



# Full wwPDB EM Validation Report ⓘ

Mar 24, 2025 – 11:05 AM EDT

PDB ID : 9NLJ  
EMDB ID : EMD-29399  
Title : E.coli Initiation complex with Uup-EQ2  
Authors : Singh, S.; Hunt, J.F.  
Deposited on : 2025-03-03  
Resolution : 3.10 Å(reported)

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

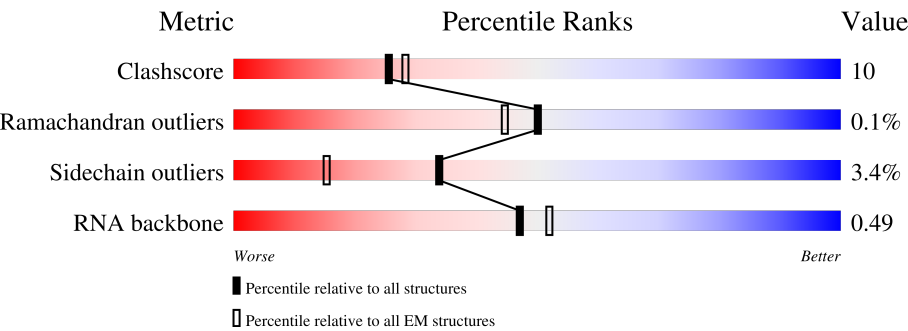
EMDB validation analysis : 0.0.1.dev117  
Mogul : 2022.3.0, CSD as543be (2022)  
MolProbity : 4.02b-467  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.41.4

# 1 Overall quality at a glance i

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

The reported resolution of this entry is 3.10 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.









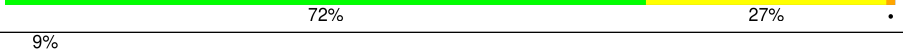
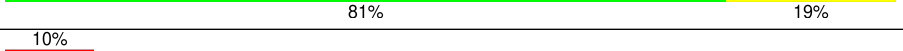
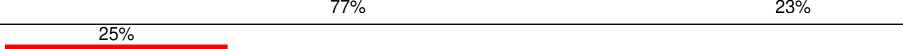
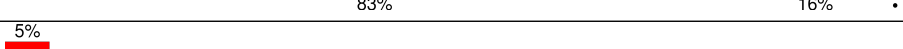
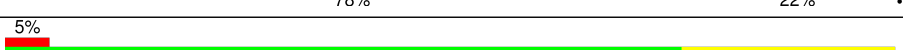

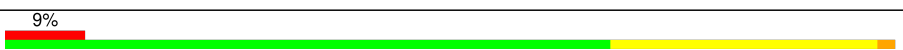

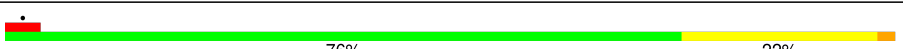






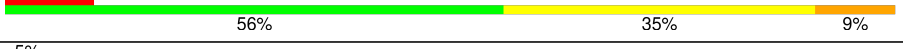



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415
RNA backbone	6643	2191

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

Mol	Chain	Length	Quality of chain
1	13	142	<div><div>6%</div><div>85%</div><div>15%</div></div>
2	14	122	<div><div>9%</div><div>85%</div><div>15%</div></div>
3	15	144	<div><div>9%</div><div>77%</div><div>23%</div></div>
4	16	136	<div><div>7%</div><div>74%</div><div>24%</div><div>.</div></div>
5	17	120	<div><div>.</div><div>68%</div><div>32%</div><div>.</div></div>
6	18	116	<div><div>20%</div><div>73%</div><div>27%</div></div>
7	19	114	<div><div>11%</div><div>72%</div><div>26%</div><div>.</div></div>

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Mol	Chain	Length	Quality of chain
8	2	271	
9	20	117	
10	21	103	
11	22	110	
12	23	93	
13	24	102	
14	25	94	
15	27	85	
16	28	77	
17	29	63	
18	3	209	
19	30	58	
20	31	66	
21	32	56	
22	33	50	
23	34	46	
24	35	64	
25	36	38	
26	4	201	
27	5	177	
28	6	176	
29	9	149	
30	R1	2903	
31	R2	119	
32	R3	1531	

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Mol	Chain	Length	Quality of chain
33	sb	218	
34	sc	206	
35	sd	205	
36	se	157	
37	sf	100	
38	sg	151	
39	sh	129	
40	si	127	
41	sj	98	
42	sk	116	
43	sl	123	
44	sm	114	
45	sn	100	
46	so	88	
47	sp	82	
48	sq	80	
49	sr	65	
50	ss	79	
51	st	85	
52	su	65	
53	T	78	
54	U	537	
55	1	220	
56	M	9	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
53	H2U	T	20	X	-	-	-
53	4OC	T	32	X	-	-	-
53	5MU	T	54	X	-	-	-
53	PSU	T	55	X	-	-	-
53	4SU	T	8	X	-	-	-

## 2 Entry composition

There are 59 unique types of molecules in this entry. The entry contains 150042 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Large ribosomal subunit protein uL13.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	13	142	Total	C	N	O	S	0	0
			1129	714	212	199	4		

- Molecule 2 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	14	122	Total	C	N	O	S	0	0
			938	587	180	165	6		

- Molecule 3 is a protein called Large ribosomal subunit protein uL15.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	15	144	Total	C	N	O	S	0	0
			1053	654	207	190	2		

- Molecule 4 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	16	136	Total	C	N	O	S	0	0
			1074	686	205	177	6		

- Molecule 5 is a protein called Large ribosomal subunit protein bL17.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	17	120	Total	C	N	O	S	0	0
			960	593	196	166	5		

- Molecule 6 is a protein called Large ribosomal subunit protein uL18.

Mol	Chain	Residues	Atoms				AltConf	Trace
6	18	116	Total	C	N	O	0	0
			892	552	178	162		

- Molecule 7 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	19	114	Total	C	N	O	S	0	0
			917	574	179	163	1		

- Molecule 8 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	2	271	Total	C	N	O	S	0	0
			2082	1288	423	364	7		

- Molecule 9 is a protein called Large ribosomal subunit protein bL20.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	20	117	Total	C	N	O	S	0	0
			947	604	192	151			

- Molecule 10 is a protein called Large ribosomal subunit protein bL21.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	21	103	Total	C	N	O	S	0	0
			816	516	153	145	2		

- Molecule 11 is a protein called Large ribosomal subunit protein uL22.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	22	110	Total	C	N	O	S	0	0
			857	532	166	156	3		

- Molecule 12 is a protein called Large ribosomal subunit protein uL23.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	23	93	Total	C	N	O	S	0	0
			738	466	139	131	2		

- Molecule 13 is a protein called Large ribosomal subunit protein uL24.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	24	102	Total	C	N	O	S	0	0
			779	492	146	141			

- Molecule 14 is a protein called Large ribosomal subunit protein bL25.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	25	94	Total	C	N	O	S	0	0
			753	479	137	134	3		

- Molecule 15 is a protein called Large ribosomal subunit protein bL27.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	27	85	Total	C	N	O	S	0	0
			642	396	130	114	2		

- Molecule 16 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	28	77	Total	C	N	O	S	0	0
			625	388	129	106	2		

- Molecule 17 is a protein called Large ribosomal subunit protein uL29.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	29	63	Total	C	N	O	S	0	0
			509	313	99	95	2		

- Molecule 18 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	3	209	Total	C	N	O	S	0	0
			1565	979	288	294	4		

- Molecule 19 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	30	58	Total	C	N	O	S	0	0
			449	281	87	79	2		

- Molecule 20 is a protein called Large ribosomal subunit protein bL31.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	31	66	Total	C	N	O	S	0	0
			522	323	99	94	6		

- Molecule 21 is a protein called 50S ribosomal protein L32.



Mol	Chain	Residues	Atoms					AltConf	Trace
21	32	56	Total	C	N	O	S	0	0
			444	269	94	80	1		

- Molecule 22 is a protein called Large ribosomal subunit protein bL33.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	33	50	Total	C	N	O		0	0
			409	263	75	71			

- Molecule 23 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	34	46	Total	C	N	O	S	0	0
			377	228	90	57	2		

- Molecule 24 is a protein called Large ribosomal subunit protein bL35.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	35	64	Total	C	N	O	S	0	0
			504	323	105	74	2		

- Molecule 25 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	36	38	Total	C	N	O	S	0	0
			302	185	65	48	4		

- Molecule 26 is a protein called Large ribosomal subunit protein uL4.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	4	201	Total	C	N	O	S	0	0
			1552	974	283	290	5		

- Molecule 27 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	5	177	Total	C	N	O	S	0	0
			1410	899	249	256	6		

- Molecule 28 is a protein called Large ribosomal subunit protein uL6.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	6	176	Total	C	N	O	S	0	0
			1323	832	243	246	2		

- Molecule 29 is a protein called Large ribosomal subunit protein bL9.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	9	149	Total	C	N	O	S	0	0
			1111	699	197	214	1		

- Molecule 30 is a RNA chain called 23S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	R1	2903	Total	C	N	O	P	0	0
			62318	27801	11467	20148	2902		

- Molecule 31 is a RNA chain called 5S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	R2	119	Total	C	N	O	P	0	0
			2546	1135	466	827	118		

- Molecule 32 is a RNA chain called 16S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	R3	1531	Total	C	N	O	P	0	0
			32850	14652	6028	10640	1530		

- Molecule 33 is a protein called Small ribosomal subunit protein uS2.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	sb	218	Total	C	N	O	S	0	0
			1704	1081	305	311	7		

- Molecule 34 is a protein called Small ribosomal subunit protein uS3.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	sc	206	Total	C	N	O	S	0	0
			1624	1028	305	288	3		

- Molecule 35 is a protein called 30S ribosomal protein S4.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	sd	205	Total	C	N	O	S	0	0
			1643	1026	315	298	4		

- Molecule 36 is a protein called Small ribosomal subunit protein uS5.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	se	157	Total	C	N	O	S	0	0
			1156	719	218	213	6		

- Molecule 37 is a protein called 30S ribosomal protein S6, non-modified isoform.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	sf	100	Total	C	N	O	S	0	0
			817	515	148	148	6		

- Molecule 38 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	sg	151	Total	C	N	O	S	0	0
			1181	735	227	215	4		

- Molecule 39 is a protein called 30S ribosomal protein S8.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	sh	129	Total	C	N	O	S	0	0
			979	616	173	184	6		

- Molecule 40 is a protein called Small ribosomal subunit protein uS9.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	si	127	Total	C	N	O	S	0	0
			1022	634	206	179	3		

- Molecule 41 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	sj	98	Total	C	N	O	S	0	0
			786	493	150	142	1		

- Molecule 42 is a protein called Small ribosomal subunit protein uS11.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	sk	116	Total	C	N	O	S	0	0
			869	535	173	158	3		

- Molecule 43 is a protein called Small ribosomal subunit protein uS12.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	sl	123	Total	C	N	O	S	0	0
			955	590	196	165	4		

- Molecule 44 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	sm	114	Total	C	N	O	S	0	0
			883	546	178	156	3		

- Molecule 45 is a protein called Small ribosomal subunit protein uS14.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	sn	100	Total	C	N	O	S	0	0
			805	499	164	139	3		

- Molecule 46 is a protein called Small ribosomal subunit protein uS15.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	so	88	Total	C	N	O	S	0	0
			714	439	144	130	1		

- Molecule 47 is a protein called Small ribosomal subunit protein bS16.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	sp	82	Total	C	N	O	S	0	0
			649	406	128	114	1		

- Molecule 48 is a protein called Small ribosomal subunit protein uS17.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	sq	80	Total	C	N	O	S	0	0
			648	411	121	113	3		

- Molecule 49 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	sr	65	Total	C	N	O	S	0	0
			535	339	100	95	1		

- Molecule 50 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	ss	79	Total	C	N	O	S	0	0
			637	408	120	107	2		

- Molecule 51 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	st	85	Total	C	N	O	S	0	0
			665	411	137	114	3		

- Molecule 52 is a protein called Small ribosomal subunit protein bS21.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	su	65	Total	C	N	O	S	0	0
			544	335	117	91	1		

- Molecule 53 is a RNA chain called tRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	T	78	Total	C	N	O	P S	0	0
			1649	740	295	536	76 2		

- Molecule 54 is a protein called Uup.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	U	537	Total	C	N	O	S	0	0
			4295	2690	778	810	17		

- Molecule 55 is a protein called Large ribosomal subunit protein uL1.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	1	220	Total	C	N	O	S	0	0
			1353	804	270	277	2		

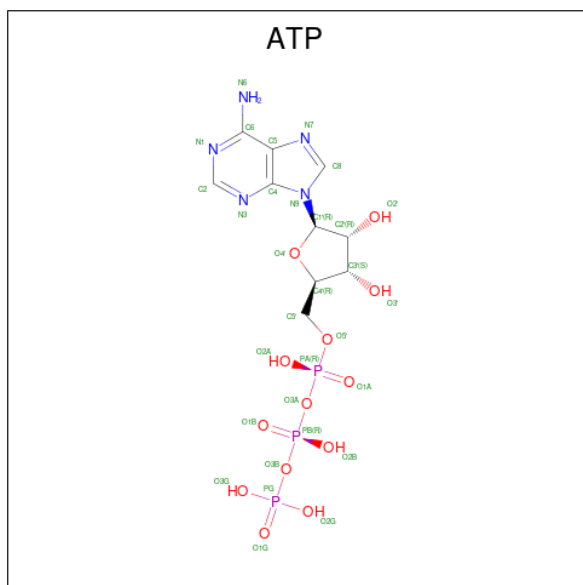
- Molecule 56 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
56	M	9	Total	C	N	O	P	0	0
			195	88	40	58	9		

- Molecule 57 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
57	15	1	Total	Mg	0
			1	1	
57	2	1	Total	Mg	0
			1	1	
57	20	1	Total	Mg	0
			1	1	
57	32	1	Total	Mg	0
			1	1	
57	R1	192	Total	Mg	0
			192	192	
57	R3	81	Total	Mg	0
			81	81	

- Molecule 58 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: C<sub>10</sub>H<sub>16</sub>N<sub>5</sub>O<sub>13</sub>P<sub>3</sub>).



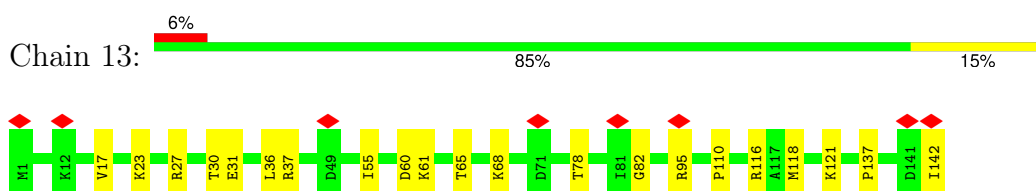
- Molecule 59 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		AltConf
59	U	2	Total	Na	0
			2	2	

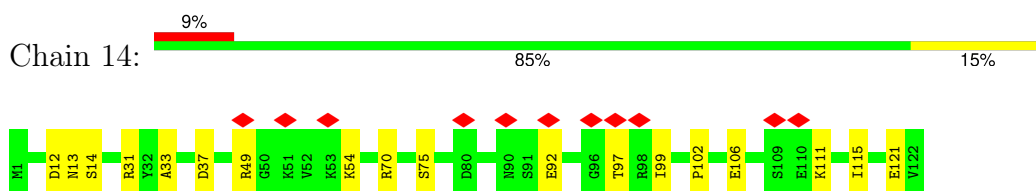
### 3 Residue-property plots [i](#)

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

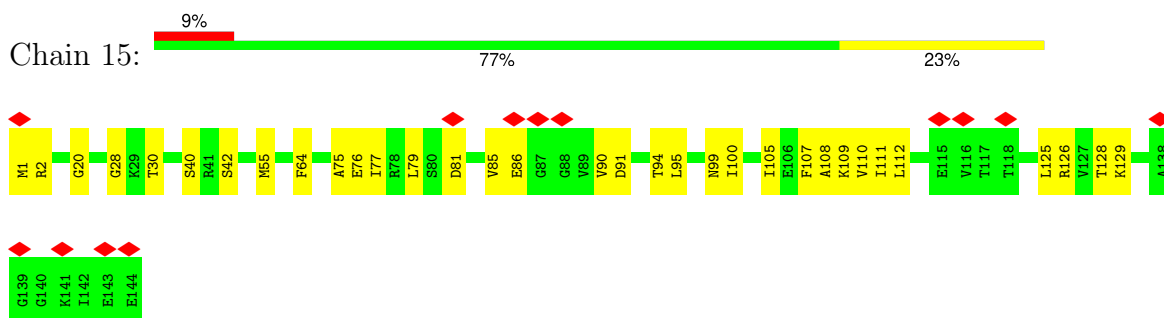
- Molecule 1: Large ribosomal subunit protein uL13



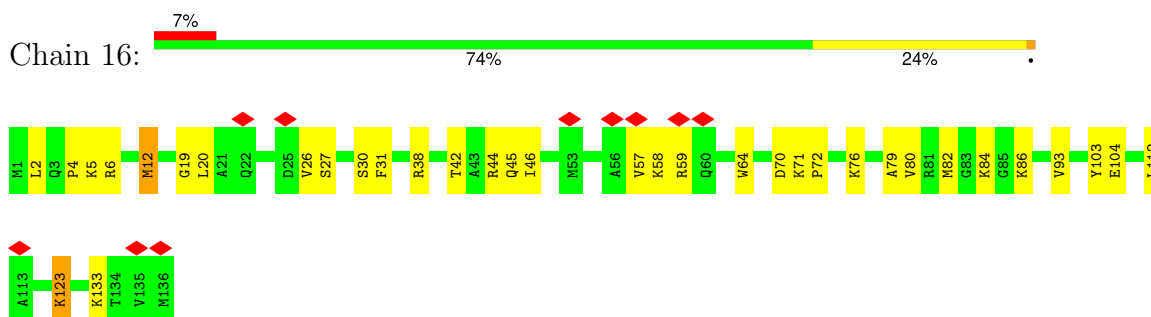
- Molecule 2: 50S ribosomal protein L14



- Molecule 3: Large ribosomal subunit protein uL15

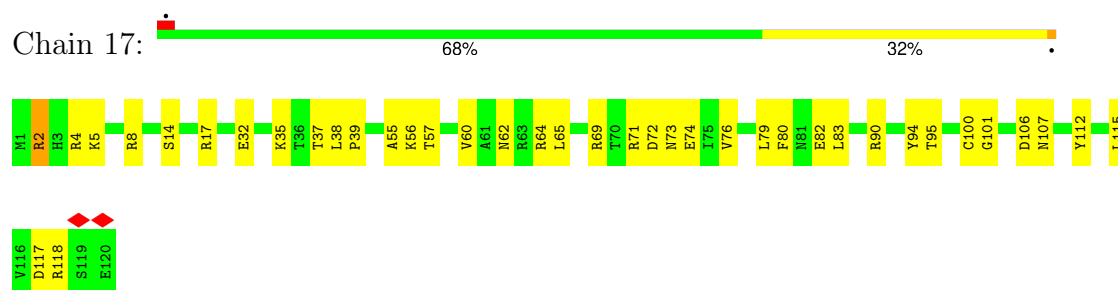


- Molecule 4: 50S ribosomal protein L16

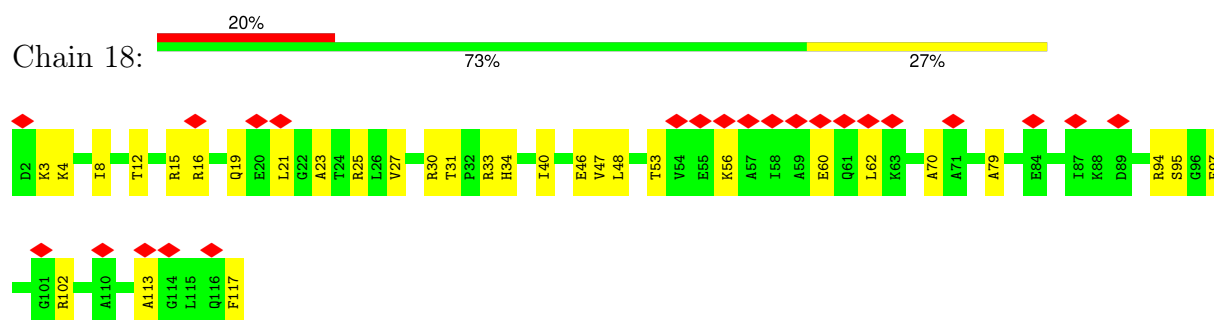




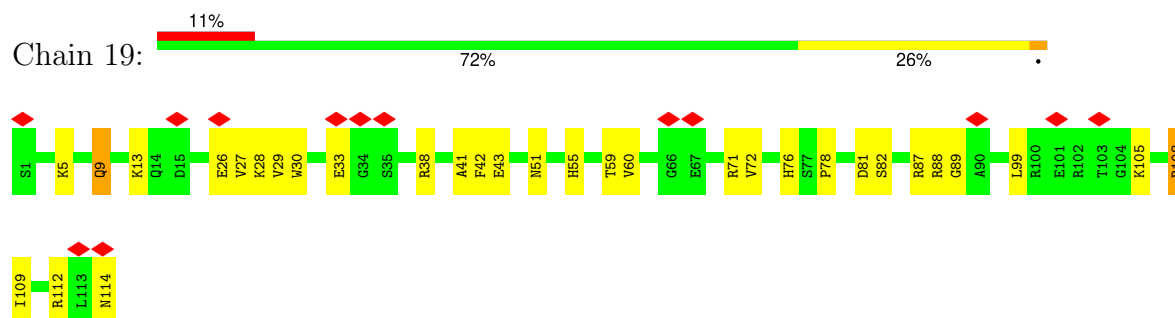
- Molecule 5: Large ribosomal subunit protein bL17



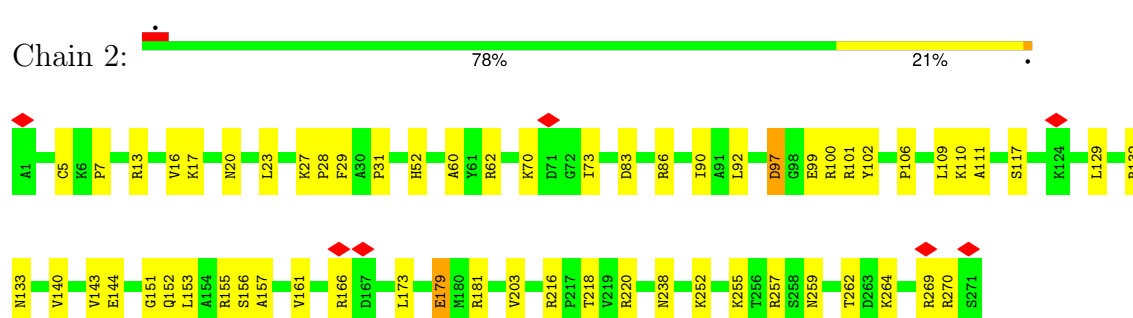
- Molecule 6: Large ribosomal subunit protein uL18



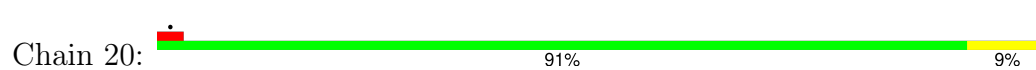
- Molecule 7: 50S ribosomal protein L19



- Molecule 8: 50S ribosomal protein L2

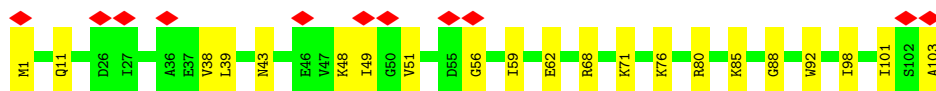
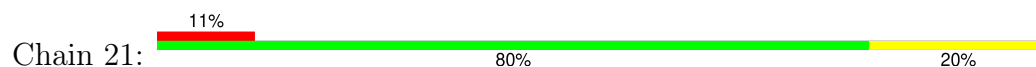


- Molecule 9: Large ribosomal subunit protein bL20

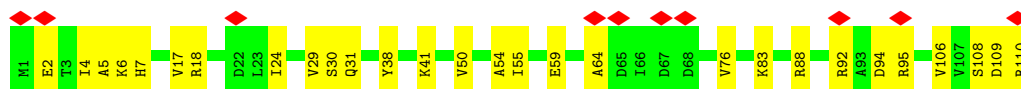
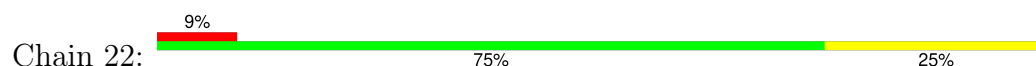




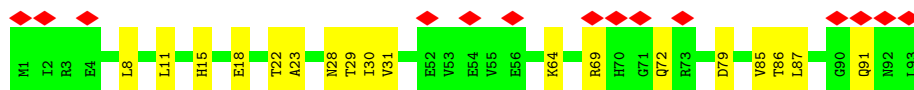
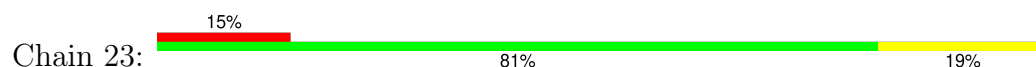
- Molecule 10: Large ribosomal subunit protein bL21



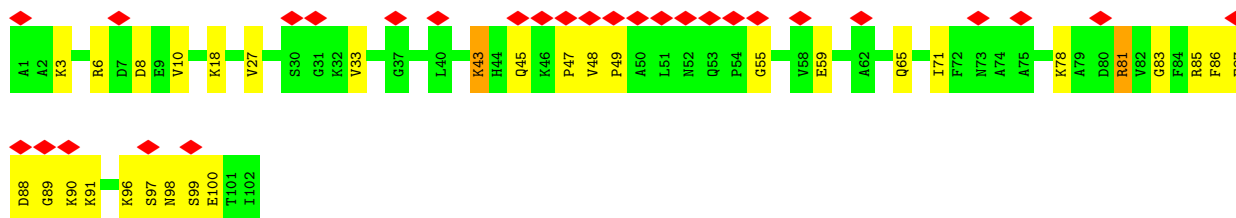
- Molecule 11: Large ribosomal subunit protein uL22



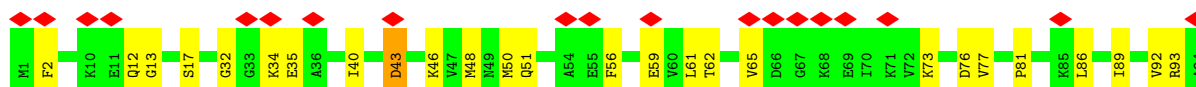
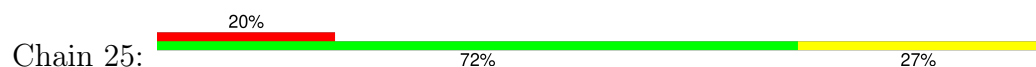
- Molecule 12: Large ribosomal subunit protein uL23



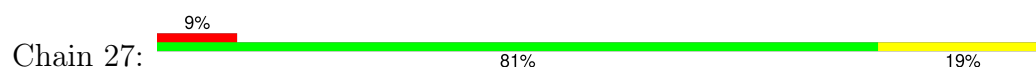
- Molecule 13: Large ribosomal subunit protein uL24



- Molecule 14: Large ribosomal subunit protein bL25

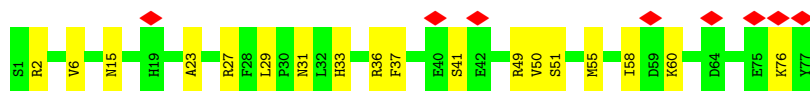
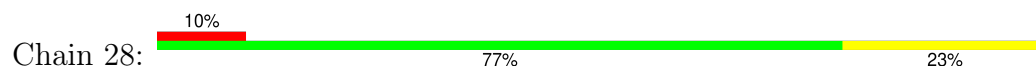


- Molecule 15: Large ribosomal subunit protein bL27

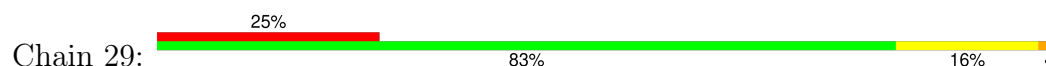




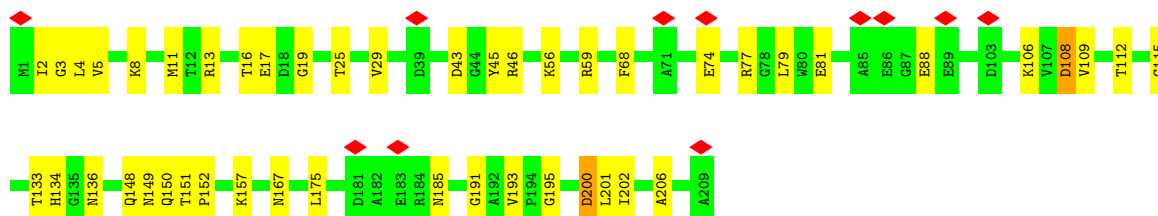
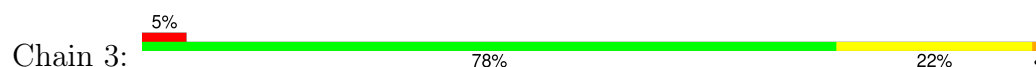
- Molecule 16: 50S ribosomal protein L28



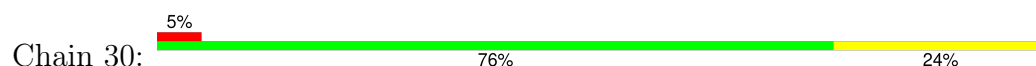
- Molecule 17: Large ribosomal subunit protein uL29



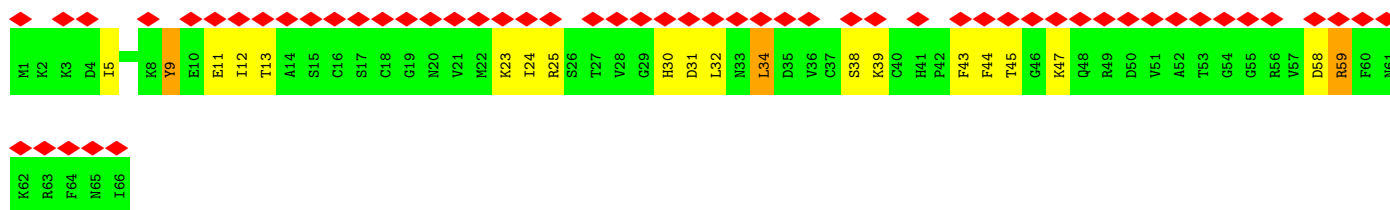
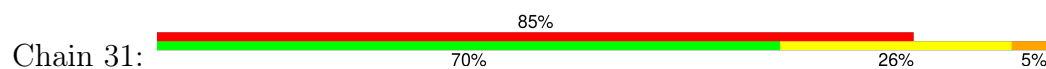
- Molecule 18: 50S ribosomal protein L3



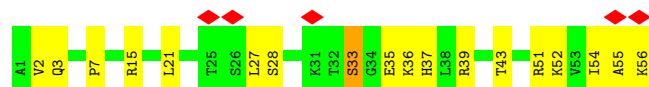
- Molecule 19: 50S ribosomal protein L30



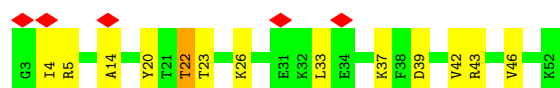
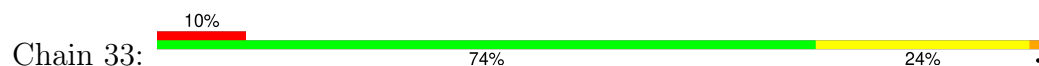
- Molecule 20: Large ribosomal subunit protein bL31



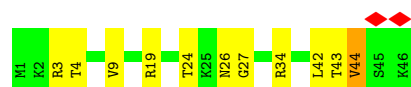
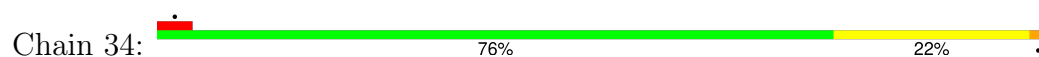
- Molecule 21: 50S ribosomal protein L32



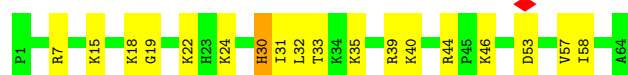
- Molecule 22: Large ribosomal subunit protein bL33



- Molecule 23: 50S ribosomal protein L34



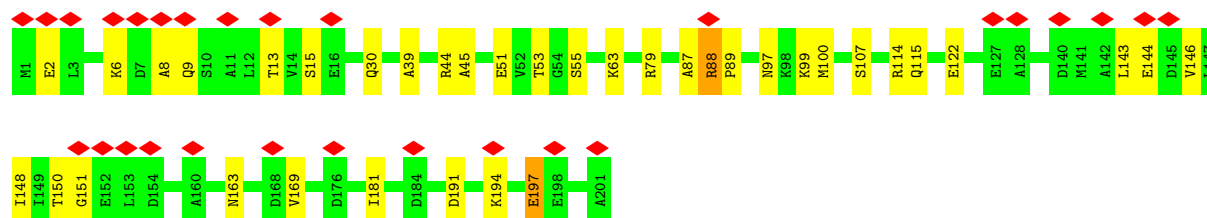
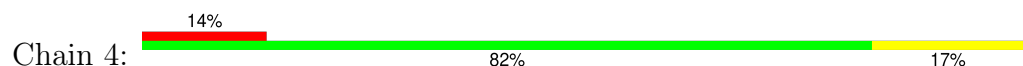
- Molecule 24: Large ribosomal subunit protein bL35



- Molecule 25: 50S ribosomal protein L36

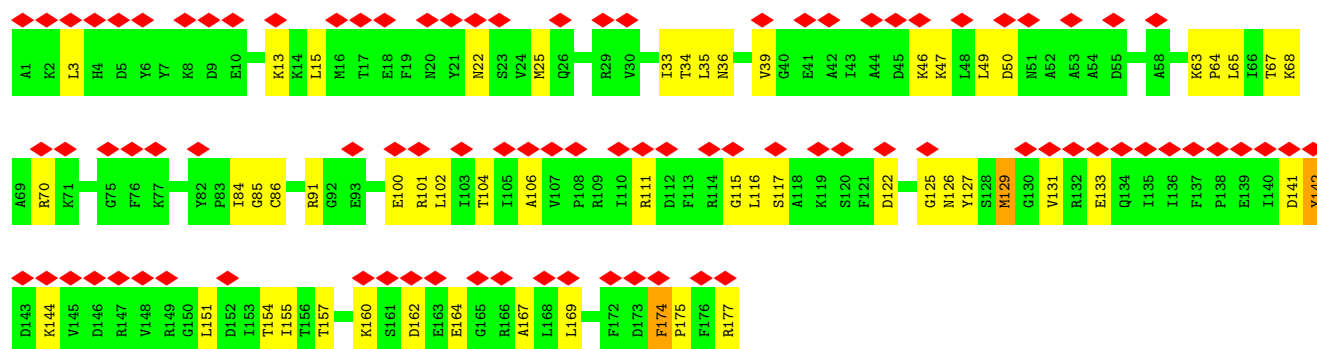


- Molecule 26: Large ribosomal subunit protein uL4

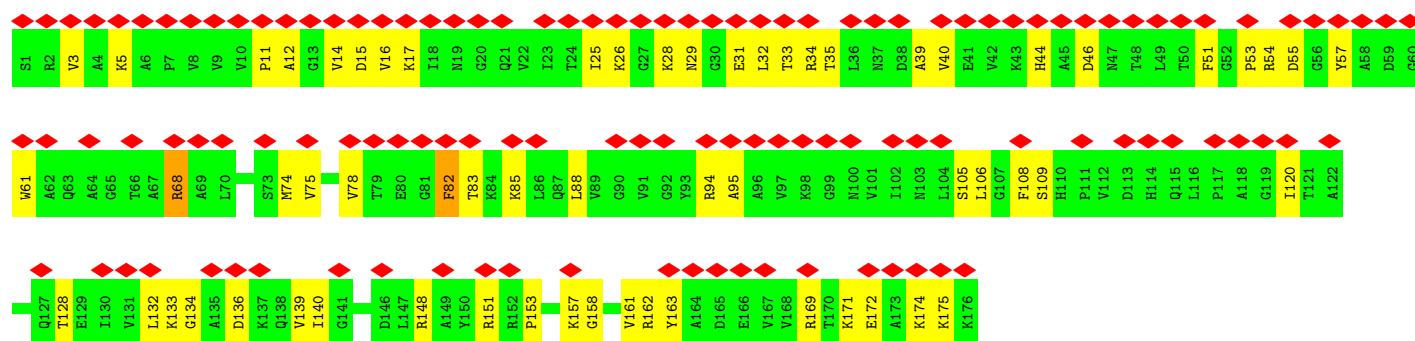


- Molecule 27: 50S ribosomal protein L5

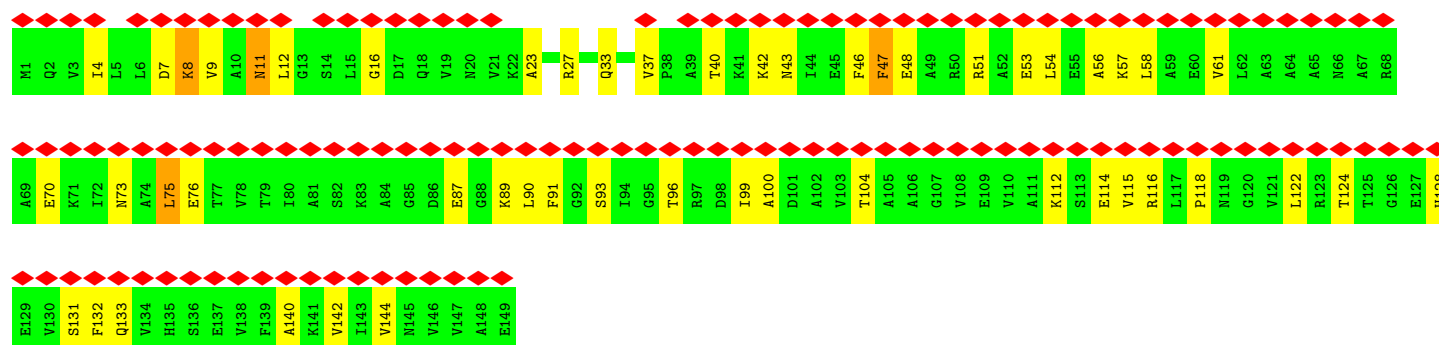
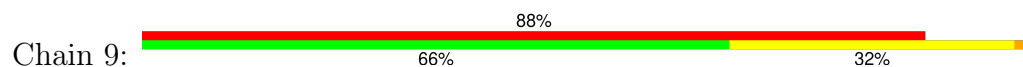




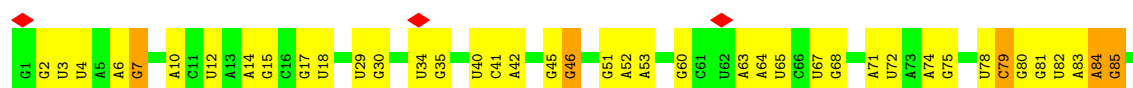
• Molecule 28: Large ribosomal subunit protein uL6

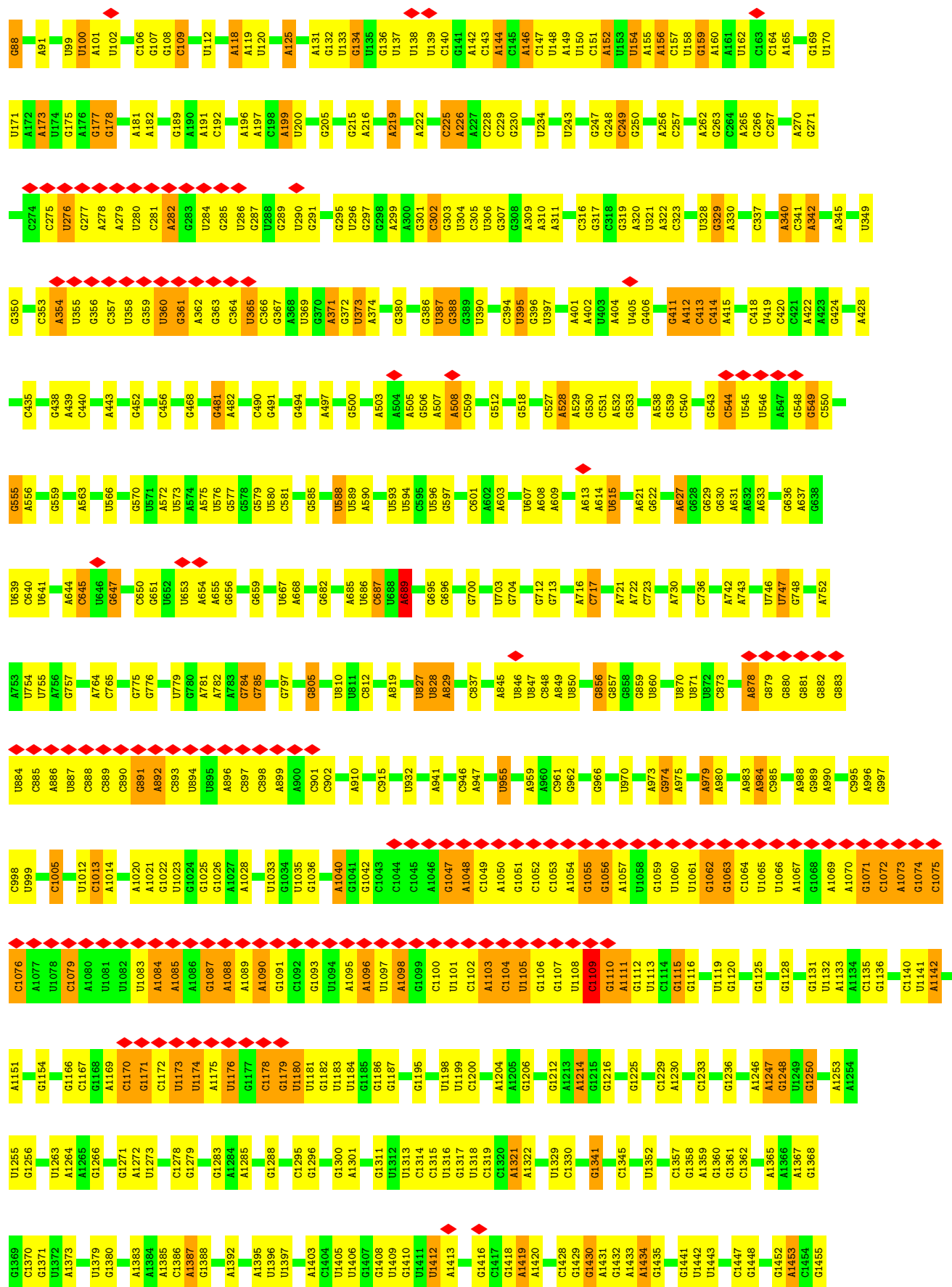


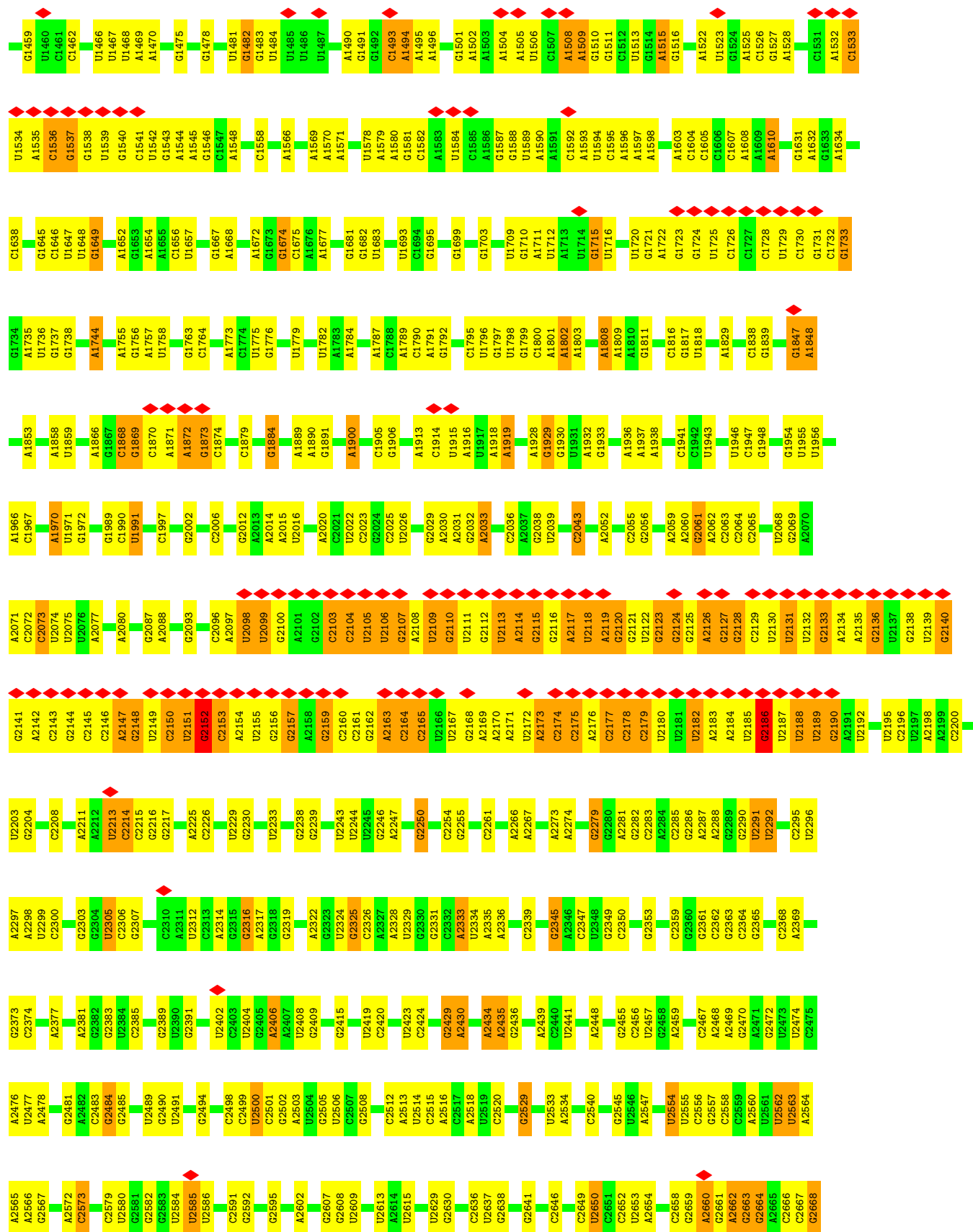
• Molecule 29: Large ribosomal subunit protein bL9

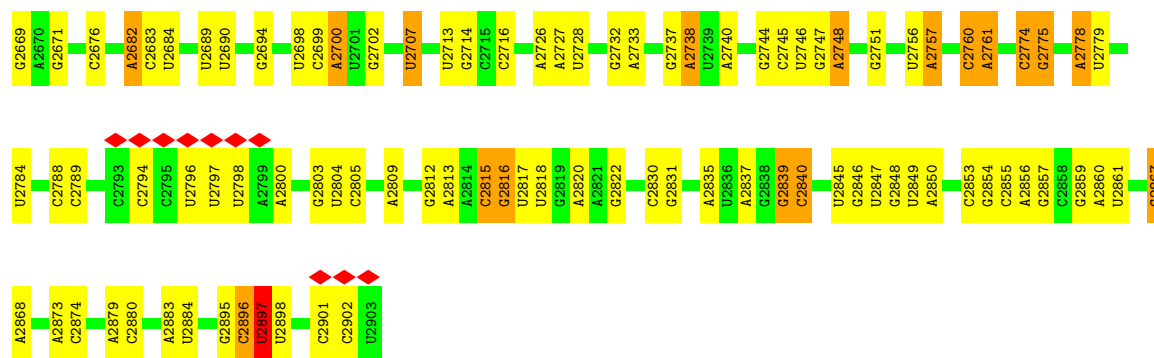


• Molecule 30: 23S ribosomal RNA

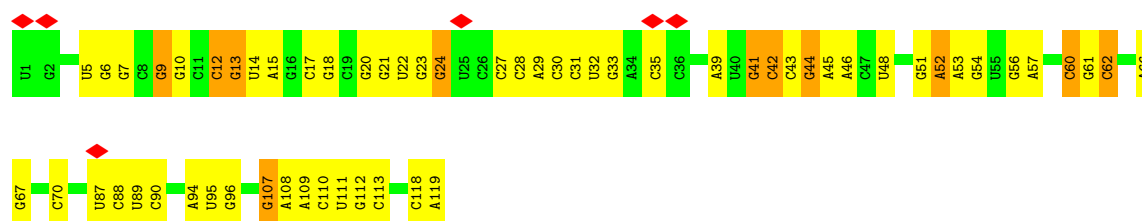




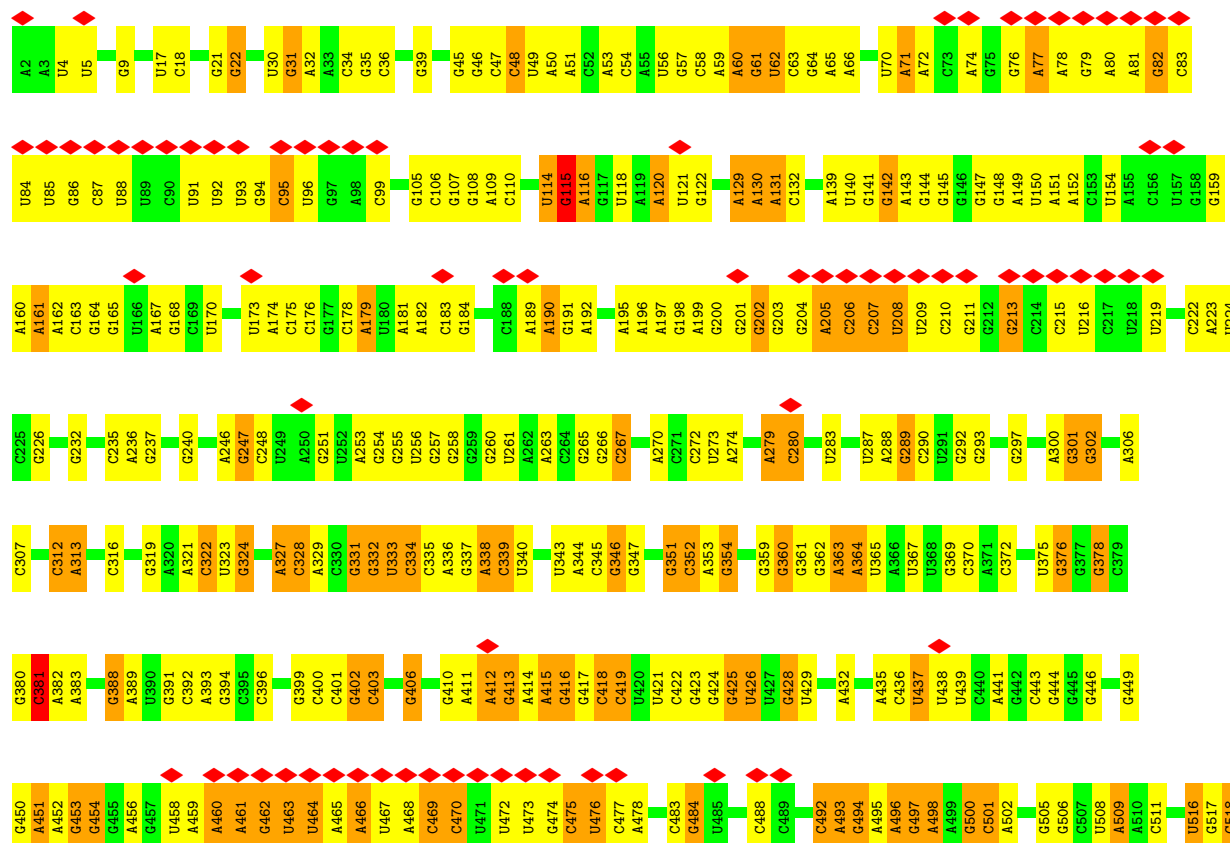




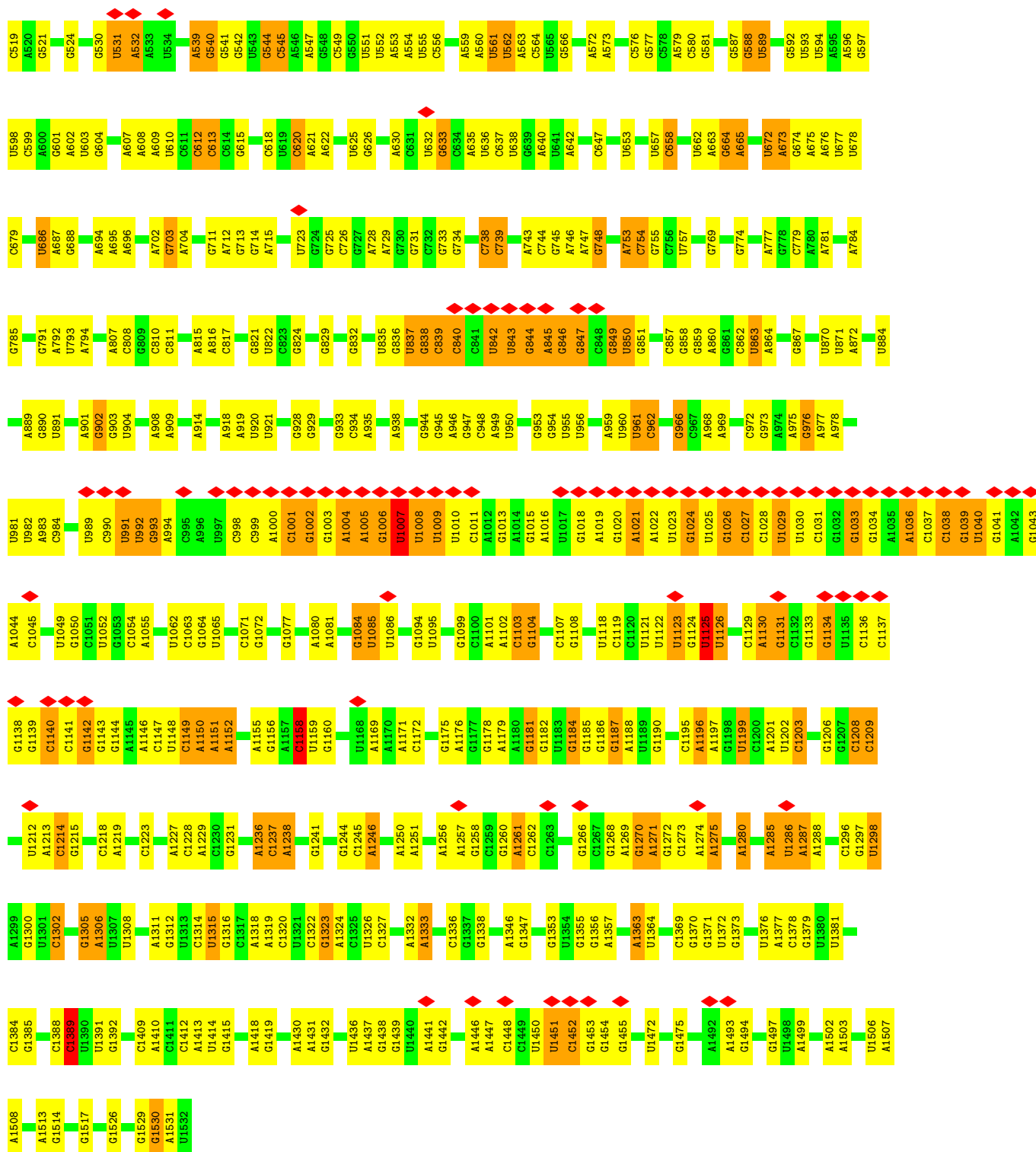
• Molecule 31: 5S ribosomal RNA



• Molecule 32: 16S ribosomal RNA

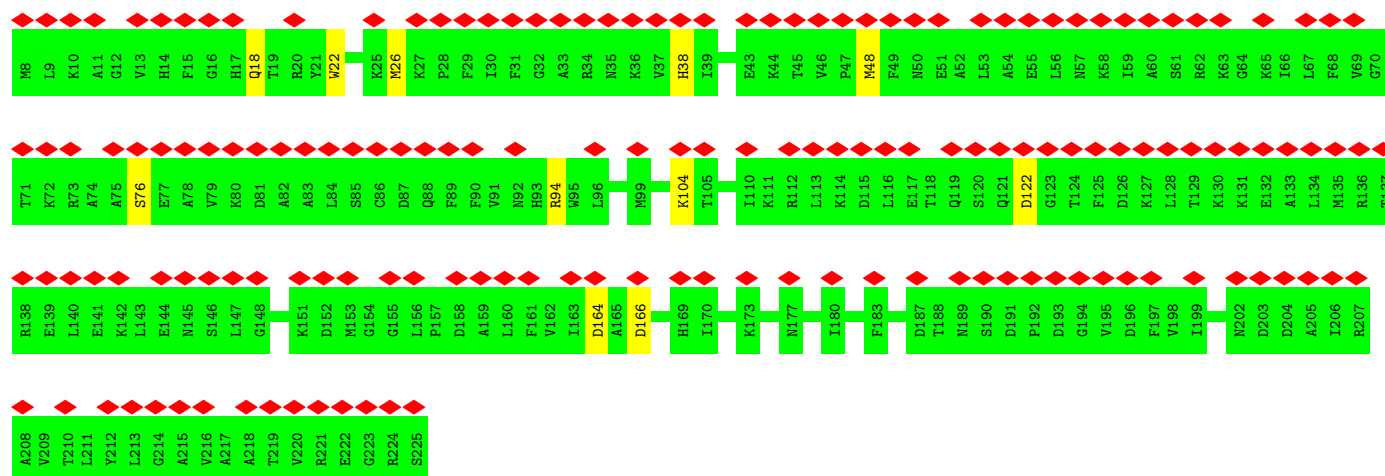






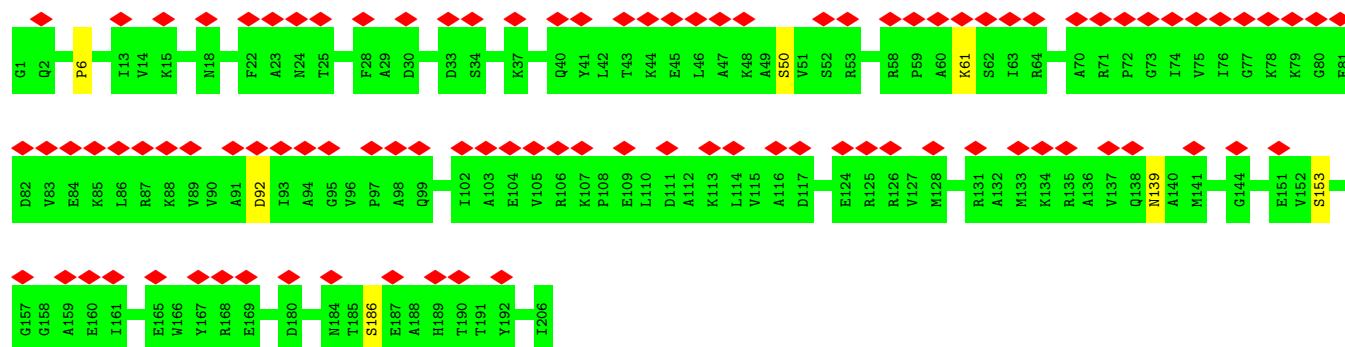
- Molecule 33: Small ribosomal subunit protein uS2





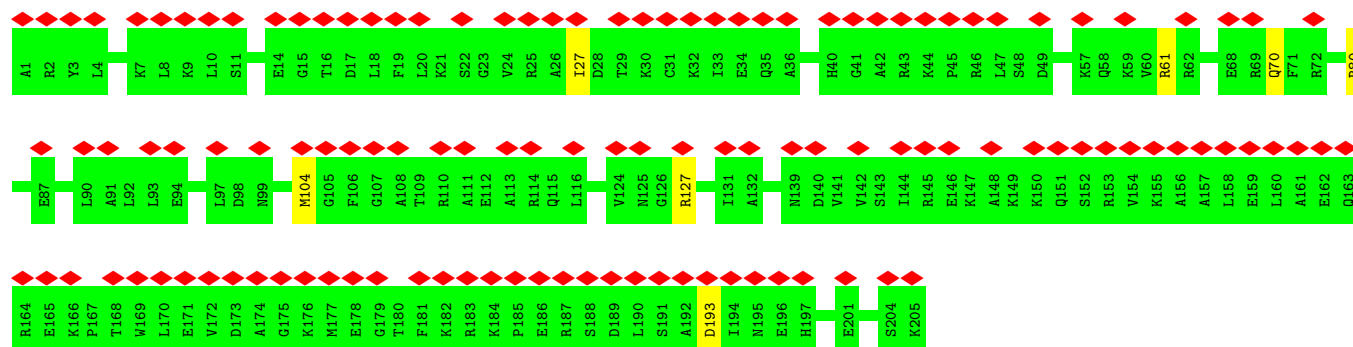
- Molecule 34: Small ribosomal subunit protein uS3

Chain sc: 47% 97%



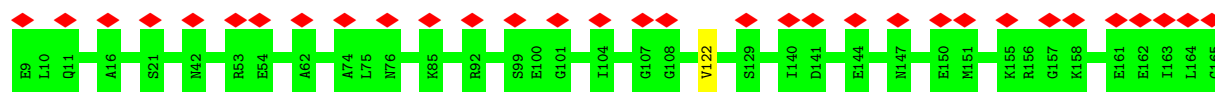
- Molecule 35: 30S ribosomal protein S4

Chain sd: 60% 97%

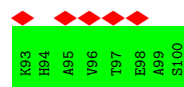
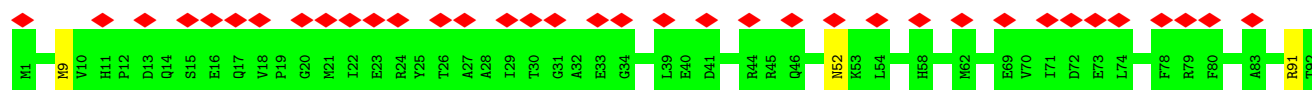
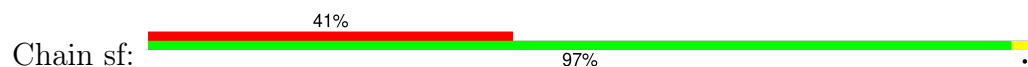


- Molecule 36: Small ribosomal subunit protein uS5

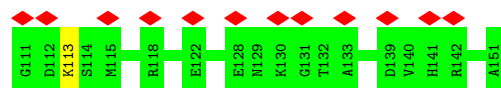
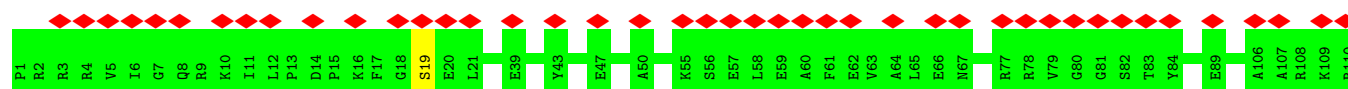
Chain se: 20% 99%



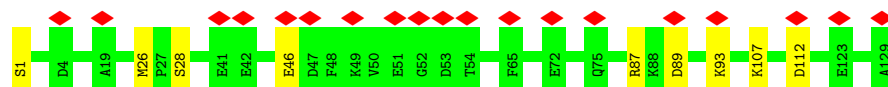
- Molecule 37: 30S ribosomal protein S6, non-modified isoform



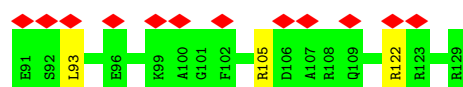
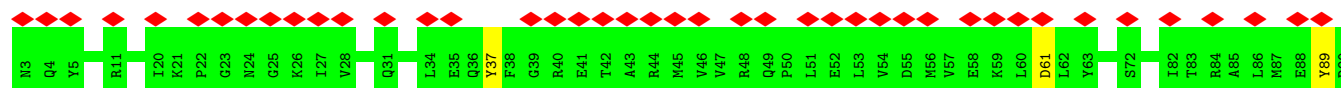
- Molecule 38: 30S ribosomal protein S7



- Molecule 39: 30S ribosomal protein S8

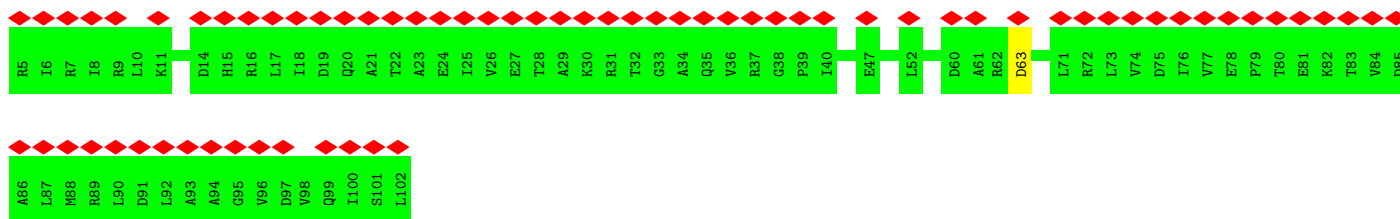


- Molecule 40: Small ribosomal subunit protein uS9



- Molecule 41: 30S ribosomal protein S10

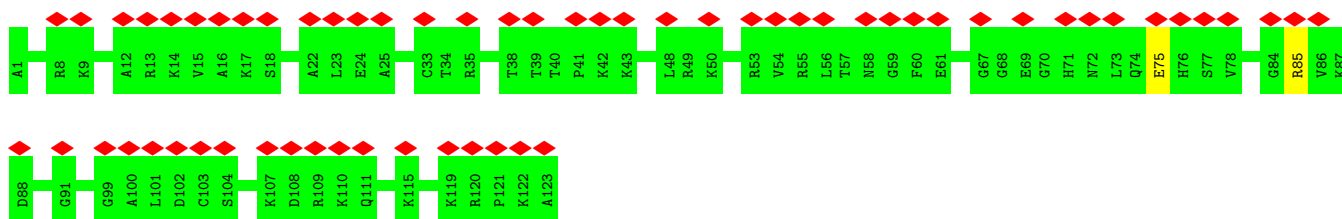




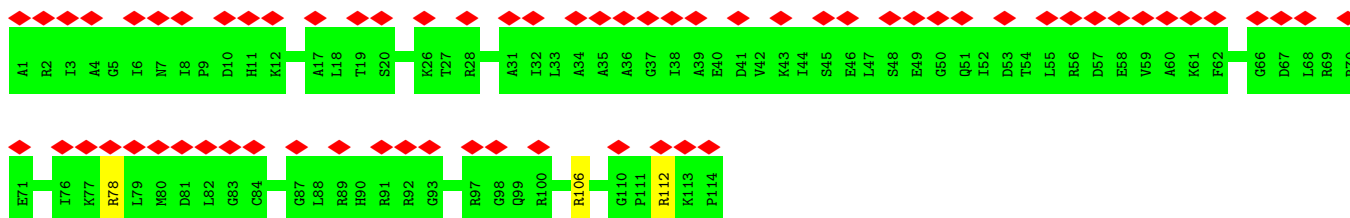
- Molecule 42: Small ribosomal subunit protein uS11



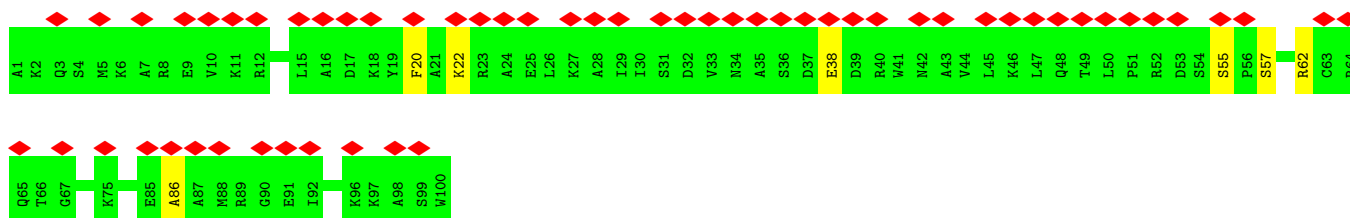
- Molecule 43: Small ribosomal subunit protein uS12



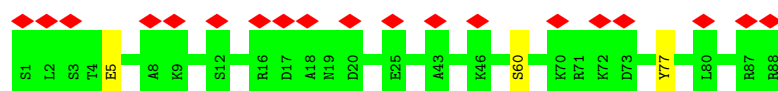
- Molecule 44: 30S ribosomal protein S13



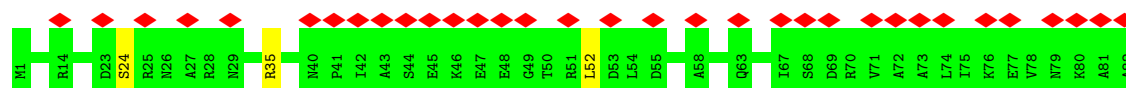
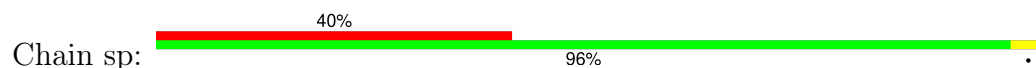
- Molecule 45: Small ribosomal subunit protein uS14



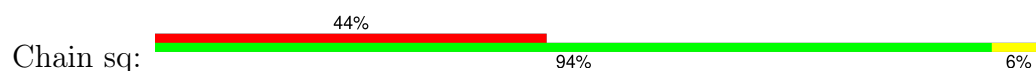
- Molecule 46: Small ribosomal subunit protein uS15



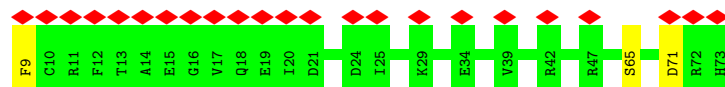
- Molecule 47: Small ribosomal subunit protein bS16



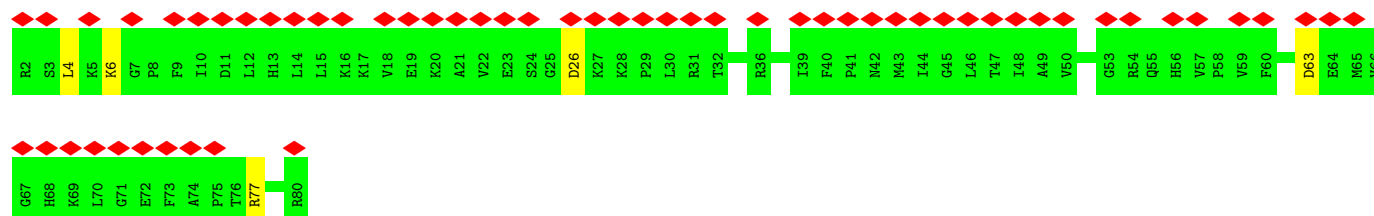
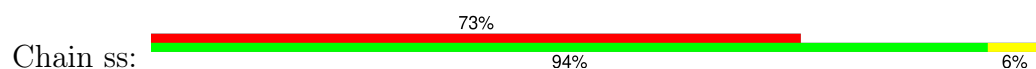
- Molecule 48: Small ribosomal subunit protein uS17



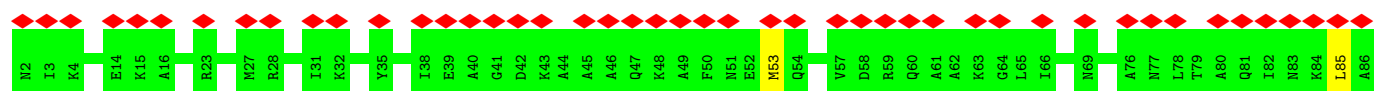
- Molecule 49: 30S ribosomal protein S18



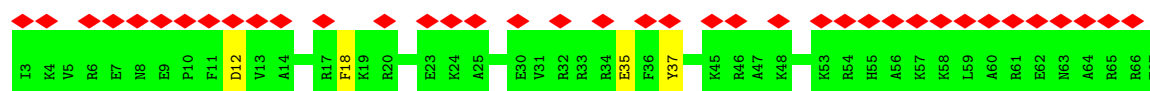
- Molecule 50: 30S ribosomal protein S19



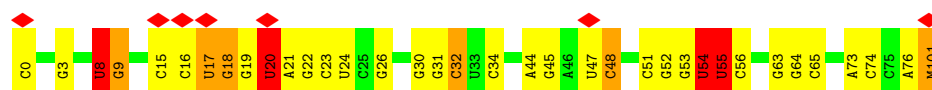
- Molecule 51: 30S ribosomal protein S20



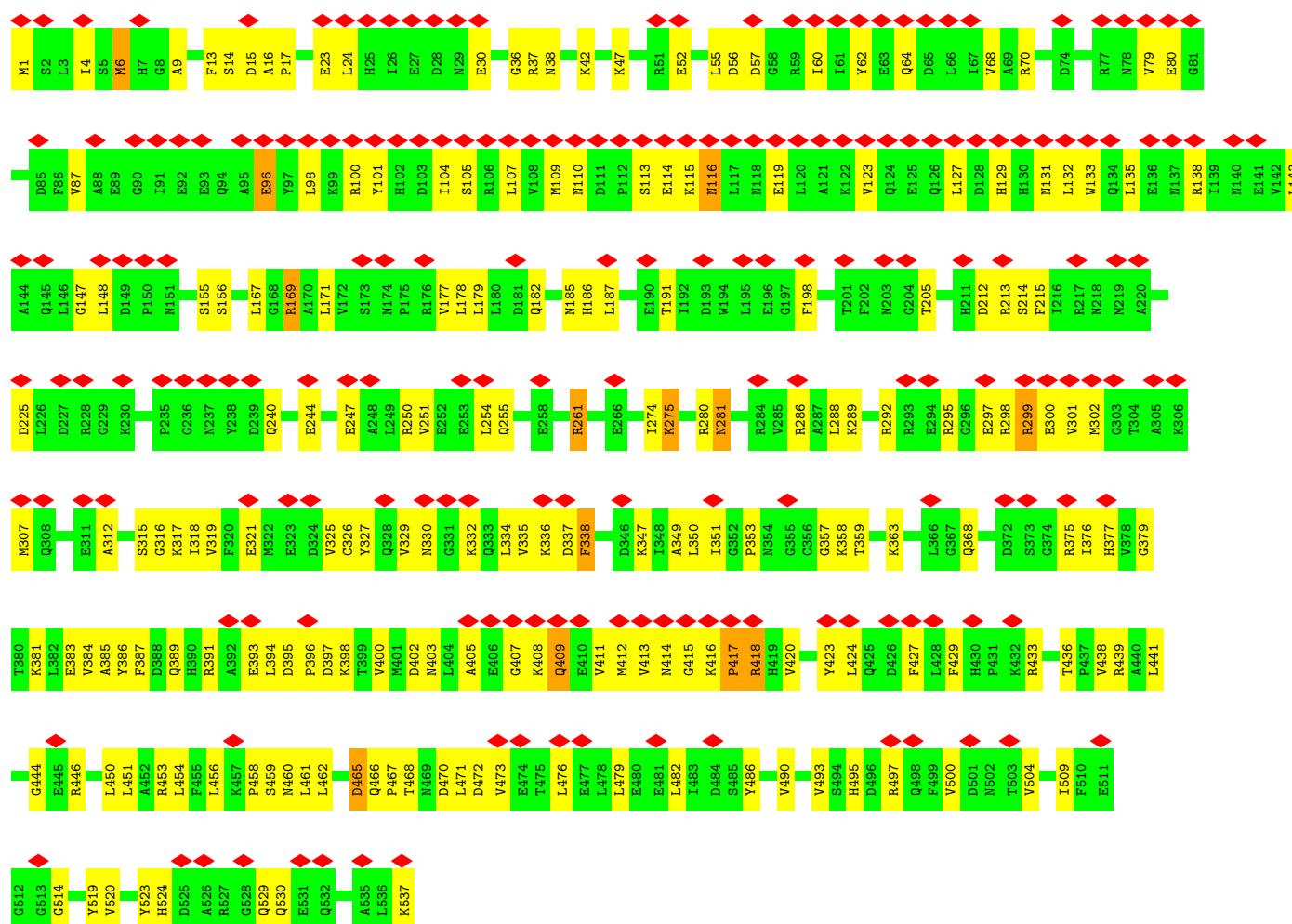
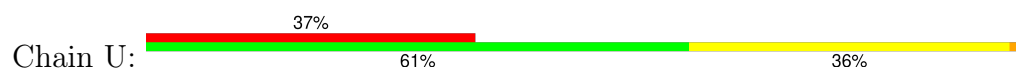
- Molecule 52: Small ribosomal subunit protein bS21



- Molecule 53: tRNA

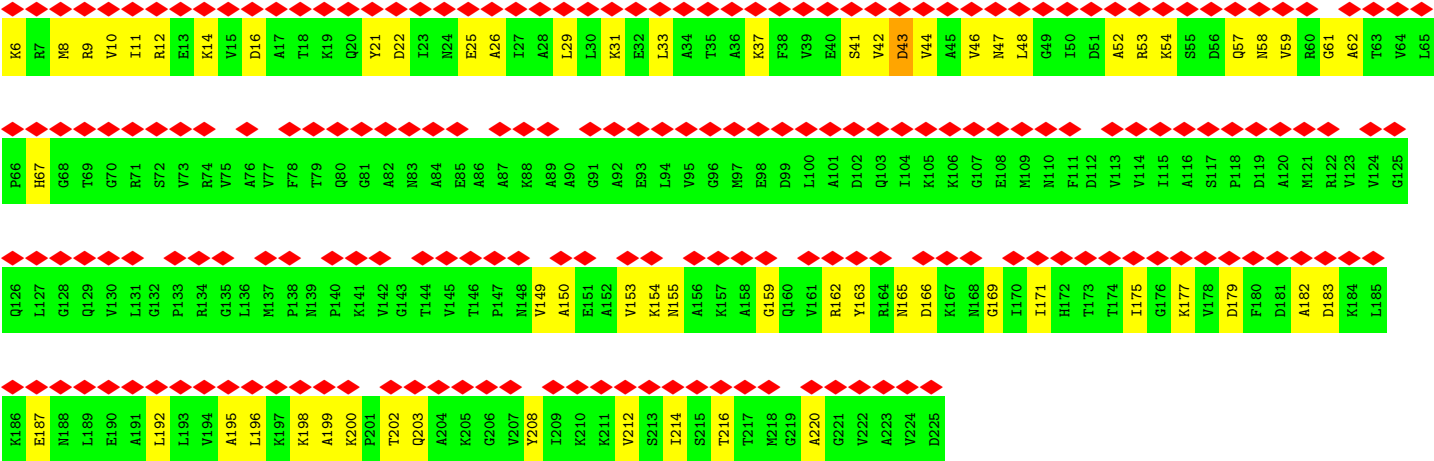


- Molecule 54: Uup

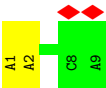
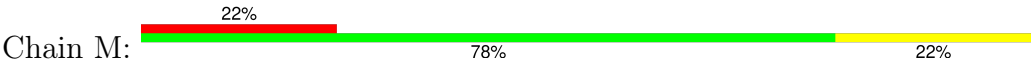


- Molecule 55: Large ribosomal subunit protein uL1





● Molecule 56: mRNA



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	61688	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI POLARA 300	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	64	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	1500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	3.670	Depositor
Minimum map value	-2.176	Depositor
Average map value	0.003	Depositor
Map value standard deviation	0.155	Depositor
Recommended contour level	0.55	Depositor
Map size (Å)	380.0, 380.0, 380.0	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.95, 0.95, 0.95	Depositor



## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 4SU, ATP, H2U, 4OC, MG, PSU, 5MU, FME, NA

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	13	0.31	0/1152	0.51	0/1551
2	14	0.32	0/947	0.61	0/1268
3	15	0.31	0/1062	0.61	0/1413
4	16	0.31	0/1093	0.60	0/1460
5	17	0.30	0/973	0.60	0/1301
6	18	0.27	0/902	0.58	0/1209
7	19	0.32	0/929	0.56	0/1242
8	2	0.33	0/2121	0.59	0/2852
9	20	0.36	0/960	0.55	0/1278
10	21	0.32	0/829	0.57	0/1107
11	22	0.31	0/864	0.55	0/1156
12	23	0.29	0/744	0.54	0/994
13	24	0.29	0/787	0.55	0/1051
14	25	0.28	0/766	0.55	0/1025
15	27	0.32	0/650	0.56	0/858
16	28	0.30	0/635	0.57	0/848
17	29	0.24	0/510	0.54	0/677
18	3	0.33	0/1586	0.56	0/2134
19	30	0.28	0/453	0.61	0/605
20	31	0.26	0/531	0.57	0/709
21	32	0.31	0/450	0.58	0/599
22	33	0.31	0/416	0.53	0/554
23	34	0.29	0/380	0.65	0/498
24	35	0.30	0/513	0.54	0/676
25	36	0.29	0/303	0.62	0/397
26	4	0.30	0/1571	0.52	0/2113
27	5	0.28	0/1434	0.54	0/1926
28	6	0.27	0/1343	0.53	0/1816
29	9	0.27	0/1122	0.56	0/1515
30	R1	0.55	0/69797	0.85	28/108890 (0.0%)
31	R2	0.39	0/2847	0.86	4/4440 (0.1%)
32	R3	0.41	0/36782	0.86	34/57377 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
33	sb	0.26	0/1735	0.51	0/2338
34	sc	0.27	0/1651	0.56	1/2225 (0.0%)
35	sd	0.27	0/1665	0.56	0/2227
36	se	0.29	0/1169	0.57	0/1573
37	sf	0.29	0/835	0.56	0/1128
38	sg	0.26	0/1195	0.55	0/1602
39	sh	0.27	0/989	0.56	0/1326
40	si	0.30	0/1034	0.64	0/1375
41	sj	0.27	0/796	0.61	0/1077
42	sk	0.28	0/885	0.56	0/1195
43	sl	0.28	0/969	0.60	0/1300
44	sm	0.26	0/892	0.60	0/1193
45	sn	0.29	0/817	0.64	1/1088 (0.1%)
46	so	0.25	0/722	0.54	0/964
47	sp	0.26	0/659	0.59	0/884
48	sq	0.30	0/657	0.59	0/881
49	sr	0.28	0/544	0.56	0/731
50	ss	0.27	0/652	0.57	0/877
51	st	0.25	0/671	0.52	0/888
52	su	0.28	0/550	0.72	0/728
53	T	0.43	0/1716	0.80	0/2672
54	U	0.28	0/4363	0.57	2/5884 (0.0%)
55	1	0.26	0/1361	0.54	0/1796
56	M	0.38	0/219	0.77	0/339
All	All	0.44	0/162198	0.78	70/241830 (0.0%)

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
29	9	0	1
35	sd	0	1
45	sn	0	1
53	T	7	0
All	All	7	3

There are no bond length outliers.

All (70) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	R1	2668	G	O4'-C1'-N9	7.95	114.56	108.20
32	R3	1208	C	C2-N1-C1'	7.58	127.14	118.80
54	U	417	PRO	N-CD-CG	-7.02	92.67	103.20
32	R3	470	C	C2-N1-C1'	6.87	126.35	118.80
30	R1	544	C	C2-N1-C1'	6.71	126.18	118.80
32	R3	470	C	N1-C2-O2	6.59	122.86	118.90
32	R3	962	C	C2-N1-C1'	6.53	125.98	118.80
32	R3	1007	U	C2-N1-C1'	6.51	125.51	117.70
34	sc	6	PRO	CA-N-CD	-6.45	102.47	111.50
30	R1	2815	C	C2-N1-C1'	6.37	125.81	118.80
30	R1	1313	U	C2-N1-C1'	6.37	125.35	117.70
30	R1	687	C	N3-C2-O2	-6.36	117.45	121.90
32	R3	1007	U	N3-C2-O2	-6.23	117.84	122.20
30	R1	512	G	O4'-C1'-N9	6.14	113.11	108.20
32	R3	1125	U	C5-C4-O4	-6.05	122.27	125.90
31	R2	60	C	N1-C2-O2	6.01	122.51	118.90
30	R1	1314	C	C2-N1-C1'	5.97	125.37	118.80
32	R3	1125	U	C2-N1-C1'	5.97	124.86	117.70
32	R3	1208	C	C6-N1-C1'	-5.97	113.64	120.80
30	R1	1109	C	N1-C2-O2	5.93	122.46	118.90
30	R1	2580	U	N3-C2-O2	-5.89	118.08	122.20
32	R3	95	C	C2-N1-C1'	5.88	125.26	118.80
32	R3	381	C	N1-C2-O2	5.81	122.39	118.90
30	R1	2573	C	C2-N1-C1'	5.80	125.18	118.80
30	R1	955	U	N3-C2-O2	-5.80	118.14	122.20
32	R3	1134	G	C5-C6-O6	5.78	132.07	128.60
32	R3	1007	U	N1-C2-O2	5.73	126.81	122.80
30	R1	2152	G	C4-N9-C1'	5.70	133.90	126.50
30	R1	544	C	C6-N1-C1'	-5.63	114.04	120.80
30	R1	2073	C	C2-N1-C1'	5.62	124.99	118.80
32	R3	1125	U	N3-C4-O4	5.62	123.33	119.40
32	R3	1134	G	N1-C6-O6	-5.57	116.56	119.90
54	U	417	PRO	CA-N-CD	-5.55	103.73	111.50
32	R3	1186	G	O4'-C1'-N9	5.54	112.63	108.20
32	R3	1389	C	N3-C2-O2	-5.54	118.02	121.90
32	R3	402	G	O4'-C1'-N9	5.54	112.63	108.20
32	R3	120	A	OP1-P-O3'	5.48	117.25	105.20
32	R3	1140	C	N1-C2-O2	5.45	122.17	118.90
30	R1	88	G	C4-N9-C1'	5.43	133.57	126.50
30	R1	837	C	N3-C2-O2	-5.42	118.11	121.90
45	sn	22	LYS	CB-CG-CD	5.40	125.63	111.60
32	R3	436	C	N1-C2-O2	5.35	122.11	118.90
32	R3	436	C	C2-N1-C1'	5.34	124.67	118.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	R1	687	C	N1-C2-O2	5.33	122.10	118.90
32	R3	1158	C	C2-N1-C1'	5.33	124.67	118.80
30	R1	748	G	O4'-C1'-N9	5.33	112.46	108.20
32	R3	381	C	C2-N1-C1'	5.33	124.66	118.80
32	R3	470	C	N3-C2-O2	-5.32	118.18	121.90
31	R2	12	C	C2-N1-C1'	5.28	124.61	118.80
30	R1	2103	C	C2-N1-C1'	5.28	124.61	118.80
32	R3	436	C	N3-C2-O2	-5.26	118.22	121.90
32	R3	1140	C	N3-C2-O2	-5.24	118.23	121.90
30	R1	2186	G	N3-C4-N9	5.24	129.14	126.00
32	R3	1208	C	N1-C2-O2	5.24	122.04	118.90
30	R1	1109	C	N3-C2-O2	-5.23	118.24	121.90
32	R3	1389	C	C2-N1-C1'	5.22	124.54	118.80
30	R1	88	G	C8-N9-C1'	-5.20	120.24	127.00
32	R3	115	G	O5'-P-OP1	-5.19	101.03	105.70
31	R2	12	C	N1-C2-O2	5.18	122.01	118.90
30	R1	7	G	O4'-C1'-N9	5.15	112.32	108.20
31	R2	60	C	N3-C2-O2	-5.13	118.31	121.90
30	R1	1170	C	O4'-C1'-N1	5.13	112.31	108.20
30	R1	689	A	N7-C8-N9	5.12	116.36	113.80
30	R1	540	C	C2-N1-C1'	5.11	124.42	118.80
32	R3	114	U	P-O3'-C3'	-5.11	113.57	119.70
32	R3	658	C	N3-C2-O2	-5.10	118.33	121.90
32	R3	1203	C	C2-N1-C1'	5.10	124.41	118.80
30	R1	2103	C	N1-C2-O2	5.09	121.95	118.90
30	R1	2897	U	C5-C6-N1	5.07	125.24	122.70
32	R3	620	C	C2-N1-C1'	5.03	124.34	118.80

All (7) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
53	T	8	4SU	C3',C2'
53	T	20	H2U	C1',C2'
53	T	32	4OC	C2'
53	T	54	5MU	C4'
53	T	55	PSU	C4'

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
29	9	8	LYS	Peptide
35	sd	27	ILE	Peptide

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Mol	Chain	Res	Type	Group
45	sn	86	ALA	Peptide

## 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	13	1129	0	1162	14	0
2	14	938	0	1012	12	0
3	15	1053	0	1129	28	0
4	16	1074	0	1157	27	0
5	17	960	0	1000	28	0
6	18	892	0	923	24	0
7	19	917	0	965	23	0
8	2	2082	0	2157	44	0
9	20	947	0	1022	14	0
10	21	816	0	839	17	0
11	22	857	0	922	20	0
12	23	738	0	807	14	0
13	24	779	0	834	22	0
14	25	753	0	780	15	0
15	27	642	0	665	15	0
16	28	625	0	655	12	0
17	29	509	0	543	9	0
18	3	1565	0	1616	33	0
19	30	449	0	491	11	0
20	31	522	0	524	16	0
21	32	444	0	461	16	0
22	33	409	0	440	10	0
23	34	377	0	418	9	0
24	35	504	0	574	13	0
25	36	302	0	343	10	0
26	4	1552	0	1619	31	0
27	5	1410	0	1447	37	0
28	6	1323	0	1374	45	0
29	9	1111	0	1148	38	0
30	R1	62318	0	31345	772	0
31	R2	2546	0	1292	42	0
32	R3	32850	0	16534	451	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
33	sb	1704	0	1732	0	0
34	sc	1624	0	1699	0	0
35	sd	1643	0	1710	0	0
36	se	1156	0	1199	0	0
37	sf	817	0	808	0	0
38	sg	1181	0	1240	0	0
39	sh	979	0	1034	0	0
40	si	1022	0	1070	0	0
41	sj	786	0	828	0	0
42	sk	869	0	878	0	0
43	sl	955	0	1019	0	0
44	sm	883	0	944	0	0
45	sn	805	0	847	0	0
46	so	714	0	737	0	0
47	sp	649	0	666	0	0
48	sq	648	0	691	0	0
49	sr	535	0	552	0	0
50	ss	637	0	665	0	0
51	st	665	0	714	0	0
52	su	544	0	579	0	0
53	T	1649	0	853	23	0
54	U	4295	0	4302	133	0
55	1	1353	0	1159	43	0
56	M	195	0	99	1	0
57	15	1	0	0	0	0
57	2	1	0	0	0	0
57	20	1	0	0	0	0
57	32	1	0	0	0	0
57	R1	192	0	0	0	0
57	R3	81	0	0	0	0
58	U	62	0	24	4	0
59	U	2	0	0	0	0
All	All	150042	0	102247	1879	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 10.

All (1879) 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)
30:R1:156:A:H2	30:R1:169:G:N1	1.28	1.26

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:R1:156:A:C2	30:R1:169:G:N1	2.03	1.24
32:R3:359:G:HO2'	32:R3:360:G:H8	1.03	0.97
30:R1:947:A:HO2'	30:R1:984:A:H2	1.09	0.92
30:R1:2073:C:H5	30:R1:2436:G:H1	1.20	0.89
32:R3:144:G:N2	32:R3:178:C:O2	2.07	0.88
32:R3:1027:C:N3	32:R3:1034:G:N1	2.23	0.87
30:R1:2127:G:N2	30:R1:2161:C:O2	2.06	0.87
1:13:31:GLU:HG2	1:13:142:ILE:HD11	1.57	0.86
30:R1:136:G:N1	30:R1:142:A:C2	2.44	0.85
29:9:9:VAL:HG12	29:9:11:ASN:H	1.42	0.85
30:R1:156:A:N1	30:R1:169:G:O6	2.09	0.85
30:R1:2545:G:H21	30:R1:2565:A:H8	1.22	0.83
6:18:16:ARG:HH12	6:18:19:GLN:HG3	1.43	0.83
30:R1:414:C:H5	30:R1:2409:G:H1	1.28	0.82
32:R3:1260:G:H21	32:R3:1275:A:H62	1.25	0.82
32:R3:592:G:N2	32:R3:647:C:O2	2.13	0.82
30:R1:79:C:H42	30:R1:107:G:H1	1.28	0.82
11:22:29:VAL:HG21	11:22:55:ILE:HD11	1.62	0.81
27:5:68:LYS:NZ	31:R2:41:G:O6	2.14	0.80
30:R1:2140:G:N2	30:R1:2151:U:O2	2.13	0.80
19:30:40:THR:HG22	19:30:42:ALA:H	1.46	0.80
9:20:57:ARG:NH1	30:R1:1154:G:OP2	2.15	0.80
30:R1:1839:G:H21	54:U:261:ARG:HH22	1.30	0.79
32:R3:592:G:N1	32:R3:647:C:N3	2.28	0.79
30:R1:2120:G:N2	30:R1:2179:C:N3	2.29	0.79
30:R1:2127:G:N1	30:R1:2161:C:N3	2.30	0.78
30:R1:2339:C:H4'	31:R2:41:G:H22	1.48	0.78
32:R3:1027:C:N4	32:R3:1034:G:O6	2.15	0.78
30:R1:1410:G:N1	30:R1:1592:C:N3	2.30	0.78
30:R1:1170:C:N4	30:R1:1176:U:O4	2.17	0.78
30:R1:371:A:H2	30:R1:402:A:H62	1.32	0.78
30:R1:1179:G:H5''	30:R1:1180:U:H6	1.47	0.77
30:R1:134:G:O6	30:R1:144:A:N1	2.17	0.77
30:R1:1216:G:N2	30:R1:1233:C:O2	2.14	0.77
30:R1:2107:G:N2	30:R1:2182:U:O2	2.17	0.77
30:R1:2136:G:H1	30:R1:2155:U:H3	1.30	0.77
30:R1:156:A:N1	30:R1:169:G:C6	2.54	0.76
30:R1:160:A:H8	30:R1:2217:G:H21	1.31	0.76
4:16:123:LYS:NZ	30:R1:2483:C:N3	2.34	0.76
11:22:5:ALA:HB2	11:22:54:ALA:HB2	1.68	0.76
30:R1:805:G:N2	30:R1:829:A:OP1	2.19	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:R1:156:A:H2	30:R1:169:G:C2	2.04	0.75
11:22:4:ILE:HG22	11:22:106:VAL:HG22	1.69	0.74
32:R3:992:U:H4'	32:R3:993:G:H5'	1.67	0.74
26:4:163:ASN:ND2	30:R1:320:A:N3	2.34	0.74
30:R1:284:U:O2	30:R1:356:G:N2	2.20	0.74
30:R1:271:G:H1	30:R1:366:C:H42	1.36	0.74
18:3:59:ARG:NH2	30:R1:2831:G:OP2	2.19	0.74
30:R1:1288:G:OP2	30:R1:1288:G:N2	2.19	0.74
28:6:172:GLU:HG2	28:6:174:LYS:H	1.51	0.73
32:R3:1149:C:H2'	32:R3:1150:A:C8	2.23	0.73
54:U:17:PRO:O	54:U:298:ARG:NH2	2.21	0.73
30:R1:1871:A:H3'	30:R1:1872:A:H8	1.53	0.73
30:R1:413:C:O2'	30:R1:414:C:O2	2.06	0.73
30:R1:856:G:H2'	30:R1:857:G:C8	2.22	0.73
32:R3:406:G:N2	32:R3:437:U:O2	2.22	0.73
32:R3:335:C:H2'	32:R3:336:A:H8	1.52	0.73
30:R1:2896:C:O2'	30:R1:2897:U:O5'	2.04	0.73
3:15:20:GLY:HA2	3:15:28:GLY:HA2	1.71	0.73
30:R1:1868:C:H42	30:R1:1873:G:H1	1.37	0.73
30:R1:1482:G:N2	30:R1:1508:A:N7	2.37	0.72
30:R1:1178:C:N3	30:R1:1179:G:O2'	2.22	0.72
30:R1:2127:G:H2'	30:R1:2128:G:C8	2.25	0.72
29:9:46:PHE:HB3	29:9:51:ARG:HH21	1.55	0.72
16:28:60:LYS:NZ	30:R1:371:A:O2'	2.23	0.72
32:R3:380:G:N2	32:R3:383:A:OP2	2.23	0.72
14:25:40:ILE:HD11	14:25:65:VAL:HG11	1.70	0.71
31:R2:112:G:O2'	31:R2:113:C:O2	2.06	0.71
28:6:3:VAL:HG21	30:R1:2748:A:H4'	1.70	0.71
30:R1:1936:A:H2	30:R1:1943:U:H3	1.39	0.71
30:R1:1063:G:N2	30:R1:1076:C:OP1	2.23	0.71
30:R1:2324:U:H3'	30:R1:2325:G:H5''	1.73	0.71
9:20:5:ARG:NH2	30:R1:585:G:N7	2.38	0.71
32:R3:1007:U:H2'	32:R3:1008:U:H4'	1.72	0.71
28:6:94:ARG:HB3	28:6:105:SER:HB2	1.73	0.71
30:R1:1528:A:OP2	30:R1:1543:G:N2	2.24	0.71
26:4:44:ARG:NH2	30:R1:1248:G:OP1	2.24	0.70
30:R1:136:G:O6	30:R1:142:A:N1	2.24	0.70
3:15:2:ARG:HD2	26:4:115:GLN:HE22	1.57	0.70
29:9:116:ARG:HB3	29:9:131:SER:HB2	1.74	0.70
54:U:424:LEU:HB3	54:U:429:PHE:HB2	1.74	0.70
32:R3:587:G:N2	32:R3:754:C:OP2	2.25	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:30:11:SER:HB2	30:R1:988:A:H5''	1.73	0.70
30:R1:247:G:OP2	30:R1:249:C:N4	2.25	0.70
14:25:77:VAL:HG23	14:25:89:ILE:HG22	1.71	0.70
29:9:7:ASP:OD1	29:9:8:LYS:N	2.25	0.70
32:R3:82:G:N1	32:R3:87:C:O2'	2.21	0.70
8:2:99:GLU:OE2	8:2:101:ARG:NH1	2.24	0.70
28:6:15:ASP:OD2	28:6:17:LYS:NZ	2.25	0.70
32:R3:990:C:H5	32:R3:1215:G:H1	1.40	0.70
1:13:23:LYS:HE3	1:13:142:ILE:HG22	1.74	0.69
30:R1:2162:G:O4'	30:R1:2173:A:N6	2.26	0.69
32:R3:1261:A:N6	32:R3:1274:A:HO2'	1.90	0.69
55:1:61:GLY:H	55:1:163:TYR:HB2	1.56	0.69
9:20:111:LYS:HG3	10:21:48:LYS:HZ3	1.57	0.69
30:R1:131:A:H61	30:R1:147:C:H42	1.39	0.69
2:14:70:ARG:NH2	30:R1:2683:C:O2	2.25	0.69
28:6:108:PHE:O	30:R1:2666:C:N4	2.22	0.69
32:R3:167:A:H2'	32:R3:168:G:C8	2.27	0.69
54:U:326:CYS:HB3	54:U:337:ASP:H	1.57	0.69
30:R1:45:G:H5''	30:R1:46:G:H5'	1.74	0.69
3:15:79:LEU:HD12	3:15:112:LEU:HA	1.75	0.69
8:2:270:ARG:NH2	30:R1:1798:U:OP2	2.23	0.69
54:U:412:MET:HG3	54:U:417:PRO:HG3	1.73	0.69
3:15:99:ASN:ND2	30:R1:621:A:OP2	2.26	0.69
9:20:90:ASP:H	10:21:11:GLN:HE22	1.40	0.68
25:36:29:ALA:O	28:6:169:ARG:NH1	2.27	0.68
30:R1:1056:G:N1	30:R1:1102:C:OP2	2.26	0.68
55:1:52:ALA:HB1	55:1:53:ARG:HH21	1.57	0.68
30:R1:848:C:H2'	30:R1:849:A:H8	1.57	0.68
30:R1:1466:U:HO2'	30:R1:1546:G:HO2'	1.37	0.68
32:R3:71:A:N6	32:R3:99:C:O2'	2.26	0.68
32:R3:1447:A:H5''	32:R3:1448:C:H5	1.58	0.68
27:5:117:SER:O	27:5:127:TYR:OH	2.12	0.68
8:2:257:ARG:NH1	30:R1:1799:G:OP1	2.26	0.68
30:R1:1802:A:H2'	30:R1:1803:A:C8	2.29	0.68
32:R3:1356:G:H2'	32:R3:1357:A:C8	2.29	0.68
14:25:76:ASP:OD1	14:25:77:VAL:N	2.26	0.68
32:R3:76:G:H21	32:R3:77:A:H62	1.42	0.68
21:32:52:LYS:HD3	21:32:55:ALA:HA	1.77	0.67
30:R1:362:A:H3'	30:R1:363:G:H8	1.58	0.67
30:R1:1410:G:N2	30:R1:1592:C:O2	2.20	0.67
32:R3:58:C:O2'	32:R3:388:G:N2	2.27	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:2:97:ASP:OD2	30:R1:1490:A:O2'	2.11	0.67
30:R1:2113:U:O2'	30:R1:2114:A:O5'	2.11	0.67
30:R1:1042:G:H1	30:R1:1113:U:H3	1.40	0.67
32:R3:1009:U:H3	32:R3:1020:G:H1	1.42	0.67
30:R1:307:G:N1	30:R1:310:A:OP2	2.24	0.67
30:R1:2699:C:O2'	30:R1:2700:A:O5'	2.12	0.67
32:R3:1218:C:H2'	32:R3:1219:A:C8	2.29	0.67
5:17:106:ASP:OD2	30:R1:1649:G:O2'	2.11	0.67
32:R3:1150:A:O2'	32:R3:1151:A:O4'	2.12	0.67
5:17:56:LYS:NZ	5:17:94:TYR:OH	2.23	0.67
14:25:35:GLU:OE1	14:25:93:ARG:NH1	2.28	0.67
20:31:25:ARG:O	27:5:101:ARG:NH2	2.27	0.67
7:19:30:TRP:NE1	7:19:81:ASP:OD2	2.28	0.66
30:R1:415:A:O2'	30:R1:1866:A:OP1	2.12	0.66
30:R1:151:C:H2'	30:R1:152:A:C8	2.30	0.66
9:20:90:ASP:OD1	10:21:11:GLN:NE2	2.28	0.66
30:R1:2788:C:O2'	30:R1:2809:A:N3	2.28	0.66
32:R3:279:A:H5''	32:R3:280:C:H3'	1.78	0.66
53:T:32:4OC:O2'	53:T:32:4OC:O2	2.12	0.66
30:R1:1478:G:H1	30:R1:1513:U:H3	1.43	0.66
32:R3:1314:C:H2'	32:R3:1315:U:H6	1.59	0.66
30:R1:1216:G:N1	30:R1:1233:C:N3	2.34	0.66
30:R1:1174:U:O2'	30:R1:1176:U:OP2	2.13	0.66
30:R1:880:G:H2'	30:R1:881:G:H8	1.61	0.66
32:R3:944:G:N1	32:R3:1338:G:OP2	2.27	0.66
32:R3:1023:U:O4	32:R3:1024:G:N2	2.29	0.66
13:24:47:PRO:HD3	13:24:55:GLY:HA2	1.78	0.65
27:5:84:ILE:HD11	30:R1:2312:U:H5'	1.77	0.65
30:R1:1022:G:N2	30:R1:1142:A:N1	2.42	0.65
30:R1:1715:G:N2	30:R1:1744:A:OP2	2.29	0.65
23:34:43:THR:OG1	23:34:44:VAL:N	2.29	0.65
30:R1:1728:C:H1'	30:R1:1733:G:H22	1.60	0.65
32:R3:501:C:H2'	32:R3:502:A:C8	2.31	0.65
32:R3:686:U:O4	32:R3:703:G:O2'	2.13	0.65
30:R1:199:A:O2'	30:R1:200:U:O2	2.14	0.65
32:R3:553:A:H2'	32:R3:554:A:H8	1.60	0.65
7:19:99:LEU:HD11	7:19:109:ILE:HD11	1.78	0.65
28:6:40:VAL:O	28:6:54:ARG:NH2	2.29	0.65
30:R1:2140:G:O6	30:R1:2142:A:N6	2.29	0.65
54:U:129:HIS:NE2	55:1:54:LYS:O	2.29	0.65
20:31:38:SER:HB3	27:5:104:THR:HA	1.77	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:R1:1900:A:H1'	30:R1:1970:A:H2'	1.78	0.65
31:R2:14:U:OP2	31:R2:70:C:O2'	2.13	0.65
30:R1:1385:A:O2'	30:R1:1396:U:O2	2.13	0.65
32:R3:674:G:H2'	32:R3:675:A:H8	1.60	0.65
32:R3:1027:C:O2	32:R3:1034:G:N2	2.23	0.65
6:18:117:PHE:O	30:R1:2377:A:O2'	2.15	0.64
30:R1:155:A:O2'	30:R1:156:A:O5'	2.15	0.64
32:R3:1356:G:H2'	32:R3:1357:A:H8	1.62	0.64
4:16:6:ARG:NH2	53:T:51:C:O2'	2.26	0.64
32:R3:257:G:H2'	32:R3:258:G:H8	1.63	0.64
4:16:30:SER:HA	4:16:133:LYS:HE2	1.79	0.64
29:9:11:ASN:O	29:9:11:ASN:ND2	2.30	0.64
32:R3:745:G:H2'	32:R3:746:A:C8	2.33	0.64
30:R1:880:G:N2	30:R1:897:C:N3	2.46	0.64
32:R3:1178:G:N2	32:R3:1181:G:OP2	2.30	0.64
29:9:87:GLU:N	29:9:87:GLU:OE1	2.31	0.64
32:R3:998:C:O2	32:R3:1043:G:N2	2.31	0.64
32:R3:1149:C:H2'	32:R3:1150:A:H8	1.62	0.64
32:R3:1260:G:N2	32:R3:1275:A:H62	1.94	0.64
17:29:9:LYS:HB2	17:29:12:GLU:HB3	1.78	0.64
18:3:133:THR:HG22	18:3:134:HIS:H	1.63	0.64
54:U:143:LEU:O	54:U:147:GLY:N	2.30	0.64
7:19:89:GLY:O	7:19:112:ARG:NH2	2.30	0.64
31:R2:30:C:H1'	31:R2:57:A:H61	1.61	0.64
12:23:11:LEU:O	17:29:29:ARG:NH1	2.30	0.64
30:R1:2255:G:OP1	54:U:280:ARG:NH1	2.31	0.64
32:R3:200:G:H2'	32:R3:201:G:C8	2.33	0.64
16:28:15:ASN:HD22	16:28:23:ALA:HB1	1.63	0.64
30:R1:1418:G:N1	30:R1:1579:A:OP2	2.26	0.64
30:R1:2848:G:O2'	30:R1:2867:G:N2	2.29	0.64
54:U:353:PRO:O	54:U:358:LYS:NZ	2.27	0.64
5:17:90:ARG:NH1	5:17:117:ASP:OD2	2.31	0.63
30:R1:2104:C:H2'	30:R1:2105:U:C6	2.33	0.63
32:R3:477:C:H2'	32:R3:478:A:C8	2.32	0.63
13:24:59:GLU:N	13:24:59:GLU:OE2	2.32	0.63
30:R1:2804:U:H2'	30:R1:2805:C:H6	1.64	0.63
32:R3:1229:A:O2'	53:T:30:G:OP1	2.16	0.63
54:U:519:TYR:HD2	54:U:529:GLN:HB2	1.64	0.63
6:18:31:THR:HG23	6:18:34:HIS:H	1.62	0.63
28:6:32:LEU:HD13	28:6:78:VAL:HG12	1.80	0.63
30:R1:286:U:H2'	30:R1:287:G:C4	2.33	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:R1:2469:A:N6	30:R1:2481:G:O2'	2.31	0.63
30:R1:2855:C:H2'	30:R1:2856:A:H8	1.62	0.63
16:28:36:ARG:NH1	30:R1:2200:C:OP2	2.31	0.63
12:23:28:ASN:HD21	12:23:91:GLN:HB3	1.61	0.63
18:3:109:VAL:HG21	18:3:193:VAL:HB	1.80	0.63
30:R1:1432:G:H2'	30:R1:1433:A:C8	2.33	0.63
30:R1:1469:A:H2'	30:R1:1470:A:C8	2.33	0.63
30:R1:2177:C:N4	30:R1:2178:C:O2	2.31	0.63
5:17:73:ASN:HA	5:17:76:VAL:HG12	1.81	0.63
30:R1:890:C:H3'	30:R1:891:G:H4'	1.81	0.63
6:18:34:HIS:ND1	6:18:53:THR:OG1	2.27	0.63
17:29:4:LYS:O	17:29:7:ARG:NH2	2.32	0.63
3:15:75:ALA:HB2	3:15:105:ILE:HD13	1.80	0.62
12:23:18:GLU:OE1	30:R1:1392:A:N6	2.32	0.62
30:R1:2139:U:O2'	30:R1:2153:C:O2	2.16	0.62
30:R1:2751:G:OP1	30:R1:2751:G:N2	2.32	0.62
28:6:172:GLU:N	28:6:172:GLU:OE2	2.29	0.62
29:9:122:LEU:HB3	29:9:128:HIS:ND1	2.14	0.62
30:R1:415:A:H62	30:R1:2408:U:H3	1.44	0.62
30:R1:1645:G:H5''	30:R1:1646:C:H5'	1.81	0.62
12:23:23:ALA:O	12:23:29:THR:OG1	2.17	0.62
32:R3:461:A:O2'	32:R3:462:G:OP1	2.18	0.62
32:R3:1129:C:H5	32:R3:1143:G:H22	1.47	0.62
3:15:91:ASP:H	3:15:94:THR:HG1	1.47	0.62
28:6:82:PHE:HB2	28:6:140:ILE:HD13	1.80	0.62
30:R1:2130:U:H1'	30:R1:2159:G:H22	1.64	0.62
32:R3:501:C:H2'	32:R3:502:A:H8	1.64	0.62
30:R1:154:U:O4	30:R1:155:A:N6	2.32	0.62
32:R3:1530:G:H2'	32:R3:1531:A:H8	1.65	0.62
30:R1:309:A:N3	30:R1:329:G:O2'	2.32	0.62
54:U:381:LYS:O	54:U:460:ASN:ND2	2.32	0.62
32:R3:154:U:O2	32:R3:168:G:N2	2.33	0.61
54:U:213:ARG:HE	54:U:473:VAL:HG11	1.65	0.61
54:U:391:ARG:NH2	54:U:470:ASP:OD2	2.32	0.61
22:33:4:ILE:O	54:U:14:SER:OG	2.17	0.61
27:5:34:THR:OG1	27:5:154:THR:OG1	2.17	0.61
30:R1:639:U:H2'	30:R1:640:C:C6	2.35	0.61
30:R1:1047:G:H21	30:R1:1110:G:H21	1.49	0.61
30:R1:1062:G:N2	30:R1:1076:C:O2	2.32	0.61
32:R3:1151:A:H2'	32:R3:1152:A:C8	2.35	0.61
5:17:57:THR:OG1	5:17:62:ASN:ND2	2.34	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:28:55:MET:SD	29:9:27:ARG:NH1	2.73	0.61
30:R1:1072:C:O2'	30:R1:1093:G:O6	2.16	0.61
32:R3:1270:G:O2'	32:R3:1271:A:OP1	2.16	0.61
54:U:64:GLN:HG2	55:1:54:LYS:HE3	1.82	0.61
30:R1:1171:G:N1	30:R1:1176:U:O2	2.33	0.61
54:U:80:GLU:N	54:U:80:GLU:OE1	2.32	0.61
28:6:174:LYS:HG3	30:R1:2529:G:H4'	1.82	0.61
30:R1:2812:G:H2'	30:R1:2813:A:C8	2.35	0.61
11:22:92:ARG:HH22	30:R1:747:U:H4'	1.66	0.61
55:1:54:LYS:O	55:1:57:GLN:NE2	2.33	0.61
1:13:17:VAL:HG22	1:13:55:ILE:HB	1.82	0.61
30:R1:881:G:H2'	30:R1:882:G:C8	2.35	0.61
30:R1:2105:U:O2'	30:R1:2106:U:OP1	2.16	0.61
30:R1:2774:C:O2'	30:R1:2775:G:H8	1.83	0.61
32:R3:254:G:H2'	32:R3:255:G:H8	1.64	0.61
32:R3:413:G:O2'	32:R3:428:G:N2	2.34	0.61
6:18:3:LYS:NZ	31:R2:46:A:OP1	2.33	0.61
10:21:59:ILE:HG12	10:21:101:ILE:HG23	1.82	0.61
30:R1:2134:A:C8	30:R1:2157:G:H4'	2.36	0.61
30:R1:2747:G:H21	30:R1:2757:A:H62	1.47	0.61
32:R3:672:U:H2'	32:R3:673:A:H8	1.66	0.61
10:21:62:GLU:N	10:21:62:GLU:OE2	2.34	0.61
30:R1:639:U:H2'	30:R1:640:C:H6	1.64	0.61
32:R3:714:G:H2'	32:R3:715:A:C8	2.36	0.61
30:R1:2638:G:H1'	30:R1:2778:A:H61	1.66	0.60
18:3:148:GLN:HB2	18:3:152:PRO:HG2	1.82	0.60
24:35:33:THR:OG1	30:R1:2420:C:OP1	2.19	0.60
30:R1:156:A:C2	30:R1:169:G:C6	2.89	0.60
30:R1:2123:G:O2'	55:1:43:ASP:OD2	2.19	0.60
13:24:6:ARG:NH1	30:R1:84:A:O2'	2.32	0.60
30:R1:136:G:C6	30:R1:142:A:N1	2.69	0.60
30:R1:1102:C:H2'	30:R1:1103:A:C8	2.35	0.60
5:17:17:ARG:NH2	30:R1:2002:G:OP1	2.34	0.60
30:R1:2760:C:H2'	30:R1:2761:A:H5''	1.81	0.60
32:R3:321:A:H62	32:R3:332:G:H1	1.47	0.60
55:1:57:GLN:NE2	55:1:58:ASN:OD1	2.34	0.60
6:18:15:ARG:NH2	6:18:95:SER:OG	2.34	0.60
30:R1:2177:C:H3'	30:R1:2178:C:H4'	1.84	0.60
32:R3:414:A:OP2	32:R3:428:G:N2	2.29	0.60
21:32:3:GLN:NE2	30:R1:2016:U:O2	2.35	0.60
26:4:143:LEU:HB3	26:4:146:VAL:HG11	1.84	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:9:128:HIS:O	29:9:144:VAL:N	2.32	0.60
30:R1:81:G:O2'	30:R1:295:G:O2'	2.19	0.60
30:R1:689:A:H8	30:R1:779:U:HO2'	1.50	0.60
30:R1:695:G:H5''	30:R1:1380:G:H4'	1.82	0.60
32:R3:745:G:H2'	32:R3:746:A:H8	1.65	0.60
28:6:5:LYS:NZ	28:6:51:PHE:O	2.34	0.60
30:R1:1522:A:H4'	30:R1:1523:U:H5'	1.83	0.60
32:R3:115:G:H8	32:R3:115:G:OP1	1.84	0.60
32:R3:746:A:H2'	32:R3:747:A:C8	2.37	0.60
32:R3:1270:G:H2'	32:R3:1271:A:C8	2.36	0.60
53:T:20:H2U:O2	53:T:20:H2U:O4'	2.17	0.60
30:R1:2174:C:C4	30:R1:2175:C:H1'	2.37	0.60
9:20:57:ARG:NH2	30:R1:998:C:OP2	2.34	0.60
21:32:33:SER:OG	21:32:35:GLU:HG3	2.02	0.60
29:9:70:GLU:HA	29:9:73:ASN:HB3	1.83	0.60
30:R1:700:G:O2'	30:R1:1632:A:N3	2.29	0.60
32:R3:505:G:H2'	32:R3:506:G:H8	1.66	0.60
32:R3:1261:A:N6	32:R3:1274:A:O2'	2.35	0.60
16:28:31:ASN:ND2	30:R1:2230:G:N3	2.50	0.59
30:R1:412:A:H2'	30:R1:413:C:H5'	1.83	0.59
32:R3:418:C:HO2'	32:R3:419:C:H6	1.50	0.59
32:R3:1285:A:H5''	32:R3:1286:U:H5	1.65	0.59
32:R3:335:C:H2'	32:R3:336:A:C8	2.37	0.59
32:R3:1013:G:N2	32:R3:1016:A:OP2	2.29	0.59
32:R3:1033:G:H2'	32:R3:1034:G:C8	2.37	0.59
30:R1:1179:G:H5''	30:R1:1180:U:C6	2.35	0.59
31:R2:23:G:H1	31:R2:60:C:H5	1.50	0.59
32:R3:508:U:H1'	32:R3:509:A:C2	2.37	0.59
32:R3:1271:A:OP1	32:R3:1314:C:H5'	2.02	0.59
54:U:402:ASP:O	54:U:407:GLY:N	2.31	0.59
28:6:26:LYS:HG3	28:6:31:GLU:HA	1.83	0.59
30:R1:2:G:H22	30:R1:2901:C:H2'	1.67	0.59
30:R1:2098:U:O2	30:R1:2099:U:N3	2.36	0.59
30:R1:2177:C:C4	30:R1:2178:C:H1'	2.37	0.59
54:U:327:TYR:H	54:U:335:VAL:HG13	1.68	0.59
1:13:30:THR:HG21	30:R1:1005:C:O2'	2.03	0.59
8:2:132:ARG:O	8:2:166:ARG:NH1	2.34	0.59
22:33:26:LYS:HB2	54:U:14:SER:HB2	1.83	0.59
30:R1:1504:A:H2'	30:R1:1505:A:C8	2.37	0.59
32:R3:142:G:H3'	32:R3:143:A:H8	1.68	0.59
54:U:30:GLU:H	54:U:205:THR:HG23	1.67	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:17:37:THR:HG22	5:17:39:PRO:HD2	1.83	0.59
10:21:1:MET:HE2	10:21:43:ASN:HB3	1.84	0.59
30:R1:1055:G:H1'	30:R1:1084:A:H61	1.65	0.59
17:29:58:ASN:ND2	30:R1:72:U:O4	2.35	0.59
29:9:89:LYS:NZ	29:9:90:LEU:O	2.25	0.59
30:R1:52:A:H2'	30:R1:53:A:H8	1.67	0.59
30:R1:2246:G:H2'	30:R1:2247:A:C8	2.38	0.59
32:R3:78:A:O2'	32:R3:93:U:N3	2.32	0.59
53:T:31:G:H2'	53:T:32:4OC:H6	1.84	0.59
54:U:13:PHE:O	54:U:15:ASP:N	2.36	0.59
54:U:325:VAL:HG12	54:U:338:PHE:HB3	1.85	0.59
55:1:195:ALA:HA	55:1:198:LYS:HE2	1.83	0.59
30:R1:2699:C:O2'	30:R1:2700:A:H8	1.86	0.59
30:R1:2774:C:O2'	30:R1:2775:G:O5'	2.21	0.59
32:R3:563:A:HO2'	32:R3:566:G:HO2'	1.50	0.59
3:15:76:GLU:OE2	30:R1:636:G:N1	2.32	0.59
4:16:4:PRO:HG2	4:16:70:ASP:HA	1.85	0.59
26:4:53:THR:HG21	30:R1:452:G:C8	2.37	0.58
55:1:192:LEU:O	55:1:196:LEU:HB3	2.03	0.58
32:R3:362:G:N1	32:R3:365:U:OP2	2.32	0.58
32:R3:811:C:O2'	32:R3:901:A:N1	2.35	0.58
54:U:129:HIS:HE1	55:1:53:ARG:HA	1.65	0.58
55:1:62:ALA:HB2	55:1:162:ARG:HH12	1.69	0.58
6:18:33:ARG:HB2	31:R2:52:A:H62	1.66	0.58
27:5:125:GLY:O	27:5:157:THR:OG1	2.20	0.58
29:9:53:GLU:HA	29:9:56:ALA:HB3	1.85	0.58
30:R1:155:A:O2'	30:R1:156:A:H8	1.85	0.58
30:R1:1755:A:N6	30:R1:2694:G:O2'	2.36	0.58
30:R1:2804:U:H2'	30:R1:2805:C:C6	2.39	0.58
54:U:56:ASP:OD1	54:U:57:ASP:N	2.35	0.58
2:14:106:GLU:N	2:14:106:GLU:OE2	2.36	0.58
8:2:143:VAL:HB	8:2:153:LEU:HB2	1.84	0.58
12:23:8:LEU:HD13	17:29:21:LEU:HB2	1.84	0.58
54:U:127:LEU:HD21	54:U:133:TRP:NE1	2.18	0.58
30:R1:106:C:H2'	30:R1:107:G:H8	1.68	0.58
20:31:31:ASP:OD2	20:31:32:LEU:N	2.34	0.58
29:9:8:LYS:O	29:9:9:VAL:HG23	2.03	0.58
32:R3:1530:G:H2'	32:R3:1531:A:C8	2.37	0.58
24:35:44:ARG:NH2	30:R1:2349:G:OP1	2.34	0.58
3:15:90:VAL:HG13	3:15:95:LEU:HD21	1.84	0.58
32:R3:816:A:OP1	32:R3:1526:G:O2'	2.21	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
54:U:104:ILE:HG23	54:U:107:LEU:HD13	1.86	0.58
6:18:30:ARG:NH2	31:R2:48:U:OP1	2.36	0.58
26:4:55:SER:OG	30:R1:797:G:OP1	2.20	0.58
30:R1:197:A:N6	30:R1:2430:A:O2'	2.36	0.58
30:R1:1410:G:O6	30:R1:1592:C:N4	2.26	0.58
32:R3:1010:U:H2'	32:R3:1011:C:C6	2.38	0.58
54:U:36:GLY:O	54:U:42:LYS:NZ	2.37	0.58
30:R1:2557:G:H2'	30:R1:2558:C:C6	2.39	0.58
30:R1:2745:C:H2'	30:R1:2746:U:C6	2.39	0.58
25:36:12:ARG:NH1	25:36:13:ASN:OD1	2.37	0.57
30:R1:301:G:N2	30:R1:316:C:O2	2.25	0.57
30:R1:1779:U:H5	30:R1:1784:A:N7	2.01	0.57
30:R1:1022:G:N2	30:R1:1023:U:O4	2.37	0.57
30:R1:1447:C:H2'	30:R1:1448:G:H8	1.68	0.57
32:R3:1266:G:N2	32:R3:1269:A:OP2	2.21	0.57
27:5:35:LEU:HD11	27:5:151:LEU:HD22	1.87	0.57
32:R3:509:A:H8	32:R3:544:G:H5'	1.69	0.57
32:R3:1144:G:N2	32:R3:1146:A:H62	2.02	0.57
14:25:43:ASP:OD1	14:25:46:LYS:N	2.32	0.57
19:30:2:LYS:O	19:30:39:ASP:N	2.34	0.57
26:4:51:GLU:OE2	26:4:88:ARG:NH2	2.37	0.57
29:9:76:GLU:HA	29:9:142:VAL:HG22	1.86	0.57
30:R1:2071:A:H2'	30:R1:2072:C:C6	2.39	0.57
30:R1:2154:A:H2'	30:R1:2155:U:C6	2.40	0.57
30:R1:219:A:N3	30:R1:234:U:O2'	2.34	0.57
30:R1:721:A:H2'	30:R1:722:A:C8	2.40	0.57
32:R3:413:G:HO2'	32:R3:428:G:N2	2.02	0.57
30:R1:353:C:H2'	30:R1:354:A:C8	2.39	0.57
32:R3:1037:C:H2'	32:R3:1038:C:C2	2.40	0.57
31:R2:6:G:H2'	31:R2:7:G:C8	2.40	0.57
4:16:64:TRP:HE1	30:R1:873:C:H4'	1.69	0.57
19:30:23:LEU:HD11	19:30:53:MET:HE1	1.86	0.57
30:R1:1087:G:O6	30:R1:1103:A:N6	2.38	0.57
30:R1:1109:C:O2'	30:R1:1110:G:OP1	2.22	0.57
30:R1:1869:G:H2'	30:R1:1872:A:N6	2.19	0.57
32:R3:466:A:N7	32:R3:468:A:N6	2.51	0.57
3:15:109:LYS:HE2	3:15:128:THR:HG22	1.87	0.56
26:4:87:ALA:O	26:4:88:ARG:HD3	2.05	0.56
8:2:106:PRO:HD2	8:2:109:LEU:HD22	1.87	0.56
30:R1:1141:U:H4'	30:R1:1142:A:O4'	2.05	0.56
11:22:5:ALA:O	30:R1:494:G:O2'	2.21	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:24:81:ARG:NH2	30:R1:301:G:OP2	2.38	0.56
14:25:51:GLN:OE1	14:25:51:GLN:N	2.38	0.56
15:27:43:THR:HG21	30:R1:2336:A:H61	1.71	0.56
18:3:74:GLU:H	18:3:74:GLU:CD	2.08	0.56
30:R1:1093:G:H21	30:R1:1098:A:H62	1.52	0.56
30:R1:1847:G:O2'	30:R1:1848:A:H8	1.87	0.56
30:R1:2063:C:H1'	53:T:101:FME:HB2	1.87	0.56
30:R1:2123:G:H2'	30:R1:2124:G:C4	2.40	0.56
30:R1:2189:U:H2'	30:R1:2190:G:C8	2.41	0.56
32:R3:908:A:H2'	32:R3:909:A:C8	2.40	0.56
32:R3:1084:G:H5''	32:R3:1085:U:H5''	1.87	0.56
32:R3:1388:C:H2'	32:R3:1389:C:O2	2.06	0.56
6:18:34:HIS:O	6:18:102:ARG:NH2	2.38	0.56
15:27:5:LYS:HG2	53:T:0:C:H5'	1.87	0.56
30:R1:340:A:H2'	30:R1:341:C:O4'	2.05	0.56
2:14:70:ARG:NH1	30:R1:2684:U:O4'	2.38	0.56
30:R1:2121:G:H2'	30:R1:2122:U:C6	2.41	0.56
32:R3:399:G:H2'	32:R3:400:C:C6	2.41	0.56
4:16:45:GLN:NE2	30:R1:2485:G:OP1	2.35	0.56
14:25:13:GLY:O	14:25:17:SER:OG	2.20	0.56
30:R1:132:G:H1	30:R1:146:A:H62	1.54	0.56
18:3:25:THR:OG1	18:3:191:GLY:O	2.24	0.56
30:R1:1266:G:O2'	30:R1:2012:G:O6	2.21	0.56
30:R1:1681:G:N2	30:R1:1763:G:OP2	2.23	0.56
8:2:129:LEU:HD13	8:2:133:ASN:HB2	1.86	0.56
13:24:43:LYS:NZ	30:R1:481:G:O5'	2.39	0.56
21:32:54:ILE:HG23	21:32:56:LYS:H	1.71	0.56
30:R1:644:A:H2'	30:R1:645:C:O4'	2.05	0.56
30:R1:1501:G:H2'	30:R1:1502:A:H8	1.71	0.56
30:R1:2154:A:H2'	30:R1:2155:U:H6	1.70	0.56
30:R1:2896:C:O2'	30:R1:2897:U:H6	1.88	0.56
32:R3:301:G:O2'	32:R3:302:G:OP1	2.24	0.56
32:R3:382:A:H2'	32:R3:383:A:H8	1.70	0.56
32:R3:402:G:H4'	32:R3:620:C:H5	1.70	0.56
54:U:384:VAL:HG22	54:U:461:LEU:HD23	1.88	0.56
28:6:39:ALA:HB2	28:6:57:TYR:HD2	1.71	0.56
30:R1:848:C:H2'	30:R1:849:A:C8	2.38	0.56
32:R3:108:G:H5'	32:R3:109:A:H5''	1.86	0.56
32:R3:553:A:H2'	32:R3:554:A:C8	2.40	0.56
5:17:38:LEU:HB3	5:17:39:PRO:HD3	1.88	0.56
28:6:136:ASP:O	28:6:140:ILE:HG12	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:14:99:ILE:HD13	2:14:115:ILE:HG23	1.88	0.55
3:15:81:ASP:OD2	3:15:100:ILE:HD13	2.06	0.55
10:21:71:LYS:NZ	30:R1:1225:G:OP1	2.30	0.55
22:33:22:THR:OG1	22:33:23:THR:N	2.39	0.55
32:R3:588:G:O2'	32:R3:589:U:OP1	2.24	0.55
7:19:13:LYS:HE3	7:19:76:HIS:HA	1.89	0.55
28:6:53:PRO:HG2	28:6:61:TRP:CE2	2.41	0.55
32:R3:45:G:H2'	32:R3:46:G:C8	2.41	0.55
32:R3:54:C:OP1	32:R3:351:G:N2	2.40	0.55
32:R3:592:G:O6	32:R3:647:C:N4	2.29	0.55
53:T:8:4SU:O2	53:T:8:4SU:O2'	2.18	0.55
8:2:13:ARG:NH2	30:R1:1695:G:N7	2.51	0.55
8:2:60:ALA:O	8:2:62:ARG:NH1	2.40	0.55
22:33:5:ARG:NH1	30:R1:2285:C:OP2	2.34	0.55
30:R1:880:G:H2'	30:R1:881:G:C8	2.39	0.55
30:R1:1176:U:O2'	30:R1:1178:C:N4	2.34	0.55
32:R3:908:A:H2'	32:R3:909:A:H8	1.71	0.55
54:U:100:ARG:O	54:U:104:ILE:HG13	2.07	0.55
30:R1:84:A:H4'	30:R1:85:G:H5'	1.88	0.55
30:R1:1040:A:H61	30:R1:1115:G:H1	1.53	0.55
32:R3:382:A:H2'	32:R3:383:A:C8	2.41	0.55
32:R3:598:U:H2'	32:R3:599:C:C6	2.41	0.55
14:25:32:GLY:HA3	14:25:93:ARG:HB2	1.87	0.55
30:R1:106:C:H2'	30:R1:107:G:C8	2.41	0.55
30:R1:1178:C:C2	30:R1:1179:G:H4'	2.42	0.55
30:R1:2176:A:O2'	55:1:47:ASN:OD1	2.24	0.55
32:R3:837:U:H2'	32:R3:838:G:C8	2.41	0.55
32:R3:928:G:H1	32:R3:1389:C:H5	1.53	0.55
30:R1:1587:G:H2'	30:R1:1588:G:H8	1.71	0.55
30:R1:2025:C:H2'	30:R1:2026:U:C6	2.42	0.55
32:R3:563:A:O2'	32:R3:566:G:O2'	2.21	0.55
11:22:108:SER:OG	11:22:109:ASP:N	2.39	0.55
13:24:87:GLU:O	13:24:90:LYS:N	2.40	0.55
18:3:45:TYR:OH	18:3:81:GLU:OE2	2.14	0.55
30:R1:2118:U:OP1	30:R1:2148:G:O2'	2.20	0.55
32:R3:321:A:C2'	32:R3:322:C:H5'	2.37	0.55
32:R3:1412:C:H2'	32:R3:1413:A:C8	2.42	0.55
30:R1:2305:U:H2'	30:R1:2306:C:C6	2.41	0.55
32:R3:532:A:N6	32:R3:1206:G:O2'	2.40	0.55
32:R3:962:C:H5	32:R3:973:G:H1	1.54	0.55
54:U:79:VAL:HG22	54:U:155:SER:HA	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:R1:277:G:H8	30:R1:361:G:C5	2.25	0.55
30:R1:482:A:O2'	30:R1:497:A:N1	2.33	0.55
32:R3:1251:A:N3	32:R3:1369:C:O2'	2.37	0.55
54:U:357:GLY:N	58:U:601:ATP:O2B	2.40	0.55
8:2:132:ARG:NH1	29:9:93:SER:OG	2.39	0.55
18:3:108:ASP:OD1	18:3:206:ALA:HA	2.06	0.55
30:R1:2430:A:H2'	30:R1:2430:A:N3	2.22	0.55
32:R3:501:C:O2	32:R3:549:C:O2'	2.25	0.55
32:R3:1326:U:H2'	32:R3:1327:C:H6	1.72	0.55
32:R3:1347:G:O2'	32:R3:1373:G:O6	2.21	0.55
54:U:411:VAL:HG23	54:U:456:LEU:HG	1.87	0.55
8:2:179:GLU:OE2	30:R1:1799:G:O2'	2.17	0.54
30:R1:2164:C:H2'	30:R1:2165:C:H4'	1.88	0.54
32:R3:1015:G:H2'	32:R3:1016:A:C8	2.42	0.54
1:13:116:ARG:NH2	30:R1:528:A:OP2	2.38	0.54
4:16:20:LEU:HD13	14:25:81:PRO:HG2	1.89	0.54
11:22:7:HIS:HB2	11:22:50:VAL:HG21	1.89	0.54
19:30:11:SER:OG	19:30:13:ILE:HG13	2.08	0.54
28:6:12:ALA:O	28:6:14:VAL:N	2.35	0.54
29:9:4:ILE:HG12	29:9:37:VAL:O	2.08	0.54
30:R1:1593:A:H2'	30:R1:1594:U:C6	2.42	0.54
30:R1:2087:G:H2'	30:R1:2088:A:C8	2.41	0.54
30:R1:2184:A:H2'	30:R1:2185:U:C6	2.42	0.54
32:R3:1250:A:H2'	32:R3:1251:A:C8	2.42	0.54
54:U:462:LEU:HB2	54:U:490:VAL:HG22	1.89	0.54
23:34:24:THR:HG23	23:34:27:GLY:H	1.72	0.54
30:R1:296:U:H2'	30:R1:297:G:H8	1.71	0.54
30:R1:1047:G:H21	30:R1:1110:G:N2	2.05	0.54
30:R1:2126:A:H61	30:R1:2163:A:H5'	1.73	0.54
55:1:149:VAL:O	55:1:153:VAL:N	2.28	0.54
4:16:6:ARG:HH21	53:T:52:G:H4'	1.72	0.54
25:36:4:ARG:HG3	25:36:4:ARG:HH11	1.71	0.54
30:R1:177:G:H3'	30:R1:178:G:H8	1.72	0.54
30:R1:593:U:H2'	30:R1:594:U:C6	2.43	0.54
30:R1:1388:G:HO2'	30:R1:1525:A:HO2'	1.55	0.54
30:R1:1441:G:H2'	30:R1:1442:U:C6	2.43	0.54
32:R3:744:C:H2'	32:R3:745:G:C8	2.42	0.54
54:U:186:HIS:HD2	54:U:389:GLN:HE21	1.56	0.54
54:U:472:ASP:OD1	54:U:473:VAL:N	2.41	0.54
30:R1:640:C:H2'	30:R1:641:U:H6	1.73	0.54
30:R1:2316:G:H2'	30:R1:2317:A:H8	1.73	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:R3:950:U:H3	32:R3:1231:G:H1	1.56	0.54
2:14:75:SER:OG	7:19:72:VAL:O	2.14	0.54
13:24:96:LYS:HE3	30:R1:299:A:H5''	1.90	0.54
26:4:55:SER:HB2	30:R1:468:G:H5''	1.90	0.54
31:R2:39:A:N1	31:R2:44:G:N1	2.55	0.54
11:22:41:LYS:HE3	21:32:21:LEU:HD11	1.88	0.54
30:R1:1110:G:O2'	30:R1:1111:A:O4'	2.25	0.54
30:R1:2457:U:H5	30:R1:2494:G:H1	1.56	0.54
30:R1:2591:C:H2'	30:R1:2592:G:H8	1.72	0.54
5:17:32:GLU:HB2	5:17:118:ARG:HD2	1.90	0.54
11:22:83:LYS:HB3	11:22:95:ARG:HE	1.73	0.54
30:R1:2254:C:H4'	54:U:274:ILE:HG13	1.89	0.54
55:1:16:ASP:O	55:1:21:TYR:OH	2.26	0.54
6:18:4:LYS:O	6:18:8:ILE:HG13	2.08	0.54
28:6:171:LYS:NZ	30:R1:2529:G:OP2	2.29	0.54
30:R1:2855:C:H2'	30:R1:2856:A:C8	2.42	0.54
32:R3:189:A:H2'	32:R3:190:A:C8	2.42	0.54
32:R3:257:G:H2'	32:R3:258:G:C8	2.43	0.54
32:R3:672:U:H2'	32:R3:673:A:C8	2.43	0.54
30:R1:191:A:H2'	30:R1:192:C:C6	2.44	0.53
30:R1:2562:U:H2'	30:R1:2563:U:H5'	1.90	0.53
32:R3:890:G:N2	32:R3:891:U:O4	2.32	0.53
32:R3:1270:G:H2'	32:R3:1271:A:H8	1.72	0.53
8:2:7:PRO:HB3	8:2:13:ARG:HG2	1.89	0.53
12:23:79:ASP:OD1	12:23:79:ASP:N	2.40	0.53
30:R1:296:U:H2'	30:R1:297:G:C8	2.44	0.53
30:R1:319:G:H1	30:R1:323:C:H5	1.55	0.53
30:R1:1408:G:H1	30:R1:1594:U:H3	1.56	0.53
30:R1:1540:G:H2'	30:R1:1541:C:C6	2.43	0.53
32:R3:352:C:O2'	32:R3:354:G:OP1	2.19	0.53
32:R3:1129:C:H1'	32:R3:1130:A:H2	1.73	0.53
6:18:30:ARG:HH22	31:R2:48:U:P	2.31	0.53
6:18:31:THR:HG21	31:R2:28:C:OP1	2.08	0.53
28:6:88:LEU:HD11	28:6:95:ALA:HB2	1.90	0.53
30:R1:152:A:H61	30:R1:173:A:H61	1.54	0.53
32:R3:674:G:H2'	32:R3:675:A:C8	2.43	0.53
32:R3:1451:U:O2'	32:R3:1453:G:N7	2.39	0.53
32:R3:1507:A:H2'	32:R3:1508:A:C8	2.44	0.53
53:T:54:5MU:OP2	53:T:54:5MU:H4'	2.08	0.53
26:4:45:ALA:HB2	26:4:89:PRO:HD3	1.90	0.53
30:R1:52:A:H2'	30:R1:53:A:C8	2.44	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:R1:411:G:OP2	30:R1:2406:A:O2'	2.26	0.53
30:R1:1482:G:H2'	30:R1:1483:G:H8	1.72	0.53
32:R3:236:A:H2'	32:R3:237:G:C8	2.44	0.53
7:19:88:ARG:NH2	7:19:114:ASN:O	2.41	0.53
8:2:99:GLU:OE1	30:R1:1491:G:O2'	2.24	0.53
12:23:28:ASN:ND2	12:23:91:GLN:HB3	2.24	0.53
12:23:87:LEU:HD12	12:23:91:GLN:HB2	1.90	0.53
32:R3:58:C:H1'	32:R3:388:G:H22	1.74	0.53
32:R3:376:G:OP1	32:R3:376:G:H4'	2.08	0.53
32:R3:1298:U:H2'	54:U:318:ILE:HD12	1.90	0.53
9:20:57:ARG:O	9:20:61:ILE:HG13	2.07	0.53
12:23:18:GLU:O	12:23:22:THR:OG1	2.25	0.53
30:R1:1418:G:O2'	30:R1:1580:A:N6	2.41	0.53
32:R3:1077:G:N2	32:R3:1080:A:OP2	2.31	0.53
32:R3:1314:C:H2'	32:R3:1315:U:C6	2.42	0.53
29:9:54:LEU:HA	29:9:57:LYS:HE3	1.91	0.53
30:R1:1594:U:H2'	30:R1:1595:C:C6	2.44	0.53
32:R3:555:U:H2'	32:R3:556:C:C6	2.44	0.53
32:R3:1305:G:H4'	32:R3:1306:A:O5'	2.06	0.53
29:9:99:ILE:HD12	29:9:115:VAL:HG11	1.90	0.53
30:R1:1667:G:O2'	30:R1:1991:U:O4	2.18	0.53
30:R1:1728:C:O2	30:R1:1733:G:N1	2.42	0.53
8:2:238:ASN:ND2	30:R1:2595:G:O6	2.42	0.53
18:3:149:ASN:OD1	18:3:150:GLN:N	2.41	0.53
30:R1:1103:A:H5''	30:R1:1104:C:H5	1.74	0.53
30:R1:1447:C:H2'	30:R1:1448:G:C8	2.44	0.53
18:3:133:THR:HG22	18:3:134:HIS:N	2.24	0.53
30:R1:289:G:H2'	30:R1:290:U:C6	2.44	0.53
30:R1:1462:C:O2'	30:R1:2702:G:O2'	2.22	0.53
32:R3:339:C:H2'	32:R3:340:U:C6	2.44	0.53
53:T:73:A:H5'	53:T:74:C:H5'	1.91	0.53
24:35:15:LYS:HE3	24:35:19:GLY:HA2	1.91	0.52
29:9:132:PHE:N	29:9:140:ALA:O	2.36	0.52
31:R2:6:G:H2'	31:R2:7:G:H8	1.74	0.52
32:R3:195:A:H2'	32:R3:196:A:C8	2.44	0.52
54:U:68:VAL:HG22	54:U:177:VAL:HB	1.91	0.52
55:1:10:VAL:O	55:1:14:LYS:NZ	2.35	0.52
3:15:30:THR:O	3:15:30:THR:OG1	2.27	0.52
15:27:14:ARG:NH1	30:R1:2279:G:N7	2.57	0.52
15:27:18:ALA:O	15:27:20:ARG:NH1	2.43	0.52
29:9:128:HIS:HB2	29:9:144:VAL:HB	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:R1:365:U:H2'	30:R1:366:C:C6	2.44	0.52
30:R1:1054:A:H2'	30:R1:1055:G:H8	1.74	0.52
2:14:102:PRO:HB3	2:14:121:GLU:HB3	1.91	0.52
3:15:108:ALA:HB3	3:15:125:LEU:HD22	1.91	0.52
14:25:59:GLU:OE1	14:25:59:GLU:N	2.41	0.52
3:15:76:GLU:CD	30:R1:636:G:H1	2.12	0.52
7:19:28:LYS:HG3	7:19:82:SER:HB3	1.92	0.52
30:R1:387:U:H4'	30:R1:388:G:H5'	1.91	0.52
30:R1:2339:C:O2'	31:R2:41:G:N2	2.43	0.52
30:R1:2638:G:H1'	30:R1:2778:A:N6	2.23	0.52
8:2:220:ARG:NH1	30:R1:1789:A:OP2	2.43	0.52
27:5:25:MET:HE3	31:R2:54:G:H21	1.75	0.52
30:R1:1341:G:OP1	30:R1:1397:U:N3	2.38	0.52
30:R1:2127:G:O6	30:R1:2161:C:N4	2.38	0.52
30:R1:2540:C:O2'	30:R1:2740:A:N3	2.38	0.52
18:3:8:LYS:HB2	18:3:201:LEU:HD11	1.92	0.52
30:R1:500:G:H22	30:R1:503:A:H5'	1.74	0.52
30:R1:1069:A:H1'	30:R1:1096:A:H4'	1.91	0.52
32:R3:261:U:HO2'	32:R3:263:A:H2	1.58	0.52
32:R3:838:G:O2'	32:R3:839:C:O5'	2.24	0.52
29:9:40:THR:OG1	29:9:43:ASN:OD1	2.27	0.52
30:R1:885:C:H1'	30:R1:892:A:C6	2.44	0.52
30:R1:1112:G:H2'	30:R1:1113:U:C6	2.45	0.52
30:R1:1954:G:O2'	30:R1:1956:U:O4	2.21	0.52
32:R3:757:U:OP1	32:R3:822:U:O2'	2.23	0.52
32:R3:966:G:N2	53:T:34:C:H5'	2.25	0.52
54:U:240:GLN:O	54:U:244:GLU:HG3	2.09	0.52
54:U:288:LEU:HG	54:U:292:ARG:HD2	1.90	0.52
29:9:16:GLY:HA2	29:9:47:PHE:HZ	1.74	0.52
30:R1:849:A:H2'	30:R1:850:U:H6	1.73	0.52
30:R1:1091:G:H22	30:R1:1100:C:H42	1.57	0.52
30:R1:1595:C:H2'	30:R1:1596:A:C8	2.45	0.52
30:R1:1725:U:H2'	30:R1:1726:C:C6	2.44	0.52
30:R1:2122:U:H3	30:R1:2176:A:H61	1.58	0.52
32:R3:253:A:H2'	32:R3:254:G:H8	1.74	0.52
32:R3:1071:C:H2'	32:R3:1072:G:C8	2.44	0.52
32:R3:1260:G:H21	32:R3:1275:A:N6	2.00	0.52
8:2:70:LYS:HG2	8:2:73:ILE:HD12	1.92	0.52
30:R1:2306:C:H3'	30:R1:2307:G:H2'	1.92	0.52
31:R2:5:U:OP1	31:R2:61:G:O2'	2.28	0.52
32:R3:203:G:O2'	32:R3:466:A:N6	2.43	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
54:U:4:ILE:HG12	54:U:62:TYR:HB3	1.91	0.52
4:16:64:TRP:NE1	30:R1:873:C:H4'	2.25	0.52
30:R1:1173:U:H3'	30:R1:1174:U:H4'	1.92	0.52
32:R3:236:A:H2'	32:R3:237:G:H8	1.75	0.52
32:R3:461:A:H5''	32:R3:463:U:C4	2.45	0.52
32:R3:1129:C:H1'	32:R3:1130:A:C2	2.45	0.52
3:15:129:LYS:NZ	30:R1:636:G:OP1	2.31	0.51
9:20:49:ARG:O	9:20:53:LYS:NZ	2.40	0.51
30:R1:1466:U:O2'	30:R1:1546:G:O2'	2.19	0.51
16:28:6:VAL:HG21	16:28:58:ILE:HD11	1.92	0.51
25:36:16:ILE:HD13	25:36:25:VAL:HG22	1.92	0.51
30:R1:528:A:C2	30:R1:2043:C:H4'	2.45	0.51
30:R1:2591:C:H2'	30:R1:2592:G:C8	2.44	0.51
32:R3:297:G:N2	32:R3:300:A:OP2	2.41	0.51
32:R3:359:G:O2'	32:R3:360:G:O5'	2.28	0.51
3:15:91:ASP:N	3:15:94:THR:OG1	2.34	0.51
12:23:29:THR:HG22	12:23:86:THR:HG22	1.91	0.51
30:R1:2554:U:H2'	30:R1:2555:U:C6	2.45	0.51
16:28:31:ASN:HB2	30:R1:397:U:H5''	1.93	0.51
30:R1:1054:A:H2'	30:R1:1055:G:C8	2.46	0.51
30:R1:1468:U:H2'	30:R1:1522:A:N6	2.25	0.51
30:R1:1589:U:H2'	30:R1:1590:A:C8	2.44	0.51
30:R1:2122:U:H2'	30:R1:2123:G:O4'	2.11	0.51
30:R1:2846:G:H2'	30:R1:2847:U:C6	2.45	0.51
32:R3:160:A:H2'	32:R3:161:A:C8	2.45	0.51
32:R3:1391:U:H2'	32:R3:1392:G:C8	2.45	0.51
53:T:54:5MU:H2'	53:T:55:PSU:O4'	2.10	0.51
32:R3:144:G:N2	32:R3:179:A:H1'	2.25	0.51
55:1:67:HIS:CE1	55:1:187:GLU:HG2	2.45	0.51
4:16:76:LYS:HB3	4:16:80:VAL:HG21	1.92	0.51
19:30:3:THR:OG1	19:30:36:GLU:OE2	2.20	0.51
21:32:2:VAL:HG13	30:R1:2015:A:C6	2.46	0.51
30:R1:1429:G:H2'	30:R1:1430:G:H8	1.75	0.51
32:R3:413:G:H22	32:R3:428:G:H1'	1.75	0.51
7:19:33:GLU:OE2	7:19:38:ARG:NH2	2.34	0.51
28:6:26:LYS:HE2	28:6:31:GLU:HB2	1.93	0.51
30:R1:2114:A:C8	30:R1:2115:G:C8	2.99	0.51
55:1:155:ASN:O	55:1:159:GLY:N	2.39	0.51
2:14:33:ALA:HB1	2:14:37:ASP:HB2	1.93	0.51
11:22:92:ARG:NH2	30:R1:747:U:H4'	2.25	0.51
18:3:2:ILE:HD12	18:3:3:GLY:N	2.25	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:5:70:ARG:HD2	30:R1:2298:A:OP1	2.11	0.51
29:9:58:LEU:HA	29:9:61:VAL:HG22	1.93	0.51
32:R3:1002:G:N2	32:R3:1039:G:N3	2.59	0.51
32:R3:1409:C:H2'	32:R3:1410:A:H8	1.75	0.51
1:13:17:VAL:HG23	1:13:137:PRO:HB2	1.92	0.51
29:9:16:GLY:HA2	29:9:47:PHE:CZ	2.46	0.51
30:R1:1581:G:H2'	30:R1:1582:C:C6	2.45	0.51
30:R1:1682:G:OP2	30:R1:1699:G:N2	2.37	0.51
32:R3:159:G:N2	32:R3:162:A:OP2	2.43	0.51
32:R3:835:U:O2	32:R3:851:G:O6	2.29	0.51
32:R3:990:C:O2'	32:R3:991:U:H5''	2.11	0.51
6:18:40:ILE:HG12	6:18:47:VAL:HG12	1.92	0.51
8:2:92:LEU:HD11	8:2:100:ARG:HB3	1.91	0.51
20:31:43:PHE:O	20:31:47:LYS:HB2	2.11	0.51
30:R1:360:U:O2'	30:R1:361:G:O5'	2.29	0.51
30:R1:1504:A:H2'	30:R1:1505:A:H8	1.75	0.51
30:R1:1515:A:H3'	30:R1:1516:G:H8	1.75	0.51
30:R1:1889:A:H2'	30:R1:1890:A:C8	2.46	0.51
30:R1:2831:G:H1'	30:R1:2883:A:H2'	1.93	0.51
32:R3:1071:C:H2'	32:R3:1072:G:H8	1.75	0.51
32:R3:1414:U:H2'	32:R3:1415:G:H8	1.76	0.51
18:3:68:PHE:HE1	18:3:79:LEU:HD11	1.76	0.50
30:R1:107:G:H2'	30:R1:108:G:H8	1.76	0.50
30:R1:1047:G:N2	30:R1:1110:G:N3	2.59	0.50
32:R3:82:G:H1'	32:R3:88:U:N3	2.25	0.50
32:R3:260:G:H2'	32:R3:261:U:C6	2.46	0.50
32:R3:1002:G:N1	32:R3:1038:C:O2'	2.42	0.50
32:R3:1062:U:H2'	32:R3:1063:C:C6	2.47	0.50
1:13:82:GLY:HA2	30:R1:1131:G:OP1	2.11	0.50
5:17:65:LEU:HD22	5:17:69:ARG:HH12	1.76	0.50
13:24:65:GLN:HG2	30:R1:328:U:H4'	1.93	0.50
25:36:15:LYS:HD2	25:36:26:ILE:HD11	1.92	0.50
30:R1:297:G:O6	30:R1:342:A:N6	2.44	0.50
30:R1:1544:A:H2'	30:R1:1545:A:C8	2.46	0.50
32:R3:662:U:H2'	32:R3:663:A:C8	2.45	0.50
32:R3:728:A:H2'	32:R3:729:A:C8	2.46	0.50
32:R3:1355:G:H2'	32:R3:1356:G:H8	1.75	0.50
55:1:163:TYR:HD2	55:1:171:ILE:HD13	1.77	0.50
8:2:90:ILE:HD12	8:2:102:TYR:CD1	2.47	0.50
22:33:33:LEU:HD21	30:R1:2286:G:C8	2.46	0.50
28:6:44:HIS:ND1	28:6:46:ASP:OD1	2.37	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:R1:181:A:H2'	30:R1:182:A:C8	2.46	0.50
30:R1:306:U:H3	30:R1:310:A:H62	1.57	0.50
30:R1:1317:G:H2'	30:R1:1318:U:C6	2.47	0.50
30:R1:1405:U:H2'	30:R1:1406:U:C6	2.46	0.50
30:R1:2637:U:H2'	30:R1:2638:G:O4'	2.11	0.50
31:R2:30:C:O2'	31:R2:57:A:N1	2.44	0.50
32:R3:232:G:H21	32:R3:263:A:H8	1.58	0.50
32:R3:500:G:HO2'	32:R3:501:C:P	2.35	0.50
32:R3:1238:A:H2	32:R3:1241:G:N3	2.08	0.50
55:1:46:VAL:HG12	55:1:212:VAL:HG13	1.93	0.50
4:16:19:GLY:O	4:16:38:ARG:NH1	2.41	0.50
7:19:87:ARG:NH2	7:19:109:ILE:O	2.33	0.50
27:5:141:ASP:HB3	27:5:144:LYS:HG2	1.93	0.50
30:R1:1316:U:N3	30:R1:1317:G:N7	2.59	0.50
30:R1:1631:G:N1	30:R1:1634:A:OP2	2.37	0.50
30:R1:1736:U:H2'	30:R1:1737:G:O4'	2.12	0.50
30:R1:2124:G:O2'	55:1:41:SER:HB3	2.12	0.50
32:R3:673:A:H2'	32:R3:674:G:C8	2.46	0.50
4:16:44:ARG:NH2	30:R1:2484:G:OP2	2.45	0.50
19:30:9:THR:OG1	19:30:53:MET:O	2.28	0.50
30:R1:1101:U:H2'	30:R1:1102:C:C6	2.47	0.50
32:R3:1001:C:N3	32:R3:1040:U:H2'	2.26	0.50
32:R3:1454:G:H2'	32:R3:1455:G:H8	1.76	0.50
18:3:77:ARG:NH1	18:3:200:ASP:OD2	2.45	0.50
30:R1:1656:C:H2'	30:R1:1657:U:H6	1.76	0.50
32:R3:1007:U:H5	32:R3:1023:U:C2	2.30	0.50
53:T:9:G:N2	53:T:26:G:H1'	2.27	0.50
54:U:350:LEU:HB2	54:U:493:VAL:HG22	1.93	0.50
20:31:23:LYS:NZ	20:31:24:ILE:O	2.42	0.50
30:R1:1103:A:H5''	30:R1:1104:C:C5	2.46	0.50
30:R1:2105:U:H2'	30:R1:2106:U:C6	2.47	0.50
32:R3:1316:G:N2	32:R3:1318:A:H3'	2.27	0.50
15:27:64:ASP:N	15:27:64:ASP:OD1	2.45	0.50
20:31:32:LEU:HG	20:31:34:LEU:HB3	1.92	0.50
30:R1:414:C:OP1	30:R1:1879:C:O2'	2.23	0.50
30:R1:1580:A:C8	30:R1:1581:G:C8	2.99	0.50
32:R3:254:G:H2'	32:R3:255:G:C8	2.45	0.50
32:R3:544:G:H2'	32:R3:545:C:C6	2.47	0.50
32:R3:1199:U:O2'	32:R3:1202:U:OP2	2.30	0.50
8:2:20:ASN:HB3	8:2:23:LEU:HG	1.93	0.50
20:31:12:ILE:HG13	20:31:24:ILE:HG13	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:35:7:ARG:NH1	30:R1:243:U:OP2	2.45	0.50
26:4:13:THR:HB	26:4:194:LYS:HE3	1.93	0.50
28:6:31:GLU:OE2	28:6:33:THR:OG1	2.29	0.50
30:R1:1071:G:H22	30:R1:1090:A:N6	2.09	0.50
30:R1:1682:G:H2'	30:R1:1683:U:C6	2.47	0.50
30:R1:2129:C:H42	30:R1:2160:C:H42	1.60	0.50
30:R1:2143:C:H2'	30:R1:2144:G:H5'	1.94	0.50
31:R2:29:A:H2'	31:R2:30:C:O4'	2.12	0.50
32:R3:954:G:H2'	32:R3:955:U:C6	2.47	0.50
54:U:55:LEU:HD22	54:U:60:ILE:HG12	1.94	0.50
26:4:122:GLU:OE1	26:4:122:GLU:N	2.44	0.49
30:R1:148:U:H2'	30:R1:149:A:C8	2.47	0.49
30:R1:1847:G:O2'	30:R1:1848:A:O5'	2.25	0.49
32:R3:508:U:H1'	32:R3:509:A:H2	1.76	0.49
32:R3:744:C:H2'	32:R3:745:G:H8	1.76	0.49
32:R3:976:G:H22	32:R3:1363:A:H5''	1.76	0.49
32:R3:1054:C:O2	32:R3:1196:A:N6	2.45	0.49
54:U:113:SER:H	54:U:116:ASN:HD22	1.60	0.49
54:U:413:VAL:O	54:U:418:ARG:NH2	2.45	0.49
12:23:64:LYS:HA	12:23:79:ASP:HB3	1.93	0.49
27:5:3:LEU:HD13	27:5:100:GLU:HB2	1.94	0.49
30:R1:1357:C:H2'	30:R1:1358:G:O4'	2.11	0.49
30:R1:1593:A:H2'	30:R1:1594:U:H6	1.76	0.49
30:R1:1796:U:H2'	30:R1:1797:G:H8	1.78	0.49
30:R1:2489:U:H2'	30:R1:2490:G:O4'	2.11	0.49
32:R3:235:C:H2'	32:R3:236:A:C8	2.47	0.49
32:R3:494:G:H2'	32:R3:496:A:H8	1.77	0.49
53:T:23:C:H2'	53:T:24:U:C6	2.47	0.49
54:U:114:GLU:HB3	54:U:115:LYS:HE2	1.94	0.49
55:1:48:LEU:HD11	55:1:171:ILE:HD12	1.94	0.49
55:1:67:HIS:HE1	55:1:187:GLU:HG2	1.77	0.49
14:25:73:LYS:HB3	14:25:92:VAL:HG12	1.93	0.49
16:28:2:ARG:HD2	16:28:29:LEU:HD22	1.93	0.49
27:5:65:LEU:HB2	31:R2:42:C:C6	2.47	0.49
27:5:142:TYR:O	27:5:142:TYR:HD1	1.95	0.49
30:R1:631:A:N3	30:R1:2415:G:O2'	2.40	0.49
30:R1:1059:G:N2	30:R1:1079:C:H2'	2.27	0.49
30:R1:1681:G:OP2	30:R1:1757:A:N6	2.44	0.49
30:R1:1858:A:H61	30:R1:1884:G:H1'	1.77	0.49
30:R1:1871:A:H3'	30:R1:1872:A:C8	2.40	0.49
30:R1:2246:G:H2'	30:R1:2247:A:H8	1.77	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:R2:31:C:H2'	31:R2:32:U:C6	2.48	0.49
32:R3:459:A:N7	32:R3:460:A:N6	2.60	0.49
32:R3:517:G:O2'	32:R3:531:U:OP2	2.30	0.49
32:R3:612:C:HO2'	32:R3:613:C:P	2.33	0.49
2:14:75:SER:OG	7:19:71:ARG:NH1	2.45	0.49
24:35:22:LYS:NZ	30:R1:631:A:OP2	2.43	0.49
30:R1:645:C:H2'	30:R1:647:G:N7	2.28	0.49
30:R1:879:G:H2'	30:R1:880:G:O4'	2.12	0.49
30:R1:2584:U:H2'	30:R1:2585:U:H2'	1.94	0.49
32:R3:580:C:H2'	32:R3:581:G:O4'	2.11	0.49
55:1:22:ASP:HB3	55:1:25:GLU:HG2	1.95	0.49
55:1:44:VAL:HG23	55:1:214:ILE:HA	1.94	0.49
6:18:94:ARG:HG2	6:18:97:PHE:O	2.12	0.49
32:R3:45:G:OP1	32:R3:307:C:O2'	2.31	0.49
32:R3:769:G:H4'	32:R3:1513:A:H4'	1.95	0.49
32:R3:1409:C:H2'	32:R3:1410:A:C8	2.47	0.49
54:U:247:GLU:OE1	54:U:250:ARG:NH2	2.36	0.49
54:U:351:ILE:HD11	54:U:509:ILE:HG12	1.94	0.49
27:5:25:MET:CE	31:R2:54:G:H21	2.26	0.49
30:R1:133:U:H2'	30:R1:134:G:O4'	2.13	0.49
30:R1:319:G:H1	30:R1:323:C:H41	1.60	0.49
30:R1:357:C:O2'	30:R1:358:U:O4'	2.24	0.49
30:R1:373:U:H2'	30:R1:374:A:H8	1.76	0.49
30:R1:1360:G:N7	30:R1:1361:G:C8	2.80	0.49
32:R3:339:C:H2'	32:R3:340:U:H6	1.78	0.49
32:R3:1355:G:H2'	32:R3:1356:G:C8	2.48	0.49
54:U:433:ARG:HH22	58:U:602:ATP:HO2'	1.56	0.49
3:15:91:ASP:O	3:15:95:LEU:HG	2.13	0.49
6:18:21:LEU:HD22	6:18:23:ALA:HB2	1.94	0.49
20:31:11:GLU:HA	20:31:25:ARG:HA	1.95	0.49
30:R1:570:G:H2'	30:R1:2030:A:N7	2.27	0.49
30:R1:1028:A:N6	30:R1:1125:G:H2'	2.28	0.49
30:R1:1434:A:H2'	30:R1:1435:G:C8	2.48	0.49
30:R1:2663:G:H2'	30:R1:2664:G:O4'	2.13	0.49
32:R3:116:A:H61	32:R3:313:A:H1'	1.78	0.49
32:R3:1323:G:H2'	32:R3:1324:A:C8	2.48	0.49
54:U:307:MET:HG2	54:U:427:PHE:CE2	2.47	0.49
6:18:12:THR:O	6:18:16:ARG:HG2	2.12	0.49
25:36:7:VAL:HG22	25:36:38:GLY:HA3	1.95	0.49
27:5:164:GLU:N	27:5:164:GLU:OE2	2.46	0.49
31:R2:94:A:H2'	31:R2:95:U:O4'	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:R3:78:A:HO2'	32:R3:93:U:H3	1.57	0.49
32:R3:255:G:H2'	32:R3:256:U:C6	2.48	0.49
2:14:12:ASP:OD2	2:14:14:SER:OG	2.26	0.49
3:15:85:VAL:HG23	3:15:86:GLU:N	2.28	0.49
30:R1:1532:A:H2'	30:R1:1533:C:C6	2.48	0.49
4:16:79:ALA:HA	30:R1:2494:G:O2'	2.12	0.49
5:17:2:ARG:NH1	30:R1:2822:G:O6	2.45	0.49
8:2:97:ASP:OD1	8:2:97:ASP:N	2.33	0.49
15:27:34:GLY:O	30:R1:2353:G:N2	2.36	0.49
18:3:56:LYS:HE3	30:R1:2830:C:H5''	1.94	0.49
25:36:19:ARG:NE	30:R1:2756:U:OP2	2.40	0.49
25:36:32:LYS:HD3	30:R1:2478:A:H5'	1.95	0.49
32:R3:53:A:N6	32:R3:359:G:O6	2.46	0.49
54:U:98:LEU:HD12	54:U:135:LEU:HD13	1.95	0.49
54:U:104:ILE:HG21	54:U:119:GLU:HG3	1.94	0.49
30:R1:282:A:C6	30:R1:359:G:C6	3.01	0.48
30:R1:974:G:H8	30:R1:990:A:H62	1.58	0.48
30:R1:1469:A:H2'	30:R1:1470:A:H8	1.77	0.48
30:R1:2316:G:H2'	30:R1:2317:A:C8	2.48	0.48
32:R3:129:A:O2'	32:R3:130:A:H5''	2.13	0.48
32:R3:844:G:H8	32:R3:845:A:N7	2.10	0.48
32:R3:1140:C:C4	32:R3:1141:C:N4	2.80	0.48
54:U:325:VAL:HG21	54:U:376:ILE:HD11	1.93	0.48
28:6:120:ILE:HG21	28:6:132:LEU:HB3	1.95	0.48
29:9:9:VAL:HB	29:9:12:LEU:C	2.33	0.48
30:R1:1429:G:H2'	30:R1:1430:G:C8	2.48	0.48
30:R1:1537:G:H3'	30:R1:1537:G:N3	2.27	0.48
32:R3:34:C:H2'	32:R3:35:G:H8	1.79	0.48
55:1:8:MET:HA	55:1:11:ILE:HG22	1.94	0.48
15:27:40:GLN:HE22	15:27:45:PHE:H	1.60	0.48
30:R1:270:A:N1	30:R1:369:U:O2'	2.46	0.48
30:R1:2213:U:H5'	30:R1:2214:C:OP2	2.12	0.48
30:R1:2774:C:O2'	30:R1:2775:G:C8	2.65	0.48
32:R3:469:C:O2'	32:R3:470:C:O5'	2.31	0.48
32:R3:603:U:H2'	32:R3:604:G:C8	2.48	0.48
32:R3:961:U:OP2	32:R3:1223:C:O2'	2.21	0.48
32:R3:978:A:C4	32:R3:1319:A:C2	3.01	0.48
32:R3:1326:U:H2'	32:R3:1327:C:C6	2.49	0.48
54:U:433:ARG:NH2	58:U:602:ATP:O2'	2.30	0.48
1:13:78:THR:HB	30:R1:2641:G:H5''	1.96	0.48
9:20:5:ARG:HD3	30:R1:1250:G:H5''	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:22:7:HIS:HB2	11:22:50:VAL:CG2	2.42	0.48
26:4:15:SER:OG	26:4:197:GLU:OE1	2.15	0.48
30:R1:1074:G:N2	30:R1:1076:C:OP2	2.46	0.48
54:U:468:THR:HB	54:U:476:LEU:HD12	1.95	0.48
55:1:8:MET:SD	55:1:9:ARG:HG3	2.53	0.48
8:2:152:GLN:O	30:R1:1818:U:O2'	2.24	0.48
13:24:3:LYS:NZ	30:R1:337:C:OP2	2.47	0.48
30:R1:2243:U:H2'	30:R1:2244:U:C6	2.48	0.48
32:R3:753:A:H4'	32:R3:754:C:O5'	2.13	0.48
32:R3:1102:A:O2'	32:R3:1103:C:H5'	2.14	0.48
8:2:156:SER:OG	8:2:157:ALA:N	2.46	0.48
15:27:19:LYS:NZ	30:R1:2261:C:OP1	2.39	0.48
15:27:77:ARG:NH1	30:R1:2333:A:OP1	2.32	0.48
25:36:18:LYS:HE2	25:36:21:GLY:HA2	1.94	0.48
32:R3:312:C:H2'	32:R3:313:A:C8	2.48	0.48
32:R3:359:G:O2'	32:R3:360:G:H8	1.82	0.48
32:R3:1019:A:H2'	32:R3:1020:G:C8	2.48	0.48
54:U:101:TYR:N	54:U:123:VAL:HG21	2.28	0.48
55:1:33:LEU:HD22	55:1:220:ALA:HB3	1.94	0.48
55:1:59:VAL:HG21	55:1:199:ALA:O	2.14	0.48
9:20:48:ASP:OD1	30:R1:559:G:N2	2.47	0.48
21:32:15:ARG:NH2	30:R1:1264:A:OP1	2.42	0.48
26:4:144:GLU:OE1	26:4:144:GLU:N	2.46	0.48
30:R1:6:A:O2'	30:R1:7:G:H5'	2.14	0.48
30:R1:191:A:H2'	30:R1:192:C:H6	1.79	0.48
30:R1:633:A:O2'	30:R1:2404:U:OP1	2.28	0.48
30:R1:1790:C:H2'	30:R1:1791:A:C5	2.49	0.48
54:U:409:GLN:HB3	54:U:420:VAL:HG21	1.96	0.48
7:19:59:THR:OG1	7:19:72:VAL:HG12	2.13	0.48
30:R1:181:A:H1'	30:R1:435:C:H5'	1.96	0.48
30:R1:1536:C:H4'	30:R1:1537:G:C2	2.49	0.48
30:R1:2029:G:N1	30:R1:2033:A:OP2	2.28	0.48
31:R2:22:U:H2'	31:R2:23:G:C8	2.49	0.48
32:R3:1038:C:O2	32:R3:1039:G:N2	2.46	0.48
27:5:102:LEU:HA	27:5:106:ALA:HB3	1.96	0.48
30:R1:593:U:H2'	30:R1:594:U:H6	1.78	0.48
30:R1:1570:A:H2'	30:R1:1571:A:C8	2.49	0.48
30:R1:2328:A:H2'	30:R1:2329:U:C6	2.49	0.48
30:R1:2646:C:OP2	30:R1:2732:G:O2'	2.28	0.48
30:R1:2747:G:N2	30:R1:2757:A:H62	2.11	0.48
31:R2:95:U:H2'	31:R2:96:G:C8	2.47	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:R3:175:C:H2'	32:R3:176:C:C6	2.48	0.48
32:R3:1129:C:H5	32:R3:1143:G:H1	1.62	0.48
54:U:186:HIS:CD2	54:U:389:GLN:HE21	2.32	0.48
25:36:11:CYS:SG	25:36:13:ASN:ND2	2.74	0.48
30:R1:754:U:H2'	30:R1:755:U:C6	2.49	0.48
30:R1:2184:A:H2'	30:R1:2185:U:H6	1.78	0.48
32:R3:147:G:H2'	32:R3:148:G:C8	2.48	0.48
32:R3:946:A:H2'	32:R3:947:G:C8	2.49	0.48
54:U:394:LEU:HD11	54:U:450:LEU:HB2	1.95	0.48
18:3:136:ASN:OD1	30:R1:2579:C:O2'	2.31	0.47
26:4:63:LYS:NZ	30:R1:2061:G:OP2	2.47	0.47
27:5:117:SER:HA	27:5:177:ARG:HH11	1.79	0.47
32:R3:456:A:N6	32:R3:476:U:H3	2.11	0.47
32:R3:821:G:H2'	32:R3:822:U:C6	2.49	0.47
32:R3:1149:C:O2'	32:R3:1150:A:OP1	2.30	0.47
12:23:30:ILE:HG12	12:23:85:VAL:HB	1.96	0.47
28:6:148:ARG:HD2	28:6:163:TYR:CE1	2.49	0.47
30:R1:159:G:N3	30:R1:2208:C:O2'	2.46	0.47
30:R1:1386:C:H2'	30:R1:1387:A:C8	2.50	0.47
32:R3:45:G:H2'	32:R3:46:G:H8	1.78	0.47
32:R3:459:A:H2'	32:R3:460:A:C4	2.49	0.47
5:17:72:ASP:OD1	5:17:74:GLU:N	2.47	0.47
11:22:18:ARG:HG3	11:22:76:VAL:HG22	1.95	0.47
30:R1:189:G:H1	30:R1:205:G:HO2'	1.62	0.47
30:R1:415:A:N6	30:R1:2408:U:H3	2.12	0.47
30:R1:1317:G:H2'	30:R1:1318:U:H6	1.78	0.47
2:14:92:GLU:HG3	2:14:111:LYS:HE3	1.95	0.47
3:15:99:ASN:HD21	30:R1:621:A:P	2.36	0.47
18:3:45:TYR:OH	30:R1:2636:C:O2'	2.31	0.47
30:R1:1597:A:H5''	30:R1:1598:A:H5'	1.97	0.47
31:R2:32:U:O2	31:R2:51:G:N2	2.47	0.47
32:R3:844:G:H2'	32:R3:845:A:C8	2.50	0.47
32:R3:1005:A:N6	32:R3:1025:U:O2'	2.34	0.47
32:R3:1377:A:H4'	32:R3:1378:C:H5	1.80	0.47
54:U:132:LEU:HA	54:U:135:LEU:HD11	1.96	0.47
54:U:274:ILE:O	54:U:275:LYS:HB2	2.13	0.47
54:U:336:LYS:N	54:U:514:GLY:O	2.38	0.47
2:14:31:ARG:HH22	30:R1:2676:C:P	2.37	0.47
30:R1:1604:C:O2'	30:R1:1610:A:N1	2.43	0.47
32:R3:424:G:H2'	32:R3:425:G:H8	1.80	0.47
32:R3:1187:G:H2'	32:R3:1188:A:H8	1.80	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:R3:1273:C:H2'	32:R3:1274:A:O4'	2.15	0.47
55:1:166:ASP:O	55:1:169:GLY:N	2.42	0.47
6:18:33:ARG:HB2	31:R2:52:A:N6	2.28	0.47
21:32:54:ILE:O	21:32:56:LYS:HE3	2.15	0.47
30:R1:2849:U:H4'	30:R1:2868:A:C2	2.50	0.47
32:R3:464:U:C6	32:R3:466:A:H5'	2.50	0.47
32:R3:695:A:H2'	32:R3:696:A:C8	2.50	0.47
3:15:30:THR:HG22	30:R1:810:U:O4	2.15	0.47
4:16:84:LYS:NZ	30:R1:2250:G:OP1	2.47	0.47
8:2:27:LYS:HD3	8:2:28:PRO:HD2	1.97	0.47
8:2:252:LYS:NZ	30:R1:1795:C:O2	2.47	0.47
18:3:5:VAL:HG22	18:3:202:ILE:HD13	1.96	0.47
18:3:133:THR:O	18:3:134:HIS:HB2	2.15	0.47
26:4:99:LYS:NZ	30:R1:601:C:O2'	2.31	0.47
27:5:67:THR:OG1	27:5:85:GLY:O	2.32	0.47
30:R1:81:G:H2'	30:R1:82:U:O4'	2.14	0.47
30:R1:287:G:H21	30:R1:354:A:N6	2.12	0.47
30:R1:1386:C:H2'	30:R1:1387:A:H8	1.80	0.47
30:R1:2273:A:H2'	30:R1:2274:A:C8	2.50	0.47
30:R1:2850:A:N7	30:R1:2868:A:O2'	2.41	0.47
32:R3:21:G:H2'	32:R3:22:G:C8	2.50	0.47
32:R3:375:U:H2'	32:R3:376:G:O4'	2.14	0.47
32:R3:678:U:H2'	32:R3:679:C:H6	1.80	0.47
32:R3:1055:A:C6	32:R3:1206:G:C5	3.03	0.47
32:R3:1150:A:O2'	32:R3:1151:A:O5'	2.32	0.47
32:R3:1285:A:H5''	32:R3:1286:U:C5	2.49	0.47
55:1:177:LYS:O	55:1:179:ASP:N	2.47	0.47
55:1:202:THR:OG1	55:1:203:GLN:OE1	2.29	0.47
4:16:82:MET:HE1	30:R1:959:A:H62	1.80	0.47
11:22:2:GLU:N	11:22:2:GLU:OE2	2.48	0.47
11:22:18:ARG:HG3	11:22:76:VAL:CG2	2.45	0.47
30:R1:880:G:H21	30:R1:898:C:H41	1.63	0.47
30:R1:2105:U:HO2'	30:R1:2106:U:P	2.38	0.47
30:R1:2112:G:H5''	30:R1:2113:U:H6	1.79	0.47
30:R1:2124:G:H2'	30:R1:2125:G:O4'	2.15	0.47
30:R1:2126:A:N1	30:R1:2162:G:O2'	2.44	0.47
32:R3:393:A:C2	32:R3:394:G:C8	3.03	0.47
32:R3:784:A:H2'	32:R3:785:G:C8	2.50	0.47
32:R3:850:U:H5	32:R3:851:G:N7	2.12	0.47
54:U:500:VAL:O	54:U:504:VAL:HG12	2.15	0.47
26:4:148:ILE:HB	26:4:169:VAL:HG22	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:6:53:PRO:HG2	28:6:61:TRP:CD2	2.49	0.47
30:R1:279:A:H2'	30:R1:280:U:O4'	2.15	0.47
30:R1:1198:U:H2'	30:R1:1199:U:C6	2.50	0.47
30:R1:1370:C:H2'	30:R1:1371:G:O4'	2.15	0.47
30:R1:1482:G:H2'	30:R1:1483:G:C8	2.48	0.47
30:R1:2087:G:H2'	30:R1:2088:A:H8	1.80	0.47
30:R1:2131:U:H5''	55:1:6:LYS:NZ	2.30	0.47
32:R3:222:C:H2'	32:R3:223:A:H8	1.79	0.47
32:R3:664:G:O2'	32:R3:725:G:O2'	2.25	0.47
32:R3:676:A:H2'	32:R3:677:U:H6	1.80	0.47
32:R3:1513:A:H2'	32:R3:1514:G:C8	2.50	0.47
15:27:40:GLN:NE2	15:27:45:PHE:O	2.48	0.47
22:33:4:ILE:HG22	54:U:14:SER:OG	2.15	0.47
24:35:18:LYS:HG3	30:R1:651:G:H5'	1.96	0.47
30:R1:2064:C:H2'	30:R1:2065:C:C6	2.50	0.47
30:R1:2853:C:H2'	30:R1:2854:G:H8	1.80	0.47
32:R3:505:G:H2'	32:R3:506:G:C8	2.48	0.47
32:R3:1184:G:C2	32:R3:1185:G:C8	3.03	0.47
4:16:58:LYS:O	4:16:59:ARG:NH1	2.48	0.46
30:R1:1526:C:H2'	30:R1:1527:G:O4'	2.15	0.46
32:R3:253:A:H2'	32:R3:254:G:C8	2.50	0.46
32:R3:1272:G:H2'	32:R3:1273:C:C6	2.49	0.46
54:U:87:VAL:HA	54:U:169:ARG:HB2	1.97	0.46
1:13:118:MET:HA	1:13:121:LYS:HE3	1.97	0.46
12:23:69:ARG:HH12	12:23:72:GLN:HA	1.80	0.46
30:R1:64:A:H2'	30:R1:65:U:C6	2.51	0.46
30:R1:891:G:H2'	30:R1:892:A:H5''	1.96	0.46
30:R1:1035:U:H2'	30:R1:1036:G:H8	1.79	0.46
30:R1:1166:G:H2'	30:R1:1167:C:C6	2.51	0.46
30:R1:1361:G:H2'	30:R1:1362:C:C6	2.50	0.46
30:R1:1442:U:H2'	30:R1:1443:U:C6	2.50	0.46
30:R1:1538:G:H2'	30:R1:1539:U:C6	2.50	0.46
30:R1:1802:A:H2'	30:R1:1803:A:H8	1.79	0.46
30:R1:2291:U:H2'	30:R1:2292:U:C6	2.50	0.46
32:R3:561:U:O2'	32:R3:562:U:OP1	2.31	0.46
32:R3:1144:G:H21	32:R3:1146:A:H62	1.61	0.46
32:R3:1156:G:H21	32:R3:1179:A:H61	1.62	0.46
54:U:359:THR:OG1	54:U:465:ASP:OD1	2.32	0.46
55:1:183:ASP:OD1	55:1:183:ASP:N	2.48	0.46
5:17:8:ARG:NH1	30:R1:1652:A:OP1	2.47	0.46
10:21:68:ARG:HD3	10:21:92:TRP:CE2	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:24:87:GLU:O	13:24:89:GLY:N	2.48	0.46
18:3:46:ARG:NH2	18:3:88:GLU:H	2.12	0.46
26:4:44:ARG:HH22	30:R1:1248:G:P	2.38	0.46
26:4:150:THR:OG1	26:4:151:GLY:N	2.48	0.46
29:9:23:ALA:O	29:9:27:ARG:HB2	2.15	0.46
30:R1:373:U:H2'	30:R1:374:A:C8	2.51	0.46
30:R1:979:A:H5'	30:R1:980:A:H5''	1.97	0.46
30:R1:1048:A:N6	30:R1:1111:A:H1'	2.30	0.46
30:R1:1709:U:H2'	30:R1:1710:G:H8	1.81	0.46
30:R1:2107:G:H1	30:R1:2182:U:H3	1.63	0.46
32:R3:464:U:C5	32:R3:466:A:H5'	2.50	0.46
32:R3:678:U:H2'	32:R3:679:C:C6	2.50	0.46
32:R3:862:C:C2'	32:R3:863:U:H5'	2.45	0.46
31:R2:13:G:O2'	31:R2:15:A:OP2	2.32	0.46
32:R3:131:A:H2'	32:R3:132:C:C6	2.50	0.46
32:R3:205:A:O2'	32:R3:206:C:H5'	2.16	0.46
32:R3:222:C:H2'	32:R3:223:A:C8	2.51	0.46
32:R3:332:G:O2'	32:R3:333:U:O2	2.22	0.46
32:R3:938:A:N3	32:R3:1376:U:O2'	2.36	0.46
32:R3:1450:U:O2'	32:R3:1453:G:O6	2.23	0.46
32:R3:1452:C:HO2'	32:R3:1453:G:N2	2.13	0.46
55:1:11:ILE:HA	55:1:14:LYS:HG2	1.97	0.46
3:15:2:ARG:HB2	26:4:181:ILE:HD11	1.97	0.46
9:20:90:ASP:H	10:21:11:GLN:NE2	2.12	0.46
11:22:59:GLU:HA	11:22:64:ALA:HA	1.98	0.46
16:28:15:ASN:ND2	16:28:23:ALA:HB1	2.29	0.46
30:R1:1071:G:H1'	30:R1:1089:A:C8	2.51	0.46
30:R1:1173:U:O2'	30:R1:1174:U:O3'	2.21	0.46
30:R1:1668:A:O2'	30:R1:1674:G:N7	2.41	0.46
30:R1:1847:G:HO2'	30:R1:1848:A:P	2.38	0.46
32:R3:115:G:OP1	32:R3:115:G:C8	2.67	0.46
32:R3:160:A:H2'	32:R3:161:A:H8	1.80	0.46
32:R3:849:G:H3'	32:R3:850:U:O2	2.16	0.46
54:U:307:MET:HB2	54:U:482:LEU:HD11	1.98	0.46
2:14:13:ASN:ND2	2:14:97:THR:OG1	2.37	0.46
5:17:79:LEU:HD23	5:17:83:LEU:HB2	1.98	0.46
22:33:20:TYR:CD1	22:33:37:LYS:HE2	2.50	0.46
30:R1:132:G:H2'	30:R1:133:U:O2	2.16	0.46
30:R1:1510:G:H2'	30:R1:1511:G:C8	2.50	0.46
30:R1:1589:U:H2'	30:R1:1590:A:H8	1.81	0.46
30:R1:2117:A:N1	30:R1:2170:A:N1	2.64	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:R2:110:C:H2'	31:R2:111:U:O4'	2.16	0.46
32:R3:17:U:H2'	32:R3:18:C:C6	2.50	0.46
32:R3:1107:C:C4	32:R3:1108:G:C8	3.03	0.46
54:U:453:ARG:HA	54:U:456:LEU:HB2	1.96	0.46
26:4:53:THR:HG21	30:R1:452:G:H8	1.77	0.46
28:6:51:PHE:CE2	28:6:68:ARG:HA	2.51	0.46
30:R1:30:G:O2'	30:R1:1214:A:N3	2.47	0.46
30:R1:2515:C:H2'	30:R1:2516:A:H8	1.80	0.46
32:R3:324:G:N1	32:R3:327:A:OP2	2.45	0.46
32:R3:401:C:H2'	32:R3:402:G:H5'	1.98	0.46
32:R3:413:G:N2	32:R3:428:G:H1'	2.30	0.46
32:R3:593:U:H2'	32:R3:594:U:C6	2.51	0.46
32:R3:1126:U:N3	32:R3:1280:A:OP1	2.48	0.46
32:R3:1195:C:H2'	32:R3:1197:A:O4'	2.16	0.46
4:16:71:LYS:HB3	4:16:93:VAL:O	2.16	0.46
5:17:4:ARG:NH1	30:R1:2874:C:H5''	2.31	0.46
8:2:203:VAL:HG12	30:R1:1792:G:H5''	1.97	0.46
14:25:56:PHE:CZ	14:25:61:LEU:HD21	2.51	0.46
23:34:34:ARG:NH2	23:34:42:LEU:O	2.38	0.46
27:5:15:LEU:HD21	27:5:167:ALA:HB1	1.96	0.46
29:9:47:PHE:CE2	29:9:48:GLU:HG2	2.51	0.46
30:R1:1318:U:H2'	30:R1:1319:C:C6	2.50	0.46
30:R1:1871:A:C8	30:R1:1872:A:C8	3.04	0.46
30:R1:2150:C:H5''	30:R1:2151:U:OP2	2.15	0.46
30:R1:2652:C:H2'	30:R1:2653:U:O4'	2.16	0.46
32:R3:31:G:O2'	32:R3:48:C:N4	2.49	0.46
32:R3:202:G:O2'	32:R3:468:A:N3	2.40	0.46
53:T:63:G:H2'	53:T:64:G:H8	1.80	0.46
54:U:387:PHE:CE1	54:U:467:PRO:HA	2.50	0.46
54:U:451:LEU:HD21	54:U:479:LEU:HD13	1.97	0.46
3:15:1:MET:SD	3:15:1:MET:N	2.75	0.46
10:21:80:ARG:HD3	30:R1:566:U:O4	2.16	0.46
19:30:9:THR:CG2	19:30:55:LYS:HE2	2.45	0.46
28:6:16:VAL:HG22	28:6:25:ILE:HG12	1.98	0.46
29:9:9:VAL:HB	29:9:12:LEU:O	2.16	0.46
30:R1:1539:U:H2'	30:R1:1540:G:H8	1.81	0.46
30:R1:2108:A:H2'	30:R1:2109:U:O4'	2.16	0.46
30:R1:2514:U:H2'	30:R1:2515:C:C6	2.51	0.46
32:R3:920:U:HO2'	32:R3:1081:A:HO2'	1.62	0.46
32:R3:945:G:C2	32:R3:946:A:C8	3.04	0.46
32:R3:1171:A:H2'	32:R3:1172:C:C6	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
53:T:48:C:OP2	53:T:48:C:H6	1.98	0.46
54:U:414:ASN:HB3	54:U:415:GLY:H	1.63	0.46
8:2:86:ARG:NH2	30:R1:1817:G:OP1	2.49	0.46
30:R1:349:U:H2'	30:R1:350:G:H8	1.80	0.46
32:R3:713:G:H2'	32:R3:714:G:C8	2.50	0.46
32:R3:1004:A:N6	32:R3:1026:G:N7	2.57	0.46
32:R3:1010:U:H2'	32:R3:1011:C:H6	1.80	0.46
32:R3:1187:G:H2'	32:R3:1188:A:C8	2.51	0.46
1:13:65:THR:O	1:13:68:LYS:HE3	2.16	0.45
6:18:79:ALA:HB3	6:18:113:ALA:HB3	1.97	0.45
8:2:5:CYS:SG	8:2:17:LYS:NZ	2.78	0.45
10:21:38:VAL:HG22	10:21:59:ILE:HD12	1.98	0.45
30:R1:1069:A:H5''	30:R1:1073:A:H61	1.81	0.45
30:R1:2118:U:O2'	30:R1:2119:A:H5''	2.16	0.45
4:16:2:LEU:HD12	4:16:46:ILE:HG21	1.98	0.45
4:16:31:PHE:O	4:16:104:GLU:HB2	2.17	0.45
5:17:95:THR:HG22	5:17:115:LEU:HD23	1.98	0.45
18:3:29:VAL:O	18:3:185:ASN:HB3	2.16	0.45
30:R1:712:G:C5	30:R1:713:G:C8	3.04	0.45
30:R1:1501:G:H2'	30:R1:1502:A:C8	2.50	0.45
32:R3:738:C:HO2'	32:R3:739:C:H6	1.64	0.45
32:R3:846:G:H2'	32:R3:847:G:C8	2.52	0.45
20:31:5:ILE:HD12	27:5:63:LYS:HD3	1.97	0.45
21:32:37:HIS:CD2	21:32:43:THR:HG22	2.50	0.45
28:6:120:ILE:HD12	28:6:134:GLY:HA3	1.98	0.45
30:R1:305:C:H2'	30:R1:306:U:C6	2.52	0.45
30:R1:878:A:H3'	30:R1:879:G:C8	2.52	0.45
30:R1:1040:A:N6	30:R1:1115:G:H1	2.14	0.45
30:R1:2014:A:H2'	30:R1:2015:A:C8	2.52	0.45
30:R1:2097:A:H5''	30:R1:2098:U:C4	2.51	0.45
30:R1:2122:U:H3	30:R1:2176:A:N6	2.14	0.45
30:R1:2123:G:H2'	30:R1:2124:G:C2	2.51	0.45
30:R1:2187:U:H2'	30:R1:2188:U:C5	2.52	0.45
32:R3:162:A:H2'	32:R3:163:C:O4'	2.17	0.45
32:R3:636:U:H2'	32:R3:637:C:C6	2.52	0.45
54:U:24:LEU:HD12	54:U:24:LEU:HA	1.86	0.45
20:31:44:PHE:CE2	20:31:45:THR:HG23	2.51	0.45
24:35:32:LEU:O	24:35:40:LYS:HE2	2.17	0.45
30:R1:412:A:C2'	30:R1:413:C:H5'	2.46	0.45
30:R1:1183:U:H2'	30:R1:1184:U:C6	2.51	0.45
31:R2:9:G:C2	31:R2:10:G:C8	3.05	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:R2:32:U:C2	31:R2:51:G:N2	2.85	0.45
32:R3:1033:G:H2'	32:R3:1034:G:N7	2.31	0.45
32:R3:1261:A:H61	32:R3:1274:A:HO2'	1.51	0.45
32:R3:1439:G:OP2	32:R3:1439:G:N2	2.49	0.45
3:15:2:ARG:HD2	26:4:115:GLN:NE2	2.29	0.45
5:17:82:GLU:N	5:17:82:GLU:OE2	2.49	0.45
30:R1:2:G:C2	30:R1:2902:C:C2	3.04	0.45
30:R1:306:U:H2'	30:R1:307:G:O4'	2.17	0.45
30:R1:2109:U:H3'	30:R1:2110:G:H5''	1.97	0.45
32:R3:412:A:H8	32:R3:413:G:H4'	1.82	0.45
32:R3:500:G:O2'	32:R3:501:C:OP1	2.26	0.45
32:R3:747:A:H2'	32:R3:748:G:O4'	2.17	0.45
32:R3:859:G:H2'	32:R3:860:A:H8	1.81	0.45
32:R3:1175:G:H2'	32:R3:1176:A:H8	1.82	0.45
54:U:433:ARG:HG3	54:U:433:ARG:O	2.16	0.45
5:17:2:ARG:HA	5:17:5:LYS:HD3	1.98	0.45
29:9:96:THR:HA	29:9:99:ILE:HD11	1.99	0.45
32:R3:199:A:H2'	32:R3:200:G:C8	2.52	0.45
32:R3:469:C:H2'	32:R3:470:C:C2	2.51	0.45
32:R3:559:A:H4'	32:R3:560:A:H3'	1.99	0.45
32:R3:1002:G:H21	32:R3:1039:G:H2'	1.81	0.45
7:19:78:PRO:HG2	18:3:19:GLY:HA2	1.98	0.45
8:2:140:VAL:O	8:2:161:VAL:N	2.44	0.45
23:34:3:ARG:HD3	23:34:3:ARG:HA	1.81	0.45
30:R1:506:G:O3'	30:R1:507:A:H8	2.00	0.45
30:R1:607:U:N3	30:R1:608:A:N7	2.64	0.45
30:R1:1311:G:H21	30:R1:1603:A:H62	1.65	0.45
30:R1:1495:A:H2'	30:R1:1496:A:C8	2.52	0.45
30:R1:2649:C:H2'	30:R1:2650:U:C6	2.51	0.45
30:R1:2897:U:H2'	30:R1:2898:U:C6	2.52	0.45
32:R3:56:U:H2'	32:R3:57:G:C8	2.52	0.45
54:U:37:ARG:NH1	54:U:302:MET:HB3	2.32	0.45
54:U:295:ARG:HD2	54:U:295:ARG:HA	1.63	0.45
1:13:27:ARG:NH1	30:R1:1140:C:O3'	2.49	0.45
20:31:39:LYS:HB2	20:31:39:LYS:HE3	1.71	0.45
27:5:115:GLY:HA3	27:5:177:ARG:HG3	1.98	0.45
28:6:109:SER:OG	30:R1:2667:C:O2	2.28	0.45
30:R1:2170:A:H2'	30:R1:2171:A:C8	2.51	0.45
32:R3:202:G:H2'	32:R3:203:G:O4'	2.17	0.45
32:R3:625:U:H2'	32:R3:626:G:H8	1.81	0.45
32:R3:850:U:H5	32:R3:851:G:C8	2.35	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:R3:1438:G:H3'	32:R3:1439:G:H21	1.81	0.45
54:U:96:GLU:O	54:U:100:ARG:HG2	2.16	0.45
54:U:523:TYR:HD1	54:U:524:HIS:ND1	2.14	0.45
8:2:144:GLU:HA	8:2:151:GLY:HA2	1.99	0.45
28:6:158:GLY:O	28:6:162:ARG:NH2	2.49	0.45
29:9:124:THR:OG1	29:9:128:HIS:NE2	2.50	0.45
30:R1:784:G:H5'	30:R1:785:G:OP1	2.16	0.45
30:R1:1594:U:H2'	30:R1:1595:C:H6	1.81	0.45
32:R3:1372:U:H2'	32:R3:1373:G:O4'	2.17	0.45
32:R3:1430:A:H2'	32:R3:1431:A:O4'	2.17	0.45
54:U:47:LYS:O	54:U:52:GLU:HB2	2.17	0.45
11:22:6:LYS:HB3	30:R1:494:G:H4'	1.99	0.45
13:24:10:VAL:HA	13:24:71:ILE:HA	1.99	0.45
29:9:42:LYS:HE3	29:9:46:PHE:CZ	2.52	0.45
30:R1:297:G:C6	30:R1:342:A:C6	3.05	0.45
30:R1:742:A:H2'	30:R1:743:A:C8	2.52	0.45
30:R1:878:A:H3'	30:R1:879:G:H8	1.81	0.45
30:R1:1918:A:O2'	30:R1:1919:A:N7	2.46	0.45
32:R3:399:G:H2'	32:R3:400:C:H6	1.81	0.45
54:U:395:ASP:HB3	54:U:398:LYS:HG3	1.98	0.45
54:U:468:THR:HA	54:U:471:LEU:HD12	1.99	0.45
14:25:2:PHE:O	14:25:62:THR:OG1	2.34	0.44
26:4:30:GLN:NE2	30:R1:659:G:H21	2.15	0.44
30:R1:170:U:H2'	30:R1:171:U:C6	2.51	0.44
30:R1:226:A:OP1	30:R1:257:C:H4'	2.17	0.44
30:R1:1062:G:OP2	30:R1:1062:G:H8	2.00	0.44
30:R1:1869:G:H22	30:R1:1872:A:H2'	1.82	0.44
30:R1:2290:G:H2'	30:R1:2291:U:C6	2.52	0.44
30:R1:2756:U:H4'	30:R1:2757:A:OP1	2.17	0.44
53:T:53:G:C5	53:T:54:5MU:H72	2.53	0.44
4:16:86:LYS:NZ	30:R1:955:U:OP1	2.33	0.44
15:27:41:ARG:HD2	15:27:41:ARG:HA	1.80	0.44
30:R1:108:G:C2'	30:R1:109:C:H5'	2.47	0.44
30:R1:160:A:H2	30:R1:165:A:H61	1.66	0.44
30:R1:1090:A:N6	30:R1:1102:C:H42	2.14	0.44
30:R1:1928:A:H2'	30:R1:1929:G:O4'	2.17	0.44
32:R3:636:U:H2'	32:R3:637:C:H6	1.82	0.44
32:R3:983:A:H5'	32:R3:984:C:OP2	2.17	0.44
32:R3:1021:A:H2'	32:R3:1022:A:O4'	2.17	0.44
54:U:459:SER:O	54:U:486:TYR:OH	2.33	0.44
9:20:61:ILE:HG23	9:20:75:TYR:CZ	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:24:6:ARG:NH2	30:R1:99:U:O2	2.50	0.44
18:3:108:ASP:OD1	18:3:108:ASP:N	2.49	0.44
18:3:133:THR:CG2	18:3:134:HIS:H	2.30	0.44
23:34:9:VAL:HG12	30:R1:125:A:H2	1.82	0.44
29:9:51:ARG:HB3	29:9:54:LEU:HB3	1.99	0.44
30:R1:276:U:H3'	30:R1:277:G:N2	2.32	0.44
30:R1:703:U:H2'	30:R1:704:G:O4'	2.17	0.44
30:R1:1604:C:H2'	30:R1:1605:C:H6	1.83	0.44
30:R1:2282:G:H4'	30:R1:2389:G:O2'	2.18	0.44
30:R1:2649:C:H2'	30:R1:2650:U:H6	1.82	0.44
30:R1:2659:G:H1'	30:R1:2662:A:H61	1.81	0.44
32:R3:208:U:H1'	32:R3:211:G:O6	2.17	0.44
32:R3:461:A:H2'	32:R3:462:G:N7	2.32	0.44
32:R3:474:G:H2'	32:R3:475:C:H5''	1.98	0.44
53:T:17:U:O2'	53:T:18:G:OP1	2.34	0.44
54:U:156:SER:HB2	58:U:601:ATP:C2	2.53	0.44
55:1:196:LEU:HA	55:1:199:ALA:HB3	1.98	0.44
30:R1:1447:C:O2'	30:R1:1544:A:N3	2.42	0.44
30:R1:1720:U:H2'	30:R1:1721:G:O4'	2.17	0.44
32:R3:363:A:O2'	32:R3:364:A:OP1	2.34	0.44
32:R3:839:C:H2'	32:R3:840:C:C6	2.52	0.44
5:17:35:LYS:HB2	5:17:112:TYR:CE1	2.52	0.44
7:19:27:VAL:HA	7:19:82:SER:O	2.18	0.44
21:32:2:VAL:HG22	30:R1:2015:A:C2	2.52	0.44
28:6:34:ARG:HG3	28:6:35:THR:O	2.18	0.44
30:R1:40:U:H2'	30:R1:41:C:C6	2.52	0.44
30:R1:1062:G:H2'	30:R1:1063:G:C8	2.53	0.44
30:R1:2281:A:O2'	30:R1:2282:G:H5'	2.17	0.44
30:R1:2339:C:H4'	31:R2:41:G:N2	2.24	0.44
32:R3:142:G:H3'	32:R3:143:A:C8	2.51	0.44
32:R3:1009:U:H2'	32:R3:1010:U:C6	2.52	0.44
32:R3:1122:U:HO2'	32:R3:1123:U:H6	1.64	0.44
54:U:329:VAL:HG22	54:U:330:ASN:OD1	2.18	0.44
4:16:12:MET:HE3	4:16:72:PRO:HD2	1.99	0.44
27:5:125:GLY:N	27:5:162:ASP:OD1	2.47	0.44
30:R1:1263:U:H2'	30:R1:1264:A:C8	2.52	0.44
30:R1:1509:A:H2'	30:R1:1510:G:H8	1.83	0.44
30:R1:2130:U:H1'	30:R1:2159:G:N2	2.30	0.44
30:R1:2146:C:H4'	30:R1:2147:A:N7	2.32	0.44
30:R1:2195:U:H2'	30:R1:2196:C:H6	1.82	0.44
30:R1:2682:A:H61	30:R1:2728:U:H1'	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:R3:663:A:H2'	32:R3:664:G:O4'	2.17	0.44
32:R3:857:C:H2'	32:R3:858:G:O4'	2.17	0.44
32:R3:1141:C:N4	32:R3:1142:G:O6	2.51	0.44
32:R3:1147:C:H2'	32:R3:1148:U:H6	1.82	0.44
54:U:519:TYR:CZ	54:U:530:GLN:HG3	2.52	0.44
4:16:26:VAL:HG13	4:16:104:GLU:OE1	2.17	0.44
5:17:55:ALA:HA	5:17:80:PHE:CE1	2.52	0.44
27:5:33:ILE:HG12	27:5:155:ILE:HD13	1.99	0.44
28:6:106:LEU:HD12	28:6:151:ARG:HG3	2.00	0.44
30:R1:321:U:O2'	30:R1:340:A:N3	2.51	0.44
30:R1:1315:C:O2'	30:R1:1392:A:N3	2.41	0.44
30:R1:2500:U:H5''	30:R1:2501:C:OP2	2.18	0.44
32:R3:203:G:H4'	32:R3:466:A:H61	1.81	0.44
32:R3:337:G:H3'	32:R3:338:A:H8	1.82	0.44
32:R3:635:A:H2'	32:R3:636:U:C6	2.52	0.44
3:15:77:ILE:HB	3:15:110:VAL:HG22	2.00	0.44
5:17:100:CYS:SG	5:17:101:GLY:N	2.90	0.44
30:R1:1057:A:H8	30:R1:1089:A:N6	2.16	0.44
30:R1:1587:G:H2'	30:R1:1588:G:C8	2.51	0.44
30:R1:2607:G:H2'	30:R1:2608:G:O4'	2.17	0.44
32:R3:150:U:H2'	32:R3:151:A:C8	2.53	0.44
54:U:393:GLU:O	54:U:453:ARG:NH2	2.51	0.44
3:15:64:PHE:HB3	24:35:24:LYS:HD2	1.99	0.44
10:21:76:LYS:HB2	10:21:85:LYS:HB2	2.00	0.44
11:22:24:ILE:O	11:22:24:ILE:HG13	2.17	0.44
20:31:11:GLU:HB2	20:31:23:LYS:NZ	2.33	0.44
24:35:46:LYS:HD3	24:35:46:LYS:HA	1.78	0.44
30:R1:134:G:C6	30:R1:144:A:N1	2.85	0.44
30:R1:354:A:H3'	30:R1:355:U:C6	2.53	0.44
30:R1:358:U:H2'	30:R1:359:G:H8	1.81	0.44
30:R1:630:G:N2	30:R1:633:A:OP2	2.42	0.44
30:R1:849:A:H2'	30:R1:850:U:C6	2.51	0.44
30:R1:1430:G:H2'	30:R1:1431:A:H8	1.82	0.44
32:R3:321:A:N6	32:R3:332:G:H1	2.16	0.44
32:R3:401:C:H1'	32:R3:622:A:H1'	2.00	0.44
32:R3:657:U:H2'	32:R3:658:C:H6	1.82	0.44
32:R3:725:G:H2'	32:R3:726:C:C6	2.53	0.44
32:R3:1287:A:H2'	32:R3:1288:A:C8	2.53	0.44
54:U:212:ASP:HB3	54:U:215:PHE:HB3	2.00	0.44
54:U:375:ARG:NH1	54:U:377:HIS:HB2	2.33	0.44
56:M:1:A:H2'	56:M:2:A:H8	1.83	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:15:55:MET:HE3	30:R1:2429:G:N7	2.33	0.43
10:21:98:ILE:HD12	10:21:98:ILE:N	2.32	0.43
24:35:30:HIS:CD2	24:35:31:ILE:HD12	2.53	0.43
26:4:53:THR:HG22	30:R1:452:G:OP1	2.18	0.43
30:R1:588:U:H2'	30:R1:589:U:C6	2.54	0.43
30:R1:131:A:H2'	30:R1:132:G:H8	1.83	0.43
30:R1:299:A:N3	30:R1:319:G:O2'	2.38	0.43
30:R1:882:G:H2'	30:R1:883:G:O4'	2.18	0.43
30:R1:2788:C:H2'	30:R1:2789:C:C6	2.53	0.43
32:R3:82:G:H1'	32:R3:88:U:H3	1.82	0.43
32:R3:849:G:C2	32:R3:850:U:H1'	2.53	0.43
54:U:398:LYS:O	54:U:438:VAL:HG23	2.18	0.43
7:19:105:LYS:O	7:19:108:ARG:NH1	2.44	0.43
26:4:51:GLU:CD	26:4:88:ARG:HH22	2.21	0.43
28:6:157:LYS:HE2	30:R1:2658:C:H5''	1.98	0.43
30:R1:354:A:H2'	30:R1:355:U:O4'	2.18	0.43
30:R1:589:U:O2'	30:R1:590:A:H5'	2.18	0.43
30:R1:596:U:H2'	30:R1:597:G:H8	1.83	0.43
32:R3:981:U:H2'	32:R3:982:U:C5	2.54	0.43
54:U:300:GLU:HG2	54:U:301:VAL:N	2.33	0.43
54:U:385:ALA:HB3	54:U:462:LEU:HD23	2.00	0.43
8:2:7:PRO:CB	8:2:13:ARG:HG2	2.49	0.43
8:2:264:LYS:HB3	8:2:264:LYS:HE3	1.67	0.43
13:24:96:LYS:O	13:24:97:SER:OG	2.32	0.43
26:4:143:LEU:HB3	26:4:146:VAL:CG1	2.47	0.43
30:R1:1055:G:H3'	30:R1:1056:G:C8	2.53	0.43
54:U:127:LEU:HD13	54:U:132:LEU:HB3	2.00	0.43
54:U:312:ALA:HB2	54:U:458:PRO:HB3	2.00	0.43
55:1:41:SER:HA	55:1:177:LYS:HD3	2.01	0.43
6:18:16:ARG:NH1	6:18:19:GLN:HG3	2.24	0.43
28:6:32:LEU:HB3	28:6:74:MET:SD	2.58	0.43
29:9:116:ARG:NH2	29:9:118:PRO:HA	2.34	0.43
30:R1:136:G:N1	30:R1:142:A:H2	2.11	0.43
30:R1:277:G:N2	30:R1:277:G:OP2	2.39	0.43
30:R1:388:G:O2'	30:R1:390:U:OP2	2.28	0.43
30:R1:1048:A:N7	30:R1:1049:C:H5	2.15	0.43
30:R1:1321:A:C4	30:R1:1322:A:C8	3.06	0.43
31:R2:17:C:C2	31:R2:18:G:C8	3.06	0.43
32:R3:312:C:H2'	32:R3:313:A:H8	1.83	0.43
32:R3:450:G:H3'	32:R3:451:A:H5''	2.01	0.43
32:R3:483:C:H5''	32:R3:484:G:OP2	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
54:U:148:LEU:H	54:U:148:LEU:HD12	1.82	0.43
54:U:405:ALA:HB1	54:U:408:LYS:HE2	1.98	0.43
6:18:46:GLU:HA	31:R2:113:C:H1'	2.00	0.43
12:23:15:HIS:HB3	12:23:31:VAL:HG12	2.00	0.43
15:27:77:ARG:HH12	30:R1:2333:A:P	2.39	0.43
24:35:35:LYS:HG2	24:35:39:ARG:NH1	2.34	0.43
27:5:91:ARG:NE	31:R2:43:C:O2	2.51	0.43
27:5:129:MET:HE2	27:5:129:MET:HB2	1.91	0.43
27:5:131:VAL:HG21	27:5:151:LEU:HD12	2.01	0.43
30:R1:284:U:N3	30:R1:356:G:N1	2.67	0.43
30:R1:419:U:H2'	30:R1:420:C:C6	2.54	0.43
30:R1:1990:C:H2'	30:R1:1991:U:O4'	2.18	0.43
30:R1:2112:G:H5''	30:R1:2113:U:C6	2.54	0.43
30:R1:2182:U:H2'	30:R1:2183:A:C8	2.53	0.43
30:R1:2266:A:H4'	30:R1:2267:A:O5'	2.17	0.43
30:R1:2556:C:H2'	30:R1:2557:G:O4'	2.18	0.43
32:R3:59:A:C6	32:R3:331:G:C8	3.07	0.43
32:R3:1141:C:C4	32:R3:1142:G:C6	3.07	0.43
32:R3:1218:C:H2'	32:R3:1219:A:H8	1.78	0.43
18:3:151:THR:OG1	30:R1:2032:G:N2	2.52	0.43
21:32:27:LEU:HD23	21:32:36:LYS:HB3	2.01	0.43
22:33:39:ASP:HB3	22:33:42:VAL:HG12	1.99	0.43
28:6:11:PRO:HG3	28:6:75:VAL:HG13	2.00	0.43
28:6:148:ARG:HA	28:6:161:VAL:HG13	2.00	0.43
28:6:148:ARG:HA	28:6:161:VAL:CG1	2.49	0.43
30:R1:225:C:O2'	30:R1:226:A:OP1	2.34	0.43
30:R1:1932:A:H2'	30:R1:1933:G:O4'	2.19	0.43
30:R1:2667:C:H2'	30:R1:2668:G:H5'	1.99	0.43
30:R1:2816:G:N3	30:R1:2883:A:O2'	2.51	0.43
32:R3:602:A:H2'	32:R3:603:U:C6	2.54	0.43
5:17:37:THR:CG2	5:17:39:PRO:HD2	2.47	0.43
14:25:34:LYS:HD2	14:25:34:LYS:HA	1.79	0.43
18:3:112:THR:O	18:3:195:GLY:HA2	2.18	0.43
23:34:4:THR:HG22	30:R1:687:C:H1'	2.01	0.43
27:5:169:LEU:O	27:5:174:PHE:HB2	2.18	0.43
30:R1:880:G:H21	30:R1:898:C:N4	2.17	0.43
30:R1:1229:C:H2'	30:R1:1230:A:C8	2.54	0.43
30:R1:1409:U:C2	30:R1:1410:G:C8	3.07	0.43
30:R1:1722:A:C4	30:R1:1723:G:C8	3.07	0.43
30:R1:1728:C:H1'	30:R1:1733:G:N2	2.31	0.43
30:R1:1989:G:H2'	30:R1:1990:C:O4'	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:R1:2121:G:H1	30:R1:2176:A:H62	1.66	0.43
30:R1:2666:C:H3'	30:R1:2667:C:H6	1.84	0.43
30:R1:2857:G:N2	30:R1:2860:A:OP2	2.40	0.43
32:R3:150:U:H2'	32:R3:151:A:H8	1.83	0.43
32:R3:909:A:N3	32:R3:1413:A:O2'	2.41	0.43
32:R3:1130:A:O2'	32:R3:1131:G:H8	2.02	0.43
32:R3:1454:G:H2'	32:R3:1455:G:C8	2.54	0.43
53:T:55:PSU:OP2	53:T:55:PSU:H4'	2.18	0.43
54:U:6:MET:HE3	54:U:24:LEU:HB2	2.00	0.43
54:U:396:PRO:O	54:U:439:ARG:N	2.45	0.43
7:19:26:GLU:OE2	7:19:41:ALA:HB1	2.19	0.43
30:R1:67:U:C2	30:R1:68:G:C8	3.07	0.43
30:R1:157:C:H1'	30:R1:169:G:N2	2.33	0.43
30:R1:387:U:C2	30:R1:388:G:N2	2.87	0.43
30:R1:827:U:O2'	30:R1:2068:U:C2	2.70	0.43
30:R1:955:U:H5	30:R1:962:G:H1	1.67	0.43
30:R1:2107:G:C2	30:R1:2182:U:O2	2.69	0.43
30:R1:2123:G:H2'	30:R1:2124:G:N3	2.33	0.43
32:R3:632:U:H3'	32:R3:633:G:H5'	2.00	0.43
32:R3:744:C:O2'	32:R3:851:G:N2	2.52	0.43
32:R3:1006:G:O2'	32:R3:1007:U:O5'	2.37	0.43
32:R3:1271:A:H2'	32:R3:1272:G:C8	2.54	0.43
54:U:131:ASN:O	54:U:133:TRP:N	2.52	0.43
11:22:17:VAL:HG12	11:22:76:VAL:HG11	2.01	0.43
24:35:53:ASP:O	24:35:57:VAL:HG23	2.18	0.43
26:4:6:LYS:HA	26:4:6:LYS:HD2	1.82	0.43
30:R1:41:C:C4	30:R1:42:A:N7	2.87	0.43
30:R1:1858:A:H2'	30:R1:1859:U:O4'	2.18	0.43
30:R1:2100:G:N2	30:R1:2190:G:H2'	2.34	0.43
30:R1:2189:U:O2'	30:R1:2190:G:OP1	2.34	0.43
30:R1:2373:G:H2'	30:R1:2374:C:C6	2.54	0.43
31:R2:66:A:H61	31:R2:107:G:H3'	1.83	0.43
32:R3:428:G:H8	32:R3:428:G:OP1	2.02	0.43
32:R3:469:C:H2'	32:R3:470:C:N3	2.33	0.43
32:R3:552:U:C4	32:R3:553:A:N7	2.86	0.43
32:R3:807:A:H2'	32:R3:808:C:C6	2.54	0.43
32:R3:920:U:H2'	32:R3:921:U:C6	2.54	0.43
54:U:9:ALA:HB1	54:U:55:LEU:HD11	2.01	0.43
54:U:261:ARG:HE	54:U:261:ARG:HB3	1.66	0.43
55:1:31:LYS:HZ1	55:1:182:ALA:HB2	1.84	0.43
1:13:60:ASP:OD2	1:13:61:LYS:HD2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:19:55:HIS:HA	18:3:13:ARG:HH21	1.84	0.42
8:2:92:LEU:HD21	8:2:100:ARG:HD3	1.99	0.42
8:2:238:ASN:HD22	30:R1:2595:G:H1	1.67	0.42
13:24:78:LYS:HE3	13:24:78:LYS:HB3	1.79	0.42
13:24:86:PHE:CE1	13:24:91:LYS:HB2	2.53	0.42
26:4:45:ALA:HA	26:4:87:ALA:O	2.19	0.42
30:R1:177:G:H3'	30:R1:178:G:C8	2.52	0.42
30:R1:1087:G:H2'	30:R1:1089:A:O4'	2.19	0.42
30:R1:1948:G:N3	32:R3:1418:A:H2	2.17	0.42
30:R1:2109:U:H5''	30:R1:2110:G:OP2	2.19	0.42
32:R3:784:A:H2'	32:R3:785:G:H8	1.84	0.42
32:R3:1155:A:H2'	32:R3:1156:G:C8	2.54	0.42
32:R3:1296:C:H4'	32:R3:1302:C:C5	2.54	0.42
54:U:315:SER:OG	54:U:316:GLY:N	2.51	0.42
54:U:383:GLU:HB2	54:U:459:SER:HA	2.00	0.42
1:13:36:LEU:HD22	1:13:121:LYS:HB2	2.00	0.42
30:R1:2164:C:C2'	30:R1:2165:C:H4'	2.49	0.42
31:R2:32:U:N3	31:R2:33:G:N7	2.68	0.42
32:R3:62:U:H5	32:R3:105:G:H1	1.67	0.42
32:R3:378:G:OP2	32:R3:378:G:N2	2.44	0.42
54:U:251:VAL:O	54:U:255:GLN:HG3	2.19	0.42
55:1:9:ARG:HA	55:1:12:ARG:HD2	2.01	0.42
1:13:37:ARG:HH11	1:13:110:PRO:HG3	1.84	0.42
5:17:60:VAL:O	5:17:64:ARG:HG2	2.19	0.42
10:21:56:GLY:HA3	10:21:103:ALA:O	2.19	0.42
14:25:48:MET:SD	14:25:86:LEU:HD23	2.60	0.42
21:32:28:SER:HB3	21:32:39:ARG:HD3	2.01	0.42
27:5:46:LYS:HD2	27:5:46:LYS:HA	1.85	0.42
30:R1:667:U:H2'	30:R1:668:A:O4'	2.19	0.42
30:R1:1112:G:H2'	30:R1:1113:U:H6	1.83	0.42
30:R1:2038:G:H2'	30:R1:2039:U:O4'	2.19	0.42
30:R1:2545:G:N2	30:R1:2565:A:H8	2.03	0.42
32:R3:178:C:H2'	32:R3:179:A:O4'	2.18	0.42
32:R3:343:U:O2'	32:R3:346:G:O6	2.24	0.42
32:R3:1245:C:H2'	32:R3:1246:A:C8	2.54	0.42
32:R3:1437:A:H2'	32:R3:1438:G:H8	1.83	0.42
54:U:171:LEU:HD23	54:U:171:LEU:O	2.19	0.42
54:U:182:GLN:HB3	54:U:185:ASN:OD1	2.19	0.42
22:33:14:ALA:HB2	22:33:46:VAL:HG11	2.01	0.42
30:R1:1468:U:H2'	30:R1:1522:A:H61	1.84	0.42
30:R1:1711:A:H2'	30:R1:1712:U:C6	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:R1:2295:C:O2'	30:R1:2296:U:H5'	2.19	0.42
32:R3:321:A:H2	32:R3:328:C:O2'	2.02	0.42
32:R3:360:G:H2'	32:R3:361:G:C8	2.54	0.42
32:R3:635:A:H2'	32:R3:636:U:H6	1.85	0.42
54:U:212:ASP:OD1	54:U:214:SER:OG	2.26	0.42
7:19:5:LYS:O	7:19:9:GLN:HB2	2.20	0.42
18:3:106:LYS:HA	18:3:175:LEU:O	2.19	0.42
30:R1:17:G:H2'	30:R1:18:U:C6	2.54	0.42
30:R1:160:A:H8	30:R1:2217:G:N2	2.07	0.42
30:R1:356:G:C8	30:R1:357:C:N3	2.87	0.42
30:R1:1047:G:N2	30:R1:1110:G:H2'	2.35	0.42
30:R1:1361:G:H2'	30:R1:1362:C:H6	1.85	0.42
30:R1:2896:C:HO2'	30:R1:2897:U:P	2.41	0.42
31:R2:24:G:H21	31:R2:27:C:H42	1.66	0.42
32:R3:60:A:H4'	32:R3:61:G:OP1	2.19	0.42
32:R3:207:C:H2'	32:R3:213:G:H1	1.85	0.42
32:R3:461:A:H2'	32:R3:462:G:C8	2.54	0.42
32:R3:497:G:H2'	32:R3:498:A:C8	2.55	0.42
32:R3:1026:G:N1	32:R3:1036:A:N1	2.68	0.42
53:T:54:5MU:C6	53:T:54:5MU:C4'	3.02	0.42
54:U:187:LEU:HD22	54:U:191:THR:HG21	2.02	0.42
55:1:42:VAL:HG21	55:1:175:ILE:HB	2.02	0.42
13:24:85:ARG:HH11	13:24:85:ARG:HG3	1.84	0.42
19:30:39:ASP:OD1	19:30:44:ARG:NE	2.51	0.42
24:35:58:ILE:H	24:35:58:ILE:HG13	1.70	0.42
27:5:111:ARG:NH2	27:5:133:GLU:OE2	2.53	0.42
30:R1:136:G:O6	30:R1:143:C:N4	2.52	0.42
30:R1:508:A:H2'	30:R1:508:A:N3	2.35	0.42
30:R1:827:U:H4'	30:R1:828:U:C6	2.54	0.42
30:R1:1108:U:H2'	30:R1:1109:C:N3	2.35	0.42
30:R1:1580:A:H8	30:R1:1581:G:C8	2.38	0.42
30:R1:2113:U:H2'	30:R1:2114:A:C5	2.55	0.42
30:R1:2185:U:H2'	30:R1:2186:G:O4'	2.19	0.42
30:R1:2368:C:C2	30:R1:2369:A:C8	3.08	0.42
30:R1:2839:G:H2'	30:R1:2840:C:O4'	2.20	0.42
32:R3:518:C:H4'	32:R3:519:C:O2	2.20	0.42
32:R3:711:G:O2'	32:R3:712:A:H5'	2.18	0.42
4:16:6:ARG:HH21	53:T:52:G:C4'	2.33	0.42
4:16:42:THR:HG22	4:16:45:GLN:CD	2.40	0.42
5:17:57:THR:OG1	5:17:57:THR:O	2.33	0.42
11:22:88:ARG:HA	11:22:88:ARG:HD2	1.82	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:24:48:VAL:HG12	13:24:49:PRO:HD2	2.01	0.42
18:3:43:ASP:OD1	30:R1:2784:U:H4'	2.19	0.42
30:R1:152:A:N6	30:R1:173:A:H61	2.17	0.42
30:R1:302:C:H2'	30:R1:303:G:H8	1.85	0.42
30:R1:608:A:H2'	30:R1:609:A:C8	2.55	0.42
30:R1:1069:A:H5''	30:R1:1073:A:N6	2.35	0.42
30:R1:1246:A:H2'	30:R1:1247:A:O4'	2.20	0.42
30:R1:1358:G:O2'	30:R1:1373:A:N6	2.53	0.42
30:R1:1412:U:H2'	30:R1:1413:A:C8	2.54	0.42
30:R1:1466:U:H5''	30:R1:1467:U:H5'	2.00	0.42
30:R1:1595:C:H2'	30:R1:1596:A:H8	1.85	0.42
32:R3:255:G:H2'	32:R3:256:U:H6	1.84	0.42
32:R3:321:A:O2'	32:R3:1436:U:H5'	2.20	0.42
32:R3:460:A:H2'	32:R3:461:A:C8	2.55	0.42
32:R3:1384:C:H2'	32:R3:1385:G:C8	2.55	0.42
54:U:15:ASP:OD1	54:U:16:ALA:N	2.42	0.42
54:U:127:LEU:HD21	54:U:133:TRP:HE1	1.82	0.42
4:16:46:ILE:HA	4:16:103:TYR:OH	2.19	0.42
18:3:157:LYS:HE2	18:3:157:LYS:HB2	1.81	0.42
30:R1:100:U:H4'	30:R1:101:A:O4'	2.20	0.42
30:R1:1430:G:H2'	30:R1:1431:A:C8	2.54	0.42
30:R1:1505:A:H2'	30:R1:1506:U:C6	2.55	0.42
30:R1:1638:C:H1'	30:R1:2698:U:O2'	2.20	0.42
30:R1:2077:A:N3	30:R1:2434:A:O2'	2.40	0.42
30:R1:2435:A:O2'	54:U:281:ASN:HB3	2.20	0.42
30:R1:2896:C:O2'	30:R1:2897:U:P	2.77	0.42
32:R3:425:G:H2'	32:R3:426:U:C6	2.54	0.42
54:U:105:SER:O	54:U:109:MET:N	2.53	0.42
7:19:42:PHE:HE1	7:19:60:VAL:HG12	1.85	0.42
8:2:110:LYS:HG3	8:2:111:ALA:N	2.35	0.42
20:31:58:ASP:HB2	20:31:59:ARG:NH1	2.35	0.42
28:6:136:ASP:HB3	28:6:139:VAL:HB	2.01	0.42
29:9:75:LEU:HD23	29:9:75:LEU:H	1.85	0.42
30:R1:966:G:O4'	30:R1:2267:A:N6	2.53	0.42
30:R1:1088:A:H5'	30:R1:1089:A:H5'	2.02	0.42
30:R1:1808:A:H3'	30:R1:1809:A:C8	2.54	0.42
30:R1:2133:G:H2'	30:R1:2157:G:H2'	2.01	0.42
32:R3:612:C:O2'	32:R3:613:C:OP1	2.30	0.42
32:R3:946:A:O2'	32:R3:1333:A:N3	2.45	0.42
32:R3:1129:C:H41	32:R3:1143:G:H1	1.68	0.42
53:T:44:A:H2'	53:T:45:G:O4'	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:18:56:LYS:O	6:18:60:GLU:HG3	2.19	0.42
17:29:58:ASN:ND2	30:R1:112:U:H5'	2.35	0.42
28:6:88:LEU:HD12	28:6:128:THR:HA	2.02	0.42
28:6:174:LYS:HE3	28:6:175:LYS:HE3	2.01	0.42
29:9:114:GLU:OE1	29:9:133:GLN:N	2.41	0.42
30:R1:640:C:H2'	30:R1:641:U:C6	2.52	0.42
30:R1:1316:U:C2	30:R1:1317:G:C8	3.07	0.42
30:R1:2299:U:H2'	30:R1:2300:C:C6	2.55	0.42
30:R1:2362:C:H2'	30:R1:2363:G:O4'	2.20	0.42
32:R3:1319:A:C8	32:R3:1323:G:C5	3.08	0.42
54:U:329:VAL:HG12	54:U:332:LYS:O	2.20	0.42
54:U:334:LEU:O	54:U:514:GLY:HA2	2.20	0.42
6:18:62:LEU:HD21	6:18:70:ALA:HA	2.01	0.41
16:28:33:HIS:NE2	30:R1:2229:U:O2	2.48	0.41
30:R1:262:A:H2'	30:R1:263:G:O4'	2.20	0.41
30:R1:319:G:H22	30:R1:323:C:H5	1.68	0.41
30:R1:548:G:H2'	30:R1:549:G:H4'	2.00	0.41
30:R1:1085:A:O4'	30:R1:1105:U:O2'	2.35	0.41
30:R1:2175:C:N4	30:R1:2178:C:H42	2.17	0.41
30:R1:2760:C:C2'	30:R1:2761:A:H5''	2.50	0.41
32:R3:807:A:H2'	32:R3:808:C:H6	1.85	0.41
32:R3:902:G:H2'	32:R3:903:G:H8	1.85	0.41
32:R3:1371:G:C6	32:R3:1372:U:C4	3.07	0.41
5:17:71:ARG:NH1	30:R1:2707:U:O2	2.54	0.41
7:19:27:VAL:HG12	7:19:29:VAL:HG23	2.02	0.41
8:2:155:ARG:NH2	30:R1:1818:U:OP2	2.39	0.41
9:20:91:ARG:HD2	30:R1:997:G:OP1	2.20	0.41
13:24:27:VAL:HG12	13:24:33:VAL:HG12	2.01	0.41
23:34:19:ARG:NE	30:R1:125:A:OP2	2.36	0.41
30:R1:118:A:N3	30:R1:178:G:H1'	2.35	0.41
30:R1:290:U:C2	30:R1:291:G:C8	3.08	0.41
30:R1:1278:C:H2'	30:R1:1279:G:H8	1.84	0.41
30:R1:1544:A:H2'	30:R1:1545:A:H8	1.85	0.41
30:R1:2215:C:H2'	30:R1:2216:G:C8	2.55	0.41
30:R1:2472:G:N1	30:R1:2477:U:OP1	2.43	0.41
32:R3:198:G:H2'	32:R3:199:A:H8	1.85	0.41
32:R3:381:C:H2'	32:R3:382:A:O4'	2.20	0.41
32:R3:416:G:O6	32:R3:417:G:O6	2.39	0.41
32:R3:1236:A:H2'	32:R3:1237:C:C6	2.55	0.41
54:U:312:ALA:HB3	54:U:460:ASN:OD1	2.20	0.41
54:U:363:LYS:HB3	54:U:368:GLN:HB2	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:18:25:ARG:HG3	6:18:27:VAL:HG13	2.02	0.41
18:3:16:THR:HG22	18:3:17:GLU:H	1.86	0.41
19:30:9:THR:HG22	19:30:55:LYS:HE2	2.02	0.41
26:4:8:ALA:O	26:4:9:GLN:HG3	2.19	0.41
30:R1:580:U:H2'	30:R1:581:C:C6	2.55	0.41
30:R1:1709:U:H2'	30:R1:1710:G:C8	2.55	0.41
30:R1:1873:G:H2'	30:R1:1874:C:C6	2.56	0.41
32:R3:34:C:H2'	32:R3:35:G:C8	2.56	0.41
32:R3:265:G:H2'	32:R3:267:C:H5	1.85	0.41
32:R3:453:G:O2'	32:R3:454:G:OP1	2.36	0.41
32:R3:462:G:H3'	32:R3:463:U:O4'	2.20	0.41
32:R3:1102:A:C6	32:R3:1103:C:N4	2.89	0.41
32:R3:1140:C:H2'	32:R3:1141:C:N1	2.34	0.41
54:U:297:GLU:O	54:U:299:ARG:NH1	2.54	0.41
3:15:109:LYS:HG3	3:15:126:ARG:O	2.21	0.41
8:2:52:HIS:NE2	8:2:218:THR:HG23	2.36	0.41
10:21:71:LYS:HZ3	10:21:88:GLY:HA3	1.85	0.41
13:24:18:LYS:HB3	13:24:18:LYS:HE2	1.90	0.41
13:24:98:ASN:HB3	13:24:100:GLU:OE2	2.20	0.41
16:28:76:LYS:HA	16:28:76:LYS:HD2	1.83	0.41
28:6:88:LEU:HD23	28:6:161:VAL:HG23	2.03	0.41
29:9:96:THR:O	29:9:112:LYS:HD2	2.20	0.41
30:R1:2152:G:N3	30:R1:2152:G:H2'	2.36	0.41
30:R1:2512:C:H2'	30:R1:2513:A:O4'	2.19	0.41
32:R3:235:C:H2'	32:R3:236:A:H8	1.83	0.41
32:R3:459:A:C5	32:R3:460:A:N6	2.88	0.41
32:R3:463:U:H2'	32:R3:464:U:C2	2.55	0.41
32:R3:1271:A:H2'	32:R3:1272:G:H8	1.84	0.41
55:1:41:SER:O	55:1:216:THR:HG23	2.20	0.41
4:16:5:LYS:HG2	30:R1:871:U:OP1	2.21	0.41
8:2:216:ARG:HH22	30:R1:781:A:P	2.40	0.41
30:R1:1013:C:H2'	30:R1:1014:A:H8	1.84	0.41
30:R1:1946:U:H2'	30:R1:1947:C:H6	1.86	0.41
30:R1:2120:G:N2	30:R1:2121:G:C6	2.88	0.41
30:R1:2514:U:H2'	30:R1:2515:C:H6	1.85	0.41
30:R1:2663:G:H2'	30:R1:2664:G:C8	2.56	0.41
32:R3:106:C:H2'	32:R3:107:G:O4'	2.21	0.41
32:R3:149:A:H2'	32:R3:150:U:C6	2.56	0.41
32:R3:198:G:H2'	32:R3:199:A:C8	2.55	0.41
32:R3:312:C:O2'	32:R3:313:A:OP1	2.36	0.41
32:R3:415:A:H3'	32:R3:416:G:H8	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:R3:1316:G:N2	32:R3:1319:A:OP2	2.27	0.41
54:U:178:LEU:HD12	54:U:178:LEU:HA	1.88	0.41
13:24:83:GLY:HA3	13:24:96:LYS:NZ	2.35	0.41
15:27:72:LYS:H	15:27:72:LYS:HG3	1.61	0.41
16:28:37:PHE:HZ	16:28:50:VAL:HG21	1.86	0.41
30:R1:152:A:H8	30:R1:152:A:OP2	2.04	0.41
30:R1:360:U:O2'	30:R1:361:G:C8	2.73	0.41
30:R1:394:C:H2'	30:R1:395:U:O4'	2.20	0.41
30:R1:1508:A:O2'	30:R1:1509:A:O5'	2.37	0.41
30:R1:2187:U:H2'	30:R1:2188:U:C6	2.55	0.41
32:R3:492:C:H5'	32:R3:493:A:OP2	2.20	0.41
32:R3:687:A:C2	32:R3:704:A:C5	3.08	0.41
32:R3:1018:G:H2'	32:R3:1019:A:O4'	2.21	0.41
32:R3:1209:C:O2'	32:R3:1214:C:N4	2.53	0.41
54:U:319:VAL:O	54:U:379:GLY:N	2.54	0.41
54:U:391:ARG:H	54:U:391:ARG:HG2	1.54	0.41
17:29:56:LEU:O	17:29:60:LYS:HB2	2.21	0.41
20:31:9:TYR:CD2	20:31:25:ARG:HG2	2.55	0.41
26:4:39:ALA:HB2	30:R1:615:U:O4	2.21	0.41
27:5:15:LEU:HD23	27:5:15:LEU:HA	1.90	0.41
27:5:22:ASN:OD1	27:5:22:ASN:N	2.49	0.41
28:6:28:LYS:HG3	28:6:29:ASN:N	2.34	0.41
30:R1:150:U:H3	30:R1:175:G:H1	1.68	0.41
30:R1:303:G:H2'	30:R1:304:U:C6	2.56	0.41
30:R1:439:A:H2'	30:R1:440:C:O4'	2.20	0.41
30:R1:722:A:H2'	30:R1:723:C:C6	2.56	0.41
30:R1:1084:A:H2'	30:R1:1105:U:O2'	2.21	0.41
30:R1:1108:U:H2'	30:R1:1109:C:C4	2.56	0.41
30:R1:2064:C:H2'	30:R1:2065:C:H6	1.84	0.41
30:R1:2189:U:O2'	30:R1:2190:G:P	2.78	0.41
32:R3:418:C:O2'	32:R3:419:C:H5''	2.20	0.41
32:R3:608:A:H2'	32:R3:609:A:O4'	2.20	0.41
32:R3:948:C:H2'	32:R3:949:A:H8	1.85	0.41
32:R3:1158:C:C4	32:R3:1160:G:C8	3.08	0.41
8:2:16:VAL:HB	8:2:203:VAL:HG22	2.02	0.41
27:5:47:LYS:HA	27:5:50:ASP:HB2	2.03	0.41
27:5:122:ASP:OD2	27:5:126:ASN:HB2	2.21	0.41
30:R1:181:A:H2'	30:R1:182:A:H8	1.84	0.41
30:R1:555:G:H5'	30:R1:556:A:OP1	2.20	0.41
30:R1:1509:A:H2'	30:R1:1510:G:C8	2.56	0.41
30:R1:2164:C:H5''	30:R1:2165:C:OP2	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:R1:2364:C:H2'	30:R1:2365:G:O4'	2.21	0.41
30:R1:2467:C:H2'	30:R1:2468:A:O4'	2.20	0.41
32:R3:35:G:H2'	32:R3:36:C:C6	2.55	0.41
32:R3:312:C:HO2'	32:R3:313:A:P	2.43	0.41
32:R3:332:G:N3	32:R3:333:U:C2	2.88	0.41
32:R3:402:G:O2'	32:R3:403:C:H6	2.04	0.41
32:R3:1064:G:O2'	32:R3:1190:G:N2	2.54	0.41
54:U:416:LYS:H	54:U:418:ARG:NH2	2.19	0.41
54:U:441:LEU:O	54:U:446:ARG:NH2	2.40	0.41
55:1:200:LYS:HG3	55:1:208:TYR:CE1	2.56	0.41
6:18:56:LYS:NZ	6:18:60:GLU:HG2	2.35	0.41
7:19:13:LYS:H	7:19:13:LYS:HG2	1.71	0.41
7:19:26:GLU:HG2	7:19:43:GLU:OE2	2.21	0.41
10:21:80:ARG:NH2	30:R1:572:A:OP2	2.54	0.41
13:24:90:LYS:HB3	13:24:90:LYS:HE3	1.88	0.41
15:27:19:LYS:HA	15:27:19:LYS:HD3	1.94	0.41
15:27:65:GLY:HA2	15:27:85:GLU:HG2	2.02	0.41
21:32:2:VAL:O	21:32:3:GLN:HB3	2.21	0.41
28:6:5:LYS:HD3	28:6:5:LYS:HA	1.88	0.41
30:R1:107:G:H2'	30:R1:108:G:C8	2.54	0.41
30:R1:271:G:C2	30:R1:367:G:C2	3.08	0.41
30:R1:322:A:C4	30:R1:340:A:N1	2.88	0.41
30:R1:362:A:C8	30:R1:363:G:C8	3.09	0.41
30:R1:438:G:H2'	30:R1:439:A:C8	2.55	0.41
30:R1:629:G:OP1	30:R1:650:C:O2'	2.30	0.41
30:R1:1295:C:C2	30:R1:1296:G:C8	3.09	0.41
30:R1:1405:U:H2'	30:R1:1406:U:H6	1.86	0.41
30:R1:1493:C:H5'	30:R1:1494:A:OP2	2.19	0.41
30:R1:1672:A:C2	30:R1:2582:G:H5'	2.56	0.41
30:R1:2074:U:H2'	30:R1:2075:U:C6	2.55	0.41
30:R1:2131:U:O2'	30:R1:2133:G:H1'	2.21	0.41
30:R1:2660:A:H2'	30:R1:2661:G:C8	2.56	0.41
31:R2:32:U:C4	31:R2:33:G:N7	2.89	0.41
32:R3:109:A:H5'	32:R3:110:C:C5	2.56	0.41
32:R3:206:C:C4	32:R3:207:C:H1'	2.56	0.41
32:R3:333:U:H2'	32:R3:334:C:C6	2.56	0.41
32:R3:459:A:H2'	32:R3:460:A:C5	2.56	0.41
32:R3:842:U:H3'	32:R3:843:U:O4'	2.21	0.41
32:R3:859:G:H2'	32:R3:860:A:C8	2.54	0.41
32:R3:903:G:H2'	32:R3:904:U:C6	2.56	0.41
32:R3:918:A:H2'	32:R3:919:A:C8	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:R3:953:G:C6	32:R3:1229:A:C6	3.09	0.41
54:U:321:GLU:CG	54:U:377:HIS:HB3	2.51	0.41
54:U:386:TYR:O	54:U:454:LEU:HD21	2.21	0.41
3:15:107:PHE:HB3	3:15:126:ARG:HH12	1.86	0.41
3:15:111:ILE:HD12	30:R1:627:A:C5	2.55	0.41
5:17:72:ASP:OD1	5:17:73:ASN:N	2.54	0.41
9:20:80:ASN:ND2	30:R1:1151:A:H4'	2.36	0.41
21:32:54:ILE:HD12	21:32:54:ILE:HA	1.92	0.41
30:R1:716:A:H2'	30:R1:717:C:O4'	2.21	0.41
30:R1:1853:A:N3	30:R1:2233:U:O2'	2.43	0.41
30:R1:2120:G:H2'	30:R1:2121:G:C8	2.56	0.41
31:R2:20:G:H2'	31:R2:21:G:H8	1.86	0.41
32:R3:116:A:N1	32:R3:313:A:O2'	2.44	0.41
32:R3:463:U:H2'	32:R3:464:U:C6	2.56	0.41
32:R3:516:U:H5''	32:R3:517:G:OP2	2.21	0.41
32:R3:849:G:N3	32:R3:850:U:H1'	2.36	0.41
32:R3:1039:G:H3'	32:R3:1040:U:C6	2.55	0.41
54:U:38:ASN:OD1	54:U:444:GLY:HA3	2.20	0.41
54:U:416:LYS:C	54:U:418:ARG:HE	2.25	0.41
54:U:537:LYS:HE2	54:U:537:LYS:HB2	1.85	0.41
8:2:161:VAL:HG11	8:2:173:LEU:HD23	2.02	0.40
18:3:115:GLY:HA3	18:3:167:ASN:HB2	2.02	0.40
21:32:7:PRO:HD2	30:R1:1263:U:O2'	2.20	0.40
27:5:63:LYS:HA	27:5:64:PRO:HD3	1.98	0.40
28:6:153:PRO:HG3	28:6:162:ARG:HB3	2.03	0.40
30:R1:576:U:H2'	30:R1:577:G:C8	2.56	0.40
30:R1:754:U:H2'	30:R1:755:U:H6	1.86	0.40
30:R1:2303:G:C6	30:R1:2314:A:C6	3.09	0.40
30:R1:2533:U:H2'	30:R1:2534:A:O4'	2.21	0.40
31:R2:61:G:H2'	31:R2:62:C:C6	2.56	0.40
31:R2:95:U:H2'	31:R2:96:G:H8	1.85	0.40
32:R3:451:A:H1'	32:R3:452:A:C2	2.56	0.40
32:R3:1009:U:H2'	32:R3:1010:U:H6	1.86	0.40
32:R3:1103:C:HO2'	32:R3:1104:G:H8	1.69	0.40
54:U:167:LEU:HD23	54:U:167:LEU:O	2.21	0.40
54:U:347:LYS:HG3	54:U:490:VAL:HB	2.01	0.40
54:U:400:VAL:HG23	54:U:436:THR:O	2.21	0.40
8:2:259:ASN:ND2	8:2:262:THR:OG1	2.37	0.40
17:29:14:LEU:HD23	17:29:14:LEU:O	2.21	0.40
22:33:39:ASP:O	22:33:43:ARG:N	2.53	0.40
23:34:26:ASN:CG	30:R1:682:G:H5'	2.42	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:4:97:ASN:HB2	26:4:100:MET:HG3	2.03	0.40
28:6:83:THR:HG23	28:6:133:LYS:HG3	2.03	0.40
30:R1:349:U:H2'	30:R1:350:G:C8	2.56	0.40
30:R1:418:C:H2'	30:R1:419:U:O4'	2.21	0.40
30:R1:1036:G:C6	30:R1:1120:G:C6	3.09	0.40
30:R1:1063:G:H22	30:R1:1075:C:H2'	1.86	0.40
30:R1:1482:G:C2	30:R1:1508:A:N7	2.89	0.40
30:R1:2130:U:H2'	30:R1:2131:U:N1	2.36	0.40
30:R1:2737:G:H2'	30:R1:2738:A:C8	2.56	0.40
32:R3:412:A:C8	32:R3:414:A:H5'	2.56	0.40
32:R3:443:C:H2'	32:R3:444:G:H8	1.85	0.40
54:U:349:ALA:HB2	54:U:504:VAL:HG21	2.03	0.40
54:U:520:VAL:O	54:U:529:GLN:NE2	2.54	0.40
55:1:150:ALA:O	55:1:154:LYS:N	2.43	0.40
5:17:74:GLU:HG3	30:R1:1453:A:N1	2.36	0.40
8:2:29:PHE:CE2	8:2:31:PRO:HD2	2.57	0.40
8:2:181:ARG:HD2	30:R1:1799:G:O2'	2.21	0.40
17:29:56:LEU:HA	17:29:59:GLU:HG2	2.03	0.40
19:30:11:SER:CB	30:R1:988:A:H5''	2.47	0.40
29:9:100:ALA:O	29:9:104:THR:OG1	2.24	0.40
30:R1:284:U:O2	30:R1:356:G:C2	2.74	0.40
30:R1:538:A:H2'	30:R1:539:G:O4'	2.22	0.40
30:R1:579:G:H2'	30:R1:580:U:C6	2.56	0.40
30:R1:1419:A:C8	30:R1:1579:A:N6	2.90	0.40
30:R1:1434:A:H2'	30:R1:1435:G:H8	1.87	0.40
30:R1:2106:U:H2'	30:R1:2107:G:H8	1.85	0.40
30:R1:2114:A:C8	30:R1:2114:A:OP2	2.75	0.40
30:R1:2115:G:C8	30:R1:2117:A:N6	2.89	0.40
30:R1:2698:U:O2'	30:R1:2699:C:H5'	2.21	0.40
32:R3:115:G:O2'	32:R3:289:G:H5'	2.21	0.40
32:R3:1125:U:O2'	32:R3:1126:U:OP1	2.30	0.40
54:U:466:GLN:HE21	54:U:495:HIS:HD2	1.69	0.40
5:17:107:ASN:ND2	5:17:107:ASN:O	2.54	0.40
10:21:49:ILE:HB	10:21:51:VAL:O	2.22	0.40
20:31:31:ASP:CG	20:31:32:LEU:H	2.24	0.40
27:5:116:LEU:HB2	27:5:175:PRO:O	2.21	0.40
29:9:100:ALA:HB2	29:9:112:LYS:HB3	2.03	0.40
30:R1:152:A:N1	30:R1:173:A:N1	2.69	0.40
30:R1:901:C:H2'	30:R1:902:C:C6	2.57	0.40
30:R1:1047:G:N2	30:R1:1110:G:H21	2.16	0.40
30:R1:2455:G:H2'	30:R1:2456:C:C6	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:R1:2846:G:H2'	30:R1:2847:U:H6	1.85	0.40
30:R1:2895:G:H2'	30:R1:2896:C:C6	2.56	0.40
32:R3:321:A:H2'	32:R3:322:C:H5'	2.04	0.40
32:R3:410:G:C2'	32:R3:432:A:H61	2.35	0.40
32:R3:501:C:H1'	32:R3:549:C:O2'	2.22	0.40
32:R3:560:A:H5''	32:R3:561:U:H3'	2.04	0.40
32:R3:665:A:H1'	32:R3:733:G:H5'	2.04	0.40
54:U:6:MET:O	54:U:23:GLU:HA	2.22	0.40
4:16:57:VAL:HG12	4:16:112:LEU:HD22	2.02	0.40
7:19:51:ASN:O	30:R1:2845:U:H5''	2.22	0.40
7:19:105:LYS:HB3	7:19:108:ARG:NH1	2.37	0.40
8:2:255:LYS:HE2	8:2:269:ARG:CZ	2.51	0.40
11:22:38:TYR:CE2	21:32:27:LEU:HD21	2.57	0.40
18:3:4:LEU:CD2	18:3:29:VAL:HG11	2.51	0.40
20:31:13:THR:OG1	20:31:31:ASP:OD1	2.38	0.40
23:34:42:LEU:HD23	23:34:42:LEU:HA	1.84	0.40
27:5:39:VAL:HG11	27:5:49:LEU:HD13	2.03	0.40
30:R1:170:U:H2'	30:R1:171:U:H6	1.86	0.40
30:R1:1283:G:N2	30:R1:1285:A:H3'	2.36	0.40
30:R1:1775:U:O4	30:R1:1789:A:H2	2.05	0.40
30:R1:2136:G:C6	30:R1:2156:G:C2	3.09	0.40
30:R1:2174:C:N4	30:R1:2175:C:O2	2.55	0.40
30:R1:2345:G:N3	30:R1:2381:A:H2'	2.37	0.40
32:R3:151:A:C5	32:R3:152:A:C8	3.09	0.40
32:R3:246:A:O3'	32:R3:247:G:H4'	2.22	0.40
32:R3:449:G:H2'	32:R3:450:G:C8	2.57	0.40
32:R3:539:A:H3'	32:R3:540:G:H8	1.85	0.40
32:R3:620:C:H2'	32:R3:621:A:O4'	2.22	0.40
32:R3:672:U:O2'	32:R3:673:A:OP1	2.36	0.40
32:R3:1029:U:H4'	32:R3:1030:U:C5	2.57	0.40
32:R3:1270:G:HO2'	32:R3:1271:A:P	2.42	0.40
54:U:70:ARG:HB2	54:U:179:LEU:HB2	2.04	0.40
55:1:26:ALA:HA	55:1:29:LEU:HB3	2.03	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	13	140/142 (99%)	139 (99%)	1 (1%)	0	100	100
2	14	120/122 (98%)	111 (92%)	9 (8%)	0	100	100
3	15	142/144 (99%)	126 (89%)	16 (11%)	0	100	100
4	16	134/136 (98%)	124 (92%)	10 (8%)	0	100	100
5	17	118/120 (98%)	108 (92%)	10 (8%)	0	100	100
6	18	114/116 (98%)	106 (93%)	8 (7%)	0	100	100
7	19	112/114 (98%)	101 (90%)	11 (10%)	0	100	100
8	2	269/271 (99%)	247 (92%)	22 (8%)	0	100	100
9	20	115/117 (98%)	113 (98%)	2 (2%)	0	100	100
10	21	101/103 (98%)	91 (90%)	10 (10%)	0	100	100
11	22	108/110 (98%)	96 (89%)	12 (11%)	0	100	100
12	23	91/93 (98%)	78 (86%)	13 (14%)	0	100	100
13	24	100/102 (98%)	88 (88%)	11 (11%)	1 (1%)	13	42
14	25	92/94 (98%)	87 (95%)	5 (5%)	0	100	100
15	27	83/85 (98%)	78 (94%)	5 (6%)	0	100	100
16	28	75/77 (97%)	73 (97%)	2 (3%)	0	100	100
17	29	61/63 (97%)	60 (98%)	1 (2%)	0	100	100
18	3	207/209 (99%)	189 (91%)	18 (9%)	0	100	100
19	30	56/58 (97%)	54 (96%)	2 (4%)	0	100	100
20	31	64/66 (97%)	52 (81%)	12 (19%)	0	100	100
21	32	54/56 (96%)	47 (87%)	7 (13%)	0	100	100
22	33	48/50 (96%)	45 (94%)	3 (6%)	0	100	100
23	34	44/46 (96%)	41 (93%)	2 (4%)	1 (2%)	5	23
24	35	62/64 (97%)	59 (95%)	3 (5%)	0	100	100
25	36	36/38 (95%)	34 (94%)	2 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
26	4	199/201 (99%)	182 (92%)	17 (8%)	0	100	100
27	5	175/177 (99%)	161 (92%)	14 (8%)	0	100	100
28	6	174/176 (99%)	156 (90%)	18 (10%)	0	100	100
29	9	147/149 (99%)	128 (87%)	19 (13%)	0	100	100
33	sb	216/218 (99%)	193 (89%)	22 (10%)	1 (0%)	25	58
34	sc	204/206 (99%)	193 (95%)	11 (5%)	0	100	100
35	sd	203/205 (99%)	177 (87%)	26 (13%)	0	100	100
36	se	155/157 (99%)	129 (83%)	25 (16%)	1 (1%)	22	53
37	sf	98/100 (98%)	85 (87%)	13 (13%)	0	100	100
38	sg	149/151 (99%)	133 (89%)	16 (11%)	0	100	100
39	sh	127/129 (98%)	121 (95%)	6 (5%)	0	100	100
40	si	125/127 (98%)	106 (85%)	19 (15%)	0	100	100
41	sj	96/98 (98%)	85 (88%)	11 (12%)	0	100	100
42	sk	114/116 (98%)	102 (90%)	12 (10%)	0	100	100
43	sl	121/123 (98%)	92 (76%)	29 (24%)	0	100	100
44	sm	112/114 (98%)	97 (87%)	15 (13%)	0	100	100
45	sn	98/100 (98%)	76 (78%)	22 (22%)	0	100	100
46	so	86/88 (98%)	81 (94%)	5 (6%)	0	100	100
47	sp	80/82 (98%)	68 (85%)	12 (15%)	0	100	100
48	sq	78/80 (98%)	66 (85%)	12 (15%)	0	100	100
49	sr	63/65 (97%)	62 (98%)	1 (2%)	0	100	100
50	ss	77/79 (98%)	68 (88%)	9 (12%)	0	100	100
51	st	83/85 (98%)	81 (98%)	2 (2%)	0	100	100
52	su	63/65 (97%)	45 (71%)	17 (27%)	1 (2%)	8	31
54	U	535/537 (100%)	484 (90%)	50 (9%)	1 (0%)	44	74
55	1	218/220 (99%)	189 (87%)	29 (13%)	0	100	100
All	All	6342/6444 (98%)	5707 (90%)	629 (10%)	6 (0%)	50	79

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
13	24	88	ASP
52	su	35	GLU

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Mol	Chain	Res	Type
54	U	275	LYS
36	se	122	VAL
33	sb	18	GLN
23	34	44	VAL

### 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	
1	13	116/116 (100%)	115 (99%)	1 (1%)	75	88
2	14	103/103 (100%)	101 (98%)	2 (2%)	52	75
3	15	103/103 (100%)	101 (98%)	2 (2%)	52	75
4	16	109/109 (100%)	106 (97%)	3 (3%)	38	66
5	17	100/100 (100%)	98 (98%)	2 (2%)	50	74
6	18	86/86 (100%)	85 (99%)	1 (1%)	67	83
7	19	99/99 (100%)	97 (98%)	2 (2%)	50	74
8	2	216/216 (100%)	212 (98%)	4 (2%)	52	75
9	20	89/89 (100%)	89 (100%)	0	100	100
10	21	84/84 (100%)	83 (99%)	1 (1%)	67	83
11	22	93/93 (100%)	89 (96%)	4 (4%)	25	55
12	23	80/80 (100%)	80 (100%)	0	100	100
13	24	83/83 (100%)	78 (94%)	5 (6%)	16	44
14	25	78/78 (100%)	75 (96%)	3 (4%)	28	59
15	27	63/63 (100%)	62 (98%)	1 (2%)	58	79
16	28	67/67 (100%)	63 (94%)	4 (6%)	16	44
17	29	55/55 (100%)	54 (98%)	1 (2%)	54	76
18	3	164/164 (100%)	161 (98%)	3 (2%)	54	76
19	30	48/48 (100%)	47 (98%)	1 (2%)	48	72
20	31	59/59 (100%)	55 (93%)	4 (7%)	13	40

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
21	32	47/47 (100%)	45 (96%)	2 (4%)	25	55
22	33	45/45 (100%)	44 (98%)	1 (2%)	47	71
23	34	38/38 (100%)	38 (100%)	0	100	100
24	35	51/51 (100%)	50 (98%)	1 (2%)	50	74
25	36	34/34 (100%)	33 (97%)	1 (3%)	37	65
26	4	165/165 (100%)	158 (96%)	7 (4%)	25	56
27	5	148/148 (100%)	141 (95%)	7 (5%)	22	52
28	6	137/137 (100%)	133 (97%)	4 (3%)	37	65
29	9	114/114 (100%)	109 (96%)	5 (4%)	24	54
33	sb	180/180 (100%)	170 (94%)	10 (6%)	17	46
34	sc	170/170 (100%)	164 (96%)	6 (4%)	31	61
35	sd	172/172 (100%)	166 (96%)	6 (4%)	31	61
36	se	119/119 (100%)	119 (100%)	0	100	100
37	sf	87/87 (100%)	84 (97%)	3 (3%)	32	62
38	sg	124/124 (100%)	122 (98%)	2 (2%)	58	79
39	sh	104/104 (100%)	95 (91%)	9 (9%)	8	31
40	si	105/105 (100%)	99 (94%)	6 (6%)	17	46
41	sj	86/86 (100%)	85 (99%)	1 (1%)	67	83
42	sk	89/89 (100%)	87 (98%)	2 (2%)	47	71
43	sl	103/103 (100%)	101 (98%)	2 (2%)	52	75
44	sm	92/92 (100%)	89 (97%)	3 (3%)	33	62
45	sn	83/83 (100%)	78 (94%)	5 (6%)	16	44
46	so	76/76 (100%)	73 (96%)	3 (4%)	27	58
47	sp	65/65 (100%)	62 (95%)	3 (5%)	23	52
48	sq	74/74 (100%)	69 (93%)	5 (7%)	13	40
49	sr	56/56 (100%)	53 (95%)	3 (5%)	18	47
50	ss	70/70 (100%)	65 (93%)	5 (7%)	12	39
51	st	65/65 (100%)	63 (97%)	2 (3%)	35	63
52	su	55/55 (100%)	52 (94%)	3 (6%)	18	47
54	U	462/462 (100%)	438 (95%)	24 (5%)	19	48
55	1	106/171 (62%)	103 (97%)	3 (3%)	38	66

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	5217/5282 (99%)	5039 (97%)	178 (3%)	34 62

All (178) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	13	95	ARG
2	14	49	ARG
2	14	54	LYS
3	15	40	SER
3	15	42	SER
4	16	12	MET
4	16	27	SER
4	16	123	LYS
5	17	2	ARG
5	17	14	SER
6	18	48	LEU
7	19	9	GLN
7	19	108	ARG
8	2	83	ASP
8	2	97	ASP
8	2	117	SER
8	2	179	GLU
10	21	39	LEU
11	22	30	SER
11	22	31	GLN
11	22	94	ASP
11	22	110	ARG
13	24	8	ASP
13	24	43	LYS
13	24	45	GLN
13	24	81	ARG
13	24	99	SER
14	25	12	GLN
14	25	43	ASP
14	25	50	MET
15	27	3	HIS
16	28	27	ARG
16	28	41	SER
16	28	49	ARG
16	28	51	SER
17	29	60	LYS
18	3	11	MET

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Mol	Chain	Res	Type
18	3	108	ASP
18	3	200	ASP
19	30	10	ARG
20	31	9	TYR
20	31	30	HIS
20	31	34	LEU
20	31	59	ARG
21	32	33	SER
21	32	51	ARG
22	33	22	THR
24	35	30	HIS
25	36	6	SER
26	4	2	GLU
26	4	79	ARG
26	4	88	ARG
26	4	107	SER
26	4	114	ARG
26	4	191	ASP
26	4	197	GLU
27	5	13	LYS
27	5	36	ASN
27	5	86	CYS
27	5	129	MET
27	5	142	TYR
27	5	160	LYS
27	5	174	PHE
28	6	55	ASP
28	6	68	ARG
28	6	82	PHE
28	6	85	LYS
29	9	11	ASN
29	9	33	GLN
29	9	47	PHE
29	9	75	LEU
29	9	91	PHE
33	sb	22	TRP
33	sb	26	MET
33	sb	38	HIS
33	sb	48	MET
33	sb	76	SER
33	sb	94	ARG
33	sb	104	LYS

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Mol	Chain	Res	Type
33	sb	122	ASP
33	sb	164	ASP
33	sb	166	ASP
34	sc	50	SER
34	sc	61	LYS
34	sc	92	ASP
34	sc	139	ASN
34	sc	153	SER
34	sc	186	SER
35	sd	61	ARG
35	sd	70	GLN
35	sd	80	ARG
35	sd	104	MET
35	sd	127	ARG
35	sd	193	ASP
37	sf	9	MET
37	sf	52	ASN
37	sf	91	ARG
38	sg	19	SER
38	sg	113	LYS
39	sh	1	SER
39	sh	26	MET
39	sh	28	SER
39	sh	46	GLU
39	sh	87	ARG
39	sh	89	ASP
39	sh	93	LYS
39	sh	107	LYS
39	sh	112	ASP
40	si	37	TYR
40	si	61	ASP
40	si	89	TYR
40	si	93	LEU
40	si	105	ARG
40	si	122	ARG
41	sj	63	ASP
42	sk	56	LYS
42	sk	126	ARG
43	sl	75	GLU
43	sl	85	ARG
44	sm	78	ARG
44	sm	106	ARG

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Mol	Chain	Res	Type
44	sm	112	ARG
45	sn	20	PHE
45	sn	38	GLU
45	sn	55	SER
45	sn	57	SER
45	sn	62	ARG
46	so	5	GLU
46	so	60	SER
46	so	77	TYR
47	sp	24	SER
47	sp	35	ARG
47	sp	52	LEU
48	sq	17	GLU
48	sq	44	HIS
48	sq	52	CYS
48	sq	61	ARG
48	sq	76	ARG
49	sr	9	PHE
49	sr	65	SER
49	sr	71	ASP
50	ss	4	LEU
50	ss	6	LYS
50	ss	26	ASP
50	ss	63	ASP
50	ss	77	ARG
51	st	53	MET
51	st	85	LEU
52	su	12	ASP
52	su	18	PHE
52	su	37	TYR
54	U	1	MET
54	U	6	MET
54	U	96	GLU
54	U	110	ASN
54	U	116	ASN
54	U	138	ARG
54	U	169	ARG
54	U	198	PHE
54	U	225	ASP
54	U	254	LEU
54	U	261	ARG
54	U	281	ASN

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Mol	Chain	Res	Type
54	U	286	ARG
54	U	289	LYS
54	U	299	ARG
54	U	317	LYS
54	U	338	PHE
54	U	397	ASP
54	U	403	ASN
54	U	409	GLN
54	U	418	ARG
54	U	423	TYR
54	U	465	ASP
54	U	497	ARG
55	1	37	LYS
55	1	43	ASP
55	1	165	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	13	58	ASN
8	2	238	ASN
10	21	11	GLN
12	23	28	ASN
17	29	58	ASN
26	4	115	GLN
34	sc	184	ASN
35	sd	115	GLN
36	se	121	ASN
45	sn	42	ASN
47	sp	63	GLN
50	ss	55	GLN
51	st	2	ASN
54	U	495	HIS
55	1	188	ASN

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
30	R1	2902/2903 (99%)	621 (21%)	13 (0%)
31	R2	118/119 (99%)	22 (18%)	1 (0%)

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
32	R3	1529/1531 (99%)	433 (28%)	24 (1%)
53	T	75/78 (96%)	18 (24%)	3 (4%)
56	M	8/9 (88%)	0	0
All	All	4632/4640 (99%)	1094 (23%)	41 (0%)

All (1094) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
30	R1	3	U
30	R1	4	U
30	R1	10	A
30	R1	12	U
30	R1	14	A
30	R1	15	G
30	R1	29	U
30	R1	34	U
30	R1	35	G
30	R1	46	G
30	R1	51	G
30	R1	60	G
30	R1	63	A
30	R1	71	A
30	R1	74	A
30	R1	75	G
30	R1	78	U
30	R1	79	C
30	R1	80	G
30	R1	83	A
30	R1	84	A
30	R1	85	G
30	R1	88	G
30	R1	91	A
30	R1	100	U
30	R1	102	U
30	R1	109	C
30	R1	118	A
30	R1	119	A
30	R1	120	U
30	R1	125	A
30	R1	134	G
30	R1	137	U
30	R1	138	U

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Mol	Chain	Res	Type
30	R1	139	U
30	R1	140	C
30	R1	144	A
30	R1	146	A
30	R1	152	A
30	R1	154	U
30	R1	156	A
30	R1	158	U
30	R1	159	G
30	R1	162	U
30	R1	164	C
30	R1	173	A
30	R1	177	G
30	R1	178	G
30	R1	196	A
30	R1	199	A
30	R1	215	G
30	R1	216	A
30	R1	219	A
30	R1	222	A
30	R1	226	A
30	R1	228	C
30	R1	229	C
30	R1	230	G
30	R1	248	G
30	R1	249	C
30	R1	250	G
30	R1	256	A
30	R1	265	A
30	R1	266	G
30	R1	267	C
30	R1	275	C
30	R1	276	U
30	R1	278	A
30	R1	281	C
30	R1	282	A
30	R1	285	G
30	R1	302	C
30	R1	311	A
30	R1	317	G
30	R1	329	G
30	R1	330	A

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Mol	Chain	Res	Type
30	R1	340	A
30	R1	342	A
30	R1	345	A
30	R1	354	A
30	R1	360	U
30	R1	361	G
30	R1	364	C
30	R1	365	U
30	R1	371	A
30	R1	372	G
30	R1	373	U
30	R1	380	G
30	R1	386	G
30	R1	387	U
30	R1	388	G
30	R1	395	U
30	R1	396	G
30	R1	401	A
30	R1	404	A
30	R1	405	U
30	R1	406	G
30	R1	411	G
30	R1	412	A
30	R1	413	C
30	R1	414	C
30	R1	422	A
30	R1	424	G
30	R1	428	A
30	R1	443	A
30	R1	456	C
30	R1	481	G
30	R1	490	C
30	R1	491	G
30	R1	505	A
30	R1	508	A
30	R1	509	C
30	R1	518	G
30	R1	527	C
30	R1	528	A
30	R1	529	A
30	R1	530	G
30	R1	531	C

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Mol	Chain	Res	Type
30	R1	532	A
30	R1	533	G
30	R1	543	G
30	R1	544	C
30	R1	545	U
30	R1	546	U
30	R1	549	G
30	R1	550	C
30	R1	555	G
30	R1	563	A
30	R1	573	U
30	R1	575	A
30	R1	588	U
30	R1	603	A
30	R1	613	A
30	R1	614	A
30	R1	615	U
30	R1	622	G
30	R1	627	A
30	R1	637	A
30	R1	645	C
30	R1	647	G
30	R1	653	U
30	R1	654	A
30	R1	655	A
30	R1	656	G
30	R1	685	A
30	R1	686	U
30	R1	689	A
30	R1	696	G
30	R1	717	C
30	R1	730	A
30	R1	736	C
30	R1	746	U
30	R1	747	U
30	R1	752	A
30	R1	757	G
30	R1	764	A
30	R1	765	C
30	R1	775	G
30	R1	776	G
30	R1	782	A

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Mol	Chain	Res	Type
30	R1	784	G
30	R1	785	G
30	R1	805	G
30	R1	812	C
30	R1	819	A
30	R1	827	U
30	R1	828	U
30	R1	829	A
30	R1	845	A
30	R1	846	U
30	R1	847	U
30	R1	856	G
30	R1	860	U
30	R1	870	U
30	R1	878	A
30	R1	884	U
30	R1	886	A
30	R1	887	U
30	R1	888	C
30	R1	889	C
30	R1	891	G
30	R1	892	A
30	R1	893	C
30	R1	894	U
30	R1	896	A
30	R1	899	A
30	R1	910	A
30	R1	915	C
30	R1	932	U
30	R1	941	A
30	R1	946	C
30	R1	961	C
30	R1	970	U
30	R1	973	A
30	R1	974	G
30	R1	975	A
30	R1	979	A
30	R1	983	A
30	R1	984	A
30	R1	985	C
30	R1	989	G
30	R1	995	C

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Mol	Chain	Res	Type
30	R1	996	A
30	R1	999	U
30	R1	1005	C
30	R1	1012	U
30	R1	1013	C
30	R1	1021	A
30	R1	1025	G
30	R1	1026	G
30	R1	1033	U
30	R1	1040	A
30	R1	1047	G
30	R1	1048	A
30	R1	1051	G
30	R1	1052	C
30	R1	1053	C
30	R1	1055	G
30	R1	1056	G
30	R1	1060	U
30	R1	1061	U
30	R1	1062	G
30	R1	1063	G
30	R1	1064	C
30	R1	1065	U
30	R1	1066	U
30	R1	1067	A
30	R1	1070	A
30	R1	1071	G
30	R1	1072	C
30	R1	1073	A
30	R1	1074	G
30	R1	1075	C
30	R1	1076	C
30	R1	1079	C
30	R1	1083	U
30	R1	1084	A
30	R1	1085	A
30	R1	1087	G
30	R1	1088	A
30	R1	1090	A
30	R1	1095	A
30	R1	1096	A
30	R1	1097	U

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Mol	Chain	Res	Type
30	R1	1098	A
30	R1	1103	A
30	R1	1104	C
30	R1	1105	U
30	R1	1106	G
30	R1	1107	G
30	R1	1109	C
30	R1	1110	G
30	R1	1111	A
30	R1	1115	G
30	R1	1116	G
30	R1	1119	U
30	R1	1128	G
30	R1	1132	U
30	R1	1133	A
30	R1	1135	C
30	R1	1136	G
30	R1	1142	A
30	R1	1169	A
30	R1	1171	G
30	R1	1172	C
30	R1	1173	U
30	R1	1174	U
30	R1	1175	A
30	R1	1176	U
30	R1	1178	C
30	R1	1179	G
30	R1	1180	U
30	R1	1181	U
30	R1	1182	G
30	R1	1186	G
30	R1	1187	G
30	R1	1195	G
30	R1	1200	C
30	R1	1204	A
30	R1	1206	G
30	R1	1212	G
30	R1	1214	A
30	R1	1236	G
30	R1	1247	A
30	R1	1248	G
30	R1	1250	G

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Mol	Chain	Res	Type
30	R1	1253	A
30	R1	1255	U
30	R1	1256	G
30	R1	1271	G
30	R1	1272	A
30	R1	1273	U
30	R1	1300	G
30	R1	1301	A
30	R1	1321	A
30	R1	1329	U
30	R1	1330	C
30	R1	1341	G
30	R1	1345	C
30	R1	1352	U
30	R1	1359	A
30	R1	1365	A
30	R1	1367	A
30	R1	1368	G
30	R1	1379	U
30	R1	1383	A
30	R1	1387	A
30	R1	1395	A
30	R1	1403	A
30	R1	1412	U
30	R1	1416	G
30	R1	1419	A
30	R1	1420	A
30	R1	1428	C
30	R1	1430	G
30	R1	1434	A
30	R1	1452	G
30	R1	1453	A
30	R1	1455	G
30	R1	1459	G
30	R1	1475	G
30	R1	1481	U
30	R1	1482	G
30	R1	1484	U
30	R1	1493	C
30	R1	1494	A
30	R1	1508	A
30	R1	1509	A

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Mol	Chain	Res	Type
30	R1	1515	A
30	R1	1533	C
30	R1	1534	U
30	R1	1535	A
30	R1	1536	C
30	R1	1537	G
30	R1	1542	U
30	R1	1548	A
30	R1	1558	C
30	R1	1566	A
30	R1	1569	A
30	R1	1578	U
30	R1	1584	U
30	R1	1607	C
30	R1	1608	A
30	R1	1610	A
30	R1	1647	U
30	R1	1648	U
30	R1	1649	G
30	R1	1654	A
30	R1	1674	G
30	R1	1675	C
30	R1	1677	A
30	R1	1693	U
30	R1	1703	G
30	R1	1715	G
30	R1	1716	U
30	R1	1724	G
30	R1	1729	U
30	R1	1730	C
30	R1	1731	G
30	R1	1732	C
30	R1	1733	G
30	R1	1735	A
30	R1	1738	G
30	R1	1744	A
30	R1	1756	G
30	R1	1758	U
30	R1	1764	C
30	R1	1773	A
30	R1	1776	G
30	R1	1782	U

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Mol	Chain	Res	Type
30	R1	1787	A
30	R1	1800	C
30	R1	1801	A
30	R1	1802	A
30	R1	1808	A
30	R1	1811	G
30	R1	1816	C
30	R1	1829	A
30	R1	1838	C
30	R1	1848	A
30	R1	1868	C
30	R1	1869	G
30	R1	1870	C
30	R1	1872	A
30	R1	1873	G
30	R1	1884	G
30	R1	1891	G
30	R1	1900	A
30	R1	1905	C
30	R1	1906	G
30	R1	1913	A
30	R1	1914	C
30	R1	1915	U
30	R1	1916	A
30	R1	1919	A
30	R1	1929	G
30	R1	1930	G
30	R1	1937	A
30	R1	1938	A
30	R1	1941	C
30	R1	1955	U
30	R1	1966	A
30	R1	1967	C
30	R1	1970	A
30	R1	1971	U
30	R1	1972	G
30	R1	1991	U
30	R1	1997	C
30	R1	2006	C
30	R1	2020	A
30	R1	2022	U
30	R1	2023	C

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Mol	Chain	Res	Type
30	R1	2031	A
30	R1	2033	A
30	R1	2036	C
30	R1	2043	C
30	R1	2052	A
30	R1	2055	C
30	R1	2056	G
30	R1	2059	A
30	R1	2060	A
30	R1	2061	G
30	R1	2062	A
30	R1	2069	G
30	R1	2080	A
30	R1	2093	G
30	R1	2096	C
30	R1	2098	U
30	R1	2099	U
30	R1	2103	C
30	R1	2104	C
30	R1	2106	U
30	R1	2107	G
30	R1	2109	U
30	R1	2110	G
30	R1	2111	U
30	R1	2113	U
30	R1	2114	A
30	R1	2115	G
30	R1	2116	G
30	R1	2117	A
30	R1	2118	U
30	R1	2119	A
30	R1	2120	G
30	R1	2123	G
30	R1	2124	G
30	R1	2126	A
30	R1	2127	G
30	R1	2128	G
30	R1	2131	U
30	R1	2132	U
30	R1	2133	G
30	R1	2135	A
30	R1	2136	G

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Mol	Chain	Res	Type
30	R1	2138	G
30	R1	2140	G
30	R1	2141	G
30	R1	2145	C
30	R1	2147	A
30	R1	2148	G
30	R1	2149	U
30	R1	2150	C
30	R1	2151	U
30	R1	2152	G
30	R1	2153	C
30	R1	2157	G
30	R1	2159	G
30	R1	2163	A
30	R1	2164	C
30	R1	2165	C
30	R1	2167	U
30	R1	2168	G
30	R1	2169	A
30	R1	2172	U
30	R1	2173	A
30	R1	2174	C
30	R1	2175	C
30	R1	2177	C
30	R1	2178	C
30	R1	2179	C
30	R1	2180	U
30	R1	2182	U
30	R1	2186	G
30	R1	2188	U
30	R1	2189	U
30	R1	2190	G
30	R1	2192	U
30	R1	2198	A
30	R1	2203	U
30	R1	2204	G
30	R1	2211	A
30	R1	2213	U
30	R1	2214	C
30	R1	2225	A
30	R1	2226	C
30	R1	2238	G

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Mol	Chain	Res	Type
30	R1	2239	G
30	R1	2250	G
30	R1	2279	G
30	R1	2283	C
30	R1	2287	A
30	R1	2288	A
30	R1	2291	U
30	R1	2292	U
30	R1	2297	A
30	R1	2305	U
30	R1	2316	G
30	R1	2319	G
30	R1	2322	A
30	R1	2325	G
30	R1	2326	C
30	R1	2331	G
30	R1	2333	A
30	R1	2334	U
30	R1	2335	A
30	R1	2345	G
30	R1	2347	C
30	R1	2350	C
30	R1	2359	C
30	R1	2361	G
30	R1	2383	G
30	R1	2385	C
30	R1	2391	G
30	R1	2402	U
30	R1	2406	A
30	R1	2419	U
30	R1	2423	U
30	R1	2424	C
30	R1	2429	G
30	R1	2430	A
30	R1	2434	A
30	R1	2435	A
30	R1	2439	A
30	R1	2441	U
30	R1	2448	A
30	R1	2459	A
30	R1	2470	G
30	R1	2474	U

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Mol	Chain	Res	Type
30	R1	2476	A
30	R1	2484	G
30	R1	2491	U
30	R1	2498	C
30	R1	2499	C
30	R1	2500	U
30	R1	2502	G
30	R1	2503	A
30	R1	2505	G
30	R1	2506	U
30	R1	2508	G
30	R1	2518	A
30	R1	2520	C
30	R1	2529	G
30	R1	2547	A
30	R1	2554	U
30	R1	2560	A
30	R1	2562	U
30	R1	2563	U
30	R1	2564	A
30	R1	2566	A
30	R1	2567	G
30	R1	2572	A
30	R1	2573	C
30	R1	2585	U
30	R1	2586	U
30	R1	2602	A
30	R1	2609	U
30	R1	2613	U
30	R1	2615	U
30	R1	2629	U
30	R1	2630	G
30	R1	2650	U
30	R1	2654	A
30	R1	2660	A
30	R1	2662	A
30	R1	2663	G
30	R1	2664	G
30	R1	2669	G
30	R1	2671	G
30	R1	2682	A
30	R1	2689	U

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Mol	Chain	Res	Type
30	R1	2690	U
30	R1	2700	A
30	R1	2707	U
30	R1	2713	U
30	R1	2714	G
30	R1	2716	C
30	R1	2726	A
30	R1	2727	A
30	R1	2733	A
30	R1	2738	A
30	R1	2744	G
30	R1	2748	A
30	R1	2757	A
30	R1	2760	C
30	R1	2761	A
30	R1	2774	C
30	R1	2775	G
30	R1	2778	A
30	R1	2779	U
30	R1	2794	C
30	R1	2796	U
30	R1	2797	U
30	R1	2798	U
30	R1	2800	A
30	R1	2803	G
30	R1	2815	C
30	R1	2816	G
30	R1	2817	U
30	R1	2818	U
30	R1	2820	A
30	R1	2835	A
30	R1	2837	A
30	R1	2840	C
30	R1	2859	G
30	R1	2861	U
30	R1	2867	G
30	R1	2873	A
30	R1	2879	A
30	R1	2880	C
30	R1	2884	U
30	R1	2897	U
31	R2	9	G

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Mol	Chain	Res	Type
31	R2	12	C
31	R2	13	G
31	R2	24	G
31	R2	35	C
31	R2	41	G
31	R2	42	C
31	R2	44	G
31	R2	45	A
31	R2	53	A
31	R2	56	G
31	R2	62	C
31	R2	67	G
31	R2	87	U
31	R2	88	C
31	R2	89	U
31	R2	90	C
31	R2	107	G
31	R2	108	A
31	R2	109	A
31	R2	118	C
31	R2	119	A
32	R3	4	U
32	R3	5	U
32	R3	9	G
32	R3	22	G
32	R3	30	U
32	R3	31	G
32	R3	32	A
32	R3	39	G
32	R3	47	C
32	R3	48	C
32	R3	49	U
32	R3	50	A
32	R3	51	A
32	R3	60	A
32	R3	61	G
32	R3	62	U
32	R3	63	C
32	R3	64	G
32	R3	65	A
32	R3	66	A
32	R3	70	U

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Mol	Chain	Res	Type
32	R3	71	A
32	R3	72	A
32	R3	74	A
32	R3	77	A
32	R3	79	G
32	R3	80	A
32	R3	81	A
32	R3	82	G
32	R3	83	C
32	R3	84	U
32	R3	85	U
32	R3	86	G
32	R3	91	U
32	R3	92	U
32	R3	94	G
32	R3	95	C
32	R3	96	U
32	R3	114	U
32	R3	115	G
32	R3	116	A
32	R3	118	U
32	R3	121	U
32	R3	122	G
32	R3	129	A
32	R3	130	A
32	R3	131	A
32	R3	139	A
32	R3	140	U
32	R3	141	G
32	R3	142	G
32	R3	145	G
32	R3	161	A
32	R3	164	G
32	R3	165	G
32	R3	170	U
32	R3	173	U
32	R3	174	A
32	R3	179	A
32	R3	181	A
32	R3	182	A
32	R3	183	C
32	R3	184	G

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Mol	Chain	Res	Type
32	R3	190	A
32	R3	191	G
32	R3	192	A
32	R3	197	A
32	R3	202	G
32	R3	204	G
32	R3	205	A
32	R3	206	C
32	R3	207	C
32	R3	208	U
32	R3	209	U
32	R3	210	C
32	R3	213	G
32	R3	215	C
32	R3	216	U
32	R3	219	U
32	R3	224	U
32	R3	226	G
32	R3	240	G
32	R3	247	G
32	R3	248	C
32	R3	251	G
32	R3	266	G
32	R3	267	C
32	R3	270	A
32	R3	272	C
32	R3	273	U
32	R3	274	A
32	R3	279	A
32	R3	280	C
32	R3	283	U
32	R3	287	U
32	R3	289	G
32	R3	290	C
32	R3	292	G
32	R3	293	G
32	R3	302	G
32	R3	306	A
32	R3	313	A
32	R3	316	C
32	R3	319	G
32	R3	322	C

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Mol	Chain	Res	Type
32	R3	323	U
32	R3	324	G
32	R3	327	A
32	R3	328	C
32	R3	329	A
32	R3	331	G
32	R3	332	G
32	R3	333	U
32	R3	334	C
32	R3	338	A
32	R3	339	C
32	R3	344	A
32	R3	345	C
32	R3	346	G
32	R3	347	G
32	R3	351	G
32	R3	352	C
32	R3	353	A
32	R3	354	G
32	R3	360	G
32	R3	363	A
32	R3	364	A
32	R3	367	U
32	R3	369	G
32	R3	370	C
32	R3	372	C
32	R3	376	G
32	R3	378	G
32	R3	381	C
32	R3	388	G
32	R3	389	A
32	R3	391	G
32	R3	392	C
32	R3	396	C
32	R3	403	C
32	R3	406	G
32	R3	411	A
32	R3	412	A
32	R3	413	G
32	R3	415	A
32	R3	416	G
32	R3	418	C

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Mol	Chain	Res	Type
32	R3	419	C
32	R3	421	U
32	R3	422	C
32	R3	423	G
32	R3	425	G
32	R3	426	U
32	R3	429	U
32	R3	435	A
32	R3	437	U
32	R3	438	U
32	R3	439	U
32	R3	441	A
32	R3	446	G
32	R3	451	A
32	R3	454	G
32	R3	458	U
32	R3	460	A
32	R3	462	G
32	R3	463	U
32	R3	464	U
32	R3	465	A
32	R3	466	A
32	R3	467	U
32	R3	469	C
32	R3	472	U
32	R3	473	U
32	R3	475	C
32	R3	476	U
32	R3	484	G
32	R3	488	C
32	R3	492	C
32	R3	493	A
32	R3	494	G
32	R3	495	A
32	R3	496	A
32	R3	497	G
32	R3	498	A
32	R3	501	C
32	R3	509	A
32	R3	511	C
32	R3	516	U
32	R3	518	C

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Mol	Chain	Res	Type
32	R3	521	G
32	R3	524	G
32	R3	530	G
32	R3	531	U
32	R3	532	A
32	R3	539	A
32	R3	540	G
32	R3	541	G
32	R3	542	G
32	R3	544	G
32	R3	545	C
32	R3	547	A
32	R3	551	U
32	R3	562	U
32	R3	564	C
32	R3	572	A
32	R3	573	A
32	R3	576	C
32	R3	577	G
32	R3	579	A
32	R3	589	U
32	R3	596	A
32	R3	597	G
32	R3	601	G
32	R3	607	A
32	R3	610	U
32	R3	613	C
32	R3	615	G
32	R3	618	C
32	R3	630	A
32	R3	633	G
32	R3	638	U
32	R3	640	A
32	R3	642	A
32	R3	653	U
32	R3	664	G
32	R3	665	A
32	R3	673	A
32	R3	686	U
32	R3	688	G
32	R3	694	A
32	R3	702	A

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Mol	Chain	Res	Type
32	R3	703	G
32	R3	723	U
32	R3	731	G
32	R3	734	G
32	R3	738	C
32	R3	739	C
32	R3	743	A
32	R3	748	G
32	R3	754	C
32	R3	755	G
32	R3	774	G
32	R3	777	A
32	R3	779	C
32	R3	781	A
32	R3	791	G
32	R3	792	A
32	R3	793	U
32	R3	794	A
32	R3	810	C
32	R3	815	A
32	R3	817	C
32	R3	824	G
32	R3	829	G
32	R3	832	G
32	R3	836	G
32	R3	838	G
32	R3	839	C
32	R3	840	C
32	R3	842	U
32	R3	843	U
32	R3	844	G
32	R3	845	A
32	R3	846	G
32	R3	847	G
32	R3	849	G
32	R3	850	U
32	R3	863	U
32	R3	864	A
32	R3	867	G
32	R3	870	U
32	R3	871	U
32	R3	872	A

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Mol	Chain	Res	Type
32	R3	884	U
32	R3	889	A
32	R3	902	G
32	R3	914	A
32	R3	929	G
32	R3	933	G
32	R3	934	C
32	R3	935	A
32	R3	956	U
32	R3	959	A
32	R3	960	U
32	R3	961	U
32	R3	966	G
32	R3	968	A
32	R3	969	A
32	R3	972	C
32	R3	975	A
32	R3	976	G
32	R3	977	A
32	R3	989	U
32	R3	991	U
32	R3	992	U
32	R3	993	G
32	R3	994	A
32	R3	999	C
32	R3	1000	A
32	R3	1001	C
32	R3	1002	G
32	R3	1003	G
32	R3	1004	A
32	R3	1005	A
32	R3	1006	G
32	R3	1007	U
32	R3	1008	U
32	R3	1009	U
32	R3	1021	A
32	R3	1024	G
32	R3	1026	G
32	R3	1027	C
32	R3	1028	C
32	R3	1029	U
32	R3	1031	C

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Mol	Chain	Res	Type
32	R3	1033	G
32	R3	1036	A
32	R3	1038	C
32	R3	1039	G
32	R3	1040	U
32	R3	1041	G
32	R3	1044	A
32	R3	1045	C
32	R3	1049	U
32	R3	1050	G
32	R3	1052	U
32	R3	1065	U
32	R3	1084	G
32	R3	1085	U
32	R3	1086	U
32	R3	1094	G
32	R3	1095	U
32	R3	1099	G
32	R3	1101	A
32	R3	1103	C
32	R3	1104	G
32	R3	1118	U
32	R3	1119	C
32	R3	1121	U
32	R3	1123	U
32	R3	1124	G
32	R3	1125	U
32	R3	1126	U
32	R3	1130	A
32	R3	1131	G
32	R3	1133	G
32	R3	1134	G
32	R3	1136	C
32	R3	1137	C
32	R3	1138	G
32	R3	1139	G
32	R3	1142	G
32	R3	1149	C
32	R3	1150	A
32	R3	1151	A
32	R3	1152	A
32	R3	1158	C

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Mol	Chain	Res	Type
32	R3	1159	U
32	R3	1169	A
32	R3	1181	G
32	R3	1182	G
32	R3	1184	G
32	R3	1187	G
32	R3	1196	A
32	R3	1199	U
32	R3	1201	A
32	R3	1203	C
32	R3	1208	C
32	R3	1209	C
32	R3	1212	U
32	R3	1213	A
32	R3	1214	C
32	R3	1227	A
32	R3	1228	C
32	R3	1236	A
32	R3	1237	C
32	R3	1238	A
32	R3	1244	G
32	R3	1246	A
32	R3	1256	A
32	R3	1257	A
32	R3	1258	G
32	R3	1261	A
32	R3	1262	C
32	R3	1268	G
32	R3	1271	A
32	R3	1275	A
32	R3	1280	A
32	R3	1285	A
32	R3	1286	U
32	R3	1287	A
32	R3	1298	U
32	R3	1300	G
32	R3	1302	C
32	R3	1305	G
32	R3	1306	A
32	R3	1308	U
32	R3	1311	A
32	R3	1312	G

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Mol	Chain	Res	Type
32	R3	1315	U
32	R3	1320	C
32	R3	1322	C
32	R3	1323	G
32	R3	1332	A
32	R3	1333	A
32	R3	1336	C
32	R3	1346	A
32	R3	1353	G
32	R3	1363	A
32	R3	1364	U
32	R3	1370	G
32	R3	1379	G
32	R3	1381	U
32	R3	1389	C
32	R3	1419	G
32	R3	1432	G
32	R3	1441	A
32	R3	1442	G
32	R3	1446	A
32	R3	1451	U
32	R3	1452	C
32	R3	1472	U
32	R3	1475	G
32	R3	1493	A
32	R3	1494	G
32	R3	1497	G
32	R3	1499	A
32	R3	1502	A
32	R3	1503	A
32	R3	1506	U
32	R3	1517	G
32	R3	1529	G
32	R3	1530	G
53	T	3	G
53	T	8	4SU
53	T	9	G
53	T	15	C
53	T	16	C
53	T	17	U
53	T	18	G
53	T	19	G

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Mol	Chain	Res	Type
53	T	20	H2U
53	T	21	A
53	T	22	G
53	T	47	U
53	T	48	C
53	T	54	5MU
53	T	55	PSU
53	T	56	C
53	T	65	C
53	T	76	A

All (41) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
30	R1	225	C
30	R1	360	U
30	R1	784	G
30	R1	859	G
30	R1	1020	A
30	R1	1050	A
30	R1	1715	G
30	R1	1847	G
30	R1	2105	U
30	R1	2189	U
30	R1	2663	G
30	R1	2839	G
30	R1	2896	C
31	R2	52	A
32	R3	120	A
32	R3	288	A
32	R3	301	G
32	R3	312	C
32	R3	363	A
32	R3	428	G
32	R3	453	G
32	R3	461	A
32	R3	497	G
32	R3	500	G
32	R3	561	U
32	R3	588	G
32	R3	612	C
32	R3	672	U

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Mol	Chain	Res	Type
32	R3	753	A
32	R3	837	U
32	R3	870	U
32	R3	1038	C
32	R3	1124	G
32	R3	1125	U
32	R3	1149	C
32	R3	1270	G
32	R3	1297	G
32	R3	1305	G
53	T	8	4SU
53	T	17	U
53	T	55	PSU

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

6 non-standard protein/DNA/RNA residues are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
53	5MU	T	54	53	19,22,23	2.72	8 (42%)	27,32,35	2.26	8 (29%)
53	PSU	T	55	53	18,21,22	2.20	9 (50%)	21,30,33	1.87	4 (19%)
53	H2U	T	20	53	18,21,22	4.33	5 (27%)	19,30,33	4.14	6 (31%)
53	4SU	T	8	53	18,21,22	3.99	7 (38%)	25,30,33	2.34	6 (24%)
53	FME	T	101	53	8,9,10	0.95	0	8,9,11	1.20	1 (12%)
53	4OC	T	32	53	20,23,24	2.38	4 (20%)	25,32,35	2.02	5 (20%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
53	5MU	T	54	53	1/1/5/5	3/7/25/26	0/2/2/2
53	PSU	T	55	53	1/1/5/5	1/7/25/26	0/2/2/2
53	H2U	T	20	53	2/2/8/9	5/7/38/39	0/2/2/2
53	4SU	T	8	53	2/2/5/5	3/7/25/26	0/2/2/2
53	FME	T	101	53	-	2/7/9/11	-
53	4OC	T	32	53	1/1/5/6	4/9/29/30	0/2/2/2

All (33) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
53	T	8	4SU	O2-C2	11.92	1.44	1.23
53	T	20	H2U	O4-C4	10.47	1.44	1.23
53	T	8	4SU	C4-S4	9.53	1.85	1.68
53	T	54	5MU	O4-C4	-9.24	1.06	1.23
53	T	20	H2U	C2-N1	9.14	1.48	1.35
53	T	20	H2U	O2-C2	7.77	1.36	1.23
53	T	32	4OC	O2-C2	7.19	1.37	1.23
53	T	20	H2U	C2-N3	7.17	1.50	1.38
53	T	32	4OC	C4-N4	5.64	1.47	1.36
53	T	20	H2U	C4-N3	5.41	1.46	1.37
53	T	8	4SU	C4-N3	-4.57	1.32	1.37
53	T	55	PSU	C2-N1	-3.96	1.31	1.36
53	T	54	5MU	C2-N1	-3.43	1.33	1.38
53	T	55	PSU	C4-N3	-3.42	1.32	1.38
53	T	55	PSU	C2-N3	-3.35	1.32	1.37
53	T	8	4SU	C2-N1	-3.28	1.33	1.38
53	T	55	PSU	C6-C5	3.18	1.38	1.35
53	T	32	4OC	C2-N1	-3.16	1.33	1.40
53	T	54	5MU	C4-C5	-3.00	1.39	1.44
53	T	55	PSU	O4'-C1'	-2.83	1.39	1.43
53	T	55	PSU	C6-N1	-2.73	1.31	1.36
53	T	54	5MU	C2-N3	-2.66	1.33	1.38
53	T	54	5MU	C6-C5	2.66	1.38	1.34
53	T	32	4OC	C6-N1	-2.66	1.31	1.38
53	T	8	4SU	C2-N3	-2.60	1.33	1.38
53	T	54	5MU	C4-N3	-2.52	1.34	1.38
53	T	55	PSU	C1'-C5	2.51	1.55	1.50
53	T	55	PSU	O4-C4	-2.48	1.18	1.23
53	T	54	5MU	C5M-C5	2.41	1.56	1.50
53	T	8	4SU	C5-C4	-2.41	1.39	1.42
53	T	55	PSU	O2-C2	-2.27	1.18	1.23
53	T	8	4SU	C6-C5	2.23	1.40	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
53	T	54	5MU	C6-N1	-2.18	1.34	1.38

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
53	T	20	H2U	O2-C2-N1	-11.63	109.12	123.10
53	T	20	H2U	O4-C4-N3	-7.68	108.45	120.30
53	T	8	4SU	C4-N3-C2	-6.65	120.94	127.31
53	T	20	H2U	O4-C4-C5	-6.62	108.65	122.20
53	T	20	H2U	O2-C2-N3	-6.23	110.00	121.49
53	T	20	H2U	N3-C2-N1	-5.97	110.65	116.65
53	T	8	4SU	N3-C2-N1	5.62	122.21	114.89
53	T	32	4OC	C1'-N1-C2	5.38	130.33	118.44
53	T	54	5MU	N3-C2-N1	5.37	121.89	114.89
53	T	54	5MU	C4-N3-C2	-5.26	120.44	127.34
53	T	55	PSU	N1-C2-N3	4.98	120.42	115.17
53	T	54	5MU	O4-C4-C5	-4.47	119.80	124.92
53	T	54	5MU	C5-C4-N3	4.47	119.21	115.32
53	T	32	4OC	O2-C2-N3	-4.46	115.30	122.33
53	T	8	4SU	C5-C4-N3	4.42	118.86	114.75
53	T	32	4OC	C1'-N1-C6	-4.10	112.01	120.78
53	T	55	PSU	C4-N3-C2	-3.92	120.98	126.37
53	T	54	5MU	C5-C6-N1	-3.76	119.23	123.31
53	T	55	PSU	O2-C2-N1	-3.54	119.14	122.79
53	T	32	4OC	C5-C4-N3	-3.23	117.55	122.60
53	T	8	4SU	C5-C4-S4	-3.21	120.64	124.31
53	T	20	H2U	C5-C4-N3	-3.12	113.37	116.69
53	T	54	5MU	O2-C2-N1	-3.06	118.82	122.80
53	T	8	4SU	C1'-N1-C2	3.04	123.05	117.59
53	T	55	PSU	C6-C5-C4	-2.56	116.44	118.17
53	T	8	4SU	O2-C2-N1	-2.54	119.49	122.80
53	T	54	5MU	C5M-C5-C4	2.48	121.43	118.78
53	T	101	FME	CA-N-CN	2.30	126.35	122.82
53	T	54	5MU	C5M-C5-C6	-2.13	119.97	122.85
53	T	32	4OC	N1-C2-N3	2.10	122.44	118.80

All (7) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
53	T	8	4SU	C3'
53	T	8	4SU	C2'
53	T	20	H2U	C1'

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Mol	Chain	Res	Type	Atom
53	T	20	H2U	C2'
53	T	32	4OC	C2'
53	T	54	5MU	C4'
53	T	55	PSU	C4'

All (18) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
53	T	20	H2U	O4'-C4'-C5'-O5'
53	T	20	H2U	O4'-C1'-N1-C6
53	T	20	H2U	C2'-C1'-N1-C2
53	T	54	5MU	C4'-C5'-O5'-P
53	T	101	FME	CB-CA-N-CN
53	T	32	4OC	O4'-C4'-C5'-O5'
53	T	55	PSU	C4'-C5'-O5'-P
53	T	20	H2U	C3'-C4'-C5'-O5'
53	T	101	FME	CB-CG-SD-CE
53	T	32	4OC	C3'-C4'-C5'-O5'
53	T	20	H2U	O4'-C1'-N1-C2
53	T	54	5MU	O4'-C4'-C5'-O5'
53	T	32	4OC	C2'-C1'-N1-C6
53	T	32	4OC	C2'-C1'-N1-C2
53	T	8	4SU	O4'-C1'-N1-C6
53	T	8	4SU	O4'-C1'-N1-C2
53	T	54	5MU	C3'-C4'-C5'-O5'
53	T	8	4SU	C2'-C1'-N1-C2

There are no ring outliers.

6 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
53	T	54	5MU	4	0
53	T	55	PSU	2	0
53	T	20	H2U	1	0
53	T	8	4SU	1	0
53	T	101	FME	1	0
53	T	32	4OC	2	0

## 5.5 Carbohydrates

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry

Of 281 ligands modelled in this entry, 279 are monoatomic - leaving 2 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
58	ATP	U	602	59	28,33,33	0.71	0	34,52,52	0.60	1 (2%)
58	ATP	U	601	59	28,33,33	0.71	0	34,52,52	0.60	1 (2%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
58	ATP	U	602	59	-	6/18/38/38	0/3/3/3
58	ATP	U	601	59	-	1/18/38/38	0/3/3/3

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
58	U	601	ATP	C5-C6-N6	2.31	123.83	120.31
58	U	602	ATP	C5-C6-N6	2.31	123.83	120.31

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
58	U	602	ATP	C5'-O5'-PA-O2A
58	U	602	ATP	O4'-C4'-C5'-O5'
58	U	602	ATP	C3'-C4'-C5'-O5'
58	U	602	ATP	C5'-O5'-PA-O1A
58	U	602	ATP	C5'-O5'-PA-O3A
58	U	602	ATP	PA-O3A-PB-O2B

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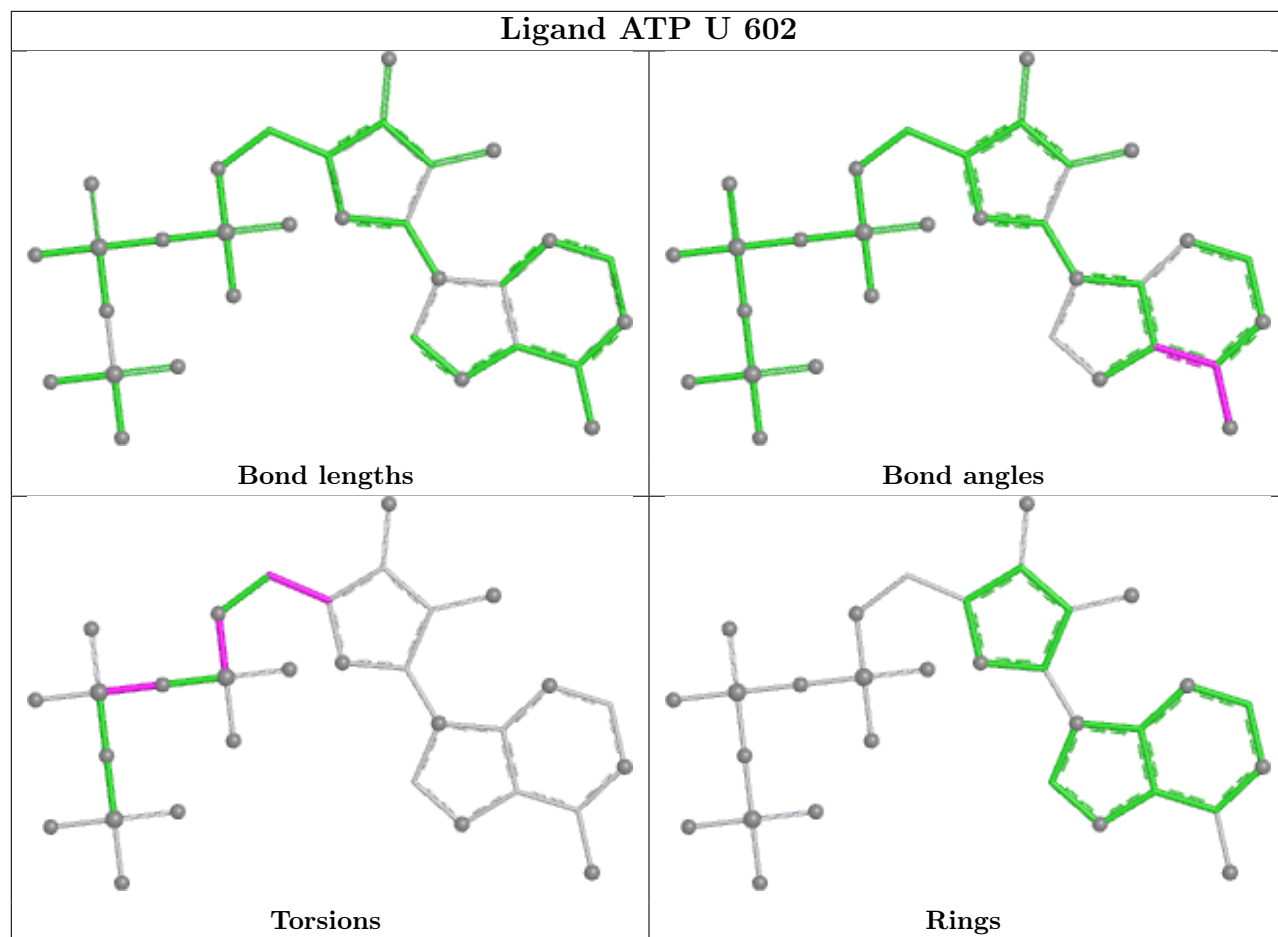
Mol	Chain	Res	Type	Atoms
58	U	601	ATP	PG-O3B-PB-O2B

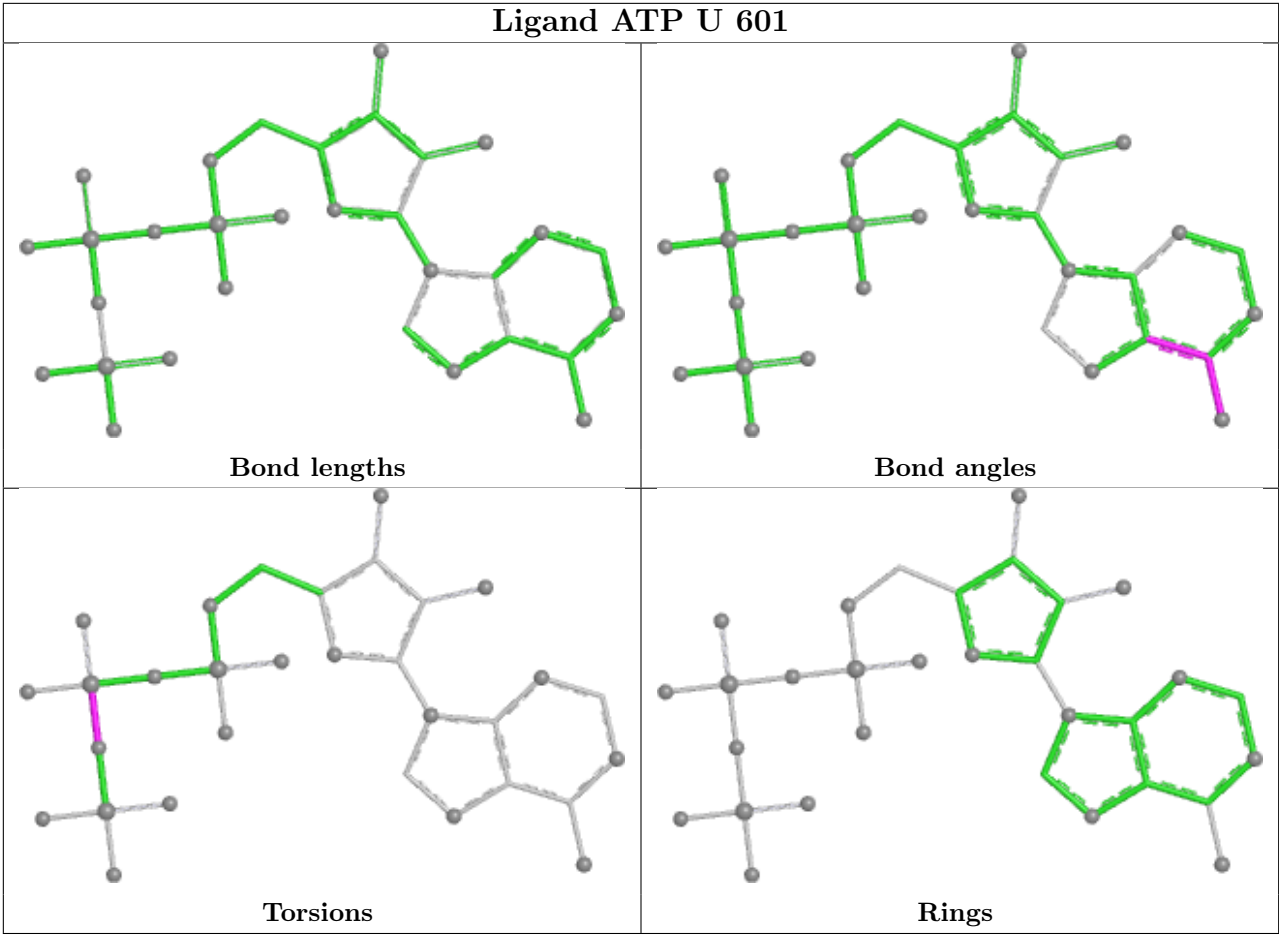
There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
58	U	602	ATP	2	0
58	U	601	ATP	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

The following chains have linkage breaks:

Mol	Chain	Number of breaks
32	R3	2

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	R3	210:C	O3'	211:G	P	7.40
1	R3	460:A	O3'	461:A	P	4.00



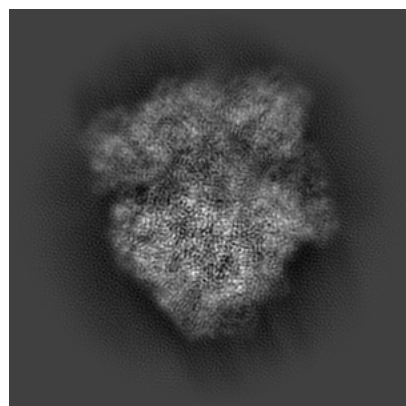
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-29399. These allow visual inspection of the internal detail of the map and identification of artifacts.

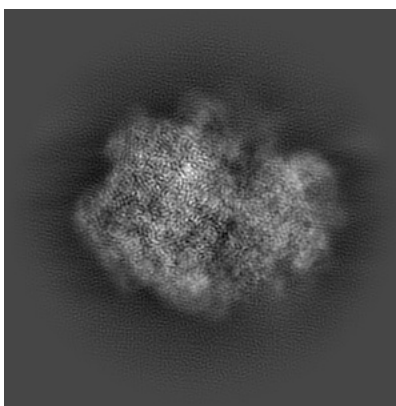
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

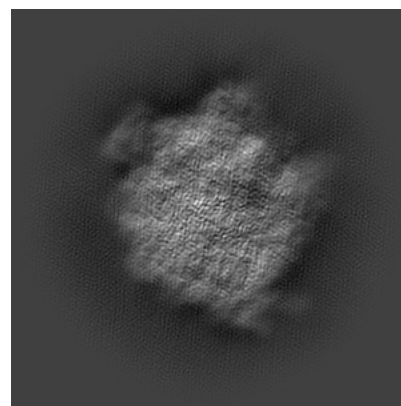
#### 6.1.1 Primary map



X

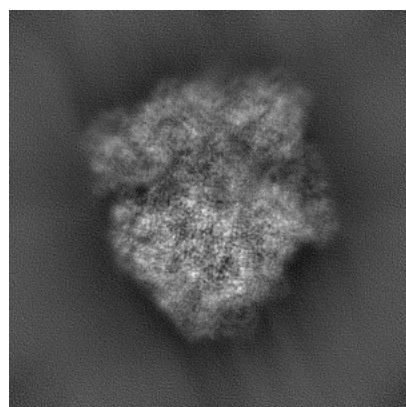


Y

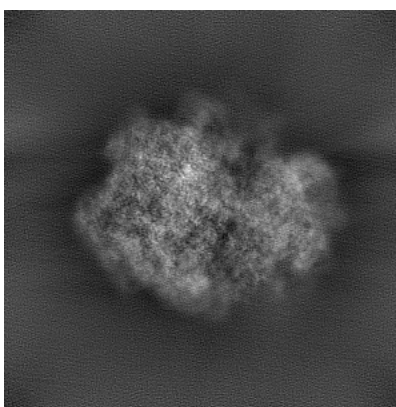


Z

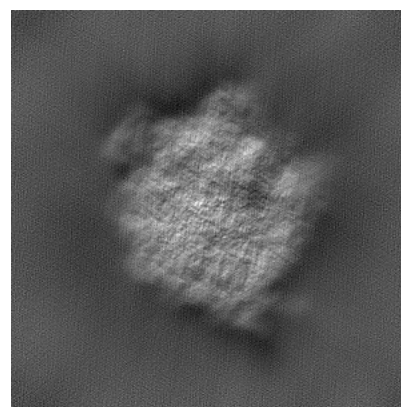
#### 6.1.2 Raw map



X



Y

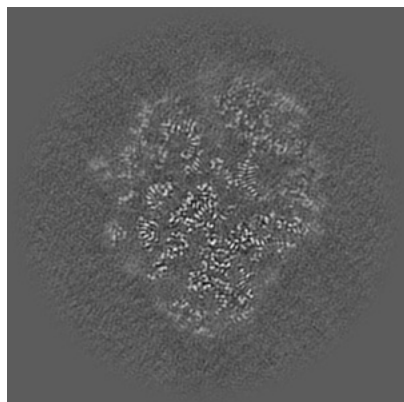


Z

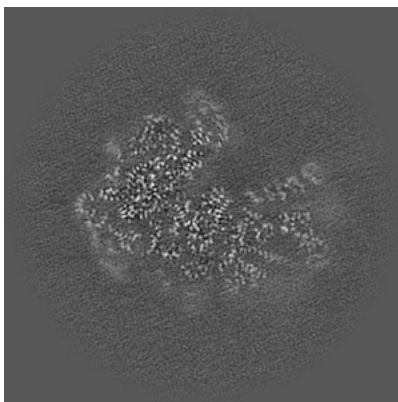
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

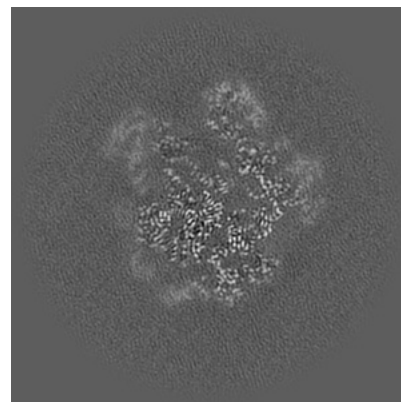
### 6.2.1 Primary map



X Index: 200

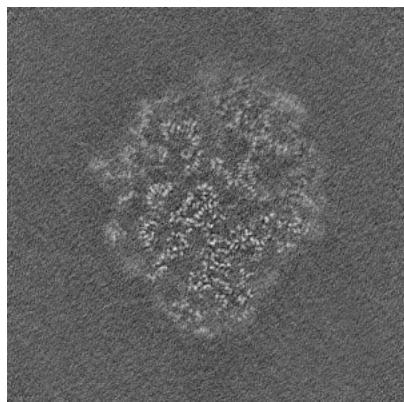


Y Index: 200

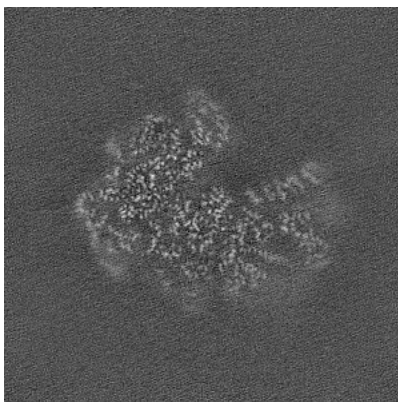


Z Index: 200

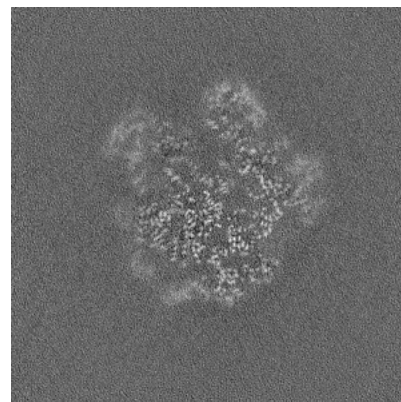
### 6.2.2 Raw map



X Index: 200



Y Index: 200

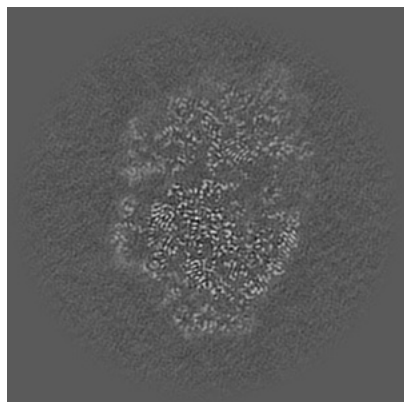


Z Index: 200

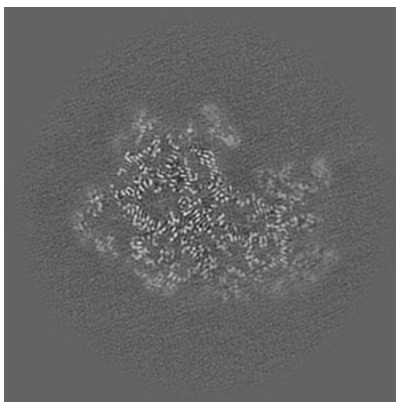
The images above show central slices of the map in three orthogonal directions.

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

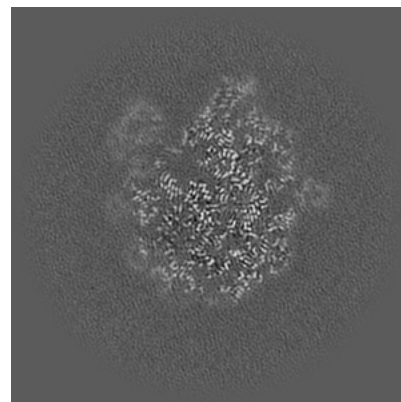
### 6.3.1 Primary map



X Index: 188

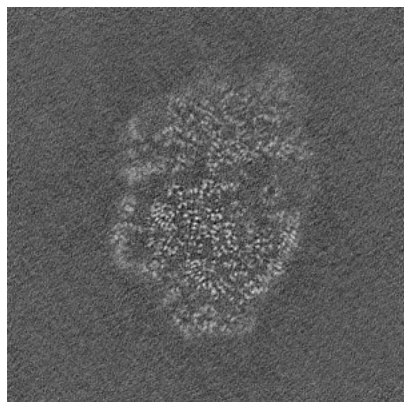


Y Index: 184

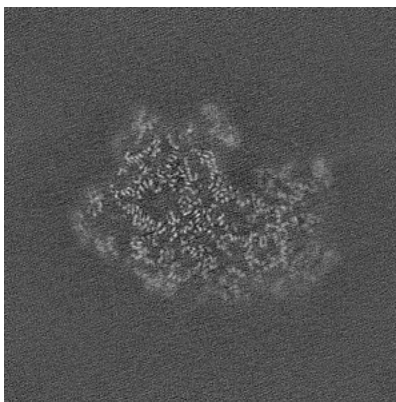


Z Index: 184

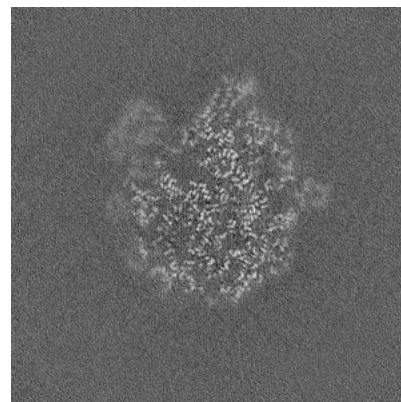
### 6.3.2 Raw map



X Index: 188



Y Index: 184



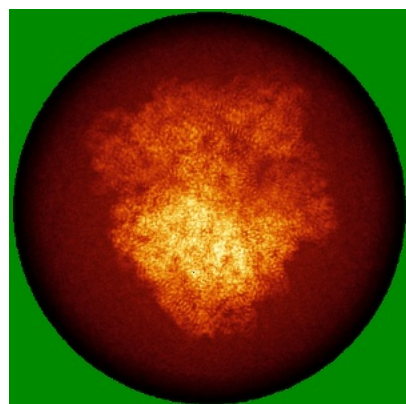
Z Index: 184

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

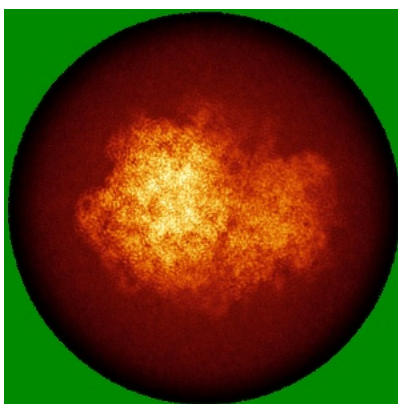


## 6.4 Orthogonal standard-deviation projections (False-color) [i](#)

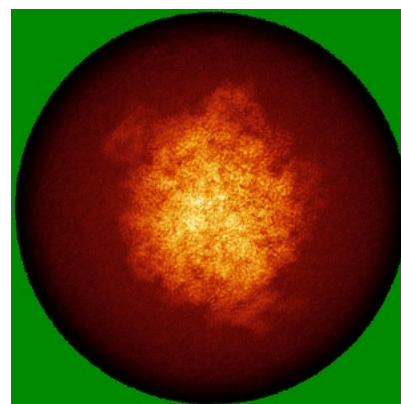
### 6.4.1 Primary map



X

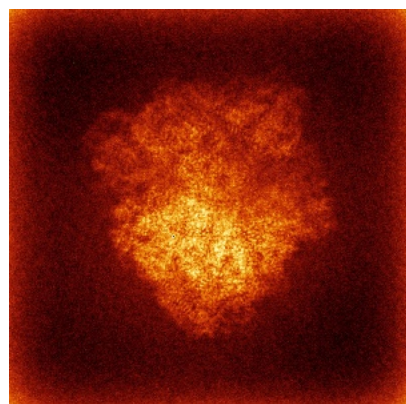


Y

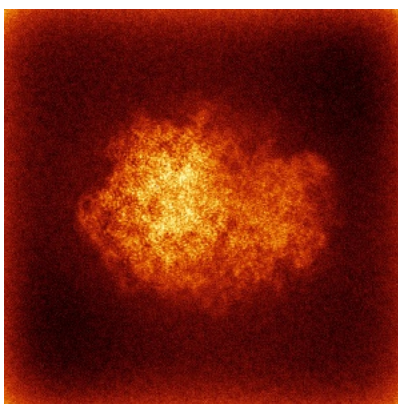


Z

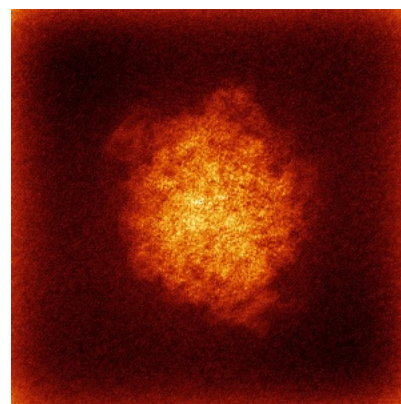
### 6.4.2 Raw map



X



Y

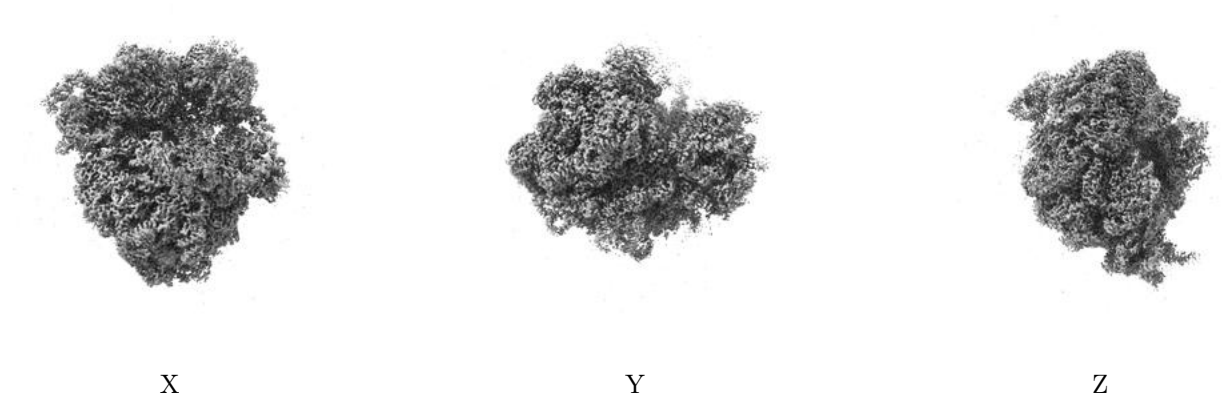


Z

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

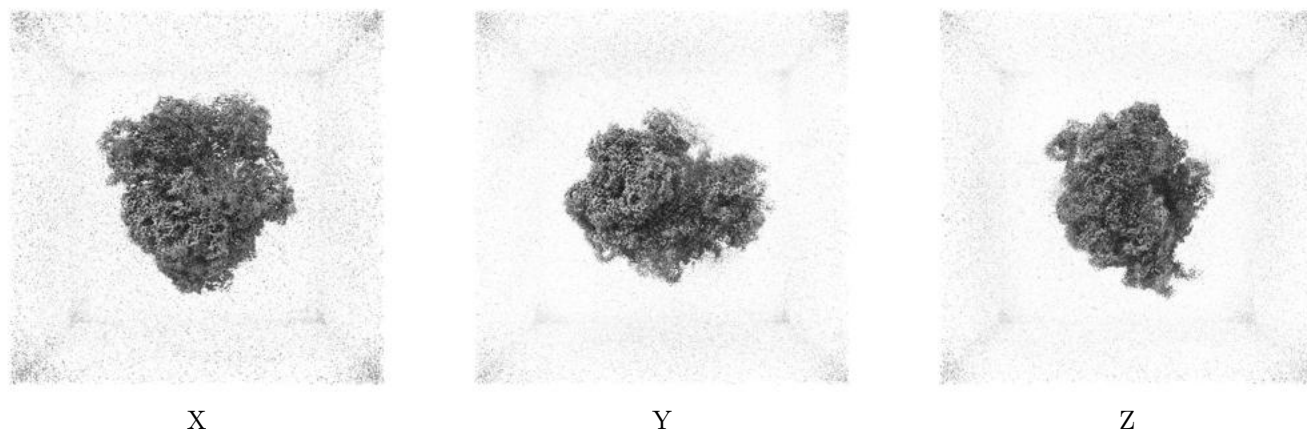
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.55. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

### 6.5.2 Raw map



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

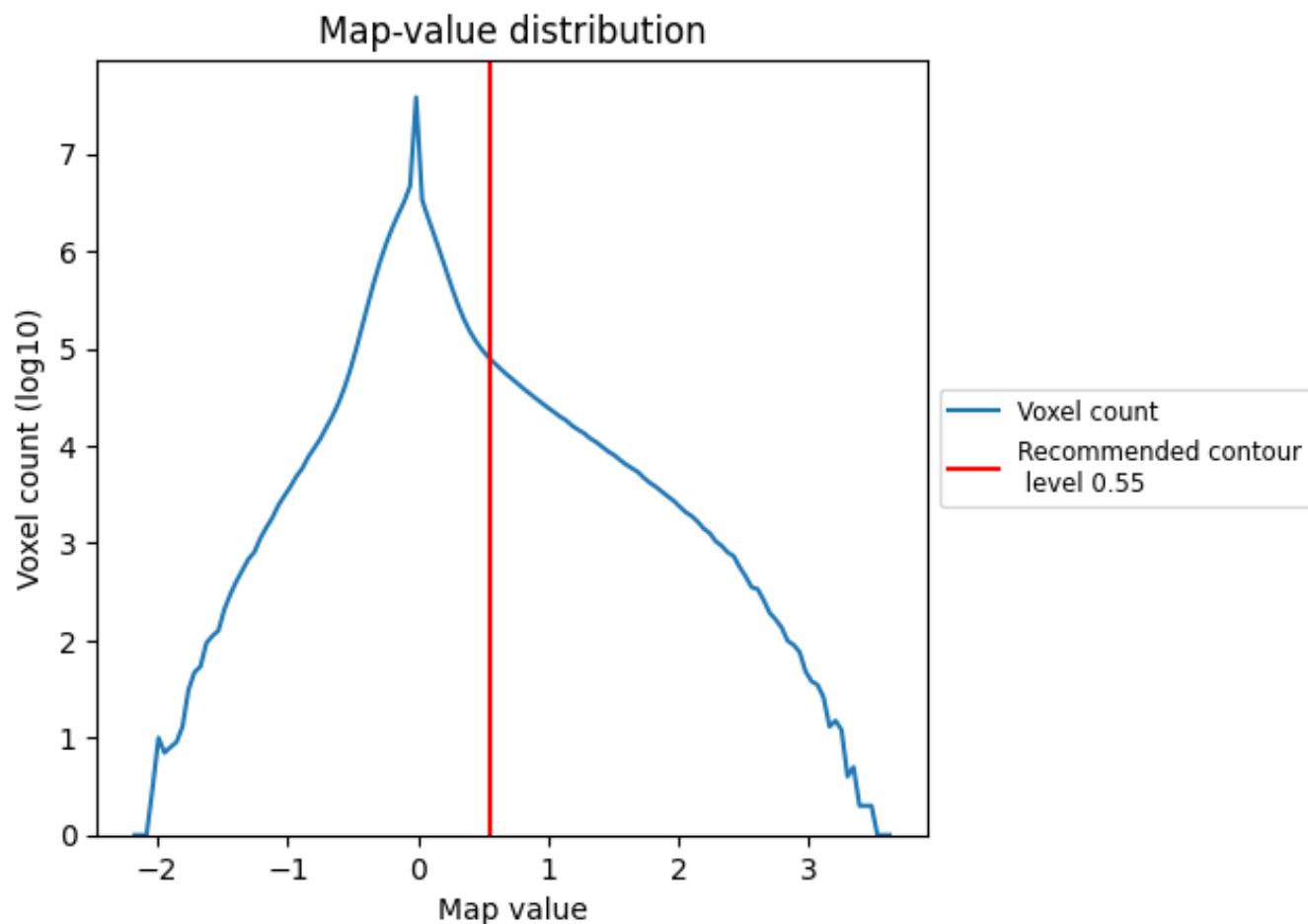
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

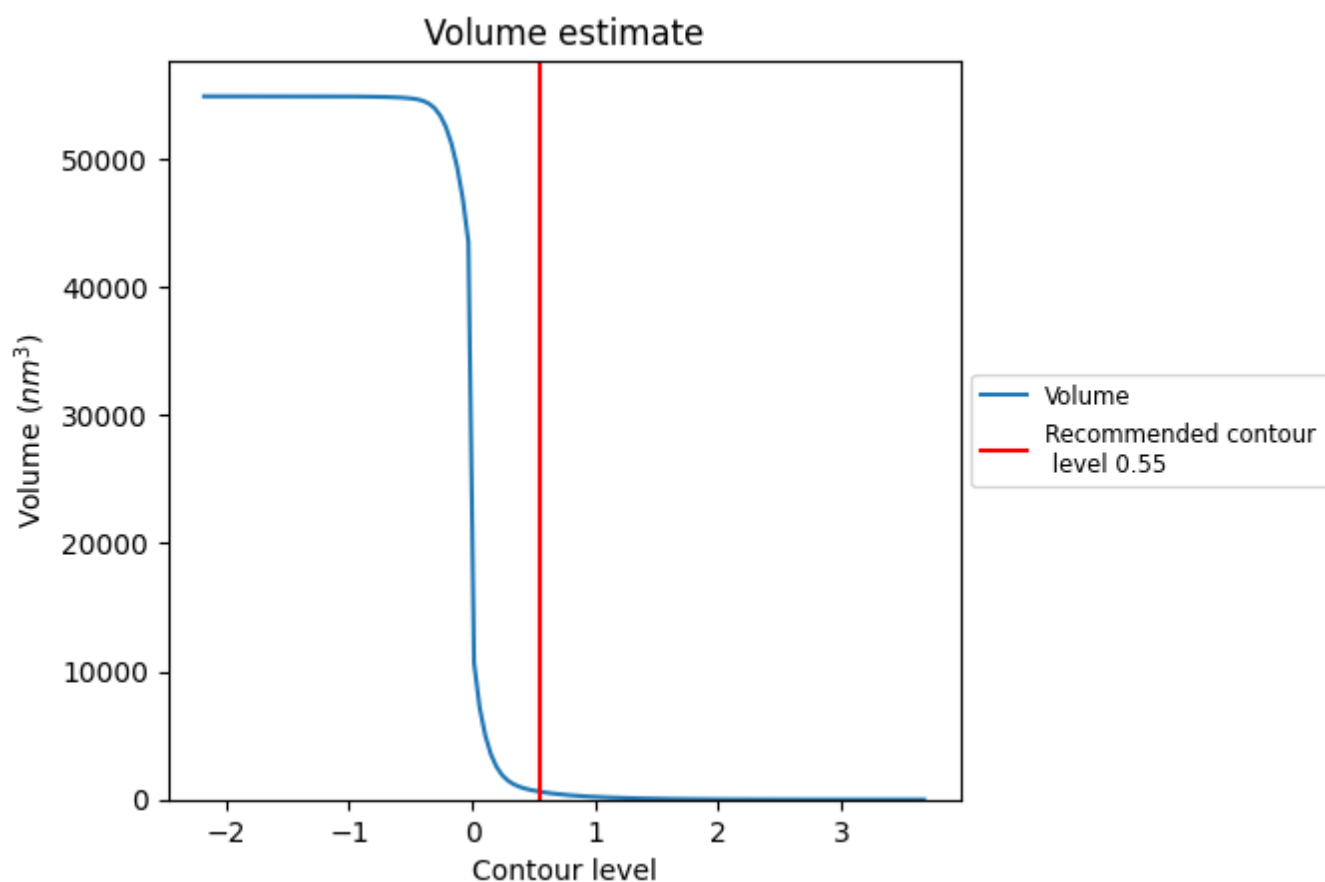
This section contains the results of statistical analysis of the map.

### 7.1 Map-value distribution [i](#)



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

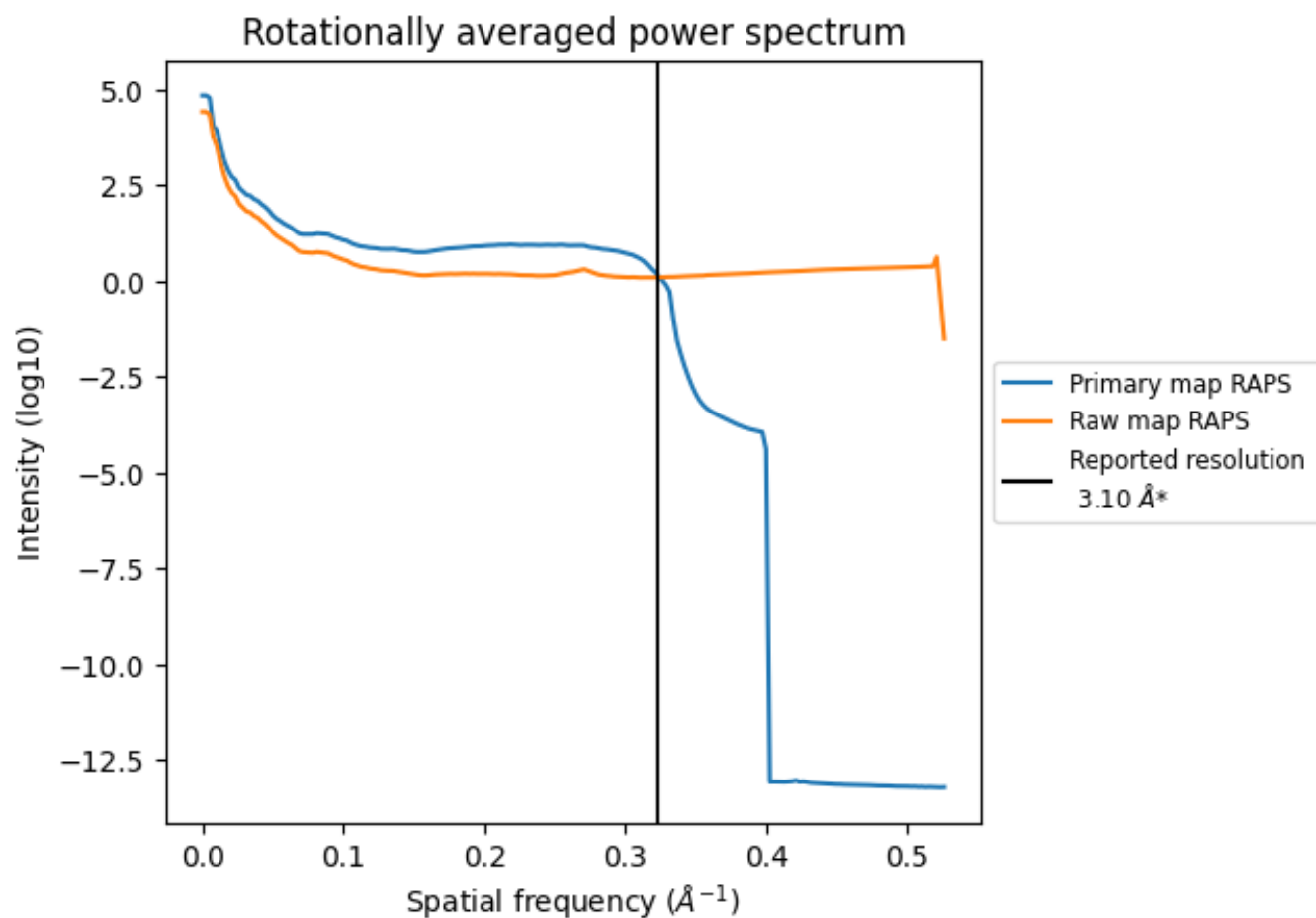
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 616 nm<sup>3</sup>; this corresponds to an approximate mass of 556 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 ⓘ



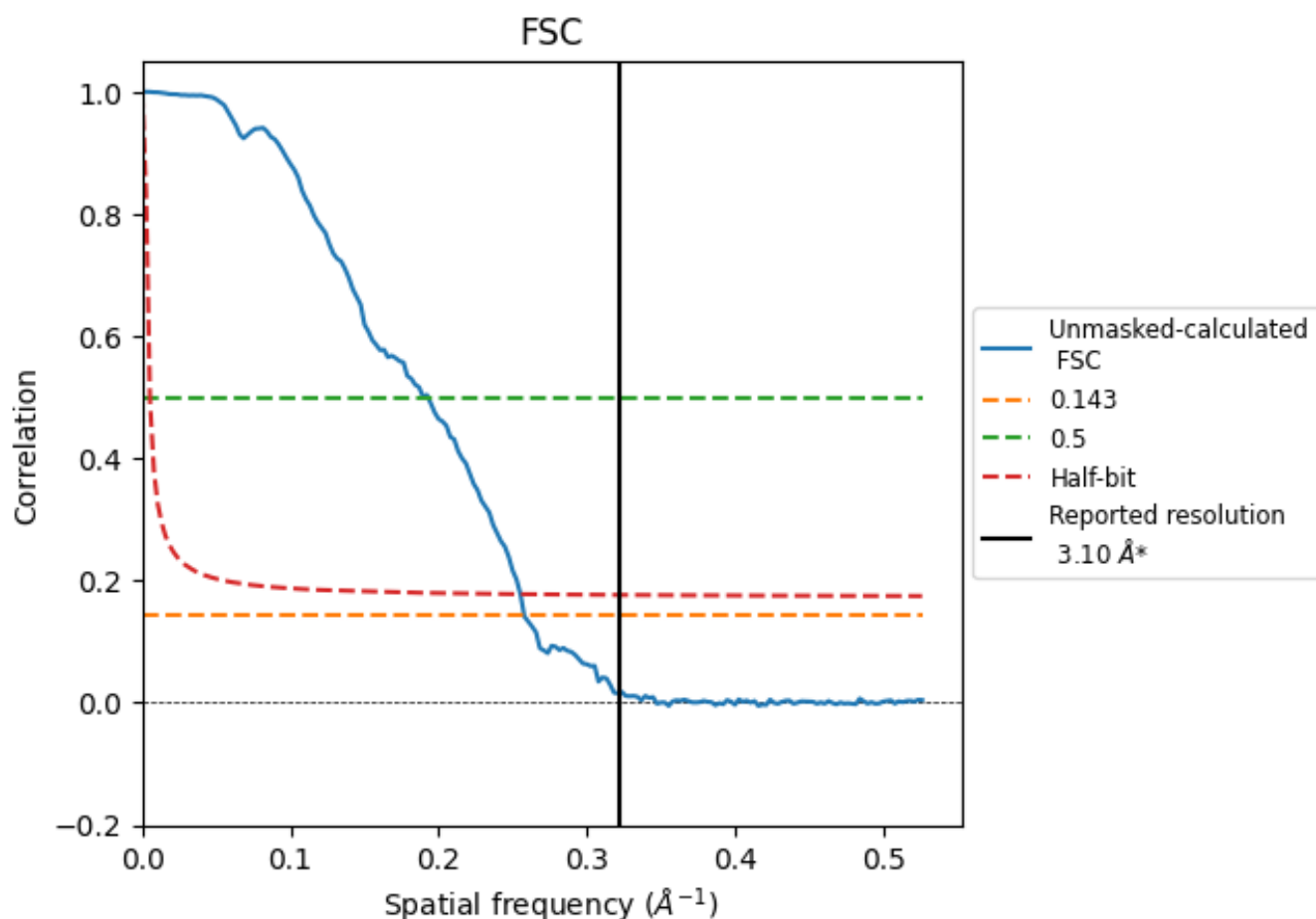
\*Reported resolution corresponds to spatial frequency of 0.323 Å<sup>-1</sup>



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

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

### 8.1 FSC [i](#)



\*Reported resolution corresponds to spatial frequency of 0.323  $\text{\AA}^{-1}$

## 8.2 Resolution estimates [i](#)

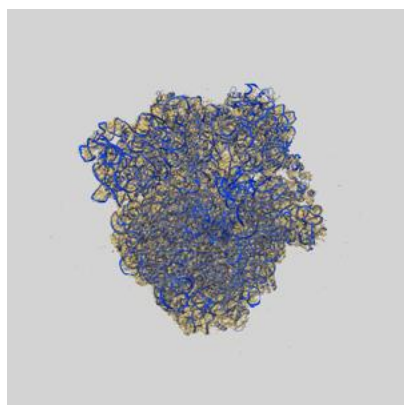
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.10	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.88	5.19	3.92

\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.88 differs from the reported value 3.1 by more than 10 %

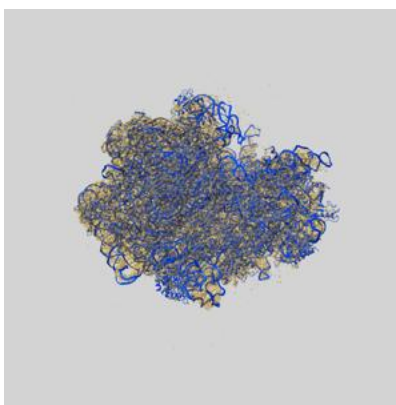
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-29399 and PDB model 9NLJ. Per-residue inclusion information can be found in section [3](#) on page [16](#).

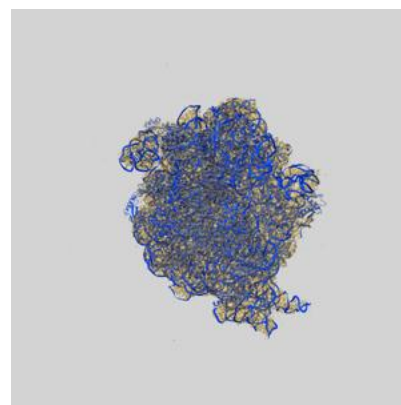
### 9.1 Map-model overlay [i](#)



X



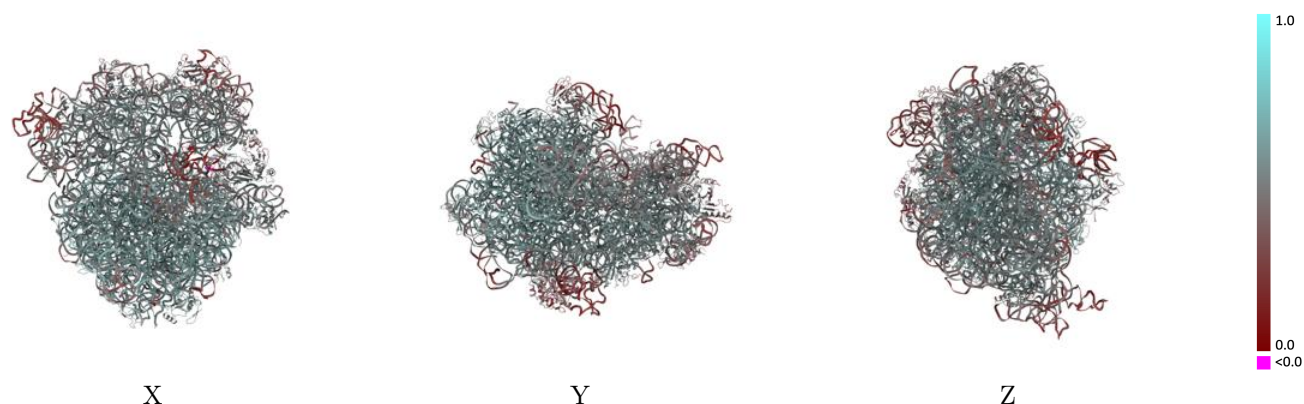
Y



Z

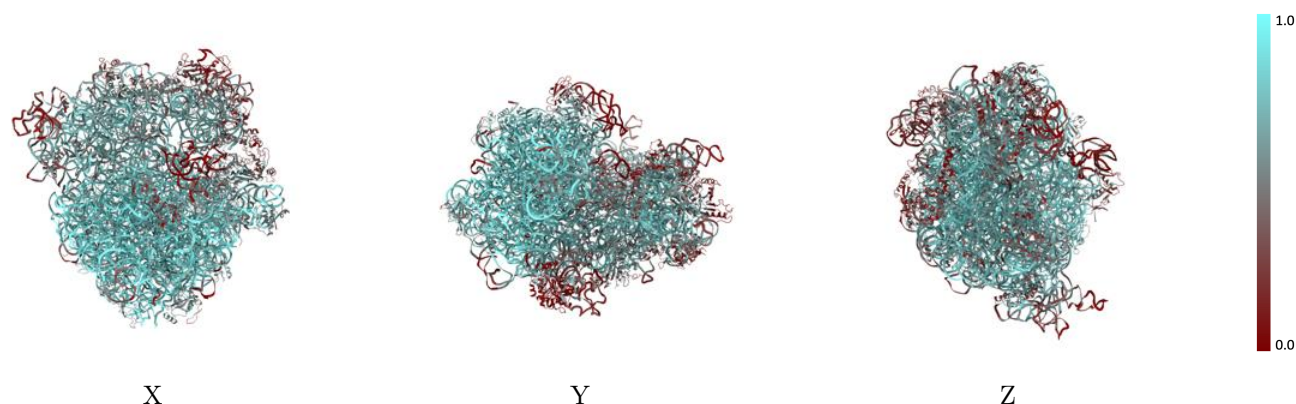
The images above show the 3D surface view of the map at the recommended contour level 0.55 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



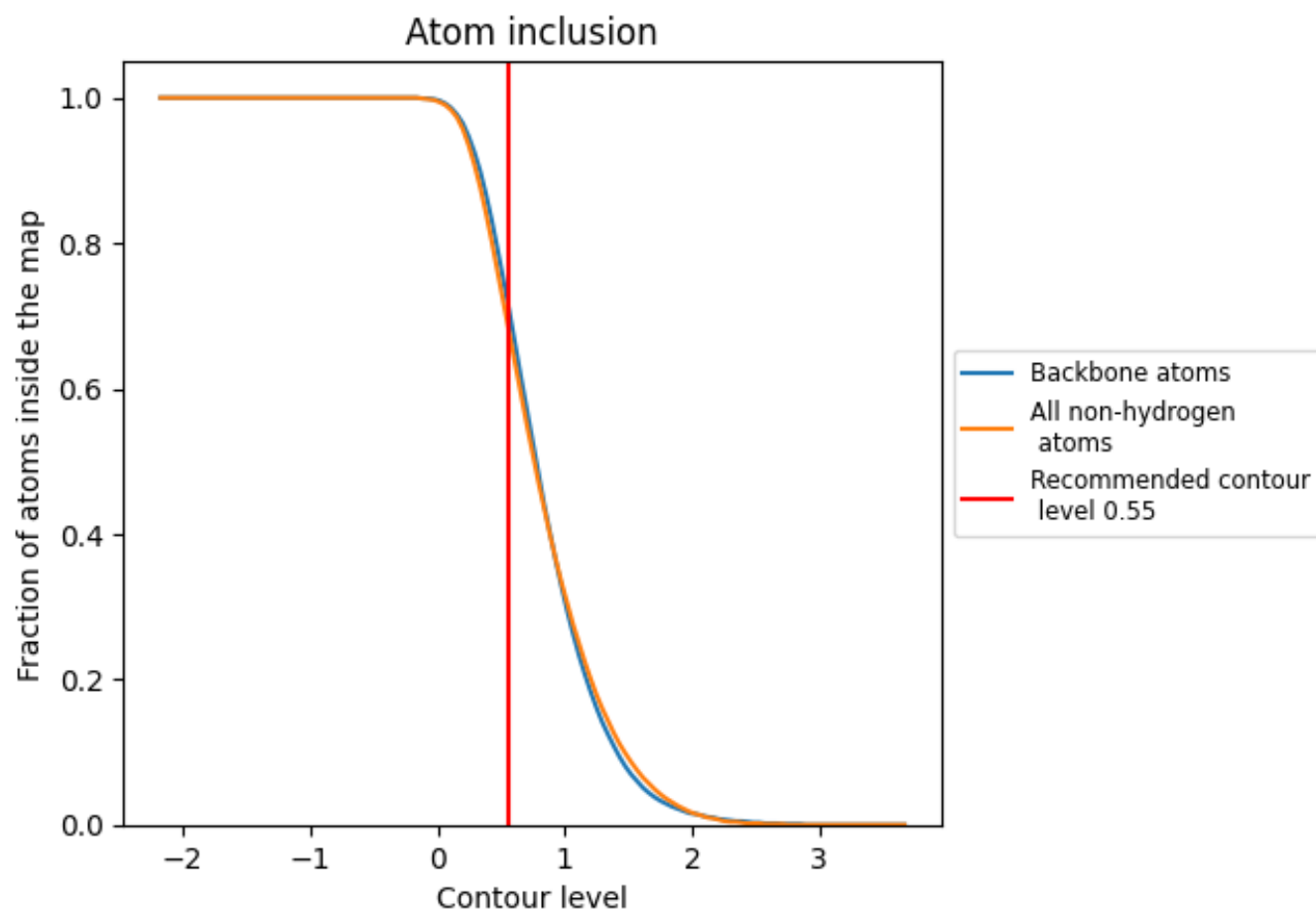
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.55).







































































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 72% of all backbone atoms, 69% 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 (0.55) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6900	 0.5200
1	 0.1170	 0.3350
13	 0.7500	 0.5890
14	 0.7150	 0.5820
15	 0.7360	 0.5620
16	 0.7170	 0.5740
17	 0.8160	 0.5810
18	 0.5540	 0.5190
19	 0.6900	 0.5700
2	 0.7360	 0.5870
20	 0.7940	 0.5910
21	 0.6670	 0.5520
22	 0.7200	 0.5710
23	 0.6190	 0.5480
24	 0.5410	 0.5200
25	 0.5980	 0.5270
27	 0.7430	 0.5800
28	 0.6960	 0.5740
29	 0.5760	 0.5130
3	 0.7740	 0.5800
30	 0.7390	 0.5700
31	 0.1740	 0.3730
32	 0.7370	 0.5750
33	 0.7080	 0.5760
34	 0.8030	 0.5970
35	 0.8310	 0.6080
36	 0.6540	 0.5610
4	 0.6520	 0.5520
5	 0.4030	 0.4830
6	 0.2940	 0.4200
9	 0.1110	 0.3510
M	 0.6560	 0.5380
R1	 0.8100	 0.5400
R2	 0.7600	 0.4990
R3	 0.6950	 0.4920



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Chain	Atom inclusion	Q-score
T	 0.7420	 0.5500
U	 0.4790	 0.5230
sb	 0.2780	 0.4310
sc	 0.4320	 0.5000
sd	 0.3490	 0.4730
se	 0.5690	 0.5190
sf	 0.4850	 0.4790
sg	 0.4850	 0.5090
sh	 0.5820	 0.5330
si	 0.4310	 0.4760
sj	 0.2820	 0.4450
sk	 0.5850	 0.5470
sl	 0.4160	 0.5130
sm	 0.3840	 0.4790
sn	 0.3760	 0.4700
so	 0.5640	 0.5170
sp	 0.4510	 0.4960
sq	 0.4640	 0.4960
sr	 0.5040	 0.5020
ss	 0.2880	 0.4460
st	 0.4080	 0.4750
su	 0.3480	 0.4410