



## Full wwPDB EM Validation Report ⓘ

May 26, 2025 – 08:05 AM EDT

PDB ID : 8T5D / pdb\_00008t5d  
EMDB ID : EMD-41049  
Title : Cryo-EM studies of the interplay between uS2 ribosomal protein and leaderless mRNA during bacterial translation initiation  
Authors : Bhattacharjee, S.; Gottesman, M.E.; Frank, J.  
Deposited on : 2023-06-13  
Resolution : 3.20 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.dev118  
MolProbity : 4-5-2 with Phenix2.0rc1  
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) : 2.43.1

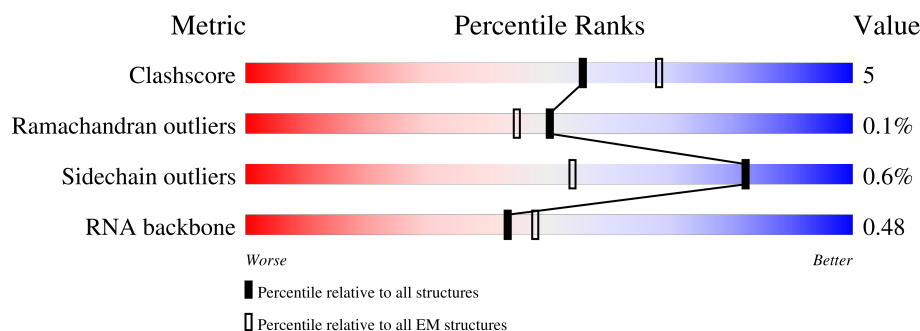
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.20 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	0	56	<div> <div>12%</div> <div>75%</div> <div>25%</div> </div>
2	1	51	<div> <div>12%</div> <div>86%</div> <div>14%</div> </div>
3	2	46	<div> <div>9%</div> <div>85%</div> <div>15%</div> </div>
4	3	64	<div> <div>80%</div> <div>20%</div> </div>
5	4	38	<div> <div>82%</div> <div>18%</div> </div>
6	A	117	<div> <div>8%</div> <div>63%</div> <div>35%</div> </div>
7	B	2903	<div> <div>11%</div> <div>67%</div> <div>30%</div> </div>




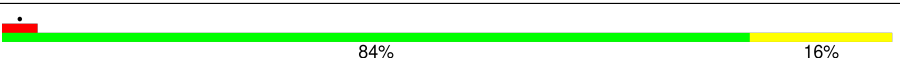
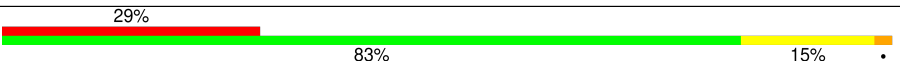

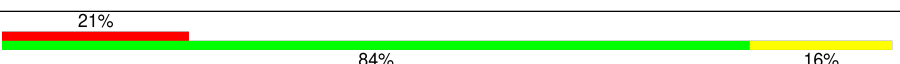
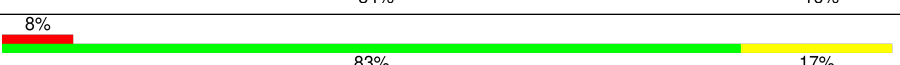

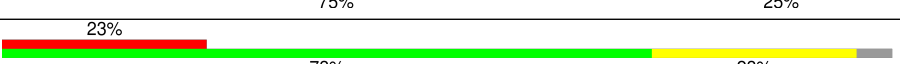
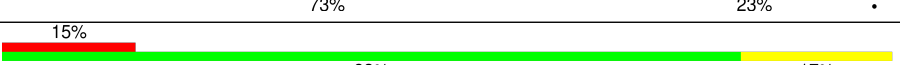
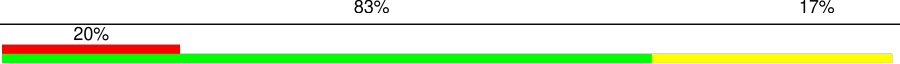
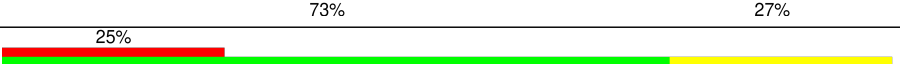
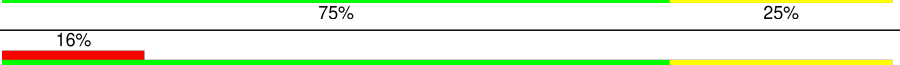







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Mol	Chain	Length	Quality of chain
8	C	272	
9	D	209	
10	E	201	
11	F	178	
12	G	176	
13	J	142	
14	K	122	
15	L	143	
16	M	136	
17	N	121	
18	O	116	
19	P	114	
20	Q	117	
21	R	103	
22	S	110	
23	T	94	
24	U	103	
25	V	94	
26	W	79	
27	X	77	
28	Y	63	
29	Z	58	
30	a	218	
31	b	206	
32	c	205	

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Mol	Chain	Length	Quality of chain
33	d	150	
34	e	100	
35	f	151	
36	g	129	
37	h	127	
38	i	98	
39	j	117	
40	k	123	
41	l	114	
42	m	100	
43	n	88	
44	o	82	
45	p	80	
46	q	55	
47	r	79	
48	s	85	
49	t	51	
50	u	59	
51	v	1539	
52	x	12	
53	5	77	

## 2 Entry composition

There are 53 unique types of molecules in this entry. The entry contains 142752 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 50S ribosomal protein L32.

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

- Molecule 2 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms				AltConf	Trace
2	1	51	Total	C	N	O	0	1
			410	263	76	71		

- Molecule 3 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	2	46	Total	C	N	O	S	0	0
			377	228	90	57	2		

- Molecule 4 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	3	64	Total	C	N	O	S	0	0
			504	323	105	74	2		

- Molecule 5 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	4	38	Total	C	N	O	S	0	0
			302	185	65	48	4		

- Molecule 6 is a RNA chain called 5S RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	A	117	Total	C	N	O	P	0	0
			2504	1116	459	813	116		

- Molecule 7 is a RNA chain called 23S RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	B	2903	Total	C	N	O	P	0	0
			62317	27801	11467	20147	2902		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
8	C	272	Total	C	N	O	S	0	1
			2083	1288	424	364	7		

- Molecule 9 is a protein called 50S ribosomal protein L3.

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

- Molecule 10 is a protein called 50S ribosomal protein L4.

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

- Molecule 11 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	F	178	Total	C	N	O	S	0	0
			1420	905	251	258	6		

- Molecule 12 is a protein called 50S ribosomal protein L6.

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

- Molecule 13 is a protein called 50S ribosomal protein L13.

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

- Molecule 14 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	K	122	Total	C	N	O	S	0	1
			931	582	180	164	5		

- Molecule 15 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	L	143	Total	C	N	O	S	0	0
			1045	649	206	189	1		

- Molecule 16 is a protein called 50S ribosomal protein L16.

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

- Molecule 17 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	N	121	Total	C	N	O	S	0	1
			961	593	197	166	5		

- Molecule 18 is a protein called 50S ribosomal protein L18.

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

- Molecule 19 is a protein called 50S ribosomal protein L19.

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

- Molecule 20 is a protein called 50S ribosomal protein L20.

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

- Molecule 21 is a protein called Ribosomal protein L21.

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

- Molecule 22 is a protein called 50S ribosomal protein L22.

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

- Molecule 23 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	T	94	Total	C	N	O	S	0	1
			739	466	140	131	2		

- Molecule 24 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	U	103	Total	C	N	O		0	1
			780	492	147	141			

- Molecule 25 is a protein called 50S ribosomal protein L25.

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

- Molecule 26 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	W	79	Total	C	N	O	S	0	0
			596	367	120	108	1		

- Molecule 27 is a protein called 50S ribosomal protein L28.

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

- Molecule 28 is a protein called 50S ribosomal protein L29.



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

- Molecule 29 is a protein called 50S ribosomal protein L30.

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

- Molecule 30 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	a	218	Total	C	N	O	S	0	0
			1705	1081	305	312	7		

- Molecule 31 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	b	206	Total	C	N	O	S	0	0
			1625	1028	305	289	3		

- Molecule 32 is a protein called 30S ribosomal protein S4.

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

- Molecule 33 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	d	150	Total	C	N	O	S	0	0
			1106	687	211	202	6		

- Molecule 34 is a protein called 30S ribosomal protein S6, non-modified isoform.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	e	100	Total	C	N	O	S	0	0
			818	515	148	149	6		

- Molecule 35 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	f	151	Total	C	N	O	S	0	0
			1182	735	227	216	4		

- Molecule 36 is a protein called 30S ribosomal protein S8.

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

- Molecule 37 is a protein called 30S ribosomal protein S9.

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

- Molecule 38 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	i	98	Total	C	N	O	S	0	0
			787	493	150	143	1		

- Molecule 39 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	j	117	Total	C	N	O	S	0	0
			877	540	174	160	3		

- Molecule 40 is a protein called 30S ribosomal protein S12.

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

- Molecule 41 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	l	114	Total	C	N	O	S	0	0
			884	546	178	157	3		

- Molecule 42 is a protein called 30S ribosomal protein S14.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	m	96	Total	C	N	O	S	0	0
			774	483	160	128	3		

- Molecule 43 is a protein called 30S ribosomal protein S15.

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

- Molecule 44 is a protein called 30S ribosomal protein S16.

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

- Molecule 45 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	p	80	Total	C	N	O	S	0	0
			649	411	121	114	3		

- Molecule 46 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms				AltConf	Trace
46	q	55	Total	C	N	O	0	0
			456	288	86	82		

- Molecule 47 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	r	79	Total	C	N	O	S	0	0
			638	408	120	108	2		

- Molecule 48 is a protein called 30S ribosomal protein S20.

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

- Molecule 49 is a protein called 30S ribosomal protein S21 (Fragment).

Mol	Chain	Residues	Atoms					AltConf	Trace
49	t	51	Total	C	N	O	S	0	0
			426	265	86	74	1		

- Molecule 50 is a protein called Transcription termination/antitermination protein NusG.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	u	59	Total	C	N	O	S	0	0
			468	297	78	92	1		

- Molecule 51 is a RNA chain called 16s RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	v	1539	Total	C	N	O	P	0	0
			33012	14725	6052	10697	1538		

- Molecule 52 is a RNA chain called lmRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	x	12	Total	C	N	O	P	0	0
			257	117	53	76	11		

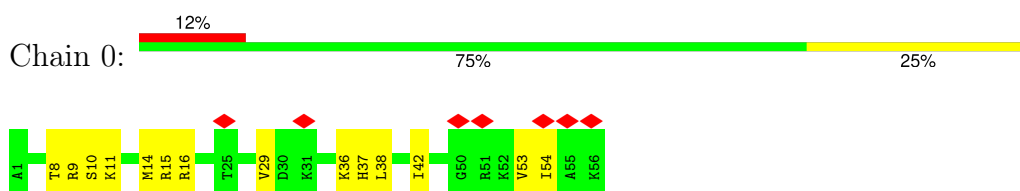
- Molecule 53 is a RNA chain called tRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	5	77	Total	C	N	O	P	0	0
			1640	732	297	535	76		

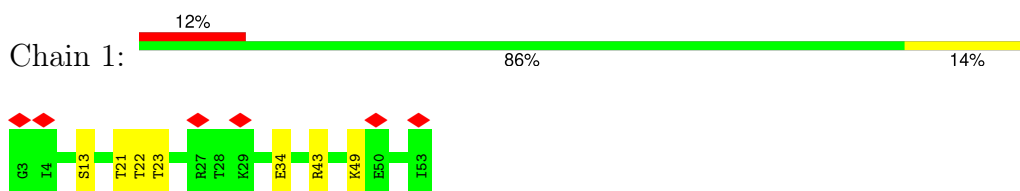
### 3 Residue-property plots [i](#)

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.

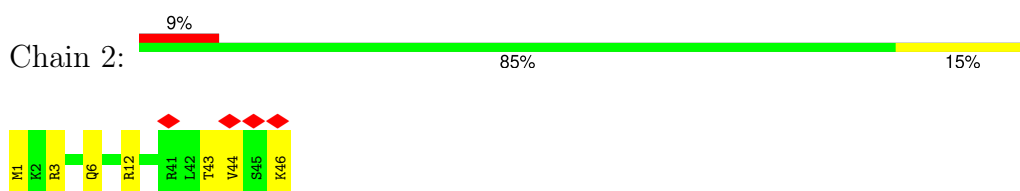
- Molecule 1: 50S ribosomal protein L32



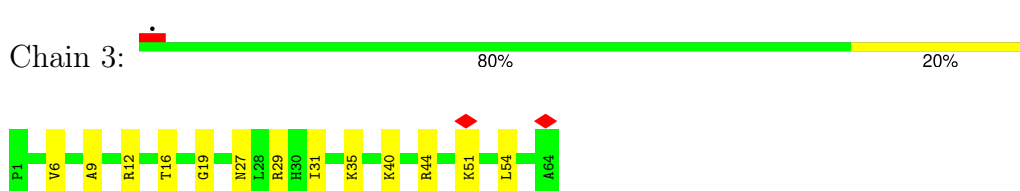
- Molecule 2: 50S ribosomal protein L33



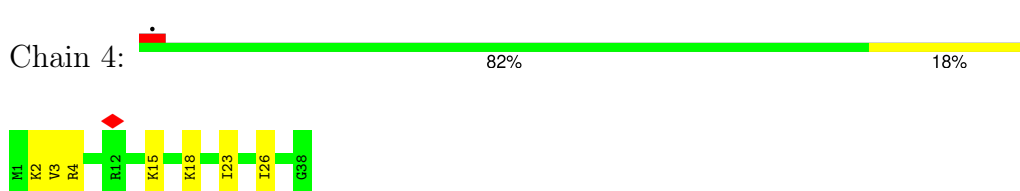
- Molecule 3: 50S ribosomal protein L34



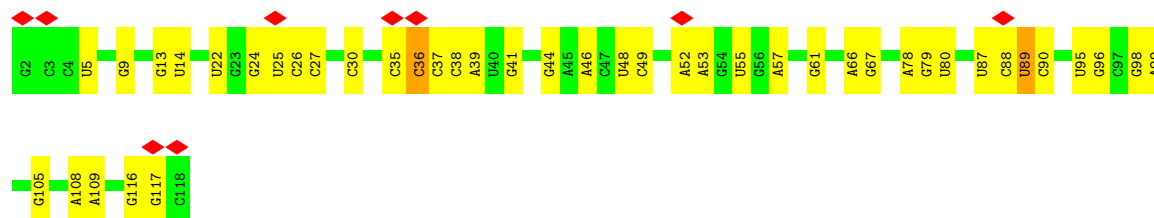
- Molecule 4: 50S ribosomal protein L35



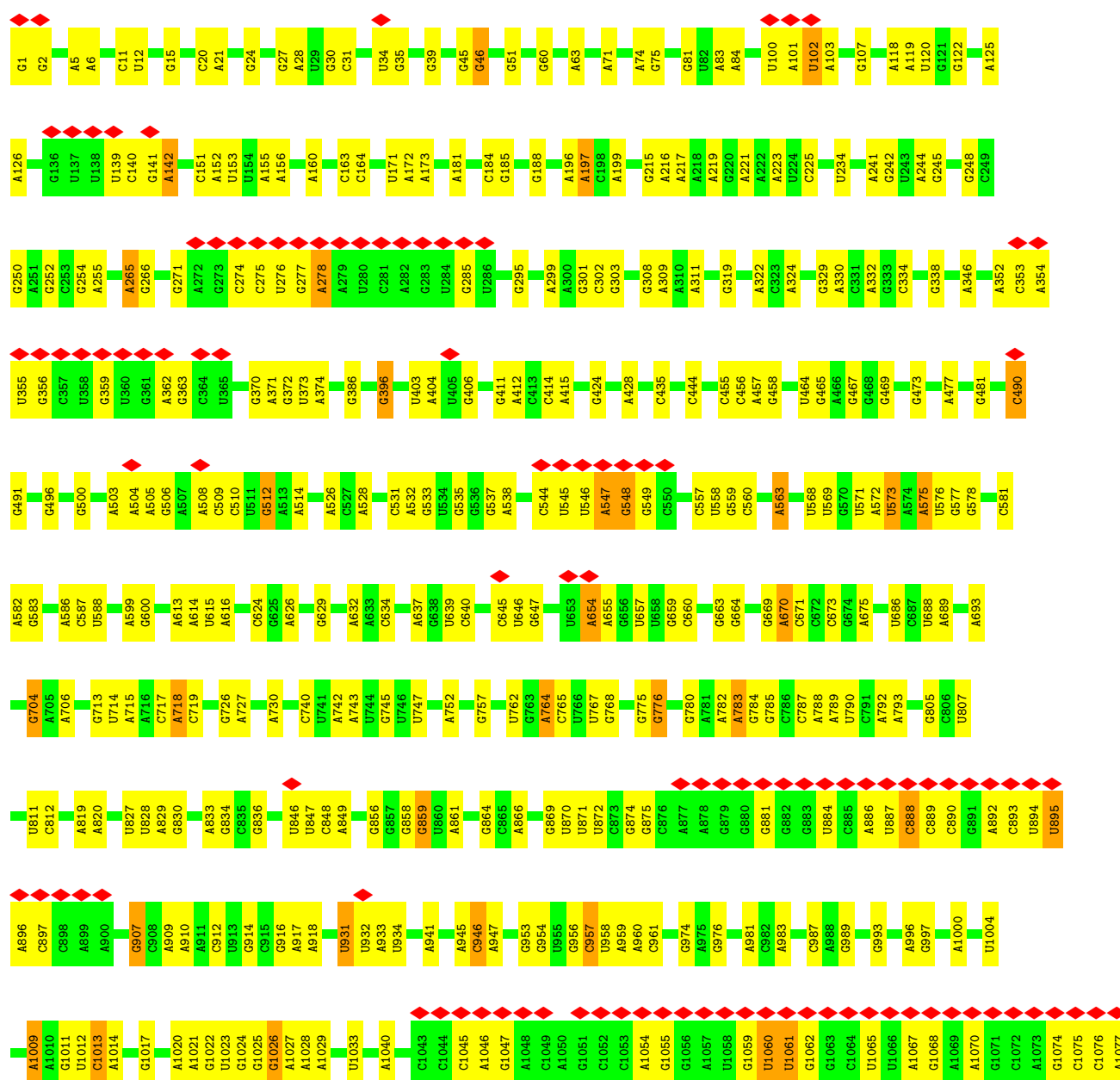
- Molecule 5: 50S ribosomal protein L36

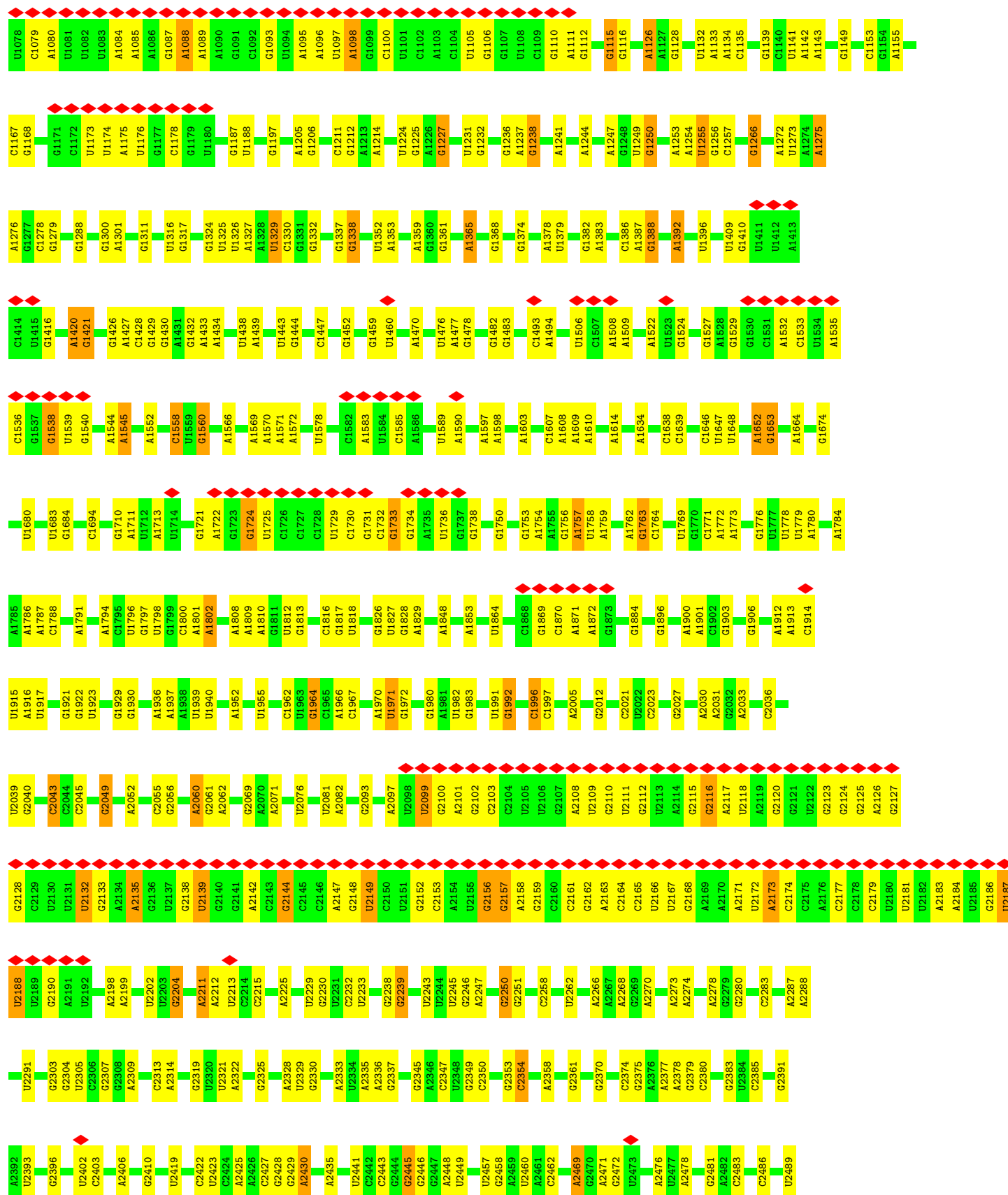


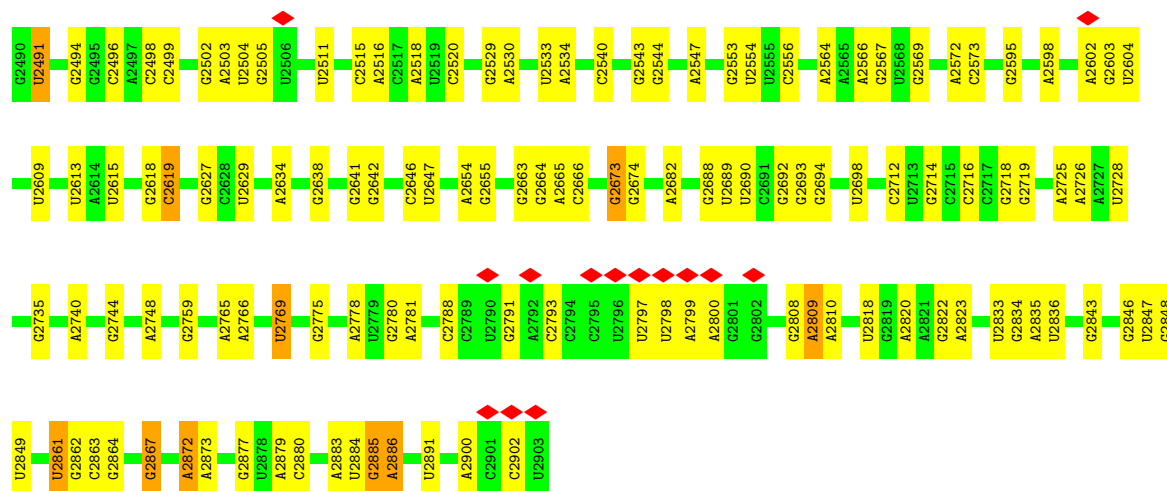
- Molecule 6: 5S RNA



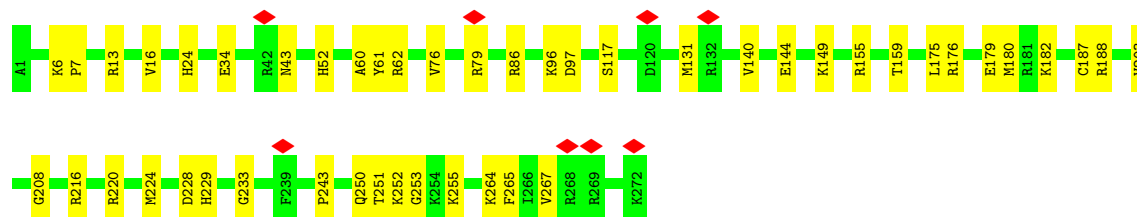
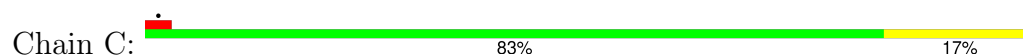
- Molecule 7: 23S RNA



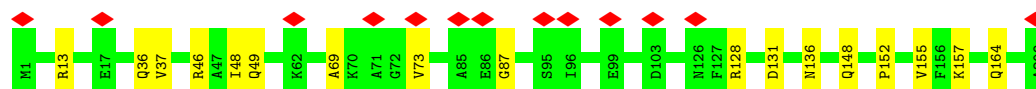
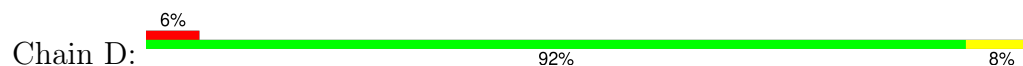




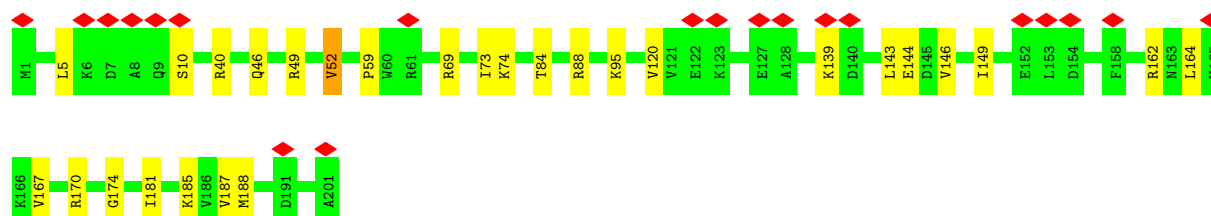
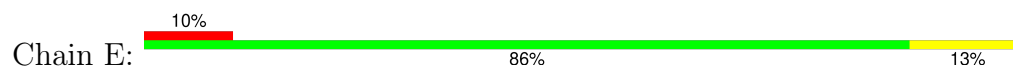
• Molecule 8: 50S ribosomal protein L2



• Molecule 9: 50S ribosomal protein L3



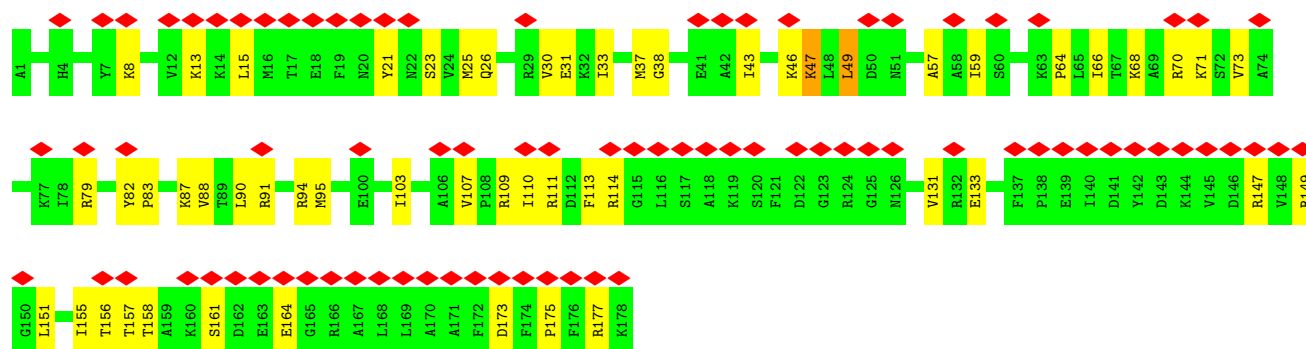
• Molecule 10: 50S ribosomal protein L4



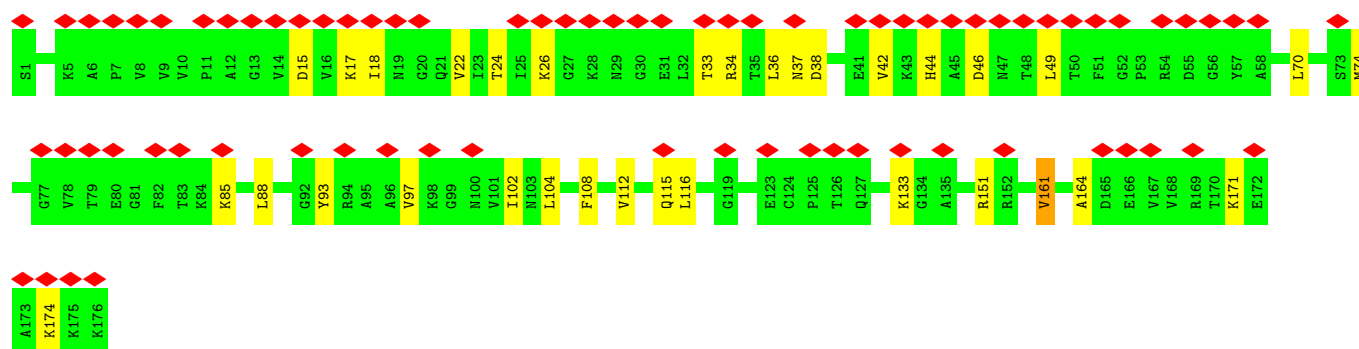
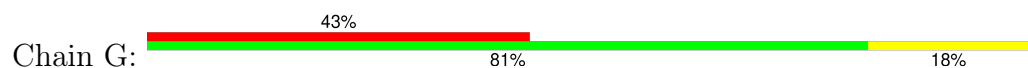
• Molecule 11: 50S ribosomal protein L5



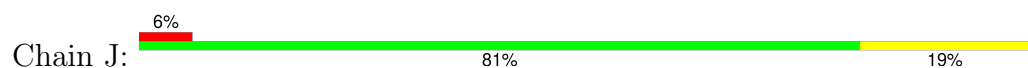




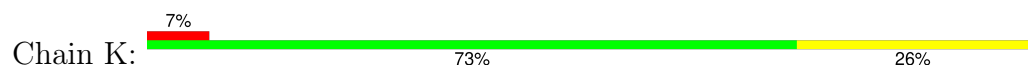
• Molecule 12: 50S ribosomal protein L6



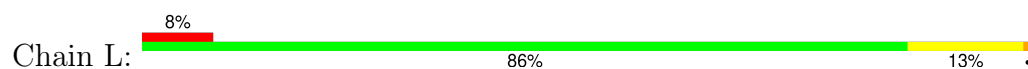
• Molecule 13: 50S ribosomal protein L13

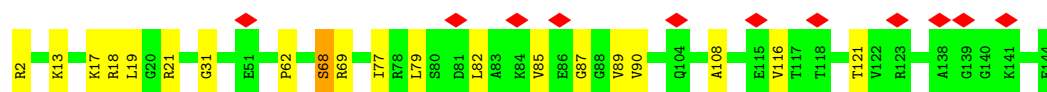


• Molecule 14: 50S ribosomal protein L14

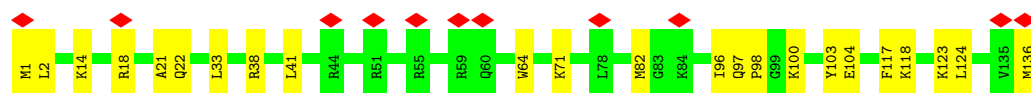
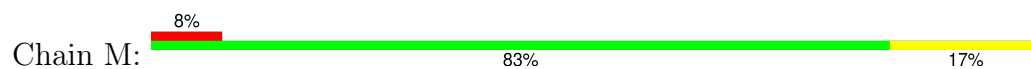


• Molecule 15: 50S ribosomal protein L15

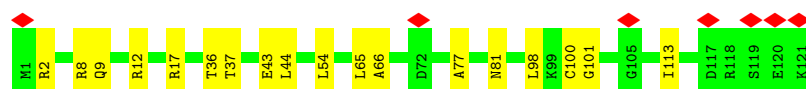
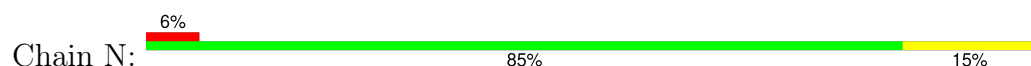




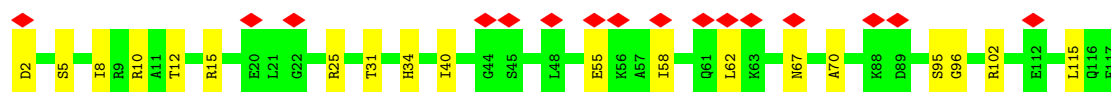
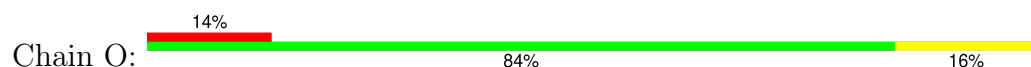
- Molecule 16: 50S ribosomal protein L16



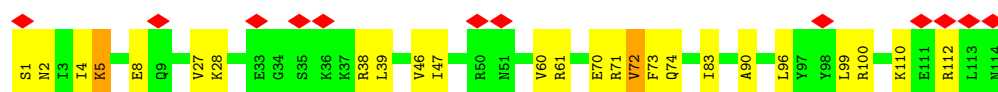
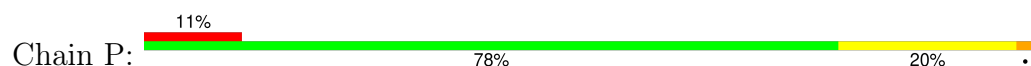
- Molecule 17: 50S ribosomal protein L17



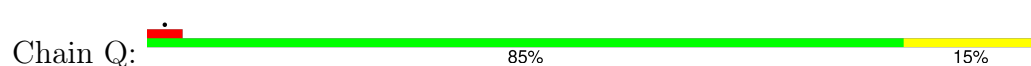
- Molecule 18: 50S ribosomal protein L18



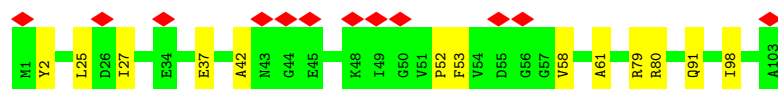
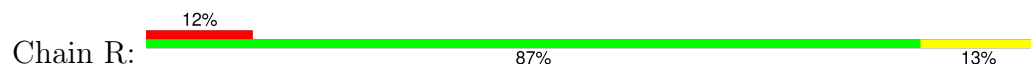
- Molecule 19: 50S ribosomal protein L19



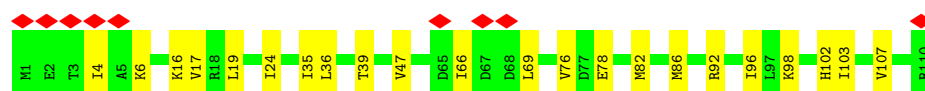
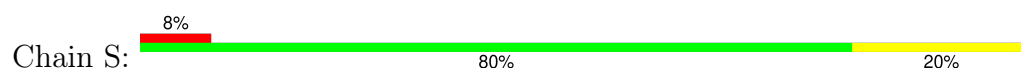
- Molecule 20: 50S ribosomal protein L20



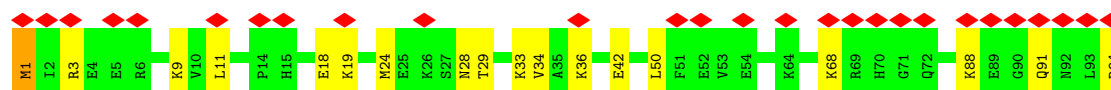
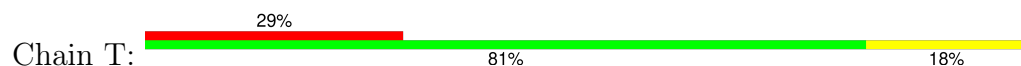
- Molecule 21: Ribosomal protein L21



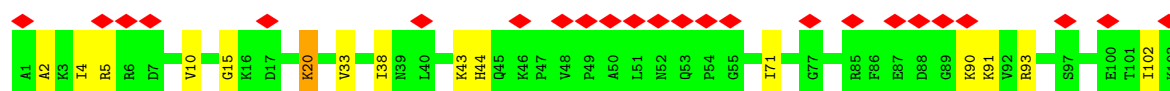
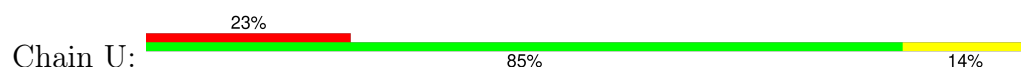
- Molecule 22: 50S ribosomal protein L22



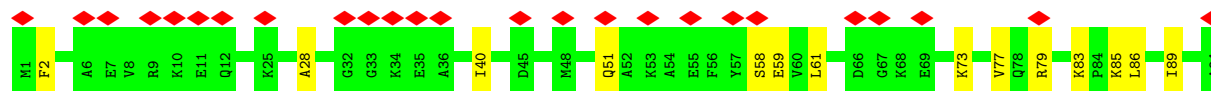
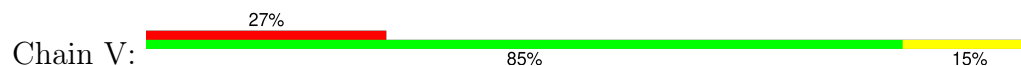
- Molecule 23: 50S ribosomal protein L23



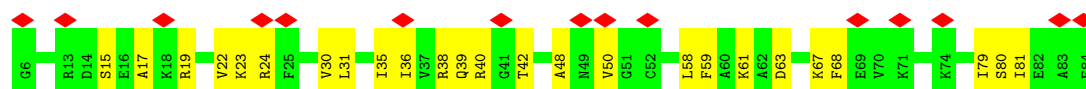
- Molecule 24: 50S ribosomal protein L24



- Molecule 25: 50S ribosomal protein L25



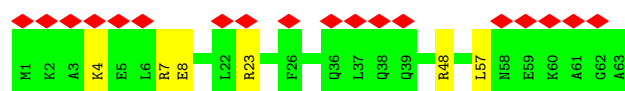
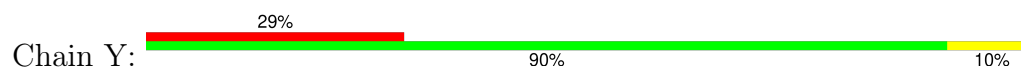
- Molecule 26: 50S ribosomal protein L27



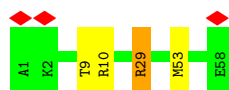
- Molecule 27: 50S ribosomal protein L28



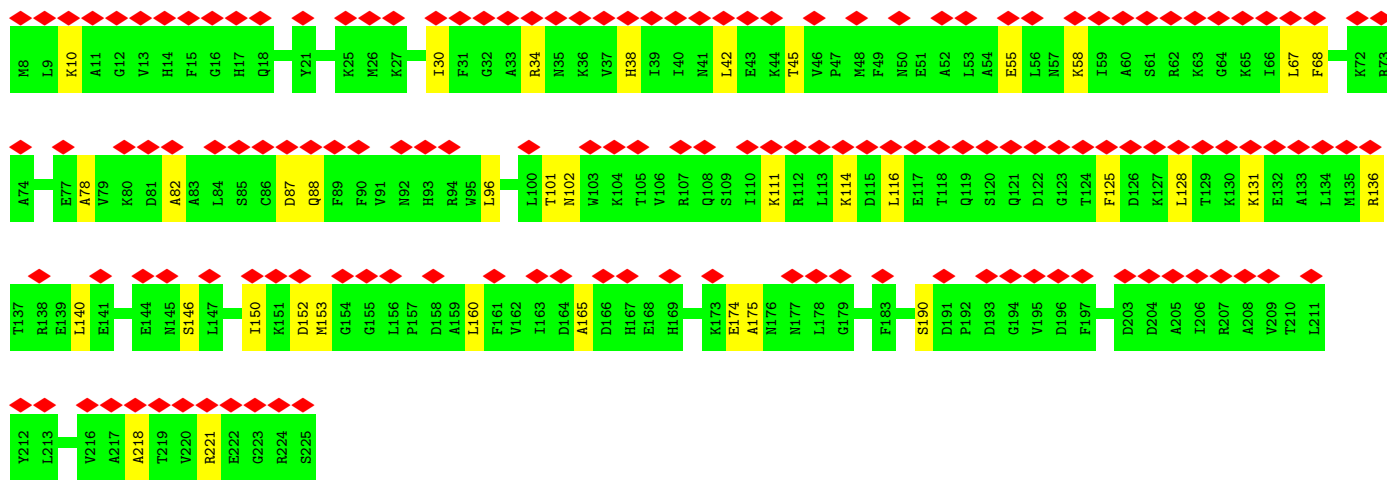
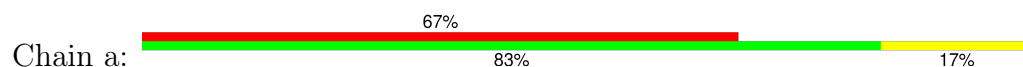
- Molecule 28: 50S ribosomal protein L29



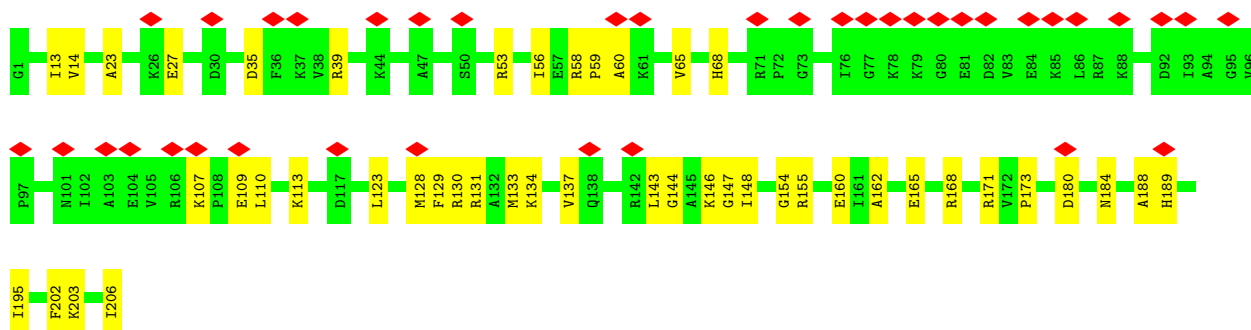
- Molecule 29: 50S ribosomal protein L30



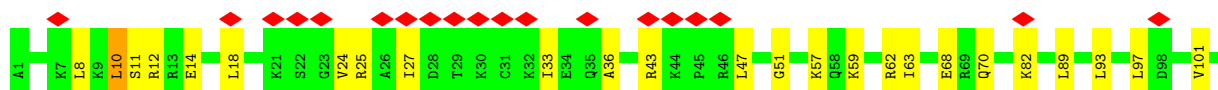
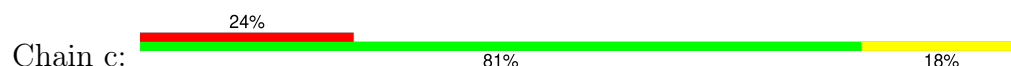
- Molecule 30: 30S ribosomal protein S2

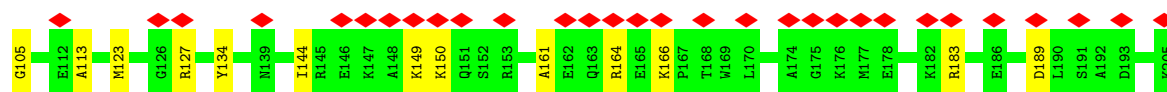


- Molecule 31: 30S ribosomal protein S3

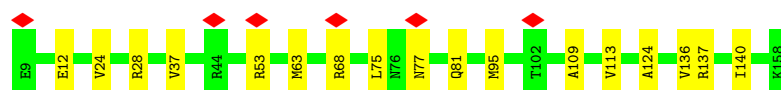
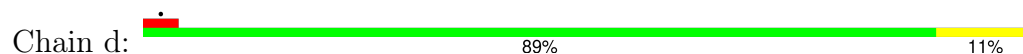


- Molecule 32: 30S ribosomal protein S4

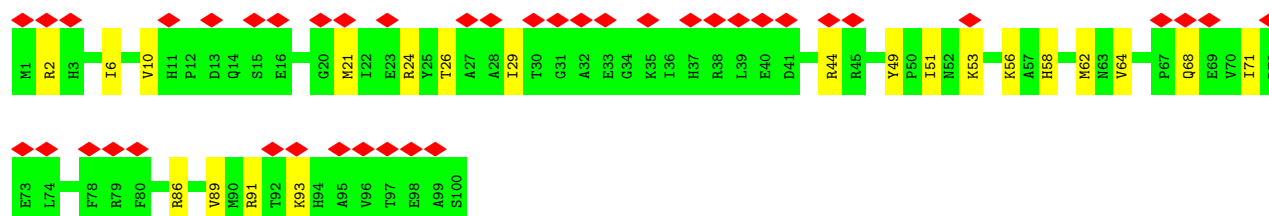
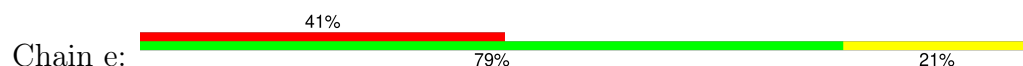




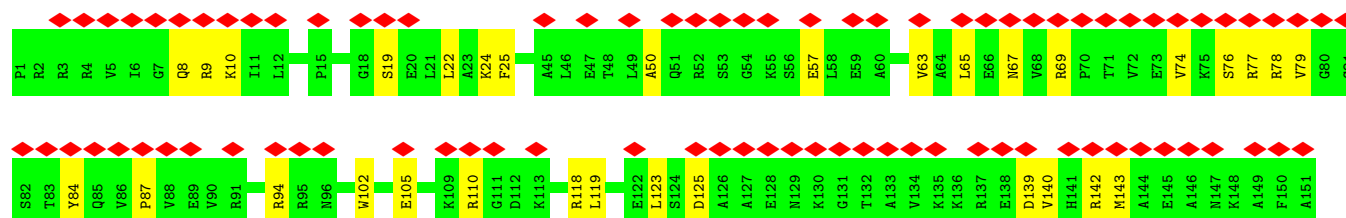
- Molecule 33: 30S ribosomal protein S5



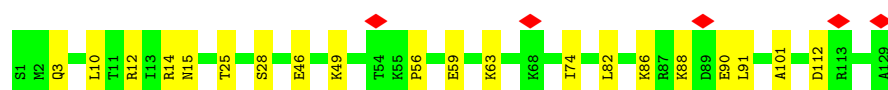
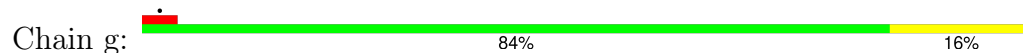
- Molecule 34: 30S ribosomal protein S6, non-modified isoform



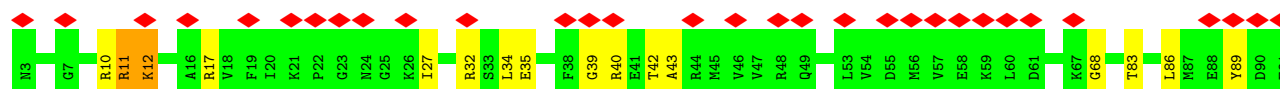
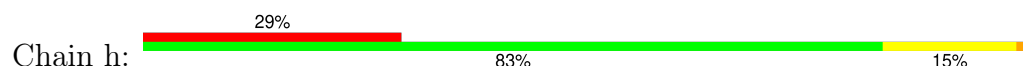
- Molecule 35: 30S ribosomal protein S7

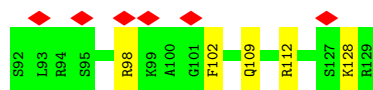


- Molecule 36: 30S ribosomal protein S8

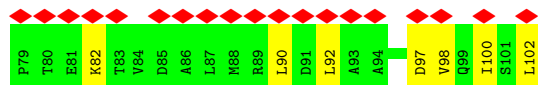
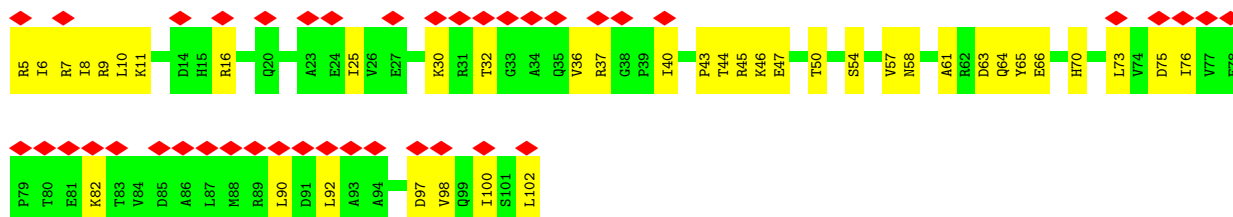
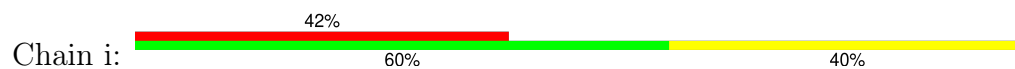


- Molecule 37: 30S ribosomal protein S9

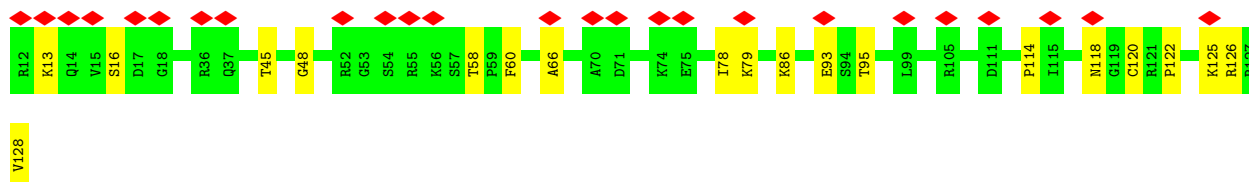
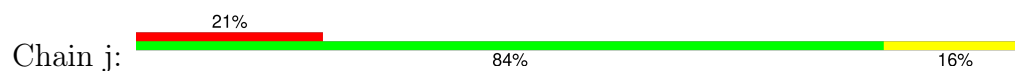




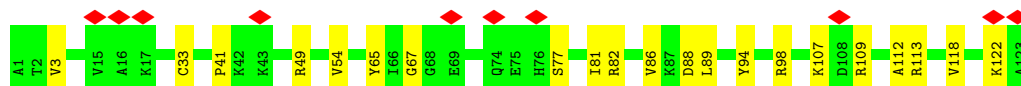
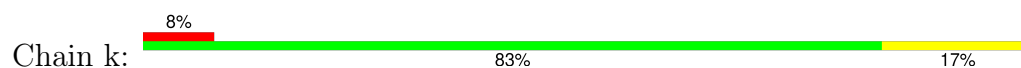
- Molecule 38: 30S ribosomal protein S10



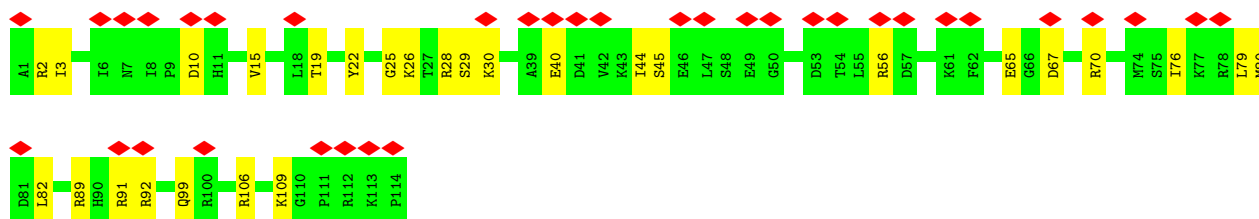
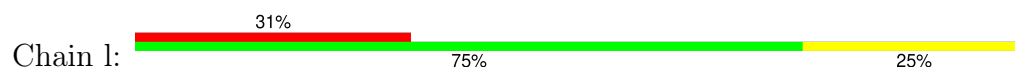
- Molecule 39: 30S ribosomal protein S11



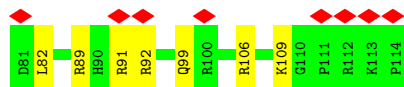
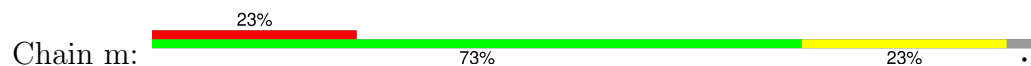
- Molecule 40: 30S ribosomal protein S12

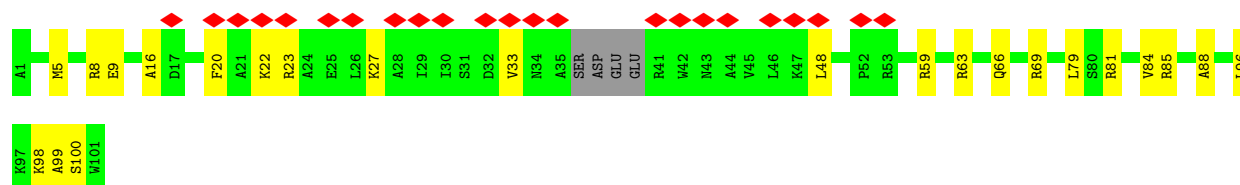


- Molecule 41: 30S ribosomal protein S13

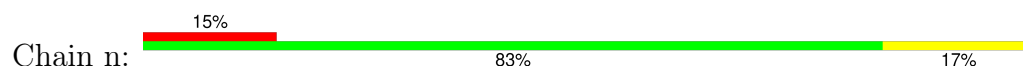


- Molecule 42: 30S ribosomal protein S14

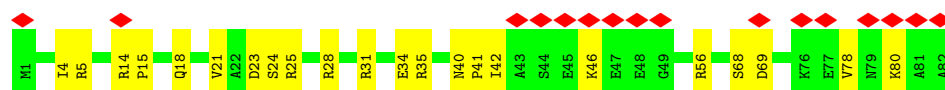
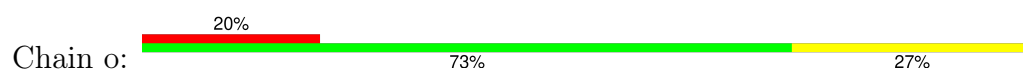




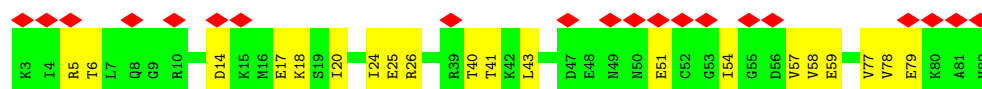
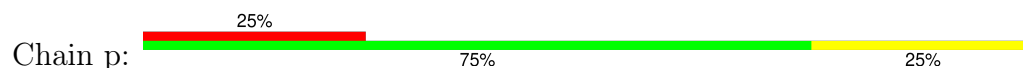
- Molecule 43: 30S ribosomal protein S15



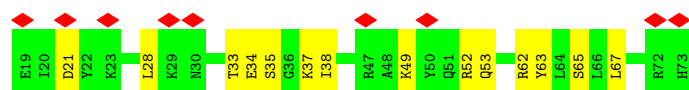
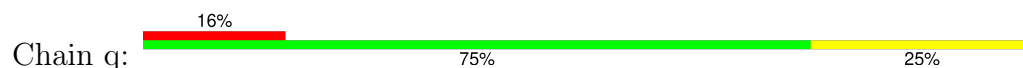
- Molecule 44: 30S ribosomal protein S16



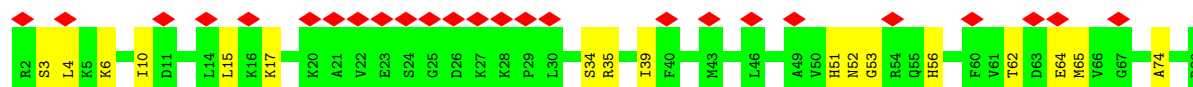
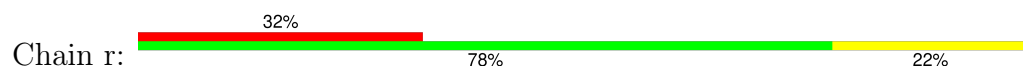
- Molecule 45: 30S ribosomal protein S17



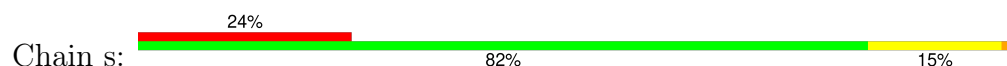
- Molecule 46: 30S ribosomal protein S18



- Molecule 47: 30S ribosomal protein S19

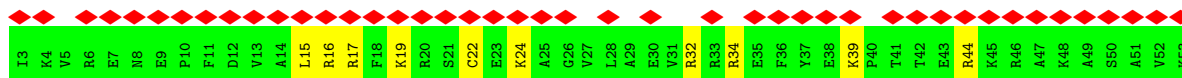
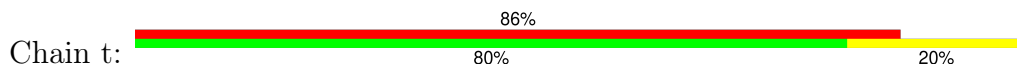


- Molecule 48: 30S ribosomal protein S20

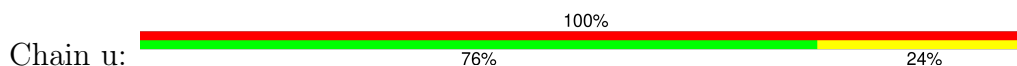




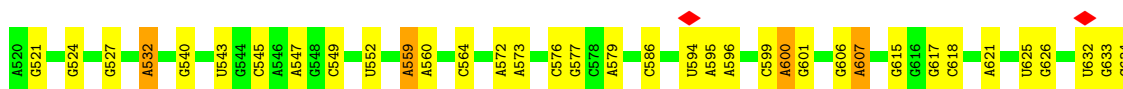
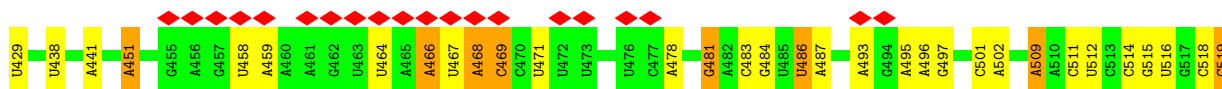
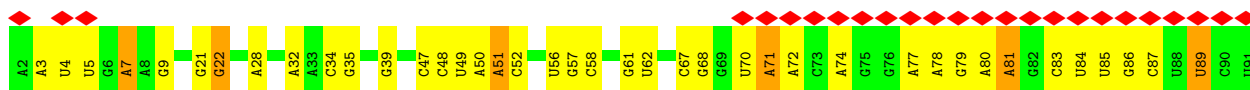
• Molecule 49: 30S ribosomal protein S21 (Fragment)



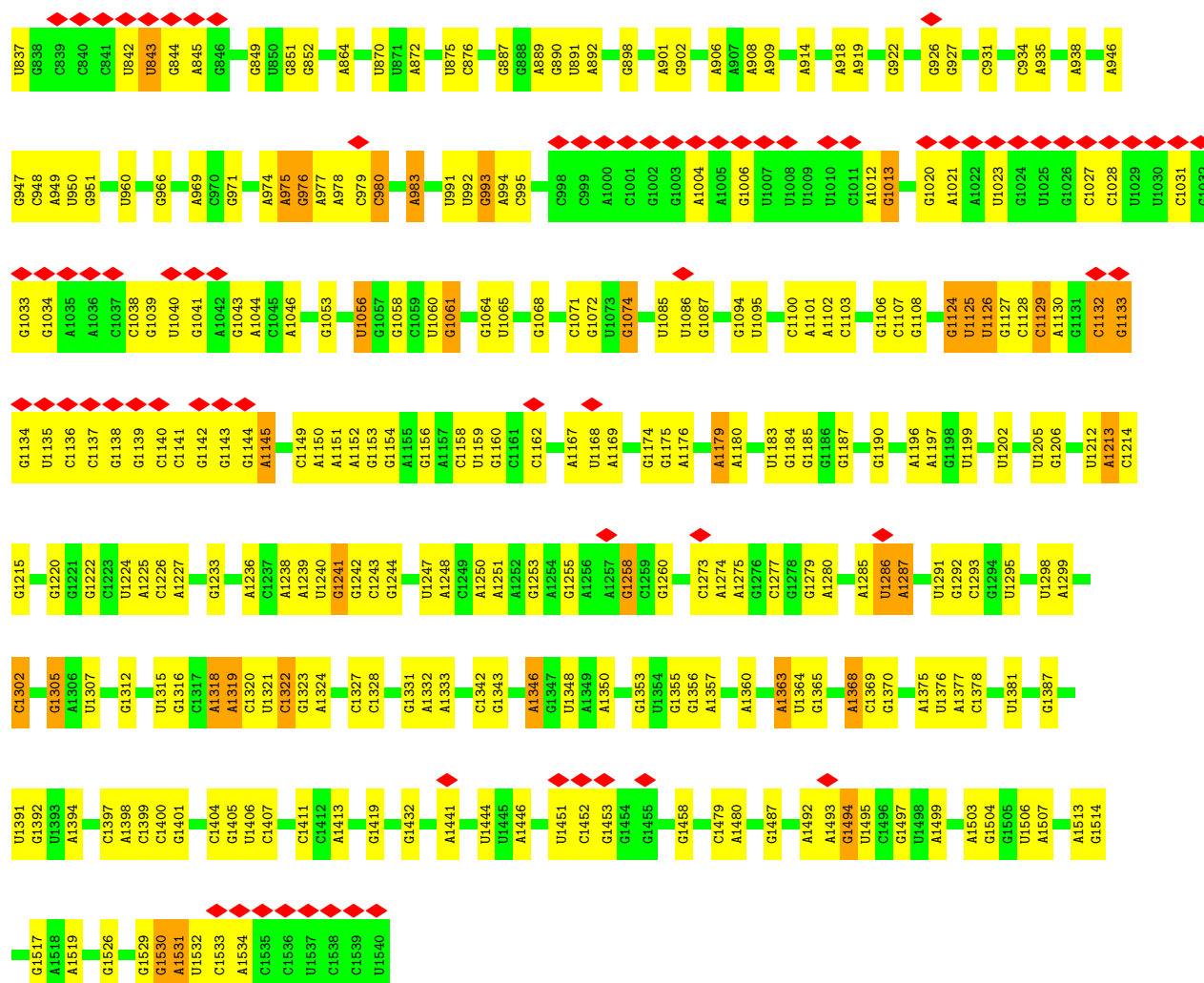
• Molecule 50: Transcription termination/antitermination protein NusG



• Molecule 51: 16s RNA



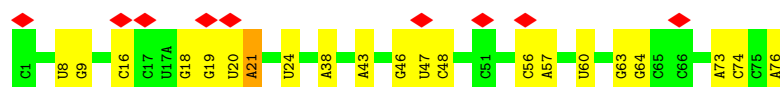
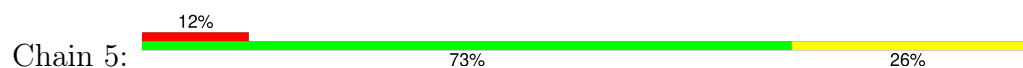




- Molecule 52: lmRNA



- Molecule 53: tRNA



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	120000	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	58	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	1.734	Depositor
Minimum map value	-0.026	Depositor
Average map value	0.007	Depositor
Map value standard deviation	0.051	Depositor
Recommended contour level	0.124	Depositor
Map size ( $\text{\AA}$ )	332.0, 332.0, 332.0	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles ( $^\circ$ )	90.0, 90.0, 90.0	wwPDB
Pixel spacing ( $\text{\AA}$ )	0.83, 0.83, 0.83	Depositor

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	0	0.24	0/450	0.53	0/599
2	1	0.19	0/417	0.49	0/556
3	2	0.28	0/380	0.59	0/498
4	3	0.29	0/513	0.68	0/676
5	4	0.28	0/303	0.73	1/397 (0.3%)
6	A	0.20	0/2800	0.35	0/4367
7	B	0.25	0/69796	0.37	3/108888 (0.0%)
8	C	0.29	0/2122	0.61	0/2854
9	D	0.28	0/1586	0.64	0/2134
10	E	0.28	0/1571	0.64	0/2113
11	F	0.23	0/1444	0.64	0/1937
12	G	0.22	0/1343	0.57	2/1816 (0.1%)
13	J	0.26	0/1152	0.60	0/1551
14	K	0.33	0/940	0.72	0/1260
15	L	0.24	0/1054	0.58	2/1403 (0.1%)
16	M	0.25	0/1093	0.53	0/1460
17	N	0.27	0/974	0.60	0/1303
18	O	0.22	0/902	0.50	0/1209
19	P	0.27	0/929	0.72	3/1242 (0.2%)
20	Q	0.26	0/960	0.54	0/1278
21	R	0.24	0/829	0.54	0/1107
22	S	0.27	0/864	0.57	0/1156
23	T	0.23	0/745	0.61	1/996 (0.1%)
24	U	0.26	0/788	0.62	0/1053
25	V	0.19	0/766	0.51	0/1025
26	W	0.26	0/603	0.76	0/797
27	X	0.23	0/635	0.53	0/848
28	Y	0.21	0/510	0.58	0/677
29	Z	0.23	0/453	0.46	0/605
30	a	0.25	0/1736	0.65	0/2338
31	b	0.26	0/1652	0.66	2/2225 (0.1%)
32	c	0.24	0/1665	0.61	0/2227
33	d	0.27	0/1119	0.66	0/1504
34	e	0.23	0/836	0.65	0/1128

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
35	f	0.20	0/1196	0.56	0/1602
36	g	0.24	0/989	0.56	0/1326
37	h	0.25	0/1034	0.65	2/1375 (0.1%)
38	i	0.26	0/797	0.57	0/1077
39	j	0.23	0/893	0.57	0/1205
40	k	0.27	0/969	0.58	0/1300
41	l	0.21	0/893	0.55	0/1193
42	m	0.24	0/785	0.58	0/1043
43	n	0.22	0/722	0.52	0/964
44	o	0.23	0/659	0.52	0/884
45	p	0.26	0/658	0.69	0/881
46	q	0.19	0/463	0.51	0/621
47	r	0.19	0/653	0.51	0/877
48	s	0.25	0/671	0.61	2/888 (0.2%)
49	t	0.28	0/431	0.63	0/570
50	u	0.24	0/477	0.60	0/642
51	v	0.27	1/36963 (0.0%)	0.38	3/57662 (0.0%)
52	x	0.16	0/289	0.29	0/449
53	5	0.17	0/1832	0.32	0/2855
All	All	0.25	1/155304 (0.0%)	0.44	21/232641 (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
23	T	0	1
30	a	0	1
31	b	0	1
37	h	0	1
39	j	0	1
All	All	0	5

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
51	v	1531	A	O3'-P	-28.53	1.18	1.61

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
51	v	1531	A	P-O3'-C3'	-12.35	101.68	120.20
19	P	4	ILE	CA-C-N	6.90	134.72	121.54
19	P	4	ILE	C-N-CA	6.90	134.72	121.54
5	4	3	VAL	CA-CB-CG1	6.59	121.61	110.40
37	h	11	ARG	CA-C-N	6.33	133.62	121.54
37	h	11	ARG	C-N-CA	6.33	133.62	121.54
51	v	1531	A	OP1-P-O3'	-5.89	90.34	108.00
51	v	1213	A	P-O3'-C3'	5.58	128.56	120.20
19	P	5	LYS	CA-CB-CG	5.46	125.03	114.10
12	G	46	ASP	CA-C-N	5.45	135.75	125.66
12	G	46	ASP	C-N-CA	5.45	135.75	125.66
7	B	490	C	P-O3'-C3'	5.35	128.23	120.20
15	L	68	SER	CA-C-N	5.26	130.81	122.61
15	L	68	SER	C-N-CA	5.26	130.81	122.61
7	B	670	A	P-O3'-C3'	5.22	128.04	120.20
31	b	59	PRO	CA-C-N	5.18	131.91	123.93
31	b	59	PRO	C-N-CA	5.18	131.91	123.93
23	T	28	ASN	N-CA-C	5.01	121.48	110.80
48	s	67	HIS	CA-C-N	5.01	131.11	121.54
48	s	67	HIS	C-N-CA	5.01	131.11	121.54
7	B	1652	A	C2'-C3'-O3'	5.01	121.21	113.70

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
23	T	1	MET	Peptide
30	a	152	ASP	Peptide
31	b	60	ALA	Peptide
37	h	11	ARG	Peptide
39	j	118	ASN	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	0	444	0	461	11	0
2	1	410	0	440	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	2	377	0	418	5	0
4	3	504	0	574	9	0
5	4	302	0	343	3	0
6	A	2504	0	1271	14	0
7	B	62317	0	31345	324	0
8	C	2083	0	2157	31	0
9	D	1565	0	1616	11	0
10	E	1552	0	1619	19	0
11	F	1420	0	1460	37	0
12	G	1323	0	1374	20	0
13	J	1129	0	1162	24	0
14	K	931	0	1003	25	0
15	L	1045	0	1117	15	0
16	M	1074	0	1157	14	0
17	N	961	0	1000	12	0
18	O	892	0	923	12	0
19	P	917	0	965	17	0
20	Q	947	0	1022	14	0
21	R	816	0	839	8	0
22	S	857	0	922	13	0
23	T	739	0	807	14	0
24	U	780	0	834	8	0
25	V	753	0	780	9	0
26	W	596	0	610	21	0
27	X	625	0	655	7	0
28	Y	509	0	543	5	0
29	Z	449	0	491	2	0
30	a	1705	0	1732	22	0
31	b	1625	0	1699	28	0
32	c	1643	0	1710	21	0
33	d	1106	0	1148	10	0
34	e	818	0	808	14	0
35	f	1182	0	1240	18	0
36	g	979	0	1034	13	0
37	h	1022	0	1070	16	0
38	i	787	0	828	33	0
39	j	877	0	887	15	0
40	k	955	0	1019	15	0
41	l	884	0	944	19	0
42	m	774	0	827	18	0
43	n	714	0	737	10	0
44	o	649	0	666	17	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
45	p	649	0	691	13	0
46	q	456	0	478	11	0
47	r	638	0	665	12	0
48	s	665	0	714	10	0
49	t	426	0	449	10	0
50	u	468	0	458	10	0
51	v	33012	0	16619	230	0
52	x	257	0	133	0	0
53	5	1640	0	837	5	0
All	All	142752	0	95301	1086	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 5.

All (1086) 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)
7:B:1311:G:H21	7:B:1603:A:H62	1.13	0.95
7:B:1021:A:H62	7:B:1141:U:H3	1.18	0.91
7:B:2735:G:H1	7:B:2769:U:H3	1.01	0.89
7:B:1311:G:N2	7:B:1603:A:H62	1.71	0.88
7:B:1483:G:H1	7:B:1506:U:H3	1.27	0.81
7:B:1664:A:H61	7:B:1996:C:H42	1.30	0.79
7:B:2099:U:H3	7:B:2190:G:H1	1.33	0.76
51:v:1156:G:H21	51:v:1179:A:H61	1.33	0.73
7:B:2125:G:H21	7:B:2173:A:N6	1.86	0.73
6:A:22:U:H3	6:A:61:G:H1	1.35	0.70
51:v:1138:G:C2	51:v:1140:C:C2	2.79	0.70
42:m:16:ALA:O	42:m:20:PHE:HB3	1.93	0.69
42:m:100:SER:HB3	51:v:1187:G:H21	1.58	0.69
31:b:107:LYS:HB3	31:b:110:LEU:HB2	1.73	0.69
19:P:90:ALA:HB2	19:P:110:LYS:HB2	1.75	0.68
11:F:147:ARG:HG3	11:F:149:ARG:H	1.59	0.68
11:F:49:LEU:HD12	11:F:64:PRO:HG2	1.77	0.67
42:m:9:GLU:HG3	42:m:63:ARG:HD2	1.77	0.67
22:S:82:MET:HG3	22:S:98:LYS:HB2	1.78	0.66
7:B:1311:G:H21	7:B:1603:A:N6	1.89	0.66
7:B:2125:G:N2	7:B:2173:A:N6	2.44	0.66
30:a:67:LEU:HD13	30:a:153:MET:HE1	1.78	0.66
37:h:12:LYS:HB2	37:h:109:GLN:HG3	1.77	0.65
37:h:12:LYS:HD3	37:h:109:GLN:HA	1.78	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:d:75:LEU:HG	33:d:77:ASN:H	1.62	0.65
7:B:981:A:H8	7:B:2027:G:H21	1.44	0.65
7:B:1664:A:H61	7:B:1996:C:N4	1.94	0.64
44:o:15:PRO:HG2	44:o:41:PRO:HG2	1.80	0.64
35:f:50:ALA:HB2	35:f:57:GLU:HB3	1.80	0.64
49:t:22:CYS:HB2	49:t:24:LYS:HD2	1.79	0.63
11:F:175:PRO:HB2	11:F:177:ARG:HH12	1.63	0.63
26:W:30:VAL:HG13	26:W:59:PHE:HB2	1.80	0.63
31:b:147:GLY:HA3	31:b:202:PHE:HB3	1.81	0.63
33:d:137:ARG:HA	33:d:140:ILE:HB	1.81	0.62
18:O:2:ASP:N	18:O:5:SER:HG	1.97	0.62
51:v:1156:G:N2	51:v:1179:A:H61	1.97	0.62
7:B:1653:G:H3'	17:N:2:ARG:HG2	1.81	0.62
6:A:55:U:H1'	11:F:25:MET:HE1	1.82	0.62
40:k:113:ARG:HG2	40:k:118:VAL:HB	1.82	0.62
37:h:112:ARG:NH2	51:v:1368:A:OP1	2.33	0.61
39:j:86:LYS:HD3	39:j:114:PRO:HD3	1.81	0.61
31:b:13:ILE:HG22	31:b:14:VAL:HG13	1.81	0.61
4:3:51:LYS:HA	4:3:54:LEU:HB2	1.81	0.61
51:v:1531:A:H2'	51:v:1532:U:O4'	2.00	0.61
51:v:532:A:N6	51:v:1206:G:O2'	2.34	0.61
7:B:1365:A:H5''	27:X:27:ARG:HH12	1.65	0.61
51:v:1132:C:N4	51:v:1133:G:O6	2.33	0.61
21:R:2:TYR:HB2	21:R:42:ALA:HB3	1.82	0.61
26:W:23:LYS:HD2	26:W:68:PHE:H	1.66	0.61
9:D:131:ASP:O	9:D:136:ASN:ND2	2.34	0.60
10:E:164:LEU:HB2	10:E:167:VAL:HG22	1.84	0.60
22:S:16:LYS:HA	22:S:19:LEU:HD12	1.82	0.60
49:t:15:LEU:HD22	49:t:19:LYS:HE2	1.83	0.60
51:v:79:G:H2'	51:v:80:A:H8	1.65	0.60
7:B:1060:U:H4'	7:B:1061:U:H3'	1.84	0.60
7:B:2864:G:OP1	19:P:112:ARG:NH1	2.35	0.60
7:B:2682:A:H61	7:B:2728:U:H1'	1.67	0.60
39:j:45:THR:HG23	39:j:48:GLY:H	1.67	0.60
47:r:51:HIS:NE2	47:r:53:GLY:O	2.32	0.60
7:B:2822:G:O6	17:N:2:ARG:NH1	2.35	0.60
16:M:64:TRP:HB2	16:M:104:GLU:HB2	1.84	0.60
27:X:4:CYS:HB3	27:X:9:LYS:H	1.66	0.60
44:o:40:ASN:ND2	44:o:42:ILE:O	2.34	0.60
32:c:10:LEU:HB2	32:c:62:ARG:HD3	1.84	0.59
51:v:980:C:N4	51:v:1318:A:N1	2.50	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:F:68:LYS:HA	11:F:83:PRO:HA	1.84	0.59
11:F:103:ILE:O	11:F:107:VAL:HB	2.03	0.59
51:v:1130:A:N1	51:v:1144:G:O6	2.35	0.59
31:b:53:ARG:HB3	31:b:68:HIS:HD2	1.67	0.59
51:v:1138:G:N1	51:v:1140:C:N3	2.51	0.59
9:D:46:ARG:NH2	9:D:87:GLY:O	2.35	0.59
14:K:70:ARG:HE	14:K:76:ILE:HD11	1.68	0.59
8:C:131:MET:HE1	8:C:140:VAL:HG21	1.85	0.59
43:n:31:LEU:HD22	43:n:58:MET:HG2	1.85	0.59
16:M:38:ARG:HG3	16:M:98:PRO:HD3	1.84	0.59
19:P:71:ARG:HH21	19:P:73:PHE:HB3	1.68	0.59
22:S:24:ILE:HD13	22:S:36:LEU:HD11	1.84	0.59
38:i:64:GLN:HG3	42:m:99:ALA:HB3	1.82	0.59
45:p:78:VAL:HG12	45:p:79:GLU:HG2	1.84	0.59
24:U:20:LYS:HD2	24:U:38:ILE:HG12	1.85	0.59
7:B:563:A:OP2	21:R:79:ARG:NH2	2.33	0.58
11:F:64:PRO:HB3	11:F:88:VAL:HB	1.85	0.58
7:B:586:A:H5'	10:E:84:THR:HG21	1.83	0.58
32:c:57:LYS:NZ	32:c:68:GLU:OE1	2.36	0.58
41:l:3:ILE:HG23	41:l:56:ARG:HG2	1.85	0.58
7:B:2103:C:H42	7:B:2187:U:H3	1.50	0.58
34:e:51:ILE:HG21	34:e:86:ARG:HH21	1.68	0.58
51:v:219:U:H2'	51:v:220:G:H8	1.68	0.58
7:B:1059:G:N1	7:B:1080:A:C2	2.72	0.58
7:B:780:G:N1	8:C:228:ASP:OD1	2.37	0.58
35:f:24:LYS:NZ	51:v:1375:A:OP1	2.36	0.58
51:v:1006:G:H1	51:v:1023:U:H3	1.52	0.58
7:B:1539:U:H2'	7:B:1540:G:H8	1.69	0.58
14:K:106:LEU:HB3	14:K:111:PHE:HB3	1.84	0.58
26:W:50:VAL:H	26:W:61:LYS:HE3	1.68	0.58
7:B:856:G:H4'	26:W:23:LYS:HD3	1.84	0.58
11:F:15:LEU:HG	11:F:21:TYR:H	1.69	0.58
49:t:39:LYS:NZ	51:v:1530:G:N7	2.52	0.57
7:B:2641:G:H5''	13:J:78:THR:HB	1.86	0.57
7:B:793:A:OP2	7:B:2071:A:O2'	2.21	0.57
7:B:1055:G:N2	7:B:1085:A:O2'	2.37	0.57
38:i:66:GLU:HB2	42:m:99:ALA:HB2	1.86	0.57
42:m:22:LYS:HD2	42:m:23:ARG:HG2	1.86	0.57
47:r:35:ARG:NH2	47:r:74:ALA:O	2.38	0.57
36:g:14:ARG:NH1	51:v:875:U:O2'	2.37	0.57
44:o:5:ARG:NH2	44:o:23:ASP:O	2.38	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:B:2861:U:H2'	7:B:2862:G:H8	1.70	0.57
8:C:175:LEU:HD12	8:C:179:GLU:HB3	1.87	0.57
31:b:146:LYS:NZ	31:b:203:LYS:O	2.37	0.57
11:F:90:LEU:HB3	11:F:95:MET:HB2	1.85	0.57
12:G:22:VAL:HA	12:G:36:LEU:HD22	1.86	0.57
44:o:31:ARG:HB3	51:v:310:G:H5''	1.87	0.57
1:0:53:VAL:HG23	1:0:54:ILE:HG12	1.86	0.57
8:C:52:HIS:HA	8:C:216:ARG:HB2	1.86	0.57
44:o:14:ARG:HH22	51:v:617:G:H21	1.52	0.57
51:v:1175:G:H2'	51:v:1176:A:H8	1.69	0.57
13:J:4:PHE:O	20:Q:63:ARG:NH2	2.38	0.56
38:i:7:ARG:NH2	51:v:1126:U:OP1	2.37	0.56
3:2:1:MET:HE2	7:B:752:A:H3'	1.86	0.56
7:B:1275:A:OP2	7:B:1646:C:N4	2.38	0.56
12:G:88:LEU:HG	12:G:161:VAL:HG12	1.86	0.56
51:v:995:C:N3	51:v:1046:A:O2'	2.38	0.56
51:v:1124:G:O2'	51:v:1127:G:O6	2.23	0.56
7:B:1794:A:HO2'	7:B:1900:A:HO2'	1.53	0.56
14:K:79:ASP:OD2	19:P:61:ARG:NH2	2.36	0.56
32:c:18:LEU:HD13	32:c:63:ILE:HG13	1.87	0.56
7:B:1664:A:N6	7:B:1996:C:H42	2.00	0.56
35:f:19:SER:HB3	35:f:22:LEU:HB2	1.86	0.56
39:j:122:PRO:HD2	49:t:34:ARG:HD3	1.88	0.56
7:B:569:U:O2'	7:B:983:A:N1	2.38	0.56
7:B:587:C:OP2	15:L:21:ARG:NH2	2.39	0.56
50:u:167:ARG:NH1	50:u:169:THR:OG1	2.39	0.56
51:v:1124:G:N2	51:v:1125:U:O4	2.37	0.56
7:B:1338:G:H4'	23:T:18:GLU:HG3	1.88	0.56
25:V:79:ARG:HA	25:V:86:LEU:HA	1.88	0.56
46:q:37:LYS:HB3	51:v:719:C:H1'	1.88	0.56
7:B:713:G:H21	7:B:718:A:H2	1.52	0.56
14:K:102:VAL:HG13	14:K:106:LEU:HD13	1.87	0.56
26:W:17:ALA:HA	26:W:36:ILE:HB	1.87	0.56
36:g:12:ARG:NH1	51:v:825:A:O2'	2.39	0.56
7:B:1361:G:HO2'	7:B:2215:C:HO2'	1.52	0.56
11:F:47:LYS:HE3	11:F:147:ARG:HB2	1.88	0.56
35:f:110:ARG:NH2	35:f:125:ASP:OD2	2.39	0.56
12:G:17:LYS:HD3	12:G:26:LYS:HE3	1.88	0.56
14:K:14:GLY:HA2	14:K:51:VAL:HG21	1.88	0.56
16:M:14:LYS:O	16:M:71:LYS:NZ	2.39	0.56
30:a:165:ALA:HB3	30:a:190:SER:HB2	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
51:v:978:A:H2'	51:v:980:C:H41	1.70	0.56
7:B:2848:G:O2'	7:B:2867:G:N2	2.36	0.55
38:i:44:THR:HG22	38:i:70:HIS:HA	1.88	0.55
7:B:1597:A:H5''	7:B:1598:A:H5'	1.88	0.55
23:T:11:LEU:HA	23:T:34:VAL:HG12	1.88	0.55
38:i:64:GLN:NE2	38:i:65:TYR:O	2.40	0.55
51:v:1251:A:N3	51:v:1369:C:O2'	2.34	0.55
51:v:1407:C:H5	51:v:1494:G:H22	1.53	0.55
4:3:6:VAL:HG12	4:3:9:ALA:H	1.70	0.55
41:l:82:LEU:HD23	47:r:65:MET:HE2	1.87	0.55
7:B:663:G:H5''	15:L:17:LYS:HD3	1.88	0.55
7:B:1420:A:H5''	7:B:2211:A:H62	1.72	0.55
23:T:24:MET:O	23:T:29:THR:N	2.37	0.55
30:a:101:THR:HG23	30:a:174:GLU:HG2	1.88	0.55
35:f:77:ARG:HB3	35:f:84:TYR:HB3	1.89	0.55
51:v:28:A:O2'	51:v:296:U:OP1	2.25	0.55
7:B:2314:A:OP2	11:F:70:ARG:NH1	2.40	0.55
16:M:103:TYR:HE2	16:M:124:LEU:HD11	1.72	0.55
36:g:88:LYS:HA	36:g:91:LEU:HD23	1.88	0.55
7:B:2081:U:H3	7:B:2239:G:H1	1.54	0.55
41:l:28:ARG:NH1	51:v:1328:C:O2'	2.40	0.55
51:v:938:A:N3	51:v:1376:U:O2'	2.37	0.55
7:B:1826:G:O2'	7:B:1971:U:OP2	2.25	0.55
13:J:6:ALA:HB2	13:J:44:TYR:HB3	1.89	0.55
31:b:155:ARG:NH2	31:b:160:GLU:OE1	2.39	0.55
7:B:1527:G:H21	7:B:1545:A:H62	1.55	0.55
38:i:10:LEU:HB3	38:i:98:VAL:HG23	1.88	0.55
7:B:1680:U:O2	7:B:1763:G:O2'	2.22	0.55
8:C:243:PRO:O	8:C:250:GLN:NE2	2.40	0.55
51:v:674:G:H2'	51:v:675:A:H8	1.72	0.55
7:B:2822:G:OP1	9:D:164:GLN:NE2	2.39	0.54
18:O:62:LEU:HD22	18:O:70:ALA:HA	1.88	0.54
44:o:25:ARG:O	51:v:110:C:O2'	2.25	0.54
45:p:24:ILE:HD12	45:p:43:LEU:HD13	1.89	0.54
6:A:39:A:O2'	6:A:46:A:N1	2.40	0.54
7:B:1059:G:C6	7:B:1080:A:N1	2.75	0.54
13:J:40:HIS:O	20:Q:70:GLN:NE2	2.40	0.54
7:B:24:G:O2'	22:S:78:GLU:O	2.25	0.54
7:B:1059:G:O6	7:B:1080:A:N1	2.41	0.54
13:J:35:ARG:HB2	13:J:54:ILE:HD11	1.89	0.54
31:b:110:LEU:HD21	31:b:144:GLY:HA3	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:f:65:LEU:HD23	35:f:69:ARG:HH12	1.72	0.54
38:i:58:ASN:OD1	51:v:1060:U:O2'	2.22	0.54
41:l:22:TYR:HB3	41:l:65:GLU:HB3	1.90	0.54
11:F:38:GLY:O	11:F:147:ARG:NH2	2.40	0.54
12:G:44:HIS:HB3	12:G:49:LEU:HD13	1.90	0.54
32:c:24:VAL:HG21	51:v:409:U:H5''	1.90	0.54
34:e:10:VAL:HG23	34:e:58:HIS:HB3	1.89	0.54
7:B:2885:G:O2'	7:B:2886:A:N3	2.40	0.54
13:J:96:ARG:NH1	13:J:98:GLU:OE1	2.40	0.54
50:u:148:VAL:HA	50:u:160:VAL:HA	1.88	0.54
7:B:2103:C:N4	7:B:2187:U:H3	2.05	0.54
38:i:57:VAL:O	38:i:58:ASN:ND2	2.40	0.54
51:v:1140:C:OP2	51:v:1141:C:N4	2.32	0.54
7:B:2258:C:O2'	7:B:2427:C:OP2	2.26	0.54
17:N:54:LEU:HD21	17:N:65:LEU:HB3	1.90	0.54
45:p:17:GLU:OE1	51:v:254:G:N2	2.38	0.54
7:B:820:A:H4'	7:B:836:G:H22	1.73	0.54
14:K:75:VAL:H	19:P:72:VAL:HG22	1.73	0.54
17:N:100:CYS:SG	17:N:101:GLY:N	2.78	0.54
30:a:160:LEU:HD22	30:a:175:ALA:HB2	1.90	0.54
13:J:41:LYS:HD2	13:J:50:THR:HG22	1.90	0.54
33:d:68:ARG:NH1	51:v:1074:G:OP1	2.41	0.54
35:f:76:SER:HB3	35:f:78:ARG:HD3	1.90	0.54
44:o:78:VAL:O	44:o:80:LYS:NZ	2.40	0.54
31:b:168:ARG:HH21	31:b:171:ARG:HA	1.73	0.54
51:v:843:U:OP1	51:v:844:G:N2	2.41	0.54
7:B:2330:G:O2'	26:W:39:GLN:NE2	2.41	0.53
32:c:12:ARG:NH2	32:c:36:ALA:O	2.39	0.53
40:k:113:ARG:NH2	51:v:501:C:OP1	2.39	0.53
51:v:413:G:N2	51:v:428:G:O2'	2.41	0.53
7:B:2619:C:OP1	9:D:157:LYS:NZ	2.41	0.53
7:B:2674:G:H4'	14:K:29:ARG:HD2	1.90	0.53
7:B:626:A:OP1	7:B:654:A:N6	2.41	0.53
37:h:98:ARG:NH2	51:v:1180:A:OP1	2.40	0.53
43:n:37:HIS:NE2	51:v:740:U:OP1	2.41	0.53
3:2:43:THR:HG22	3:2:46:LYS:H	1.73	0.53
38:i:9:ARG:NH2	51:v:1126:U:O4	2.41	0.53
53:5:63:G:H2'	53:5:64:G:H8	1.74	0.53
7:B:704:G:O2'	7:B:727:A:N6	2.41	0.53
23:T:91:GLN:OE1	23:T:94:ASP:N	2.42	0.53
31:b:56:ILE:HG12	31:b:65:VAL:HG12	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:b:168:ARG:HH22	51:v:1107:C:H5'	1.73	0.53
36:g:3:GLN:NE2	51:v:586:C:O2	2.42	0.53
41:l:67:ASP:OD1	41:l:70:ARG:NH2	2.39	0.53
7:B:578:G:OP1	7:B:1255:U:O2'	2.25	0.53
7:B:1028:A:OP2	7:B:1126:A:N6	2.42	0.53
7:B:2540:C:O2'	7:B:2740:A:N3	2.41	0.53
17:N:36:THR:OG1	17:N:37:THR:N	2.42	0.53
7:B:660:C:O2'	15:L:13:LYS:NZ	2.41	0.53
42:m:5:MET:SD	42:m:8:ARG:NH2	2.78	0.53
5:4:18:LYS:HG3	5:4:23:ILE:HG13	1.90	0.53
7:B:560:C:O2	20:Q:47:ARG:NH2	2.40	0.53
7:B:693:A:O2'	7:B:1353:A:N3	2.40	0.53
14:K:15:ALA:HB1	14:K:46:ILE:H	1.74	0.53
51:v:401:C:O2'	51:v:621:A:N3	2.37	0.53
10:E:139:LYS:NZ	10:E:144:GLU:OE2	2.38	0.53
36:g:101:ALA:HB3	36:g:112:ASP:HB3	1.91	0.53
51:v:744:C:H2'	51:v:745:G:H8	1.73	0.53
7:B:2469:A:N6	7:B:2481:G:O2'	2.42	0.52
13:J:14:ASP:OD1	13:J:14:ASP:N	2.41	0.52
7:B:577:G:O2'	7:B:1254:A:OP1	2.27	0.52
38:i:61:ALA:HB2	51:v:1061:G:H5'	1.92	0.52
17:N:54:LEU:HD23	17:N:66:ALA:HB2	1.91	0.52
47:r:17:LYS:NZ	51:v:1013:G:OP1	2.42	0.52
50:u:157:ARG:HE	50:u:172:GLU:HG2	1.74	0.52
7:B:30:G:O2'	7:B:1214:A:N3	2.37	0.52
38:i:6:ILE:HD13	50:u:140:PRO:HD3	1.91	0.52
2:1:21:THR:HG21	7:B:2419:U:H4'	1.91	0.52
7:B:1798:U:O2'	7:B:1802:A:N3	2.42	0.52
16:M:41:LEU:HD13	16:M:96:ILE:HG13	1.90	0.52
51:v:216:U:H4'	51:v:464:U:H4'	1.89	0.52
7:B:2125:G:N2	7:B:2173:A:C6	2.77	0.52
11:F:31:GLU:OE2	11:F:156:THR:N	2.41	0.52
7:B:987:C:O2'	7:B:1000:A:N3	2.39	0.52
18:O:8:ILE:O	18:O:12:THR:OG1	2.28	0.52
31:b:128:MET:H	31:b:131:ARG:HH21	1.58	0.52
42:m:69:ARG:NH2	51:v:974:A:OP1	2.43	0.52
51:v:1315:U:O2'	51:v:1360:A:N3	2.42	0.52
7:B:1817:G:OP1	8:C:86:ARG:NH2	2.42	0.52
7:B:2692:G:N3	7:B:2847:U:O2'	2.42	0.52
18:O:31:THR:O	18:O:102:ARG:NH2	2.39	0.52
31:b:180:ASP:HB2	31:b:206:ILE:HD11	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
51:v:1006:G:N2	51:v:1023:U:O2	2.38	0.52
2:l:34:GLU:HG2	2:l:49:LYS:HB2	1.91	0.52
7:B:2314:A:HO2'	11:F:156:THR:HG1	1.58	0.52
31:b:35:ASP:OD1	31:b:58:ARG:NH2	2.43	0.52
32:c:70:GLN:NE2	51:v:402:G:OP1	2.41	0.52
51:v:80:A:N6	51:v:89:U:O4	2.43	0.52
7:B:1026:G:H2'	7:B:1027:A:H8	1.73	0.51
7:B:1812:U:O2	8:C:43:ASN:ND2	2.40	0.51
21:R:37:GLU:HB3	21:R:53:PHE:HB3	1.92	0.51
51:v:834:U:H3	51:v:852:G:H1	1.58	0.51
7:B:2102:G:N1	7:B:2188:U:N3	2.58	0.51
35:f:118:ARG:NH2	51:v:1240:U:OP1	2.43	0.51
41:l:99:GLN:NE2	51:v:1307:U:OP1	2.39	0.51
8:C:60:ALA:O	8:C:62:ARG:NH1	2.43	0.51
10:E:181:ILE:HG23	15:L:2:ARG:HB3	1.92	0.51
14:K:40:ILE:HD13	14:K:59:ALA:HB2	1.93	0.51
43:n:57:ARG:NH1	43:n:61:GLN:OE1	2.44	0.51
51:v:983:A:H2	51:v:1222:G:H22	1.56	0.51
6:A:89:U:O2	7:B:958:U:O2'	2.28	0.51
7:B:888:C:H1'	41:l:91:ARG:HD3	1.92	0.51
7:B:1791:A:N6	7:B:1828:G:O2'	2.38	0.51
51:v:1071:C:H2'	51:v:1072:G:H8	1.74	0.51
51:v:1100:C:N4	51:v:1103:C:OP1	2.44	0.51
38:i:98:VAL:O	50:u:167:ARG:NH1	2.44	0.51
3:2:3:ARG:O	3:2:6:GLN:NE2	2.42	0.51
7:B:807:U:O2'	7:B:2060:A:N1	2.42	0.51
7:B:1197:G:N2	7:B:1249:U:O2'	2.44	0.51
7:B:1227:G:OP2	20:Q:15:LYS:NZ	2.43	0.51
7:B:1992:G:N2	7:B:1996:C:O2'	2.44	0.51
7:B:2081:U:H2'	7:B:2082:A:H8	1.76	0.51
22:S:35:ILE:O	22:S:39:THR:OG1	2.26	0.51
32:c:25:ARG:NH2	51:v:411:A:OP2	2.42	0.51
35:f:8:GLN:O	35:f:10:LYS:NZ	2.43	0.51
44:o:28:ARG:NH1	51:v:375:U:O2	2.43	0.51
7:B:1093:G:H21	7:B:1098:A:H62	1.58	0.51
43:n:21:THR:HA	43:n:26:VAL:HG11	1.93	0.51
48:s:54:GLN:HG3	48:s:75:LYS:HE3	1.93	0.51
7:B:309:A:H4'	24:U:15:GLY:HA2	1.92	0.51
7:B:500:G:N1	7:B:503:A:OP2	2.43	0.51
7:B:2666:C:H41	12:G:108:PHE:HA	1.76	0.51
7:B:2780:G:O6	13:J:99:ARG:NH1	2.42	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:e:6:ILE:HG13	34:e:89:VAL:HG23	1.91	0.51
8:C:159:THR:HG22	8:C:176:ARG:HG3	1.92	0.51
11:F:23:SER:HB2	11:F:26:GLN:HB2	1.93	0.51
13:J:99:ARG:HE	13:J:103:ILE:HG13	1.76	0.51
25:V:51:GLN:HE22	25:V:77:VAL:HG21	1.76	0.51
30:a:55:GLU:HA	30:a:58:LYS:HD3	1.93	0.51
41:l:30:LYS:NZ	41:l:40:GLU:OE1	2.44	0.51
51:v:1356:G:H2'	51:v:1357:A:H8	1.76	0.51
7:B:1438:U:H2'	7:B:1439:A:H8	1.76	0.51
11:F:33:ILE:HG23	11:F:155:ILE:HG23	1.93	0.51
15:L:19:LEU:HB3	15:L:31:GLY:HA3	1.93	0.51
32:c:183:ARG:NH2	32:c:189:ASP:OD2	2.43	0.51
7:B:881:G:N7	7:B:895:U:N3	2.58	0.50
22:S:47:VAL:HG12	22:S:103:ILE:HG21	1.92	0.50
26:W:19:ARG:O	26:W:19:ARG:NH1	2.38	0.50
45:p:18:LYS:HG3	51:v:255:G:H4'	1.93	0.50
46:q:52:ARG:NE	51:v:664:G:OP1	2.45	0.50
51:v:1241:G:H2'	51:v:1242:G:H8	1.76	0.50
7:B:629:G:N3	7:B:639:U:O2'	2.44	0.50
7:B:2627:G:O2'	7:B:2781:A:N1	2.43	0.50
25:V:2:PHE:HB3	25:V:61:LEU:HD23	1.93	0.50
33:d:28:ARG:NH2	51:v:1397:C:OP2	2.39	0.50
48:s:5:SER:OG	51:v:61:G:N7	2.45	0.50
51:v:909:A:N3	51:v:1413:A:O2'	2.39	0.50
3:2:44:VAL:HG21	7:B:465:G:H5''	1.92	0.50
7:B:1434:A:H62	7:B:1558:C:H42	1.59	0.50
7:B:1788:C:OP1	8:C:220:ARG:NH2	2.43	0.50
35:f:94:ARG:NH2	51:v:938:A:O3'	2.44	0.50
36:g:46:GLU:HG3	36:g:63:LYS:HB3	1.92	0.50
2:1:13:SER:OG	2:1:49:LYS:NZ	2.38	0.50
19:P:46:VAL:HG22	19:P:60:VAL:HG12	1.93	0.50
51:v:837:U:H3	51:v:849:G:H1	1.58	0.50
7:B:547:A:H5'	7:B:548:G:H21	1.76	0.50
7:B:953:G:H2'	7:B:954:G:H8	1.76	0.50
31:b:188:ALA:HB3	31:b:195:ILE:HG23	1.93	0.50
42:m:33:VAL:HG23	47:r:6:LYS:HD3	1.93	0.50
51:v:201:G:HO2'	51:v:469:C:HO2'	1.53	0.50
51:v:373:A:O2'	51:v:451:A:N7	2.44	0.50
7:B:514:A:N3	7:B:581:C:O2'	2.42	0.50
11:F:31:GLU:OE1	11:F:157:THR:OG1	2.30	0.50
14:K:115:ILE:HG23	14:K:121:VAL:HG21	1.91	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:b:154:GLY:HA2	31:b:162:ALA:HB1	1.93	0.50
36:g:28:SER:HB3	36:g:56:PRO:HB2	1.93	0.50
44:o:34:GLU:OE2	44:o:56:ARG:NH2	2.45	0.50
51:v:1156:G:H21	51:v:1179:A:N6	2.04	0.50
30:a:30:ILE:HD12	30:a:38:HIS:HB3	1.94	0.50
32:c:164:ARG:O	32:c:166:LYS:NZ	2.44	0.50
51:v:677:U:O2	51:v:777:A:O2'	2.29	0.50
51:v:975:A:H4'	51:v:976:G:H5''	1.93	0.50
7:B:142:A:N3	23:T:1:MET:N	2.58	0.50
9:D:37:VAL:HG22	9:D:48:ILE:HG22	1.93	0.50
23:T:3:ARG:HH11	23:T:42:GLU:HG3	1.77	0.50
42:m:79:LEU:HB2	42:m:84:VAL:HG23	1.92	0.50
11:F:91:ARG:HB2	11:F:94:ARG:HB2	1.92	0.50
45:p:58:VAL:HG12	45:p:77:VAL:HA	1.94	0.50
49:t:16:ARG:HB3	49:t:19:LYS:HB3	1.93	0.50
7:B:1187:G:N2	7:B:1188:U:O4	2.45	0.49
7:B:1869:G:N2	7:B:1872:A:OP2	2.40	0.49
8:C:24:HIS:HA	8:C:79:ARG:HE	1.76	0.49
7:B:1288:G:OP2	7:B:1288:G:N2	2.39	0.49
38:i:45:ARG:NH2	38:i:47:GLU:OE2	2.45	0.49
51:v:1233:G:O2'	51:v:1365:G:OP1	2.31	0.49
11:F:131:VAL:HG12	11:F:133:GLU:H	1.77	0.49
37:h:10:ARG:NH1	51:v:1149:C:OP1	2.46	0.49
37:h:42:THR:OG1	37:h:43:ALA:N	2.45	0.49
40:k:33:CYS:SG	40:k:77:SER:OG	2.70	0.49
51:v:946:A:H2'	51:v:947:G:C8	2.48	0.49
7:B:909:A:OP1	16:M:18:ARG:NH2	2.44	0.49
7:B:917:A:H5''	7:B:2268:A:H61	1.77	0.49
7:B:2719:G:H21	7:B:2872:A:H61	1.58	0.49
51:v:201:G:H22	51:v:468:A:H62	1.58	0.49
7:B:848:C:H2'	7:B:849:A:H8	1.77	0.49
9:D:13:ARG:NH1	19:P:74:GLN:OE1	2.43	0.49
39:j:120:CYS:SG	51:v:714:G:N2	2.85	0.49
45:p:57:VAL:HG13	45:p:78:VAL:HB	1.94	0.49
51:v:765:G:N1	51:v:812:G:O2'	2.37	0.49
51:v:890:G:O2'	51:v:906:A:N6	2.46	0.49
6:A:79:G:O2'	7:B:861:A:N3	2.44	0.49
14:K:18:VAL:HG12	14:K:42:ILE:HA	1.94	0.49
14:K:69:ARG:HG2	14:K:75:VAL:HG12	1.93	0.49
28:Y:4:LYS:O	28:Y:7:ARG:NH1	2.46	0.49
49:t:44:ARG:NH1	51:v:1534:A:C2	2.80	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
51:v:776:G:N2	51:v:802:A:OP2	2.44	0.49
7:B:2788:C:O2'	7:B:2809:A:N3	2.38	0.49
10:E:46:GLN:O	10:E:88:ARG:NH2	2.46	0.49
18:O:15:ARG:HH22	18:O:95:SER:HG	1.56	0.49
51:v:1183:U:O2'	51:v:1185:G:OP2	2.30	0.49
7:B:1421:G:H4'	7:B:1493:C:H41	1.76	0.49
7:B:2099:U:H2'	7:B:2100:G:H8	1.78	0.49
10:E:5:LEU:HB2	10:E:10:SER:HB3	1.93	0.49
30:a:116:LEU:HB3	30:a:140:LEU:HD13	1.94	0.49
35:f:25:PHE:HZ	35:f:119:LEU:HD11	1.77	0.49
51:v:417:G:N2	51:v:540:G:O2'	2.44	0.49
7:B:1028:A:H2'	7:B:1029:A:C8	2.48	0.49
38:i:16:ARG:NH2	51:v:1153:G:OP1	2.46	0.49
39:j:13:LYS:HG2	39:j:16:SER:H	1.78	0.49
7:B:1508:A:H4'	7:B:1509:A:H5'	1.94	0.48
7:B:2885:G:O2'	7:B:2886:A:O4'	2.29	0.48
16:M:1:MET:HG3	16:M:2:LEU:H	1.78	0.48
26:W:35:ILE:HG12	26:W:36:ILE:HG12	1.95	0.48
47:r:10:ILE:HG12	47:r:15:LEU:HD13	1.95	0.48
51:v:1295:U:O2'	51:v:1302:C:N4	2.46	0.48
7:B:673:C:OP1	10:E:49:ARG:NH1	2.46	0.48
7:B:1721:G:H22	7:B:1738:G:H1'	1.78	0.48
7:B:1753:G:N2	7:B:1756:G:OP2	2.43	0.48
26:W:23:LYS:HG3	26:W:68:PHE:HD1	1.77	0.48
35:f:9:ARG:NH1	51:v:1376:U:O4	2.46	0.48
43:n:57:ARG:NH2	51:v:742:G:OP1	2.41	0.48
51:v:946:A:O2'	51:v:1333:A:N3	2.39	0.48
7:B:2598:A:H5''	8:C:233:GLY:HA3	1.95	0.48
12:G:104:LEU:HB2	12:G:112:VAL:HG13	1.95	0.48
31:b:113:LYS:HE2	31:b:184:ASN:HB3	1.95	0.48
31:b:162:ALA:N	51:v:1056:U:OP1	2.47	0.48
50:u:149:GLU:HB3	50:u:159:LYS:HB3	1.93	0.48
7:B:1901:A:OP2	8:C:252:LYS:NZ	2.46	0.48
7:B:2229:U:H2'	7:B:2230:G:H8	1.79	0.48
11:F:57:ALA:HA	11:F:94:ARG:HH22	1.78	0.48
14:K:36:ASP:OD1	14:K:36:ASP:N	2.38	0.48
51:v:356:A:N3	51:v:368:U:O2'	2.39	0.48
51:v:713:G:H2'	51:v:714:G:C8	2.49	0.48
51:v:714:G:H2'	51:v:715:A:C8	2.49	0.48
37:h:83:THR:HG21	37:h:102:PHE:HB3	1.94	0.48
51:v:1222:G:OP1	51:v:1321:U:O2'	2.29	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:P:96:LEU:HD22	19:P:99:LEU:HD13	1.95	0.48
30:a:87:ASP:OD1	30:a:87:ASP:N	2.46	0.48
38:i:43:PRO:HG3	51:v:1150:A:H4'	1.95	0.48
7:B:2135:A:OP2	7:B:2156:G:N2	2.46	0.48
19:P:28:LYS:HB3	19:P:39:LEU:HD22	1.95	0.48
47:r:51:HIS:HB2	47:r:56:HIS:CE1	2.49	0.48
51:v:1058:G:H1	51:v:1199:U:H3	1.60	0.48
51:v:1363:A:O2'	51:v:1365:G:N7	2.41	0.48
7:B:107:G:H21	7:B:346:A:N6	2.12	0.48
7:B:1028:A:N3	7:B:2486:C:O2'	2.42	0.48
11:F:71:LYS:HG3	11:F:73:VAL:HB	1.96	0.48
18:O:25:ARG:HH21	18:O:40:ILE:HG21	1.78	0.48
51:v:309:A:O2'	51:v:607:A:N1	2.45	0.48
7:B:538:A:H4'	13:J:7:LYS:HG3	1.95	0.48
7:B:1433:A:H61	7:B:1560:G:H1	1.62	0.48
19:P:38:ARG:NH2	51:v:346:G:OP1	2.47	0.48
51:v:1068:G:OP1	51:v:1387:G:O2'	2.32	0.48
51:v:1305:G:N2	51:v:1331:G:O2'	2.42	0.48
7:B:1733:G:H2'	7:B:1734:G:H8	1.79	0.48
22:S:6:LYS:HD2	22:S:102:HIS:HB3	1.96	0.48
7:B:776:G:OP2	7:B:776:G:N2	2.44	0.47
7:B:993:G:N3	21:R:91:GLN:NE2	2.61	0.47
11:F:161:SER:HB2	11:F:164:GLU:HB3	1.96	0.47
32:c:105:GLY:HA3	32:c:161:ALA:HB2	1.95	0.47
51:v:123:U:OP1	51:v:311:C:O2'	2.30	0.47
51:v:182:A:H1'	51:v:183:C:H2'	1.96	0.47
8:C:180:MET:HB3	8:C:267:VAL:HB	1.96	0.47
37:h:35:GLU:HA	37:h:39:GLY:HA3	1.95	0.47
11:F:30:VAL:HG13	11:F:95:MET:HE1	1.96	0.47
12:G:93:TYR:OH	12:G:151:ARG:NH1	2.46	0.47
24:U:4:ILE:HG21	24:U:33:VAL:HG11	1.95	0.47
6:A:5:U:OP1	6:A:61:G:O2'	2.26	0.47
7:B:2515:C:H2'	7:B:2516:A:H8	1.79	0.47
11:F:111:ARG:HH11	11:F:114:ARG:HH12	1.61	0.47
15:L:85:VAL:HG12	15:L:87:GLY:H	1.79	0.47
17:N:44:LEU:HD23	17:N:113:ILE:HG21	1.96	0.47
26:W:48:ALA:HB2	26:W:81:ILE:HB	1.96	0.47
33:d:53:ARG:NH1	51:v:1071:C:OP1	2.47	0.47
51:v:1128:C:N3	51:v:1145:A:N6	2.62	0.47
51:v:1224:U:O2'	51:v:1322:C:OP1	2.25	0.47
23:T:36:LYS:HD2	23:T:36:LYS:HA	1.72	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:i:8:ILE:HG23	38:i:100:ILE:HG13	1.97	0.47
41:l:106:ARG:HA	41:l:109:LYS:HB2	1.97	0.47
47:r:62:THR:HG23	47:r:64:GLU:HG2	1.95	0.47
26:W:58:LEU:HD22	26:W:79:ILE:HD12	1.97	0.47
38:i:11:LYS:HG3	38:i:97:ASP:HB3	1.96	0.47
51:v:715:A:H2'	51:v:716:A:C8	2.50	0.47
51:v:757:U:OP1	51:v:822:U:O2'	2.31	0.47
7:B:1962:C:O2'	7:B:1964:G:OP2	2.30	0.47
7:B:2638:G:O2'	7:B:2775:G:N2	2.40	0.47
13:J:118:MET:HA	13:J:121:LYS:HE2	1.97	0.47
19:P:61:ARG:HD2	19:P:100:ARG:HB2	1.95	0.47
34:e:6:ILE:HD13	34:e:62:MET:HE2	1.97	0.47
36:g:86:LYS:HE2	36:g:90:GLU:HG3	1.96	0.47
37:h:17:ARG:HH12	51:v:1129:C:H5'	1.80	0.47
38:i:30:LYS:HD2	38:i:30:LYS:HA	1.69	0.47
51:v:34:C:H2'	51:v:35:G:H8	1.80	0.47
51:v:948:C:H2'	51:v:949:A:H8	1.79	0.47
7:B:715:A:OP2	43:n:87:ARG:NH2	2.48	0.47
13:J:96:ARG:HH12	13:J:98:GLU:HB2	1.80	0.47
29:Z:9:THR:N	29:Z:53:MET:O	2.42	0.47
30:a:34:ARG:NH1	30:a:34:ARG:O	2.47	0.47
30:a:68:PHE:HE1	30:a:88:GLN:HB3	1.80	0.47
48:s:67:HIS:O	48:s:67:HIS:ND1	2.47	0.47
51:v:715:A:OP1	51:v:805:C:O2'	2.31	0.47
7:B:184:C:O2'	7:B:217:A:N3	2.42	0.47
7:B:558:U:H5''	13:J:111:LYS:HD3	1.97	0.47
7:B:1250:G:N7	15:L:18:ARG:NH2	2.49	0.47
11:F:109:ARG:NH2	11:F:173:ASP:OD1	2.48	0.47
41:l:76:ILE:HG22	41:l:80:MET:HE2	1.96	0.47
53:5:21:A:H61	53:5:46:G:H2'	1.80	0.47
7:B:2270:A:O2'	26:W:15:SER:O	2.28	0.47
32:c:97:LEU:HD22	32:c:134:TYR:HD2	1.80	0.47
34:e:49:TYR:OH	46:q:62:ARG:O	2.28	0.47
38:i:63:ASP:OD1	42:m:98:LYS:NZ	2.48	0.47
39:j:16:SER:OG	39:j:79:LYS:NZ	2.42	0.47
51:v:652:U:O4	51:v:752:G:O2'	2.33	0.47
51:v:1479:C:H2'	51:v:1480:A:H8	1.80	0.47
7:B:859:G:O2'	7:B:916:G:O6	2.27	0.46
7:B:1864:U:OP1	7:B:2410:G:O2'	2.29	0.46
38:i:44:THR:OG1	38:i:46:LYS:NZ	2.49	0.46
51:v:21:G:H2'	51:v:22:G:C8	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
51:v:946:A:H2'	51:v:947:G:H8	1.80	0.46
51:v:1255:G:O2'	51:v:1258:G:N3	2.42	0.46
7:B:83:A:N6	7:B:102:U:OP2	2.47	0.46
11:F:43:ILE:HG13	11:F:82:TYR:HB3	1.97	0.46
30:a:42:LEU:HA	30:a:45:THR:HG22	1.97	0.46
38:i:37:ARG:HB2	38:i:75:ASP:HB3	1.96	0.46
38:i:44:THR:HG23	51:v:1151:A:H5''	1.96	0.46
40:k:49:ARG:HB3	40:k:65:TYR:HE1	1.79	0.46
48:s:35:TYR:OH	51:v:259:G:OP1	2.32	0.46
7:B:548:G:OP2	7:B:549:G:N2	2.48	0.46
7:B:1076:C:H2'	7:B:1077:A:H8	1.80	0.46
7:B:1939:U:OP1	7:B:2604:U:O2'	2.31	0.46
7:B:2250:G:H21	7:B:2496:C:H4'	1.81	0.46
24:U:93:ARG:HB3	24:U:102:ILE:HD12	1.98	0.46
39:j:93:GLU:HG3	49:t:19:LYS:HD2	1.98	0.46
7:B:572:A:OP2	21:R:80:ARG:NH2	2.46	0.46
7:B:1923:U:OP1	53:5:24:U:O2'	2.34	0.46
31:b:23:ALA:HB1	31:b:27:GLU:HB2	1.97	0.46
36:g:15:ASN:ND2	51:v:826:C:O2	2.48	0.46
51:v:673:A:H2'	51:v:674:G:C8	2.49	0.46
7:B:81:G:HO2'	7:B:295:G:HO2'	1.62	0.46
7:B:833:A:H2'	7:B:834:G:C8	2.50	0.46
7:B:2132:U:O4'	7:B:2157:G:N2	2.48	0.46
7:B:2313:C:H5'	11:F:87:LYS:HD3	1.98	0.46
38:i:50:THR:OG1	38:i:64:GLN:OE1	2.29	0.46
39:j:66:ALA:HB2	39:j:95:THR:HG23	1.96	0.46
51:v:816:A:OP1	51:v:1526:G:O2'	2.34	0.46
7:B:219:A:N3	7:B:234:U:O2'	2.40	0.46
7:B:1080:A:N6	7:B:1088:A:OP1	2.49	0.46
7:B:2647:U:O2	7:B:2673:G:O6	2.34	0.46
11:F:46:LYS:HB3	11:F:49:LEU:HD23	1.97	0.46
12:G:70:LEU:O	12:G:74:MET:HG2	2.15	0.46
40:k:49:ARG:NH2	40:k:88:ASP:OD2	2.49	0.46
9:D:148:GLN:HB2	9:D:152:PRO:HG2	1.97	0.46
30:a:96:LEU:HD21	30:a:146:SER:HB2	1.97	0.46
34:e:26:THR:HA	34:e:29:ILE:HD12	1.97	0.46
34:e:93:LYS:HE3	46:q:21:ASP:HA	1.98	0.46
51:v:1243:C:H2'	51:v:1244:G:H8	1.80	0.46
7:B:1614:A:N6	22:S:92:ARG:O	2.48	0.46
24:U:43:LYS:NZ	24:U:44:HIS:O	2.48	0.46
33:d:124:ALA:O	51:v:7:A:O2'	2.33	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
46:q:33:THR:HG23	46:q:35:SER:H	1.81	0.46
47:r:3:SER:OG	47:r:4:LEU:N	2.48	0.46
51:v:559:A:H4'	51:v:560:A:H3'	1.97	0.46
51:v:1327:C:H2'	51:v:1328:C:H6	1.81	0.46
53:5:73:A:H5''	53:5:74:C:H5'	1.98	0.46
1:0:29:VAL:HG22	1:0:36:LYS:HG2	1.96	0.46
4:3:29:ARG:HE	15:L:62:PRO:HB3	1.81	0.46
7:B:2116:G:O2'	7:B:2144:G:O2'	2.28	0.46
7:B:2462:C:H1'	7:B:2491:U:H5	1.81	0.46
22:S:86:MET:HE3	22:S:96:ILE:HG13	1.96	0.46
35:f:139:ASP:OD1	35:f:142:ARG:NH2	2.48	0.46
46:q:33:THR:OG1	46:q:34:GLU:N	2.49	0.46
51:v:362:G:N2	51:v:365:U:OP2	2.47	0.46
51:v:1138:G:C2	51:v:1140:C:N3	2.84	0.46
51:v:1356:G:H2'	51:v:1357:A:C8	2.51	0.46
7:B:788:A:H5''	7:B:790:U:H3	1.80	0.46
7:B:1316:U:H2'	7:B:1317:G:H8	1.80	0.46
7:B:2250:G:O2'	7:B:2496:C:OP1	2.30	0.46
51:v:1342:C:H2'	51:v:1343:G:C8	2.51	0.46
51:v:1391:U:H2'	51:v:1392:G:C8	2.51	0.46
7:B:1769:U:H3	7:B:1983:G:H1	1.64	0.45
14:K:63:ARG:HB2	14:K:82:ALA:HB3	1.97	0.45
17:N:12:ARG:O	17:N:17:ARG:NH1	2.49	0.45
38:i:25:ILE:HA	38:i:90:LEU:HD13	1.97	0.45
39:j:122:PRO:HG2	49:t:34:ARG:HB2	1.98	0.45
40:k:109:ARG:HH22	40:k:112:ALA:HB3	1.81	0.45
2:1:22:THR:OG1	2:1:23:THR:N	2.48	0.45
7:B:537:G:H4'	13:J:5:THR:HG21	1.98	0.45
20:Q:94:LEU:HD13	20:Q:94:LEU:HA	1.79	0.45
22:S:66:ILE:HA	22:S:69:LEU:HD12	1.97	0.45
23:T:9:LYS:HB2	23:T:9:LYS:HE3	1.77	0.45
26:W:63:ASP:OD1	26:W:63:ASP:N	2.49	0.45
48:s:38:ILE:HD13	48:s:85:LEU:HD22	1.99	0.45
51:v:696:A:N3	51:v:786:G:O2'	2.45	0.45
34:e:21:MET:HA	34:e:24:ARG:HG3	1.98	0.45
39:j:128:VAL:OXT	51:v:795:C:O2'	2.29	0.45
41:l:10:ASP:HA	41:l:44:ILE:HG23	1.98	0.45
41:l:26:LYS:HD3	41:l:30:LYS:HD2	1.97	0.45
46:q:28:LEU:HD23	46:q:67:LEU:HD11	1.98	0.45
51:v:501:C:H2'	51:v:502:A:C8	2.51	0.45
7:B:414:C:H2'	7:B:415:A:H8	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:C:144:GLU:HB2	8:C:187:CYS:HB2	1.98	0.45
11:F:13:LYS:HA	11:F:13:LYS:HD3	1.68	0.45
19:P:1:SER:OG	19:P:2:ASN:N	2.50	0.45
34:e:68:GLN:HA	34:e:71:ILE:HB	1.97	0.45
38:i:90:LEU:HD23	38:i:90:LEU:HA	1.78	0.45
46:q:65:SER:O	46:q:65:SER:OG	2.28	0.45
51:v:606:G:N2	51:v:632:U:OP1	2.40	0.45
51:v:1513:A:H2'	51:v:1514:G:C8	2.52	0.45
6:A:27:C:OP1	18:O:34:HIS:NE2	2.46	0.45
7:B:742:A:H2'	7:B:743:A:C8	2.52	0.45
7:B:931:U:OP1	29:Z:29:ARG:NH2	2.50	0.45
7:B:1812:U:H2'	7:B:1813:G:H8	1.82	0.45
7:B:2125:G:N2	7:B:2173:A:H62	2.15	0.45
30:a:218:ALA:HA	30:a:221:ARG:HG3	1.99	0.45
35:f:74:VAL:HA	35:f:87:PRO:HA	1.97	0.45
38:i:32:THR:HB	38:i:82:LYS:HD2	1.98	0.45
44:o:5:ARG:HB2	51:v:376:G:H5''	1.98	0.45
50:u:148:VAL:HG12	50:u:160:VAL:HG22	1.97	0.45
51:v:1138:G:N1	51:v:1140:C:C2	2.83	0.45
4:3:44:ARG:NH2	7:B:2349:G:OP1	2.50	0.45
7:B:396:G:OP2	27:X:9:LYS:NZ	2.50	0.45
12:G:85:LYS:HB3	12:G:164:ALA:HA	1.99	0.45
13:J:69:ARG:HG2	13:J:90:GLU:HG3	1.99	0.45
16:M:136:MET:HE2	25:V:79:ARG:HH11	1.81	0.45
31:b:109:GLU:HB3	31:b:143:LEU:HD22	1.98	0.45
32:c:11:SER:HA	32:c:18:LEU:HD23	1.98	0.45
39:j:13:LYS:HE3	39:j:13:LYS:HB2	1.84	0.45
51:v:407:U:H2'	51:v:408:A:H8	1.82	0.45
51:v:1444:U:H3	51:v:1458:G:H1	1.64	0.45
7:B:373:U:H2'	7:B:374:A:H8	1.82	0.45
7:B:1952:A:C8	14:K:41:THR:HG21	2.52	0.45
25:V:28:ALA:HB3	25:V:40:ILE:HD12	1.98	0.45
32:c:47:LEU:HD22	32:c:51:GLY:HA3	1.98	0.45
51:v:62:U:OP1	51:v:385:C:O2'	2.34	0.45
51:v:1346:A:N6	51:v:1376:U:O4	2.50	0.45
6:A:36:C:N4	6:A:49:C:O2	2.50	0.45
7:B:265:A:N6	7:B:428:A:N7	2.65	0.45
7:B:458:G:O2'	7:B:469:G:O6	2.28	0.45
10:E:5:LEU:HA	10:E:120:VAL:HG23	1.99	0.45
11:F:8:LYS:HA	11:F:8:LYS:HD2	1.78	0.45
14:K:42:ILE:HD11	14:K:57:LEU:HD21	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
51:v:451:A:H61	51:v:481:G:H5'	1.81	0.45
7:B:244:A:O2'	15:L:69:ARG:NH2	2.50	0.45
7:B:1231:U:H2'	7:B:1232:G:H8	1.82	0.45
7:B:1332:G:N7	7:B:1609:A:O2'	2.39	0.45
7:B:1757:A:H62	7:B:1762:A:H2	1.64	0.45
15:L:77:ILE:HD11	15:L:108:ALA:HB1	1.97	0.45
16:M:118:LYS:HB3	16:M:118:LYS:HE2	1.71	0.45
23:T:68:LYS:HD2	23:T:68:LYS:HA	1.85	0.45
25:V:58:SER:OG	25:V:59:GLU:OE1	2.34	0.45
47:r:52:ASN:HB3	47:r:74:ALA:HB1	1.99	0.45
50:u:128:PHE:HE1	50:u:180:LYS:HB3	1.82	0.45
51:v:672:U:H2'	51:v:673:A:H8	1.81	0.45
4:3:27:ASN:O	4:3:35:LYS:NZ	2.48	0.44
7:B:184:C:H2'	7:B:185:G:H8	1.81	0.44
31:b:39:ARG:HH21	31:b:56:ILE:HD12	1.82	0.44
31:b:129:PHE:O	31:b:133:MET:HG3	2.17	0.44
37:h:32:ARG:HH22	51:v:1248:A:H4'	1.82	0.44
41:l:79:LEU:HA	41:l:82:LEU:HD12	1.99	0.44
42:m:27:LYS:HD3	42:m:48:LEU:HD23	1.97	0.44
49:t:15:LEU:HB2	49:t:17:ARG:HH22	1.82	0.44
51:v:1401:G:O6	51:v:1504:G:N2	2.50	0.44
9:D:69:ALA:HA	9:D:73:VAL:HB	1.99	0.44
25:V:77:VAL:HG22	25:V:89:ILE:HG12	1.99	0.44
25:V:83:LYS:HB3	25:V:85:LYS:HD2	2.00	0.44
30:a:150:ILE:HA	30:a:153:MET:HB2	1.98	0.44
31:b:137:VAL:HG22	31:b:148:ILE:HG13	1.99	0.44
40:k:122:LYS:HD3	40:k:122:LYS:HA	1.77	0.44
51:v:769:G:H4'	51:v:1513:A:H4'	1.98	0.44
51:v:1040:U:H2'	51:v:1041:G:C8	2.52	0.44
7:B:1432:G:H2'	7:B:1433:A:C8	2.52	0.44
7:B:2533:U:OP1	7:B:2665:A:O2'	2.34	0.44
45:p:54:ILE:HD12	45:p:54:ILE:HA	1.86	0.44
50:u:138:ASP:OD1	50:u:177:GLN:NE2	2.49	0.44
51:v:599:C:H2'	51:v:600:A:H8	1.83	0.44
7:B:1570:A:H2'	7:B:1571:A:C8	2.52	0.44
10:E:146:VAL:HG12	10:E:185:LYS:HB2	1.99	0.44
14:K:52:LYS:HA	14:K:52:LYS:HD3	1.73	0.44
23:T:88:LYS:HA	23:T:91:GLN:HE21	1.82	0.44
31:b:130:ARG:O	31:b:134:LYS:HB2	2.17	0.44
34:e:29:ILE:HG12	34:e:64:VAL:HG11	1.99	0.44
38:i:5:ARG:HG3	38:i:102:LEU:HD11	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
51:v:358:U:H2'	51:v:359:G:H8	1.83	0.44
7:B:1724:G:H1	7:B:1736:U:H3	1.66	0.44
7:B:1921:G:H2'	7:B:1922:G:H8	1.83	0.44
7:B:2693:G:H2'	7:B:2694:G:H8	1.83	0.44
8:C:182:LYS:N	8:C:265:PHE:O	2.49	0.44
20:Q:86:SER:HB3	21:R:52:PRO:HD3	1.98	0.44
36:g:82:LEU:HD22	40:k:3:VAL:HG21	1.98	0.44
44:o:46:LYS:HB3	44:o:46:LYS:HE2	1.78	0.44
7:B:557:C:O2'	13:J:47:HIS:O	2.34	0.44
7:B:706:A:OP1	8:C:6:LYS:NZ	2.36	0.44
7:B:1539:U:H2'	7:B:1540:G:C8	2.51	0.44
26:W:24:ARG:HD3	26:W:24:ARG:HA	1.85	0.44
35:f:63:VAL:O	35:f:67:ASN:ND2	2.50	0.44
40:k:81:ILE:HG23	40:k:94:TYR:HB3	2.00	0.44
7:B:576:U:H2'	7:B:577:G:C8	2.53	0.44
7:B:1818:U:OP2	8:C:155:ARG:NH1	2.51	0.44
7:B:2759:G:H21	12:G:34:ARG:HH22	1.66	0.44
14:K:16:ARG:HD2	14:K:16:ARG:HA	1.76	0.44
16:M:33:LEU:HD13	16:M:117:PHE:HB3	2.00	0.44
42:m:88:ALA:HB2	42:m:96:LEU:HD23	1.98	0.44
3:2:12:ARG:NH2	7:B:464:U:O3'	2.50	0.44
7:B:526:A:O2'	7:B:2043:C:O2	2.32	0.44
7:B:632:A:H4'	15:L:68:SER:HB3	1.99	0.44
7:B:1796:U:H2'	7:B:1797:G:C8	2.52	0.44
7:B:2005:A:O2'	7:B:2049:G:OP1	2.32	0.44
24:U:2:ALA:O	24:U:5:ARG:NH2	2.51	0.44
30:a:131:LYS:HA	30:a:131:LYS:HD3	1.69	0.44
33:d:109:ALA:HB1	33:d:136:VAL:HG23	1.98	0.44
39:j:16:SER:HA	39:j:78:ILE:HG22	2.00	0.44
7:B:1:G:H2'	7:B:2:G:H8	1.83	0.44
7:B:322:A:OP1	10:E:162:ARG:NH1	2.51	0.44
7:B:1710:G:H2'	7:B:1711:A:C8	2.53	0.44
11:F:33:ILE:HG13	11:F:95:MET:HG3	2.00	0.44
51:v:94:G:H4'	51:v:95:C:H5'	2.00	0.44
51:v:662:U:H2'	51:v:663:A:C8	2.53	0.44
6:A:36:C:H5''	6:A:38:C:H41	1.83	0.43
6:A:78:A:H62	6:A:98:G:H21	1.65	0.43
7:B:581:C:H2'	7:B:582:A:C8	2.53	0.43
7:B:659:G:O2'	10:E:95:LYS:O	2.28	0.43
7:B:1443:U:H2'	7:B:1444:G:H8	1.83	0.43
7:B:2511:U:OP1	9:D:128:ARG:NE	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:W:39:GLN:NE2	26:W:42:THR:OG1	2.46	0.43
41:l:10:ASP:HB3	41:l:45:SER:HB3	2.00	0.43
7:B:45:G:H5''	7:B:46:G:H5'	2.00	0.43
7:B:1224:U:H2'	7:B:1225:G:C8	2.53	0.43
7:B:1329:U:H5''	7:B:1330:C:H5	1.83	0.43
11:F:59:ILE:H	11:F:94:ARG:HH21	1.66	0.43
16:M:22:GLN:O	16:M:100:LYS:NZ	2.49	0.43
30:a:128:LEU:HD23	30:a:128:LEU:HA	1.88	0.43
32:c:82:LYS:HA	32:c:82:LYS:HD2	1.88	0.43
45:p:26:ARG:NH1	45:p:41:THR:OG1	2.51	0.43
7:B:764:A:H5''	8:C:208:GLY:HA3	2.01	0.43
7:B:864:G:O2'	7:B:914:G:O6	2.36	0.43
7:B:1392:A:H62	23:T:19:LYS:HD3	1.83	0.43
7:B:2328:A:H2'	7:B:2329:U:C6	2.53	0.43
8:C:182:LYS:HB3	8:C:182:LYS:HE3	1.75	0.43
25:V:58:SER:O	25:V:73:LYS:NZ	2.52	0.43
47:r:34:SER:O	47:r:34:SER:OG	2.35	0.43
51:v:481:G:O2'	51:v:483:C:N4	2.51	0.43
51:v:625:U:H2'	51:v:626:G:H8	1.83	0.43
7:B:197:A:N6	7:B:2430:A:O2'	2.51	0.43
7:B:960:A:H61	16:M:82:MET:HE2	1.84	0.43
7:B:1020:A:N1	7:B:1141:U:O2'	2.47	0.43
7:B:1059:G:C6	7:B:1080:A:C2	3.06	0.43
7:B:1278:C:H2'	7:B:1279:G:H8	1.83	0.43
7:B:2167:U:H2'	7:B:2168:G:C8	2.53	0.43
7:B:2202:U:O2'	7:B:2204:G:OP1	2.35	0.43
12:G:133:LYS:HA	12:G:133:LYS:HD3	1.78	0.43
28:Y:23:ARG:HA	28:Y:23:ARG:HD3	1.85	0.43
30:a:111:LYS:HA	30:a:114:LYS:HE3	1.99	0.43
31:b:133:MET:HE1	31:b:165:GLU:HG3	2.00	0.43
41:l:2:ARG:O	41:l:56:ARG:NH2	2.44	0.43
45:p:5:ARG:HH22	51:v:127:G:H4'	1.83	0.43
48:s:63:LYS:HD3	48:s:63:LYS:HA	1.74	0.43
51:v:1138:G:N2	51:v:1140:C:C4	2.86	0.43
6:A:80:U:O2'	7:B:918:A:N3	2.49	0.43
7:B:414:C:H2'	7:B:415:A:C8	2.54	0.43
7:B:582:A:H2'	7:B:583:G:H8	1.82	0.43
7:B:1128:G:N7	7:B:2489:U:O2'	2.50	0.43
7:B:2458:G:O2'	7:B:2460:U:O4	2.32	0.43
12:G:37:ASN:N	12:G:37:ASN:OD1	2.51	0.43
28:Y:7:ARG:HG2	28:Y:8:GLU:HG3	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:B:444:C:OP1	10:E:40:ARG:NH2	2.51	0.43
8:C:7:PRO:HB3	8:C:13:ARG:HG3	2.00	0.43
28:Y:48:ARG:HD3	28:Y:48:ARG:HA	1.72	0.43
33:d:95:MET:HE3	33:d:95:MET:HB2	1.91	0.43
37:h:40:ARG:NH2	51:v:1291:U:O2	2.52	0.43
51:v:56:U:H2'	51:v:57:G:H8	1.84	0.43
5:4:15:LYS:HG2	5:4:26:ILE:HG13	2.00	0.43
7:B:2102:G:N2	7:B:2188:U:O2	2.51	0.43
7:B:2809:A:H2'	7:B:2810:A:C8	2.54	0.43
12:G:15:ASP:HB3	12:G:26:LYS:HB2	2.01	0.43
21:R:25:LEU:HB2	21:R:27:ILE:HG22	1.98	0.43
22:S:4:ILE:HG12	22:S:6:LYS:HE2	2.00	0.43
33:d:12:GLU:HB3	33:d:63:MET:HE2	2.00	0.43
44:o:5:ARG:HD3	51:v:376:G:H4'	1.99	0.43
44:o:69:ASP:OD1	44:o:69:ASP:N	2.50	0.43
7:B:675:A:N3	7:B:2443:C:O2'	2.44	0.43
7:B:1009:A:N3	7:B:1153:C:O2'	2.42	0.43
7:B:1796:U:H2'	7:B:1797:G:H8	1.84	0.43
20:Q:71:ASN:HB3	20:Q:109:VAL:HG11	1.99	0.43
34:e:53:LYS:HE3	51:v:710:G:H5''	2.01	0.43
40:k:82:ARG:O	51:v:552:U:O2'	2.33	0.43
44:o:68:SER:OG	44:o:69:ASP:N	2.51	0.43
51:v:501:C:H2'	51:v:502:A:H8	1.83	0.43
51:v:918:A:H2'	51:v:919:A:C8	2.54	0.43
7:B:276:U:O2'	7:B:278:A:N6	2.48	0.43
7:B:870:U:H3	7:B:907:G:H1	1.67	0.43
7:B:1115:G:H2'	7:B:1116:G:H8	1.82	0.43
7:B:1683:U:H2'	7:B:1684:G:H8	1.84	0.43
18:O:55:GLU:HG2	18:O:58:ILE:HB	2.00	0.43
51:v:514:C:H2'	51:v:515:G:H8	1.83	0.43
51:v:891:U:H2'	51:v:892:A:H8	1.83	0.43
1:O:15:ARG:NH1	7:B:1266:G:OP1	2.52	0.43
5:4:2:LYS:HD2	5:4:4:ARG:HH21	1.82	0.43
7:B:787:C:H5''	7:B:788:A:H5'	2.01	0.43
7:B:976:G:O2'	7:B:1155:A:O2'	2.33	0.43
7:B:1105:U:H2'	7:B:1106:G:H8	1.84	0.43
7:B:2148:G:H2'	7:B:2149:U:H4'	2.00	0.43
7:B:2291:U:O2'	7:B:2374:C:O2	2.36	0.43
8:C:16:VAL:HG22	8:C:203:VAL:HG22	2.01	0.43
24:U:90:LYS:NZ	24:U:91:LYS:O	2.39	0.43
31:b:168:ARG:NH2	51:v:1106:G:O2'	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:c:101:VAL:HB	32:c:113:ALA:HB1	2.01	0.43
35:f:102:TRP:HA	35:f:105:GLU:HG2	2.01	0.43
39:j:58:THR:HG22	39:j:60:PHE:H	1.84	0.43
41:l:92:ARG:HA	41:l:92:ARG:HD2	1.89	0.43
48:s:61:ALA:HB1	48:s:68:LYS:HB3	2.01	0.43
7:B:302:C:H2'	7:B:303:G:H8	1.84	0.42
7:B:581:C:H2'	7:B:582:A:H8	1.83	0.42
7:B:1167:C:H2'	7:B:1168:G:H8	1.84	0.42
7:B:1638:C:O2	7:B:2698:U:O2'	2.37	0.42
7:B:2039:U:H2'	7:B:2040:G:C8	2.54	0.42
12:G:115:GLN:NE2	12:G:116:LEU:O	2.52	0.42
13:J:60:ASP:OD1	13:J:60:ASP:N	2.48	0.42
30:a:30:ILE:HD13	30:a:30:ILE:HA	1.91	0.42
51:v:898:G:N2	51:v:901:A:OP2	2.51	0.42
1:O:14:MET:HB3	7:B:2045:C:H4'	2.00	0.42
12:G:18:ILE:HD13	12:G:42:VAL:HG13	2.00	0.42
17:N:77:ALA:O	17:N:81:ASN:HB2	2.19	0.42
22:S:17:VAL:HB	22:S:76:VAL:HG11	2.00	0.42
41:l:25:GLY:O	41:l:29:SER:CB	2.67	0.42
48:s:17:ARG:HG3	51:v:322:C:H4'	2.00	0.42
51:v:579:A:H5'	51:v:728:A:H1'	2.00	0.42
4:3:12:ARG:NH1	7:B:250:G:OP2	2.44	0.42
6:A:95:U:H2'	6:A:96:G:H8	1.84	0.42
7:B:2483:C:N3	16:M:123:LYS:NZ	2.64	0.42
7:B:2543:G:H2'	7:B:2544:G:C8	2.54	0.42
7:B:2595:G:N2	7:B:2598:A:OP2	2.42	0.42
10:E:170:ARG:NH1	10:E:174:GLY:O	2.52	0.42
11:F:110:ILE:HG22	11:F:113:PHE:H	1.83	0.42
15:L:82:LEU:HD22	15:L:90:VAL:HG11	2.01	0.42
20:Q:97:ILE:HA	20:Q:100:PHE:O	2.19	0.42
36:g:49:LYS:HE3	36:g:49:LYS:HB3	1.75	0.42
37:h:17:ARG:HH22	51:v:1129:C:H4'	1.83	0.42
51:v:657:U:H2'	51:v:658:C:H6	1.84	0.42
2:1:43:ARG:NH2	7:B:2370:G:O2'	2.52	0.42
12:G:174:LYS:HD3	12:G:174:LYS:HA	1.89	0.42
14:K:46:ILE:HD13	14:K:46:ILE:HA	1.96	0.42
20:Q:82:LEU:HD22	20:Q:88:GLU:HB3	2.02	0.42
32:c:27:ILE:HD12	32:c:27:ILE:HA	1.88	0.42
43:n:42:PHE:HE1	43:n:48:ASP:HB3	1.84	0.42
51:v:509:A:N3	51:v:543:U:O2'	2.44	0.42
51:v:834:U:O2	51:v:852:G:N2	2.47	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
51:v:1133:G:H2'	51:v:1134:G:C8	2.54	0.42
7:B:1447:C:O2'	7:B:1544:A:N3	2.46	0.42
7:B:2446:G:N2	7:B:2449:U:O2	2.44	0.42
23:T:50:LEU:O	28:Y:23:ARG:NH2	2.52	0.42
38:i:36:VAL:HG22	38:i:76:ILE:HG23	2.01	0.42
38:i:40:ILE:HD11	38:i:73:LEU:HD23	2.02	0.42
40:k:33:CYS:HA	40:k:54:VAL:HA	2.01	0.42
51:v:219:U:H2'	51:v:220:G:C8	2.53	0.42
51:v:358:U:H2'	51:v:359:G:C8	2.54	0.42
51:v:950:U:H2'	51:v:951:G:C8	2.55	0.42
7:B:151:C:H2'	7:B:152:A:H8	1.85	0.42
7:B:1266:G:O2'	7:B:2012:G:O6	2.35	0.42
7:B:1912:A:H2	7:B:1917:U:H3	1.66	0.42
7:B:2246:G:H2'	7:B:2247:A:H8	1.85	0.42
10:E:59:PRO:HG3	10:E:73:ILE:HG13	2.00	0.42
36:g:25:THR:HG22	36:g:59:GLU:HG3	2.01	0.42
39:j:125:LYS:O	49:t:32:ARG:NH1	2.52	0.42
45:p:51:GLU:H	45:p:51:GLU:HG3	1.71	0.42
51:v:1355:G:H2'	51:v:1356:G:C8	2.55	0.42
7:B:573:U:O2'	7:B:575:A:OP1	2.31	0.42
7:B:1827:U:H5'	7:B:1971:U:H5'	2.01	0.42
8:C:251:THR:OG1	8:C:252:LYS:N	2.52	0.42
19:P:27:VAL:HG22	19:P:83:ILE:HG23	2.02	0.42
19:P:70:GLU:OE1	19:P:100:ARG:NH1	2.52	0.42
46:q:38:ILE:O	51:v:719:C:O2'	2.33	0.42
1:0:16:ARG:NE	7:B:1266:G:OP2	2.53	0.42
7:B:956:G:H2'	7:B:957:C:H2'	2.02	0.42
7:B:1429:G:H2'	7:B:1430:G:H8	1.84	0.42
7:B:1571:A:H2'	7:B:1572:A:C8	2.55	0.42
7:B:2204:G:H4'	8:C:149:LYS:HG3	2.02	0.42
7:B:2329:U:H2'	7:B:2330:G:C8	2.55	0.42
8:C:224:MET:SD	8:C:229:HIS:HB2	2.59	0.42
20:Q:16:ILE:HD12	20:Q:38:VAL:HG21	2.02	0.42
26:W:67:LYS:N	26:W:80:SER:O	2.48	0.42
34:e:2:ARG:HB2	34:e:91:ARG:HH12	1.85	0.42
45:p:14:ASP:HA	45:p:20:ILE:HG22	2.02	0.42
51:v:993:G:O2'	51:v:994:A:N7	2.53	0.42
7:B:171:U:H2'	7:B:172:A:H8	1.85	0.42
7:B:1338:G:O2'	23:T:18:GLU:OE2	2.37	0.42
7:B:1386:C:H2'	7:B:1387:A:C8	2.55	0.42
7:B:2861:U:H2'	7:B:2862:G:C8	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:L:79:LEU:HD13	15:L:116:VAL:HG12	2.01	0.42
31:b:189:HIS:NE2	51:v:1205:U:O3'	2.53	0.42
38:i:92:LEU:HD23	38:i:92:LEU:HA	1.92	0.42
45:p:25:GLU:HG2	45:p:40:THR:HG23	2.01	0.42
51:v:335:C:H2'	51:v:336:A:C8	2.55	0.42
51:v:824:G:H2'	51:v:825:A:H8	1.85	0.42
4:3:12:ARG:NH2	7:B:2393:U:O2'	2.53	0.42
7:B:829:A:N7	7:B:2247:A:O2'	2.45	0.42
7:B:1004:U:H2'	7:B:1011:G:H2'	2.02	0.42
7:B:1409:U:H2'	7:B:1410:G:H8	1.85	0.42
7:B:1980:G:O2'	7:B:1982:U:OP2	2.34	0.42
10:E:143:LEU:HD22	10:E:185:LYS:HD2	2.01	0.42
11:F:37:MET:HG3	11:F:151:LEU:HB3	2.02	0.42
38:i:16:ARG:HD3	38:i:16:ARG:HA	1.74	0.42
44:o:5:ARG:HH21	44:o:24:SER:HA	1.85	0.42
48:s:45:ALA:HA	48:s:48:LYS:HG2	2.02	0.42
51:v:790:A:OP1	53:5:38:A:O2'	2.32	0.42
51:v:1316:G:N1	51:v:1319:A:OP2	2.47	0.42
7:B:2262:U:H5''	26:W:38:ARG:HH22	1.85	0.41
13:J:57:LEU:HD23	13:J:57:LEU:HA	1.84	0.41
14:K:59:ALA:HB1	14:K:83:CYS:HB2	2.02	0.41
14:K:70:ARG:HH22	14:K:104:ARG:HB2	1.85	0.41
17:N:8:ARG:NH1	17:N:43:GLU:OE2	2.50	0.41
30:a:102:ASN:N	30:a:102:ASN:OD1	2.52	0.41
34:e:86:ARG:NH1	46:q:63:TYR:O	2.53	0.41
51:v:744:C:H2'	51:v:745:G:C8	2.55	0.41
51:v:745:G:H2'	51:v:746:A:C8	2.55	0.41
51:v:908:A:H2'	51:v:909:A:H8	1.85	0.41
7:B:767:U:H2'	7:B:768:G:H8	1.85	0.41
7:B:1060:U:H3	7:B:1079:C:H42	1.68	0.41
7:B:1853:A:N3	7:B:2233:U:O2'	2.41	0.41
7:B:2735:G:O6	7:B:2769:U:O4	2.38	0.41
19:P:47:ILE:HG23	19:P:96:LEU:H	1.84	0.41
33:d:37:VAL:HG11	33:d:113:VAL:HG22	2.03	0.41
42:m:23:ARG:HA	42:m:23:ARG:HD2	1.75	0.41
44:o:4:ILE:HG12	44:o:21:VAL:HG12	2.01	0.41
1:0:10:SER:O	1:0:14:MET:HG3	2.20	0.41
1:0:36:LYS:HB2	1:0:36:LYS:HE2	1.86	0.41
7:B:2229:U:H2'	7:B:2230:G:C8	2.55	0.41
7:B:2245:U:H5''	7:B:2246:G:H5'	2.03	0.41
11:F:43:ILE:HG21	11:F:83:PRO:HG2	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:N:9:GLN:O	17:N:17:ARG:NH1	2.48	0.41
36:g:10:LEU:HD22	36:g:74:ILE:HG21	2.01	0.41
51:v:201:G:N2	51:v:469:C:O2	2.50	0.41
51:v:746:A:H2'	51:v:747:A:C8	2.55	0.41
7:B:599:A:H2'	7:B:600:G:H8	1.85	0.41
8:C:176:ARG:HD2	8:C:176:ARG:HA	1.81	0.41
10:E:143:LEU:HD13	10:E:146:VAL:HG11	2.02	0.41
10:E:149:ILE:HD13	10:E:188:MET:HG2	2.02	0.41
11:F:49:LEU:HD13	11:F:66:ILE:HG12	2.02	0.41
13:J:96:ARG:HG3	13:J:99:ARG:HB2	2.01	0.41
15:L:89:VAL:HA	15:L:121:THR:HG23	2.03	0.41
19:P:5:LYS:HA	19:P:8:GLU:HB2	2.02	0.41
32:c:43:ARG:H	32:c:43:ARG:HG3	1.74	0.41
40:k:107:LYS:HE2	40:k:107:LYS:HB2	1.88	0.41
42:m:85:ARG:NH2	51:v:1060:U:OP1	2.54	0.41
4:3:16:THR:OG1	4:3:19:GLY:O	2.29	0.41
7:B:2457:U:H3	7:B:2494:G:H1	1.68	0.41
8:C:34:GLU:HG3	8:C:61:TYR:HB3	2.02	0.41
9:D:36:GLN:HB3	9:D:49:GLN:HE21	1.86	0.41
13:J:31:GLU:O	13:J:35:ARG:HG2	2.20	0.41
22:S:69:LEU:HD22	22:S:107:VAL:HB	2.03	0.41
34:e:44:ARG:HH21	34:e:56:LYS:HE2	1.86	0.41
42:m:66:GLN:HG2	42:m:79:LEU:HD22	2.01	0.41
50:u:155:LYS:HB3	50:u:157:ARG:HG2	2.01	0.41
51:v:81:A:H61	51:v:87:C:H42	1.68	0.41
51:v:1286:U:H2'	51:v:1287:A:H4'	2.02	0.41
51:v:1342:C:H2'	51:v:1343:G:H8	1.84	0.41
7:B:1797:G:H5''	8:C:255:LYS:HG2	2.01	0.41
38:i:54:SER:O	42:m:81:ARG:NH1	2.51	0.41
51:v:600:A:H2'	51:v:601:G:H8	1.86	0.41
7:B:5:A:H2'	7:B:6:A:C8	2.55	0.41
7:B:1421:G:H5'	7:B:2211:A:C8	2.55	0.41
7:B:1532:A:H2'	7:B:1533:C:C6	2.56	0.41
7:B:2125:G:N1	7:B:2174:C:N3	2.66	0.41
7:B:2139:U:H3	7:B:2152:G:H2'	1.85	0.41
14:K:22:LYS:HB2	14:K:22:LYS:HE2	1.87	0.41
14:K:110:LYS:HB2	14:K:110:LYS:HE2	1.75	0.41
14:K:113:LYS:O	14:K:116:SER:OG	2.36	0.41
18:O:67:ASN:H	18:O:70:ALA:HB3	1.85	0.41
31:b:123:LEU:HD13	31:b:123:LEU:HA	1.92	0.41
43:n:24:THR:HG21	43:n:69:LEU:HB2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
44:o:18:GLN:HG2	44:o:35:ARG:HE	1.84	0.41
51:v:1130:A:H2	51:v:1144:G:H1	1.64	0.41
1:0:37:HIS:ND1	1:0:38:LEU:O	2.54	0.41
7:B:1538:G:H2'	7:B:1539:U:C6	2.55	0.41
7:B:2377:A:H2'	7:B:2378:A:C8	2.56	0.41
7:B:2618:G:H21	9:D:155:VAL:HG21	1.86	0.41
8:C:76:VAL:HG23	8:C:96:LYS:HZ2	1.86	0.41
14:K:111:PHE:O	14:K:115:ILE:HG12	2.20	0.41
32:c:89:LEU:O	32:c:93:LEU:HD12	2.21	0.41
35:f:140:VAL:HA	35:f:143:MET:HE3	2.02	0.41
40:k:67:GLY:O	40:k:98:ARG:NH1	2.53	0.41
41:l:15:VAL:O	41:l:19:THR:HG23	2.21	0.41
51:v:235:C:H2'	51:v:236:A:C8	2.56	0.41
51:v:545:C:O2'	51:v:549:C:OP1	2.39	0.41
51:v:1038:C:H2'	51:v:1039:G:C8	2.56	0.41
1:0:8:THR:OG1	1:0:9:ARG:N	2.53	0.41
1:0:11:LYS:HD2	1:0:11:LYS:HA	1.86	0.41
7:B:28:A:N6	7:B:512:G:O2'	2.54	0.41
7:B:155:A:H2'	7:B:156:A:H8	1.85	0.41
7:B:624:C:O2'	7:B:657:U:OP1	2.37	0.41
7:B:688:U:H2'	7:B:689:A:H8	1.85	0.41
7:B:1754:A:H5'	19:P:99:LEU:HD21	2.02	0.41
7:B:1796:U:H4'	8:C:253:GLY:H	1.85	0.41
7:B:1912:A:N6	51:v:1407:C:O2'	2.54	0.41
7:B:2232:C:P	27:X:26:ARG:HH12	2.43	0.41
7:B:2354:C:H4'	26:W:31:LEU:HD22	2.03	0.41
7:B:2530:A:N7	12:G:171:LYS:NZ	2.51	0.41
7:B:2655:G:O2'	7:B:2664:G:O6	2.29	0.41
11:F:79:ARG:HD2	11:F:79:ARG:HA	1.82	0.41
12:G:38:ASP:OD1	12:G:38:ASP:N	2.53	0.41
13:J:41:LYS:HB2	13:J:41:LYS:HE2	1.77	0.41
16:M:21:ALA:HB2	16:M:97:GLN:HB2	2.03	0.41
18:O:25:ARG:O	18:O:40:ILE:N	2.52	0.41
20:Q:30:VAL:HG12	20:Q:33:VAL:H	1.86	0.41
26:W:39:GLN:OE1	26:W:42:THR:N	2.47	0.41
27:X:42:GLU:HB3	27:X:44:ARG:HG2	2.03	0.41
27:X:55:MET:HE2	27:X:55:MET:HB3	1.85	0.41
31:b:171:ARG:NH1	31:b:173:PRO:HG3	2.36	0.41
32:c:144:ILE:HB	32:c:149:LYS:HE2	2.02	0.41
35:f:79:VAL:H	35:f:84:TYR:HB2	1.85	0.41
47:r:39:ILE:HD11	47:r:65:MET:HB2	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
51:v:51:A:N7	51:v:114:U:O2'	2.53	0.41
51:v:197:A:O2'	51:v:220:G:N2	2.54	0.41
51:v:352:C:O2	51:v:355:C:N4	2.52	0.41
51:v:407:U:H2'	51:v:408:A:C8	2.56	0.41
51:v:486:U:H2'	51:v:487:A:H8	1.85	0.41
51:v:1355:G:H2'	51:v:1356:G:H8	1.85	0.41
6:A:95:U:H2'	6:A:96:G:C8	2.56	0.41
7:B:242:G:O2'	7:B:254:G:O6	2.32	0.41
7:B:299:A:N3	7:B:319:G:O2'	2.44	0.41
7:B:2099:U:H2'	7:B:2100:G:C8	2.56	0.41
7:B:2291:U:OP1	7:B:2380:C:O2'	2.39	0.41
7:B:2353:G:H21	26:W:30:VAL:HG12	1.86	0.41
10:E:52:VAL:HG13	10:E:74:LYS:HG2	2.02	0.41
12:G:97:VAL:HG22	12:G:102:ILE:HG23	2.02	0.41
20:Q:16:ILE:HD13	20:Q:16:ILE:HA	1.91	0.41
40:k:41:PRO:HB3	40:k:88:ASP:HB3	2.02	0.41
51:v:216:U:H2'	51:v:217:C:C6	2.56	0.41
51:v:634:C:H2'	51:v:635:A:C8	2.56	0.41
6:A:116:G:H2'	6:A:117:G:C8	2.56	0.40
7:B:31:C:O2'	7:B:1238:G:OP1	2.36	0.40
7:B:172:A:H2'	7:B:173:A:C8	2.56	0.40
7:B:783:A:H2	7:B:1778:U:H4'	1.86	0.40
7:B:2863:C:H2'	7:B:2864:G:H8	1.86	0.40
18:O:10:ARG:NH1	18:O:96:GLY:O	2.54	0.40
23:T:33:LYS:HE2	23:T:33:LYS:HB2	1.96	0.40
37:h:68:GLY:HA2	51:v:1250:A:H4'	2.03	0.40
38:i:58:ASN:HD22	38:i:58:ASN:HA	1.62	0.40
42:m:59:ARG:HD2	51:v:980:C:H1'	2.03	0.40
43:n:2:LEU:HD23	43:n:2:LEU:HA	1.94	0.40
51:v:67:C:H2'	51:v:68:G:C8	2.56	0.40
51:v:1323:G:H2'	51:v:1324:A:C8	2.56	0.40
7:B:20:C:H2'	7:B:21:A:H8	1.87	0.40
7:B:946:C:H2'	7:B:947:A:H8	1.86	0.40
7:B:1278:C:H2'	7:B:1279:G:C8	2.57	0.40
39:j:126:ARG:NH2	51:v:796:C:O2'	2.54	0.40
46:q:49:LYS:O	46:q:53:GLN:HG3	2.21	0.40
51:v:34:C:H2'	51:v:35:G:C8	2.56	0.40
51:v:516:U:O2'	51:v:519:C:N3	2.49	0.40
51:v:908:A:H2'	51:v:909:A:C8	2.56	0.40
7:B:1013:C:H2'	7:B:1014:A:H8	1.86	0.40
7:B:1387:A:H2'	7:B:1388:G:H8	1.86	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:B:2273:A:H2'	7:B:2274:A:C8	2.57	0.40
13:J:44:TYR:O	20:Q:63:ARG:NH2	2.53	0.40
15:L:69:ARG:HE	15:L:69:ARG:HB3	1.64	0.40
37:h:27:ILE:HD11	37:h:34:LEU:HD13	2.03	0.40
40:k:86:VAL:HG21	40:k:89:LEU:HD12	2.02	0.40
43:n:81:ILE:O	43:n:88:ARG:NH1	2.54	0.40
45:p:6:THR:HB	45:p:59:GLU:HG2	2.04	0.40
51:v:202:G:H21	51:v:466:A:H61	1.69	0.40
7:B:153:U:OP1	27:X:76:LYS:NZ	2.45	0.40
7:B:874:G:H2'	7:B:875:G:C8	2.56	0.40
7:B:874:G:H2'	7:B:875:G:H8	1.86	0.40
7:B:1326:U:H2'	7:B:1327:A:H8	1.87	0.40
18:O:115:LEU:HD12	18:O:115:LEU:HA	1.91	0.40
24:U:10:VAL:HG12	24:U:71:ILE:HD13	2.03	0.40
30:a:10:LYS:HD2	30:a:10:LYS:HA	1.84	0.40
32:c:150:LYS:HD3	32:c:150:LYS:HA	1.72	0.40
48:s:29:THR:OG1	51:v:1458:G:OP1	2.40	0.40
51:v:216:U:H2'	51:v:217:C:H6	1.85	0.40
51:v:257:G:H2'	51:v:258:G:H8	1.86	0.40
1:O:42:ILE:HD11	17:N:98:LEU:HB3	2.03	0.40
4:3:40:LYS:NZ	7:B:2419:U:OP1	2.39	0.40
7:B:559:G:N3	20:Q:55:GLN:NE2	2.70	0.40
7:B:1771:C:H2'	7:B:1772:A:H8	1.87	0.40
7:B:2445:G:OP1	10:E:69:ARG:NH1	2.50	0.40
8:C:117:SER:O	8:C:188:ARG:NH2	2.55	0.40
12:G:24:THR:HG23	12:G:33:THR:HB	2.03	0.40
13:J:96:ARG:HD2	13:J:96:ARG:HA	1.88	0.40
21:R:61:ALA:HB2	21:R:98:ILE:HD13	2.03	0.40
26:W:40:ARG:HD3	26:W:40:ARG:H	1.85	0.40
30:a:78:ALA:O	30:a:82:ALA:HB3	2.21	0.40
30:a:125:PHE:O	30:a:136:ARG:NH2	2.47	0.40
32:c:14:GLU:HG3	32:c:59:LYS:HA	2.03	0.40
37:h:86:LEU:HA	37:h:89:TYR:HB2	2.03	0.40
37:h:128:LYS:O	51:v:966:G:O2'	2.38	0.40
41:l:89:ARG:NH2	51:v:1226:C:OP2	2.54	0.40
51:v:71:A:H61	51:v:99:C:H1'	1.87	0.40
51:v:672:U:H2'	51:v:673:A:C8	2.56	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	0	54/56 (96%)	52 (96%)	2 (4%)	0	100	100
2	1	49/51 (96%)	49 (100%)	0	0	100	100
3	2	44/46 (96%)	44 (100%)	0	0	100	100
4	3	62/64 (97%)	59 (95%)	2 (3%)	1 (2%)	8	37
5	4	36/38 (95%)	34 (94%)	2 (6%)	0	100	100
8	C	270/272 (99%)	260 (96%)	10 (4%)	0	100	100
9	D	207/209 (99%)	192 (93%)	15 (7%)	0	100	100
10	E	199/201 (99%)	190 (96%)	9 (4%)	0	100	100
11	F	176/178 (99%)	165 (94%)	11 (6%)	0	100	100
12	G	174/176 (99%)	170 (98%)	4 (2%)	0	100	100
13	J	140/142 (99%)	130 (93%)	9 (6%)	1 (1%)	19	54
14	K	120/122 (98%)	111 (92%)	8 (7%)	1 (1%)	16	51
15	L	141/143 (99%)	133 (94%)	8 (6%)	0	100	100
16	M	134/136 (98%)	134 (100%)	0	0	100	100
17	N	119/121 (98%)	112 (94%)	7 (6%)	0	100	100
18	O	114/116 (98%)	114 (100%)	0	0	100	100
19	P	112/114 (98%)	104 (93%)	8 (7%)	0	100	100
20	Q	115/117 (98%)	112 (97%)	3 (3%)	0	100	100
21	R	101/103 (98%)	93 (92%)	7 (7%)	1 (1%)	13	47
22	S	108/110 (98%)	104 (96%)	4 (4%)	0	100	100
23	T	92/94 (98%)	85 (92%)	7 (8%)	0	100	100
24	U	101/103 (98%)	94 (93%)	7 (7%)	0	100	100
25	V	92/94 (98%)	90 (98%)	2 (2%)	0	100	100
26	W	77/79 (98%)	69 (90%)	8 (10%)	0	100	100
27	X	75/77 (97%)	74 (99%)	1 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
28	Y	61/63 (97%)	57 (93%)	4 (7%)	0	100	100
29	Z	56/58 (97%)	55 (98%)	1 (2%)	0	100	100
30	a	216/218 (99%)	203 (94%)	13 (6%)	0	100	100
31	b	204/206 (99%)	196 (96%)	8 (4%)	0	100	100
32	c	203/205 (99%)	197 (97%)	6 (3%)	0	100	100
33	d	148/150 (99%)	144 (97%)	4 (3%)	0	100	100
34	e	98/100 (98%)	95 (97%)	3 (3%)	0	100	100
35	f	149/151 (99%)	148 (99%)	1 (1%)	0	100	100
36	g	127/129 (98%)	125 (98%)	2 (2%)	0	100	100
37	h	125/127 (98%)	116 (93%)	8 (6%)	1 (1%)	16	51
38	i	96/98 (98%)	89 (93%)	7 (7%)	0	100	100
39	j	115/117 (98%)	112 (97%)	3 (3%)	0	100	100
40	k	121/123 (98%)	112 (93%)	9 (7%)	0	100	100
41	l	112/114 (98%)	109 (97%)	3 (3%)	0	100	100
42	m	92/100 (92%)	87 (95%)	5 (5%)	0	100	100
43	n	86/88 (98%)	83 (96%)	3 (4%)	0	100	100
44	o	80/82 (98%)	77 (96%)	3 (4%)	0	100	100
45	p	78/80 (98%)	75 (96%)	3 (4%)	0	100	100
46	q	53/55 (96%)	50 (94%)	3 (6%)	0	100	100
47	r	77/79 (98%)	73 (95%)	4 (5%)	0	100	100
48	s	83/85 (98%)	81 (98%)	1 (1%)	1 (1%)	11	43
49	t	49/51 (96%)	46 (94%)	3 (6%)	0	100	100
50	u	57/59 (97%)	55 (96%)	2 (4%)	0	100	100
All	All	5398/5500 (98%)	5159 (96%)	233 (4%)	6 (0%)	50	80

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
14	K	109	GLU
37	h	12	LYS
48	s	68	LYS
21	R	58	VAL
4	3	31	ILE
13	J	110	PRO

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	0	47/47 (100%)	47 (100%)	0	100	100
2	1	45/46 (98%)	45 (100%)	0	100	100
3	2	38/38 (100%)	38 (100%)	0	100	100
4	3	51/51 (100%)	51 (100%)	0	100	100
5	4	34/34 (100%)	34 (100%)	0	100	100
8	C	216/217 (100%)	214 (99%)	2 (1%)	75	89
9	D	164/164 (100%)	164 (100%)	0	100	100
10	E	165/165 (100%)	163 (99%)	2 (1%)	67	85
11	F	149/149 (100%)	146 (98%)	3 (2%)	50	75
12	G	137/137 (100%)	136 (99%)	1 (1%)	81	92
13	J	116/116 (100%)	115 (99%)	1 (1%)	75	89
14	K	102/103 (99%)	101 (99%)	1 (1%)	73	87
15	L	102/102 (100%)	102 (100%)	0	100	100
16	M	109/109 (100%)	109 (100%)	0	100	100
17	N	100/101 (99%)	100 (100%)	0	100	100
18	O	86/86 (100%)	86 (100%)	0	100	100
19	P	99/99 (100%)	98 (99%)	1 (1%)	73	87
20	Q	89/89 (100%)	89 (100%)	0	100	100
21	R	84/84 (100%)	84 (100%)	0	100	100
22	S	93/93 (100%)	93 (100%)	0	100	100
23	T	80/81 (99%)	80 (100%)	0	100	100
24	U	83/84 (99%)	82 (99%)	1 (1%)	67	85
25	V	78/78 (100%)	78 (100%)	0	100	100
26	W	59/59 (100%)	58 (98%)	1 (2%)	56	78
27	X	67/67 (100%)	67 (100%)	0	100	100
28	Y	55/55 (100%)	54 (98%)	1 (2%)	54	77

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
29	Z	48/48 (100%)	46 (96%)	2 (4%)	25	58
30	a	180/180 (100%)	180 (100%)	0	100	100
31	b	170/170 (100%)	170 (100%)	0	100	100
32	c	172/172 (100%)	167 (97%)	5 (3%)	37	67
33	d	113/113 (100%)	111 (98%)	2 (2%)	54	77
34	e	87/87 (100%)	87 (100%)	0	100	100
35	f	124/124 (100%)	123 (99%)	1 (1%)	79	90
36	g	104/104 (100%)	104 (100%)	0	100	100
37	h	105/105 (100%)	105 (100%)	0	100	100
38	i	86/86 (100%)	86 (100%)	0	100	100
39	j	90/90 (100%)	90 (100%)	0	100	100
40	k	103/103 (100%)	103 (100%)	0	100	100
41	l	92/92 (100%)	92 (100%)	0	100	100
42	m	79/83 (95%)	79 (100%)	0	100	100
43	n	76/76 (100%)	76 (100%)	0	100	100
44	o	65/65 (100%)	65 (100%)	0	100	100
45	p	74/74 (100%)	74 (100%)	0	100	100
46	q	48/48 (100%)	48 (100%)	0	100	100
47	r	70/70 (100%)	70 (100%)	0	100	100
48	s	65/65 (100%)	64 (98%)	1 (2%)	60	81
49	t	44/44 (100%)	44 (100%)	0	100	100
50	u	52/52 (100%)	52 (100%)	0	100	100
All	All	4495/4505 (100%)	4470 (99%)	25 (1%)	82	92

All (25) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
8	C	97	ASP
8	C	264	LYS
10	E	52	VAL
10	E	187	VAL
11	F	47	LYS
11	F	49	LEU
11	F	158	THR

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Mol	Chain	Res	Type
12	G	161	VAL
13	J	142	ILE
14	K	51	VAL
19	P	72	VAL
24	U	20	LYS
26	W	22	VAL
28	Y	57	LEU
29	Z	10	ARG
29	Z	29	ARG
32	c	8	LEU
32	c	10	LEU
32	c	33	ILE
32	c	123	MET
32	c	127	ARG
33	d	24	VAL
33	d	81	GLN
35	f	123	LEU
48	s	26	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (53) such sidechains are listed below:

Mol	Chain	Res	Type
3	2	29	GLN
8	C	85	ASN
9	D	49	GLN
9	D	58	ASN
9	D	150	GLN
10	E	90	GLN
10	E	92	HIS
10	E	94	GLN
12	G	19	ASN
12	G	44	HIS
12	G	103	ASN
13	J	58	ASN
13	J	67	ASN
13	J	135	GLN
15	L	4	ASN
15	L	35	HIS
15	L	54	GLN
16	M	17	ASN
18	O	29	HIS
19	P	65	ASN

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Mol	Chain	Res	Type
19	P	76	HIS
24	U	45	GLN
25	V	49	ASN
25	V	51	GLN
25	V	80	HIS
28	Y	20	ASN
30	a	18	GLN
30	a	50	ASN
30	a	92	ASN
30	a	93	HIS
30	a	145	ASN
31	b	99	GLN
31	b	101	ASN
31	b	138	GLN
32	c	40	HIS
32	c	139	ASN
32	c	151	GLN
33	d	18	ASN
34	e	81	ASN
35	f	8	GLN
36	g	17	GLN
37	h	31	GLN
37	h	49	GLN
37	h	74	GLN
37	h	125	GLN
39	j	23	HIS
40	k	95	HIS
42	m	49	GLN
42	m	62	ASN
43	n	39	GLN
45	p	49	ASN
46	q	53	GLN
48	s	81	GLN

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
51	v	1538/1539 (99%)	332 (21%)	0
52	x	11/12 (91%)	5 (45%)	0
53	5	76/77 (98%)	14 (18%)	0
6	A	116/117 (99%)	25 (21%)	1 (0%)

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
7	B	2902/2903 (99%)	598 (20%)	5 (0%)
All	All	4643/4648 (99%)	974 (20%)	6 (0%)

All (974) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
6	A	9	G
6	A	13	G
6	A	14	U
6	A	24	G
6	A	25	U
6	A	26	C
6	A	30	C
6	A	35	C
6	A	36	C
6	A	37	C
6	A	41	G
6	A	44	G
6	A	48	U
6	A	52	A
6	A	53	A
6	A	57	A
6	A	67	G
6	A	87	U
6	A	88	C
6	A	89	U
6	A	90	C
6	A	99	A
6	A	105	G
6	A	108	A
6	A	109	A
7	B	11	C
7	B	12	U
7	B	15	G
7	B	27	G
7	B	34	U
7	B	35	G
7	B	39	G
7	B	46	G
7	B	51	G
7	B	60	G
7	B	63	A

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Mol	Chain	Res	Type
7	B	71	A
7	B	74	A
7	B	75	G
7	B	84	A
7	B	100	U
7	B	101	A
7	B	102	U
7	B	103	A
7	B	118	A
7	B	119	A
7	B	120	U
7	B	122	G
7	B	125	A
7	B	126	A
7	B	139	U
7	B	140	C
7	B	141	G
7	B	142	A
7	B	160	A
7	B	163	C
7	B	164	C
7	B	181	A
7	B	188	G
7	B	196	A
7	B	197	A
7	B	199	A
7	B	215	G
7	B	216	A
7	B	221	A
7	B	223	A
7	B	225	C
7	B	241	A
7	B	245	G
7	B	248	G
7	B	252	G
7	B	255	A
7	B	265	A
7	B	266	G
7	B	271	G
7	B	274	C
7	B	275	C
7	B	277	G

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Mol	Chain	Res	Type
7	B	278	A
7	B	285	G
7	B	301	G
7	B	308	G
7	B	311	A
7	B	324	A
7	B	329	G
7	B	330	A
7	B	332	A
7	B	334	C
7	B	338	G
7	B	352	A
7	B	353	C
7	B	354	A
7	B	355	U
7	B	356	G
7	B	359	G
7	B	362	A
7	B	363	G
7	B	370	G
7	B	371	A
7	B	372	G
7	B	386	G
7	B	396	G
7	B	403	U
7	B	404	A
7	B	406	G
7	B	411	G
7	B	412	A
7	B	424	G
7	B	435	C
7	B	455	C
7	B	456	C
7	B	457	A
7	B	467	G
7	B	473	G
7	B	477	A
7	B	481	G
7	B	490	C
7	B	491	G
7	B	496	G
7	B	504	A

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Mol	Chain	Res	Type
7	B	505	A
7	B	506	G
7	B	508	A
7	B	509	C
7	B	510	C
7	B	512	G
7	B	528	A
7	B	531	C
7	B	532	A
7	B	533	G
7	B	535	G
7	B	544	C
7	B	545	U
7	B	546	U
7	B	547	A
7	B	548	G
7	B	563	A
7	B	568	U
7	B	571	U
7	B	573	U
7	B	575	A
7	B	588	U
7	B	613	A
7	B	614	A
7	B	615	U
7	B	616	A
7	B	634	C
7	B	637	A
7	B	640	C
7	B	645	C
7	B	646	U
7	B	647	G
7	B	654	A
7	B	655	A
7	B	664	G
7	B	669	G
7	B	670	A
7	B	671	C
7	B	686	U
7	B	704	G
7	B	714	U
7	B	717	C

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Mol	Chain	Res	Type
7	B	718	A
7	B	719	C
7	B	726	G
7	B	730	A
7	B	740	C
7	B	745	G
7	B	747	U
7	B	757	G
7	B	762	U
7	B	764	A
7	B	765	C
7	B	775	G
7	B	776	G
7	B	782	A
7	B	783	A
7	B	784	G
7	B	785	G
7	B	789	A
7	B	792	A
7	B	805	G
7	B	811	U
7	B	812	C
7	B	819	A
7	B	827	U
7	B	828	U
7	B	830	G
7	B	846	U
7	B	847	U
7	B	858	G
7	B	859	G
7	B	866	A
7	B	869	G
7	B	871	U
7	B	872	U
7	B	884	U
7	B	886	A
7	B	887	U
7	B	888	C
7	B	889	C
7	B	890	C
7	B	892	A
7	B	893	C

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Mol	Chain	Res	Type
7	B	894	U
7	B	895	U
7	B	896	A
7	B	897	C
7	B	907	G
7	B	910	A
7	B	912	C
7	B	931	U
7	B	932	U
7	B	933	A
7	B	934	U
7	B	941	A
7	B	945	A
7	B	946	C
7	B	957	C
7	B	959	A
7	B	961	C
7	B	974	G
7	B	989	G
7	B	996	A
7	B	997	G
7	B	1009	A
7	B	1012	U
7	B	1013	C
7	B	1017	G
7	B	1022	G
7	B	1023	U
7	B	1024	G
7	B	1025	G
7	B	1026	G
7	B	1033	U
7	B	1040	A
7	B	1045	C
7	B	1046	A
7	B	1047	G
7	B	1054	A
7	B	1060	U
7	B	1061	U
7	B	1062	G
7	B	1065	U
7	B	1067	A
7	B	1068	G

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Mol	Chain	Res	Type
7	B	1070	A
7	B	1074	G
7	B	1075	C
7	B	1084	A
7	B	1087	G
7	B	1088	A
7	B	1089	A
7	B	1095	A
7	B	1096	A
7	B	1097	U
7	B	1098	A
7	B	1100	C
7	B	1110	G
7	B	1111	A
7	B	1112	G
7	B	1115	G
7	B	1126	A
7	B	1132	U
7	B	1133	A
7	B	1134	A
7	B	1135	C
7	B	1139	G
7	B	1142	A
7	B	1143	A
7	B	1149	G
7	B	1173	U
7	B	1174	U
7	B	1175	A
7	B	1176	U
7	B	1178	C
7	B	1205	A
7	B	1206	G
7	B	1211	C
7	B	1212	G
7	B	1227	G
7	B	1236	G
7	B	1237	A
7	B	1238	G
7	B	1241	A
7	B	1244	A
7	B	1247	A
7	B	1250	G

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Mol	Chain	Res	Type
7	B	1253	A
7	B	1255	U
7	B	1256	G
7	B	1257	C
7	B	1266	G
7	B	1272	A
7	B	1273	U
7	B	1275	A
7	B	1276	A
7	B	1300	G
7	B	1301	A
7	B	1324	G
7	B	1325	U
7	B	1329	U
7	B	1337	G
7	B	1338	G
7	B	1352	U
7	B	1359	A
7	B	1365	A
7	B	1368	G
7	B	1374	G
7	B	1378	A
7	B	1379	U
7	B	1382	G
7	B	1383	A
7	B	1388	G
7	B	1392	A
7	B	1396	U
7	B	1416	G
7	B	1420	A
7	B	1421	G
7	B	1426	G
7	B	1427	A
7	B	1428	C
7	B	1452	G
7	B	1459	G
7	B	1460	U
7	B	1470	A
7	B	1476	U
7	B	1477	A
7	B	1478	G
7	B	1482	G

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Mol	Chain	Res	Type
7	B	1494	A
7	B	1522	A
7	B	1524	G
7	B	1529	G
7	B	1535	A
7	B	1536	C
7	B	1538	G
7	B	1545	A
7	B	1552	A
7	B	1558	C
7	B	1560	G
7	B	1566	A
7	B	1569	A
7	B	1578	U
7	B	1583	A
7	B	1585	C
7	B	1589	U
7	B	1590	A
7	B	1607	C
7	B	1608	A
7	B	1610	A
7	B	1634	A
7	B	1639	C
7	B	1647	U
7	B	1648	U
7	B	1653	G
7	B	1674	G
7	B	1694	C
7	B	1713	A
7	B	1722	A
7	B	1724	G
7	B	1725	U
7	B	1729	U
7	B	1730	C
7	B	1731	G
7	B	1732	C
7	B	1733	G
7	B	1750	G
7	B	1757	A
7	B	1758	U
7	B	1759	A
7	B	1763	G

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Mol	Chain	Res	Type
7	B	1764	C
7	B	1773	A
7	B	1776	G
7	B	1779	U
7	B	1780	A
7	B	1784	A
7	B	1786	A
7	B	1787	A
7	B	1800	C
7	B	1801	A
7	B	1802	A
7	B	1808	A
7	B	1809	A
7	B	1810	A
7	B	1816	C
7	B	1829	A
7	B	1848	A
7	B	1870	C
7	B	1871	A
7	B	1884	G
7	B	1896	G
7	B	1903	G
7	B	1906	G
7	B	1913	A
7	B	1914	C
7	B	1915	U
7	B	1916	A
7	B	1929	G
7	B	1930	G
7	B	1936	A
7	B	1937	A
7	B	1940	U
7	B	1955	U
7	B	1964	G
7	B	1966	A
7	B	1967	C
7	B	1970	A
7	B	1971	U
7	B	1972	G
7	B	1991	U
7	B	1992	G
7	B	1996	C

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Mol	Chain	Res	Type
7	B	1997	C
7	B	2021	C
7	B	2023	C
7	B	2030	A
7	B	2031	A
7	B	2033	A
7	B	2036	C
7	B	2043	C
7	B	2049	G
7	B	2052	A
7	B	2055	C
7	B	2056	G
7	B	2060	A
7	B	2061	G
7	B	2062	A
7	B	2069	G
7	B	2076	U
7	B	2093	G
7	B	2097	A
7	B	2099	U
7	B	2101	A
7	B	2108	A
7	B	2109	U
7	B	2110	G
7	B	2111	U
7	B	2112	G
7	B	2115	G
7	B	2116	G
7	B	2117	A
7	B	2118	U
7	B	2120	G
7	B	2123	G
7	B	2124	G
7	B	2126	A
7	B	2127	G
7	B	2128	G
7	B	2132	U
7	B	2133	G
7	B	2135	A
7	B	2138	G
7	B	2139	U
7	B	2142	A

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Mol	Chain	Res	Type
7	B	2144	G
7	B	2147	A
7	B	2149	U
7	B	2153	C
7	B	2156	G
7	B	2157	G
7	B	2158	A
7	B	2159	G
7	B	2161	C
7	B	2162	G
7	B	2163	A
7	B	2164	C
7	B	2165	C
7	B	2166	U
7	B	2171	A
7	B	2172	U
7	B	2173	A
7	B	2177	C
7	B	2179	C
7	B	2181	U
7	B	2183	A
7	B	2184	A
7	B	2186	G
7	B	2187	U
7	B	2188	U
7	B	2198	A
7	B	2199	A
7	B	2204	G
7	B	2211	A
7	B	2212	A
7	B	2213	U
7	B	2225	A
7	B	2238	G
7	B	2239	G
7	B	2243	U
7	B	2250	G
7	B	2251	G
7	B	2266	A
7	B	2278	A
7	B	2280	G
7	B	2283	C
7	B	2287	A

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Mol	Chain	Res	Type
7	B	2288	A
7	B	2303	G
7	B	2304	G
7	B	2305	U
7	B	2307	G
7	B	2309	A
7	B	2319	G
7	B	2321	U
7	B	2322	A
7	B	2325	G
7	B	2333	A
7	B	2335	A
7	B	2336	A
7	B	2337	G
7	B	2345	G
7	B	2347	C
7	B	2350	C
7	B	2354	C
7	B	2358	A
7	B	2361	G
7	B	2375	G
7	B	2379	G
7	B	2383	G
7	B	2385	C
7	B	2391	G
7	B	2396	G
7	B	2402	U
7	B	2403	C
7	B	2406	A
7	B	2422	C
7	B	2423	U
7	B	2425	A
7	B	2428	G
7	B	2429	G
7	B	2430	A
7	B	2435	A
7	B	2441	U
7	B	2445	G
7	B	2448	A
7	B	2469	A
7	B	2471	A
7	B	2472	G

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Mol	Chain	Res	Type
7	B	2476	A
7	B	2478	A
7	B	2491	U
7	B	2498	C
7	B	2499	C
7	B	2502	G
7	B	2503	A
7	B	2504	U
7	B	2505	G
7	B	2518	A
7	B	2520	C
7	B	2529	G
7	B	2534	A
7	B	2547	A
7	B	2553	G
7	B	2554	U
7	B	2556	C
7	B	2564	A
7	B	2566	A
7	B	2567	G
7	B	2569	G
7	B	2572	A
7	B	2573	C
7	B	2602	A
7	B	2603	G
7	B	2609	U
7	B	2613	U
7	B	2615	U
7	B	2619	C
7	B	2629	U
7	B	2634	A
7	B	2642	G
7	B	2646	C
7	B	2654	A
7	B	2663	G
7	B	2673	G
7	B	2688	G
7	B	2689	U
7	B	2690	U
7	B	2712	C
7	B	2714	G
7	B	2716	C

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Mol	Chain	Res	Type
7	B	2718	G
7	B	2725	A
7	B	2726	A
7	B	2744	G
7	B	2748	A
7	B	2765	A
7	B	2766	A
7	B	2769	U
7	B	2778	A
7	B	2791	G
7	B	2793	C
7	B	2797	U
7	B	2798	U
7	B	2799	A
7	B	2800	A
7	B	2808	G
7	B	2809	A
7	B	2818	U
7	B	2820	A
7	B	2823	A
7	B	2833	U
7	B	2834	G
7	B	2835	A
7	B	2836	U
7	B	2843	G
7	B	2846	G
7	B	2849	U
7	B	2861	U
7	B	2867	G
7	B	2872	A
7	B	2873	A
7	B	2877	G
7	B	2879	A
7	B	2880	C
7	B	2883	A
7	B	2884	U
7	B	2885	G
7	B	2886	A
7	B	2891	U
7	B	2900	A
7	B	2902	C
51	v	3	A

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Mol	Chain	Res	Type
51	v	4	U
51	v	5	U
51	v	7	A
51	v	9	G
51	v	22	G
51	v	32	A
51	v	39	G
51	v	47	C
51	v	48	C
51	v	49	U
51	v	50	A
51	v	51	A
51	v	52	C
51	v	58	C
51	v	70	U
51	v	71	A
51	v	72	A
51	v	74	A
51	v	77	A
51	v	78	A
51	v	81	A
51	v	83	C
51	v	84	U
51	v	85	U
51	v	86	G
51	v	89	U
51	v	92	U
51	v	94	G
51	v	95	C
51	v	108	G
51	v	110	C
51	v	116	A
51	v	119	A
51	v	120	A
51	v	121	U
51	v	122	G
51	v	127	G
51	v	130	A
51	v	131	A
51	v	132	C
51	v	138	G
51	v	142	G

*Continued on next page...*

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Mol	Chain	Res	Type
51	v	144	G
51	v	146	G
51	v	159	G
51	v	163	C
51	v	171	A
51	v	177	G
51	v	181	A
51	v	182	A
51	v	183	C
51	v	190	A
51	v	191	G
51	v	197	A
51	v	203	G
51	v	204	G
51	v	205	A
51	v	207	C
51	v	210	C
51	v	211	G
51	v	212	G
51	v	213	G
51	v	226	G
51	v	245	U
51	v	247	G
51	v	251	G
51	v	266	G
51	v	267	C
51	v	268	U
51	v	278	G
51	v	281	G
51	v	289	G
51	v	321	A
51	v	327	A
51	v	328	C
51	v	330	C
51	v	332	G
51	v	345	C
51	v	347	G
51	v	351	G
51	v	352	C
51	v	354	G
51	v	367	U
51	v	372	C

*Continued on next page...*



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Mol	Chain	Res	Type
51	v	378	G
51	v	388	G
51	v	398	U
51	v	406	G
51	v	413	G
51	v	421	U
51	v	422	C
51	v	423	G
51	v	424	G
51	v	425	G
51	v	428	G
51	v	429	U
51	v	438	U
51	v	441	A
51	v	451	A
51	v	458	U
51	v	459	A
51	v	466	A
51	v	467	U
51	v	468	A
51	v	469	C
51	v	471	U
51	v	478	A
51	v	481	G
51	v	484	G
51	v	486	U
51	v	493	A
51	v	495	A
51	v	496	A
51	v	497	G
51	v	509	A
51	v	511	C
51	v	512	U
51	v	518	C
51	v	519	C
51	v	521	G
51	v	524	G
51	v	527	G
51	v	532	A
51	v	547	A
51	v	559	A
51	v	564	C

*Continued on next page...*

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Mol	Chain	Res	Type
51	v	572	A
51	v	573	A
51	v	576	C
51	v	577	G
51	v	594	U
51	v	595	A
51	v	596	A
51	v	600	A
51	v	607	A
51	v	615	G
51	v	618	C
51	v	633	G
51	v	640	A
51	v	642	A
51	v	650	G
51	v	653	U
51	v	665	A
51	v	682	G
51	v	686	U
51	v	695	A
51	v	702	A
51	v	703	G
51	v	721	G
51	v	723	U
51	v	731	G
51	v	734	G
51	v	755	G
51	v	778	G
51	v	781	A
51	v	782	A
51	v	793	U
51	v	794	A
51	v	799	G
51	v	814	A
51	v	815	A
51	v	817	C
51	v	819	A
51	v	820	U
51	v	821	G
51	v	828	U
51	v	829	G
51	v	832	G

*Continued on next page...*

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Mol	Chain	Res	Type
51	v	836	G
51	v	842	U
51	v	843	U
51	v	845	A
51	v	851	G
51	v	864	A
51	v	870	U
51	v	872	A
51	v	876	C
51	v	887	G
51	v	889	A
51	v	902	G
51	v	914	A
51	v	922	G
51	v	926	G
51	v	927	G
51	v	931	C
51	v	934	C
51	v	935	A
51	v	960	U
51	v	969	A
51	v	971	G
51	v	975	A
51	v	976	G
51	v	977	A
51	v	979	C
51	v	980	C
51	v	983	A
51	v	991	U
51	v	992	U
51	v	993	G
51	v	1004	A
51	v	1012	A
51	v	1013	G
51	v	1020	G
51	v	1021	A
51	v	1027	C
51	v	1028	C
51	v	1031	C
51	v	1033	G
51	v	1034	G
51	v	1043	G

*Continued on next page...*

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Mol	Chain	Res	Type
51	v	1044	A
51	v	1053	G
51	v	1056	U
51	v	1061	G
51	v	1064	G
51	v	1065	U
51	v	1074	G
51	v	1085	U
51	v	1086	U
51	v	1087	G
51	v	1094	G
51	v	1095	U
51	v	1101	A
51	v	1102	A
51	v	1108	G
51	v	1124	G
51	v	1125	U
51	v	1126	U
51	v	1129	C
51	v	1132	C
51	v	1133	G
51	v	1135	U
51	v	1136	C
51	v	1137	C
51	v	1139	G
51	v	1142	G
51	v	1143	G
51	v	1145	A
51	v	1152	A
51	v	1154	G
51	v	1158	C
51	v	1159	U
51	v	1160	G
51	v	1162	C
51	v	1167	A
51	v	1168	U
51	v	1169	A
51	v	1174	G
51	v	1179	A
51	v	1184	G
51	v	1190	G
51	v	1196	A

*Continued on next page...*

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Mol	Chain	Res	Type
51	v	1197	A
51	v	1202	U
51	v	1212	U
51	v	1213	A
51	v	1214	C
51	v	1215	G
51	v	1220	G
51	v	1225	A
51	v	1227	A
51	v	1236	A
51	v	1238	A
51	v	1239	A
51	v	1241	G
51	v	1247	U
51	v	1253	G
51	v	1258	G
51	v	1260	G
51	v	1273	C
51	v	1274	A
51	v	1275	A
51	v	1277	C
51	v	1279	G
51	v	1280	A
51	v	1285	A
51	v	1286	U
51	v	1287	A
51	v	1292	G
51	v	1293	C
51	v	1298	U
51	v	1299	A
51	v	1302	C
51	v	1305	G
51	v	1312	G
51	v	1318	A
51	v	1319	A
51	v	1320	C
51	v	1322	C
51	v	1332	A
51	v	1346	A
51	v	1348	U
51	v	1350	A
51	v	1353	G

*Continued on next page...*

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Mol	Chain	Res	Type
51	v	1363	A
51	v	1364	U
51	v	1368	A
51	v	1370	G
51	v	1377	A
51	v	1378	C
51	v	1381	U
51	v	1394	A
51	v	1398	A
51	v	1399	C
51	v	1400	C
51	v	1404	C
51	v	1405	G
51	v	1406	U
51	v	1411	C
51	v	1419	G
51	v	1432	G
51	v	1441	A
51	v	1446	A
51	v	1451	U
51	v	1452	C
51	v	1453	G
51	v	1487	G
51	v	1492	A
51	v	1493	A
51	v	1494	G
51	v	1495	U
51	v	1497	G
51	v	1499	A
51	v	1503	A
51	v	1506	U
51	v	1507	A
51	v	1517	G
51	v	1519	A
51	v	1529	G
51	v	1530	G
51	v	1533	C
52	x	4	A
52	x	8	C
52	x	9	A
52	x	10	A
52	x	12	A

*Continued on next page...*

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Mol	Chain	Res	Type
53	5	8	U
53	5	9	G
53	5	16	C
53	5	18	G
53	5	19	G
53	5	20	U
53	5	21	A
53	5	43	A
53	5	47	U
53	5	48	C
53	5	56	C
53	5	57	A
53	5	60	U
53	5	76	A

All (6) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
6	A	66	A
7	B	490	C
7	B	669	G
7	B	670	A
7	B	1652	A
7	B	2808	G

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

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

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues

The following chains have linkage breaks:

Mol	Chain	Number of breaks
51	v	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	v	1531:A	O3'	1532:U	P	1.18



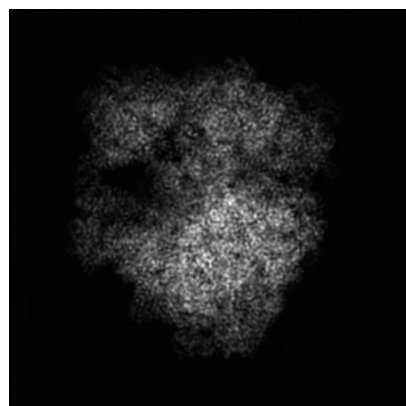
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-41049. These allow visual inspection of the internal detail of the map and identification of artifacts.

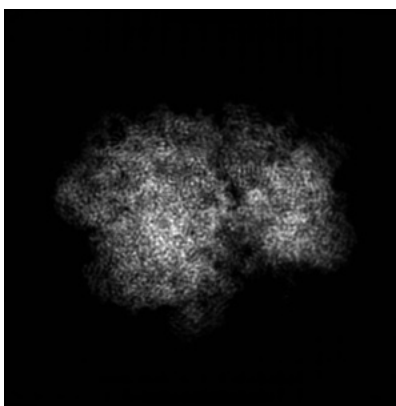
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

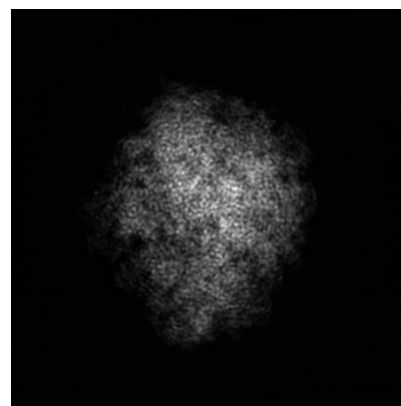
#### 6.1.1 Primary map



X

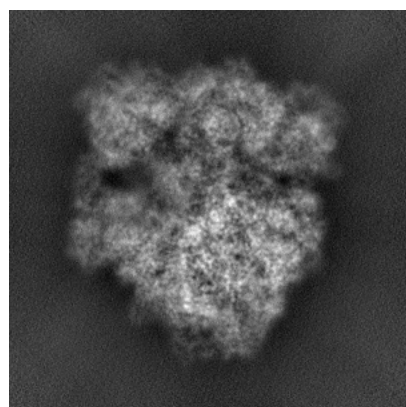


Y

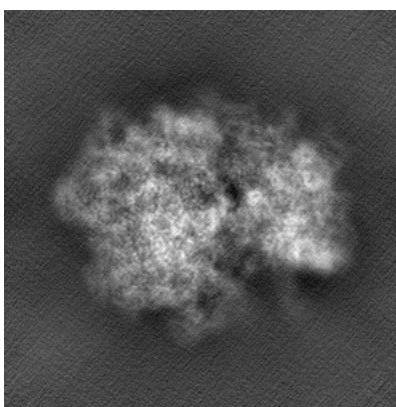


Z

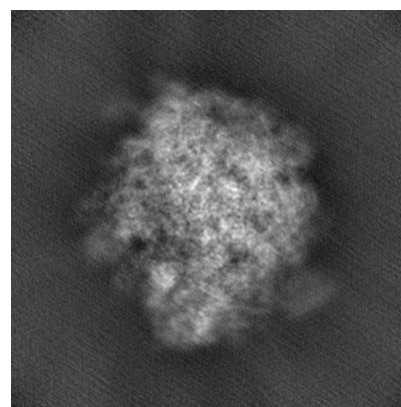
#### 6.1.2 Raw map



X



Y

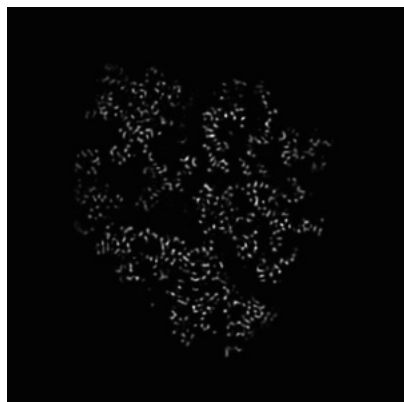


Z

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

## 6.2 Central slices [i](#)

### 6.2.1 Primary map



X Index: 200

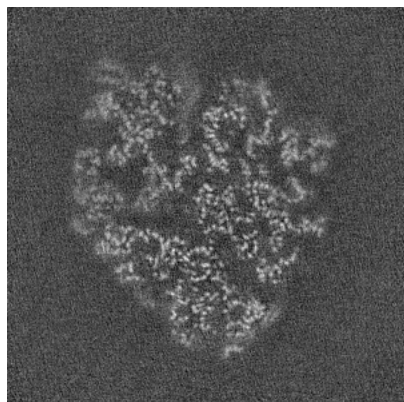


Y Index: 200

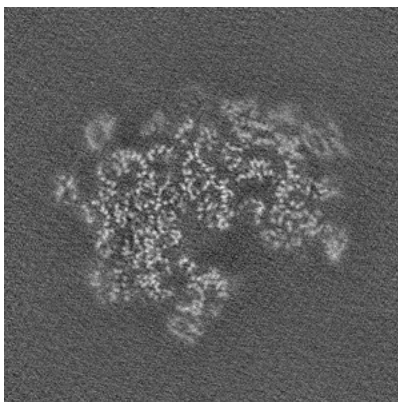


Z Index: 200

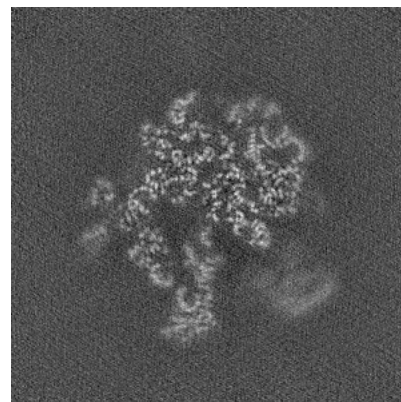
### 6.2.2 Raw map



X Index: 200



Y Index: 200

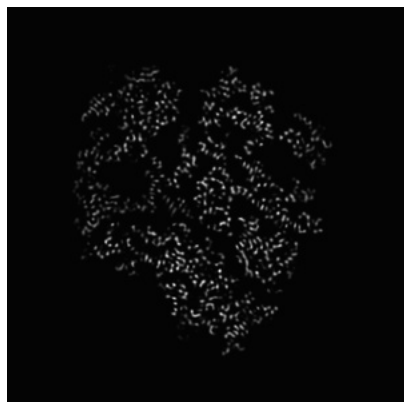


Z Index: 200

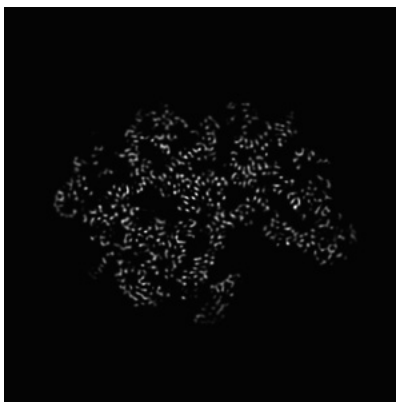
The images above show central slices of the map in three orthogonal directions.

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

### 6.3.1 Primary map



X Index: 195

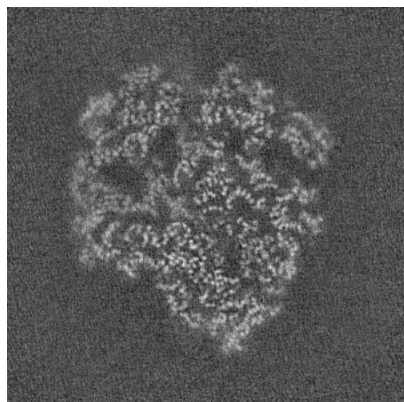


Y Index: 218

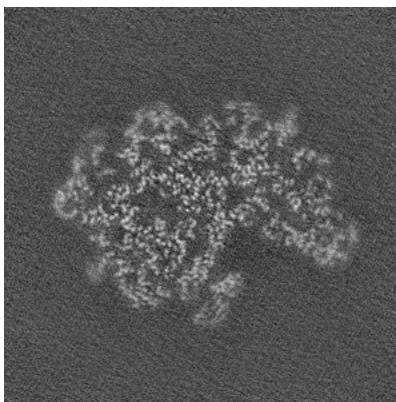


Z Index: 165

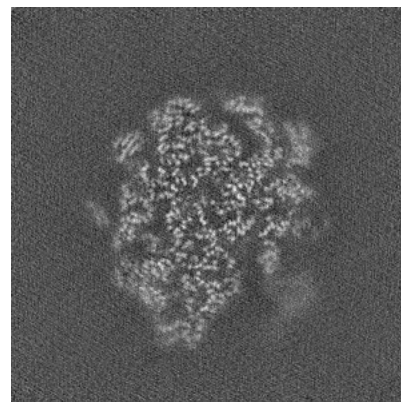
### 6.3.2 Raw map



X Index: 193



Y Index: 218

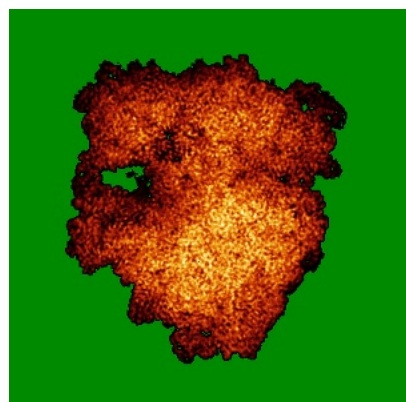


Z Index: 165

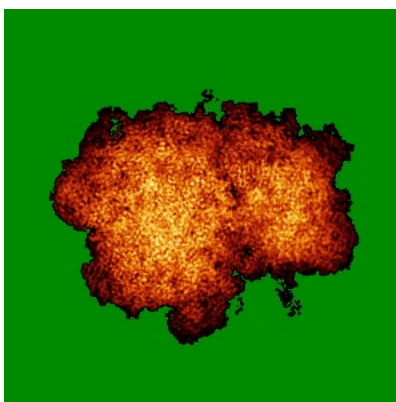
The images above show the largest variance slices of the map in three orthogonal directions.

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

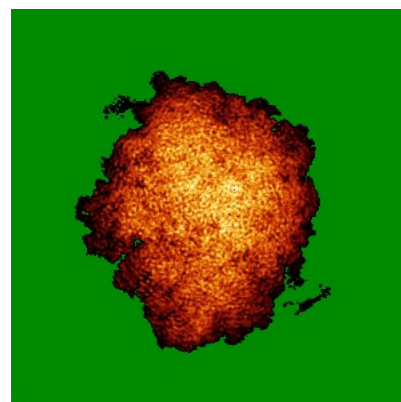
### 6.4.1 Primary map



X

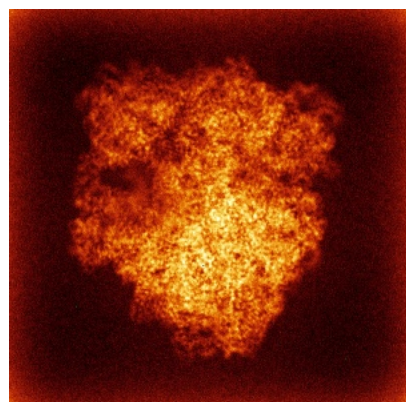


Y

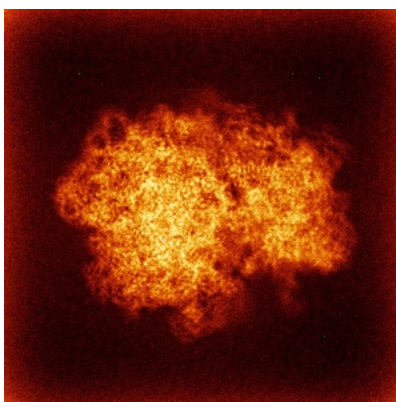


Z

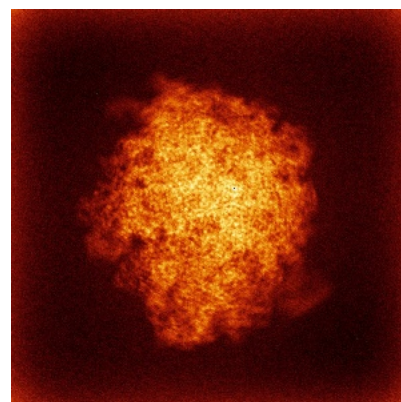
### 6.4.2 Raw map



X



Y



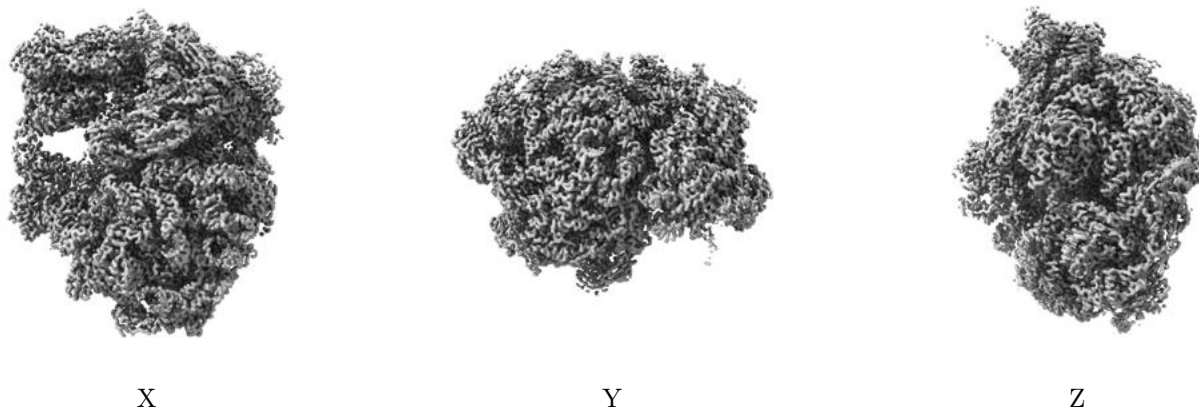
Z

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.



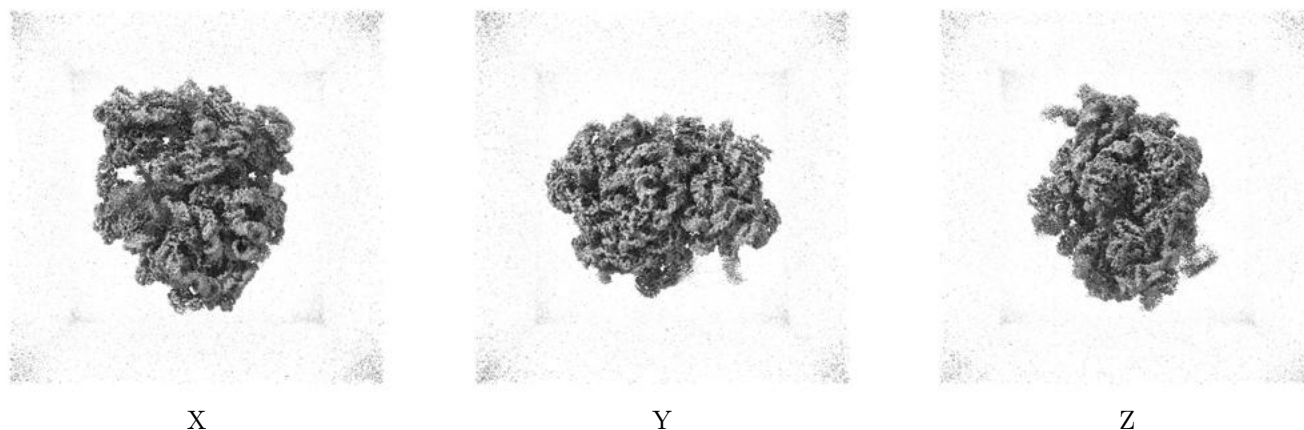
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.124. 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.

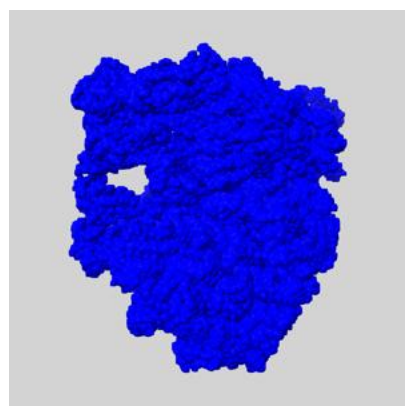
## 6.6 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

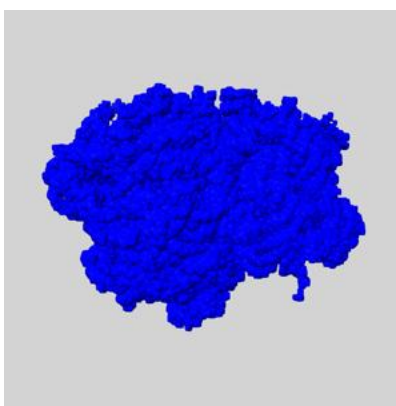
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

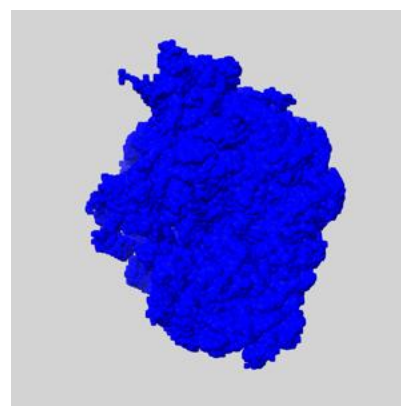
### 6.6.1 emd\_41049\_msk\_1.map [i](#)



X



Y

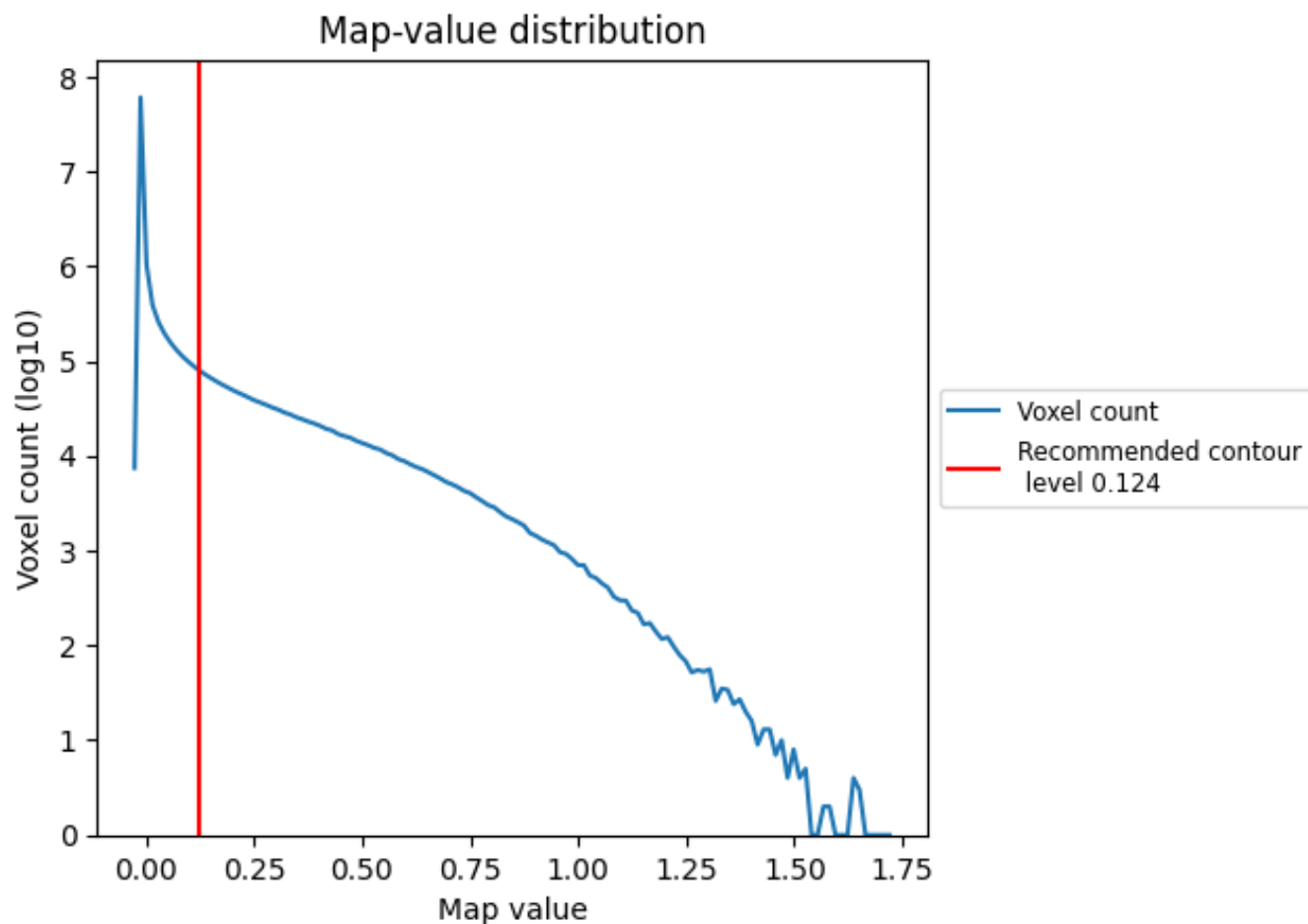


Z

## 7 Map analysis [i](#)

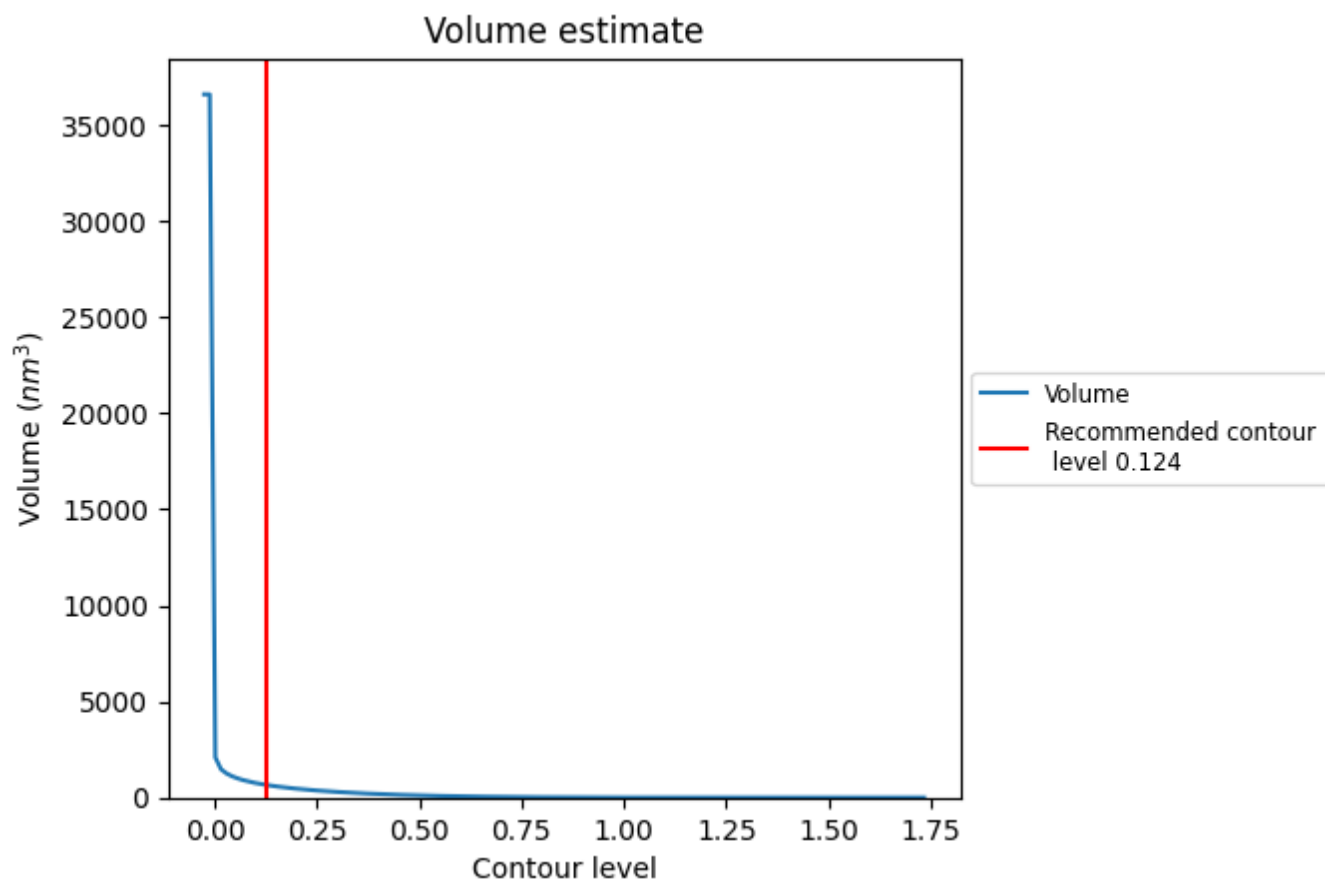
This section contains the results of statistical analysis of the map.

### 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](#)

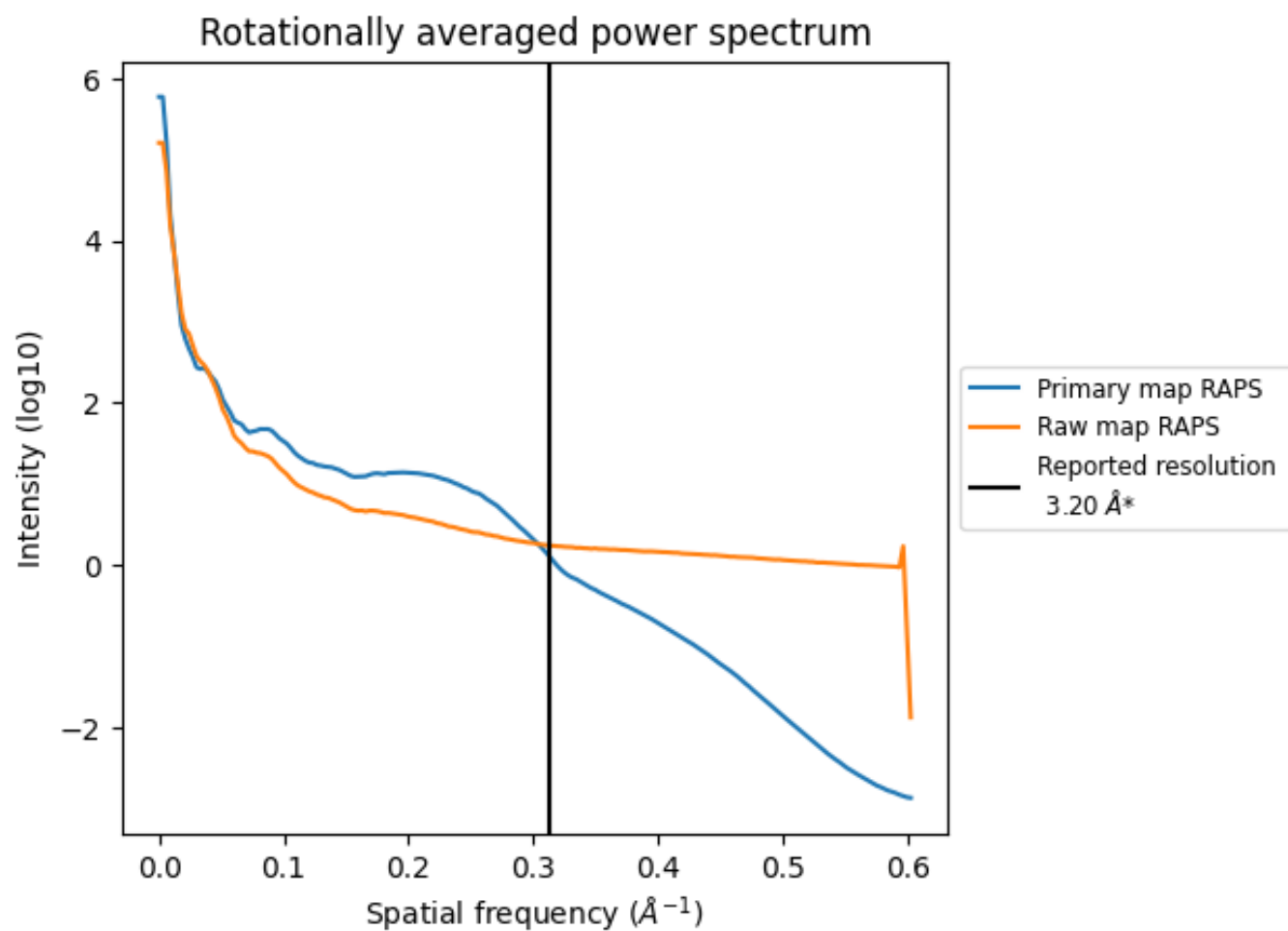


The volume at the recommended contour level is  $665 \text{ nm}^3$ ; this corresponds to an approximate mass of 601 kDa.

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 ⓘ

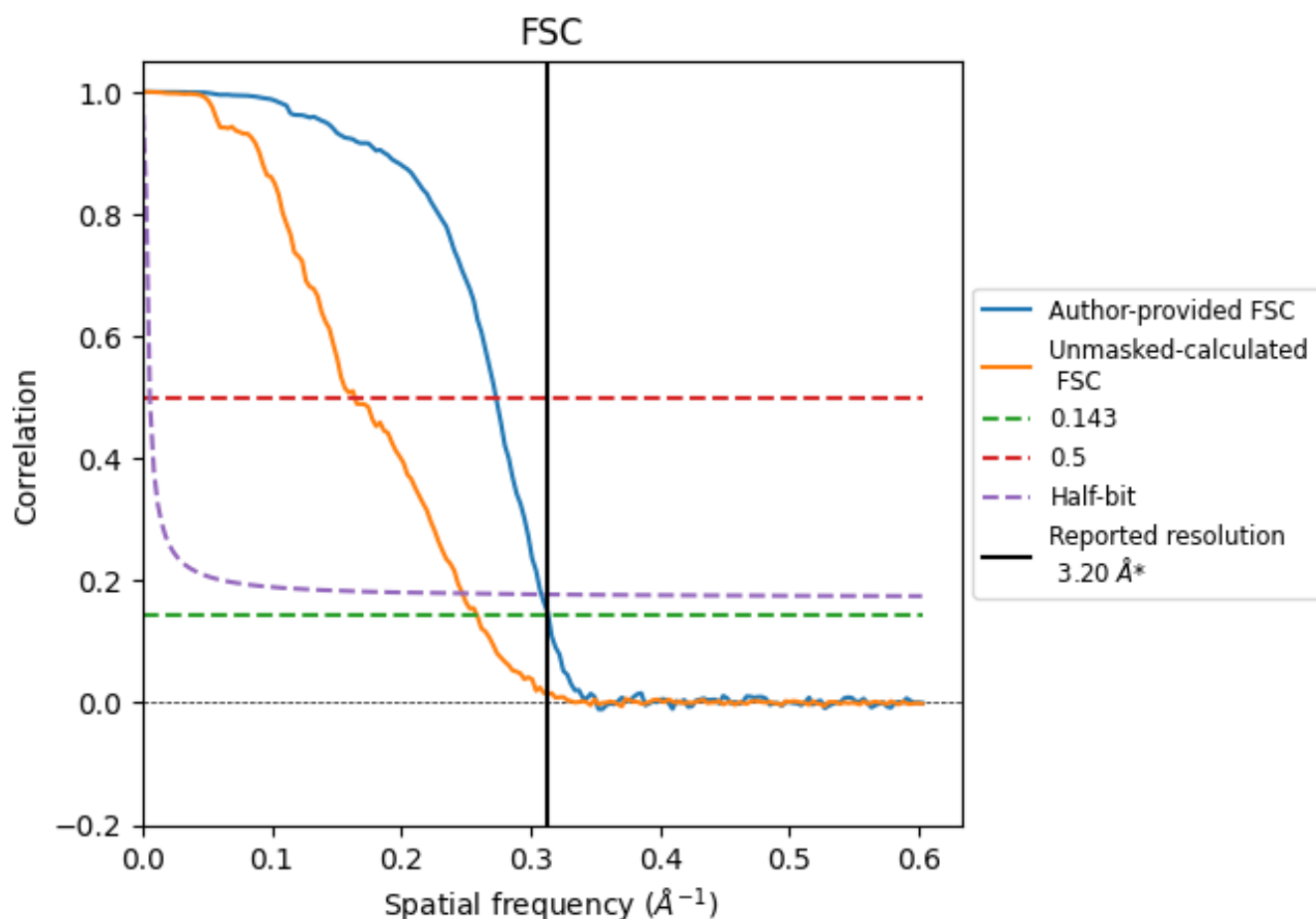


\*Reported resolution corresponds to spatial frequency of 0.312  $\text{\AA}^{-1}$

## 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  $0.312 \text{ \AA}^{-1}$

## 8.2 Resolution estimates [i](#)

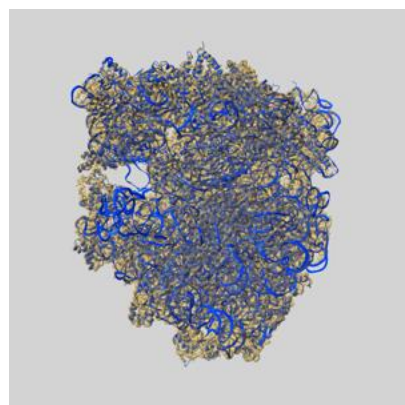
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.20	-	-
Author-provided FSC curve	3.19	3.66	3.24
Unmasked-calculated*	3.87	6.09	4.04

\*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 3.87 differs from the reported value 3.2 by more than 10 %

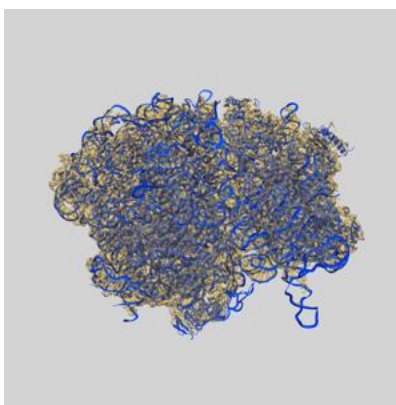
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-41049 and PDB model 8T5D. Per-residue inclusion information can be found in [section 3](#) on [page 13](#).

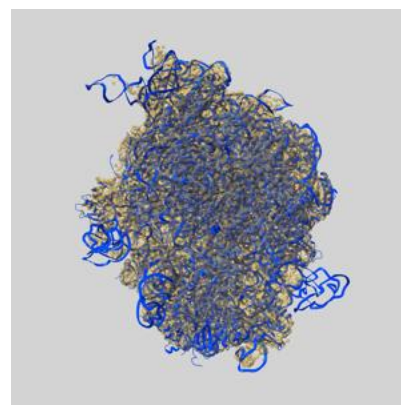
### 9.1 Map-model overlay [i](#)



X



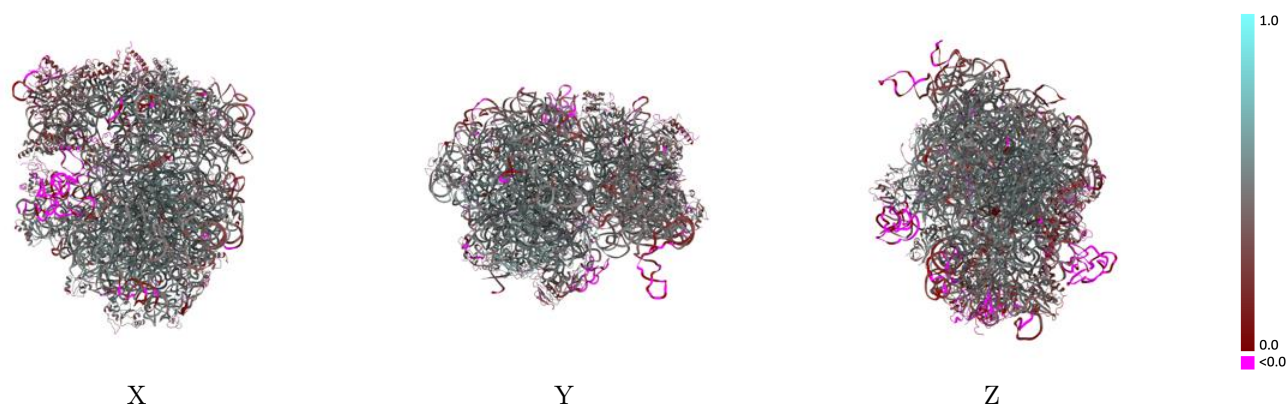
Y



Z

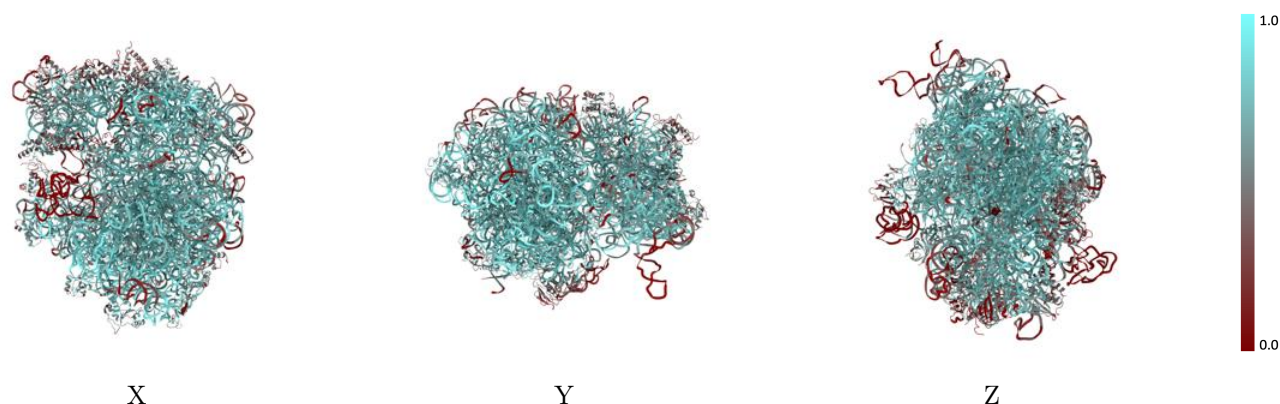
The images above show the 3D surface view of the map at the recommended contour level 0.124 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



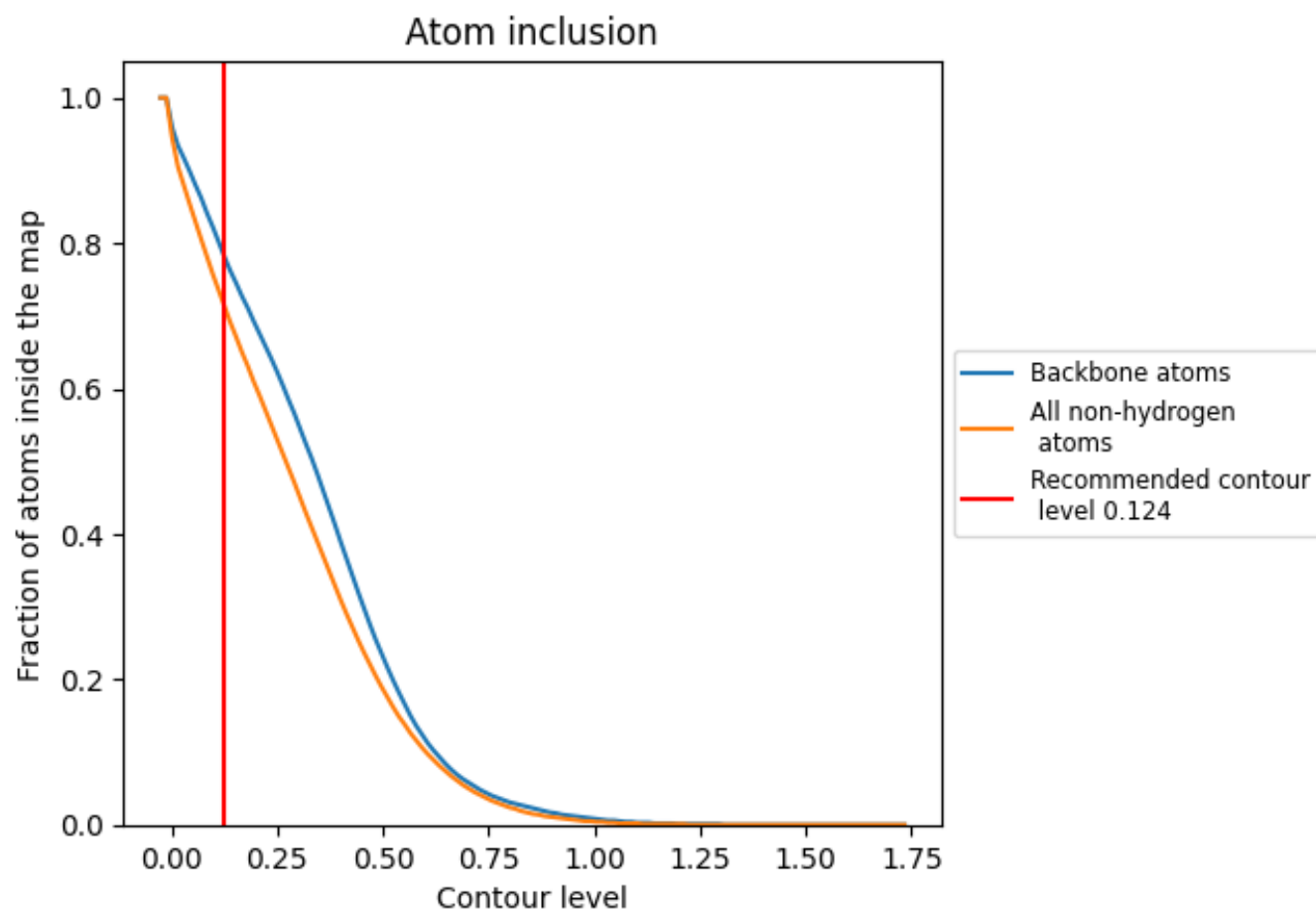
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.124).







































































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 78% of all backbone atoms, 72% 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 (0.124) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7150	 0.4360
0	 0.6920	 0.4730
1	 0.6470	 0.4380
2	 0.7890	 0.5200
3	 0.8290	 0.5590
4	 0.7360	 0.5210
5	 0.6360	 0.4160
A	 0.7220	 0.4280
B	 0.7740	 0.4580
C	 0.7880	 0.5200
D	 0.7460	 0.4940
E	 0.6970	 0.4640
F	 0.3930	 0.1950
G	 0.4260	 0.3290
J	 0.7360	 0.4790
K	 0.7310	 0.4770
L	 0.7090	 0.4740
M	 0.7190	 0.4840
N	 0.7760	 0.5150
O	 0.6170	 0.4220
P	 0.6910	 0.4260
Q	 0.7610	 0.5110
R	 0.6850	 0.4600
S	 0.7210	 0.4690
T	 0.5480	 0.3430
U	 0.5690	 0.3890
V	 0.5220	 0.3980
W	 0.6450	 0.3720
X	 0.6640	 0.4840
Y	 0.5210	 0.3350
Z	 0.7090	 0.4800
a	 0.3180	 0.2320
b	 0.6190	 0.4080
c	 0.5840	 0.3900
d	 0.7090	 0.4730



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Chain	Atom inclusion	Q-score
e	 0.4520	 0.3310
f	 0.3380	 0.2560
g	 0.7160	 0.4650
h	 0.5130	 0.3320
i	 0.4720	 0.3010
j	 0.5670	 0.3830
k	 0.6910	 0.4790
l	 0.5010	 0.3450
m	 0.5530	 0.3660
n	 0.6390	 0.4180
o	 0.6410	 0.4350
p	 0.5610	 0.3830
q	 0.6060	 0.4150
r	 0.5210	 0.3640
s	 0.5570	 0.3870
t	 0.1670	 0.1190
u	 0.0020	 -0.0270
v	 0.7510	 0.4400
x	 0.3110	 0.2350