



Full wwPDB EM Validation Report ⓘ

Mar 6, 2026 – 01:57 PM UTC

PDB ID : 8G2U / pdb_00008g2u
EMDB ID : EMD-29681
Title : Time-resolved cryo-EM study of the 70S recycling by the HflX:control-apo-70S at 900ms
Authors : Bhattacharjee, S.; Brown, P.Z.; Frank, J.
Deposited on : 2023-02-06
Resolution : 3.00 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

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

The types of validation reports are described at
<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

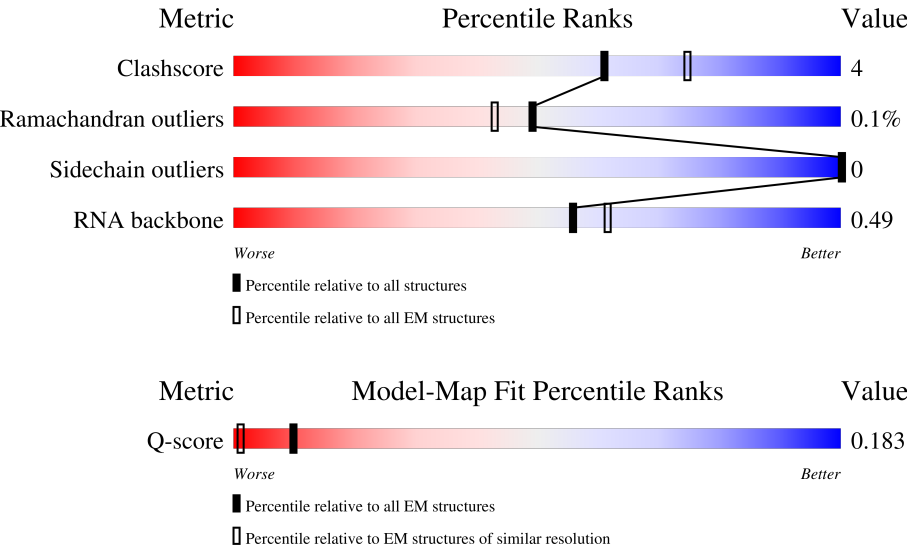
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh &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

1 Overall quality at a glance i

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

The reported resolution of this entry is 3.00 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	14081 (2.50 - 3.50)

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

Mol	Chain	Length	Quality of chain
1	0	56	55% 77% 23%
2	1	51	49% 86% 14%
3	2	46	48% 91% 9%

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Mol	Chain	Length	Quality of chain
4	3	64	39% 88% 11%
5	4	38	55% 84% 16%
6	A	117	46% 68% 31%
7	B	2903	40% 68% 28%
8	C	272	36% 82% 18%
9	D	209	52% 90% 10%
10	E	201	72% 86% 14%
11	F	178	99% 85% 14%
12	G	176	89% 86% 14%
13	J	142	62% 85% 15%
14	K	122	56% 79% 20%
15	L	143	57% 86% 14%
16	M	136	49% 83% 17%
17	N	121	55% 91% 9%
18	O	116	72% 89% 11%
19	P	114	58% 86% 14%
20	Q	117	60% 84% 16%
21	R	103	58% 85% 15%
22	S	110	60% 79% 21%
23	T	94	82% 85% 15%
24	U	103	79% 83% 17%
25	V	94	72% 82% 18%
26	W	79	48% 72% 27%
27	X	77	44% 87% 13%
28	Y	63	81% 79% 21%

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Mol	Chain	Length	Quality of chain
29	Z	58	
30	a	218	
31	b	206	
32	c	205	
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	

2 Entry composition

There are 51 unique types of molecules in this entry. The entry contains 140855 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 rRNA.

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 rRNA.

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		

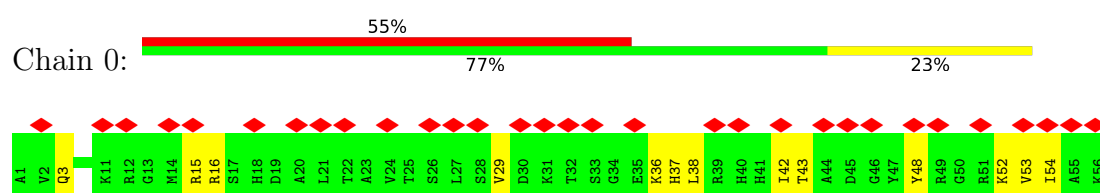
- Molecule 51 is a RNA chain called 16S rRNA.

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

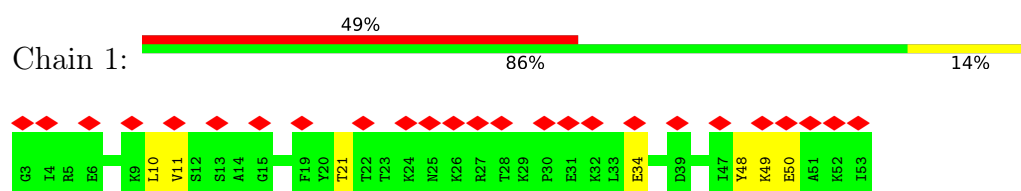
3 Residue-property plots [i](#)

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.

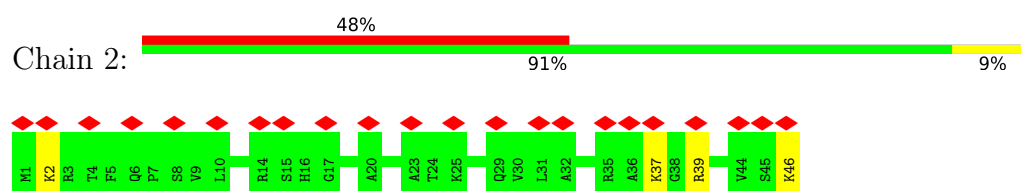
- Molecule 1: 50S ribosomal protein L32



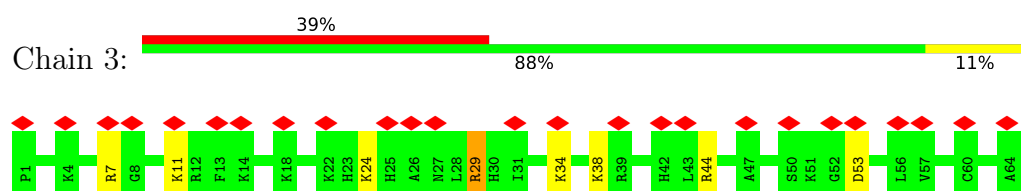
- Molecule 2: 50S ribosomal protein L33



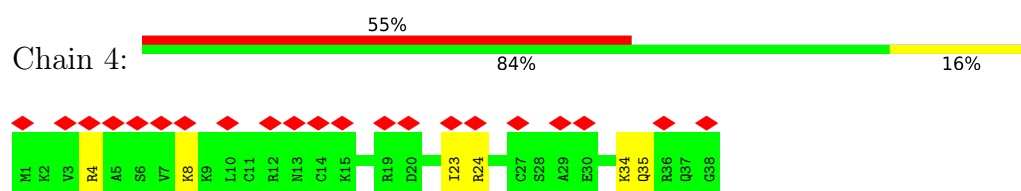
- Molecule 3: 50S ribosomal protein L34



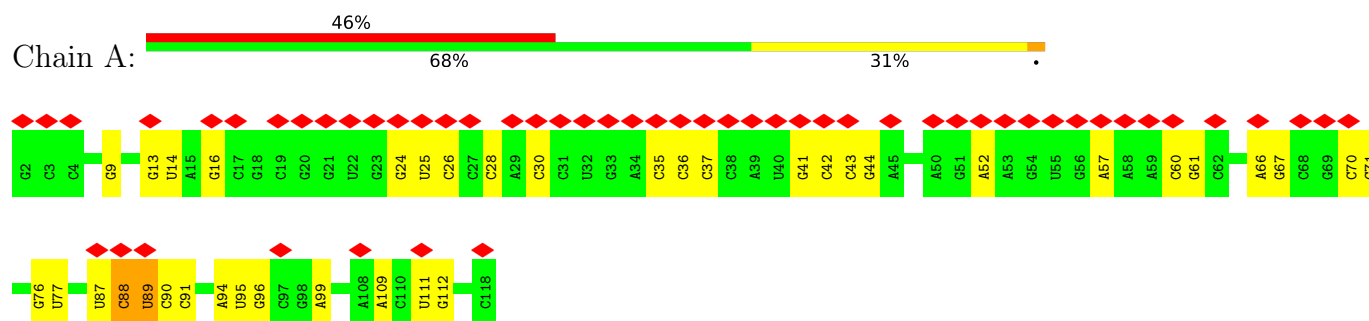
- Molecule 4: 50S ribosomal protein L35



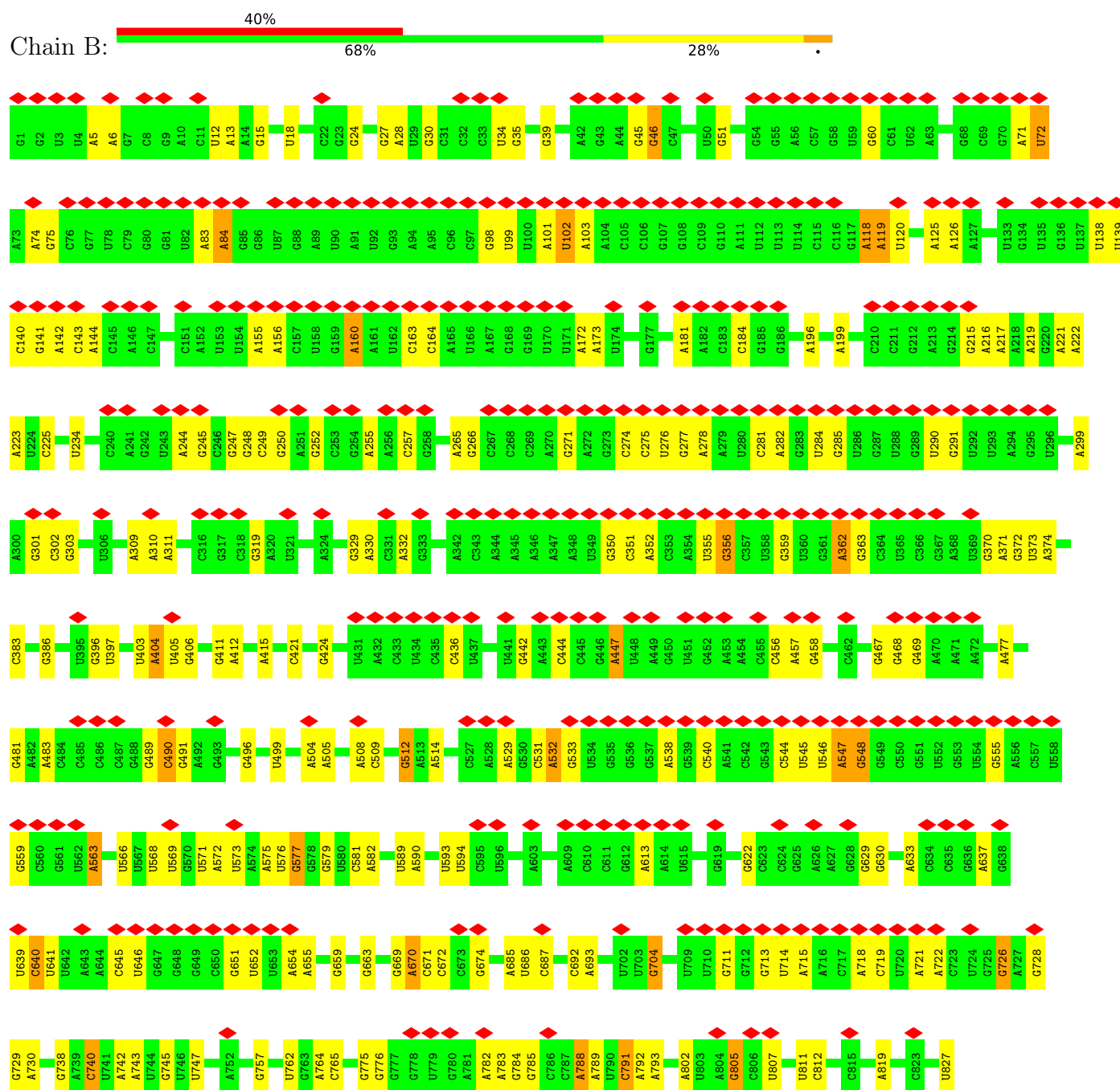
- Molecule 5: 50S ribosomal protein L36

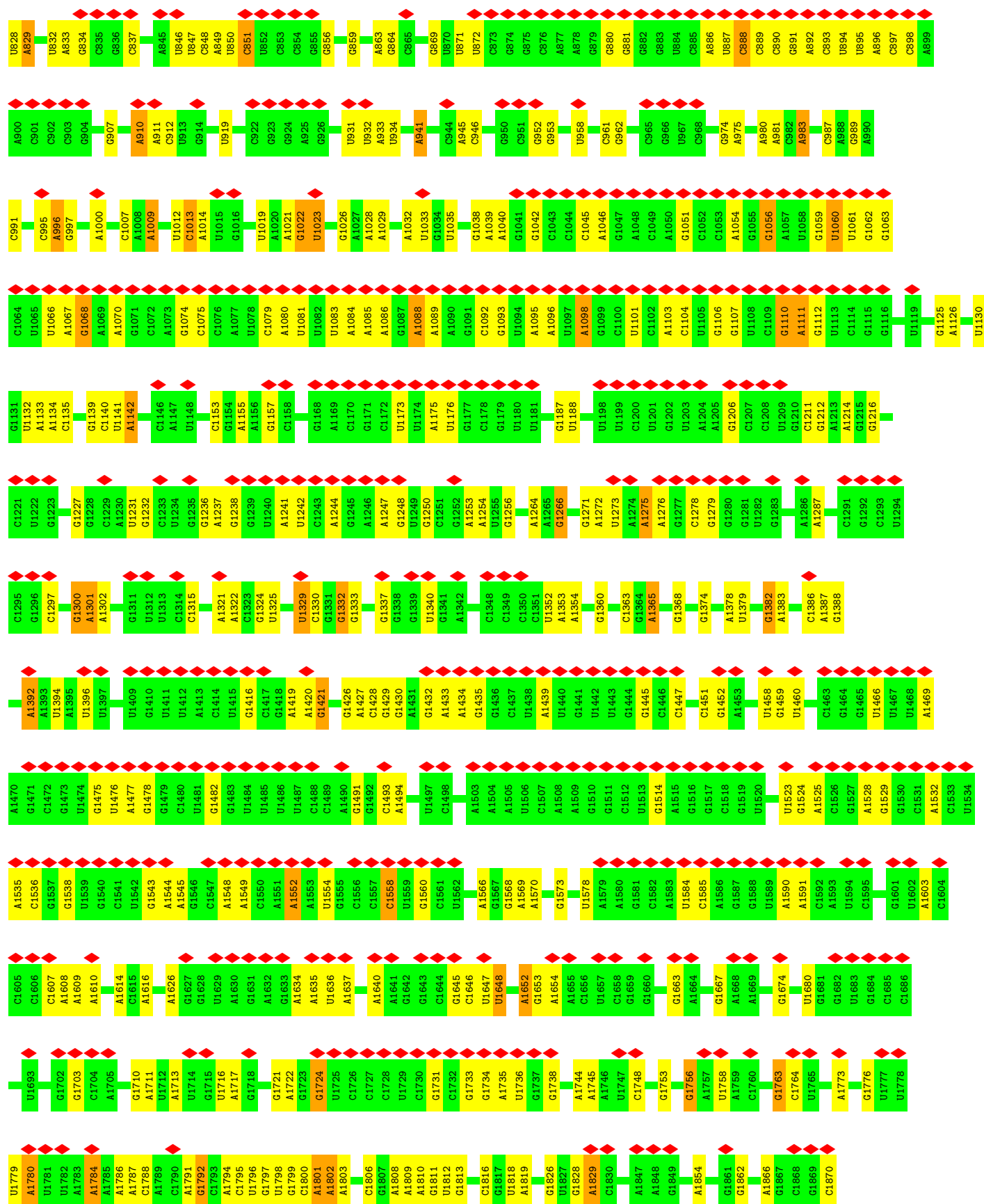


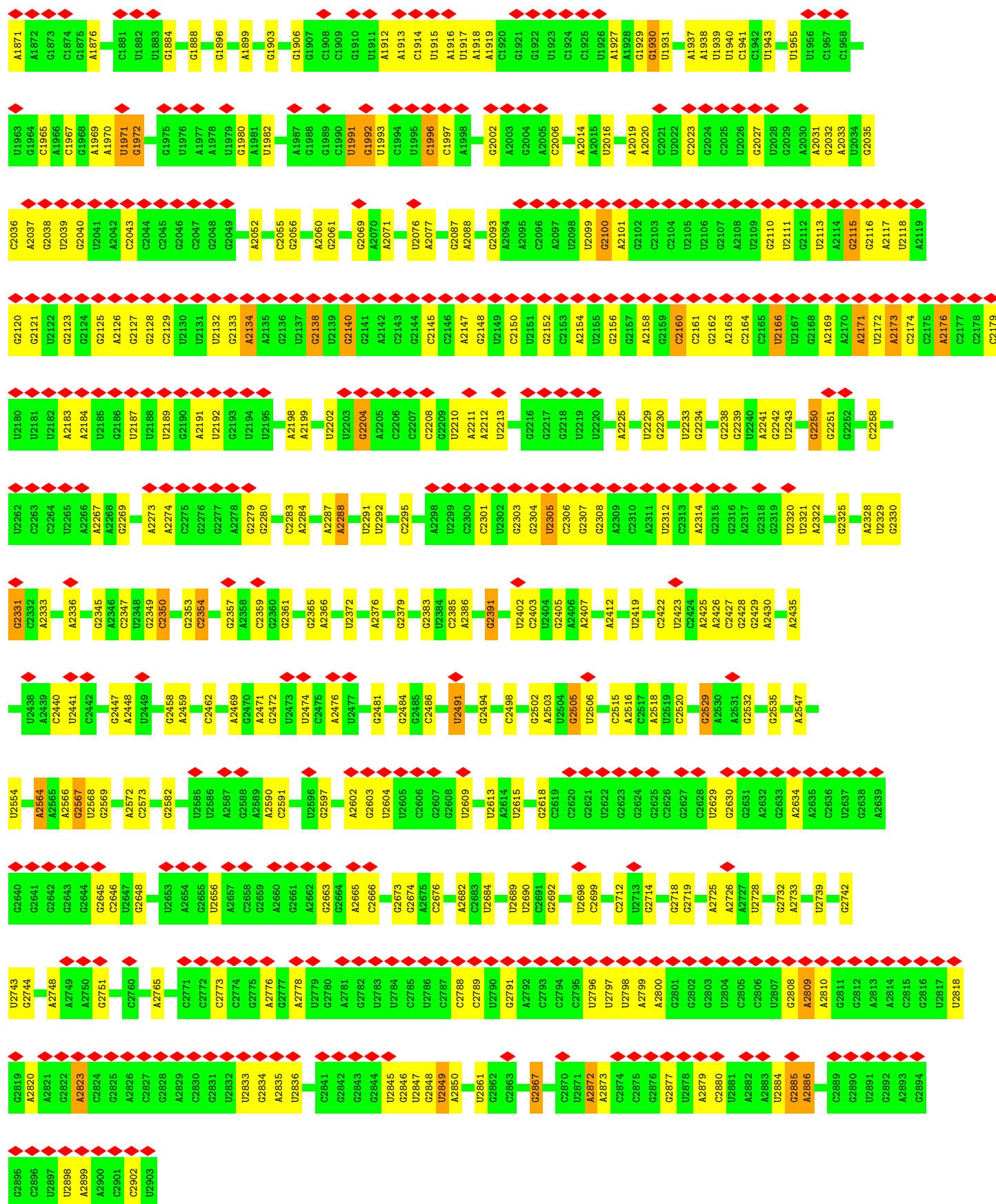
- Molecule 6: 5S rRNA



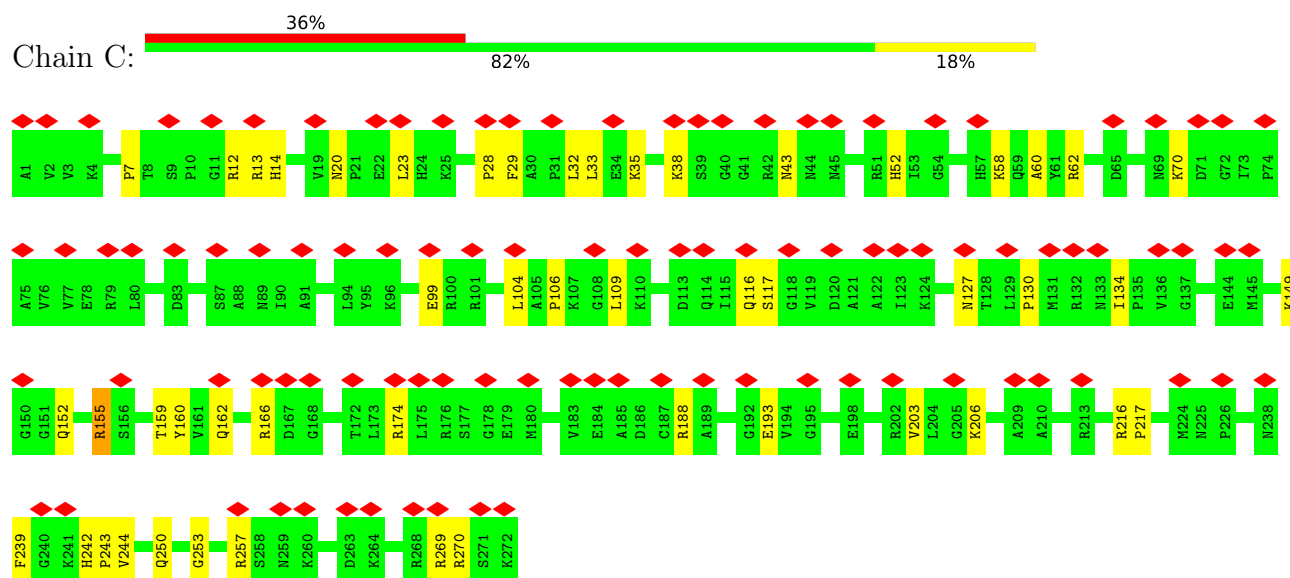
- Molecule 7: 23S rRNA



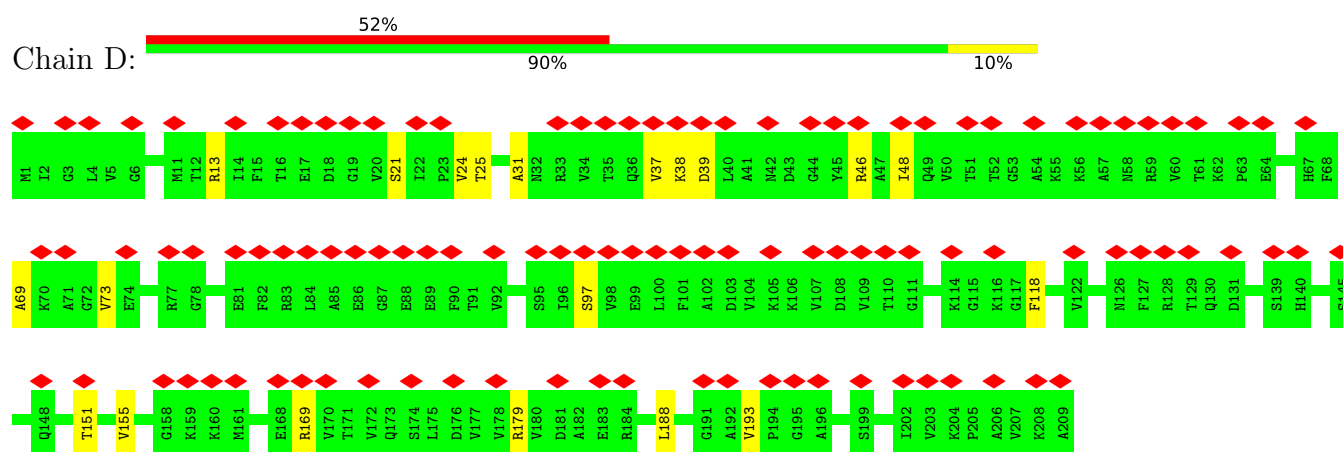




• Molecule 8: 50S ribosomal protein L2

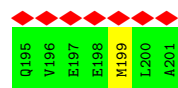


• Molecule 9: 50S ribosomal protein L3

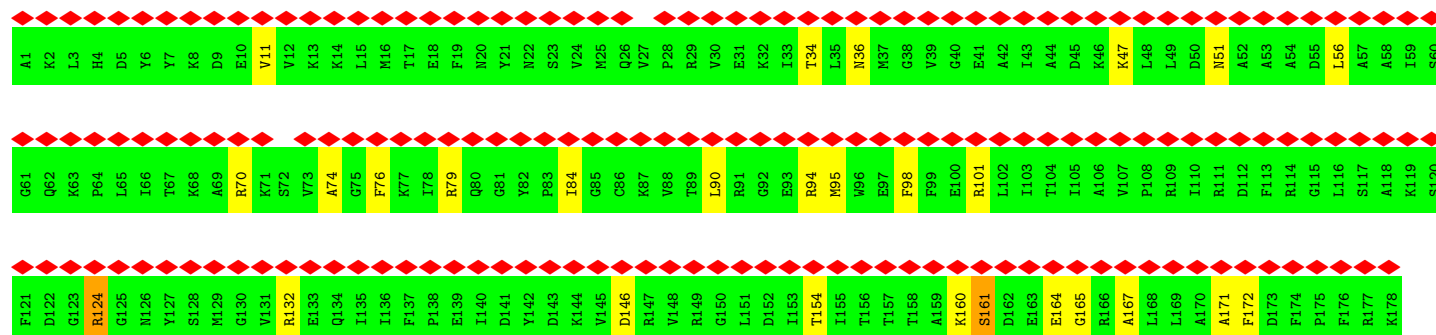
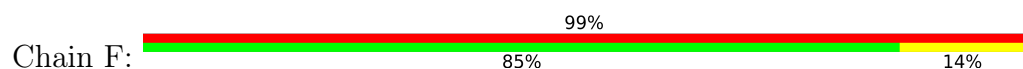


• Molecule 10: 50S ribosomal protein L4

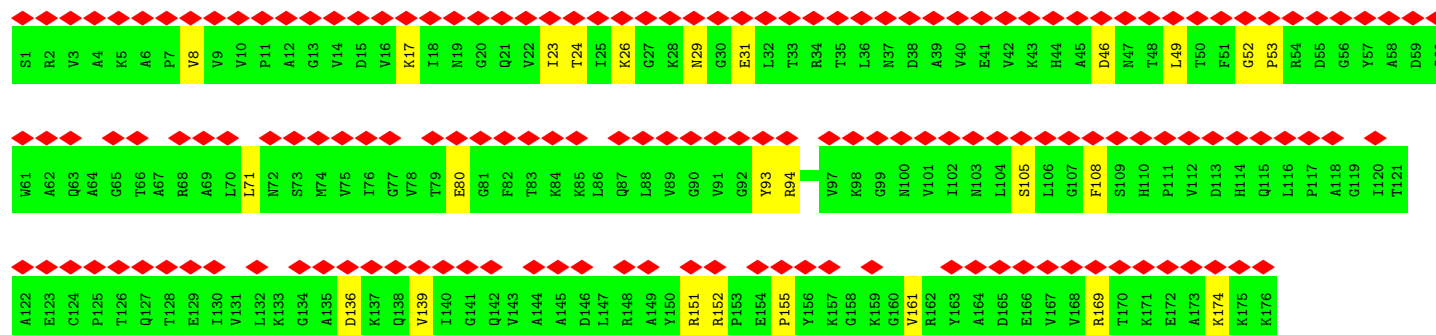
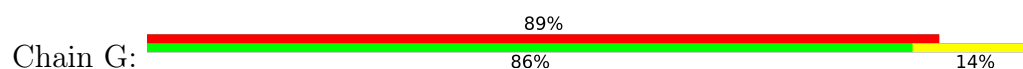




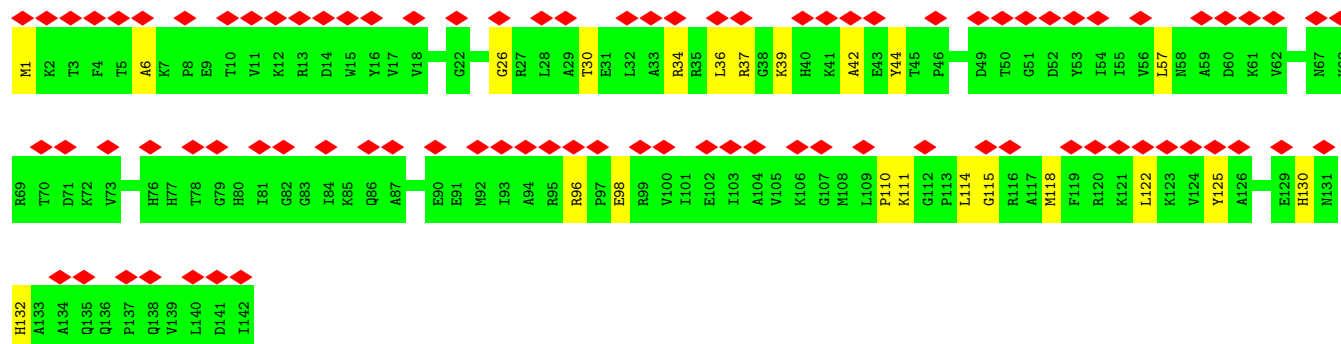
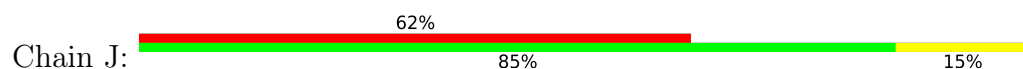
• Molecule 11: 50S ribosomal protein L5



• Molecule 12: 50S ribosomal protein L6

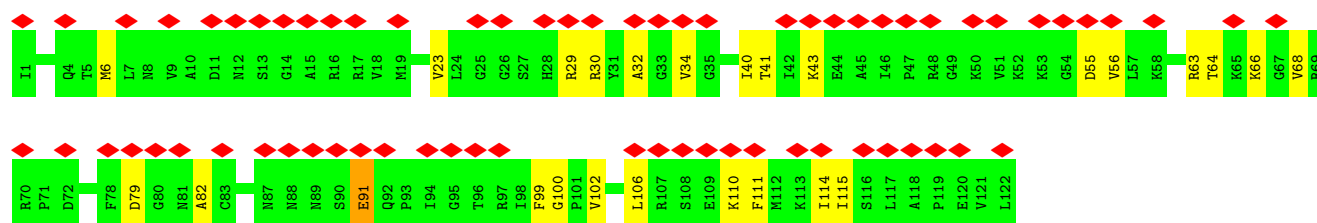


• Molecule 13: 50S ribosomal protein L13



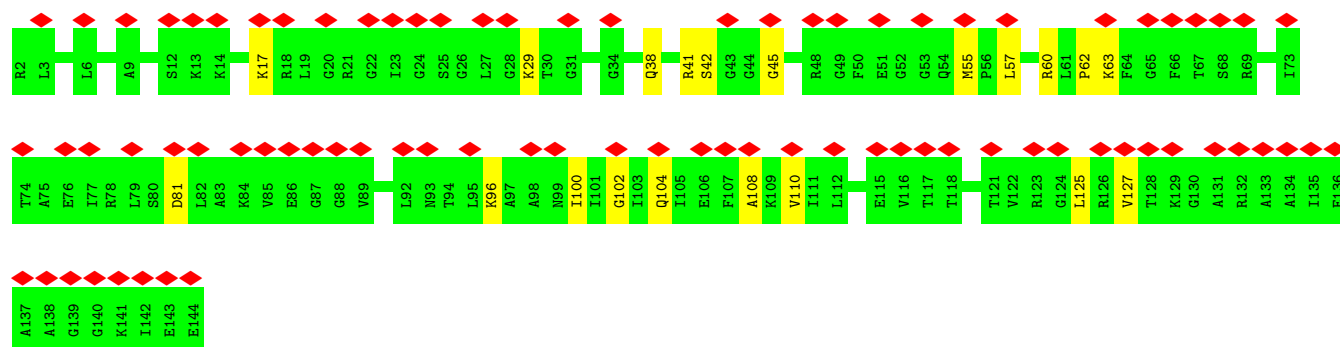
• Molecule 14: 50S ribosomal protein L14

Chain K: 



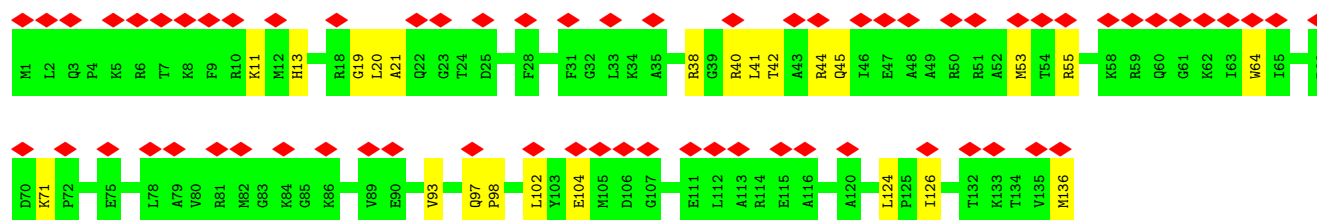
• Molecule 15: 50S ribosomal protein L15

Chain L: 

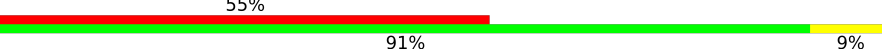


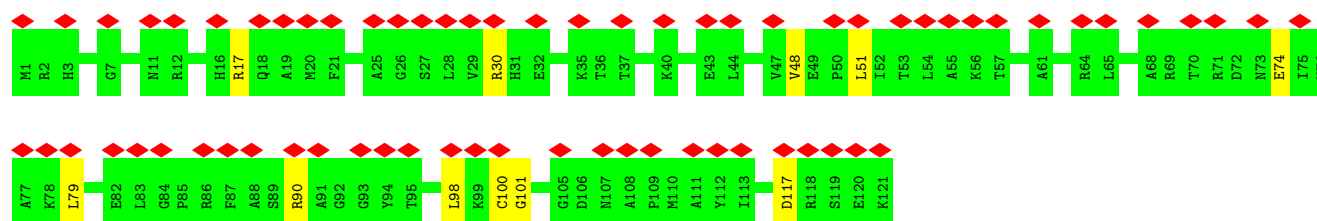
• Molecule 16: 50S ribosomal protein L16

Chain M: 



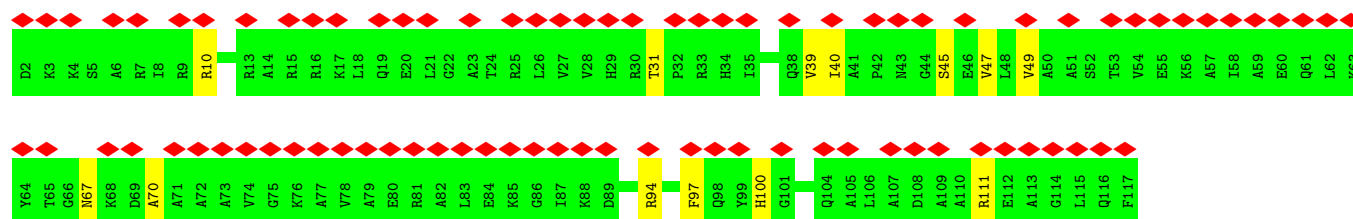
• Molecule 17: 50S ribosomal protein L17

Chain N: 

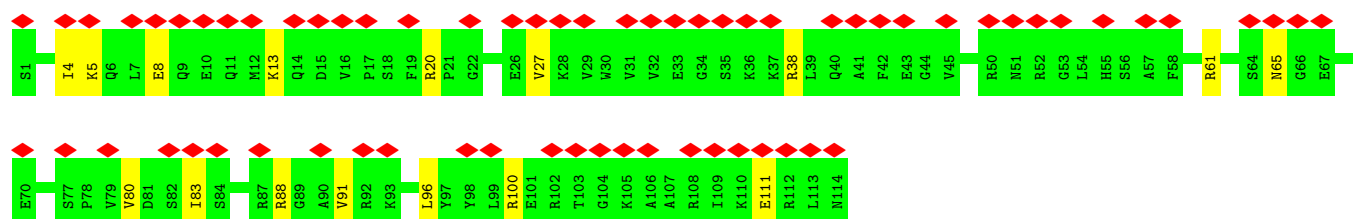
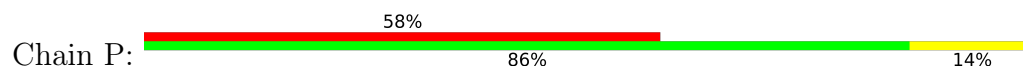


• Molecule 18: 50S ribosomal protein L18

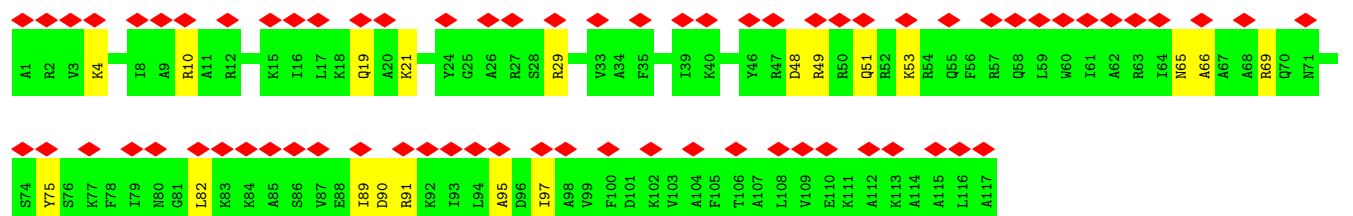
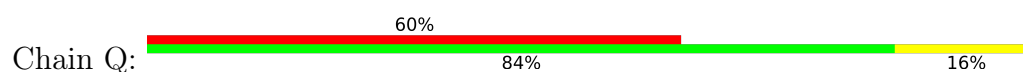
Chain O: 



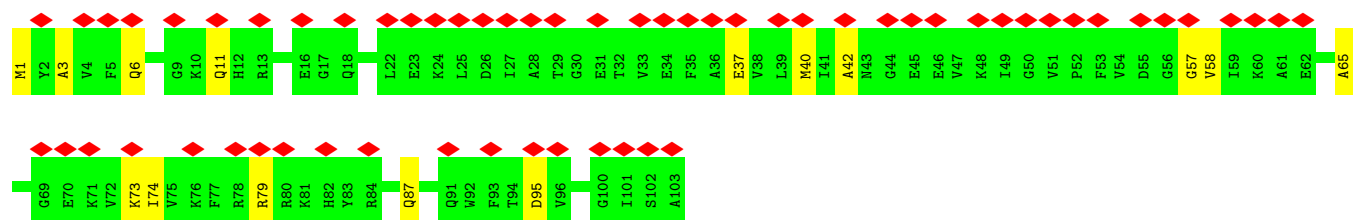
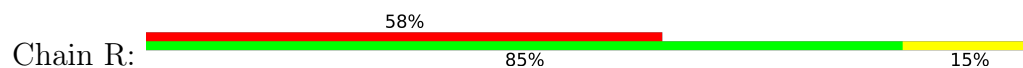
• Molecule 19: 50S ribosomal protein L19



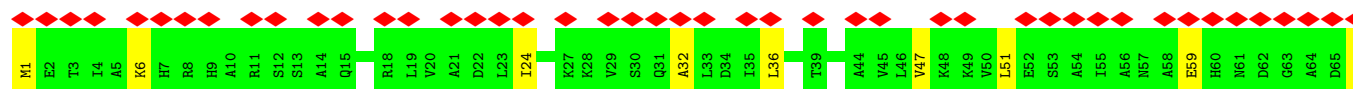
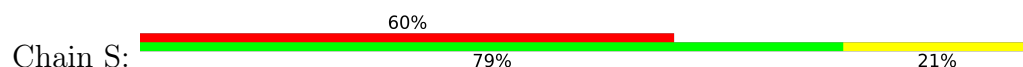
• Molecule 20: 50S ribosomal protein L20

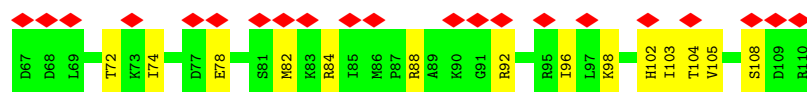


• Molecule 21: Ribosomal protein L21

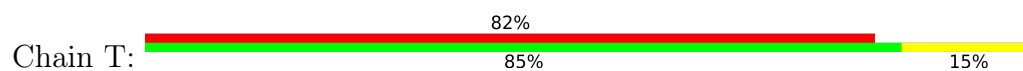


• Molecule 22: 50S ribosomal protein L22

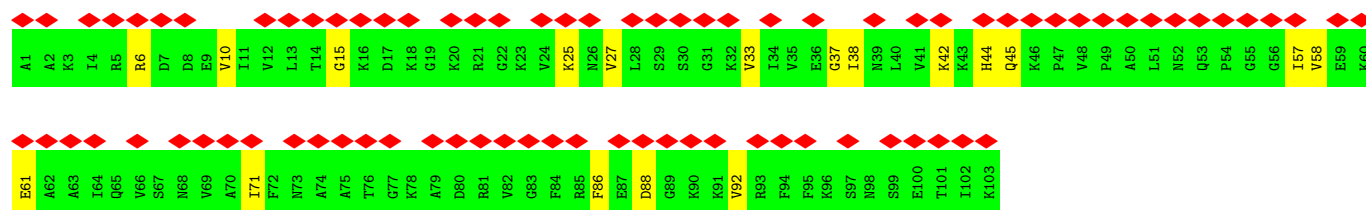
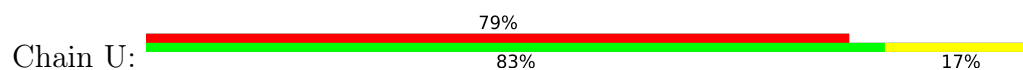




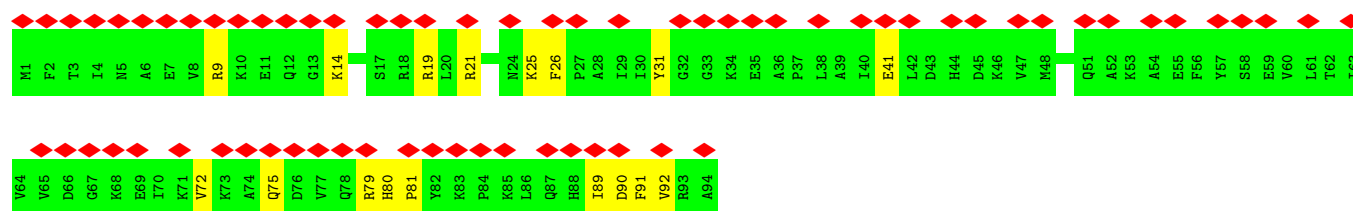
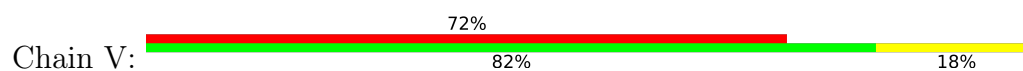
• Molecule 23: 50S ribosomal protein L23



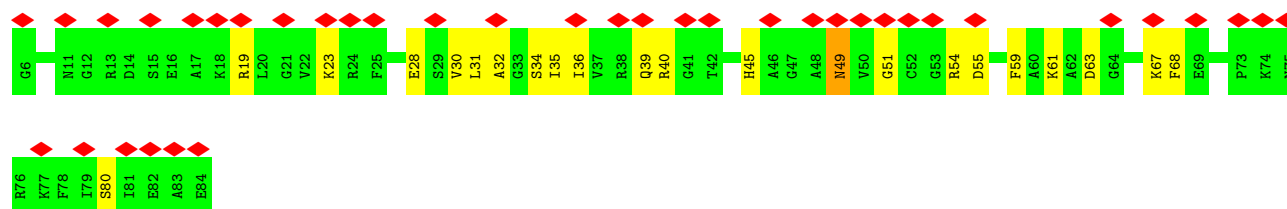
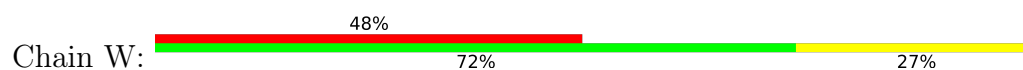
• Molecule 24: 50S ribosomal protein L24



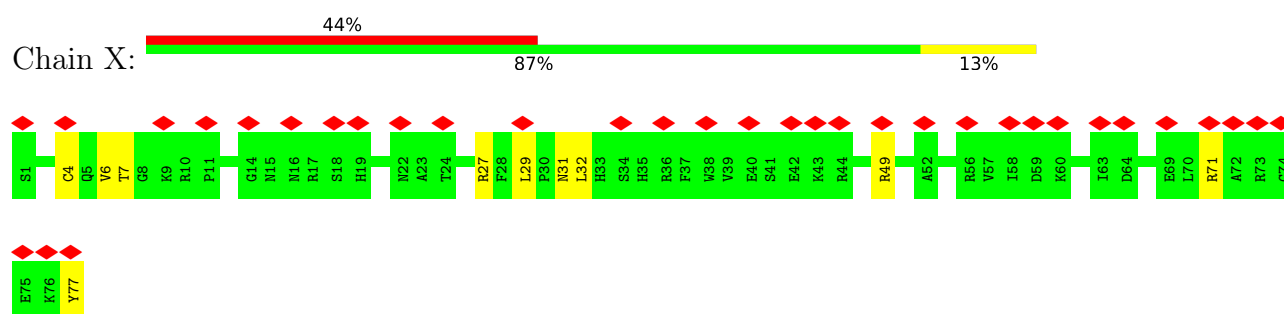
• Molecule 25: 50S ribosomal protein L25



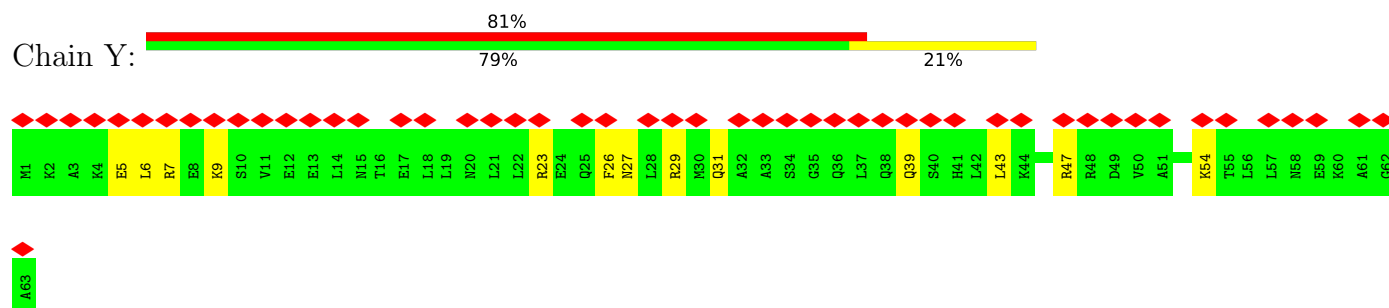
• Molecule 26: 50S ribosomal protein L27



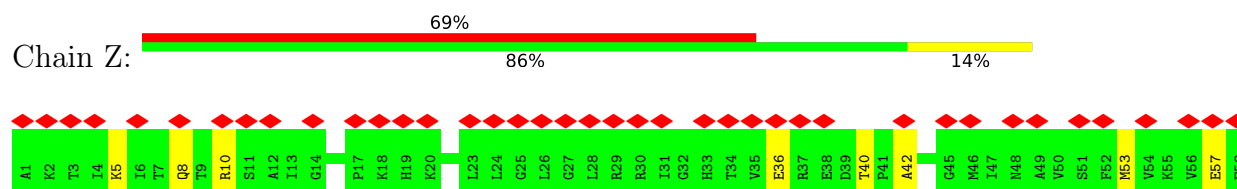
• Molecule 27: 50S ribosomal protein L28



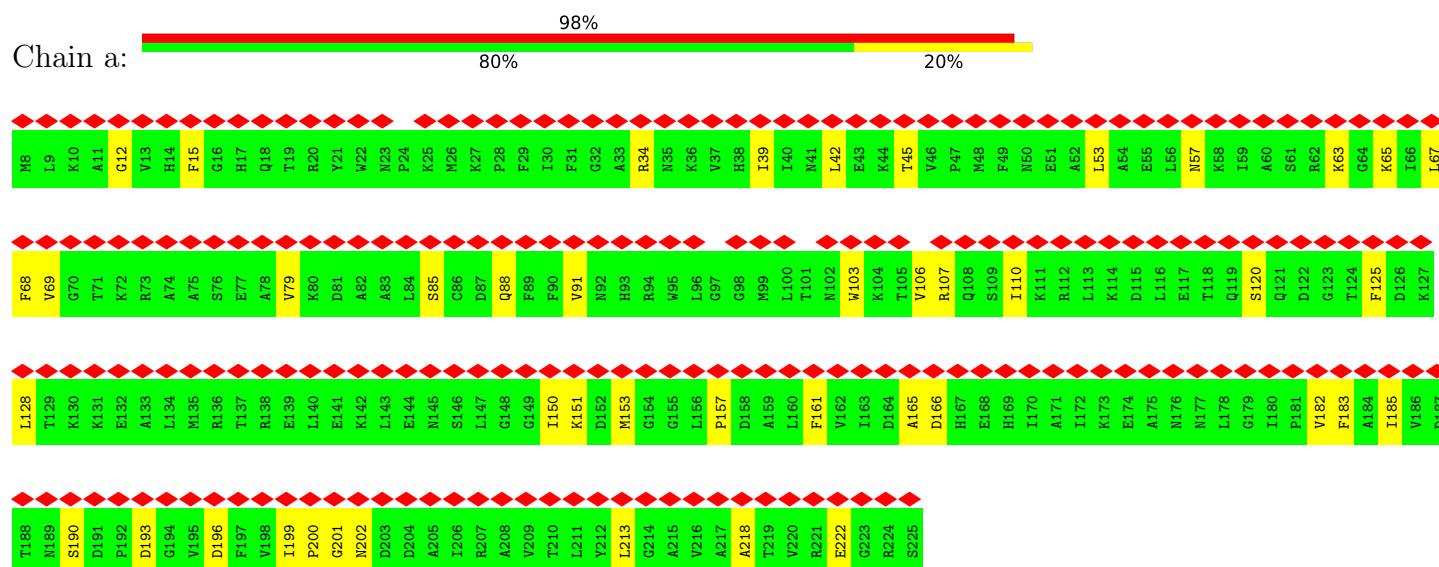
- Molecule 28: 50S ribosomal protein L29



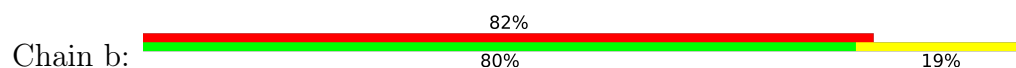
- Molecule 29: 50S ribosomal protein L30

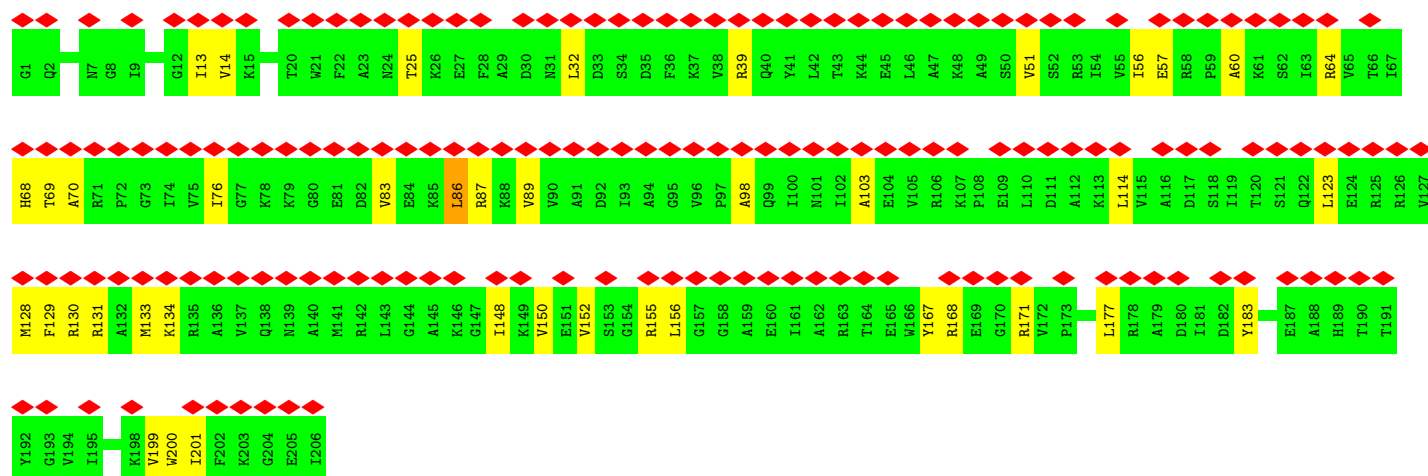


- Molecule 30: 30S ribosomal protein S2

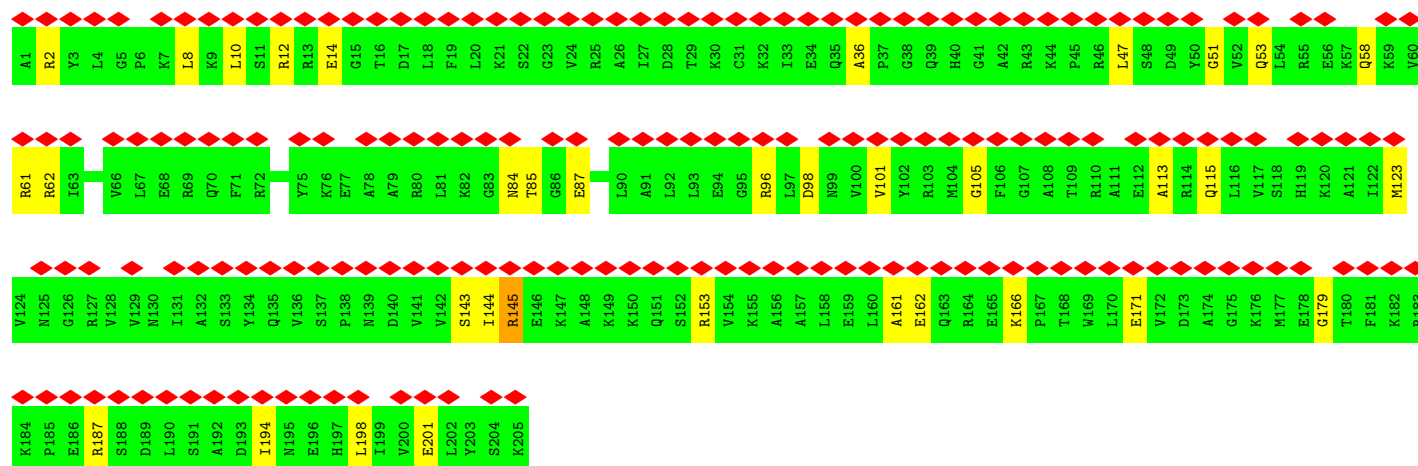
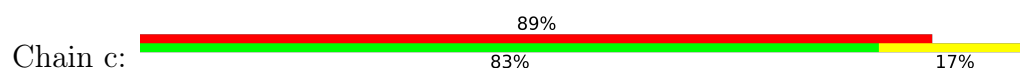


- Molecule 31: 30S ribosomal protein S3

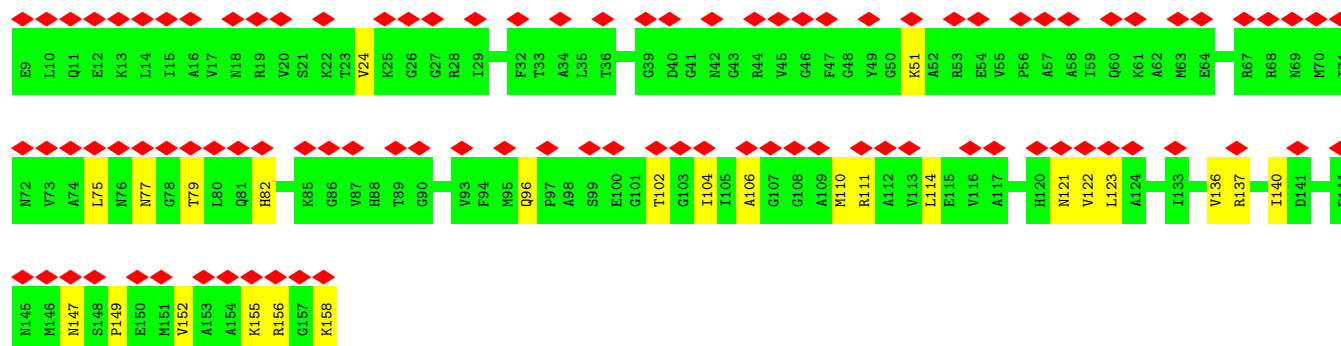
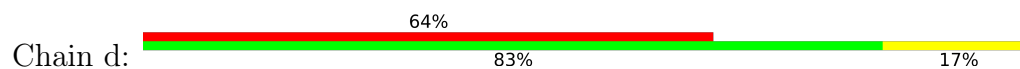




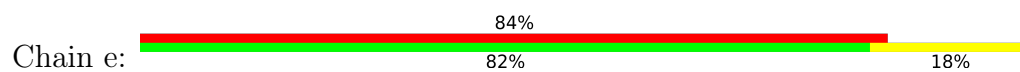
• Molecule 32: 30S ribosomal protein S4



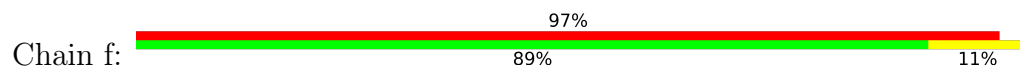
• Molecule 33: 30S ribosomal protein S5



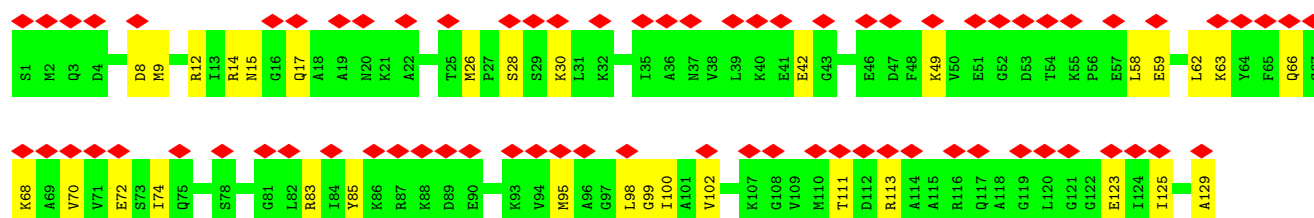
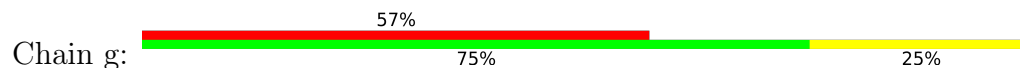
• Molecule 34: 30S ribosomal protein S6, non-modified isoform



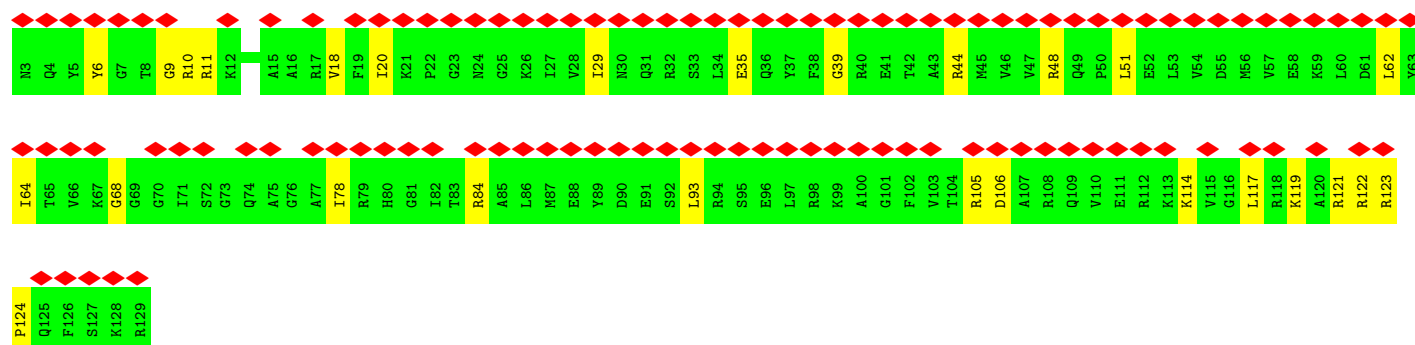
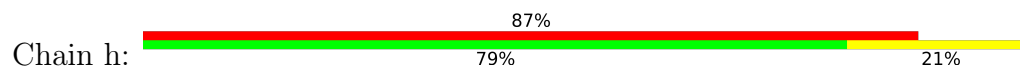
• Molecule 35: 30S ribosomal protein S7



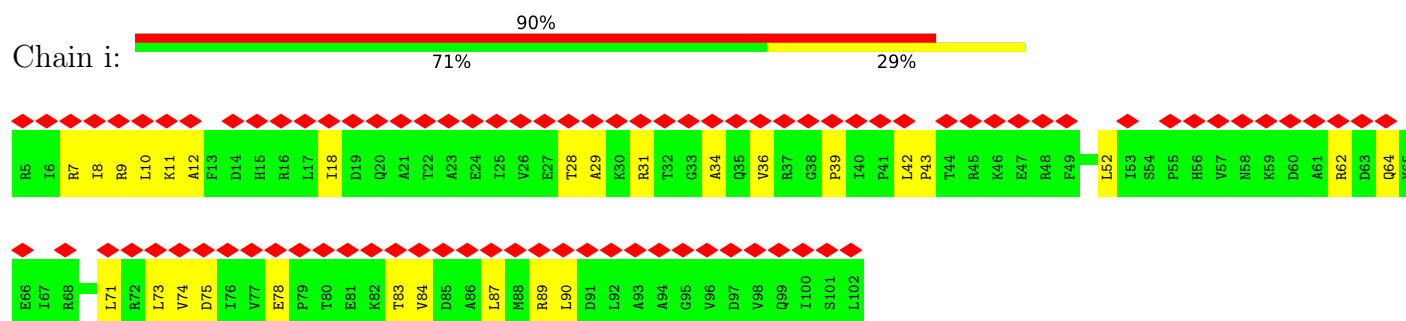
• Molecule 36: 30S ribosomal protein S8



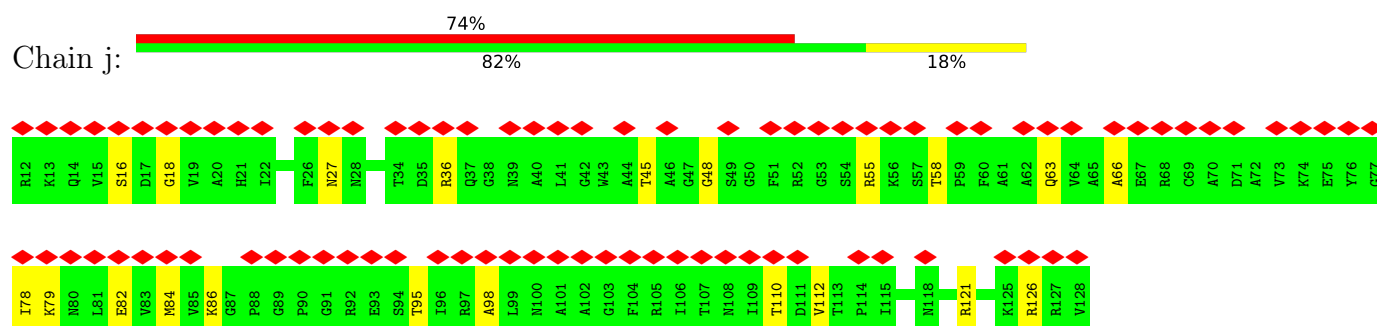
• Molecule 37: 30S ribosomal protein S9



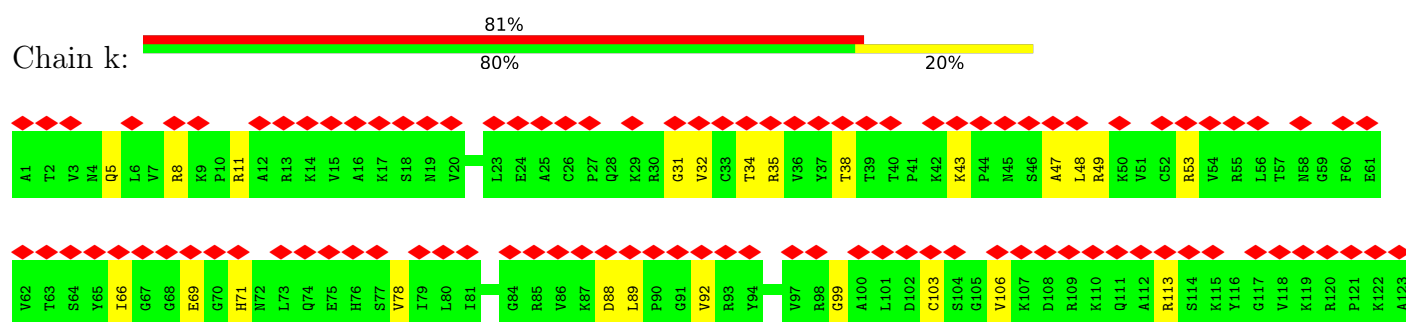
• Molecule 38: 30S ribosomal protein S10



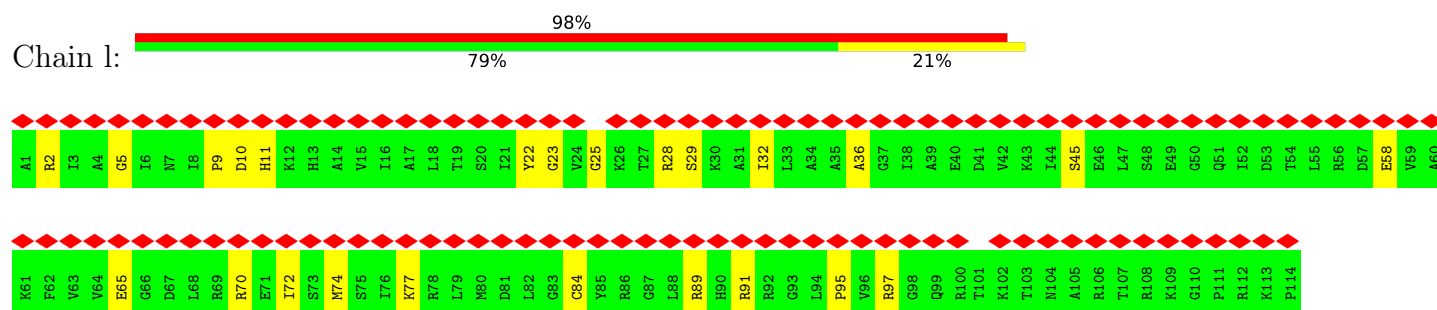
• Molecule 39: 30S ribosomal protein S11



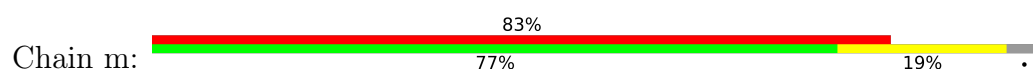
• Molecule 40: 30S ribosomal protein S12

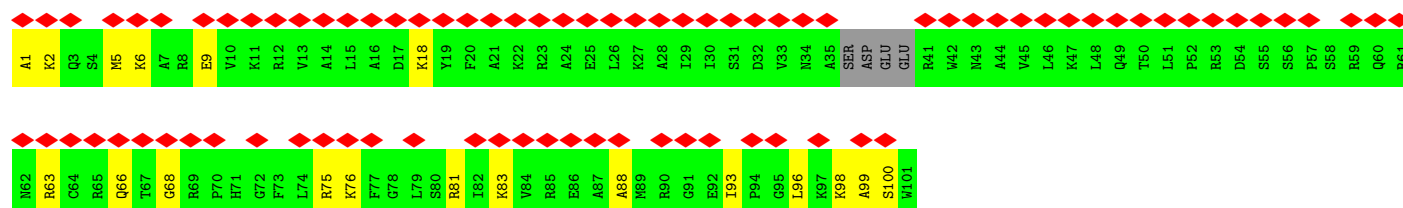


• Molecule 41: 30S ribosomal protein S13

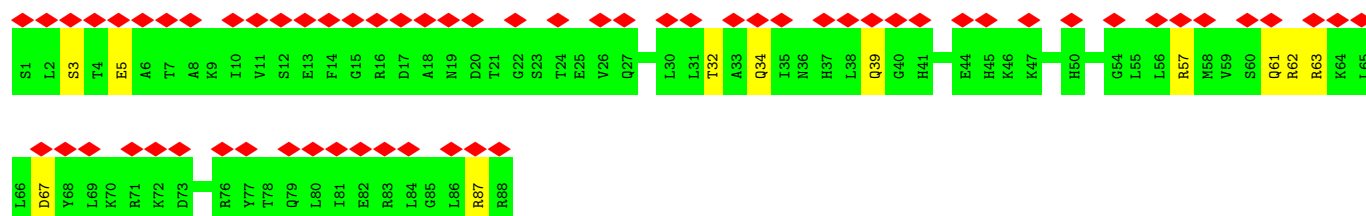
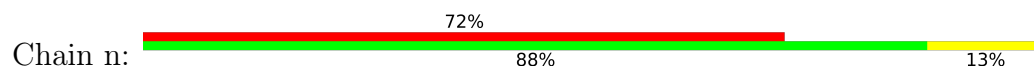


• Molecule 42: 30S ribosomal protein S14

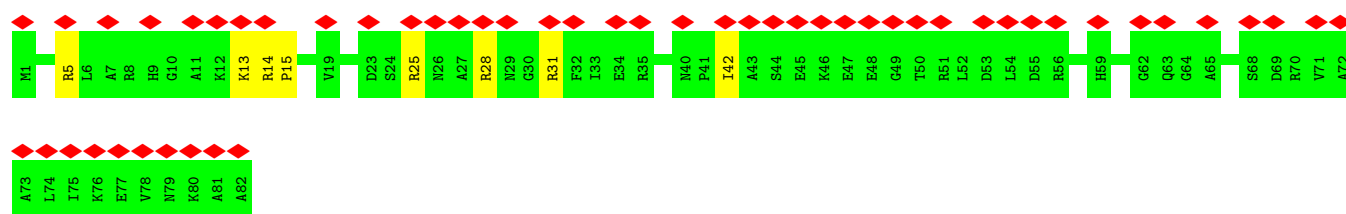
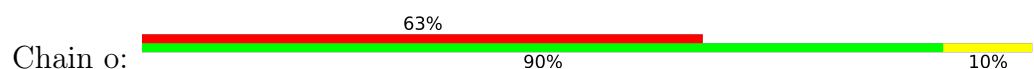




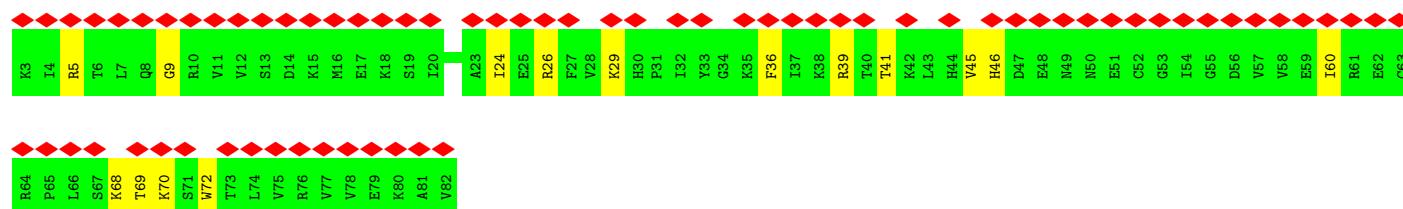
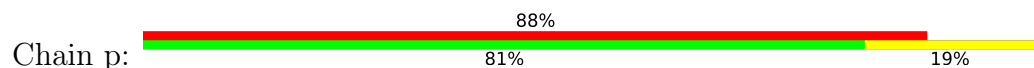
• Molecule 43: 30S ribosomal protein S15



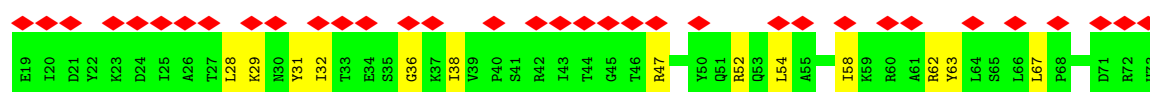
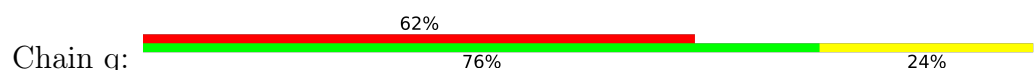
• Molecule 44: 30S ribosomal protein S16



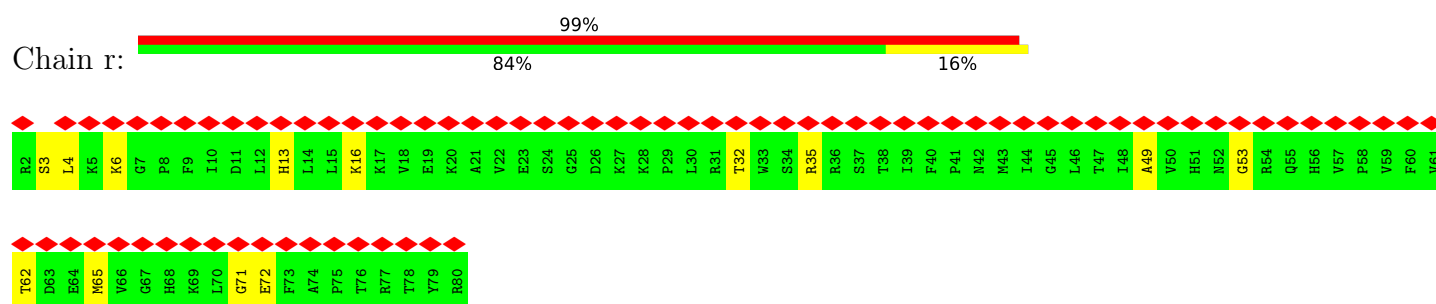
• Molecule 45: 30S ribosomal protein S17



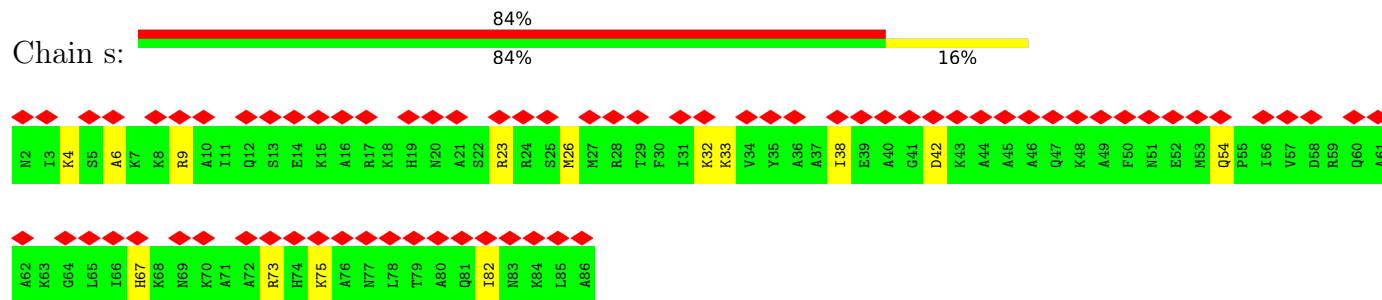
• Molecule 46: 30S ribosomal protein S18



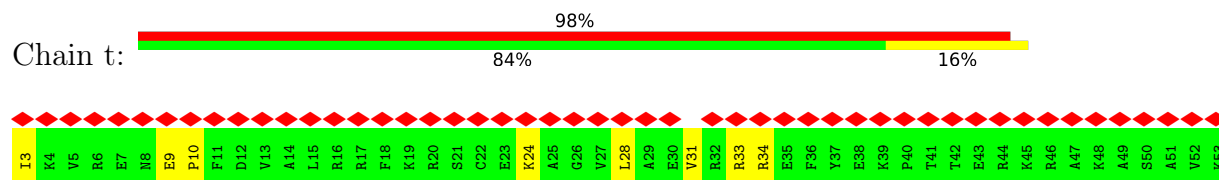
• Molecule 47: 30S ribosomal protein S19



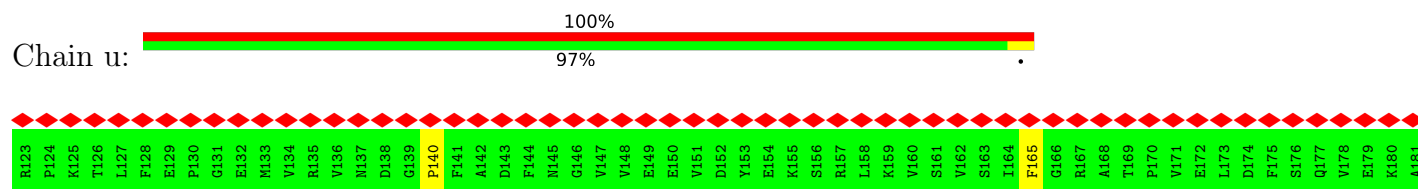
• Molecule 48: 30S ribosomal protein S20



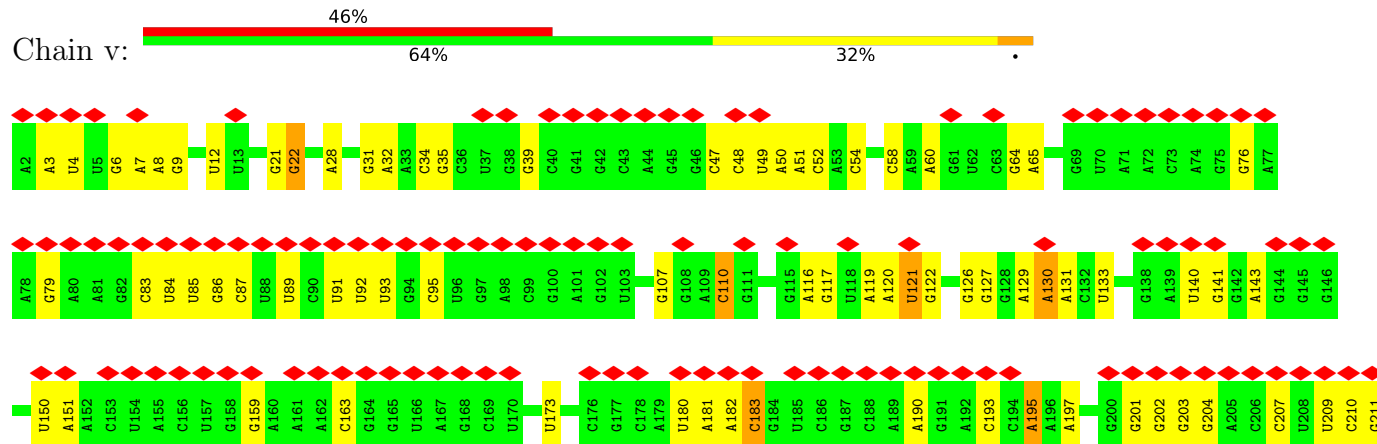
• Molecule 49: 30S ribosomal protein S21 (Fragment)

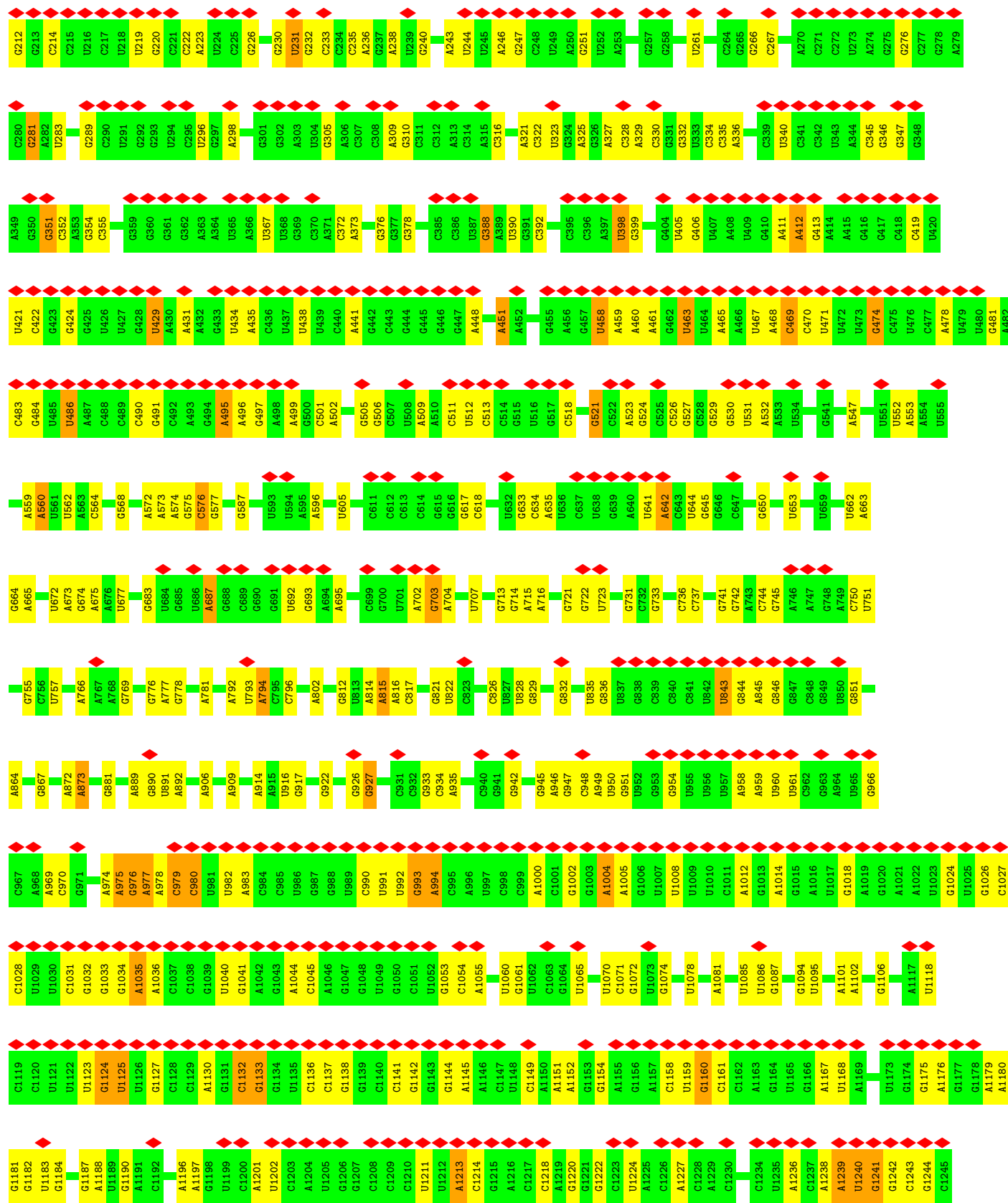


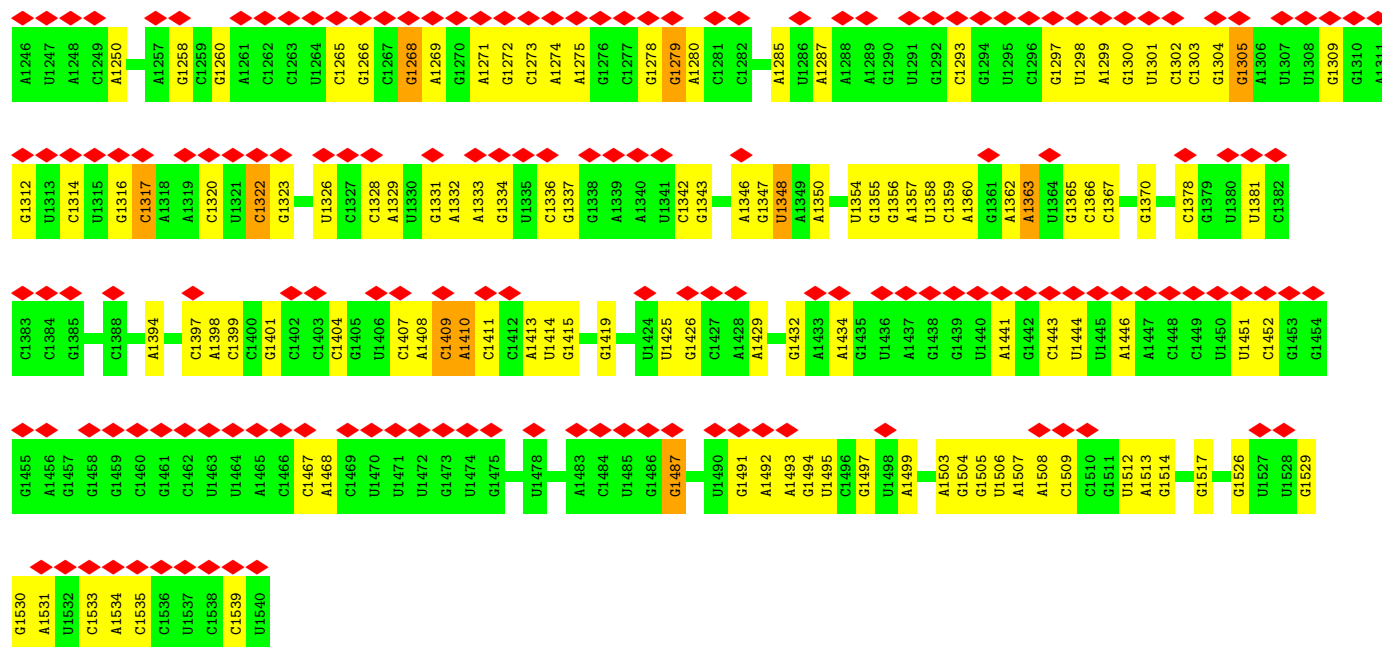
• Molecule 50: Transcription termination/antitermination protein NusG



• Molecule 51: 16S rRNA







4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	140338	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	1.664	Depositor
Minimum map value	-0.277	Depositor
Average map value	0.012	Depositor
Map value standard deviation	0.049	Depositor
Recommended contour level	0.193	Depositor
Map size (Å)	350.19998, 350.19998, 350.19998	wwPDB
Map dimensions	340, 340, 340	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.03, 1.03, 1.03	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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	0.33	0/450	0.73	1/599 (0.2%)
2	1	0.19	0/417	0.43	0/556
3	2	0.26	0/380	0.47	0/498
4	3	0.29	0/513	0.64	0/676
5	4	0.26	0/303	0.68	0/397
6	A	0.19	0/2800	0.36	0/4367
7	B	0.24	0/69796	0.38	3/108888 (0.0%)
8	C	0.28	0/2122	0.57	0/2854
9	D	0.28	0/1586	0.58	0/2134
10	E	0.26	0/1571	0.54	0/2113
11	F	0.25	0/1444	0.71	0/1937
12	G	0.22	0/1343	0.54	2/1816 (0.1%)
13	J	0.27	0/1152	0.58	0/1551
14	K	0.31	0/940	0.75	2/1260 (0.2%)
15	L	0.27	0/1054	0.56	0/1403
16	M	0.26	0/1093	0.52	1/1460 (0.1%)
17	N	0.30	0/974	0.58	0/1303
18	O	0.18	0/902	0.46	0/1209
19	P	0.26	0/929	0.66	2/1242 (0.2%)
20	Q	0.31	0/960	0.57	0/1278
21	R	0.26	0/829	0.54	0/1107
22	S	0.29	0/864	0.57	0/1156
23	T	0.26	0/745	0.67	0/996
24	U	0.25	0/788	0.58	0/1053
25	V	0.24	0/766	0.58	0/1025
26	W	0.35	0/603	0.90	3/797 (0.4%)
27	X	0.27	0/635	0.55	0/848
28	Y	0.27	0/510	0.68	0/677
29	Z	0.24	0/453	0.48	0/605
30	a	0.25	0/1736	0.66	4/2338 (0.2%)
31	b	0.24	0/1652	0.60	1/2225 (0.0%)
32	c	0.22	0/1665	0.61	1/2227 (0.0%)
33	d	0.24	0/1119	0.62	2/1504 (0.1%)
34	e	0.21	0/836	0.56	0/1128

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
35	f	0.25	0/1196	0.58	0/1602
36	g	0.20	0/989	0.48	0/1326
37	h	0.22	0/1034	0.57	0/1375
38	i	0.21	0/797	0.62	0/1077
39	j	0.24	0/893	0.56	0/1205
40	k	0.19	0/969	0.53	0/1300
41	l	0.21	0/893	0.52	0/1193
42	m	0.22	0/785	0.53	0/1043
43	n	0.21	0/722	0.50	0/964
44	o	0.15	0/659	0.42	0/884
45	p	0.22	0/658	0.54	0/881
46	q	0.18	0/463	0.40	0/621
47	r	0.18	0/653	0.46	0/877
48	s	0.26	0/671	0.68	2/888 (0.2%)
49	t	0.24	0/431	0.63	0/570
50	u	0.19	0/477	0.53	0/642
51	v	0.17	0/36963	0.34	1/57662 (0.0%)
All	All	0.23	0/153183	0.43	25/229337 (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
1	0	0	1
4	3	0	1
8	C	0	1
11	F	0	5
31	b	0	1
49	t	0	1
All	All	0	10

There are no bond length outliers.

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	P	4	ILE	CA-C-N	7.20	139.19	126.45
19	P	4	ILE	C-N-CA	7.20	139.19	126.45
14	K	91	GLU	CA-C-N	6.90	131.17	120.68
14	K	91	GLU	C-N-CA	6.90	131.17	120.68
48	s	67	HIS	CA-C-N	6.73	134.40	121.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
48	s	67	HIS	C-N-CA	6.73	134.40	121.54
16	M	53	MET	CB-CG-SD	-6.37	93.59	112.70
30	a	218	ALA	CA-C-N	5.56	131.28	122.61
30	a	218	ALA	C-N-CA	5.56	131.28	122.61
31	b	86	LEU	CA-CB-CG	5.52	135.63	116.30
30	a	128	LEU	CA-C-N	5.45	127.85	120.38
30	a	128	LEU	C-N-CA	5.45	127.85	120.38
1	0	43	THR	OG1-CB-CG2	-5.30	98.71	109.30
51	v	1213	A	P-O3'-C3'	5.27	128.11	120.20
26	W	54	ARG	CA-C-N	5.24	133.06	124.31
26	W	54	ARG	C-N-CA	5.24	133.06	124.31
7	B	490	C	P-O3'-C3'	5.21	128.02	120.20
7	B	670	A	P-O3'-C3'	5.21	128.02	120.20
26	W	49	ASN	CB-CA-C	-5.17	110.63	116.63
32	c	145	ARG	CA-CB-CG	5.14	124.38	114.10
33	d	136	VAL	CA-C-N	5.11	131.31	121.54
33	d	136	VAL	C-N-CA	5.11	131.31	121.54
7	B	1652	A	C2'-C3'-O3'	5.10	121.36	113.70
12	G	46	ASP	CA-C-N	5.08	135.06	125.66
12	G	46	ASP	C-N-CA	5.08	135.06	125.66

There are no chirality outliers.

All (10) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	0	48	TYR	Peptide
4	3	29	ARG	Peptide
8	C	155	ARG	Sidechain
11	F	11	VAL	Peptide
11	F	124	ARG	Peptide
11	F	160	LYS	Peptide
11	F	171	ALA	Peptide
11	F	172	PHE	Peptide
31	b	60	ALA	Peptide
49	t	33	ARG	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	9	0
2	1	410	0	440	5	0
3	2	377	0	418	3	0
4	3	504	0	574	10	0
5	4	302	0	343	5	0
6	A	2504	0	1271	12	0
7	B	62317	0	31345	304	0
8	C	2083	0	2157	37	0
9	D	1565	0	1616	13	0
10	E	1552	0	1619	19	0
11	F	1420	0	1460	16	0
12	G	1323	0	1374	14	0
13	J	1129	0	1162	15	0
14	K	931	0	1003	18	0
15	L	1045	0	1117	14	0
16	M	1074	0	1157	15	0
17	N	961	0	1000	7	0
18	O	892	0	923	9	0
19	P	917	0	965	10	0
20	Q	947	0	1022	16	0
21	R	816	0	839	9	0
22	S	857	0	922	17	0
23	T	739	0	807	10	0
24	U	780	0	834	12	0
25	V	753	0	780	12	0
26	W	596	0	610	17	0
27	X	625	0	655	7	0
28	Y	509	0	543	8	0
29	Z	449	0	491	6	0
30	a	1705	0	1732	25	0
31	b	1625	0	1699	26	0
32	c	1643	0	1710	22	0
33	d	1106	0	1148	20	0
34	e	818	0	808	11	0
35	f	1182	0	1240	10	0
36	g	979	0	1034	26	0
37	h	1022	0	1070	18	0
38	i	787	0	828	23	0
39	j	877	0	887	14	0
40	k	955	0	1019	21	0
41	l	884	0	944	19	0
42	m	774	0	827	14	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
43	n	714	0	737	8	0
44	o	649	0	666	9	0
45	p	649	0	691	9	0
46	q	456	0	478	10	0
47	r	638	0	665	9	0
48	s	665	0	714	9	0
49	t	426	0	449	4	0
50	u	468	0	458	2	0
51	v	33012	0	16618	230	0
All	All	140855	0	94330	980	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 4.

All (980) 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:1093:G:H21	7:B:1098:A:N6	1.55	1.02
7:B:1093:G:N2	7:B:1098:A:H62	1.56	1.02
51:v:1304:G:H21	51:v:1333:A:H62	1.06	0.97
51:v:143:A:H2	51:v:220:G:N1	1.63	0.96
7:B:2166:U:H3	7:B:2171:A:H62	1.15	0.95
51:v:1304:G:N2	51:v:1333:A:H62	1.64	0.94
51:v:412:A:H62	51:v:431:A:H2	1.13	0.93
7:B:1056:G:H21	7:B:1103:A:H62	0.95	0.93
51:v:143:A:C2	51:v:220:G:N1	2.37	0.89
51:v:1304:G:H21	51:v:1333:A:N6	1.70	0.89
7:B:1724:G:H1	7:B:1736:U:H3	1.19	0.88
7:B:1056:G:N2	7:B:1103:A:H62	1.72	0.87
51:v:180:U:H3	51:v:195:A:H62	1.24	0.86
7:B:1056:G:H21	7:B:1103:A:N6	1.74	0.83
51:v:143:A:H2	51:v:220:G:H1	0.89	0.80
51:v:683:G:H1	51:v:707:U:H3	1.30	0.79
51:v:1160:G:H1	51:v:1176:A:N6	1.82	0.78
51:v:246:A:N6	51:v:281:G:C2	2.55	0.75
51:v:1160:G:H1	51:v:1176:A:H61	1.35	0.75
11:F:161:SER:O	11:F:165:GLY:HA3	1.87	0.74
7:B:2138:G:O6	7:B:2154:A:C6	2.43	0.72
7:B:2125:G:H21	7:B:2173:A:H62	1.35	0.72
51:v:412:A:N6	51:v:431:A:H2	1.88	0.72
16:M:64:TRP:HB2	16:M:104:GLU:HB2	1.71	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:B:1792:G:H5'	8:C:203:VAL:HG23	1.72	0.71
51:v:982:U:N3	51:v:1222:G:N1	2.38	0.71
21:R:1:MET:HA	21:R:42:ALA:O	1.90	0.71
33:d:75:LEU:HG	33:d:77:ASN:H	1.57	0.69
7:B:1439:A:H62	7:B:1552:A:H8	1.40	0.68
22:S:24:ILE:HD12	22:S:36:LEU:HD11	1.74	0.68
36:g:28:SER:HB3	36:g:58:LEU:HB2	1.74	0.68
42:m:100:SER:HB3	51:v:1187:G:H21	1.60	0.67
7:B:715:A:N7	43:n:39:GLN:NE2	2.43	0.67
7:B:1912:A:H2	7:B:1917:U:H3	1.44	0.66
51:v:412:A:N7	51:v:431:A:N1	2.44	0.65
32:c:53:GLN:HE22	51:v:8:A:H61	1.45	0.65
7:B:881:G:O6	7:B:895:U:C2	2.51	0.64
31:b:168:ARG:NH2	51:v:1106:G:N3	2.46	0.64
14:K:106:LEU:HG	14:K:111:PHE:HB3	1.80	0.64
45:p:46:HIS:HB2	45:p:70:LYS:HD3	1.79	0.64
7:B:2848:G:O2'	7:B:2867:G:N2	2.30	0.63
26:W:67:LYS:HB3	26:W:80:SER:HB2	1.80	0.63
7:B:2002:G:OP1	17:N:17:ARG:NH2	2.31	0.63
29:Z:10:ARG:HB2	29:Z:53:MET:HG2	1.80	0.63
7:B:1060:U:H4'	7:B:1061:U:H3'	1.81	0.63
7:B:997:G:H5'	20:Q:91:ARG:HD2	1.81	0.63
7:B:1680:U:O2	7:B:1763:G:O2'	2.14	0.63
38:i:52:LEU:HB2	42:m:81:ARG:HE	1.65	0.62
22:S:82:MET:HB2	22:S:98:LYS:HB2	1.80	0.62
40:k:49:ARG:NH2	51:v:521:G:N7	2.47	0.62
51:v:463:U:H3	51:v:469:C:H42	1.44	0.62
28:Y:23:ARG:O	28:Y:27:ASN:HB2	1.98	0.62
29:Z:5:LYS:NZ	29:Z:36:GLU:OE1	2.33	0.62
7:B:27:G:N2	7:B:512:G:O2'	2.34	0.61
51:v:1026:G:O6	51:v:1035:A:C6	2.53	0.61
36:g:9:MET:HG3	36:g:26:MET:HE1	1.82	0.61
32:c:10:LEU:HB2	32:c:62:ARG:HD3	1.82	0.61
41:l:2:ARG:HD3	41:l:9:PRO:HD3	1.83	0.61
14:K:40:ILE:O	14:K:56:VAL:HA	2.01	0.60
51:v:201:G:H21	51:v:469:C:H1'	1.65	0.60
16:M:20:LEU:HD13	25:V:81:PRO:HG2	1.83	0.60
22:S:6:LYS:HD3	22:S:102:HIS:HB3	1.82	0.60
40:k:69:GLU:H	40:k:106:VAL:HG22	1.67	0.60
15:L:81:ASP:HB3	15:L:100:ILE:HG12	1.83	0.60
35:f:2:ARG:NH2	51:v:933:G:N7	2.50	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:42:ILE:HD11	17:N:98:LEU:HB3	1.85	0.59
7:B:807:U:OP2	15:L:41:ARG:NH2	2.36	0.59
19:P:27:VAL:HG22	19:P:83:ILE:HG23	1.83	0.59
38:i:10:LEU:HB3	38:i:18:ILE:HD11	1.84	0.59
7:B:663:G:H5''	15:L:17:LYS:HG3	1.83	0.59
51:v:663:A:H61	51:v:742:G:H1	1.51	0.59
32:c:53:GLN:OE1	33:d:111:ARG:NH2	2.35	0.59
44:o:5:ARG:HB2	51:v:376:G:H5''	1.84	0.59
7:B:981:A:H8	7:B:2027:G:H21	1.50	0.59
32:c:201:GLU:OE1	33:d:111:ARG:NH2	2.36	0.59
7:B:2366:A:H4'	26:W:61:LYS:HE2	1.85	0.59
34:e:22:ILE:HD11	34:e:60:VAL:HG11	1.84	0.59
16:M:19:GLY:O	16:M:38:ARG:NH2	2.35	0.58
18:O:40:ILE:HG12	18:O:47:VAL:HG22	1.84	0.58
39:j:45:THR:HG23	39:j:48:GLY:H	1.67	0.58
7:B:257:C:O2	15:L:104:GLN:NE2	2.36	0.58
48:s:9:ARG:NH2	51:v:107:G:N7	2.51	0.58
51:v:143:A:N1	51:v:220:G:O6	2.36	0.58
38:i:89:ARG:H	50:u:165:PHE:HE1	1.51	0.58
41:l:23:GLY:O	41:l:28:ARG:NH2	2.35	0.58
7:B:563:A:OP2	21:R:79:ARG:NH2	2.36	0.58
40:k:66:ILE:HG21	40:k:71:HIS:HB3	1.85	0.58
51:v:978:A:C2	51:v:1316:G:N2	2.71	0.58
6:A:76:G:OP1	25:V:9:ARG:NH2	2.37	0.58
7:B:888:C:O2	41:l:91:ARG:NH2	2.37	0.58
17:N:51:LEU:HB3	17:N:79:LEU:HD21	1.86	0.58
36:g:95:MET:HB2	36:g:99:GLY:H	1.68	0.58
7:B:2125:G:N2	7:B:2173:A:H62	2.02	0.58
16:M:13:HIS:O	16:M:71:LYS:NZ	2.37	0.58
33:d:147:ASN:HB3	36:g:95:MET:HE1	1.84	0.58
43:n:57:ARG:NH2	51:v:742:G:OP1	2.37	0.58
51:v:1026:G:O6	51:v:1035:A:N1	2.37	0.58
7:B:547:A:H5'	7:B:548:G:H21	1.70	0.57
13:J:111:LYS:HB2	13:J:115:GLY:H	1.68	0.57
42:m:98:LYS:NZ	51:v:1188:A:O2'	2.37	0.57
7:B:1007:C:OP1	13:J:37:ARG:NH1	2.37	0.57
34:e:9:MET:HA	34:e:58:HIS:O	2.04	0.57
37:h:29:ILE:HG22	37:h:64:ILE:HB	1.84	0.57
48:s:23:ARG:HG2	48:s:26:MET:HE2	1.85	0.57
8:C:117:SER:O	8:C:188:ARG:NH2	2.37	0.57
34:e:36:ILE:HG22	34:e:64:VAL:HG22	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:B:1818:U:OP2	8:C:155:ARG:NH1	2.38	0.57
10:E:149:ILE:HB	10:E:188:MET:HG3	1.86	0.57
29:Z:5:LYS:HB2	29:Z:57:GLU:HB2	1.86	0.57
33:d:51:LYS:NZ	51:v:1081:A:OP2	2.36	0.57
7:B:987:C:O2'	7:B:1000:A:N3	2.36	0.57
7:B:1022:G:N2	7:B:1023:U:O4	2.36	0.57
28:Y:23:ARG:HA	28:Y:26:PHE:HB2	1.86	0.57
7:B:2618:G:H21	9:D:155:VAL:HG21	1.68	0.57
7:B:83:A:N6	7:B:102:U:OP2	2.37	0.56
40:k:5:GLN:HG2	40:k:8:ARG:HH21	1.70	0.56
51:v:180:U:H3	51:v:195:A:N6	1.98	0.56
8:C:134:ILE:O	8:C:166:ARG:NH2	2.35	0.56
7:B:309:A:H4'	24:U:15:GLY:HA2	1.87	0.56
7:B:2849:U:O4	19:P:20:ARG:NH1	2.37	0.56
4:3:44:ARG:NH2	7:B:2349:G:OP1	2.38	0.56
7:B:2121:G:O6	7:B:2176:A:N1	2.38	0.56
39:j:121:ARG:HE	49:t:34:ARG:HH22	1.54	0.56
51:v:993:G:O2'	51:v:994:A:N7	2.37	0.56
19:P:38:ARG:NH2	51:v:346:G:OP1	2.38	0.56
37:h:35:GLU:HA	37:h:39:GLY:HA3	1.87	0.56
7:B:2125:G:H21	7:B:2173:A:N6	2.03	0.56
7:B:2330:G:H21	26:W:39:GLN:HB3	1.69	0.56
40:k:69:GLU:HB2	40:k:106:VAL:HG13	1.87	0.56
7:B:141:G:O6	23:T:1:MET:N	2.39	0.56
14:K:79:ASP:OD2	19:P:61:ARG:NH2	2.39	0.56
36:g:42:GLU:HG3	36:g:100:ILE:HD13	1.85	0.56
39:j:126:ARG:NH2	51:v:796:C:O2'	2.38	0.56
13:J:125:TYR:OH	13:J:132:HIS:NE2	2.38	0.56
47:r:35:ARG:NH1	51:v:1320:C:N3	2.53	0.56
7:B:2682:A:H61	7:B:2728:U:H1'	1.70	0.56
31:b:148:ILE:HD12	31:b:201:ILE:HD12	1.88	0.56
36:g:15:ASN:ND2	51:v:826:C:O2	2.38	0.56
38:i:84:VAL:HG13	50:u:140:PRO:HA	1.88	0.56
7:B:2314:A:OP2	11:F:70:ARG:NH1	2.40	0.55
31:b:152:VAL:HG12	31:b:156:LEU:HD11	1.89	0.55
36:g:8:ASP:OD2	36:g:12:ARG:NH1	2.39	0.55
43:n:57:ARG:NH1	43:n:61:GLN:OE1	2.39	0.55
28:Y:6:LEU:HD12	28:Y:9:LYS:HG3	1.87	0.55
7:B:2354:C:H4'	26:W:31:LEU:HG	1.88	0.55
14:K:63:ARG:NH2	14:K:99:PHE:O	2.39	0.55
41:l:10:ASP:HB3	41:l:45:SER:HB3	1.87	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:B:2885:G:O2'	7:B:2886:A:N3	2.40	0.55
31:b:155:ARG:NH1	51:v:1055:A:N3	2.55	0.55
7:B:397:U:H5''	27:X:31:ASN:HB2	1.89	0.55
7:B:1801:A:OP2	8:C:152:GLN:NE2	2.38	0.55
19:P:91:VAL:HG11	19:P:96:LEU:HD21	1.88	0.55
32:c:171:GLU:O	32:c:179:GLY:HA2	2.07	0.55
41:l:28:ARG:NH1	51:v:1328:C:O2'	2.40	0.55
46:q:38:ILE:HG12	46:q:58:ILE:HD13	1.89	0.55
51:v:1363:A:O2'	51:v:1365:G:N7	2.34	0.55
15:L:108:ALA:HB3	15:L:125:LEU:HD22	1.87	0.55
7:B:1083:U:N3	7:B:1086:A:OP2	2.40	0.55
10:E:173:THR:HA	10:E:199:MET:HE1	1.87	0.55
31:b:13:ILE:HD11	31:b:177:LEU:HB3	1.89	0.55
51:v:246:A:H62	51:v:281:G:N2	2.04	0.55
7:B:962:G:H21	7:B:2250:G:H1	1.53	0.55
10:E:5:LEU:HD23	10:E:122:GLU:HB3	1.87	0.55
51:v:1268:G:O2'	51:v:1326:U:O2'	2.25	0.55
7:B:1187:G:N2	7:B:1188:U:O4	2.40	0.55
7:B:2312:U:O2	11:F:36:ASN:ND2	2.39	0.55
7:B:2469:A:H4'	16:M:55:ARG:HD2	1.89	0.55
41:l:36:ALA:HB2	41:l:58:GLU:HG3	1.88	0.55
19:P:13:LYS:NZ	19:P:80:VAL:O	2.40	0.55
41:l:2:ARG:HE	41:l:5:GLY:HA3	1.71	0.55
51:v:1060:U:H2'	51:v:1061:G:H8	1.70	0.55
7:B:2166:U:O4	7:B:2171:A:N7	2.40	0.54
7:B:2656:U:O2	7:B:2665:A:N7	2.40	0.54
40:k:49:ARG:NH1	40:k:88:ASP:OD2	2.40	0.54
32:c:115:GLN:OE1	32:c:153:ARG:NH1	2.40	0.54
7:B:911:A:N6	16:M:11:LYS:O	2.39	0.54
45:p:39:ARG:NH2	51:v:238:A:OP1	2.40	0.54
51:v:1071:C:H2'	51:v:1072:G:H8	1.73	0.54
7:B:1080:A:N6	7:B:1088:A:OP1	2.40	0.54
7:B:1365:A:H5''	27:X:27:ARG:HH22	1.72	0.54
7:B:2140:G:OP2	7:B:2152:G:N2	2.41	0.54
11:F:47:LYS:HE2	11:F:146:ASP:HB2	1.89	0.54
12:G:29:ASN:HD22	12:G:80:GLU:HA	1.73	0.54
17:N:30:ARG:NH1	17:N:74:GLU:OE1	2.40	0.54
8:C:20:ASN:HB3	8:C:23:LEU:HG	1.90	0.54
8:C:28:PRO:HG2	8:C:33:LEU:HD11	1.88	0.54
7:B:1421:G:O3'	7:B:1493:C:N4	2.41	0.54
35:f:110:ARG:NH2	35:f:125:ASP:OD2	2.40	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:B:1798:U:OP2	8:C:270:ARG:NH2	2.40	0.54
21:R:37:GLU:HG2	21:R:57:GLY:H	1.73	0.54
24:U:86:PHE:HB2	24:U:92:VAL:HG22	1.90	0.54
31:b:83:VAL:HA	31:b:86:LEU:HD23	1.90	0.54
36:g:83:ARG:NH2	51:v:587:G:OP1	2.41	0.54
32:c:8:LEU:HD12	51:v:429:U:H3'	1.89	0.54
37:h:64:ILE:HG21	37:h:78:ILE:HG12	1.89	0.54
39:j:36:ARG:NH1	39:j:82:GLU:OE2	2.41	0.54
41:l:84:CYS:HB2	47:r:72:GLU:HB3	1.89	0.54
51:v:126:G:OP1	51:v:605:U:O2'	2.24	0.54
45:p:45:VAL:HG12	45:p:72:TRP:HB2	1.89	0.54
46:q:36:GLY:O	46:q:62:ARG:NH2	2.41	0.54
30:a:107:ARG:HA	30:a:110:ILE:HG22	1.90	0.54
44:o:14:ARG:HH12	51:v:617:G:H21	1.56	0.54
4:3:11:LYS:NZ	7:B:249:C:O2	2.40	0.53
7:B:629:G:N3	7:B:639:U:O2'	2.41	0.53
16:M:136:MET:HE2	25:V:79:ARG:HH11	1.73	0.53
41:l:2:ARG:HH21	41:l:5:GLY:HA3	1.73	0.53
7:B:1918:A:O2'	7:B:1919:A:N7	2.40	0.53
31:b:86:LEU:HA	31:b:89:VAL:HG12	1.89	0.53
38:i:64:GLN:HG3	42:m:99:ALA:HB3	1.91	0.53
7:B:514:A:N3	7:B:581:C:O2'	2.36	0.53
31:b:130:ARG:NH1	31:b:167:TYR:OH	2.41	0.53
5:4:4:ARG:NH1	5:4:35:GLN:OE1	2.41	0.53
6:A:77:U:OP1	25:V:21:ARG:NH1	2.40	0.53
7:B:793:A:OP2	7:B:2071:A:O2'	2.26	0.53
15:L:55:MET:O	15:L:60:ARG:NH1	2.42	0.53
30:a:79:VAL:HG22	30:a:213:LEU:HD11	1.90	0.53
6:A:89:U:O2	7:B:958:U:O2'	2.26	0.53
7:B:1819:A:H5''	8:C:159:THR:HG21	1.90	0.53
44:o:13:LYS:NZ	51:v:483:C:O2	2.41	0.53
48:s:54:GLN:HG3	48:s:75:LYS:HD3	1.91	0.53
20:Q:48:ASP:HA	20:Q:51:GLN:HB2	1.89	0.53
22:S:47:VAL:HG12	22:S:103:ILE:HG21	1.90	0.53
42:m:63:ARG:NH1	42:m:68:GLY:O	2.41	0.53
51:v:766:A:OP2	51:v:812:G:N2	2.41	0.53
44:o:31:ARG:NH2	51:v:231:U:OP2	2.41	0.53
46:q:29:LYS:HA	46:q:32:ILE:HG12	1.90	0.53
51:v:843:U:OP1	51:v:844:G:N2	2.41	0.53
7:B:952:G:H21	7:B:2267:A:H2	1.56	0.53
7:B:2014:A:O2'	22:S:92:ARG:NH2	2.42	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
51:v:335:C:H2'	51:v:336:A:H8	1.74	0.53
7:B:674:G:H1'	10:E:69:ARG:HD3	1.91	0.53
23:T:12:ARG:HG2	23:T:35:ALA:H	1.74	0.53
39:j:16:SER:HB2	39:j:79:LYS:HB2	1.90	0.53
5:4:23:ILE:HD13	7:B:1032:A:H1'	1.90	0.53
7:B:1315:C:O2'	7:B:1392:A:N3	2.41	0.53
7:B:2032:G:N2	9:D:151:THR:OG1	2.42	0.53
7:B:2692:G:N3	7:B:2847:U:O2'	2.42	0.53
7:B:2743:U:O2'	12:G:152:ARG:NH2	2.39	0.53
38:i:34:ALA:HB1	38:i:78:GLU:HG2	1.91	0.53
51:v:687:A:N6	51:v:703:G:C2	2.77	0.53
23:T:24:MET:O	23:T:29:THR:N	2.41	0.52
36:g:102:VAL:O	36:g:125:ILE:N	2.41	0.52
7:B:1826:G:O2'	7:B:1971:U:OP2	2.26	0.52
30:a:15:PHE:O	30:a:202:ASN:ND2	2.40	0.52
30:a:185:ILE:HD11	30:a:201:GLY:HA3	1.90	0.52
43:n:34:GLN:NE2	51:v:741:G:OP1	2.42	0.52
1:0:52:LYS:NZ	1:0:54:ILE:O	2.43	0.52
7:B:284:U:O2	7:B:356:G:O6	2.27	0.52
7:B:2100:G:O6	7:B:2189:U:O2	2.26	0.52
33:d:137:ARG:HA	33:d:140:ILE:HB	1.91	0.52
51:v:1414:U:H2'	51:v:1415:G:H8	1.74	0.52
2:1:34:GLU:HG2	2:1:49:LYS:HB3	1.91	0.52
19:P:5:LYS:HA	19:P:8:GLU:HB2	1.91	0.52
23:T:34:VAL:HG11	23:T:43:ILE:HG12	1.89	0.52
26:W:23:LYS:HG3	26:W:67:LYS:HA	1.91	0.52
33:d:106:ALA:HB1	33:d:110:MET:HG2	1.91	0.52
51:v:309:A:H2'	51:v:310:G:H8	1.74	0.52
1:0:3:GLN:O	7:B:2016:U:O2'	2.28	0.52
7:B:247:G:OP2	7:B:249:C:N4	2.38	0.52
7:B:1528:A:N6	7:B:1543:G:O2'	2.42	0.52
8:C:106:PRO:HD2	8:C:109:LEU:HD22	1.90	0.52
8:C:160:TYR:HB3	8:C:193:GLU:HB3	1.91	0.52
51:v:978:A:H61	51:v:1316:G:H1'	1.75	0.52
4:3:7:ARG:NH2	7:B:244:A:OP2	2.39	0.52
26:W:30:VAL:HG13	26:W:59:PHE:HB2	1.92	0.52
51:v:1239:A:H4'	51:v:1240:U:H5''	1.92	0.52
7:B:2458:G:H8	7:B:2459:A:H62	1.56	0.52
30:a:63:LYS:NZ	30:a:222:GLU:O	2.43	0.52
40:k:89:LEU:HB2	40:k:92:VAL:HG12	1.90	0.52
7:B:1854:A:H62	7:B:1888:G:H8	1.57	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:B:2376:A:N3	18:O:111:ARG:NH2	2.58	0.52
30:a:68:PHE:HE1	30:a:88:GLN:HB3	1.74	0.52
33:d:158:LYS:NZ	36:g:42:GLU:O	2.42	0.52
47:r:62:THR:H	47:r:65:MET:HE3	1.74	0.52
51:v:890:G:O2'	51:v:906:A:N6	2.43	0.52
39:j:84:MET:HE3	39:j:112:VAL:HG11	1.91	0.52
51:v:246:A:N6	51:v:281:G:N2	2.57	0.52
7:B:1568:G:H4'	8:C:58:LYS:HG2	1.92	0.51
34:e:8:PHE:HE1	34:e:62:MET:HE3	1.75	0.51
38:i:7:ARG:HD3	38:i:73:LEU:HD11	1.91	0.51
51:v:411:A:N6	51:v:429:U:OP2	2.44	0.51
51:v:1409:C:H4'	51:v:1410:A:H5'	1.92	0.51
3:2:2:LYS:HE2	7:B:687:C:H5''	1.92	0.51
7:B:805:G:N2	7:B:829:A:OP1	2.43	0.51
32:c:162:GLU:O	32:c:166:LYS:NZ	2.43	0.51
38:i:62:ARG:HH12	51:v:1367:C:H5'	1.74	0.51
51:v:672:U:H2'	51:v:673:A:H8	1.74	0.51
7:B:641:U:O2'	7:B:2350:C:OP1	2.28	0.51
30:a:67:LEU:HD22	30:a:157:PRO:HG3	1.92	0.51
31:b:171:ARG:HB3	51:v:1106:G:H5''	1.93	0.51
32:c:96:ARG:NH2	32:c:98:ASP:OD2	2.44	0.51
38:i:8:ILE:HB	38:i:74:VAL:HG12	1.93	0.51
51:v:150:U:H2'	51:v:151:A:H8	1.76	0.51
26:W:35:ILE:HG12	26:W:36:ILE:HG13	1.91	0.51
7:B:118:A:H5'	7:B:119:A:H8	1.75	0.51
7:B:1392:A:N6	23:T:18:GLU:OE2	2.38	0.51
9:D:39:ASP:OD1	9:D:39:ASP:N	2.43	0.51
23:T:11:LEU:O	28:Y:29:ARG:NH1	2.39	0.51
51:v:140:U:O2'	51:v:183:C:N4	2.43	0.51
51:v:1323:G:O2'	51:v:1362:A:O2'	2.28	0.51
7:B:84:A:N1	7:B:98:G:O2'	2.40	0.51
7:B:559:G:N2	20:Q:48:ASP:OD1	2.43	0.51
44:o:15:PRO:HD2	44:o:42:ILE:HD11	1.93	0.51
51:v:664:G:H22	51:v:741:G:H1	1.59	0.51
7:B:299:A:N3	7:B:319:G:O2'	2.43	0.51
7:B:692:C:H5''	8:C:38:LYS:HB2	1.91	0.51
7:B:693:A:O2'	7:B:1353:A:N3	2.41	0.51
14:K:29:ARG:HH21	14:K:32:ALA:HB1	1.75	0.51
7:B:1791:A:N6	7:B:1828:G:O2'	2.35	0.51
47:r:6:LYS:NZ	51:v:1314:C:OP2	2.42	0.51
3:2:46:LYS:HE3	7:B:126:A:H3'	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:B:2666:C:H41	12:G:108:PHE:HA	1.75	0.51
31:b:87:ARG:NE	31:b:98:ALA:O	2.42	0.51
2:1:49:LYS:HG3	2:1:50:GLU:HG2	1.92	0.51
7:B:45:G:H5''	7:B:46:G:H5'	1.93	0.51
7:B:2202:U:O2'	7:B:2204:G:OP1	2.25	0.51
30:a:12:GLY:HA3	30:a:42:LEU:HD12	1.92	0.51
42:m:1:ALA:O	42:m:6:LYS:NZ	2.44	0.51
7:B:2258:C:O2'	7:B:2427:C:OP2	2.29	0.50
8:C:70:LYS:NZ	8:C:99:GLU:OE1	2.41	0.50
13:J:96:ARG:NH1	13:J:98:GLU:OE1	2.40	0.50
8:C:60:ALA:O	8:C:62:ARG:NH1	2.44	0.50
38:i:7:ARG:HA	38:i:75:ASP:HA	1.92	0.50
51:v:673:A:H2'	51:v:674:G:C8	2.46	0.50
8:C:7:PRO:HB3	8:C:13:ARG:HD3	1.93	0.50
18:O:94:ARG:NH1	18:O:97:PHE:O	2.42	0.50
20:Q:19:GLN:OE1	21:R:73:LYS:NZ	2.43	0.50
23:T:25:GLU:HG2	23:T:30:ILE:HD13	1.94	0.50
32:c:58:GLN:OE1	32:c:61:ARG:NH1	2.44	0.50
36:g:63:LYS:HG3	36:g:70:VAL:HG21	1.93	0.50
51:v:117:G:N2	51:v:121:U:O4	2.45	0.50
1:O:15:ARG:NE	7:B:1266:G:OP1	2.44	0.50
7:B:881:G:O6	7:B:895:U:O2	2.30	0.50
7:B:1275:A:OP2	7:B:1646:C:N4	2.36	0.50
24:U:6:ARG:NH1	24:U:25:LYS:O	2.44	0.50
46:q:52:ARG:NH2	51:v:835:U:OP1	2.42	0.50
7:B:659:G:O2'	10:E:95:LYS:O	2.29	0.50
10:E:148:ILE:HB	10:E:169:VAL:HG22	1.94	0.50
39:j:18:GLY:HA3	39:j:78:ILE:HD13	1.93	0.50
1:O:53:VAL:HG23	1:O:54:ILE:HD12	1.94	0.50
6:A:37:C:O2	18:O:100:HIS:NE2	2.41	0.50
7:B:275:C:O2'	7:B:362:A:N6	2.43	0.50
7:B:566:U:H5''	15:L:29:LYS:HE3	1.94	0.50
7:B:1021:A:H61	7:B:1142:A:H61	1.60	0.50
45:p:9:GLY:HA3	45:p:24:ILE:HG22	1.94	0.50
45:p:29:LYS:HA	45:p:36:PHE:HA	1.94	0.50
4:3:29:ARG:NH2	15:L:63:LYS:O	2.44	0.50
7:B:2301:C:O2	11:F:124:ARG:NH2	2.45	0.50
7:B:2462:C:H1'	7:B:2491:U:H5	1.77	0.50
10:E:46:GLN:O	10:E:88:ARG:NH2	2.44	0.50
38:i:28:THR:O	38:i:31:ARG:NH1	2.44	0.50
1:O:37:HIS:ND1	1:O:38:LEU:O	2.44	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:B:290:U:O2	7:B:350:G:O6	2.30	0.50
7:B:1724:G:O6	7:B:1736:U:O4	2.29	0.50
32:c:123:MET:HA	32:c:145:ARG:HH21	1.77	0.50
37:h:6:TYR:HA	37:h:18:VAL:O	2.12	0.50
51:v:28:A:O2'	51:v:296:U:OP1	2.29	0.50
7:B:851:C:O2'	29:Z:42:ALA:O	2.29	0.49
12:G:94:ARG:HG2	12:G:105:SER:HB2	1.93	0.49
40:k:38:THR:HB	40:k:48:LEU:HG	1.94	0.49
31:b:128:MET:HE3	31:b:131:ARG:HH11	1.76	0.49
7:B:1930:G:N2	7:B:1931:U:O4	2.44	0.49
8:C:52:HIS:HA	8:C:216:ARG:HB2	1.94	0.49
11:F:47:LYS:O	11:F:51:ASN:ND2	2.46	0.49
51:v:34:C:H2'	51:v:35:G:H8	1.77	0.49
18:O:67:ASN:H	18:O:70:ALA:HB3	1.77	0.49
41:l:97:ARG:NH1	51:v:1309:G:OP2	2.45	0.49
31:b:51:VAL:HG12	31:b:69:THR:HG23	1.95	0.49
36:g:14:ARG:HH11	36:g:74:ILE:HG23	1.78	0.49
36:g:14:ARG:NH1	36:g:74:ILE:O	2.45	0.49
51:v:769:G:H4'	51:v:1513:A:H4'	1.93	0.49
51:v:982:U:C4	51:v:1222:G:O6	2.65	0.49
7:B:630:G:N2	7:B:633:A:OP2	2.39	0.49
7:B:1068:G:H21	7:B:1095:A:HO2'	1.60	0.49
34:e:51:ILE:HD11	34:e:85:ILE:HD12	1.95	0.49
35:f:69:ARG:HD3	35:f:95:ARG:HD3	1.94	0.49
39:j:126:ARG:NH1	51:v:693:G:OP1	2.45	0.49
51:v:60:A:N1	51:v:107:G:O2'	2.41	0.49
51:v:977:A:N6	51:v:1224:U:O4'	2.45	0.49
7:B:837:C:N3	7:B:941:A:N6	2.61	0.49
10:E:1:MET:HE1	10:E:114:ARG:HG3	1.95	0.49
11:F:90:LEU:HB3	11:F:95:MET:HA	1.94	0.49
24:U:45:GLN:HE22	24:U:58:VAL:HB	1.77	0.49
33:d:96:GLN:HB2	33:d:123:LEU:HB2	1.94	0.49
7:B:577:G:O2'	7:B:1254:A:OP1	2.30	0.49
10:E:21:ARG:HH12	10:E:24:ASN:HB2	1.78	0.49
15:L:110:VAL:HB	15:L:127:VAL:HG12	1.94	0.49
46:q:28:LEU:HD12	46:q:58:ILE:HG13	1.95	0.49
7:B:995:C:O2'	13:J:1:MET:N	2.46	0.49
7:B:1110:G:H1'	7:B:1111:A:H8	1.77	0.49
31:b:183:TYR:HA	31:b:199:VAL:O	2.11	0.49
41:l:11:HIS:H	41:l:45:SER:HB3	1.78	0.49
2:l:11:VAL:HB	2:l:50:GLU:HB2	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:B:2295:C:OP1	18:O:10:ARG:NH1	2.45	0.49
14:K:23:VAL:HG11	14:K:32:ALA:HB3	1.94	0.49
44:o:28:ARG:NH2	51:v:390:U:O3'	2.45	0.49
51:v:1000:A:N6	51:v:1041:G:O6	2.46	0.49
4:3:53:ASP:OD2	7:B:2359:C:O2'	2.29	0.48
29:Z:40:THR:HG22	29:Z:42:ALA:H	1.78	0.48
30:a:65:LYS:HG2	30:a:153:MET:HG2	1.94	0.48
40:k:47:ALA:HB2	51:v:529:G:H1	1.77	0.48
7:B:581:C:H2'	7:B:582:A:C8	2.48	0.48
19:P:88:ARG:NH2	19:P:111:GLU:OE1	2.47	0.48
22:S:24:ILE:HG23	22:S:74:ILE:HG21	1.95	0.48
26:W:45:HIS:HB3	26:W:51:GLY:H	1.77	0.48
51:v:867:G:O2'	51:v:873:A:N1	2.44	0.48
5:4:34:LYS:NZ	7:B:2743:U:OP1	2.44	0.48
7:B:704:G:H2'	7:B:726:G:H22	1.78	0.48
13:J:6:ALA:HB2	13:J:44:TYR:HB3	1.95	0.48
21:R:74:ILE:HB	21:R:87:GLN:HB3	1.94	0.48
28:Y:31:GLN:OE1	28:Y:39:GLN:NE2	2.46	0.48
40:k:34:THR:N	40:k:53:ARG:O	2.46	0.48
7:B:538:A:N6	7:B:555:G:O2'	2.46	0.48
7:B:788:A:OP1	7:B:791:C:N4	2.42	0.48
7:B:1419:A:O2'	7:B:1421:G:N7	2.38	0.48
7:B:1432:G:H2'	7:B:1433:A:C8	2.48	0.48
9:D:37:VAL:HG22	9:D:48:ILE:HG22	1.96	0.48
9:D:69:ALA:HA	9:D:73:VAL:HB	1.96	0.48
27:X:71:ARG:NE	27:X:77:TYR:OH	2.44	0.48
7:B:1388:G:HO2'	7:B:1525:A:HO2'	1.62	0.48
7:B:2331:G:H21	26:W:40:ARG:HH22	1.60	0.48
10:E:154:ASP:OD1	10:E:154:ASP:N	2.43	0.48
7:B:1434:A:H62	7:B:1558:C:H42	1.60	0.48
7:B:2885:G:O2'	7:B:2886:A:O4'	2.30	0.48
7:B:1912:A:H8	51:v:1495:U:H1'	1.77	0.48
9:D:13:ARG:HD2	9:D:21:SER:HB2	1.96	0.48
30:a:103:TRP:HA	30:a:106:VAL:HB	1.96	0.48
40:k:8:ARG:NH2	51:v:881:G:OP2	2.44	0.48
7:B:458:G:O2'	7:B:469:G:O6	2.30	0.48
7:B:833:A:H2'	7:B:834:G:C8	2.49	0.48
33:d:137:ARG:NH2	51:v:1078:U:O2'	2.47	0.48
35:f:87:PRO:HG3	35:f:148:LYS:HB2	1.95	0.48
7:B:504:A:O3'	22:S:1:MET:N	2.47	0.48
7:B:2405:G:O2'	7:B:2412:A:N6	2.47	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
51:v:411:A:H5''	51:v:429:U:H5	1.79	0.48
51:v:1130:A:H61	51:v:1144:G:H1	1.62	0.48
51:v:1266:G:N2	51:v:1269:A:OP2	2.47	0.48
7:B:1753:G:N2	7:B:1756:G:OP2	2.36	0.47
40:k:38:THR:HA	40:k:49:ARG:O	2.14	0.47
48:s:4:LYS:HG3	48:s:6:ALA:H	1.79	0.47
51:v:677:U:O2	51:v:777:A:O2'	2.30	0.47
7:B:2134:A:O2'	7:B:2160:C:O2	2.29	0.47
26:W:28:GLU:HA	26:W:63:ASP:HA	1.96	0.47
30:a:69:VAL:HG23	30:a:91:VAL:HB	1.95	0.47
32:c:143:SER:OG	32:c:144:ILE:N	2.47	0.47
37:h:10:ARG:NH2	51:v:1149:C:OP2	2.45	0.47
9:D:179:ARG:HB3	9:D:188:LEU:HD13	1.96	0.47
30:a:166:ASP:HB2	30:a:190:SER:HB3	1.96	0.47
33:d:156:ARG:NH1	36:g:98:LEU:O	2.47	0.47
34:e:82:ASP:OD1	34:e:82:ASP:N	2.46	0.47
7:B:2515:C:H2'	7:B:2516:A:H8	1.80	0.47
16:M:21:ALA:HB2	16:M:97:GLN:HB2	1.96	0.47
33:d:114:LEU:HD13	33:d:122:VAL:HG11	1.96	0.47
51:v:458:U:O2	51:v:474:G:O6	2.32	0.47
51:v:552:U:H2'	51:v:553:A:H8	1.79	0.47
51:v:1175:G:H2'	51:v:1176:A:H8	1.79	0.47
7:B:1068:G:N2	7:B:1095:A:O2'	2.39	0.47
7:B:1140:C:H5'	13:J:26:GLY:HA3	1.96	0.47
7:B:1796:U:H2'	7:B:1797:G:H8	1.78	0.47
38:i:11:LYS:HG2	38:i:71:LEU:HD13	1.96	0.47
51:v:975:A:N1	51:v:1366:C:O2'	2.44	0.47
7:B:2564:A:OP1	7:B:2648:G:O2'	2.27	0.47
12:G:136:ASP:HB3	12:G:139:VAL:HB	1.97	0.47
33:d:155:LYS:HD2	36:g:70:VAL:HA	1.96	0.47
36:g:17:GLN:HG2	36:g:62:LEU:HD13	1.96	0.47
51:v:1241:G:H2'	51:v:1242:G:H8	1.78	0.47
7:B:18:U:OP1	20:Q:29:ARG:NH1	2.48	0.47
22:S:24:ILE:HG13	22:S:32:ALA:HB1	1.96	0.47
30:a:110:ILE:HD11	30:a:151:LYS:HA	1.97	0.47
33:d:24:VAL:HA	51:v:922:G:H4'	1.97	0.47
34:e:12:PRO:HD2	34:e:54:LEU:HD11	1.96	0.47
37:h:11:ARG:NH2	51:v:1347:G:O6	2.45	0.47
51:v:54:C:OP1	51:v:351:G:N2	2.45	0.47
51:v:130:A:N6	51:v:233:C:O2	2.48	0.47
51:v:674:G:H2'	51:v:675:A:H8	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
51:v:1012:A:N6	51:v:1018:G:O6	2.48	0.47
7:B:373:U:H2'	7:B:374:A:H8	1.80	0.47
7:B:572:A:H5'	21:R:79:ARG:NH2	2.30	0.47
7:B:1019:U:OP1	7:B:1035:U:O2'	2.29	0.47
19:P:61:ARG:HD2	19:P:100:ARG:HB2	1.97	0.47
30:a:193:ASP:OD1	30:a:193:ASP:N	2.45	0.47
51:v:713:G:H2'	51:v:714:G:C8	2.50	0.47
5:4:24:ARG:NH2	7:B:2742:G:OP2	2.47	0.47
7:B:1447:C:O2'	7:B:1544:A:N3	2.42	0.47
31:b:25:THR:HG23	42:m:76:LYS:HA	1.97	0.47
47:r:53:GLY:HA3	51:v:958:A:H2	1.79	0.47
28:Y:5:GLU:OE1	28:Y:7:ARG:NH2	2.47	0.47
40:k:99:GLY:H	40:k:103:CYS:HB3	1.79	0.47
51:v:982:U:O4	51:v:1222:G:O6	2.33	0.47
51:v:1222:G:OP2	51:v:1322:C:N4	2.47	0.47
4:3:53:ASP:HB3	15:L:57:LEU:HD22	1.97	0.46
7:B:2312:U:H5'	11:F:84:ILE:HD11	1.97	0.46
8:C:162:GLN:OE1	8:C:174:ARG:NE	2.43	0.46
42:m:66:GLN:HG2	42:m:83:LYS:HG3	1.97	0.46
6:A:28:C:H5''	18:O:31:THR:HG21	1.97	0.46
9:D:38:LYS:O	9:D:46:ARG:HA	2.15	0.46
15:L:38:GLN:HG2	15:L:45:GLY:HA2	1.96	0.46
25:V:75:GLN:HB2	25:V:92:VAL:HG23	1.98	0.46
51:v:222:C:H2'	51:v:223:A:H8	1.79	0.46
4:3:44:ARG:NH1	7:B:2350:C:OP2	2.48	0.46
7:B:2039:U:H2'	7:B:2040:G:C8	2.50	0.46
12:G:8:VAL:HB	12:G:49:LEU:HB2	1.96	0.46
13:J:42:ALA:HA	20:Q:66:ALA:HB3	1.97	0.46
45:p:45:VAL:HG11	45:p:60:ILE:HG21	1.98	0.46
51:v:419:C:OP1	51:v:513:C:O2'	2.33	0.46
51:v:1160:G:O6	51:v:1182:G:O6	2.34	0.46
7:B:404:A:N6	7:B:421:C:O2'	2.46	0.46
7:B:1721:G:H22	7:B:1738:G:H1'	1.80	0.46
12:G:23:ILE:HG21	12:G:71:LEU:HD11	1.96	0.46
14:K:41:THR:HG23	14:K:43:LYS:HD3	1.98	0.46
14:K:63:ARG:HB2	14:K:82:ALA:HB3	1.98	0.46
14:K:111:PHE:HD1	14:K:114:ILE:HD12	1.81	0.46
34:e:91:ARG:N	51:v:737:C:OP1	2.46	0.46
43:n:63:ARG:NH1	43:n:67:ASP:OD1	2.46	0.46
7:B:856:G:H21	26:W:19:ARG:HH21	1.62	0.46
7:B:1363:C:O2'	7:B:1809:A:N3	2.43	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:C:116:GLN:N	8:C:127:ASN:OD1	2.46	0.46
18:O:39:VAL:HB	18:O:49:VAL:HB	1.98	0.46
37:h:44:ARG:HH22	37:h:48:ARG:HH11	1.62	0.46
51:v:235:C:H2'	51:v:236:A:H8	1.81	0.46
9:D:25:THR:HG21	9:D:193:VAL:HG22	1.98	0.46
22:S:74:ILE:HD12	22:S:105:VAL:HG22	1.97	0.46
41:l:25:GLY:H	51:v:1329:A:H5''	1.80	0.46
51:v:1305:G:N2	51:v:1332:A:OP2	2.49	0.46
7:B:184:C:O2'	7:B:217:A:N3	2.46	0.46
7:B:740:C:H5'	7:B:1784:A:H3'	1.97	0.46
27:X:32:LEU:HD22	27:X:49:ARG:HG2	1.98	0.46
28:Y:43:LEU:HB3	28:Y:47:ARG:HH21	1.80	0.46
30:a:120:SER:HA	30:a:125:PHE:HD2	1.81	0.46
35:f:113:LYS:HB3	51:v:1297:G:H21	1.79	0.46
41:l:32:ILE:HD12	41:l:58:GLU:HB3	1.97	0.46
51:v:6:G:H4'	51:v:298:A:H4'	1.98	0.46
7:B:1013:C:H2'	7:B:1014:A:H8	1.80	0.46
30:a:151:LYS:HB3	30:a:151:LYS:HE2	1.69	0.46
51:v:501:C:H2'	51:v:502:A:C8	2.51	0.46
51:v:559:A:H4'	51:v:560:A:H3'	1.98	0.46
7:B:540:C:OP1	7:B:2799:A:N6	2.49	0.46
7:B:1667:G:O2'	7:B:1991:U:O4	2.29	0.46
32:c:85:THR:H	33:d:102:THR:HG21	1.81	0.46
33:d:104:ILE:HG22	33:d:122:VAL:HG12	1.97	0.46
38:i:29:ALA:HB1	38:i:36:VAL:HG21	1.98	0.46
51:v:133:U:H4'	51:v:325:A:H1'	1.98	0.46
7:B:1429:G:H2'	7:B:1430:G:H8	1.80	0.46
7:B:1802:A:H2'	7:B:1803:A:C8	2.51	0.46
7:B:2674:G:H4'	14:K:29:ARG:HG2	1.97	0.46
7:B:2773:C:H5''	9:D:169:ARG:HG2	1.98	0.46
20:Q:95:ALA:HA	20:Q:97:ILE:HG12	1.98	0.46
37:h:93:LEU:HD12	37:h:93:LEU:HA	1.81	0.46
7:B:848:C:H2'	7:B:849:A:H8	1.81	0.45
7:B:1445:G:O6	7:B:1466:U:O2	2.34	0.45
37:h:68:GLY:HA2	51:v:1250:A:H4'	1.98	0.45
37:h:105:ARG:NH1	37:h:106:ASP:O	2.49	0.45
38:i:39:PRO:O	51:v:1123:U:O2'	2.30	0.45
46:q:28:LEU:HB3	46:q:67:LEU:HD11	1.97	0.45
51:v:945:G:N2	51:v:1334:G:O2'	2.48	0.45
7:B:569:U:O2'	7:B:983:A:N1	2.45	0.45
13:J:36:LEU:HD11	13:J:122:LEU:HB2	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:b:13:ILE:HG13	31:b:14:VAL:HG23	1.97	0.45
31:b:39:ARG:HG3	31:b:56:ILE:HD11	1.99	0.45
32:c:84:ASN:HB2	32:c:87:GLU:HG2	1.97	0.45
39:j:55:ARG:O	39:j:58:THR:OG1	2.34	0.45
49:t:28:LEU:HA	49:t:31:VAL:HG12	1.98	0.45
51:v:1356:G:H2'	51:v:1357:A:C8	2.50	0.45
26:W:49:ASN:HB2	26:W:61:LYS:HD2	1.99	0.45
32:c:2:ARG:NH1	51:v:405:U:OP2	2.50	0.45
32:c:101:VAL:HB	32:c:113:ALA:HB1	1.98	0.45
7:B:30:G:O2'	7:B:1214:A:N3	2.42	0.45
7:B:958:U:OP1	16:M:40:ARG:NH2	2.49	0.45
7:B:1332:G:N7	7:B:1609:A:O2'	2.39	0.45
16:M:41:LEU:HD11	16:M:124:LEU:HD22	1.97	0.45
32:c:47:LEU:HD12	32:c:51:GLY:HA3	1.99	0.45
33:d:155:LYS:HG2	36:g:70:VAL:HG13	1.97	0.45
41:l:22:TYR:HD2	41:l:65:GLU:HB2	1.82	0.45
45:p:5:ARG:NH1	51:v:127:G:O2'	2.50	0.45
51:v:946:A:H2'	51:v:947:G:C8	2.52	0.45
7:B:1028:A:H2'	7:B:1029:A:C8	2.51	0.45
7:B:2353:G:H21	26:W:30:VAL:HG12	1.81	0.45
23:T:85:VAL:HG12	23:T:87:LEU:HD23	1.98	0.45
24:U:10:VAL:HG12	24:U:71:ILE:HA	1.98	0.45
31:b:32:LEU:HD11	42:m:93:ILE:HG12	1.98	0.45
48:s:42:ASP:OD1	48:s:42:ASP:N	2.50	0.45
51:v:714:G:H2'	51:v:715:A:C8	2.52	0.45
7:B:589:U:H2'	7:B:590:A:C8	2.52	0.45
7:B:1329:U:H5''	7:B:1330:C:H5	1.81	0.45
16:M:102:LEU:HD11	16:M:126:ILE:HD11	1.98	0.45
32:c:105:GLY:HA3	32:c:161:ALA:HB2	1.99	0.45
51:v:979:C:H41	51:v:1317:C:H42	1.64	0.45
7:B:1278:C:H2'	7:B:1279:G:H8	1.81	0.45
11:F:164:GLU:HA	11:F:167:ALA:HB3	1.97	0.45
22:S:59:GLU:HG3	22:S:66:ILE:HD11	1.98	0.45
37:h:20:ILE:HG12	37:h:62:LEU:HG	1.98	0.45
46:q:47:ARG:NH2	51:v:845:A:N3	2.65	0.45
51:v:335:C:H2'	51:v:336:A:C8	2.51	0.45
51:v:398:U:H2'	51:v:399:G:H8	1.80	0.45
7:B:143:C:H2'	7:B:144:A:H8	1.82	0.45
7:B:1716:U:H2'	7:B:1717:A:H8	1.82	0.45
7:B:2204:G:H4'	8:C:149:LYS:HG3	1.98	0.45
20:Q:65:ASN:O	20:Q:69:ARG:HG2	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:Z:8:GLN:NE2	29:Z:10:ARG:O	2.41	0.45
36:g:66:GLN:HB2	36:g:68:LYS:HG2	1.99	0.45
37:h:119:LYS:HB2	37:h:122:ARG:HB3	1.99	0.45
40:k:11:ARG:HD2	51:v:562:U:H1'	1.98	0.45
51:v:76:G:O6	51:v:93:U:O2	2.34	0.45
51:v:1243:C:H2'	51:v:1244:G:H8	1.82	0.45
7:B:1980:G:O2'	7:B:1982:U:OP2	2.34	0.45
11:F:76:PHE:O	11:F:79:ARG:NH1	2.49	0.45
36:g:72:GLU:N	36:g:129:ALA:O	2.50	0.45
42:m:18:LYS:HE2	42:m:18:LYS:HB3	1.83	0.45
51:v:950:U:H2'	51:v:951:G:H8	1.81	0.45
51:v:1236:A:H4'	51:v:1304:G:H4'	1.98	0.45
7:B:5:A:H2'	7:B:6:A:C8	2.52	0.45
7:B:1798:U:OP2	8:C:269:ARG:NH2	2.49	0.45
12:G:93:TYR:HA	12:G:105:SER:O	2.17	0.45
14:K:64:THR:HG22	14:K:66:LYS:H	1.82	0.45
24:U:42:LYS:HB3	24:U:57:ILE:HG22	1.98	0.45
30:a:53:LEU:O	30:a:57:ASN:ND2	2.48	0.45
39:j:27:ASN:ND2	51:v:692:U:O4	2.49	0.45
51:v:982:U:O2	51:v:1222:G:N2	2.40	0.45
7:B:672:C:H5	15:L:42:SER:HB2	1.82	0.44
7:B:1386:C:H2'	7:B:1387:A:C8	2.52	0.44
7:B:2241:A:H2'	7:B:2242:G:C8	2.52	0.44
38:i:9:ARG:NH2	51:v:1279:G:O5'	2.50	0.44
42:m:9:GLU:HG2	42:m:63:ARG:HD2	1.98	0.44
51:v:1425:U:H2'	51:v:1426:G:H8	1.81	0.44
44:o:31:ARG:HB3	51:v:310:G:H5''	1.99	0.44
48:s:38:ILE:HD11	48:s:82:ILE:HG13	1.99	0.44
51:v:1224:U:O2'	51:v:1322:C:OP1	2.32	0.44
7:B:468:G:H5''	10:E:55:SER:HB3	1.99	0.44
7:B:2305:U:H5'	11:F:132:ARG:HH11	1.83	0.44
7:B:2751:G:OP1	7:B:2751:G:N2	2.49	0.44
38:i:42:LEU:HD23	38:i:71:LEU:HG	2.00	0.44
1:O:16:ARG:NE	7:B:1266:G:OP2	2.47	0.44
7:B:1028:A:N3	7:B:2486:C:O2'	2.43	0.44
37:h:9:GLY:H	37:h:84:ARG:HH11	1.66	0.44
41:l:72:ILE:HD12	51:v:1309:G:H1'	2.00	0.44
51:v:1005:A:C5	51:v:1024:G:N2	2.86	0.44
7:B:2386:A:H4'	26:W:55:ASP:HA	1.98	0.44
21:R:3:ALA:HA	21:R:40:MET:O	2.16	0.44
34:e:88:MET:HB2	46:q:63:TYR:HE2	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:h:114:LYS:HB2	37:h:117:LEU:HD12	1.99	0.44
39:j:66:ALA:HB2	39:j:95:THR:HG23	2.00	0.44
42:m:88:ALA:HB2	42:m:96:LEU:HD23	2.00	0.44
51:v:243:A:H4'	51:v:244:U:H3'	2.00	0.44
51:v:373:A:O2'	51:v:451:A:N7	2.51	0.44
51:v:909:A:N3	51:v:1413:A:O2'	2.44	0.44
7:B:687:C:O2'	7:B:1780:A:N6	2.50	0.44
7:B:1382:G:O2'	7:B:1573:G:N3	2.51	0.44
30:a:34:ARG:HB2	30:a:39:ILE:HD11	2.00	0.44
30:a:45:THR:HG23	30:a:200:PRO:HD2	2.00	0.44
30:a:182:VAL:H	30:a:196:ASP:HB2	1.82	0.44
33:d:82:HIS:CE1	36:g:95:MET:HE3	2.52	0.44
36:g:15:ASN:HD22	51:v:826:C:H1'	1.81	0.44
36:g:49:LYS:NZ	36:g:59:GLU:OE2	2.45	0.44
43:n:32:THR:OG1	43:n:62:ARG:NH1	2.50	0.44
7:B:1806:C:O2	8:C:43:ASN:ND2	2.49	0.44
30:a:185:ILE:HA	30:a:199:ILE:O	2.17	0.44
40:k:32:VAL:HG22	40:k:78:VAL:HG12	2.00	0.44
41:l:70:ARG:O	41:l:74:MET:HG2	2.17	0.44
46:q:31:TYR:HB3	46:q:54:LEU:HD21	1.99	0.44
51:v:1160:G:N2	51:v:1176:A:N1	2.64	0.44
7:B:2532:G:N2	7:B:2663:G:O2'	2.51	0.44
14:K:100:GLY:HA2	19:P:65:ASN:HB2	2.00	0.44
51:v:12:U:H4'	51:v:526:C:H4'	1.99	0.44
51:v:950:U:H2'	51:v:951:G:C8	2.53	0.44
51:v:1354:U:H2'	51:v:1355:G:H8	1.82	0.44
7:B:1654:A:O2'	9:D:118:PHE:O	2.32	0.44
7:B:1969:A:H2'	7:B:1972:G:H21	1.82	0.44
7:B:2115:G:O2'	7:B:2171:A:N6	2.47	0.44
7:B:2484:G:OP1	16:M:44:ARG:NE	2.51	0.44
10:E:159:LEU:HD22	10:E:162:ARG:HH21	1.83	0.44
20:Q:82:LEU:HD13	20:Q:89:ILE:HA	1.99	0.44
51:v:21:G:H2'	51:v:22:G:C8	2.53	0.44
51:v:219:U:H2'	51:v:220:G:H8	1.82	0.44
51:v:976:G:OP2	51:v:1358:U:O2'	2.35	0.44
6:A:94:A:OP1	25:V:19:ARG:NH1	2.44	0.43
13:J:34:ARG:HG3	13:J:39:LYS:HB2	2.00	0.43
31:b:70:ALA:HB2	31:b:114:LEU:HD21	1.99	0.43
51:v:143:A:N1	51:v:220:G:C6	2.86	0.43
51:v:715:A:H2'	51:v:716:A:C8	2.53	0.43
7:B:579:G:O2'	7:B:2019:A:OP1	2.36	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:B:1710:G:H2'	7:B:1711:A:C8	2.52	0.43
32:c:12:ARG:NH1	32:c:36:ALA:O	2.40	0.43
36:g:95:MET:HE2	36:g:95:MET:HB3	1.73	0.43
6:A:111:U:H2'	6:A:112:G:H8	1.83	0.43
7:B:1216:G:OP1	20:Q:10:ARG:NH1	2.48	0.43
7:B:2505:G:N2	7:B:2506:U:O4	2.49	0.43
7:B:2809:A:H2'	7:B:2810:A:C8	2.53	0.43
8:C:130:PRO:HA	8:C:188:ARG:HA	2.00	0.43
21:R:6:GLN:HG2	21:R:11:GLN:HG2	2.01	0.43
51:v:722:G:H1	51:v:733:G:H1	1.66	0.43
51:v:916:U:H2'	51:v:917:G:H8	1.83	0.43
51:v:927:G:O2'	51:v:1503:A:N7	2.48	0.43
3:2:37:LYS:HD3	3:2:39:ARG:HD3	2.00	0.43
31:b:76:ILE:HA	31:b:83:VAL:HB	2.00	0.43
31:b:129:PHE:O	31:b:133:MET:HG3	2.19	0.43
35:f:139:ASP:OD1	35:f:142:ARG:NH1	2.52	0.43
51:v:982:U:N3	51:v:1222:G:C6	2.86	0.43
7:B:1125:G:OP2	7:B:1126:A:O2'	2.34	0.43
7:B:2121:G:H1	7:B:2176:A:H2	1.61	0.43
7:B:2291:U:H2'	7:B:2292:U:C6	2.52	0.43
7:B:2328:A:H2'	7:B:2329:U:C6	2.53	0.43
27:X:4:CYS:HA	27:X:32:LEU:HD21	1.99	0.43
33:d:79:THR:HB	33:d:121:ASN:HB2	2.01	0.43
42:m:75:ARG:NE	51:v:1359:C:OP2	2.51	0.43
45:p:26:ARG:NH1	45:p:41:THR:OG1	2.51	0.43
46:q:32:ILE:HD12	46:q:36:GLY:HA2	1.99	0.43
49:t:9:GLU:HG2	49:t:10:PRO:HD3	2.00	0.43
51:v:322:C:H2'	51:v:323:U:C6	2.53	0.43
7:B:1231:U:H2'	7:B:1232:G:H8	1.84	0.43
7:B:1794:A:H2'	7:B:1795:C:C6	2.54	0.43
7:B:1796:U:H2'	7:B:1797:G:C8	2.53	0.43
7:B:2329:U:H2'	7:B:2330:G:C8	2.54	0.43
10:E:188:MET:HE3	10:E:193:VAL:HA	1.99	0.43
14:K:102:VAL:HG21	14:K:115:ILE:HG22	2.00	0.43
31:b:57:GLU:HB2	31:b:64:ARG:HG3	2.00	0.43
39:j:86:LYS:HB2	39:j:86:LYS:HE2	1.79	0.43
47:r:13:HIS:HA	47:r:16:LYS:HG2	2.01	0.43
51:v:946:A:O2'	51:v:1333:A:N3	2.40	0.43
7:B:1093:G:H21	7:B:1098:A:H62	0.73	0.43
7:B:1287:A:N1	7:B:1648:U:O2'	2.47	0.43
7:B:1297:C:O2'	7:B:1302:A:N1	2.43	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:S:24:ILE:HD11	22:S:51:LEU:HD22	2.00	0.43
51:v:334:C:HO2'	51:v:1434:A:HO2'	1.60	0.43
51:v:1004:A:N3	51:v:1036:A:N6	2.67	0.43
7:B:2597:G:H5''	8:C:239:PHE:O	2.18	0.43
13:J:57:LEU:HD23	13:J:57:LEU:HA	1.89	0.43
25:V:72:VAL:HB	25:V:91:PHE:HB3	2.01	0.43
44:o:25:ARG:O	51:v:110:C:O2'	2.28	0.43
51:v:1413:A:H2	51:v:1487:G:H22	1.65	0.43
7:B:1021:A:H2'	7:B:1022:G:H4'	1.99	0.43
13:J:57:LEU:HD21	13:J:130:HIS:HD2	1.83	0.43
17:N:48:VAL:HA	17:N:51:LEU:HD12	2.01	0.43
40:k:113:ARG:NH2	51:v:501:C:OP1	2.42	0.43
43:n:3:SER:OG	43:n:5:GLU:OE1	2.37	0.43
51:v:460:A:H2'	51:v:461:A:H8	1.84	0.43
51:v:744:C:H2'	51:v:745:G:H8	1.84	0.43
7:B:2529:G:H4'	12:G:174:LYS:HE3	2.01	0.43
8:C:29:PHE:HD2	8:C:32:LEU:HD12	1.84	0.43
11:F:34:THR:HG22	11:F:154:THR:HB	2.01	0.43
17:N:90:ARG:NH1	17:N:117:ASP:OD2	2.51	0.43
22:S:74:ILE:HA	22:S:104:THR:O	2.19	0.43
30:a:161:PHE:HA	30:a:183:PHE:O	2.19	0.43
31:b:68:HIS:HA	31:b:103:ALA:O	2.19	0.43
51:v:129:A:H2	51:v:232:G:H22	1.66	0.43
6:A:112:G:N2	18:O:45:SER:O	2.40	0.42
7:B:302:C:H2'	7:B:303:G:H8	1.84	0.42
7:B:2719:G:H21	7:B:2872:A:H61	1.67	0.42
10:E:83:VAL:HB	10:E:86:ALA:HB2	2.00	0.42
11:F:56:LEU:HD12	11:F:94:ARG:HH22	1.83	0.42
12:G:52:GLY:HA2	12:G:53:PRO:HD3	1.90	0.42
51:v:448:A:H62	51:v:486:U:H3	1.65	0.42
51:v:815:A:N7	51:v:1509:C:O2'	2.48	0.42
7:B:24:G:O2'	22:S:78:GLU:O	2.33	0.42
7:B:581:C:H2'	7:B:582:A:H8	1.83	0.42
7:B:721:A:H2'	7:B:722:A:C8	2.54	0.42
7:B:996:A:O2'	20:Q:91:ARG:NE	2.52	0.42
7:B:1038:G:H2'	7:B:1039:A:C8	2.55	0.42
7:B:1322:A:N1	7:B:1333:G:O2'	2.48	0.42
7:B:1939:U:OP1	7:B:2604:U:O2'	2.35	0.42
44:o:31:ARG:HH21	51:v:230:G:H5''	1.84	0.42
48:s:32:LYS:HB3	48:s:32:LYS:HE2	1.81	0.42
51:v:672:U:H2'	51:v:673:A:C8	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
51:v:891:U:H2'	51:v:892:A:H8	1.84	0.42
7:B:881:G:C6	7:B:895:U:O2	2.72	0.42
7:B:2284:A:O2'	7:B:2288:A:N1	2.49	0.42
40:k:31:GLY:O	40:k:78:VAL:HA	2.19	0.42
48:s:33:LYS:HA	48:s:33:LYS:HD3	1.86	0.42
51:v:1512:U:H2'	51:v:1513:A:C8	2.55	0.42
7:B:1796:U:H4'	8:C:253:GLY:H	1.83	0.42
7:B:1812:U:H2'	7:B:1813:G:C8	2.54	0.42
7:B:2229:U:H2'	7:B:2230:G:H8	1.84	0.42
7:B:2314:A:H1'	11:F:154:THR:HG21	2.00	0.42
7:B:2898:U:H2'	7:B:2899:A:C8	2.54	0.42
16:M:40:ARG:HD2	16:M:93:VAL:HG21	2.00	0.42
37:h:123:ARG:HB2	51:v:1343:G:H4'	2.00	0.42
51:v:316:C:OP2	51:v:351:G:O2'	2.36	0.42
7:B:910:A:H2'	7:B:911:A:C8	2.54	0.42
7:B:1021:A:H62	7:B:1141:U:H3	1.67	0.42
7:B:1614:A:N6	22:S:92:ARG:O	2.53	0.42
7:B:2590:A:H2'	7:B:2591:C:H6	1.85	0.42
7:B:2645:G:H4'	7:B:2732:G:H2'	2.01	0.42
33:d:149:PRO:HA	33:d:152:VAL:HG12	1.99	0.42
48:s:73:ARG:NH1	51:v:261:U:OP2	2.41	0.42
51:v:309:A:H2'	51:v:310:G:C8	2.54	0.42
51:v:501:C:H2'	51:v:502:A:H8	1.83	0.42
51:v:634:C:H2'	51:v:635:A:H8	1.84	0.42
7:B:155:A:H2'	7:B:156:A:C8	2.55	0.42
7:B:483:A:C8	24:U:44:HIS:HD2	2.37	0.42
7:B:532:A:H4'	7:B:533:G:C8	2.55	0.42
7:B:1829:A:N3	8:C:14:HIS:NE2	2.59	0.42
13:J:114:LEU:HG	13:J:118:MET:HE3	2.02	0.42
51:v:958:A:O2'	51:v:959:A:O4'	2.33	0.42
7:B:28:A:N6	7:B:512:G:H1'	2.33	0.42
13:J:42:ALA:HB3	13:J:44:TYR:CE1	2.54	0.42
16:M:42:THR:HB	16:M:45:GLN:HG3	2.01	0.42
32:c:187:ARG:NH2	32:c:194:ILE:O	2.46	0.42
35:f:25:PHE:HZ	35:f:119:LEU:HD11	1.84	0.42
37:h:51:LEU:HD23	37:h:51:LEU:HA	1.93	0.42
37:h:121:ARG:HD2	51:v:1348:U:H4'	2.02	0.42
51:v:405:U:H5''	51:v:495:A:H2	1.84	0.42
51:v:816:A:OP1	51:v:1526:G:O2'	2.36	0.42
51:v:1124:G:N2	51:v:1125:U:O4	2.53	0.42
7:B:1590:A:H2'	7:B:1591:A:H8	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:B:1744:A:H3'	7:B:1745:A:H8	1.84	0.42
7:B:2230:G:H5''	27:X:29:LEU:HD12	2.02	0.42
7:B:2273:A:H2'	7:B:2274:A:C8	2.54	0.42
8:C:242:HIS:HA	8:C:243:PRO:HD3	1.94	0.42
14:K:6:MET:HE3	14:K:6:MET:HB3	1.84	0.42
20:Q:49:ARG:O	20:Q:53:LYS:NZ	2.48	0.42
25:V:31:TYR:OH	25:V:90:ASP:OD2	2.31	0.42
31:b:150:VAL:HG22	31:b:199:VAL:HG12	2.00	0.42
32:c:53:GLN:HA	32:c:198:LEU:HD23	2.01	0.42
51:v:776:G:N2	51:v:802:A:OP2	2.49	0.42
51:v:1342:C:H2'	51:v:1343:G:C8	2.54	0.42
51:v:1401:G:O6	51:v:1504:G:N2	2.53	0.42
7:B:447:A:OP1	20:Q:4:LYS:NZ	2.53	0.42
7:B:728:G:H4'	8:C:12:ARG:HD3	2.01	0.42
7:B:1278:C:H2'	7:B:1279:G:C8	2.54	0.42
7:B:1734:G:H2'	7:B:1735:A:H8	1.85	0.42
7:B:2233:U:H2'	7:B:2234:G:C8	2.55	0.42
9:D:31:ALA:HA	9:D:97:SER:HB3	2.01	0.42
22:S:72:THR:HG21	22:S:108:SER:HB3	2.01	0.42
25:V:26:PHE:HE2	25:V:89:ILE:HG13	1.85	0.42
2:1:10:LEU:HB3	2:1:48:TYR:HB3	2.01	0.42
7:B:742:A:H2'	7:B:743:A:C8	2.55	0.42
7:B:1570:A:H5'	8:C:35:LYS:HB2	2.02	0.42
7:B:2788:C:H2'	7:B:2789:C:C6	2.55	0.42
11:F:98:PHE:HA	11:F:101:ARG:HG2	2.02	0.42
12:G:17:LYS:HG2	12:G:24:THR:HB	2.02	0.42
34:e:89:VAL:O	51:v:736:C:O2'	2.36	0.42
51:v:644:U:H2'	51:v:645:G:H8	1.84	0.42
51:v:792:A:O2'	51:v:794:A:N7	2.49	0.42
7:B:172:A:H2'	7:B:173:A:C8	2.54	0.41
7:B:729:G:C6	8:C:206:LYS:HB2	2.55	0.41
7:B:1009:A:N3	7:B:1153:C:O2'	2.49	0.41
12:G:151:ARG:HB2	12:G:161:VAL:HG23	2.01	0.41
30:a:150:ILE:HG23	30:a:153:MET:HE3	2.01	0.41
37:h:117:LEU:HA	37:h:124:PRO:HD3	2.01	0.41
40:k:43:LYS:NZ	51:v:1491:G:OP1	2.38	0.41
41:l:74:MET:HA	41:l:77:LYS:HB2	2.02	0.41
51:v:1507:A:H2'	51:v:1508:A:C8	2.56	0.41
4:3:34:LYS:NZ	7:B:2391:G:OP2	2.50	0.41
4:3:38:LYS:NZ	7:B:2365:G:N7	2.55	0.41
7:B:593:U:H2'	7:B:594:U:C6	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:Q:21:LYS:HB3	20:Q:21:LYS:HE2	1.83	0.41
22:S:88:ARG:HA	22:S:88:ARG:HD2	1.85	0.41
38:i:28:THR:HG21	38:i:90:LEU:HD22	2.01	0.41
51:v:1071:C:H2'	51:v:1072:G:C8	2.52	0.41
51:v:1243:C:H2'	51:v:1244:G:C8	2.55	0.41
51:v:1467:C:H2'	51:v:1468:A:H8	1.85	0.41
5:4:8:LYS:H	5:4:35:GLN:HE21	1.68	0.41
7:B:2698:U:H2'	7:B:2699:C:C6	2.55	0.41
10:E:2:GLU:HA	10:E:14:VAL:HG22	2.02	0.41
30:a:85:SER:N	30:a:88:GLN:OE1	2.50	0.41
32:c:14:GLU:HG2	32:c:62:ARG:HD2	2.01	0.41
51:v:505:G:H2'	51:v:506:G:C8	2.55	0.41
51:v:662:U:H2'	51:v:663:A:C8	2.55	0.41
51:v:978:A:H2'	51:v:980:C:N4	2.34	0.41
7:B:1394:U:H4'	7:B:1603:A:H4'	2.03	0.41
7:B:2037:A:H2'	7:B:2038:G:C8	2.56	0.41
7:B:2676:C:P	14:K:30:ARG:HH22	2.43	0.41
12:G:155:PRO:HB3	12:G:169:ARG:HE	1.85	0.41
31:b:148:ILE:HA	31:b:200:TRP:O	2.20	0.41
7:B:219:A:N3	7:B:234:U:O2'	2.41	0.41
7:B:764:A:H2	8:C:217:PRO:HG3	1.86	0.41
7:B:1799:G:OP1	8:C:257:ARG:NH1	2.42	0.41
7:B:1992:G:N2	7:B:1996:C:O2'	2.53	0.41
7:B:2087:G:H2'	7:B:2088:A:C8	2.54	0.41
9:D:24:VAL:HG21	9:D:188:LEU:HD23	2.02	0.41
45:p:68:LYS:HG2	45:p:69:THR:HG23	2.03	0.41
51:v:1312:G:N2	51:v:1326:U:O2	2.53	0.41
1:O:15:ARG:NH2	7:B:1264:A:OP1	2.36	0.41
2:1:21:THR:HG21	7:B:2419:U:H4'	2.03	0.41
7:B:138:U:O2'	23:T:1:MET:N	2.38	0.41
7:B:160:A:N3	7:B:2208:C:O2'	2.46	0.41
7:B:281:C:H2'	7:B:282:A:C8	2.56	0.41
7:B:639:U:H2'	7:B:640:C:C6	2.55	0.41
8:C:104:LEU:HD23	8:C:104:LEU:HA	1.92	0.41
14:K:91:GLU:HG2	14:K:110:LYS:HE3	2.02	0.41
25:V:14:LYS:HE3	25:V:14:LYS:HB2	1.79	0.41
39:j:84:MET:HG2	39:j:110:THR:HB	2.01	0.41
42:m:2:LYS:HB2	42:m:5:MET:HB2	2.02	0.41
51:v:235:C:H2'	51:v:236:A:C8	2.56	0.41
51:v:490:C:H2'	51:v:491:G:H8	1.85	0.41
51:v:1355:G:H2'	51:v:1356:G:H8	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:29:VAL:HG22	1:0:36:LYS:HG2	2.01	0.41
7:B:72:U:H5'	28:Y:54:LYS:HD3	2.03	0.41
7:B:1300:G:H4'	7:B:1301:A:H5''	2.03	0.41
25:V:80:HIS:HA	25:V:81:PRO:HD3	1.96	0.41
35:f:32:ASP:OD1	51:v:1350:A:O2'	2.35	0.41
4:3:24:LYS:HD3	15:L:62:PRO:HB2	2.02	0.41
7:B:576:U:H2'	7:B:577:G:C8	2.56	0.41
7:B:714:U:OP2	43:n:87:ARG:NH1	2.47	0.41
7:B:1733:G:H2'	7:B:1734:G:H8	1.85	0.41
8:C:244:VAL:HG12	8:C:250:GLN:HA	2.03	0.41
12:G:26:LYS:HZ2	12:G:31:GLU:HB3	1.85	0.41
14:K:55:ASP:OD1	14:K:55:ASP:N	2.54	0.41
20:Q:65:ASN:HA	20:Q:75:TYR:HB2	2.03	0.41
22:S:84:ARG:HB2	22:S:96:ILE:HB	2.02	0.41
38:i:8:ILE:O	38:i:73:LEU:HA	2.21	0.41
38:i:12:ALA:HB2	38:i:18:ILE:HD13	2.03	0.41
51:v:181:A:O2'	51:v:193:C:N4	2.54	0.41
51:v:750:C:H2'	51:v:751:U:H6	1.85	0.41
51:v:1265:C:N3	51:v:1271:A:N6	2.68	0.41
7:B:442:G:N2	10:E:43:THR:O	2.52	0.41
7:B:832:U:H2'	7:B:833:A:C8	2.56	0.41
7:B:863:A:H2'	7:B:864:G:C8	2.56	0.41
7:B:1354:A:OP1	8:C:35:LYS:NZ	2.45	0.41
7:B:1636:U:H2'	7:B:1637:A:C8	2.55	0.41
7:B:1645:G:H5''	7:B:1646:C:H5'	2.03	0.41
11:F:74:ALA:HB3	11:F:79:ARG:HA	2.01	0.41
13:J:26:GLY:O	13:J:30:THR:HG23	2.20	0.41
17:N:100:CYS:SG	17:N:101:GLY:N	2.93	0.41
21:R:65:ALA:HB3	21:R:95:ASP:HB2	2.02	0.41
26:W:19:ARG:HA	26:W:34:SER:HA	2.02	0.41
30:a:165:ALA:HB3	30:a:190:SER:HB2	2.02	0.41
31:b:130:ARG:O	31:b:134:LYS:HG2	2.21	0.41
35:f:14:ASP:N	35:f:14:ASP:OD1	2.51	0.41
35:f:68:VAL:HG11	35:f:103:ILE:HG13	2.03	0.41
36:g:111:THR:HG22	36:g:113:ARG:H	1.84	0.41
39:j:63:GLN:HG3	39:j:98:ALA:HB2	2.02	0.41
41:l:25:GLY:O	41:l:29:SER:HB3	2.21	0.41
51:v:64:G:H4'	51:v:65:A:H3'	2.02	0.41
51:v:355:C:H1'	51:v:388:G:H1'	2.03	0.41
51:v:398:U:H2'	51:v:399:G:C8	2.56	0.41
51:v:434:U:H2'	51:v:435:A:C8	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:B:444:C:OP1	10:E:40:ARG:NH2	2.50	0.41
7:B:674:G:H5''	10:E:71:GLY:N	2.36	0.41
7:B:1475:G:O2'	7:B:1514:G:O6	2.35	0.41
7:B:2006:C:O2'	7:B:2823:A:N3	2.49	0.41
7:B:2133:G:N2	7:B:2174:C:O5'	2.53	0.41
24:U:37:GLY:N	24:U:61:GLU:OE2	2.39	0.41
24:U:38:ILE:HD13	24:U:38:ILE:HA	1.93	0.41
40:k:35:ARG:HB2	40:k:53:ARG:HB2	2.02	0.41
41:l:89:ARG:NE	41:l:95:PRO:O	2.49	0.41
51:v:948:C:H2'	51:v:949:A:H8	1.86	0.41
51:v:1179:A:H2'	51:v:1180:A:C8	2.55	0.41
6:A:88:C:H6	6:A:88:C:H2'	1.70	0.40
7:B:1548:A:H2'	7:B:1549:A:C8	2.56	0.40
7:B:2204:G:OP2	8:C:149:LYS:NZ	2.45	0.40
7:B:2229:U:H2'	7:B:2230:G:C8	2.56	0.40
14:K:34:VAL:HG23	14:K:68:VAL:HG12	2.02	0.40
16:M:38:ARG:HG3	16:M:98:PRO:HD3	2.03	0.40
34:e:11:HIS:HB2	34:e:14:GLN:H	1.87	0.40
40:k:43:LYS:HB2	40:k:43:LYS:HE2	1.89	0.40
47:r:3:SER:OG	47:r:4:LEU:N	2.54	0.40
51:v:1513:A:H2'	51:v:1514:G:C8	2.56	0.40
7:B:1429:G:H2'	7:B:1430:G:C8	2.56	0.40
15:L:96:LYS:NZ	15:L:102:GLY:O	2.53	0.40
27:X:6:VAL:HG13	27:X:7:THR:HG23	2.03	0.40
38:i:28:THR:HA	38:i:31:ARG:HD3	2.04	0.40
38:i:83:THR:O	38:i:87:LEU:HB3	2.21	0.40
51:v:575:G:H4'	51:v:576:C:H5''	2.03	0.40
6:A:60:C:H2'	6:A:61:G:H8	1.86	0.40
6:A:95:U:H2'	6:A:96:G:H8	1.86	0.40
7:B:1590:A:H2'	7:B:1591:A:C8	2.56	0.40
24:U:27:VAL:HG22	24:U:33:VAL:HG12	2.03	0.40
25:V:25:LYS:HE2	25:V:41:GLU:HG3	2.03	0.40
31:b:123:LEU:HD11	31:b:129:PHE:HB3	2.02	0.40
38:i:62:ARG:NH1	51:v:1367:C:H5'	2.35	0.40
51:v:1132:C:N4	51:v:1133:G:O6	2.54	0.40
6:A:70:C:H2'	6:A:71:C:H6	1.86	0.40
7:B:2567:G:H2'	7:B:2568:U:C6	2.56	0.40
23:T:39:THR:O	23:T:43:ILE:HG13	2.22	0.40
24:U:88:ASP:OD1	24:U:88:ASP:N	2.54	0.40
26:W:32:ALA:HB1	26:W:35:ILE:HB	2.04	0.40
36:g:30:LYS:NZ	51:v:642:A:OP2	2.54	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:k:88:ASP:HB2	51:v:523:A:H61	1.86	0.40
47:r:35:ARG:NH2	47:r:71:GLY:O	2.54	0.40
49:t:3:ILE:HD13	49:t:24:LYS:HE3	2.02	0.40
51:v:1305:G:H1	51:v:1331:G:HO2'	1.69	0.40
51:v:1355:G:H2'	51:v:1356:G:C8	2.57	0.40
7:B:499:U:H5''	24:U:42:LYS:HE3	2.02	0.40
10:E:1:MET:HE2	10:E:20:GLY:HA2	2.03	0.40
20:Q:90:ASP:O	20:Q:91:ARG:HD3	2.21	0.40
26:W:23:LYS:HB2	26:W:68:PHE:HD1	1.87	0.40
36:g:85:TYR:CD1	36:g:123:GLU:HB3	2.57	0.40
38:i:42:LEU:HA	38:i:43:PRO:HD3	1.96	0.40
47:r:32:THR:OG1	47:r:49:ALA:O	2.34	0.40
51:v:757:U:OP1	51:v:822:U:O2'	2.37	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	0	54/56 (96%)	47 (87%)	7 (13%)	0	100	100
2	1	49/51 (96%)	48 (98%)	1 (2%)	0	100	100
3	2	44/46 (96%)	43 (98%)	1 (2%)	0	100	100
4	3	62/64 (97%)	58 (94%)	4 (6%)	0	100	100
5	4	36/38 (95%)	33 (92%)	3 (8%)	0	100	100
8	C	270/272 (99%)	265 (98%)	5 (2%)	0	100	100
9	D	207/209 (99%)	195 (94%)	12 (6%)	0	100	100
10	E	199/201 (99%)	186 (94%)	13 (6%)	0	100	100
11	F	176/178 (99%)	151 (86%)	24 (14%)	1 (1%)	21	56
12	G	174/176 (99%)	169 (97%)	5 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
13	J	140/142 (99%)	133 (95%)	6 (4%)	1 (1%)	18	53
14	K	120/122 (98%)	110 (92%)	10 (8%)	0	100	100
15	L	141/143 (99%)	132 (94%)	9 (6%)	0	100	100
16	M	134/136 (98%)	132 (98%)	2 (2%)	0	100	100
17	N	119/121 (98%)	110 (92%)	9 (8%)	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%)	111 (96%)	4 (4%)	0	100	100
21	R	101/103 (98%)	94 (93%)	6 (6%)	1 (1%)	12	45
22	S	108/110 (98%)	104 (96%)	4 (4%)	0	100	100
23	T	92/94 (98%)	83 (90%)	9 (10%)	0	100	100
24	U	101/103 (98%)	95 (94%)	6 (6%)	0	100	100
25	V	92/94 (98%)	88 (96%)	4 (4%)	0	100	100
26	W	77/79 (98%)	66 (86%)	11 (14%)	0	100	100
27	X	75/77 (97%)	71 (95%)	4 (5%)	0	100	100
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%)	199 (92%)	17 (8%)	0	100	100
31	b	204/206 (99%)	195 (96%)	9 (4%)	0	100	100
32	c	203/205 (99%)	196 (97%)	7 (3%)	0	100	100
33	d	148/150 (99%)	137 (93%)	11 (7%)	0	100	100
34	e	98/100 (98%)	96 (98%)	2 (2%)	0	100	100
35	f	149/151 (99%)	144 (97%)	5 (3%)	0	100	100
36	g	127/129 (98%)	124 (98%)	3 (2%)	0	100	100
37	h	125/127 (98%)	114 (91%)	11 (9%)	0	100	100
38	i	96/98 (98%)	94 (98%)	2 (2%)	0	100	100
39	j	115/117 (98%)	108 (94%)	7 (6%)	0	100	100
40	k	121/123 (98%)	117 (97%)	4 (3%)	0	100	100
41	l	112/114 (98%)	110 (98%)	2 (2%)	0	100	100
42	m	92/100 (92%)	89 (97%)	3 (3%)	0	100	100
43	n	86/88 (98%)	82 (95%)	4 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
44	o	80/82 (98%)	78 (98%)	2 (2%)	0	100	100
45	p	78/80 (98%)	73 (94%)	5 (6%)	0	100	100
46	q	53/55 (96%)	51 (96%)	2 (4%)	0	100	100
47	r	77/79 (98%)	74 (96%)	3 (4%)	0	100	100
48	s	83/85 (98%)	82 (99%)	1 (1%)	0	100	100
49	t	49/51 (96%)	43 (88%)	6 (12%)	0	100	100
50	u	57/59 (97%)	56 (98%)	1 (2%)	0	100	100
All	All	5398/5500 (98%)	5116 (95%)	279 (5%)	3 (0%)	49	80

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
11	F	161	SER
21	R	58	VAL
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%)	216 (100%)	0	100	100
9	D	164/164 (100%)	164 (100%)	0	100	100
10	E	165/165 (100%)	165 (100%)	0	100	100
11	F	149/149 (100%)	149 (100%)	0	100	100
12	G	137/137 (100%)	137 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
13	J	116/116 (100%)	116 (100%)	0	100	100
14	K	102/103 (99%)	102 (100%)	0	100	100
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%)	99 (100%)	0	100	100
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%)	83 (100%)	0	100	100
25	V	78/78 (100%)	78 (100%)	0	100	100
26	W	59/59 (100%)	59 (100%)	0	100	100
27	X	67/67 (100%)	67 (100%)	0	100	100
28	Y	55/55 (100%)	55 (100%)	0	100	100
29	Z	48/48 (100%)	48 (100%)	0	100	100
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%)	172 (100%)	0	100	100
33	d	113/113 (100%)	113 (100%)	0	100	100
34	e	87/87 (100%)	87 (100%)	0	100	100
35	f	124/124 (100%)	124 (100%)	0	100	100
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

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
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%)	65 (100%)	0	100	100
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%)	4495 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (40) such sidechains are listed below:

Mol	Chain	Res	Type
5	4	13	ASN
5	4	33	HIS
8	C	85	ASN
8	C	114	GLN
9	D	173	GLN
11	F	4	HIS
11	F	36	ASN
11	F	62	GLN
12	G	29	ASN
12	G	72	ASN
12	G	138	GLN
13	J	47	HIS
13	J	67	ASN
13	J	138	GLN
14	K	2	GLN
15	L	35	HIS
16	M	22	GLN
19	P	40	GLN
20	Q	43	GLN
20	Q	80	ASN
24	U	52	ASN
24	U	53	GLN
28	Y	15	ASN
28	Y	36	GLN
28	Y	58	ASN

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Mol	Chain	Res	Type
29	Z	19	HIS
30	a	41	ASN
32	c	53	GLN
33	d	72	ASN
34	e	46	GLN
34	e	68	GLN
34	e	81	ASN
35	f	121	ASN
41	l	104	ASN
42	m	62	ASN
43	n	39	GLN
43	n	79	GLN
44	o	26	ASN
46	q	30	ASN
48	s	2	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
51	v	1538/1539 (99%)	319 (20%)	0
6	A	116/117 (99%)	24 (20%)	1 (0%)
7	B	2902/2903 (99%)	591 (20%)	7 (0%)
All	All	4556/4559 (99%)	934 (20%)	8 (0%)

All (934) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
6	A	9	G
6	A	13	G
6	A	14	U
6	A	16	G
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	41	G
6	A	42	C
6	A	43	C
6	A	44	G

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Mol	Chain	Res	Type
6	A	52	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	91	C
6	A	99	A
6	A	109	A
7	B	12	U
7	B	13	A
7	B	15	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	71	A
7	B	72	U
7	B	74	A
7	B	75	G
7	B	84	A
7	B	99	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	125	A
7	B	139	U
7	B	140	C
7	B	142	A
7	B	160	A
7	B	163	C
7	B	164	C
7	B	181	A
7	B	196	A
7	B	199	A
7	B	215	G

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Mol	Chain	Res	Type
7	B	216	A
7	B	221	A
7	B	222	A
7	B	223	A
7	B	225	C
7	B	245	G
7	B	248	G
7	B	250	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	276	U
7	B	277	G
7	B	278	A
7	B	285	G
7	B	291	G
7	B	301	G
7	B	310	A
7	B	311	A
7	B	329	G
7	B	330	A
7	B	332	A
7	B	351	C
7	B	352	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	383	C
7	B	386	G
7	B	396	G
7	B	403	U
7	B	404	A
7	B	405	U
7	B	406	G

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Mol	Chain	Res	Type
7	B	411	G
7	B	412	A
7	B	415	A
7	B	424	G
7	B	436	C
7	B	447	A
7	B	456	C
7	B	457	A
7	B	467	G
7	B	477	A
7	B	481	G
7	B	489	G
7	B	490	C
7	B	491	G
7	B	496	G
7	B	505	A
7	B	508	A
7	B	509	C
7	B	512	G
7	B	529	A
7	B	531	C
7	B	532	A
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	577	G
7	B	613	A
7	B	622	G
7	B	637	A
7	B	640	C
7	B	645	C
7	B	646	U
7	B	651	G
7	B	652	U
7	B	654	A

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Mol	Chain	Res	Type
7	B	655	A
7	B	669	G
7	B	670	A
7	B	671	C
7	B	685	A
7	B	686	U
7	B	704	G
7	B	711	G
7	B	713	G
7	B	718	A
7	B	719	C
7	B	726	G
7	B	730	A
7	B	738	G
7	B	740	C
7	B	745	G
7	B	747	U
7	B	757	G
7	B	762	U
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	788	A
7	B	789	A
7	B	791	C
7	B	792	A
7	B	802	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	829	A
7	B	846	U
7	B	847	U
7	B	850	U
7	B	851	C

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Mol	Chain	Res	Type
7	B	859	G
7	B	869	G
7	B	871	U
7	B	872	U
7	B	880	G
7	B	886	A
7	B	887	U
7	B	888	C
7	B	889	C
7	B	890	C
7	B	891	G
7	B	892	A
7	B	893	C
7	B	894	U
7	B	896	A
7	B	897	C
7	B	898	C
7	B	907	G
7	B	910	A
7	B	912	C
7	B	919	U
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	953	G
7	B	961	C
7	B	974	G
7	B	975	A
7	B	980	A
7	B	983	A
7	B	989	G
7	B	991	C
7	B	996	A
7	B	1009	A
7	B	1012	U
7	B	1013	C
7	B	1022	G
7	B	1023	U

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Mol	Chain	Res	Type
7	B	1026	G
7	B	1033	U
7	B	1040	A
7	B	1042	G
7	B	1045	C
7	B	1046	A
7	B	1051	G
7	B	1054	A
7	B	1056	G
7	B	1059	G
7	B	1060	U
7	B	1062	G
7	B	1063	G
7	B	1066	U
7	B	1067	A
7	B	1068	G
7	B	1070	A
7	B	1074	G
7	B	1075	C
7	B	1079	C
7	B	1081	U
7	B	1084	A
7	B	1085	A
7	B	1088	A
7	B	1089	A
7	B	1092	C
7	B	1096	A
7	B	1098	A
7	B	1101	U
7	B	1104	C
7	B	1106	G
7	B	1107	G
7	B	1110	G
7	B	1111	A
7	B	1112	G
7	B	1130	U
7	B	1132	U
7	B	1133	A
7	B	1134	A
7	B	1135	C
7	B	1139	G
7	B	1142	A

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Mol	Chain	Res	Type
7	B	1155	A
7	B	1157	G
7	B	1173	U
7	B	1175	A
7	B	1176	U
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	1242	U
7	B	1244	A
7	B	1247	A
7	B	1248	G
7	B	1250	G
7	B	1253	A
7	B	1256	G
7	B	1266	G
7	B	1271	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	1321	A
7	B	1324	G
7	B	1325	U
7	B	1329	U
7	B	1332	G
7	B	1337	G
7	B	1340	U
7	B	1352	U
7	B	1360	G
7	B	1365	A
7	B	1368	G
7	B	1374	G
7	B	1378	A
7	B	1379	U

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Mol	Chain	Res	Type
7	B	1382	G
7	B	1383	A
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	1435	G
7	B	1451	C
7	B	1452	G
7	B	1458	U
7	B	1459	G
7	B	1460	U
7	B	1469	A
7	B	1476	U
7	B	1477	A
7	B	1478	G
7	B	1482	G
7	B	1491	G
7	B	1494	A
7	B	1523	U
7	B	1524	G
7	B	1529	G
7	B	1532	A
7	B	1535	A
7	B	1536	C
7	B	1538	G
7	B	1545	A
7	B	1552	A
7	B	1554	U
7	B	1558	C
7	B	1560	G
7	B	1566	A
7	B	1569	A
7	B	1578	U
7	B	1584	U
7	B	1585	C
7	B	1607	C
7	B	1608	A

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Mol	Chain	Res	Type
7	B	1610	A
7	B	1616	A
7	B	1626	A
7	B	1634	A
7	B	1635	A
7	B	1640	A
7	B	1647	U
7	B	1648	U
7	B	1653	G
7	B	1663	G
7	B	1674	G
7	B	1703	G
7	B	1713	A
7	B	1722	A
7	B	1724	G
7	B	1731	G
7	B	1748	C
7	B	1756	G
7	B	1758	U
7	B	1763	G
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	1788	C
7	B	1792	G
7	B	1800	C
7	B	1801	A
7	B	1802	A
7	B	1808	A
7	B	1810	A
7	B	1811	G
7	B	1816	C
7	B	1829	A
7	B	1862	G
7	B	1866	A
7	B	1870	C
7	B	1871	A

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Mol	Chain	Res	Type
7	B	1876	A
7	B	1884	G
7	B	1896	G
7	B	1899	A
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	1927	A
7	B	1929	G
7	B	1930	G
7	B	1937	A
7	B	1938	A
7	B	1940	U
7	B	1941	C
7	B	1943	U
7	B	1955	U
7	B	1965	C
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	1993	U
7	B	1996	C
7	B	1997	C
7	B	2020	A
7	B	2023	C
7	B	2031	A
7	B	2033	A
7	B	2035	G
7	B	2036	C
7	B	2043	C
7	B	2052	A
7	B	2055	C
7	B	2056	G
7	B	2060	A
7	B	2061	G
7	B	2069	G

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Mol	Chain	Res	Type
7	B	2076	U
7	B	2077	A
7	B	2093	G
7	B	2099	U
7	B	2100	G
7	B	2101	A
7	B	2110	G
7	B	2111	U
7	B	2113	U
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	2126	A
7	B	2127	G
7	B	2128	G
7	B	2129	C
7	B	2132	U
7	B	2134	A
7	B	2138	G
7	B	2140	G
7	B	2145	C
7	B	2147	A
7	B	2148	G
7	B	2150	C
7	B	2156	G
7	B	2158	A
7	B	2160	C
7	B	2161	C
7	B	2162	G
7	B	2163	A
7	B	2164	C
7	B	2166	U
7	B	2169	A
7	B	2171	A
7	B	2172	U
7	B	2173	A
7	B	2176	A
7	B	2179	C
7	B	2183	A

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Mol	Chain	Res	Type
7	B	2184	A
7	B	2187	U
7	B	2191	A
7	B	2192	U
7	B	2198	A
7	B	2199	A
7	B	2204	G
7	B	2210	U
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	2269	G
7	B	2279	G
7	B	2280	G
7	B	2283	C
7	B	2287	A
7	B	2288	A
7	B	2303	G
7	B	2304	G
7	B	2305	U
7	B	2306	C
7	B	2307	G
7	B	2308	G
7	B	2320	U
7	B	2321	U
7	B	2322	A
7	B	2325	G
7	B	2331	G
7	B	2333	A
7	B	2336	A
7	B	2345	G
7	B	2347	C
7	B	2350	C
7	B	2354	C
7	B	2357	G
7	B	2361	G

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Mol	Chain	Res	Type
7	B	2372	U
7	B	2379	G
7	B	2383	G
7	B	2385	C
7	B	2391	G
7	B	2402	U
7	B	2403	C
7	B	2407	A
7	B	2422	C
7	B	2423	U
7	B	2425	A
7	B	2426	A
7	B	2428	G
7	B	2429	G
7	B	2430	A
7	B	2435	A
7	B	2440	C
7	B	2441	U
7	B	2447	G
7	B	2448	A
7	B	2471	A
7	B	2472	G
7	B	2474	U
7	B	2476	A
7	B	2481	G
7	B	2491	U
7	B	2494	G
7	B	2498	C
7	B	2502	G
7	B	2503	A
7	B	2505	G
7	B	2518	A
7	B	2520	C
7	B	2529	G
7	B	2535	G
7	B	2547	A
7	B	2554	U
7	B	2564	A
7	B	2566	A
7	B	2567	G
7	B	2569	G
7	B	2572	A

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Mol	Chain	Res	Type
7	B	2573	C
7	B	2582	G
7	B	2602	A
7	B	2603	G
7	B	2609	U
7	B	2613	U
7	B	2615	U
7	B	2629	U
7	B	2630	G
7	B	2634	A
7	B	2646	C
7	B	2673	G
7	B	2684	U
7	B	2689	U
7	B	2690	U
7	B	2712	C
7	B	2714	G
7	B	2718	G
7	B	2725	A
7	B	2726	A
7	B	2733	A
7	B	2739	U
7	B	2744	G
7	B	2748	A
7	B	2765	A
7	B	2776	A
7	B	2778	A
7	B	2791	G
7	B	2796	U
7	B	2797	U
7	B	2798	U
7	B	2800	A
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	2845	U
7	B	2846	G

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Mol	Chain	Res	Type
7	B	2849	U
7	B	2850	A
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	2884	U
7	B	2885	G
7	B	2886	A
7	B	2902	C
51	v	3	A
51	v	4	U
51	v	7	A
51	v	9	G
51	v	22	G
51	v	31	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	79	G
51	v	83	C
51	v	84	U
51	v	85	U
51	v	86	G
51	v	87	C
51	v	89	U
51	v	91	U
51	v	92	U
51	v	95	C
51	v	110	C
51	v	116	A
51	v	119	A
51	v	120	A

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Mol	Chain	Res	Type
51	v	121	U
51	v	122	G
51	v	130	A
51	v	131	A
51	v	141	G
51	v	159	G
51	v	163	C
51	v	173	U
51	v	182	A
51	v	183	C
51	v	190	A
51	v	195	A
51	v	197	A
51	v	202	G
51	v	203	G
51	v	204	G
51	v	207	C
51	v	209	U
51	v	210	C
51	v	211	G
51	v	212	G
51	v	214	C
51	v	226	G
51	v	231	U
51	v	240	G
51	v	247	G
51	v	251	G
51	v	266	G
51	v	267	C
51	v	276	G
51	v	281	G
51	v	283	U
51	v	289	G
51	v	305	G
51	v	321	A
51	v	327	A
51	v	328	C
51	v	329	A
51	v	330	C
51	v	332	G
51	v	340	U
51	v	345	C

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Mol	Chain	Res	Type
51	v	347	G
51	v	351	G
51	v	352	C
51	v	354	G
51	v	367	U
51	v	372	C
51	v	378	G
51	v	388	G
51	v	392	C
51	v	398	U
51	v	406	G
51	v	412	A
51	v	413	G
51	v	421	U
51	v	422	C
51	v	424	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	463	U
51	v	465	A
51	v	467	U
51	v	468	A
51	v	469	C
51	v	470	C
51	v	471	U
51	v	474	G
51	v	478	A
51	v	481	G
51	v	484	G
51	v	486	U
51	v	495	A
51	v	496	A
51	v	497	G
51	v	499	A
51	v	509	A
51	v	511	C
51	v	512	U
51	v	518	C

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Mol	Chain	Res	Type
51	v	521	G
51	v	524	G
51	v	527	G
51	v	530	G
51	v	531	U
51	v	532	A
51	v	547	A
51	v	560	A
51	v	564	C
51	v	568	G
51	v	572	A
51	v	573	A
51	v	574	A
51	v	576	C
51	v	577	G
51	v	596	A
51	v	618	C
51	v	633	G
51	v	641	U
51	v	642	A
51	v	650	G
51	v	653	U
51	v	665	A
51	v	687	A
51	v	695	A
51	v	702	A
51	v	703	G
51	v	704	A
51	v	721	G
51	v	723	U
51	v	731	G
51	v	755	G
51	v	778	G
51	v	781	A
51	v	793	U
51	v	794	A
51	v	814	A
51	v	815	A
51	v	817	C
51	v	821	G
51	v	828	U
51	v	829	G

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Mol	Chain	Res	Type
51	v	832	G
51	v	836	G
51	v	843	U
51	v	846	G
51	v	851	G
51	v	864	A
51	v	872	A
51	v	873	A
51	v	889	A
51	v	914	A
51	v	926	G
51	v	927	G
51	v	934	C
51	v	935	A
51	v	942	G
51	v	954	G
51	v	960	U
51	v	961	U
51	v	966	G
51	v	969	A
51	v	970	C
51	v	974	A
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	990	C
51	v	991	U
51	v	992	U
51	v	993	G
51	v	994	A
51	v	1002	G
51	v	1004	A
51	v	1008	U
51	v	1014	A
51	v	1027	C
51	v	1028	C
51	v	1031	C
51	v	1032	G
51	v	1033	G

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Mol	Chain	Res	Type
51	v	1034	G
51	v	1035	A
51	v	1040	U
51	v	1044	A
51	v	1045	C
51	v	1053	G
51	v	1054	C
51	v	1065	U
51	v	1070	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	1118	U
51	v	1124	G
51	v	1125	U
51	v	1127	G
51	v	1132	C
51	v	1133	G
51	v	1136	C
51	v	1137	C
51	v	1138	G
51	v	1141	C
51	v	1142	G
51	v	1145	A
51	v	1151	A
51	v	1152	A
51	v	1154	G
51	v	1158	C
51	v	1159	U
51	v	1160	G
51	v	1161	C
51	v	1167	A
51	v	1168	U
51	v	1181	G
51	v	1183	U
51	v	1184	G
51	v	1190	G

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Mol	Chain	Res	Type
51	v	1196	A
51	v	1197	A
51	v	1201	A
51	v	1202	U
51	v	1211	U
51	v	1213	A
51	v	1214	C
51	v	1218	C
51	v	1220	G
51	v	1227	A
51	v	1238	A
51	v	1239	A
51	v	1240	U
51	v	1241	G
51	v	1258	G
51	v	1260	G
51	v	1268	G
51	v	1272	G
51	v	1273	C
51	v	1274	A
51	v	1275	A
51	v	1278	G
51	v	1279	G
51	v	1280	A
51	v	1285	A
51	v	1287	A
51	v	1293	C
51	v	1298	U
51	v	1299	A
51	v	1300	G
51	v	1301	U
51	v	1302	C
51	v	1303	C
51	v	1305	G
51	v	1317	C
51	v	1322	C
51	v	1336	C
51	v	1337	G
51	v	1346	A
51	v	1348	U
51	v	1360	A
51	v	1363	A

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Mol	Chain	Res	Type
51	v	1370	G
51	v	1378	C
51	v	1381	U
51	v	1394	A
51	v	1397	C
51	v	1398	A
51	v	1399	C
51	v	1404	C
51	v	1407	C
51	v	1408	A
51	v	1409	C
51	v	1410	A
51	v	1411	C
51	v	1419	G
51	v	1429	A
51	v	1432	G
51	v	1441	A
51	v	1443	C
51	v	1444	U
51	v	1446	A
51	v	1451	U
51	v	1452	C
51	v	1487	G
51	v	1492	A
51	v	1493	A
51	v	1494	G
51	v	1497	G
51	v	1499	A
51	v	1505	G
51	v	1506	U
51	v	1517	G
51	v	1529	G
51	v	1530	G
51	v	1531	A
51	v	1533	C
51	v	1534	A
51	v	1535	C
51	v	1539	C

All (8) RNA pucker outliers are listed below:

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Mol	Chain	Res	Type
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Mol	Chain	Res	Type
6	A	66	A
7	B	490	C
7	B	669	G
7	B	670	A
7	B	827	U
7	B	1652	A
7	B	2147	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 [i](#)

There are no chain breaks in this entry.

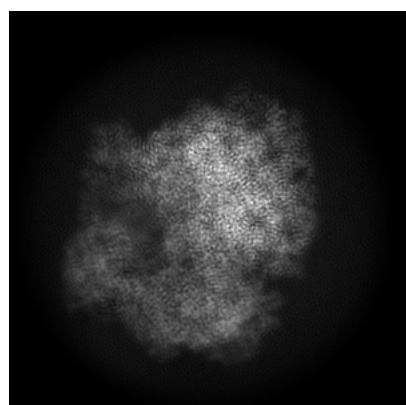
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-29681. These allow visual inspection of the internal detail of the map and identification of artifacts.

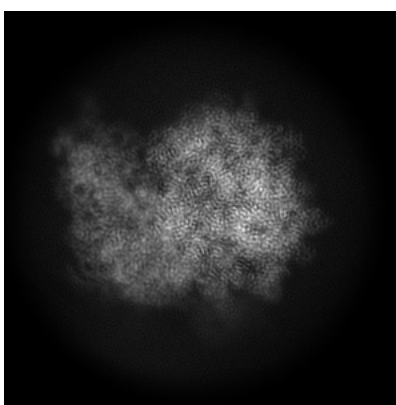
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

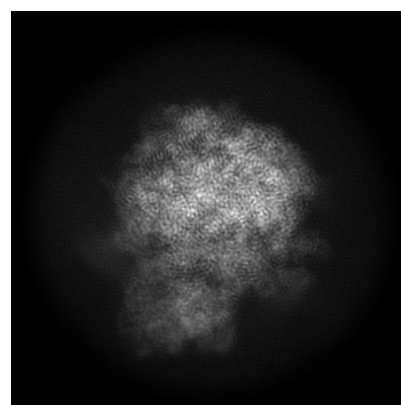
6.1.1 Primary map



X



Y

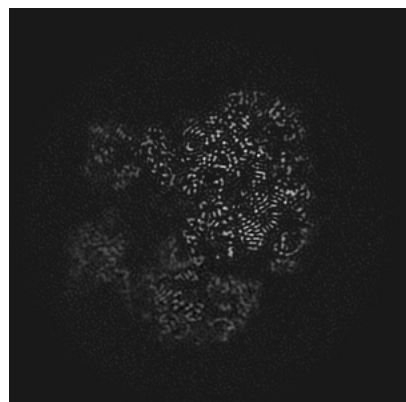


Z

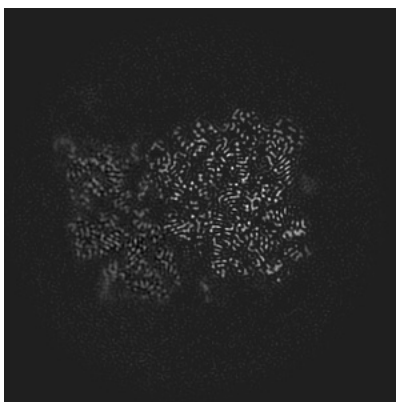
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

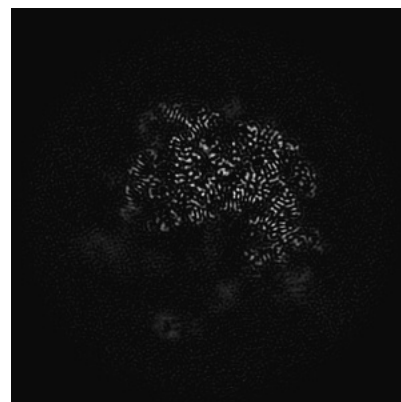
6.2.1 Primary map



X Index: 170



Y Index: 170

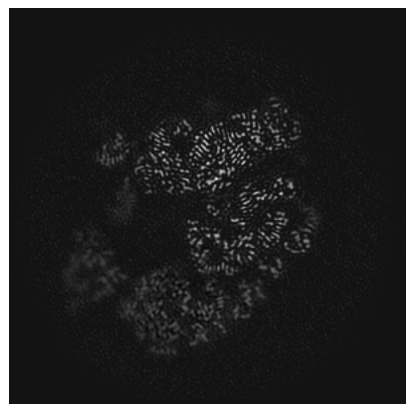


Z Index: 170

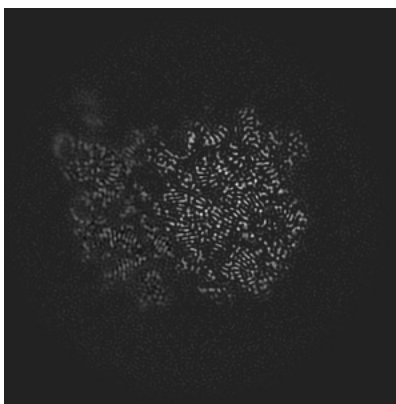
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

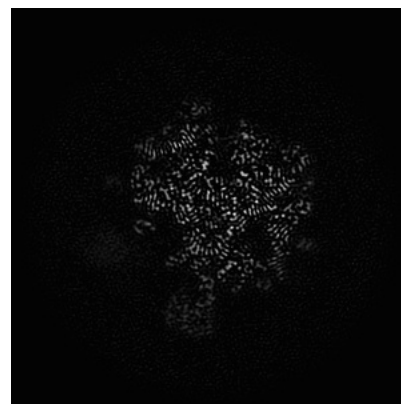
6.3.1 Primary map



X Index: 182



Y Index: 178

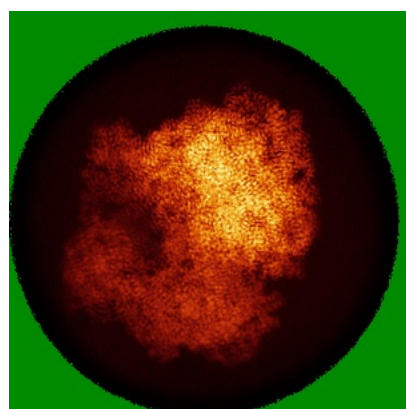


Z Index: 198

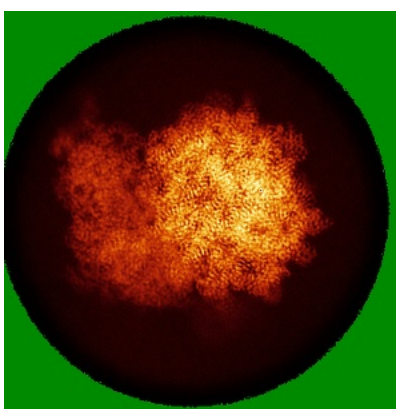
The images above show the largest variance slices of the map in three orthogonal directions.

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

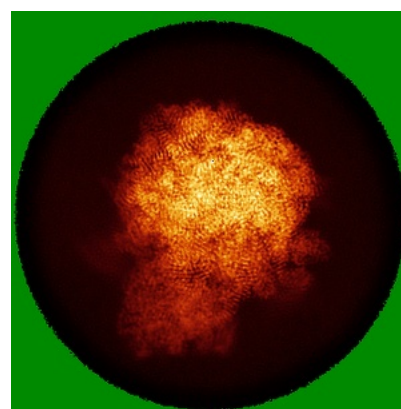
6.4.1 Primary map



X



Y

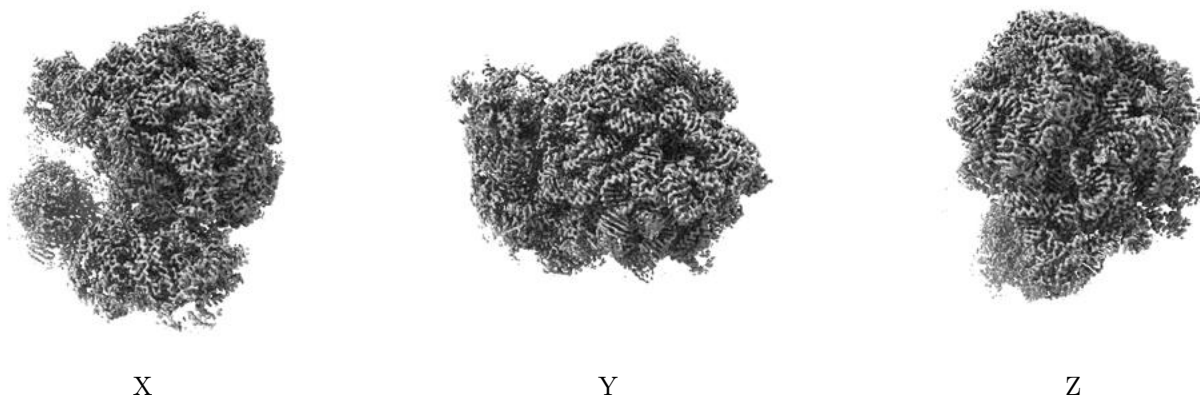


Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.193. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

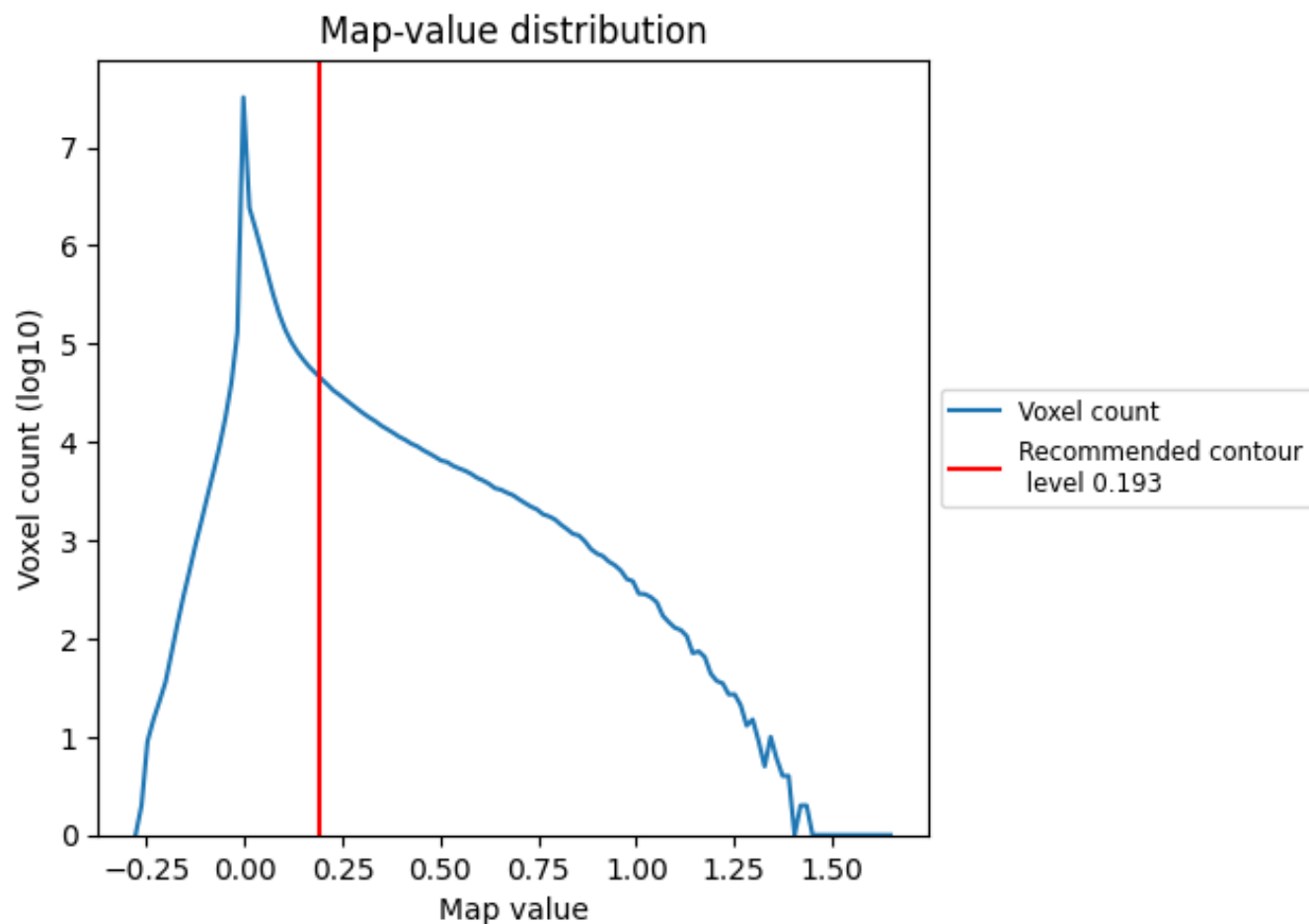
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

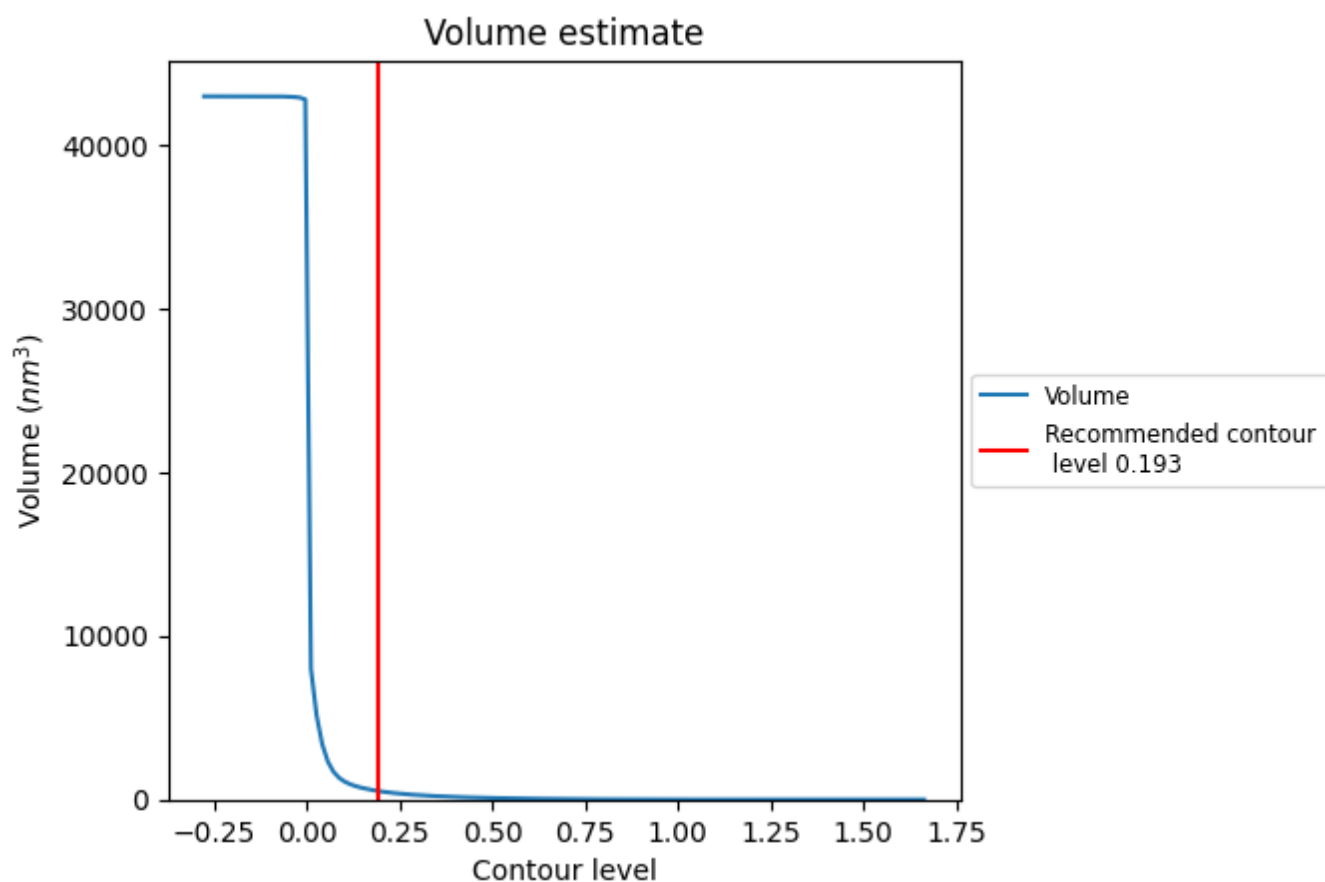
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

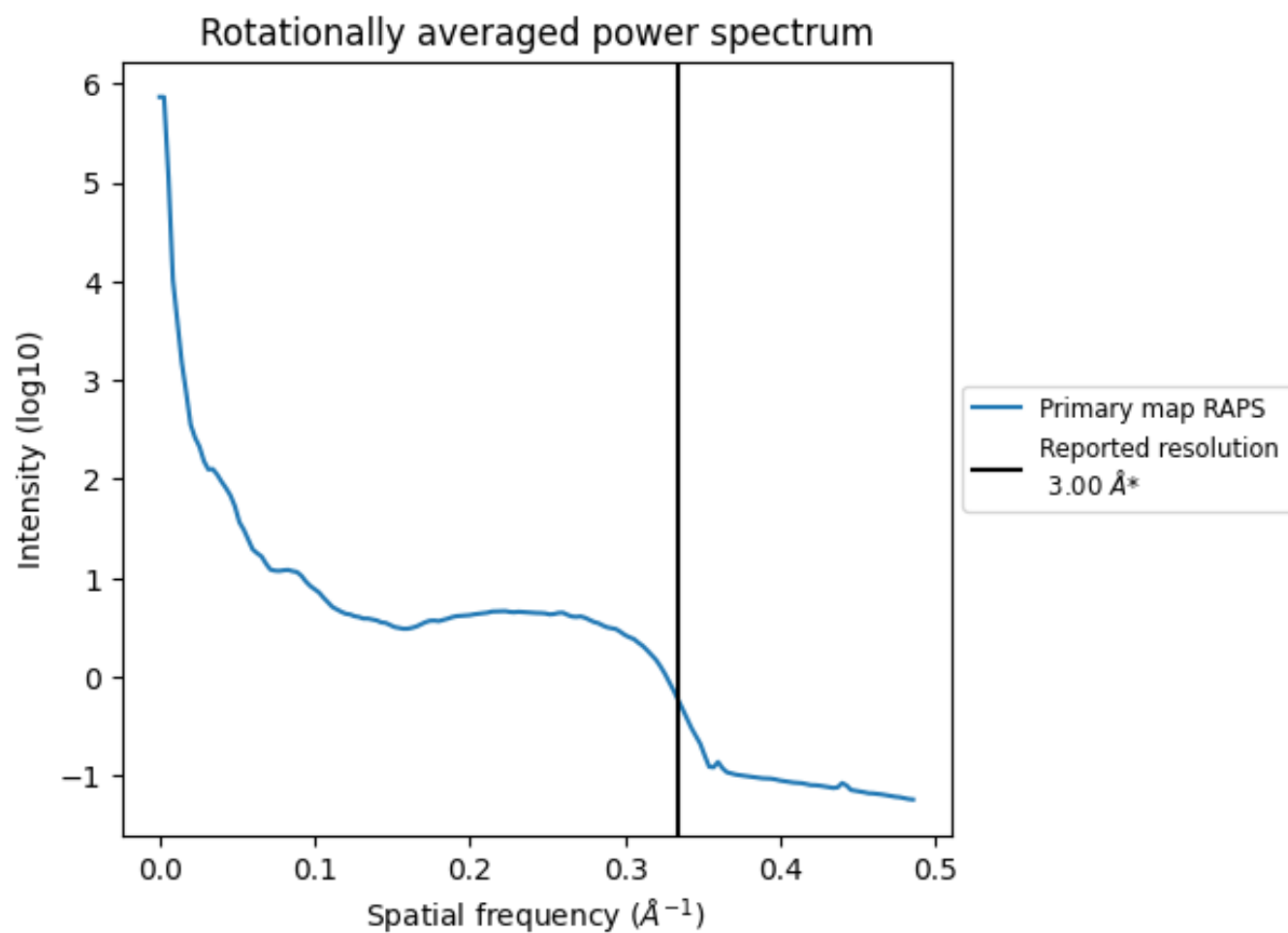
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 519 nm³; this corresponds to an approximate mass of 469 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 0.333 Å⁻¹

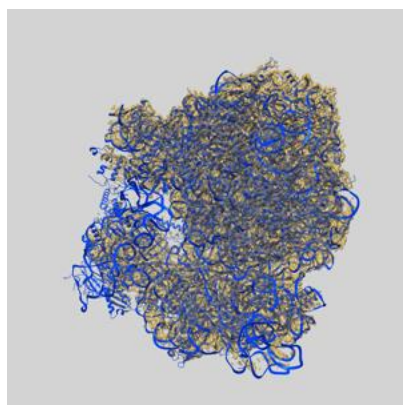
8 Fourier-Shell correlation ⓘ

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

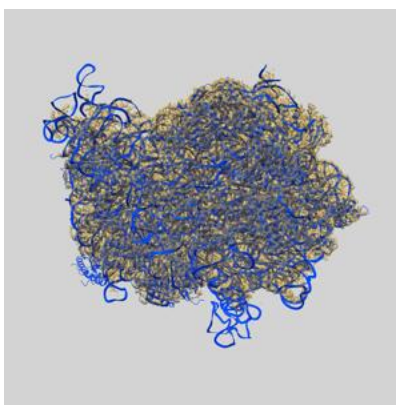
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-29681 and PDB model 8G2U. Per-residue inclusion information can be found in section 3 on page 13.

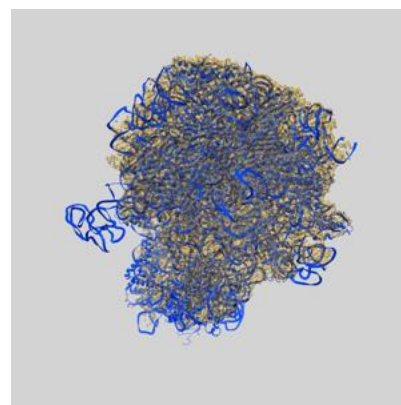
9.1 Map-model overlay [i](#)



X



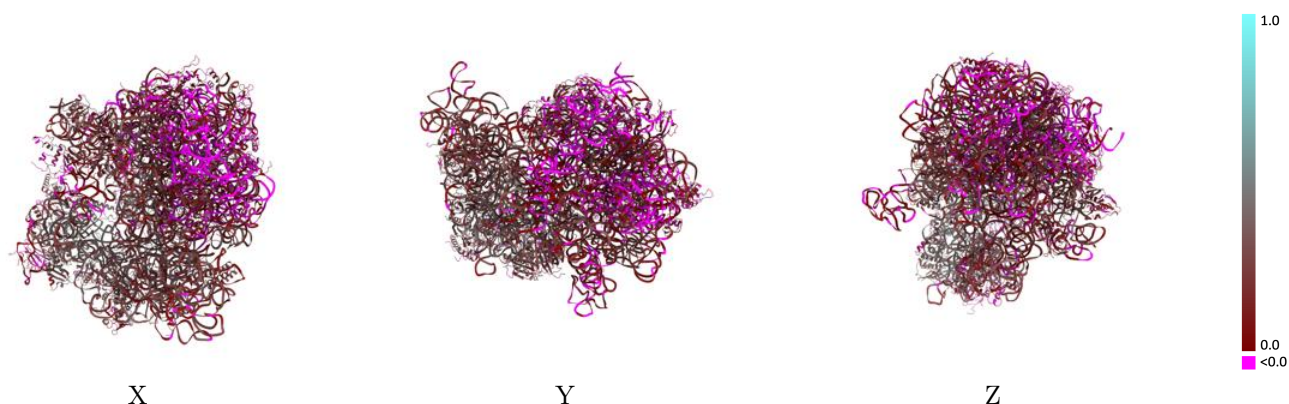
Y



Z

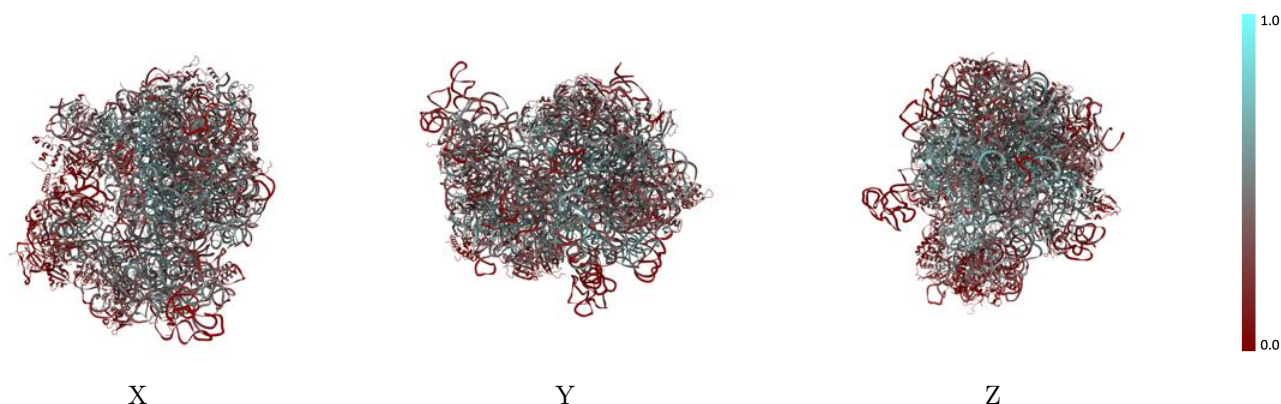
The images above show the 3D surface view of the map at the recommended contour level 0.193 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



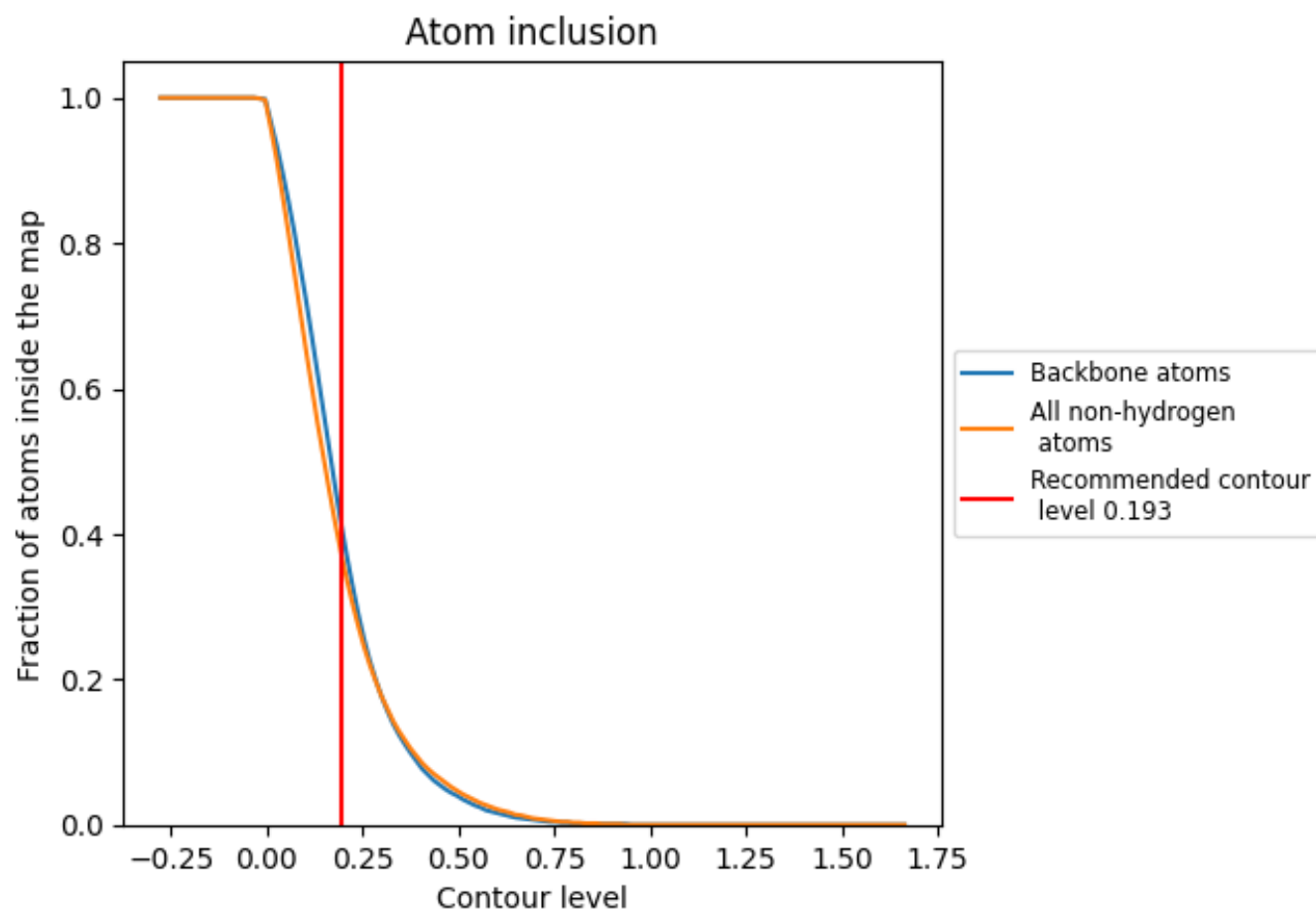
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.193).

9.4 Atom inclusion ⓘ



At the recommended contour level, 42% of all backbone atoms, 38% 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 (0.193) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.3760	 0.1830
0	 0.3600	 0.0450
1	 0.3980	 0.2200
2	 0.4620	 0.1310
3	 0.4810	 0.1670
4	 0.3770	 0.1890
A	 0.4050	 0.2180
B	 0.4310	 0.1250
C	 0.4900	 0.1980
D	 0.3970	 0.1040
E	 0.3030	 0.0600
F	 0.0570	 0.0820
G	 0.1800	 0.1730
J	 0.3760	 0.0960
K	 0.3870	 0.1480
L	 0.3800	 0.1110
M	 0.4050	 0.1880
N	 0.3810	 0.0740
O	 0.3060	 0.2040
P	 0.3550	 0.1330
Q	 0.3770	 0.0530
R	 0.3590	 0.0710
S	 0.3650	 0.0730
T	 0.2640	 0.0410
U	 0.2410	 0.0720
V	 0.3020	 0.1770
W	 0.3950	 0.1350
X	 0.4290	 0.1680
Y	 0.2560	 0.0710
Z	 0.3480	 0.1100
a	 0.0460	 0.2450
b	 0.1860	 0.3160
c	 0.1560	 0.2350
d	 0.3440	 0.3330
e	 0.2160	 0.2580



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Chain	Atom inclusion	Q-score
f	 0.0920	 0.3190
g	 0.3780	 0.3450
h	 0.1690	 0.3410
i	 0.1350	 0.2280
j	 0.2360	 0.2740
k	 0.2390	 0.2630
l	 0.0580	 0.2690
m	 0.1820	 0.2870
n	 0.3230	 0.2740
o	 0.3410	 0.2480
p	 0.1990	 0.2610
q	 0.3410	 0.2970
r	 0.0470	 0.2420
s	 0.2370	 0.2190
t	 0.0340	 0.1430
u	 0.0000	 0.0100
v	 0.3990	 0.2860