



Full wwPDB EM Validation Report ⓘ

Mar 27, 2026 – 02:10 AM UTC

PDB ID : 7NSP / pdb_00007nsp
EMDB ID : EMD-12574
Title : Structure of ErmDL-Erythromycin-stalled 70S E. coli ribosomal complex with A and P-tRNA
Authors : Beckert, B.; Wilson, D.N.
Deposited on : 2021-03-08
Resolution : 3.50 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:

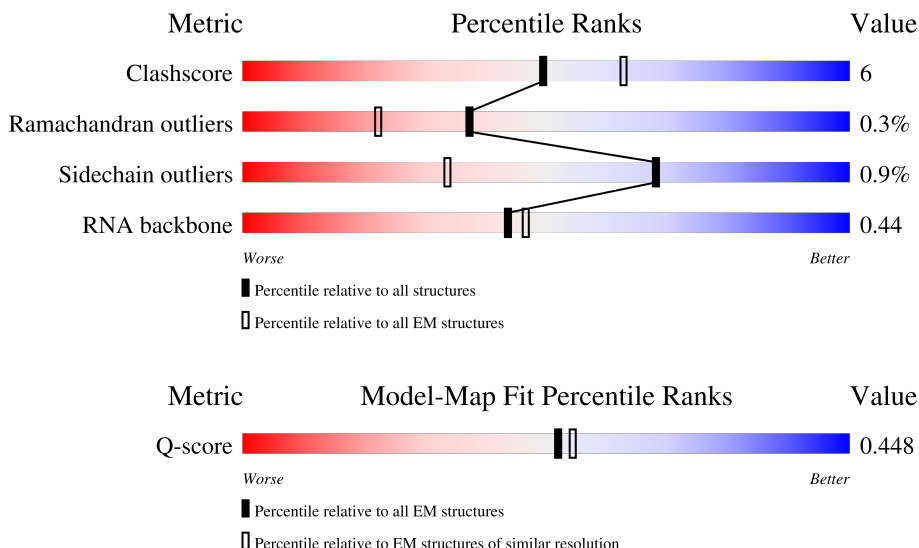
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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

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

The reported resolution of this entry is 3.50 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	13950 (3.00 - 4.00)

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

Mol	Chain	Length	Quality of chain
1	A	2903	14% 63% 33% .
2	B	120	15% 51% 48% .
3	C	271	27% 82% 18%

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Mol	Chain	Length	Quality of chain
4	D	209	
5	E	201	
6	F	177	
7	G	174	
8	H	149	
9	J	142	
10	K	122	
11	L	144	
12	M	136	
13	N	118	
14	O	116	
15	P	114	
16	Q	117	
17	R	103	
18	S	110	
19	T	89	
20	U	102	
21	V	94	
22	W	75	
23	X	77	
24	Y	63	
25	Z	58	
26	0	55	
27	1	50	
28	2	46	

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Mol	Chain	Length	Quality of chain
29	3	64	
30	4	38	
31	5	65	
32	6	6	
33	7	7	
34	8	87	
35	a	1540	
36	b	224	
37	c	206	
38	d	205	
39	e	157	
40	f	99	
41	g	151	
42	h	129	
43	i	127	
44	j	98	
45	k	117	
46	l	123	
47	m	114	
48	n	100	
49	o	88	
50	p	82	
51	q	80	
52	r	66	
53	s	83	

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Mol	Chain	Length	Quality of chain
54	t	86	56%
			87%13%
55	u	70	99%
			86%14%
56	v	77	92%
			34%49%17%

2 Entry composition

There are 57 unique types of molecules in this entry. The entry contains 146148 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a RNA chain called 23S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	2903	Total	C	N	O	P	0	0
			62320	27801	11467	20149	2903		

- Molecule 2 is a RNA chain called 5S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	120	Total	C	N	O	P	0	0
			2570	1144	468	838	120		

- Molecule 3 is a protein called 50S ribosomal protein L2.

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

- Molecule 4 is a protein called 50S ribosomal protein L3.

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

- Molecule 5 is a protein called 50S ribosomal protein L4.

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

- Molecule 6 is a protein called 50S ribosomal protein L5.

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

- Molecule 7 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	174	Total	C	N	O	S	0	0
			1304	820	239	243	2		

- Molecule 8 is a protein called 50S ribosomal protein L9.

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

- Molecule 9 is a protein called 50S ribosomal protein L13.

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

- Molecule 10 is a protein called 50S ribosomal protein L14.

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

- Molecule 11 is a protein called 50S ribosomal protein L15.

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

- Molecule 12 is a protein called 50S ribosomal protein L16.

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

- Molecule 13 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	N	118	Total	C	N	O	S	0	0
			945	585	194	161	5		

- Molecule 14 is a protein called 50S ribosomal protein L18.

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

- Molecule 15 is a protein called 50S ribosomal protein L19.

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

- Molecule 16 is a protein called 50S ribosomal protein L20.

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

- Molecule 17 is a protein called 50S ribosomal protein L21.

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

- Molecule 18 is a protein called 50S ribosomal protein L22.

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

- Molecule 19 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	T	89	Total	C	N	O	S	0	0
			709	449	133	125	2		

- Molecule 20 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms				AltConf	Trace
20	U	102	Total	C	N	O	0	0
			779	492	146	141		

- Molecule 21 is a protein called 50S ribosomal protein L25.

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

- Molecule 22 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	W	75	Total	C	N	O	S	0	0
			575	356	116	102	1		

- Molecule 23 is a protein called 50S ribosomal protein L28.

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

- Molecule 24 is a protein called 50S ribosomal protein L29.

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

- Molecule 25 is a protein called 50S ribosomal protein L30.

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

- Molecule 26 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	0	55	Total	C	N	O	S	0	0
			434	263	92	78	1		

- Molecule 27 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms				AltConf	Trace
27	1	50	Total	C	N	O	0	0
			409	263	75	71		

- Molecule 28 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	2	46	Total	C	N	O	S	0	0
			377	228	90	57	2		

- Molecule 29 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	3	64	Total	C	N	O	S	0	0
			504	323	105	74	2		

- Molecule 30 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	4	38	Total	C	N	O	S	0	0
			302	185	65	48	4		

- Molecule 31 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	5	65	Total	C	N	O	S	0	0
			514	317	98	93	6		

- Molecule 32 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	6	6	Total	C	N	O	P	0	0
			123	55	17	45	6		

- Molecule 33 is a protein called ermDL.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	7	7	Total	C	N	O	S	0	0
			58	35	12	9	2		

- Molecule 34 is a RNA chain called P-tRNA (leu).

Mol	Chain	Residues	Atoms					AltConf	Trace
34	8	87	Total	C	N	O	P	0	0
			1861	829	333	612	87		

- Molecule 35 is a RNA chain called 16S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	a	1540	Total	C	N	O	P	0	0
			33037	14735	6057	10705	1540		

- Molecule 36 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	b	224	Total	C	N	O	S	0	0
			1753	1109	315	321	8		

- Molecule 37 is a protein called 30S ribosomal protein S3.

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

- Molecule 38 is a protein called 30S ribosomal protein S4.

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

- Molecule 39 is a protein called 30S ribosomal protein S5.

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

- Molecule 40 is a protein called 30S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	f	99	Total	C	N	O	S	0	0
			811	512	147	146	6		

- Molecule 41 is a protein called 30S ribosomal protein S7.

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

- Molecule 42 is a protein called 30S ribosomal protein S8.

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

- Molecule 43 is a protein called 30S ribosomal protein S9.

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

- Molecule 44 is a protein called 30S ribosomal protein S10.

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

- Molecule 45 is a protein called 30S ribosomal protein S11.

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

- Molecule 46 is a protein called 30S ribosomal protein S12.

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

- Molecule 47 is a protein called 30S ribosomal protein S13.

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

- Molecule 48 is a protein called 30S ribosomal protein S14.

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

- Molecule 49 is a protein called 30S ribosomal protein S15.

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

- Molecule 50 is a protein called 30S ribosomal protein S16.

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

- Molecule 51 is a protein called 30S ribosomal protein S17.

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

- Molecule 52 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	r	66	Total	C	N	O	S	0	0
			545	344	102	98	1		

- Molecule 53 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	s	83	Total	C	N	O	S	0	0
			663	424	126	111	2		

- Molecule 54 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	t	86	Total	C	N	O	S	0	0
			670	414	138	115	3		

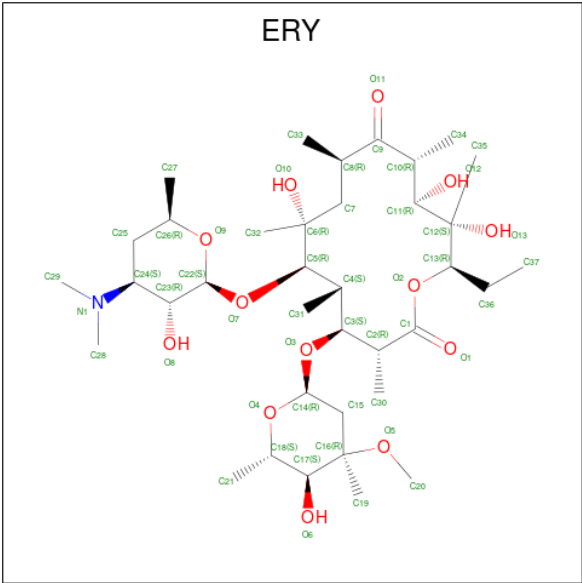
- Molecule 55 is a protein called 30S ribosomal protein S21.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	u	70	Total	C	N	O	S	0	0
			590	366	125	98	1		

- Molecule 56 is a RNA chain called A-tRNA (Arg).

Mol	Chain	Residues	Atoms					AltConf	Trace
56	v	77	Total	C	N	O	P	0	0
			1643	733	297	536	77		

- Molecule 57 is ERYTHROMYCIN A (CCD ID: ERY) (formula: C₃₇H₆₇NO₁₃) (labeled as "Ligand of Interest" by depositor).

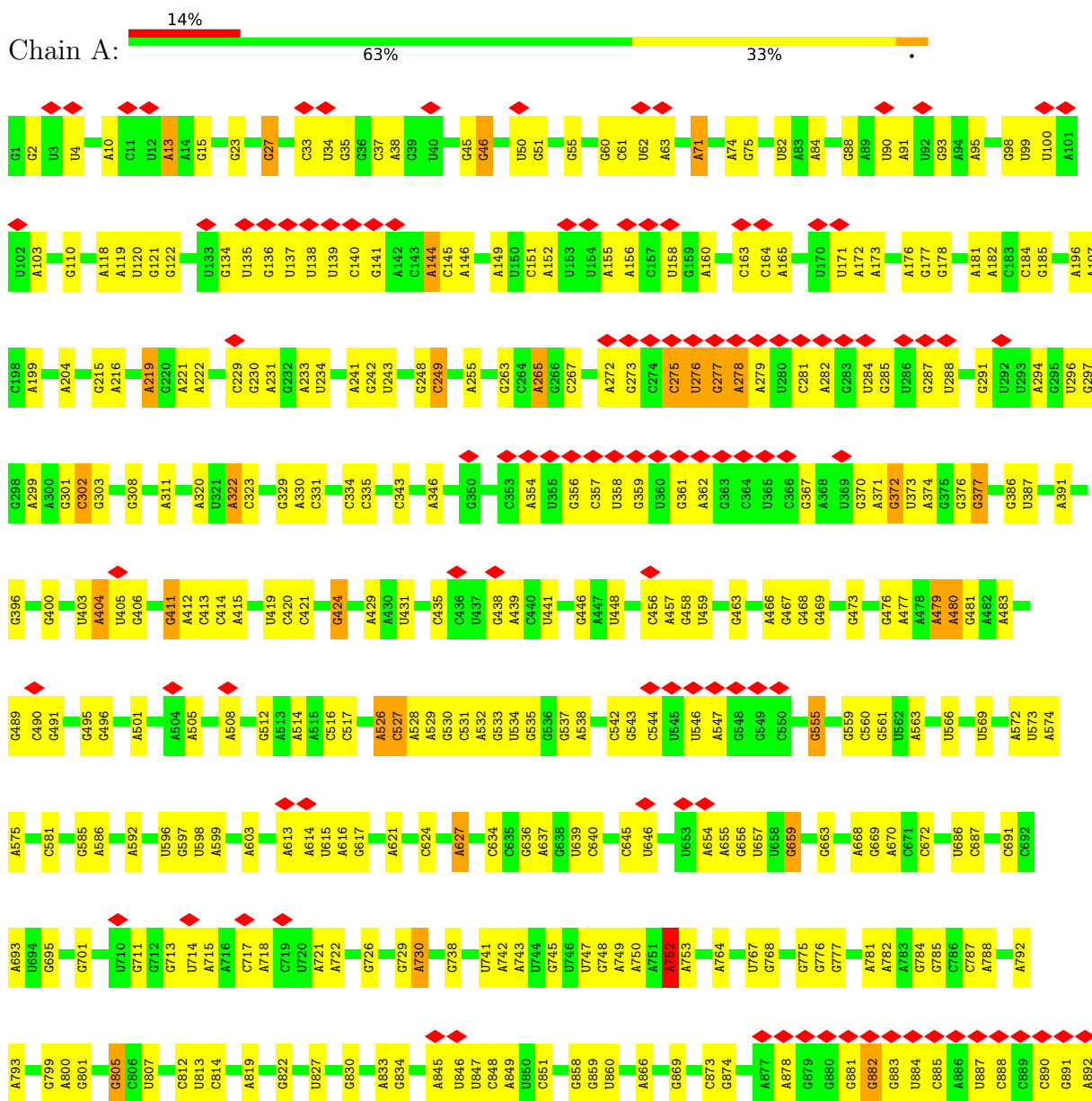


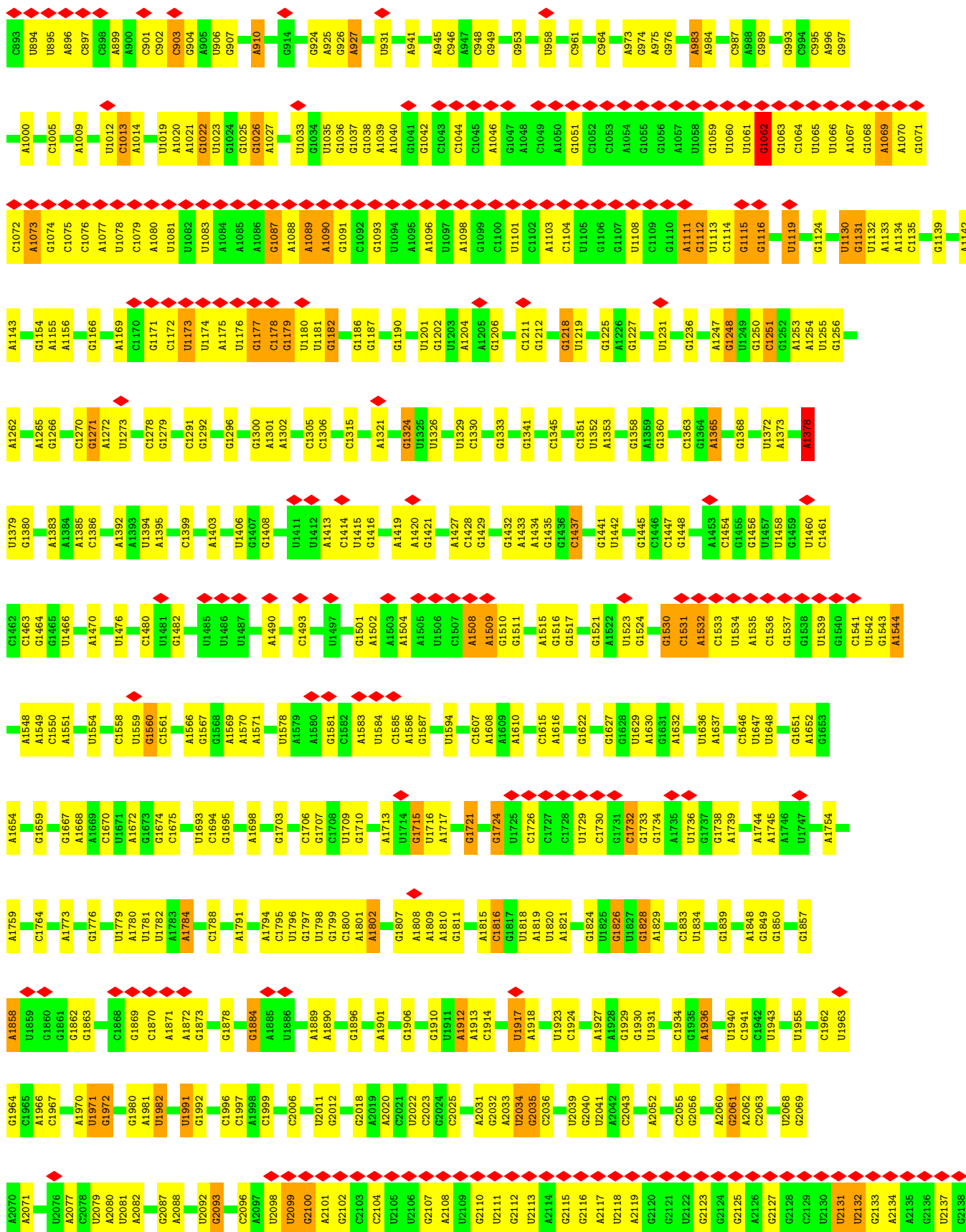
Mol	Chain	Residues	Atoms				AltConf
57	7	1	Total	C	N	O	0
			51	37	1	13	

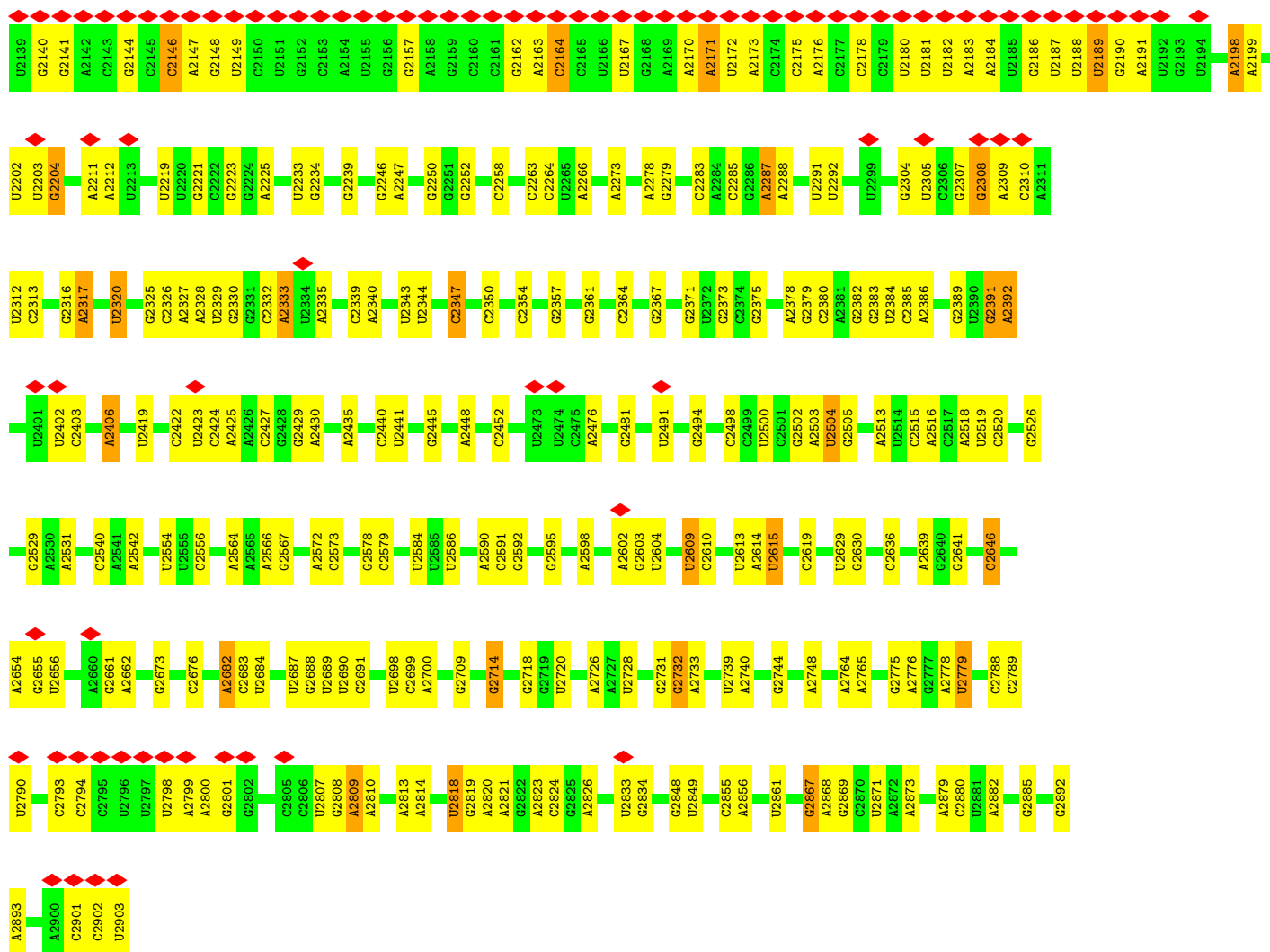
3 Residue-property plots

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

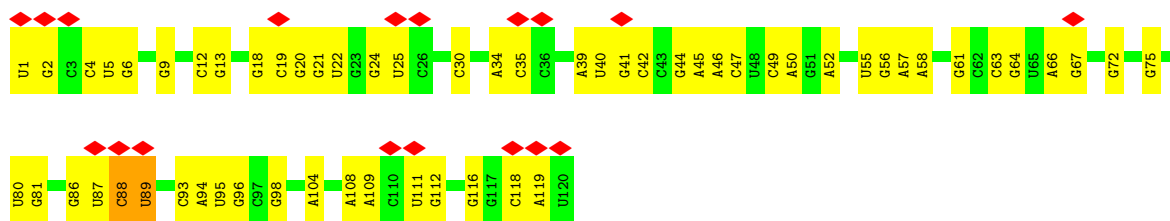
• Molecule 1: 23S rRNA



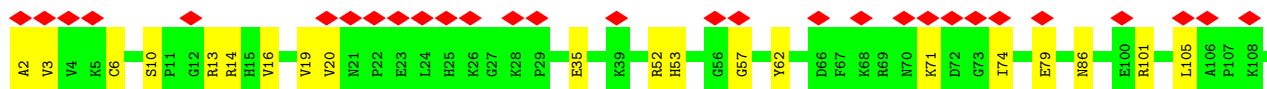
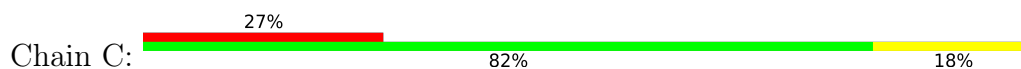


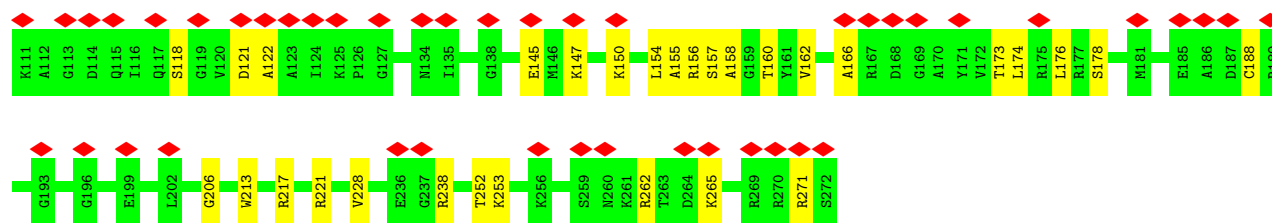


- Molecule 2: 5S rRNA

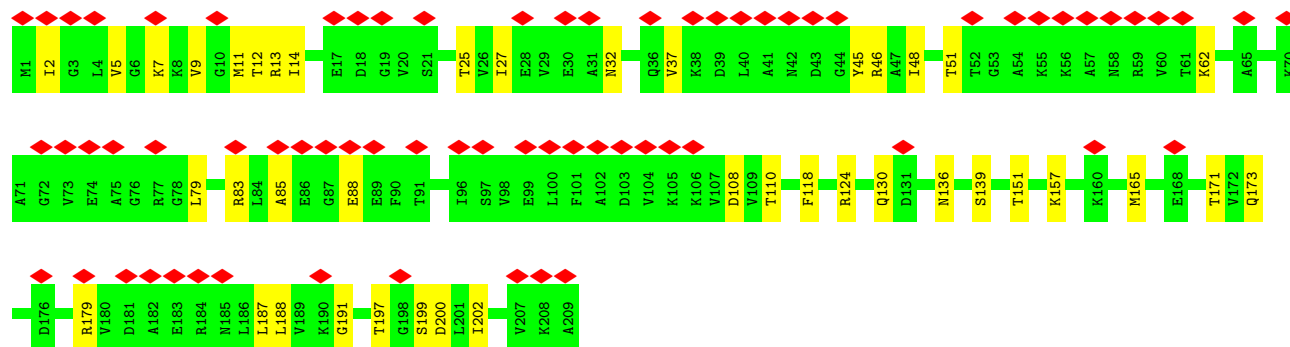
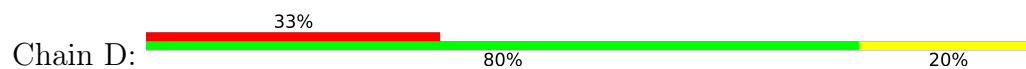


- Molecule 3: 50S ribosomal protein L2

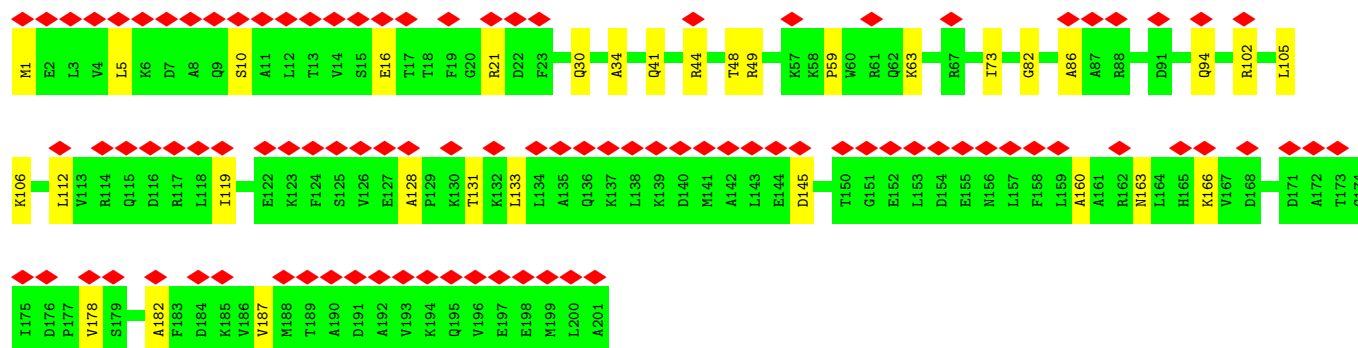
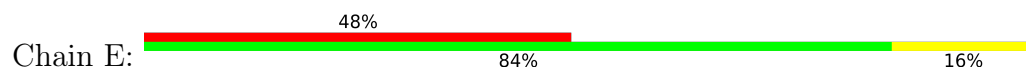




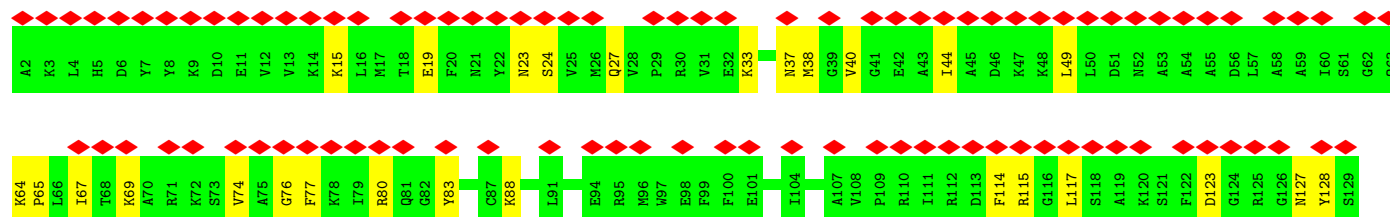
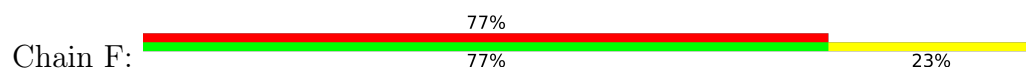
• Molecule 4: 50S ribosomal protein L3



• Molecule 5: 50S ribosomal protein L4

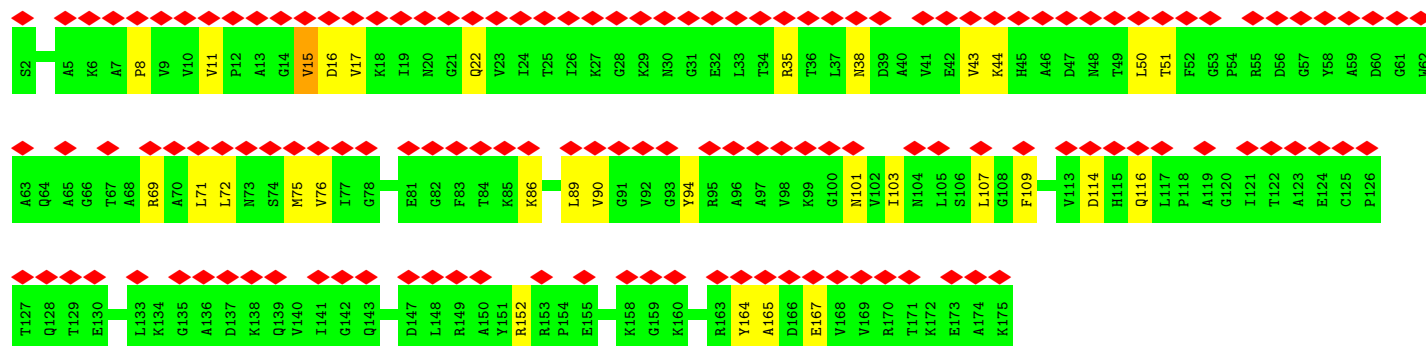
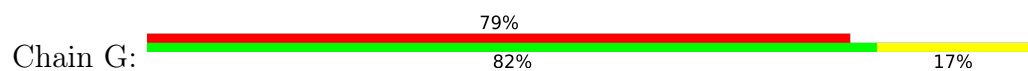


• Molecule 6: 50S ribosomal protein L5

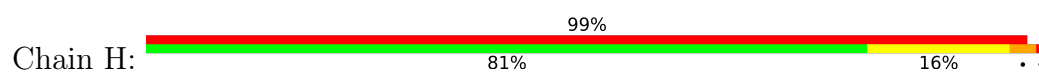




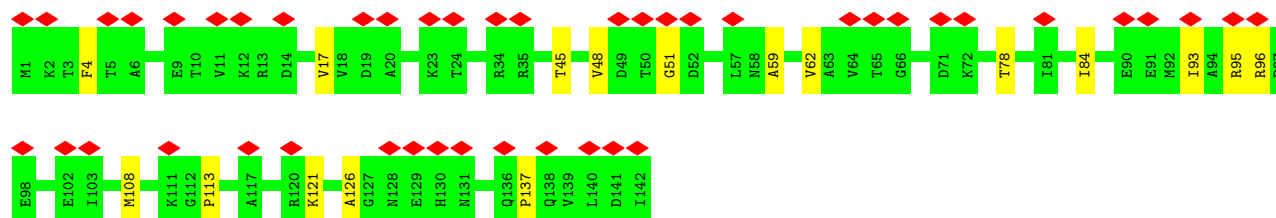
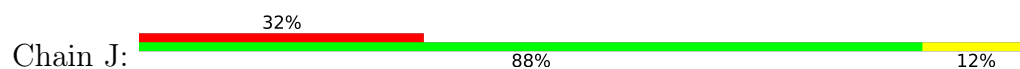
• Molecule 7: 50S ribosomal protein L6



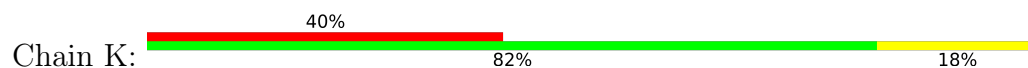
• Molecule 8: 50S ribosomal protein L9

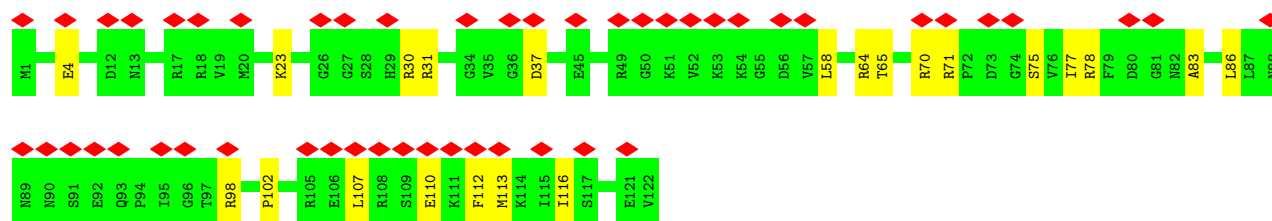


• Molecule 9: 50S ribosomal protein L13

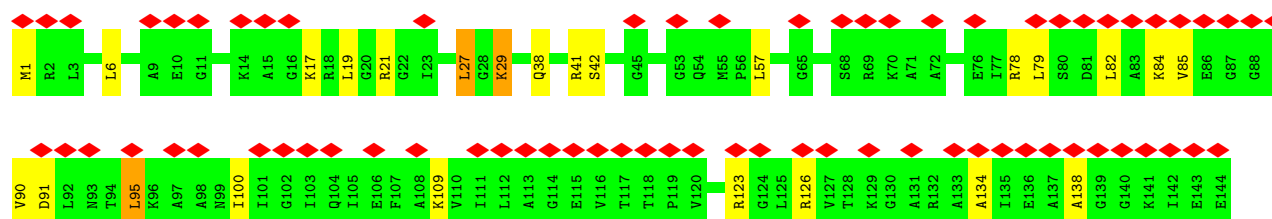
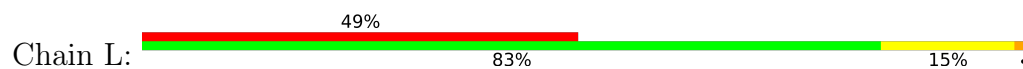


• Molecule 10: 50S ribosomal protein L14

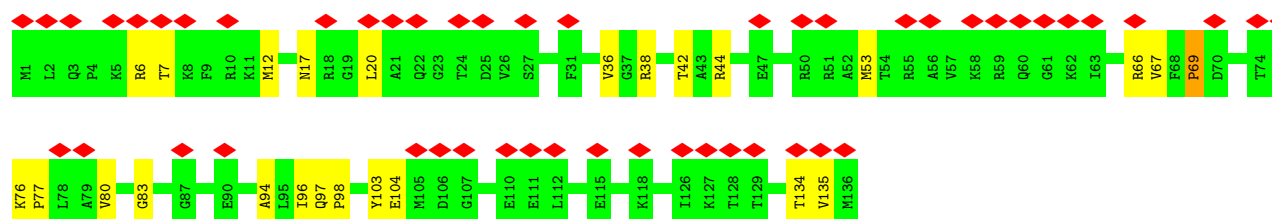
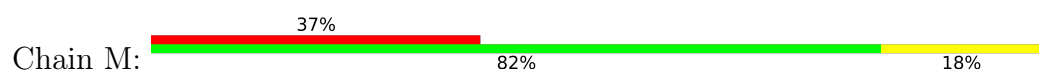




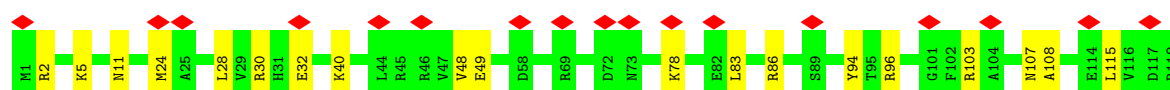
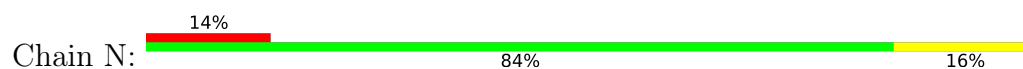
• Molecule 11: 50S ribosomal protein L15



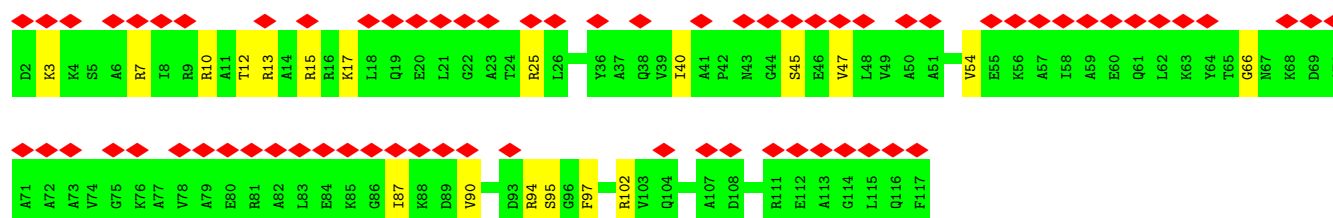
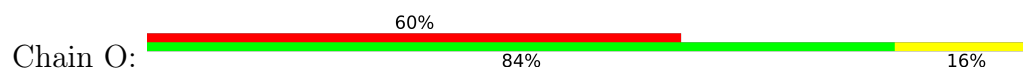
• Molecule 12: 50S ribosomal protein L16



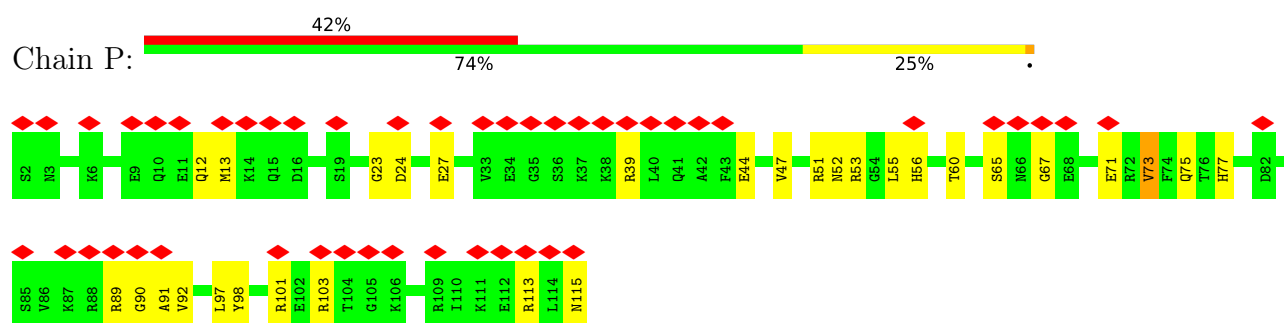
• Molecule 13: 50S ribosomal protein L17



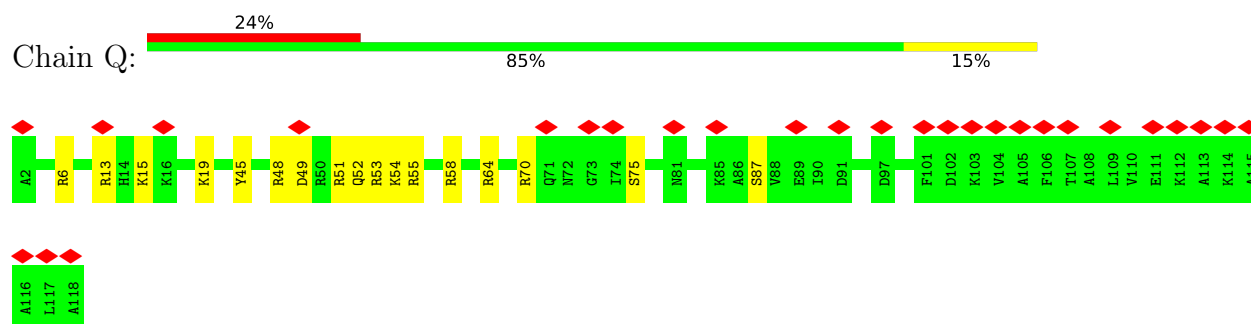
• Molecule 14: 50S ribosomal protein L18



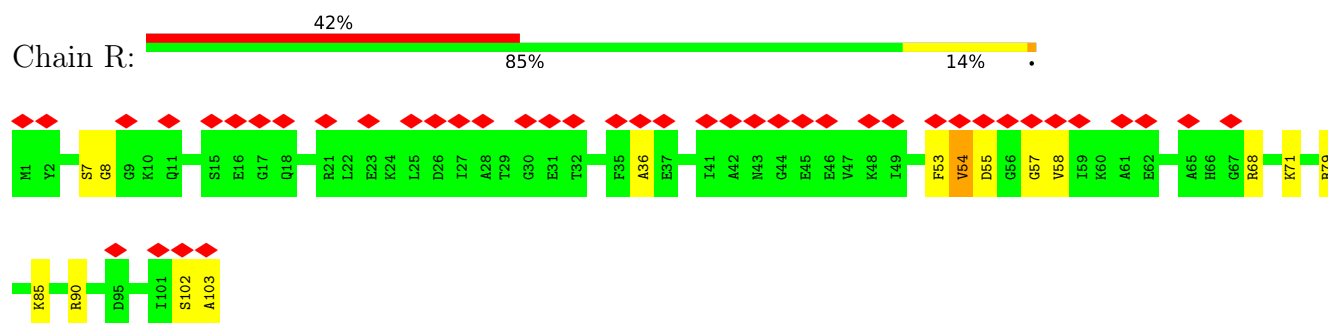
• Molecule 15: 50S ribosomal protein L19



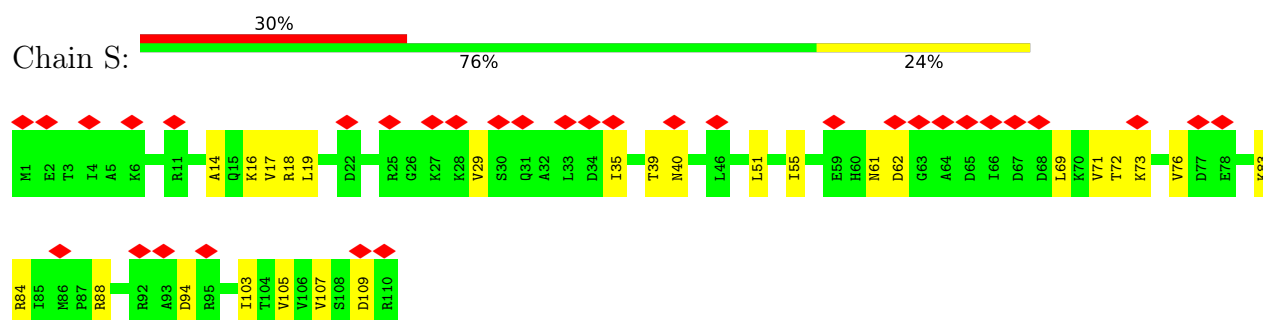
- Molecule 16: 50S ribosomal protein L20



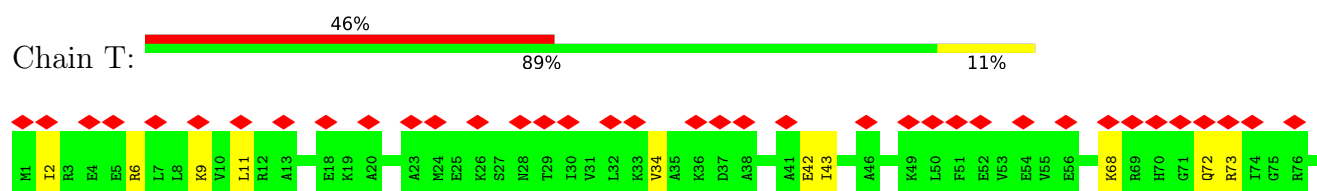
- Molecule 17: 50S ribosomal protein L21

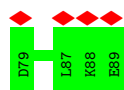


- Molecule 18: 50S ribosomal protein L22

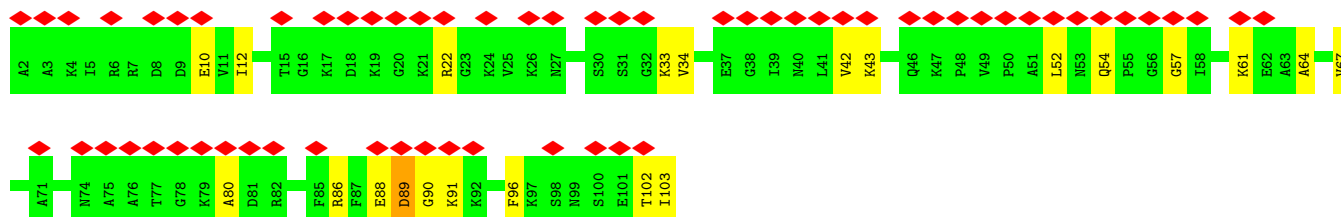
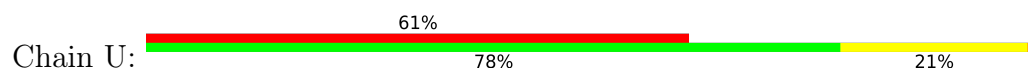


- Molecule 19: 50S ribosomal protein L23

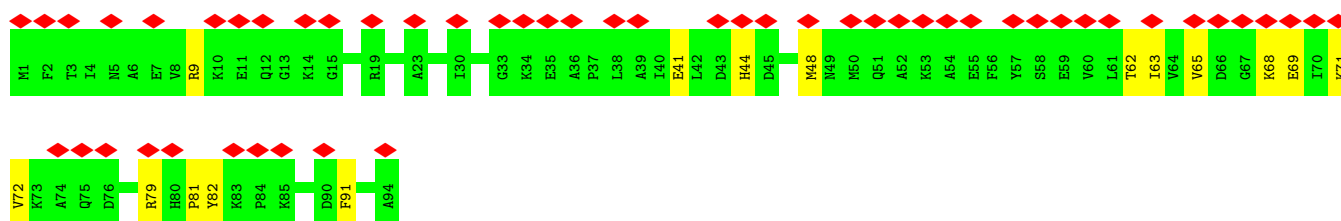
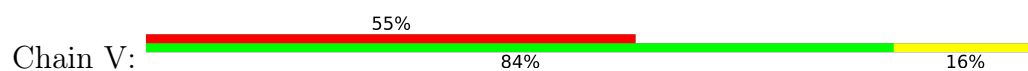




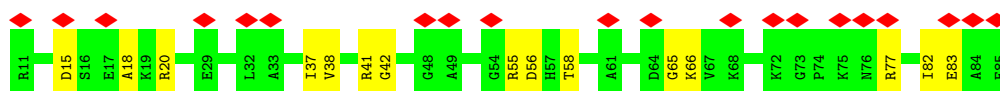
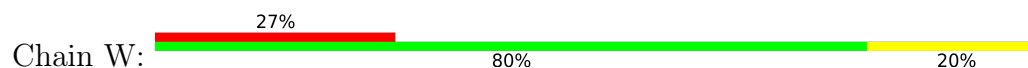
- Molecule 20: 50S ribosomal protein L24



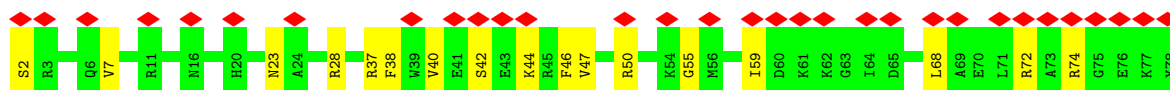
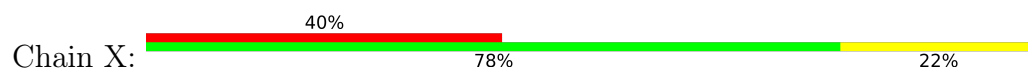
- Molecule 21: 50S ribosomal protein L25



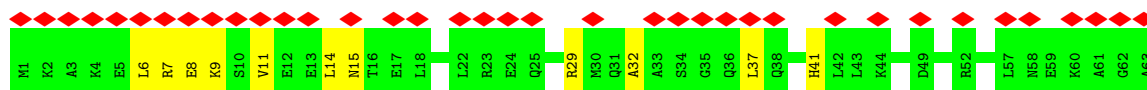
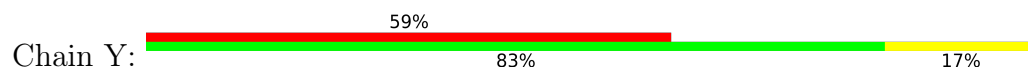
- Molecule 22: 50S ribosomal protein L27



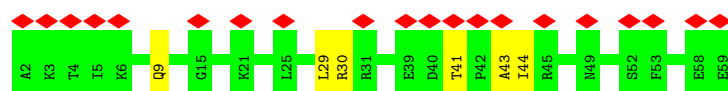
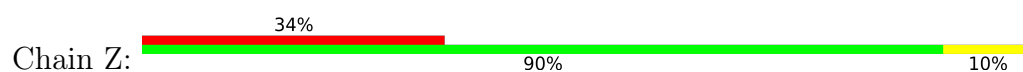
- Molecule 23: 50S ribosomal protein L28



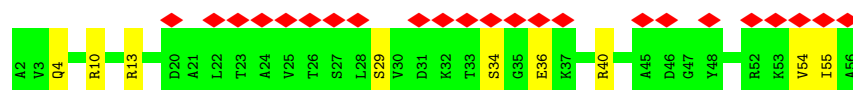
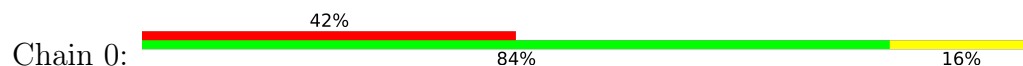
- Molecule 24: 50S ribosomal protein L29



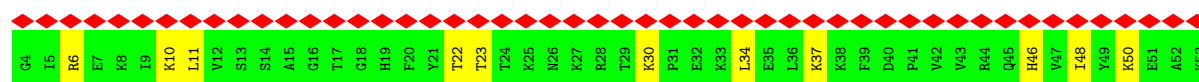
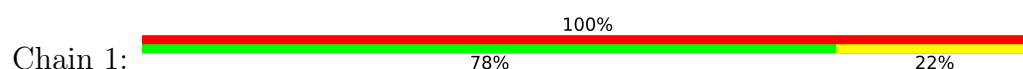
- Molecule 25: 50S ribosomal protein L30



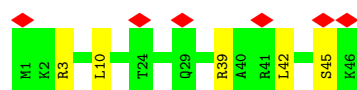
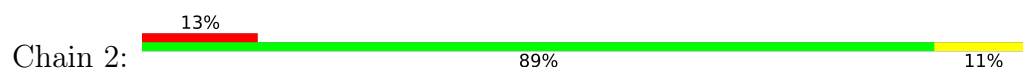
- Molecule 26: 50S ribosomal protein L32



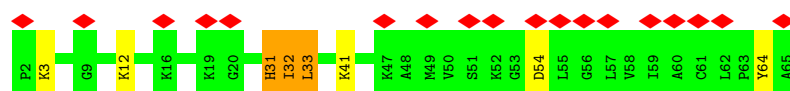
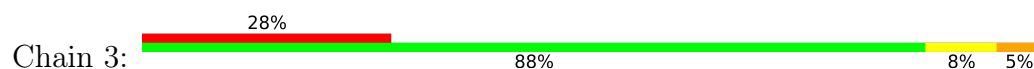
- Molecule 27: 50S ribosomal protein L33



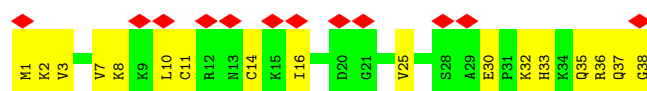
- Molecule 28: 50S ribosomal protein L34



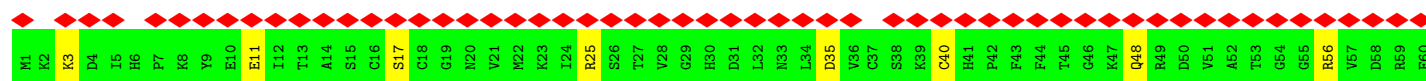
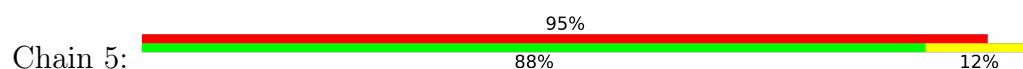
- Molecule 29: 50S ribosomal protein L35

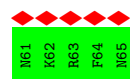


- Molecule 30: 50S ribosomal protein L36

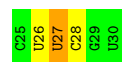


- Molecule 31: 50S ribosomal protein L31

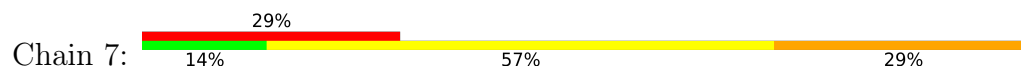




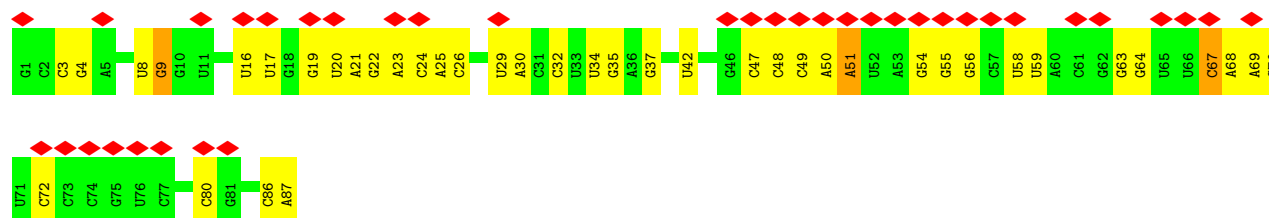
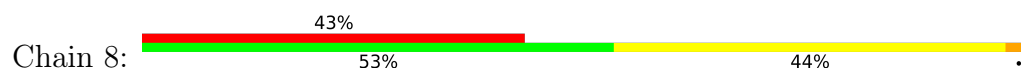
• Molecule 32: mRNA



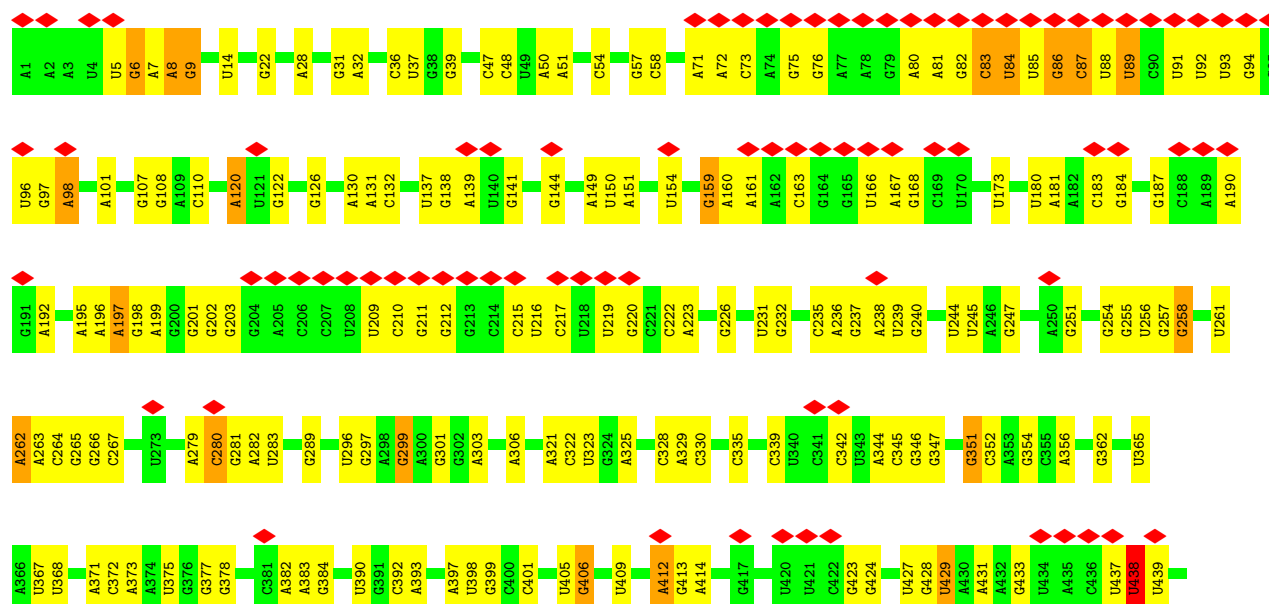
• Molecule 33: ermDL

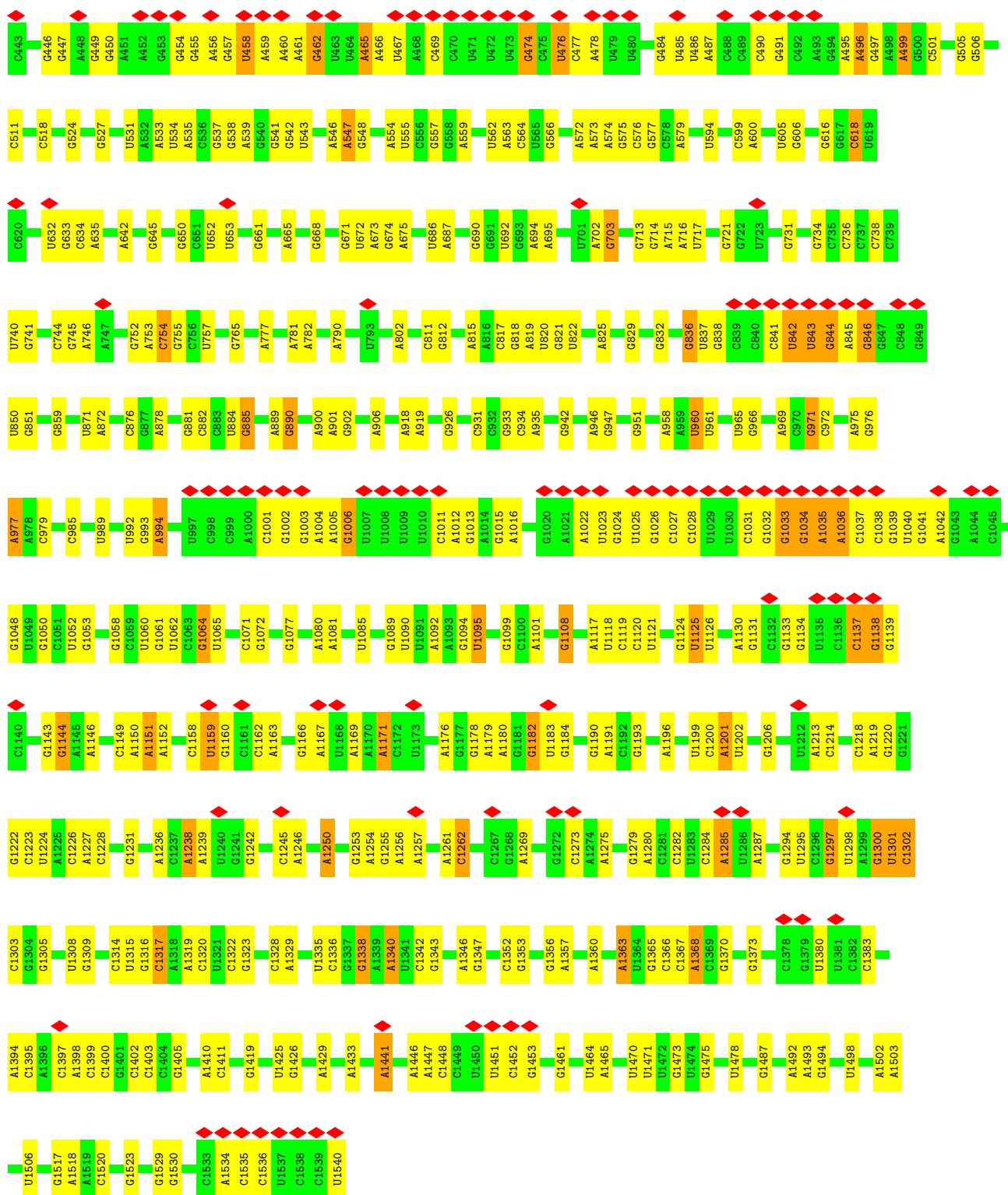


• Molecule 34: P-tRNA (leu)

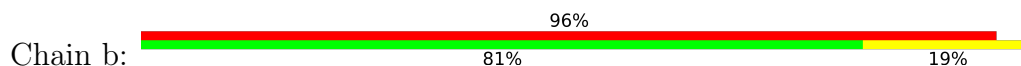


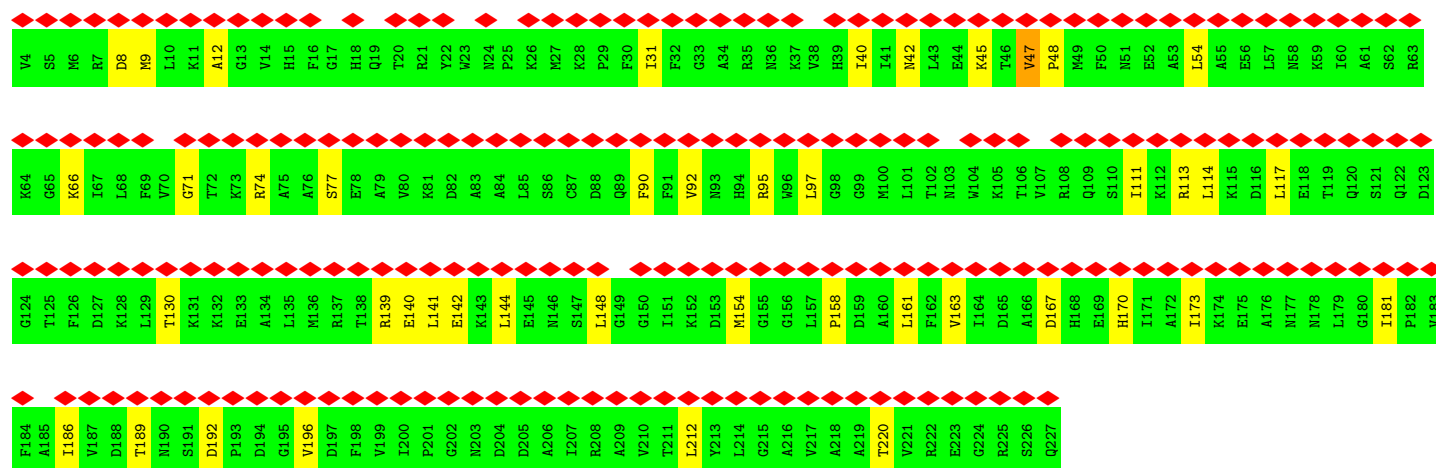
• Molecule 35: 16S rRNA



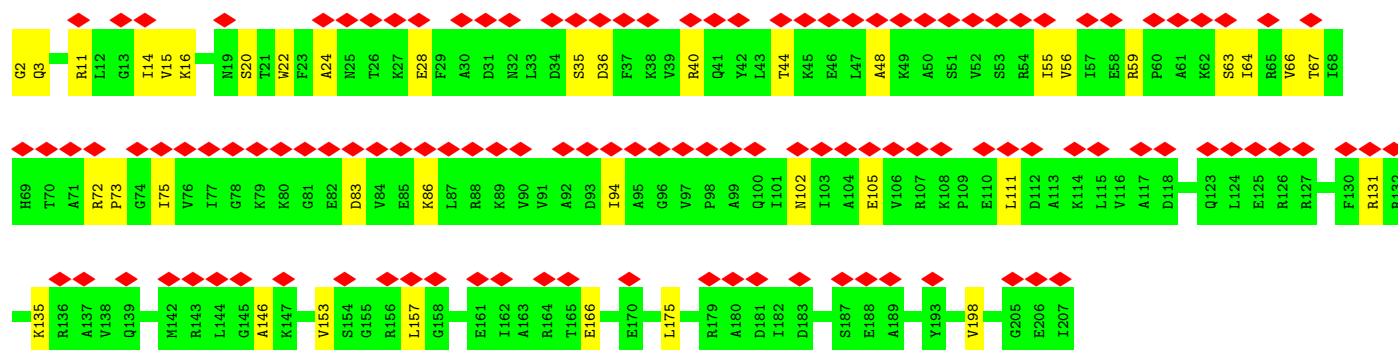
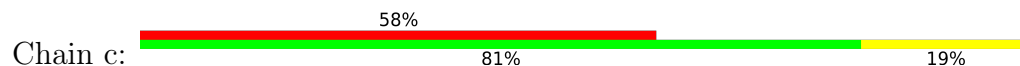


• Molecule 36: 30S ribosomal protein S2

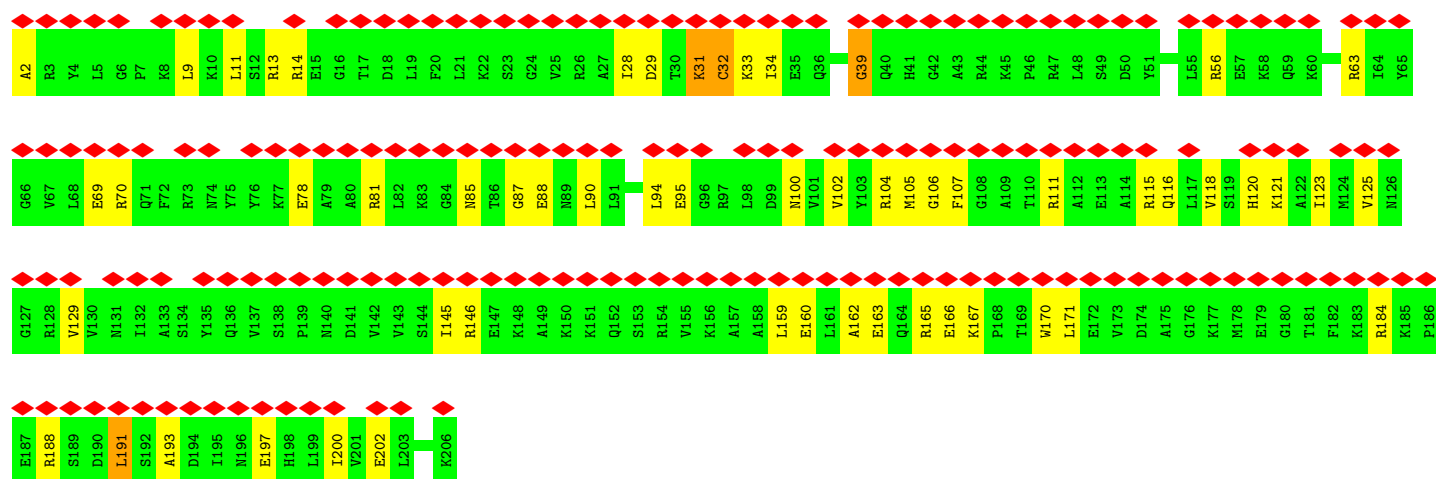
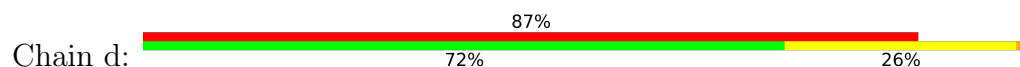




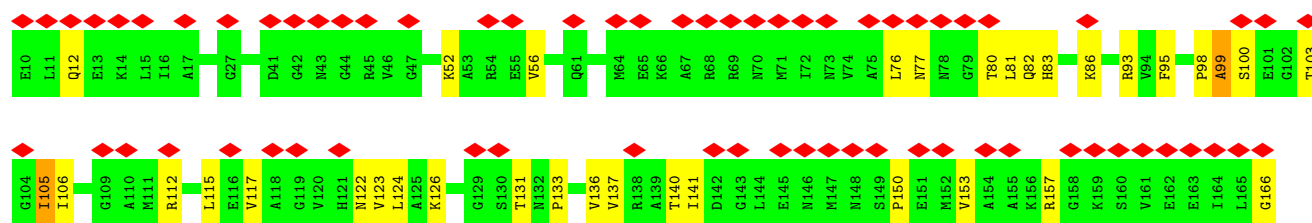
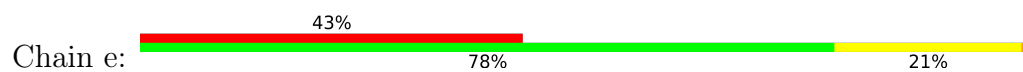
• Molecule 37: 30S ribosomal protein S3



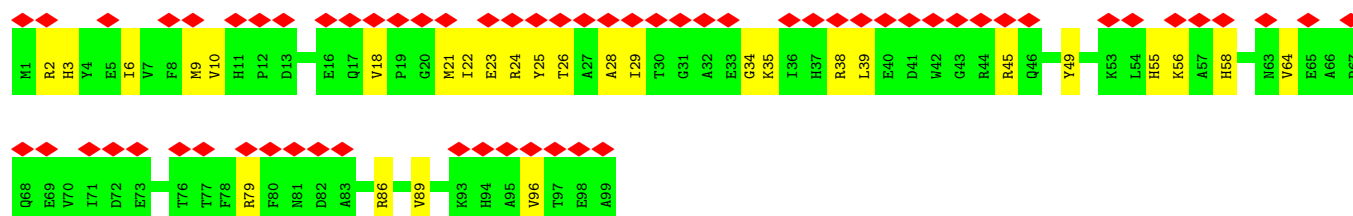
• Molecule 38: 30S ribosomal protein S4



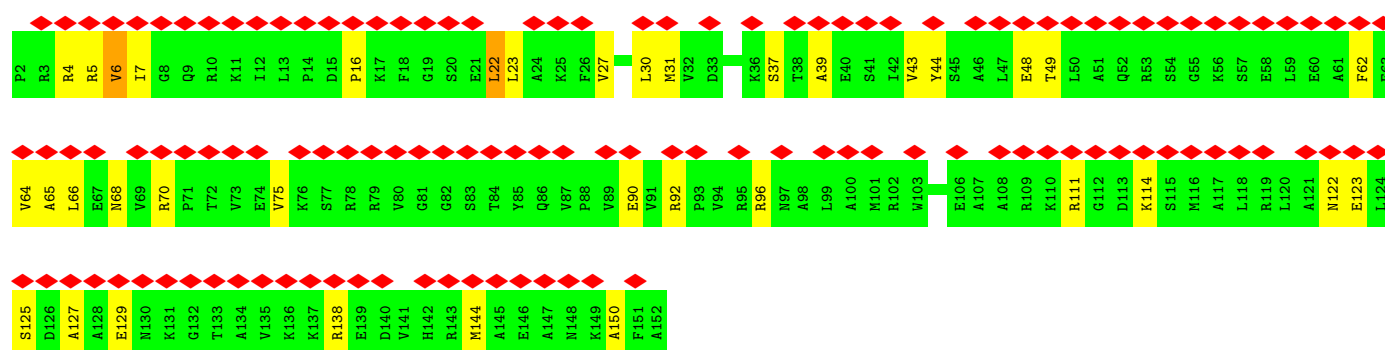
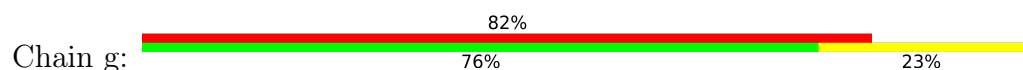
• Molecule 39: 30S ribosomal protein S5



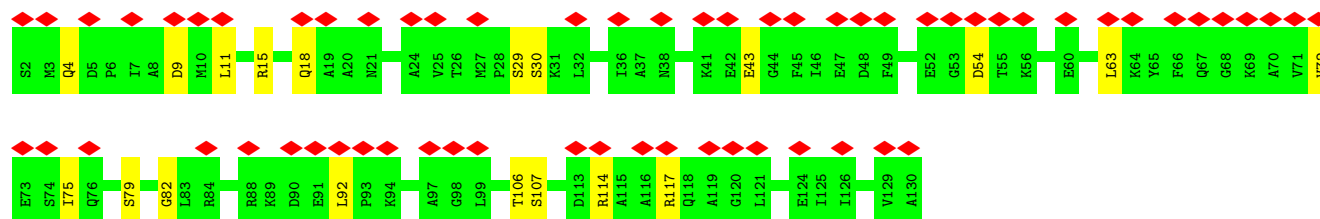
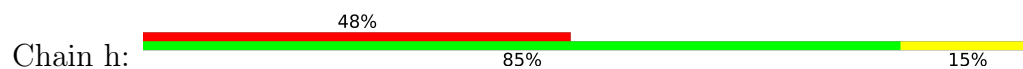
• Molecule 40: 30S ribosomal protein S6



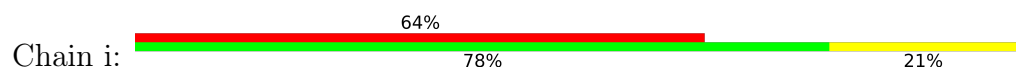
• Molecule 41: 30S ribosomal protein S7

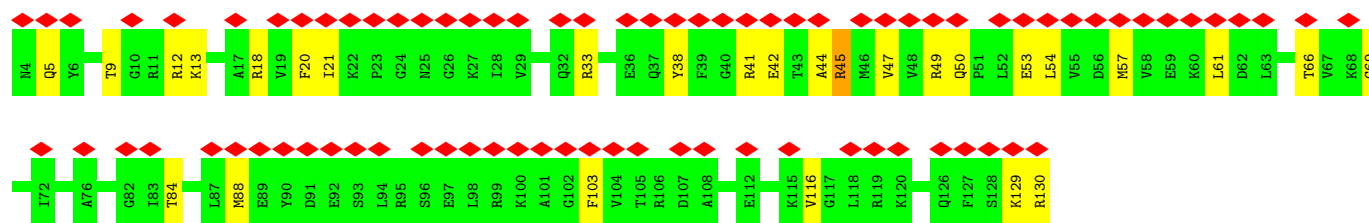


• Molecule 42: 30S ribosomal protein S8

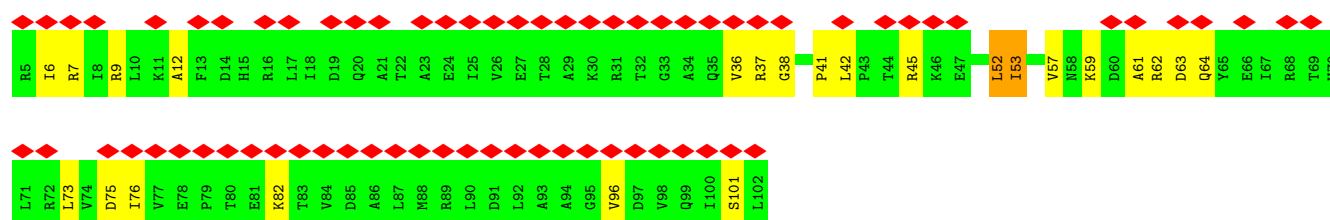
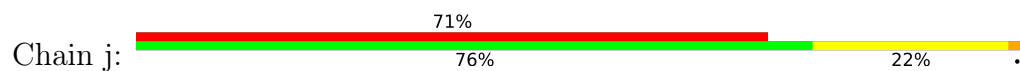


• Molecule 43: 30S ribosomal protein S9

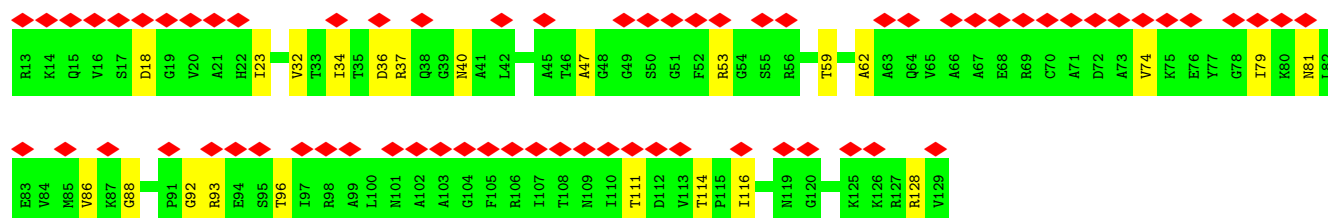
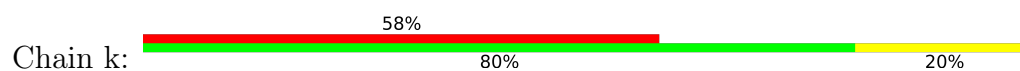




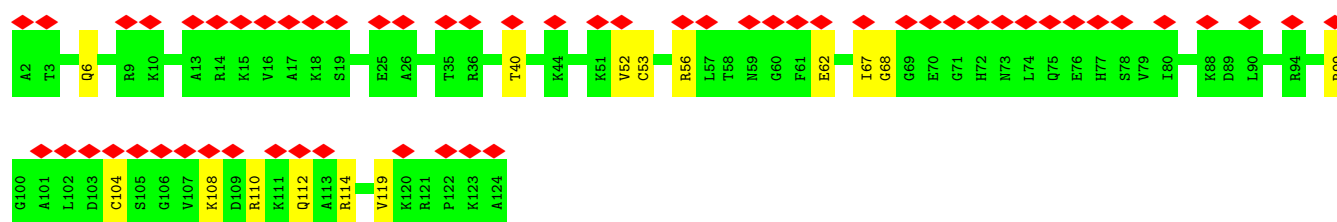
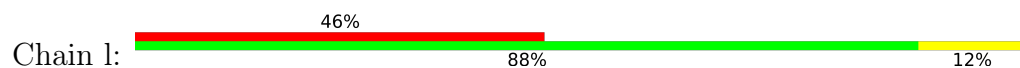
• Molecule 44: 30S ribosomal protein S10



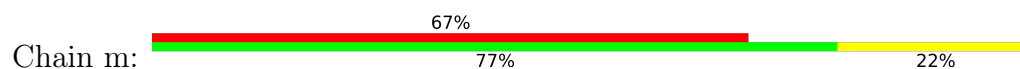
• Molecule 45: 30S ribosomal protein S11

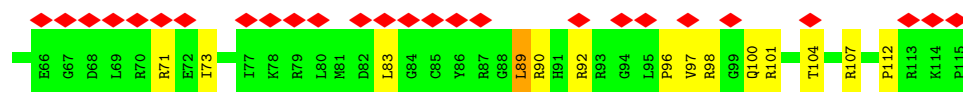


• Molecule 46: 30S ribosomal protein S12

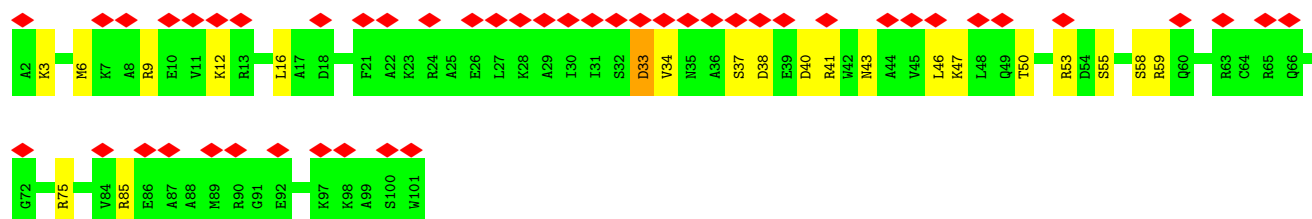
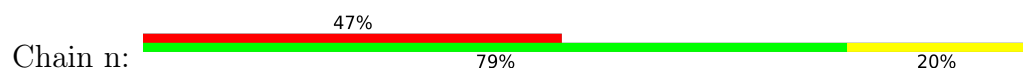


• Molecule 47: 30S ribosomal protein S13

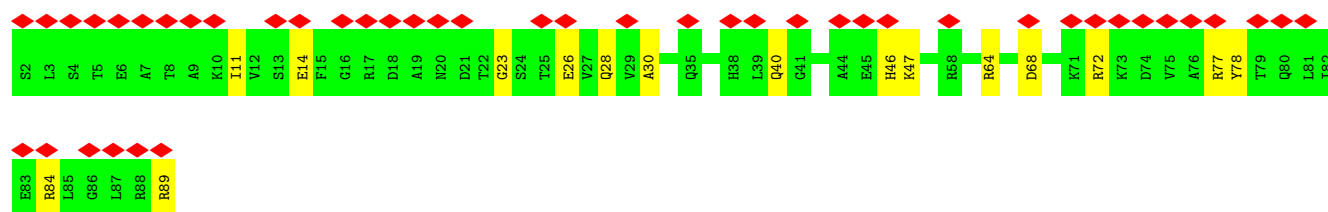
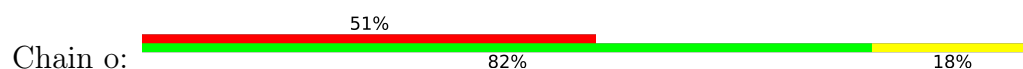




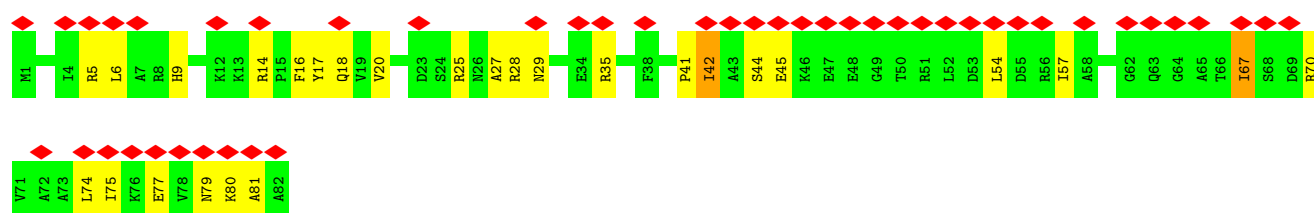
- Molecule 48: 30S ribosomal protein S14



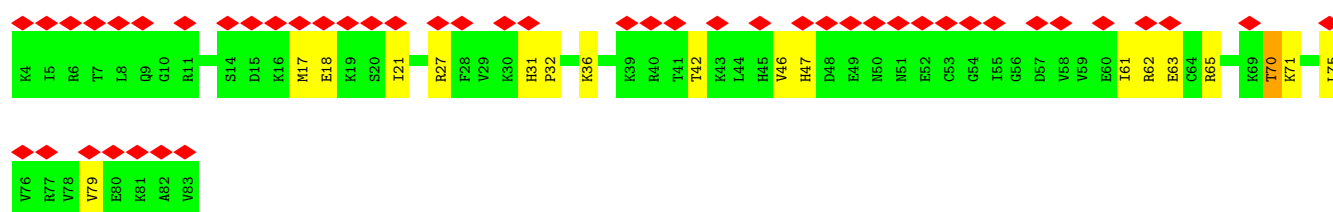
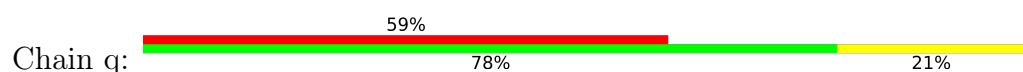
- Molecule 49: 30S ribosomal protein S15



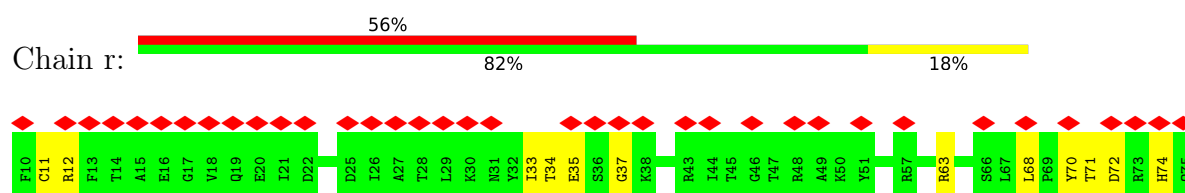
- Molecule 50: 30S ribosomal protein S16



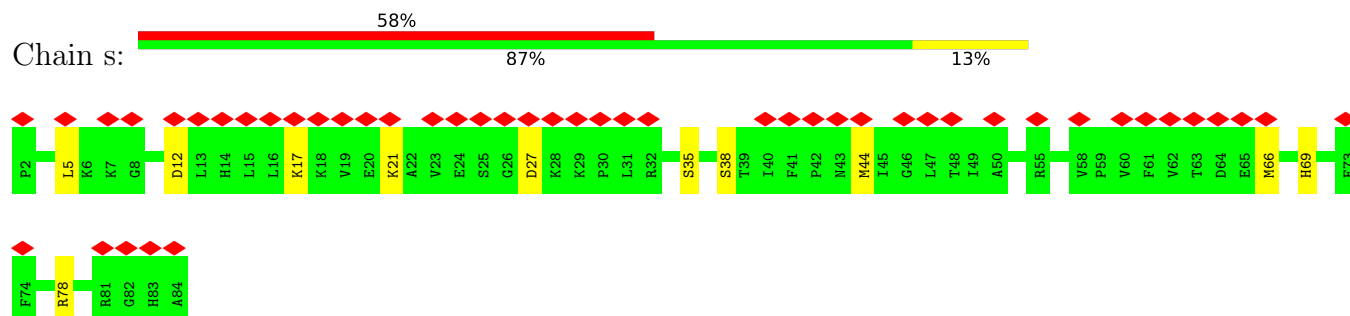
- Molecule 51: 30S ribosomal protein S17



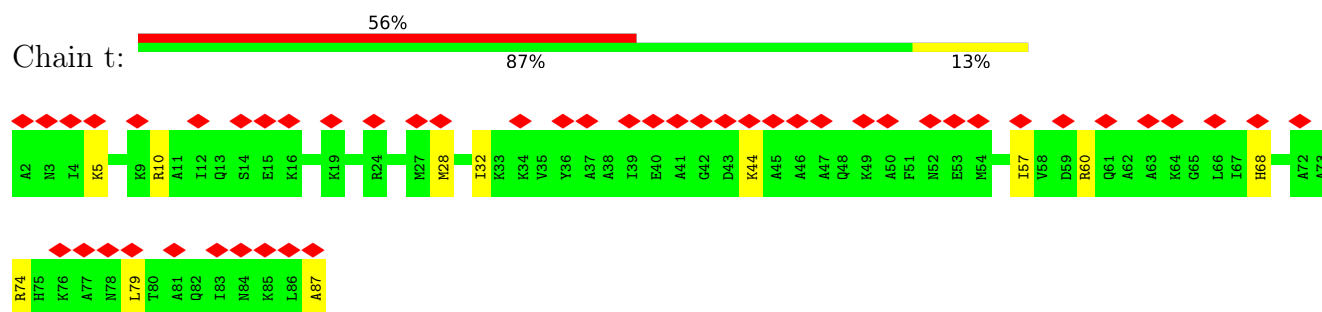
- Molecule 52: 30S ribosomal protein S18



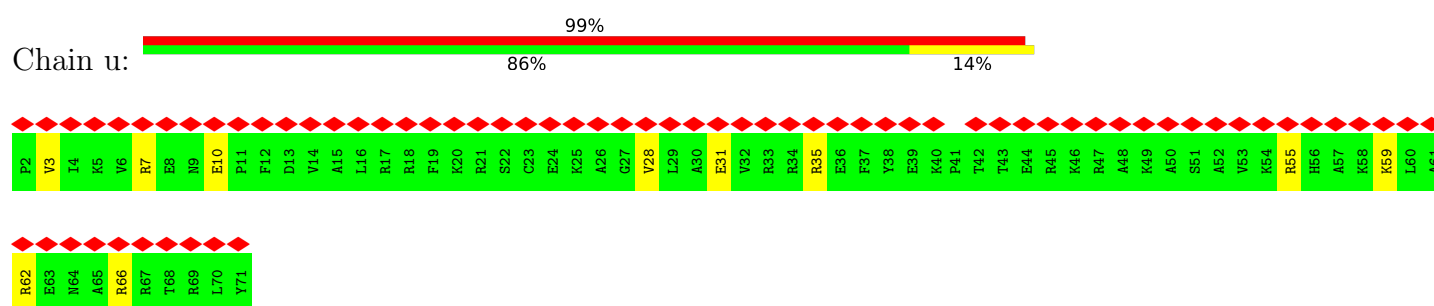
- Molecule 53: 30S ribosomal protein S19



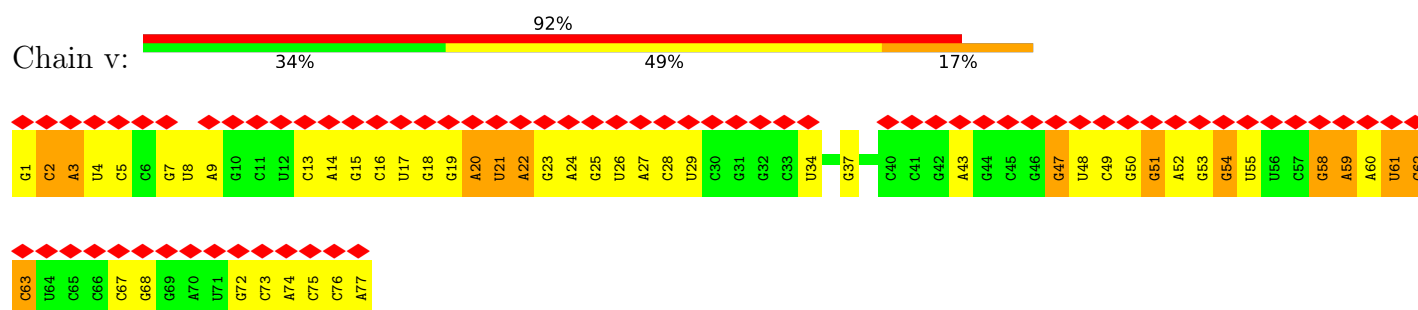
- Molecule 54: 30S ribosomal protein S20



- Molecule 55: 30S ribosomal protein S21



- Molecule 56: A-tRNA (Arg)



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	27397	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 ($e^-/\text{\AA}^2$)	1.0	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	FEI FALCON II (4k x 4k)	Depositor
Maximum map value	0.318	Depositor
Minimum map value	-0.153	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.012	Depositor
Recommended contour level	0.07	Depositor
Map size (Å)	398.88, 398.88, 398.88	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.108, 1.108, 1.108	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.40	0/69799	0.47	6/108892 (0.0%)
2	B	0.31	0/2873	0.47	0/4478
3	C	0.42	0/2121	0.67	0/2852
4	D	0.39	0/1586	0.70	0/2134
5	E	0.34	0/1571	0.63	0/2113
6	F	0.32	0/1434	0.72	1/1926 (0.1%)
7	G	0.29	0/1324	0.70	2/1794 (0.1%)
8	H	0.30	0/1122	0.79	2/1515 (0.1%)
9	J	0.40	1/1152 (0.1%)	0.62	0/1551
10	K	0.38	0/947	0.77	0/1268
11	L	0.38	0/1062	0.78	2/1413 (0.1%)
12	M	0.37	0/1093	0.67	0/1460
13	N	0.37	0/958	0.73	0/1281
14	O	0.32	0/902	0.68	0/1209
15	P	0.37	0/929	0.65	0/1242
16	Q	0.40	0/960	0.51	0/1278
17	R	0.39	0/829	0.70	0/1107
18	S	0.37	0/864	0.69	0/1156
19	T	0.30	0/715	0.65	0/955
20	U	0.33	0/787	0.73	2/1051 (0.2%)
21	V	0.31	0/766	0.62	0/1025
22	W	0.36	0/582	0.57	0/769
23	X	0.37	0/635	0.61	0/848
24	Y	0.32	0/510	0.70	0/677
25	Z	0.32	0/453	0.56	0/605
26	0	0.37	0/440	0.59	0/588
27	1	0.31	0/416	0.75	0/554
28	2	0.41	0/380	0.71	1/498 (0.2%)
29	3	0.38	0/513	0.82	1/676 (0.1%)
30	4	0.40	0/303	0.78	0/397
31	5	0.29	0/523	0.80	2/698 (0.3%)
32	6	0.48	0/135	0.86	2/207 (1.0%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	7	1.81	2/58 (3.4%)	2.00	2/75 (2.7%)
34	8	0.29	0/2080	0.45	0/3242
35	a	0.47	0/36991	0.51	2/57705 (0.0%)
36	b	0.35	0/1784	0.75	2/2403 (0.1%)
37	c	0.42	0/1651	0.72	0/2225
38	d	0.37	0/1665	0.76	2/2227 (0.1%)
39	e	0.46	0/1169	0.80	5/1573 (0.3%)
40	f	0.39	0/829	0.79	0/1120
41	g	0.32	0/1195	0.80	3/1602 (0.2%)
42	h	0.46	0/989	0.74	0/1326
43	i	0.41	0/1034	0.84	1/1375 (0.1%)
44	j	0.42	0/796	0.75	1/1077 (0.1%)
45	k	0.41	0/893	0.73	2/1205 (0.2%)
46	l	0.44	0/969	0.83	2/1300 (0.2%)
47	m	0.40	0/892	0.74	2/1193 (0.2%)
48	n	0.42	0/817	0.71	0/1088
49	o	0.39	0/722	0.72	0/964
50	p	0.39	0/659	0.80	0/884
51	q	0.42	0/657	0.89	1/881 (0.1%)
52	r	0.38	0/554	0.69	0/743
53	s	0.38	0/680	0.67	0/915
54	t	0.34	0/676	0.61	0/895
55	u	0.29	0/598	0.62	0/792
56	v	0.26	0/1836	0.54	0/2860
All	All	0.41	3/158878 (0.0%)	0.55	46/237887 (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
3	C	0	1
5	E	0	1
6	F	0	1
8	H	0	3
14	O	0	1
17	R	0	1
20	U	0	1
27	1	0	1
29	3	0	1
38	d	0	2

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Mol	Chain	#Chirality outliers	#Planarity outliers
39	e	0	1
41	g	0	1
48	n	0	2
50	p	0	1
All	All	0	18

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
33	7	5	MET	CA-C	-8.84	1.41	1.52
9	J	108	MET	C-N	-6.41	1.25	1.32
33	7	5	MET	N-CA	-5.92	1.38	1.46

All (46) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
41	g	65	ALA	N-CA-C	-8.03	104.63	114.75
46	l	40	THR	CA-C-N	7.87	135.90	120.94
46	l	40	THR	C-N-CA	7.87	135.90	120.94
33	7	2	THR	N-CA-C	7.70	127.20	110.80
28	2	45	SER	N-CA-C	-6.93	104.70	113.43
33	7	4	SER	CB-CA-C	-6.60	100.47	110.90
39	e	99	ALA	N-CA-C	6.51	118.22	107.73
36	b	130	THR	CA-C-N	6.37	133.70	121.54
36	b	130	THR	C-N-CA	6.37	133.70	121.54
6	F	177	PHE	N-CA-C	6.31	118.29	110.91
39	e	77	ASN	CA-C-N	6.08	129.95	120.82
39	e	77	ASN	C-N-CA	6.08	129.95	120.82
29	3	32	ILE	N-CA-C	6.08	121.98	109.34
32	6	27	U	C2'-C3'-O3'	6.06	118.59	109.50
20	U	88	GLU	CA-C-N	5.86	129.43	120.82
20	U	88	GLU	C-N-CA	5.86	129.43	120.82
45	k	92	GLY	CA-C-N	5.82	129.55	120.82
45	k	92	GLY	C-N-CA	5.82	129.55	120.82
31	5	40	CYS	CA-C-N	5.79	139.99	121.98
31	5	40	CYS	C-N-CA	5.79	139.99	121.98
38	d	34	ILE	CA-C-N	5.70	133.37	123.91
38	d	34	ILE	C-N-CA	5.70	133.37	123.91
41	g	6	VAL	CA-C-N	5.60	128.22	120.49
41	g	6	VAL	C-N-CA	5.60	128.22	120.49
32	6	27	U	C4'-C3'-O3'	5.42	117.52	109.40
1	A	1062	G	P-O3'-C3'	5.35	128.22	120.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	L	29	LYS	CA-C-N	5.33	135.24	126.86
11	L	29	LYS	C-N-CA	5.33	135.24	126.86
8	H	8	LYS	CA-C-N	5.29	131.49	121.97
8	H	8	LYS	C-N-CA	5.29	131.49	121.97
1	A	752	A	P-O3'-C3'	5.28	128.12	120.20
35	a	438	U	P-O3'-C3'	5.21	128.02	120.20
39	e	93	ARG	CA-C-N	5.19	127.65	120.49
39	e	93	ARG	C-N-CA	5.19	127.65	120.49
7	G	90	VAL	CA-C-N	-5.18	115.54	122.54
7	G	90	VAL	C-N-CA	-5.18	115.54	122.54
47	m	4	ILE	CA-C-N	5.14	127.17	120.28
47	m	4	ILE	C-N-CA	5.14	127.17	120.28
1	A	1173	U	P-O3'-C3'	5.12	127.88	120.20
51	q	70	THR	N-CA-C	-5.12	101.59	108.19
1	A	1130	U	P-O3'-C3'	5.08	127.82	120.20
35	a	960	U	P-O3'-C3'	5.07	127.80	120.20
1	A	1022	G	P-O3'-C3'	5.05	127.78	120.20
43	i	45	ARG	N-CA-C	-5.05	107.67	113.88
1	A	1378	A	P-O3'-C3'	5.05	127.77	120.20
44	j	53	ILE	N-CA-C	5.01	117.00	112.29

There are no chirality outliers.

All (18) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
27	1	34	LEU	Peptide
29	3	31	HIS	Peptide
3	C	121	ASP	Peptide
5	E	82	GLY	Peptide
6	F	145	LYS	Peptide
8	H	3	VAL	Peptide
8	H	39	ALA	Peptide
8	H	8	LYS	Peptide
14	O	87	ILE	Peptide
17	R	53	PHE	Peptide
20	U	89	ASP	Peptide
38	d	31	LYS	Peptide
38	d	39	GLY	Peptide
39	e	99	ALA	Peptide
41	g	64	VAL	Peptide
48	n	33	ASP	Peptide
48	n	34	VAL	Peptide

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Mol	Chain	Res	Type	Group
50	p	42	ILE	Peptide

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	62320	0	31344	369	0
2	B	2570	0	1301	23	0
3	C	2082	0	2154	32	0
4	D	1565	0	1616	32	0
5	E	1552	0	1619	20	0
6	F	1410	0	1444	27	0
7	G	1304	0	1345	17	0
8	H	1111	0	1148	19	0
9	J	1129	0	1162	9	0
10	K	938	0	1012	14	0
11	L	1053	0	1129	20	0
12	M	1074	0	1157	14	0
13	N	945	0	989	12	0
14	O	892	0	923	15	0
15	P	917	0	962	22	0
16	Q	947	0	1019	18	0
17	R	816	0	839	10	0
18	S	857	0	922	16	0
19	T	709	0	779	7	0
20	U	779	0	831	12	0
21	V	753	0	780	11	0
22	W	575	0	592	12	0
23	X	625	0	652	11	0
24	Y	509	0	543	7	0
25	Z	449	0	488	4	0
26	0	434	0	445	8	0
27	1	409	0	440	6	0
28	2	377	0	418	5	0
29	3	504	0	572	7	0
30	4	302	0	340	11	0
31	5	514	0	509	5	0
32	6	123	0	64	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
33	7	58	0	63	23	0
34	8	1861	0	937	18	0
35	a	33037	0	16628	249	0
36	b	1753	0	1780	24	0
37	c	1624	0	1696	29	0
38	d	1643	0	1707	39	0
39	e	1156	0	1199	19	0
40	f	811	0	803	21	0
41	g	1181	0	1238	23	0
42	h	979	0	1031	14	0
43	i	1022	0	1070	20	0
44	j	786	0	828	19	0
45	k	877	0	887	18	0
46	l	955	0	1016	10	0
47	m	883	0	941	27	0
48	n	805	0	844	15	0
49	o	714	0	734	10	0
50	p	649	0	666	17	0
51	q	648	0	691	10	0
52	r	545	0	560	8	0
53	s	663	0	688	10	0
54	t	670	0	719	8	0
55	u	590	0	629	6	0
56	v	1643	0	834	43	0
57	7	51	0	67	11	0
All	All	146148	0	97794	1255	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 6.

All (1255) 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)
1:A:2609:U:H6	33:7:1:MET:CE	1.48	1.25
1:A:2609:U:C6	33:7:1:MET:CE	2.30	1.13
34:8:51:A:H1'	47:m:112:PRO:HD2	1.25	1.12
1:A:2609:U:H6	33:7:1:MET:HE3	1.17	1.05
1:A:1093:G:H21	1:A:1098:A:H62	1.06	1.00
1:A:2609:U:C6	33:7:1:MET:HE1	1.95	0.98
1:A:2609:U:C6	33:7:1:MET:HE3	1.98	0.96
35:a:76:G:H1	35:a:93:U:H3	0.95	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:87:GLU:OE1	40:f:21:MET:CG	2.15	0.94
1:A:2609:U:H6	33:7:1:MET:HE1	1.28	0.92
1:A:1530:G:C8	1:A:1530:G:H5''	2.04	0.92
33:7:1:MET:HB2	57:7:101:ERY:H17	1.53	0.91
1:A:1093:G:N2	1:A:1098:A:H62	1.70	0.88
56:v:1:G:N2	56:v:73:C:O2	2.07	0.86
8:H:87:GLU:OE1	40:f:21:MET:HG3	1.74	0.86
34:8:51:A:C1'	47:m:112:PRO:HD2	2.05	0.85
33:7:1:MET:CB	57:7:101:ERY:H17	2.07	0.85
57:7:101:ERY:O3	57:7:101:ERY:H202	1.78	0.83
1:A:284:U:H3	1:A:356:G:H1	0.84	0.83
56:v:1:G:H2'	56:v:2:C:C6	2.15	0.82
1:A:2584:U:O4	33:7:3:HIS:NE2	2.12	0.82
1:A:1093:G:H21	1:A:1098:A:N6	1.77	0.81
34:8:51:A:H1'	47:m:112:PRO:CD	2.10	0.81
56:v:22:A:C6	56:v:47:G:C2	2.70	0.80
1:A:1724:G:H1	1:A:1736:U:H3	1.31	0.78
7:G:44:LYS:O	7:G:50:LEU:HA	1.82	0.78
1:A:1912:A:N7	1:A:1917:U:O4	2.17	0.78
56:v:22:A:C5	56:v:47:G:C2	2.72	0.77
35:a:83:C:O2	35:a:86:G:N2	2.18	0.76
35:a:447:G:H21	35:a:487:A:H62	1.34	0.76
1:A:1517:G:N2	1:A:1732:C:O2	2.19	0.76
56:v:22:A:C2	56:v:47:G:N2	2.54	0.76
1:A:2610:C:N4	33:7:3:HIS:ND1	2.34	0.75
1:A:1042:G:H1	1:A:1113:U:H3	1.32	0.75
1:A:1530:G:H5''	1:A:1530:G:H8	1.46	0.75
56:v:2:C:H42	56:v:72:G:H1	1.34	0.74
22:W:65:GLY:HA3	22:W:83:GLU:O	1.87	0.73
11:L:79:LEU:O	11:L:82:LEU:HB3	1.89	0.72
50:p:9:HIS:O	50:p:16:PHE:HB3	1.89	0.72
56:v:1:G:N1	56:v:73:C:N3	2.31	0.71
56:v:25:G:C2	56:v:26:U:H1'	2.24	0.71
35:a:198:G:H1	35:a:219:U:H3	1.38	0.71
41:g:70:ARG:H	41:g:138:ARG:HD3	1.56	0.71
56:v:22:A:N1	56:v:47:G:N2	2.39	0.70
8:H:87:GLU:OE1	40:f:21:MET:HG2	1.92	0.70
1:A:1531:C:H2'	1:A:1532:A:C8	2.28	0.69
2:B:72:G:H21	2:B:104:A:H62	1.40	0.69
1:A:2609:U:H5	33:7:1:MET:SD	2.16	0.69
15:P:27:GLU:HG2	15:P:44:GLU:HG2	1.75	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
43:i:5:GLN:HE21	43:i:20:PHE:HB3	1.58	0.68
42:h:11:LEU:HD22	42:h:75:ILE:HD11	1.76	0.68
35:a:84:U:H2'	35:a:86:G:H21	1.59	0.68
50:p:28:ARG:HH11	50:p:29:ASN:HD21	1.40	0.68
34:8:34:U:OP2	43:i:130:ARG:NH2	2.18	0.67
35:a:490:C:H2'	35:a:491:G:H8	1.59	0.67
41:g:62:PHE:O	41:g:66:LEU:HB2	1.93	0.67
40:f:45:ARG:O	40:f:56:LYS:HA	1.93	0.67
44:j:42:LEU:HD11	44:j:73:LEU:HB2	1.77	0.67
35:a:201:G:H1	35:a:216:U:H3	1.40	0.66
1:A:1408:G:H1	1:A:1594:U:H3	1.43	0.66
1:A:2609:U:C5	33:7:1:MET:SD	2.89	0.66
35:a:454:G:H2'	35:a:455:G:H8	1.61	0.66
1:A:1818:U:OP2	3:C:156:ARG:NH1	2.29	0.66
10:K:98:ARG:NH2	35:a:339:C:OP2	2.28	0.66
37:c:111:LEU:HD11	37:c:146:ALA:HB2	1.78	0.66
1:A:1270:C:H5''	1:A:1271:G:H5'	1.77	0.65
12:M:20:LEU:HD13	21:V:81:PRO:HG2	1.79	0.65
56:v:2:C:H2'	56:v:2:C:O2	1.97	0.65
35:a:107:G:N7	54:t:10:ARG:NH2	2.44	0.65
1:A:2332:C:OP1	22:W:77:ARG:NH1	2.31	0.64
6:F:115:ARG:HH12	31:5:48:GLN:HB2	1.62	0.64
4:D:5:VAL:H	4:D:32:ASN:HD21	1.46	0.64
56:v:1:G:H2'	56:v:2:C:H6	1.61	0.64
8:H:39:ALA:HA	8:H:43:ASN:HB2	1.80	0.64
35:a:201:G:N2	35:a:216:U:O2	2.29	0.64
20:U:12:ILE:HG22	20:U:22:ARG:HB3	1.79	0.64
1:A:1799:G:N2	1:A:1818:U:O2'	2.30	0.63
1:A:1869:G:N2	1:A:1872:A:OP2	2.31	0.63
56:v:25:G:N2	56:v:26:U:H1'	2.13	0.63
3:C:6:CYS:SG	3:C:13:ARG:NH2	2.71	0.63
6:F:80:ARG:NH2	34:8:67:C:C4	2.66	0.63
35:a:537:G:H5''	46:l:110:ARG:HH12	1.62	0.63
2:B:30:C:H1'	2:B:57:A:H61	1.63	0.63
8:H:85:GLY:H	8:H:90:LEU:HA	1.63	0.63
47:m:30:SER:HA	47:m:33:ILE:HD12	1.81	0.63
37:c:22:TRP:HB3	37:c:59:ARG:HB2	1.81	0.63
1:A:627:A:OP1	11:L:78:ARG:NH1	2.30	0.63
38:d:123:ILE:HG22	38:d:145:ILE:HG22	1.79	0.62
35:a:1081:A:OP2	39:e:52:LYS:NZ	2.32	0.62
41:g:125:SER:O	41:g:129:GLU:HB2	1.99	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2788:C:O2'	1:A:2809:A:N3	2.31	0.62
41:g:37:SER:OG	43:i:41:ARG:NH1	2.32	0.62
41:g:75:VAL:HG21	41:g:144:MET:HG2	1.82	0.62
1:A:1779:U:OP2	1:A:1784:A:N6	2.31	0.62
8:H:3:VAL:HG12	8:H:19:VAL:H	1.64	0.62
1:A:1062:G:C6	1:A:1077:A:C6	2.87	0.62
1:A:2609:U:C5	33:7:1:MET:CE	2.82	0.62
10:K:64:ARG:NH1	10:K:102:PRO:O	2.32	0.62
12:M:6:ARG:NH1	12:M:7:THR:O	2.33	0.62
38:d:105:MET:HE2	38:d:171:LEU:HD22	1.81	0.61
42:h:92:LEU:O	42:h:117:ARG:NH2	2.33	0.61
51:q:27:ARG:NH2	51:q:42:THR:OG1	2.33	0.61
52:r:37:GLY:O	52:r:63:ARG:NH2	2.31	0.61
36:b:8:ASP:HB3	36:b:212:LEU:HD21	1.81	0.61
9:J:4:PHE:O	16:Q:64:ARG:NH2	2.34	0.61
1:A:2202:U:H3	1:A:2221:G:H1	1.49	0.61
49:o:78:TYR:OH	49:o:89:ARG:NH1	2.34	0.61
6:F:15:LYS:O	6:F:19:GLU:HB2	2.01	0.61
12:M:36:VAL:HG12	21:V:82:TYR:HB2	1.83	0.61
30:4:30:GLU:HG3	30:4:32:LYS:H	1.66	0.61
35:a:1064:G:O2'	35:a:1190:G:N2	2.33	0.61
51:q:21:ILE:HD11	51:q:75:LEU:HD11	1.82	0.61
1:A:873:C:H2'	1:A:874:G:H8	1.66	0.60
1:A:2144:G:H1'	1:A:2147:A:H61	1.65	0.60
8:H:40:THR:OG1	8:H:43:ASN:ND2	2.34	0.60
6:F:64:LYS:NZ	6:F:65:PRO:O	2.33	0.60
38:d:11:LEU:HD13	38:d:63:ARG:HG2	1.83	0.60
13:N:24:MET:HE1	13:N:40:LYS:HD3	1.83	0.60
3:C:154:LEU:HD13	3:C:176:LEU:HD21	1.83	0.60
1:A:2526:G:N3	30:4:1:MET:N	2.50	0.60
35:a:1025:U:H5''	35:a:1026:G:H5'	1.83	0.60
1:A:2163:A:OP1	1:A:2171:A:N6	2.34	0.60
35:a:215:C:O2'	35:a:465:A:N7	2.35	0.60
35:a:437:U:N3	35:a:495:A:C8	2.70	0.60
8:H:77:THR:HG22	8:H:143:ILE:HB	1.82	0.59
56:v:59:A:O2'	56:v:61:U:OP2	2.19	0.59
35:a:126:G:OP1	35:a:605:U:O2'	2.19	0.59
35:a:618:C:O2'	50:p:14:ARG:NH1	2.35	0.59
1:A:1754:A:O2'	15:P:103:ARG:NH2	2.35	0.59
7:G:22:GLN:NE2	7:G:38:ASN:O	2.35	0.59
11:L:19:LEU:HD23	11:L:27:LEU:HD13	1.83	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:a:1015:G:N2	35:a:1218:C:O2	2.35	0.59
56:v:4:U:H2'	56:v:5:C:C6	2.38	0.59
12:M:69:PRO:HA	12:M:94:ALA:HB2	1.84	0.59
14:O:94:ARG:NH2	14:O:97:PHE:O	2.36	0.59
35:a:8:A:N6	38:d:202:GLU:O	2.36	0.59
35:a:405:U:O4	38:d:2:ALA:N	2.36	0.59
37:c:36:ASP:OD2	37:c:59:ARG:NH1	2.34	0.59
1:A:2144:G:N2	1:A:2146:C:O2	2.36	0.59
41:g:68:ASN:ND2	41:g:127:ALA:O	2.36	0.59
1:A:320:A:N3	5:E:163:ASN:ND2	2.43	0.59
13:N:32:GLU:OE1	13:N:86:ARG:NH2	2.36	0.59
30:4:16:ILE:HG12	30:4:25:VAL:HG22	1.84	0.59
35:a:36:C:O2'	46:l:114:ARG:NH2	2.36	0.59
42:h:15:ARG:HE	42:h:75:ILE:HG23	1.66	0.59
46:l:68:GLY:O	46:l:99:ARG:NH1	2.36	0.59
50:p:5:ARG:NH2	50:p:27:ALA:O	2.35	0.59
35:a:668:G:H21	49:o:46:HIS:HE1	1.51	0.59
35:a:837:U:H2'	35:a:838:G:H8	1.68	0.59
42:h:82:GLY:O	51:q:36:LYS:NZ	2.36	0.59
56:v:62:C:C2	56:v:63:C:C5	2.91	0.59
43:i:44:ALA:HA	43:i:47:VAL:HG22	1.85	0.59
44:j:52:LEU:HD21	44:j:59:LYS:HD2	1.84	0.59
1:A:99:U:H5''	1:A:100:U:H5'	1.86	0.58
35:a:1006:G:O6	35:a:1023:U:O2	2.21	0.58
35:a:1368:A:OP1	44:j:64:GLN:NE2	2.35	0.58
1:A:538:A:N6	1:A:555:G:O2'	2.34	0.58
1:A:2285:C:OP2	27:1:6:ARG:NH1	2.36	0.58
11:L:57:LEU:HD22	29:3:54:ASP:HB3	1.84	0.58
13:N:28:LEU:HD23	13:N:48:VAL:HG21	1.84	0.58
14:O:12:THR:HA	14:O:15:ARG:HB2	1.84	0.58
35:a:9:G:OP2	39:e:126:LYS:NZ	2.35	0.58
7:G:8:PRO:O	7:G:69:ARG:NH2	2.36	0.58
35:a:437:U:C2	35:a:495:A:N7	2.71	0.58
51:q:62:ARG:NH1	51:q:63:GLU:O	2.36	0.58
10:K:71:ARG:HD2	10:K:77:ILE:HD11	1.85	0.58
1:A:284:U:O4	1:A:356:G:O6	2.21	0.58
35:a:890:G:O2'	35:a:906:A:N6	2.36	0.58
35:a:414:A:OP2	35:a:428:G:N1	2.34	0.58
10:K:58:LEU:HD11	10:K:86:LEU:HD23	1.85	0.58
8:H:87:GLU:HB2	40:f:24:ARG:HH22	1.67	0.58
35:a:371:A:O2'	35:a:373:A:N7	2.37	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:d:188:ARG:HH12	38:d:193:ALA:HA	1.67	0.58
47:m:83:LEU:HD11	53:s:66:MET:HG2	1.85	0.58
1:A:560:C:O2'	16:Q:48:ARG:NH2	2.37	0.58
33:7:1:MET:HE2	57:7:101:ERY:H152	1.84	0.58
34:8:51:A:N3	47:m:112:PRO:HD3	2.18	0.58
35:a:159:G:O2'	35:a:161:A:N7	2.36	0.58
34:8:22:G:H5'	34:8:23:A:H5'	1.85	0.57
39:e:80:THR:OG1	39:e:81:LEU:N	2.38	0.57
45:k:18:ASP:OD2	45:k:37:ARG:NH1	2.37	0.57
45:k:34:ILE:HD13	45:k:74:VAL:HG21	1.86	0.57
4:D:130:GLN:NE2	4:D:139:SER:O	2.37	0.57
15:P:55:LEU:HA	15:P:77:HIS:HD2	1.68	0.57
40:f:23:GLU:O	40:f:26:THR:HB	2.04	0.57
1:A:559:G:N2	16:Q:49:ASP:OD2	2.37	0.57
4:D:46:ARG:NH2	4:D:88:GLU:O	2.37	0.57
35:a:409:U:H3	35:a:433:G:H1	1.52	0.57
36:b:47:VAL:HG23	36:b:48:PRO:HD3	1.86	0.57
45:k:111:THR:HB	55:u:3:VAL:HG23	1.86	0.57
1:A:275:C:O2'	1:A:362:A:N6	2.35	0.57
1:A:527:C:N4	1:A:2779:U:OP2	2.38	0.57
4:D:14:ILE:HG22	15:P:12:GLN:HE22	1.70	0.57
35:a:6:G:H1	39:e:103:THR:HG21	1.69	0.57
48:n:37:SER:HB3	48:n:40:ASP:H	1.69	0.57
1:A:2183:A:H2'	1:A:2184:A:H8	1.68	0.57
56:v:22:A:C6	56:v:47:G:N3	2.73	0.57
1:A:468:G:N7	28:2:39:ARG:NH2	2.52	0.57
35:a:490:C:OP1	38:d:146:ARG:NH1	2.36	0.57
1:A:663:G:H5''	11:L:17:LYS:HD3	1.87	0.57
1:A:1798:U:OP2	3:C:271:ARG:NH2	2.36	0.57
1:A:1972:G:OP2	3:C:238:ARG:NH1	2.37	0.57
1:A:2504:U:H2'	1:A:2504:U:O2	2.04	0.57
1:A:569:U:O2'	1:A:983:A:N1	2.37	0.57
1:A:1858:A:N6	1:A:1884:G:O2'	2.37	0.57
1:A:27:G:N2	1:A:512:G:O2'	2.38	0.57
1:A:145:C:H2'	1:A:146:A:H8	1.69	0.57
23:X:2:SER:O	23:X:50:ARG:NH1	2.38	0.57
35:a:1048:G:H5''	48:n:3:LYS:HD2	1.87	0.57
38:d:165:ARG:O	38:d:167:LYS:NZ	2.37	0.56
1:A:1039:A:N1	1:A:1116:G:O6	2.38	0.56
1:A:2848:G:O2'	1:A:2867:G:N2	2.37	0.56
4:D:12:THR:OG1	4:D:13:ARG:N	2.39	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:a:979:C:O2	48:m:59:ARG:NH1	2.39	0.56
35:a:1279:G:H5''	44:j:9:ARG:HH12	1.70	0.56
47:m:104:THR:O	47:m:107:ARG:NH2	2.39	0.56
1:A:71:A:O2'	19:T:9:LYS:NZ	2.38	0.56
1:A:1154:G:OP2	16:Q:58:ARG:NH1	2.38	0.56
1:A:2500:U:O2'	1:A:2504:U:OP1	2.24	0.56
35:a:599:C:H2'	35:a:600:A:H8	1.70	0.56
39:e:166:GLY:HA2	42:h:114:ARG:HD2	1.88	0.56
56:v:26:U:C2	56:v:27:A:C8	2.93	0.56
1:A:1218:G:OP2	16:Q:15:LYS:NZ	2.38	0.56
11:L:95:LEU:HG	11:L:100:ILE:HD11	1.86	0.56
35:a:1005:A:OP2	35:a:1024:G:N2	2.38	0.56
1:A:672:C:OP2	11:L:42:SER:OG	2.21	0.56
1:A:1248:G:OP1	5:E:44:ARG:NH1	2.39	0.56
1:A:2590:A:N1	1:A:2604:U:C4	2.73	0.56
9:J:51:GLY:O	9:J:121:LYS:NZ	2.39	0.56
18:S:62:ASP:N	18:S:62:ASP:OD1	2.37	0.56
38:d:188:ARG:O	38:d:188:ARG:NH1	2.38	0.56
1:A:2540:C:O2'	1:A:2740:A:N3	2.35	0.56
1:A:2609:U:H2'	33:7:1:MET:HE1	1.87	0.56
20:U:10:GLU:OE2	20:U:22:ARG:NH2	2.39	0.56
39:e:100:SER:O	39:e:122:ASN:ND2	2.38	0.56
49:o:64:ARG:HH21	49:o:68:ASP:HB3	1.71	0.56
5:E:178:VAL:O	5:E:182:ALA:HB2	2.05	0.56
35:a:427:U:O2'	35:a:541:G:OP1	2.24	0.56
35:a:542:G:O3'	38:d:14:ARG:NH2	2.38	0.56
1:A:715:A:H2	49:o:40:GLN:HE22	1.54	0.55
1:A:848:C:H2'	1:A:849:A:H8	1.71	0.55
25:Z:41:THR:HG23	25:Z:44:ILE:H	1.70	0.55
35:a:201:G:HO2'	35:a:469:C:HO2'	1.54	0.55
35:a:427:U:OP1	38:d:13:ARG:NH2	2.35	0.55
35:a:994:A:O2'	48:n:12:LYS:NZ	2.39	0.55
54:t:44:LYS:HD2	54:t:87:ALA:HB3	1.87	0.55
1:A:2392:A:OP2	29:3:31:HIS:NE2	2.38	0.55
1:A:2636:C:O2'	4:D:45:TYR:OH	2.22	0.55
35:a:1250:A:H4'	43:i:69:GLY:HA2	1.88	0.55
1:A:888:C:C5	47:m:92:ARG:HD2	2.42	0.55
1:A:1051:G:H22	1:A:1108:U:H3	1.53	0.55
1:A:2691:C:HO2'	1:A:2871:U:HO2'	1.54	0.55
35:a:1151:A:H1'	44:j:41:PRO:HB2	1.88	0.55
39:e:105:ILE:O	39:e:112:ARG:NH2	2.40	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1530:G:C8	1:A:1530:G:C5'	2.85	0.55
44:j:37:ARG:HB2	44:j:75:ASP:HB2	1.88	0.55
56:v:26:U:H2'	56:v:27:A:H8	1.72	0.55
1:A:90:U:H3'	1:A:91:A:H2'	1.87	0.55
1:A:1062:G:C6	1:A:1077:A:N6	2.74	0.55
1:A:1365:A:OP1	23:X:28:ARG:NH2	2.40	0.55
1:A:1715:G:N2	1:A:1716:U:O4	2.39	0.55
33:7:4:SER:HB3	57:7:101:ERY:H24	1.87	0.55
35:a:690:G:O6	45:k:53:ARG:NH2	2.39	0.55
35:a:1193:G:O6	37:c:3:GLN:NE2	2.40	0.55
4:D:13:ARG:NH1	15:P:75:GLN:OE1	2.40	0.55
56:v:26:U:C2	56:v:27:A:N7	2.75	0.55
1:A:1962:C:O2'	1:A:1964:G:OP2	2.23	0.55
23:X:38:PHE:O	23:X:46:PHE:HA	2.07	0.55
35:a:543:U:OP1	38:d:14:ARG:NE	2.37	0.55
37:c:72:ARG:HB3	37:c:75:ILE:HD13	1.89	0.55
46:l:110:ARG:NH2	46:l:112:GLN:O	2.35	0.55
1:A:277:G:N2	1:A:357:C:OP1	2.39	0.55
38:d:100:ASN:OD1	38:d:111:ARG:NH1	2.40	0.55
6:F:74:VAL:HG22	6:F:76:GLY:H	1.71	0.55
35:a:671:G:O2'	40:f:79:ARG:NH2	2.40	0.55
1:A:495:G:H21	18:S:61:ASN:HD21	1.55	0.54
8:H:75:LEU:HG	8:H:77:THR:H	1.73	0.54
56:v:22:A:C6	56:v:47:G:N2	2.73	0.54
35:a:1013:G:N2	35:a:1016:A:OP2	2.40	0.54
36:b:71:GLY:N	36:b:92:VAL:O	2.36	0.54
6:F:115:ARG:HG3	47:m:71:ARG:HH22	1.71	0.54
34:8:16:U:O4'	34:8:70:G:N2	2.41	0.54
42:h:29:SER:OG	42:h:30:SER:N	2.39	0.54
42:h:106:THR:OG1	42:h:107:SER:N	2.40	0.54
45:k:23:ILE:HG12	45:k:32:VAL:HG13	1.88	0.54
47:m:89:LEU:HG	47:m:92:ARG:HH21	1.72	0.54
6:F:67:ILE:O	6:F:69:LYS:NZ	2.40	0.54
43:i:84:THR:HG21	43:i:103:PHE:HB3	1.89	0.54
49:o:14:GLU:O	49:o:84:ARG:NH2	2.40	0.54
1:A:2636:C:HO2'	4:D:45:TYR:HH	1.54	0.54
18:S:83:LYS:O	18:S:84:ARG:NH2	2.40	0.54
35:a:843:U:H5'	35:a:844:G:H8	1.73	0.54
1:A:976:G:HO2'	1:A:1155:A:HO2'	1.53	0.54
35:a:76:G:O6	35:a:93:U:O4	2.25	0.54
35:a:673:A:H4'	40:f:86:ARG:HH12	1.73	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
56:v:26:U:N3	56:v:27:A:N7	2.55	0.54
5:E:5:LEU:HD22	5:E:10:SER:HB3	1.88	0.54
1:A:592:A:HO2'	29:3:64:TYR:HH	1.51	0.54
8:H:94:ILE:HD11	8:H:122:LEU:HD12	1.90	0.54
30:4:7:VAL:HG22	30:4:38:GLY:HA3	1.90	0.54
35:a:447:G:N2	35:a:487:A:H62	2.03	0.54
35:a:1300:G:O2'	35:a:1303:C:N4	2.41	0.54
37:c:20:SER:OG	37:c:40:ARG:NH2	2.41	0.54
41:g:44:TYR:O	41:g:48:GLU:HB2	2.08	0.54
33:7:1:MET:HB3	57:7:101:ERY:H17	1.87	0.54
35:a:1302:C:OP2	47:m:13:LYS:NZ	2.39	0.54
37:c:44:THR:O	37:c:48:ALA:HB2	2.08	0.54
1:A:1716:U:H2'	1:A:1717:A:H8	1.73	0.53
24:Y:32:ALA:HB2	24:Y:37:LEU:HD12	1.89	0.53
43:i:18:ARG:NE	43:i:66:THR:OG1	2.39	0.53
1:A:2061:G:OP1	5:E:63:LYS:NZ	2.38	0.53
35:a:1226:C:OP2	47:m:90:ARG:NH2	2.35	0.53
35:a:1367:C:H5''	43:i:116:VAL:HG23	1.91	0.53
38:d:32:CYS:SG	38:d:33:LYS:N	2.81	0.53
45:k:88:GLY:O	45:k:93:ARG:NH1	2.42	0.53
19:T:34:VAL:HG21	19:T:43:ILE:HD11	1.89	0.53
35:a:335:C:O2'	35:a:1433:A:N3	2.36	0.53
1:A:2116:G:H1	1:A:2164:C:H42	1.56	0.53
2:B:72:G:N2	2:B:104:A:H62	2.05	0.53
36:b:8:ASP:O	36:b:12:ALA:HB2	2.08	0.53
43:i:49:ARG:O	43:i:53:GLU:N	2.40	0.53
48:n:38:ASP:OD2	48:n:41:ARG:NH1	2.37	0.53
49:o:23:GLY:O	49:o:28:GLN:NE2	2.42	0.53
1:A:517:C:OP1	26:0:13:ARG:NH2	2.41	0.53
1:A:1445:G:O6	1:A:1466:U:C2	2.61	0.53
35:a:54:C:OP1	35:a:351:G:N2	2.42	0.53
35:a:195:A:N3	35:a:222:C:O2'	2.40	0.53
35:a:458:U:H3	35:a:474:G:H1	1.56	0.53
35:a:881:G:OP2	46:l:6:GLN:NE2	2.39	0.53
45:k:23:ILE:HG21	45:k:96:THR:HG21	1.90	0.53
56:v:24:A:H2'	56:v:25:G:H8	1.72	0.53
1:A:931:U:O4	1:A:1166:G:N2	2.41	0.53
35:a:401:C:OP2	38:d:70:ARG:NH1	2.42	0.53
35:a:1366:C:O2'	44:j:62:ARG:NH2	2.41	0.53
50:p:18:GLN:OE1	50:p:35:ARG:NE	2.41	0.53
1:A:2379:G:O2'	14:O:17:LYS:NZ	2.39	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:a:563:A:HO2'	35:a:566:G:HO2'	1.54	0.53
35:a:1464:U:H2'	35:a:1465:A:H8	1.73	0.53
1:A:574:A:N6	1:A:2034:U:OP1	2.38	0.53
1:A:1826:G:O2'	1:A:1971:U:OP2	2.24	0.53
1:A:2676:C:OP1	10:K:31:ARG:NH2	2.42	0.53
31:5:17:SER:OG	31:5:35:ASP:O	2.27	0.53
35:a:447:G:H21	35:a:487:A:N6	2.04	0.53
38:d:9:LEU:HD11	38:d:28:ILE:HG23	1.91	0.53
1:A:1087:G:H2'	1:A:1089:A:H5''	1.90	0.53
17:R:58:VAL:H	17:R:102:SER:HB3	1.73	0.53
35:a:541:G:O2'	38:d:39:GLY:O	2.26	0.53
56:v:1:G:C4	56:v:2:C:C5	2.97	0.53
1:A:1470:A:N6	1:A:1521:G:O2'	2.42	0.52
1:A:2313:C:H5''	6:F:88:LYS:HD2	1.89	0.52
1:A:2579:C:O2'	4:D:136:ASN:OD1	2.28	0.52
1:A:2682:A:H61	1:A:2728:U:H1'	1.75	0.52
3:C:71:LYS:HB3	3:C:74:ILE:HD11	1.89	0.52
41:g:68:ASN:O	41:g:138:ARG:NE	2.42	0.52
1:A:221:A:N1	1:A:265:A:O2'	2.41	0.52
1:A:534:U:H2'	1:A:535:G:H8	1.74	0.52
1:A:2258:C:O2'	1:A:2427:C:OP2	2.25	0.52
36:b:42:ASN:OD1	36:b:45:LYS:N	2.40	0.52
41:g:90:GLU:OE1	41:g:92:ARG:NH2	2.40	0.52
1:A:807:U:OP2	11:L:41:ARG:NH1	2.39	0.52
1:A:1819:A:H5''	3:C:160:THR:HG21	1.91	0.52
1:A:1315:C:O2'	1:A:1392:A:N3	2.36	0.52
35:a:1328:C:H2'	35:a:1329:A:H8	1.75	0.52
41:g:16:PRO:HG3	43:i:42:GLU:HG3	1.92	0.52
41:g:27:VAL:HG22	41:g:43:VAL:HG11	1.91	0.52
56:v:16:C:N4	56:v:21:U:OP2	2.43	0.52
1:A:750:A:OP1	1:A:1615:C:N4	2.41	0.52
1:A:2006:C:O2'	1:A:2823:A:N3	2.42	0.52
10:K:113:MET:HA	10:K:116:ILE:HG12	1.90	0.52
1:A:1036:G:H1	1:A:1119:U:H3	1.57	0.52
35:a:392:C:H2'	35:a:393:A:H8	1.74	0.52
39:e:115:LEU:HD13	39:e:123:VAL:HG21	1.92	0.52
2:B:9:G:OP2	14:O:15:ARG:NH1	2.42	0.52
35:a:1218:C:H2'	35:a:1219:A:C8	2.45	0.52
1:A:1807:G:N2	1:A:1810:A:OP2	2.42	0.52
1:A:2578:G:OP1	1:A:2614:A:N6	2.43	0.52
7:G:17:VAL:HG21	7:G:50:LEU:HD21	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:a:574:A:HO2'	35:a:882:C:HO2'	1.54	0.52
36:b:31:ILE:HG21	36:b:189:THR:HG22	1.92	0.52
37:c:35:SER:OG	37:c:59:ARG:NH2	2.42	0.52
35:a:28:A:O2'	35:a:296:U:OP1	2.26	0.52
35:a:437:U:O2	35:a:495:A:N7	2.43	0.52
35:a:1035:A:H3'	35:a:1036:A:H8	1.75	0.52
35:a:1356:G:H2'	35:a:1357:A:H8	1.74	0.52
43:i:45:ARG:O	43:i:49:ARG:NH2	2.39	0.52
2:B:22:U:H3	2:B:61:G:H1	1.57	0.52
2:B:47:C:OP2	14:O:3:LYS:NZ	2.43	0.52
35:a:180:U:O2	35:a:195:A:N7	2.43	0.52
35:a:429:U:O2'	38:d:31:LYS:NZ	2.43	0.52
35:a:842:U:OP2	35:a:846:G:N1	2.42	0.52
38:d:102:VAL:HG22	38:d:107:PHE:HB2	1.91	0.52
1:A:1654:A:O2'	4:D:118:PHE:O	2.26	0.51
1:A:1936:A:H2	1:A:1943:U:H3	1.58	0.51
35:a:594:U:H3	35:a:645:G:H1	1.58	0.51
37:c:56:VAL:O	37:c:66:VAL:HA	2.10	0.51
1:A:781:A:OP1	3:C:217:ARG:NH2	2.43	0.51
1:A:2099:U:O2	1:A:2190:G:N2	2.41	0.51
3:C:79:GLU:OE2	3:C:101:ARG:NH2	2.42	0.51
44:j:53:ILE:CG2	44:j:63:ASP:HB2	2.40	0.51
1:A:296:U:H2'	1:A:297:G:H8	1.76	0.51
1:A:1816:C:N4	3:C:35:GLU:OE2	2.36	0.51
1:A:95:A:O2'	24:Y:41:HIS:ND1	2.43	0.51
6:F:115:ARG:HG3	47:m:71:ARG:NH2	2.26	0.51
14:O:7:ARG:HA	14:O:10:ARG:HE	1.74	0.51
35:a:1137:C:H5'	35:a:1138:G:H5'	1.92	0.51
35:a:1220:G:OP1	48:n:53:ARG:NH2	2.40	0.51
44:j:7:ARG:CB	44:j:101:SER:O	2.59	0.51
36:b:111:ILE:HG22	36:b:148:LEU:HD13	1.92	0.51
35:a:299:G:N2	35:a:566:G:O6	2.42	0.51
35:a:692:U:O2'	35:a:694:A:N7	2.38	0.51
36:b:8:ASP:O	36:b:12:ALA:CB	2.59	0.51
1:A:2683:C:OP1	15:P:51:ARG:NH2	2.43	0.51
1:A:2882:A:OP1	13:N:96:ARG:NH2	2.44	0.51
30:4:2:LYS:O	30:4:35:GLN:HA	2.11	0.51
39:e:157:ARG:NH1	42:h:43:GLU:OE2	2.44	0.51
1:A:370:G:O2'	1:A:424:G:OP1	2.29	0.51
1:A:1447:C:O2'	1:A:1544:A:N3	2.37	0.51
1:A:1980:G:O2'	1:A:1982:U:OP2	2.29	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2531:A:H61	1:A:2662:A:H61	1.59	0.51
1:A:1026:G:H2'	1:A:1027:A:H8	1.76	0.51
1:A:1090:A:H2'	1:A:1091:G:H8	1.76	0.51
1:A:2347:C:N3	1:A:2371:G:N2	2.59	0.51
2:B:111:U:H2'	2:B:112:G:H8	1.76	0.51
7:G:164:TYR:HB2	7:G:167:GLU:HB2	1.92	0.51
24:Y:11:VAL:HA	24:Y:14:LEU:HD12	1.93	0.51
41:g:90:GLU:OE2	41:g:96:ARG:NH2	2.44	0.51
42:h:18:GLN:HE21	42:h:72:VAL:HG22	1.76	0.51
47:m:13:LYS:HB2	47:m:18:ALA:HB2	1.92	0.51
1:A:1607:C:N4	1:A:1622:G:OP2	2.38	0.51
1:A:2609:U:H2'	33:7:1:MET:CE	2.40	0.51
14:O:66:GLY:O	14:O:102:ARG:NH2	2.43	0.51
42:h:54:ASP:OD1	42:h:54:ASP:N	2.36	0.51
1:A:2855:C:H2'	1:A:2856:A:H8	1.76	0.50
15:P:113:ARG:HG2	15:P:115:ASN:HB3	1.93	0.50
35:a:1038:C:H2'	35:a:1039:G:C8	2.46	0.50
1:A:2364:C:OP1	22:W:55:ARG:NH1	2.40	0.50
7:G:103:ILE:O	7:G:114:ASP:HA	2.11	0.50
35:a:110:C:O2'	50:p:25:ARG:O	2.27	0.50
35:a:235:C:H2'	35:a:236:A:C8	2.46	0.50
35:a:458:U:O4	35:a:474:G:O6	2.29	0.50
39:e:150:PRO:HA	39:e:153:VAL:HG12	1.93	0.50
6:F:23:ASN:N	6:F:27:GLN:OE1	2.44	0.50
12:M:66:ARG:NH1	12:M:104:GLU:OE2	2.43	0.50
24:Y:11:VAL:O	24:Y:15:ASN:ND2	2.44	0.50
55:u:55:ARG:O	55:u:59:LYS:HB2	2.11	0.50
56:v:26:U:O2	56:v:27:A:C8	2.65	0.50
1:A:537:G:H22	1:A:555:G:H2'	1.77	0.50
1:A:1363:C:O2'	1:A:1809:A:N3	2.35	0.50
35:a:1090:U:O2'	35:a:1171:A:O2'	2.29	0.50
47:m:25:VAL:HG23	47:m:29:ARG:HB3	1.94	0.50
1:A:1266:G:O2'	1:A:2012:G:O6	2.27	0.50
1:A:1788:C:OP1	3:C:221:ARG:NH2	2.44	0.50
6:F:33:LYS:HE2	6:F:157:THR:HG21	1.94	0.50
35:a:1356:G:H2'	35:a:1357:A:C8	2.47	0.50
50:p:14:ARG:HE	50:p:42:ILE:HD11	1.76	0.50
53:s:12:ASP:OD1	53:s:38:SER:OG	2.27	0.50
10:K:107:LEU:HG	10:K:112:PHE:HB3	1.93	0.50
30:4:8:LYS:O	30:4:35:GLN:NE2	2.45	0.50
35:a:1052:U:H3	35:a:1206:G:H1	1.59	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:c:24:ALA:HB1	37:c:28:GLU:HB3	1.93	0.50
41:g:150:ALA:HB1	45:k:59:THR:HG21	1.94	0.50
47:m:90:ARG:HB2	47:m:97:VAL:HG12	1.92	0.50
1:A:931:U:OP1	25:Z:30:ARG:NH1	2.41	0.50
45:k:47:ALA:HB1	45:k:62:ALA:HB1	1.93	0.50
1:A:1218:G:O6	1:A:1231:U:O2	2.29	0.50
1:A:1652:A:N6	13:N:11:ASN:OD1	2.41	0.50
35:a:745:G:H2'	35:a:746:A:H8	1.76	0.50
36:b:74:ARG:O	36:b:77:SER:OG	2.21	0.50
40:f:25:TYR:O	40:f:28:ALA:HB3	2.12	0.50
45:k:36:ASP:OD1	45:k:40:ASN:N	2.44	0.50
45:k:86:VAL:HG21	45:k:93:ARG:HB3	1.94	0.50
1:A:441:U:O2'	5:E:41:GLN:NE2	2.45	0.50
1:A:1013:C:H2'	1:A:1014:A:H8	1.76	0.50
7:G:43:VAL:HA	7:G:51:THR:O	2.12	0.50
20:U:33:LYS:HB3	20:U:64:ALA:HB1	1.94	0.50
37:c:67:THR:HA	37:c:102:ASN:O	2.11	0.50
40:f:9:MET:HA	40:f:58:HIS:O	2.12	0.50
1:A:151:C:H2'	1:A:152:A:H8	1.77	0.49
1:A:561:G:HO2'	16:Q:45:TYR:HH	1.60	0.49
1:A:1062:G:O6	1:A:1077:A:N6	2.45	0.49
1:A:2263:C:N4	22:W:15:ASP:OD1	2.42	0.49
2:B:5:U:OP1	2:B:61:G:O2'	2.29	0.49
3:C:57:GLY:HA2	3:C:213:TRP:HA	1.94	0.49
27:1:37:LYS:HA	27:1:48:ILE:HA	1.94	0.49
34:8:34:U:H5''	43:i:130:ARG:NH2	2.27	0.49
35:a:356:A:N3	35:a:368:U:O2'	2.40	0.49
35:a:1360:A:OP2	48:n:75:ARG:NH2	2.43	0.49
47:m:96:PRO:HB2	47:m:100:GLN:HE21	1.76	0.49
52:r:71:THR:OG1	52:r:72:ASP:N	2.45	0.49
1:A:2140:G:H2'	1:A:2141:G:H8	1.77	0.49
15:P:98:TYR:HA	15:P:101:ARG:HG3	1.94	0.49
34:8:42:U:O2'	35:a:1338:G:N2	2.41	0.49
35:a:673:A:H2'	35:a:674:G:C8	2.47	0.49
1:A:1501:G:H2'	1:A:1502:A:H8	1.77	0.49
8:H:30:LEU:HB3	8:H:36:ALA:HB3	1.93	0.49
13:N:30:ARG:O	13:N:78:LYS:NZ	2.45	0.49
35:a:1062:U:O4	37:c:2:GLY:N	2.44	0.49
41:g:22:LEU:HD12	41:g:23:LEU:HG	1.94	0.49
49:o:26:GLU:OE2	49:o:77:ARG:NH1	2.45	0.49
50:p:41:PRO:HG2	50:p:42:ILE:HG23	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:184:C:H2'	1:A:185:G:H8	1.76	0.49
1:A:787:C:H5''	1:A:788:A:H5'	1.94	0.49
1:A:1040:A:H2	1:A:1115:G:H22	1.60	0.49
4:D:9:VAL:HA	4:D:197:THR:HG23	1.94	0.49
6:F:148:ARG:HB3	6:F:150:ARG:HG3	1.94	0.49
33:7:1:MET:HB2	57:7:101:ERY:C17	2.34	0.49
3:C:62:TYR:HA	3:C:86:ASN:HD21	1.78	0.49
23:X:40:VAL:HG12	23:X:42:SER:H	1.76	0.49
35:a:437:U:O2'	38:d:120:HIS:ND1	2.41	0.49
35:a:1316:G:N1	35:a:1319:A:OP2	2.44	0.49
1:A:1433:A:N1	1:A:1560:G:O6	2.45	0.49
18:S:35:ILE:O	18:S:39:THR:OG1	2.31	0.49
50:p:54:LEU:HA	50:p:57:ILE:HG12	1.95	0.49
1:A:276:U:O2'	1:A:278:A:N6	2.46	0.49
1:A:404:A:N6	1:A:421:C:O2'	2.46	0.49
1:A:516:C:OP1	26:0:10:ARG:NH1	2.46	0.49
10:K:4:GLU:HG2	10:K:23:LYS:HA	1.94	0.49
1:A:1225:G:OP1	17:R:71:LYS:NZ	2.43	0.49
1:A:2391:G:H2'	1:A:2424:C:H41	1.77	0.49
15:P:23:GLY:H	15:P:47:VAL:HG23	1.76	0.49
1:A:1744:A:H3'	1:A:1745:A:H8	1.77	0.49
1:A:2375:G:N2	1:A:2378:A:OP2	2.44	0.49
35:a:505:G:H5'	35:a:534:U:H2'	1.94	0.49
1:A:572:A:H5'	17:R:79:ARG:HH12	1.78	0.49
7:G:101:ASN:ND2	7:G:116:GLN:OE1	2.46	0.49
1:A:299:A:N1	1:A:322:A:O2'	2.42	0.48
1:A:1131:G:O2'	1:A:2025:C:O2'	2.23	0.48
1:A:1434:A:H2'	1:A:1435:G:C8	2.48	0.48
5:E:119:ILE:HB	5:E:187:VAL:HG12	1.95	0.48
6:F:160:ALA:HB1	6:F:165:GLU:HB3	1.95	0.48
11:L:91:ASP:HB3	11:L:123:ARG:HB3	1.95	0.48
35:a:1523:G:OP2	45:k:128:ARG:NH2	2.46	0.48
52:r:11:CYS:SG	52:r:12:ARG:N	2.86	0.48
1:A:372:G:O2'	1:A:400:G:O6	2.31	0.48
1:A:2101:A:N6	1:A:2189:U:O4	2.46	0.48
1:A:2312:U:O2	6:F:37:ASN:ND2	2.43	0.48
2:B:95:U:H2'	2:B:96:G:H8	1.77	0.48
34:8:35:G:OP2	43:i:129:LYS:NZ	2.45	0.48
35:a:1317:C:N3	48:n:53:ARG:NH1	2.61	0.48
1:A:691:C:OP1	3:C:217:ARG:NH1	2.46	0.48
1:A:964:C:O2'	1:A:2273:A:N3	2.40	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1227:G:OP1	16:Q:13:ARG:NH2	2.46	0.48
15:P:60:THR:HA	15:P:73:VAL:HA	1.95	0.48
15:P:91:ALA:HB2	15:P:113:ARG:HA	1.95	0.48
22:W:66:LYS:O	22:W:82:ILE:HA	2.14	0.48
35:a:714:G:H2'	35:a:715:A:C8	2.48	0.48
35:a:836:G:O6	35:a:850:U:O4	2.31	0.48
35:a:946:A:H2'	35:a:947:G:H8	1.77	0.48
35:a:1297:G:N2	41:g:114:LYS:O	2.47	0.48
1:A:480:A:O2'	20:U:43:LYS:O	2.30	0.48
1:A:1508:A:O2'	1:A:1509:A:O4'	2.31	0.48
20:U:86:ARG:NH2	20:U:102:THR:OG1	2.46	0.48
35:a:1242:G:H1	35:a:1295:U:H3	1.60	0.48
45:k:81:ASN:N	45:k:81:ASN:OD1	2.46	0.48
48:n:12:LYS:HB2	48:n:12:LYS:HE3	1.60	0.48
1:A:514:A:N3	1:A:581:C:O2'	2.40	0.48
1:A:1434:A:H2'	1:A:1435:G:H8	1.77	0.48
1:A:1791:A:N6	1:A:1828:G:O2'	2.43	0.48
18:S:88:ARG:NH2	18:S:94:ASP:OD1	2.47	0.48
30:4:3:VAL:HG12	30:4:36:ARG:HB3	1.96	0.48
35:a:1061:G:N7	37:c:2:GLY:N	2.61	0.48
52:r:70:TYR:H	52:r:74:HIS:HE1	1.61	0.48
1:A:145:C:H2'	1:A:146:A:C8	2.48	0.48
1:A:1181:U:H2'	1:A:1182:G:C8	2.48	0.48
1:A:1187:G:OP1	17:R:85:LYS:NZ	2.35	0.48
1:A:1296:G:OP1	1:A:2709:G:O2'	2.24	0.48
7:G:11:VAL:HG23	7:G:76:VAL:HG21	1.95	0.48
15:P:53:ARG:HB2	15:P:56:HIS:HB2	1.95	0.48
35:a:972:C:OP2	44:j:59:LYS:NZ	2.46	0.48
35:a:1200:C:H5''	35:a:1201:A:H3'	1.95	0.48
35:a:1347:G:O2'	35:a:1373:G:O6	2.30	0.48
39:e:122:ASN:N	39:e:122:ASN:OD1	2.44	0.48
56:v:59:A:C2	56:v:62:C:C6	3.01	0.48
1:A:888:C:C6	47:m:92:ARG:HD2	2.49	0.48
3:C:71:LYS:O	3:C:118:SER:OG	2.26	0.48
26:0:54:VAL:HG23	26:0:55:ILE:HD12	1.96	0.48
35:a:362:G:N2	35:a:365:U:OP2	2.47	0.48
36:b:9:MET:HE3	36:b:9:MET:HB2	1.80	0.48
1:A:483:A:O2'	20:U:57:GLY:N	2.47	0.48
1:A:2419:U:OP1	29:3:41:LYS:NZ	2.47	0.48
16:Q:70:ARG:NH2	16:Q:75:SER:OG	2.47	0.48
34:8:9:G:O4'	34:8:22:G:N2	2.47	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:a:754:C:OP1	49:o:72:ARG:NH2	2.47	0.48
35:a:1254:A:H2'	35:a:1255:G:H8	1.79	0.48
12:M:17:ASN:OD1	12:M:97:GLN:NE2	2.46	0.48
13:N:49:GLU:HG2	13:N:94:TYR:HD2	1.78	0.48
35:a:1425:U:H2'	35:a:1426:G:H8	1.79	0.48
53:s:44:MET:HE2	53:s:44:MET:HB3	1.72	0.48
1:A:2504:U:H3	33:7:6:ARG:HH12	1.60	0.47
10:K:64:ARG:HB2	10:K:83:ALA:HB3	1.95	0.47
37:c:153:VAL:HG22	37:c:198:VAL:HG22	1.95	0.47
1:A:411:G:OP2	1:A:2406:A:O2'	2.31	0.47
1:A:721:A:H2'	1:A:722:A:C8	2.50	0.47
1:A:1629:U:O4	1:A:1630:A:N6	2.47	0.47
8:H:96:THR:HA	8:H:99:ILE:HG22	1.96	0.47
40:f:49:TYR:OH	52:r:63:ARG:O	2.28	0.47
1:A:249:C:O2	29:3:12:LYS:NZ	2.47	0.47
1:A:1378:A:O2'	1:A:1380:G:OP2	2.31	0.47
6:F:24:SER:N	6:F:27:GLN:OE1	2.47	0.47
7:G:86:LYS:HB3	7:G:165:ALA:HB2	1.95	0.47
35:a:843:U:H5'	35:a:844:G:C8	2.49	0.47
35:a:958:A:N3	35:a:985:C:O2'	2.47	0.47
36:b:66:LYS:HB3	36:b:90:PHE:HE2	1.79	0.47
1:A:910:A:N3	1:A:2264:C:O2'	2.46	0.47
1:A:2291:U:OP1	1:A:2380:C:O2'	2.33	0.47
35:a:107:G:OP1	35:a:325:A:N6	2.47	0.47
39:e:131:THR:O	39:e:131:THR:OG1	2.32	0.47
40:f:6:ILE:HG12	40:f:89:VAL:HG22	1.96	0.47
1:A:1155:A:H5''	16:Q:55:ARG:HD3	1.97	0.47
1:A:1178:C:H2'	1:A:1179:G:H8	1.79	0.47
3:C:262:ARG:O	3:C:265:LYS:NZ	2.48	0.47
14:O:95:SER:O	14:O:95:SER:OG	2.30	0.47
35:a:1058:G:H1	35:a:1199:U:H3	1.60	0.47
35:a:1060:U:OP1	48:n:85:ARG:NH2	2.47	0.47
39:e:12:GLN:HG3	39:e:117:VAL:HG23	1.95	0.47
56:v:28:C:H2'	56:v:29:U:H6	1.79	0.47
1:A:45:G:H5''	1:A:46:G:H5'	1.96	0.47
1:A:636:G:OP2	11:L:109:LYS:NZ	2.45	0.47
1:A:1124:G:O2'	30:4:37:GLN:O	2.33	0.47
1:A:1721:G:O2'	1:A:1739:A:N6	2.48	0.47
35:a:231:U:H2'	35:a:232:G:H8	1.79	0.47
36:b:139:ARG:O	36:b:142:GLU:HB3	2.15	0.47
1:A:1177:G:O2'	1:A:1178:C:O5'	2.28	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1668:A:N3	1:A:1670:C:N4	2.62	0.47
1:A:1709:U:H2'	1:A:1710:G:H8	1.80	0.47
1:A:1857:G:H22	1:A:1884:G:H2'	1.79	0.47
1:A:2032:G:N2	4:D:151:THR:OG1	2.47	0.47
10:K:30:ARG:NH2	10:K:37:ASP:OD2	2.48	0.47
13:N:32:GLU:HG3	13:N:115:LEU:HD12	1.96	0.47
35:a:459:A:H2'	35:a:460:A:H8	1.80	0.47
35:a:675:A:O2'	45:k:116:ILE:O	2.29	0.47
35:a:836:G:H1	35:a:850:U:H3	1.63	0.47
37:c:44:THR:O	37:c:48:ALA:CB	2.62	0.47
45:k:114:THR:HG21	55:u:28:VAL:HG13	1.96	0.47
1:A:585:G:N7	16:Q:6:ARG:NH1	2.62	0.47
1:A:2595:G:N2	1:A:2598:A:OP2	2.40	0.47
2:B:39:A:O2'	2:B:46:A:N1	2.45	0.47
4:D:25:THR:OG1	4:D:191:GLY:O	2.30	0.47
34:8:51:A:C2'	47:m:112:PRO:HD2	2.45	0.47
35:a:195:A:H2'	35:a:196:A:C8	2.50	0.47
36:b:114:LEU:HD12	36:b:144:LEU:HD22	1.96	0.47
1:A:851:C:O2'	25:Z:43:ALA:O	2.33	0.47
35:a:122:G:O6	35:a:239:U:O2	2.33	0.47
35:a:1011:C:H2'	35:a:1012:A:H8	1.80	0.47
37:c:153:VAL:HG12	37:c:157:LEU:HD22	1.97	0.47
38:d:85:ASN:HD22	38:d:88:GLU:HB2	1.79	0.47
38:d:95:GLU:HG3	38:d:191:LEU:HD22	1.96	0.47
45:k:59:THR:HG23	45:k:62:ALA:H	1.79	0.47
50:p:70:ARG:HH21	50:p:74:LEU:HD21	1.80	0.47
1:A:752:A:OP1	28:2:3:ARG:NH1	2.47	0.47
13:N:83:LEU:HD21	13:N:115:LEU:HD13	1.96	0.47
15:P:65:SER:O	15:P:67:GLY:N	2.48	0.47
35:a:279:A:H5''	35:a:280:C:H3'	1.96	0.47
35:a:297:G:H4'	35:a:557:G:H4'	1.96	0.47
36:b:74:ARG:O	36:b:77:SER:CB	2.62	0.47
1:A:1433:A:H2'	1:A:1434:A:C8	2.50	0.46
1:A:1999:C:O2	1:A:2687:U:O2'	2.30	0.46
1:A:2204:G:H4'	3:C:150:LYS:HD3	1.96	0.46
1:A:2500:U:O2	1:A:2504:U:C5	2.68	0.46
4:D:108:ASP:HB2	4:D:173:GLN:HA	1.96	0.46
4:D:139:SER:O	4:D:139:SER:OG	2.28	0.46
6:F:163:ASP:O	6:F:167:ARG:HB2	2.15	0.46
35:a:977:A:O2'	35:a:979:C:OP2	2.33	0.46
1:A:476:G:N1	1:A:479:A:OP2	2.42	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:535:G:O3'	16:Q:53:ARG:NH1	2.48	0.46
1:A:1090:A:H2'	1:A:1091:G:C8	2.51	0.46
1:A:2123:G:O2'	1:A:2176:A:N1	2.48	0.46
1:A:2343:U:O2'	1:A:2373:G:O2'	2.31	0.46
21:V:9:ARG:HG2	21:V:41:GLU:HB2	1.96	0.46
21:V:44:HIS:O	21:V:48:MET:HB2	2.15	0.46
35:a:83:C:O2	35:a:86:G:C2	2.67	0.46
35:a:606:G:N2	35:a:632:U:OP1	2.33	0.46
55:u:7:ARG:NH1	55:u:10:GLU:OE1	2.49	0.46
1:A:1437:C:HO2'	1:A:1516:G:HO2'	1.60	0.46
1:A:2035:G:H5''	1:A:2036:C:H5	1.79	0.46
2:B:5:U:H2'	2:B:6:G:H8	1.81	0.46
3:C:162:VAL:HG11	3:C:174:LEU:HD13	1.98	0.46
5:E:34:ALA:HA	5:E:94:GLN:HE21	1.80	0.46
35:a:1033:G:H3'	35:a:1034:G:H8	1.80	0.46
35:a:1254:A:H2'	35:a:1255:G:C8	2.51	0.46
40:f:22:ILE:HA	40:f:25:TYR:HB2	1.97	0.46
40:f:35:LYS:HE3	40:f:35:LYS:HB3	1.81	0.46
52:r:72:ASP:N	52:r:72:ASP:OD1	2.46	0.46
53:s:27:ASP:OD1	53:s:27:ASP:N	2.43	0.46
2:B:93:C:H2'	2:B:94:A:H8	1.81	0.46
7:G:71:LEU:O	7:G:75:MET:HB2	2.15	0.46
13:N:2:ARG:NH2	13:N:5:LYS:O	2.47	0.46
16:Q:49:ASP:HA	16:Q:52:GLN:HB2	1.97	0.46
35:a:946:A:H2'	35:a:947:G:C8	2.51	0.46
46:l:114:ARG:HB3	46:l:119:VAL:HB	1.97	0.46
53:s:35:SER:O	53:s:35:SER:OG	2.29	0.46
1:A:276:U:H4'	1:A:278:A:H62	1.80	0.46
1:A:1026:G:H2'	1:A:1027:A:C8	2.51	0.46
1:A:1037:G:H2'	1:A:1038:G:H8	1.81	0.46
1:A:1824:G:OP1	3:C:52:ARG:NH2	2.49	0.46
1:A:2131:U:H5'	1:A:2132:U:H5''	1.96	0.46
2:B:116:G:H4'	14:O:54:VAL:HG12	1.98	0.46
18:S:29:VAL:HB	18:S:55:ILE:HD11	1.96	0.46
35:a:715:A:H2'	35:a:716:A:C8	2.50	0.46
48:n:16:LEU:HB3	48:n:55:SER:HB3	1.98	0.46
52:r:34:THR:OG1	52:r:35:GLU:N	2.49	0.46
1:A:566:U:H5''	11:L:29:LYS:HE3	1.98	0.46
35:a:262:A:H5'	54:t:68:HIS:HB3	1.97	0.46
35:a:538:G:H2'	35:a:539:A:H8	1.80	0.46
1:A:414:C:H2'	1:A:415:A:C8	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1798:U:O2'	1:A:1802:A:N3	2.43	0.46
49:o:64:ARG:NH1	49:o:89:ARG:OXT	2.48	0.46
1:A:617:G:OP1	5:E:102:ARG:NH1	2.49	0.46
34:8:51:A:O2'	47:m:112:PRO:HD2	2.16	0.46
35:a:1125:U:H2'	35:a:1126:U:H2'	1.98	0.46
35:a:1144:G:N2	35:a:1146:A:H62	2.14	0.46
36:b:95:ARG:HG2	36:b:97:LEU:H	1.80	0.46
38:d:29:ASP:OD2	38:d:29:ASP:N	2.47	0.46
1:A:882:G:H22	1:A:894:U:H3	1.63	0.46
1:A:948:C:H2'	1:A:949:G:H8	1.81	0.46
1:A:2371:G:O2'	27:1:46:HIS:ND1	2.43	0.46
3:C:157:SER:OG	3:C:158:ALA:N	2.46	0.46
35:a:377:G:H2'	35:a:378:G:H8	1.81	0.46
35:a:740:U:H2'	35:a:741:G:H8	1.81	0.46
38:d:56:ARG:HD3	38:d:56:ARG:HA	1.66	0.46
40:f:3:HIS:HA	40:f:64:VAL:O	2.16	0.46
50:p:44:SER:OG	50:p:45:GLU:O	2.30	0.46
1:A:458:G:O2'	1:A:469:G:O6	2.31	0.46
1:A:793:A:OP2	1:A:2071:A:O2'	2.33	0.46
1:A:2100:G:H2'	1:A:2101:A:H8	1.81	0.46
26:0:29:SER:HB3	26:0:40:ARG:HD3	1.98	0.46
35:a:951:G:N7	47:m:101:ARG:NH2	2.63	0.46
38:d:170:TRP:HA	38:d:184:ARG:HG2	1.98	0.46
56:v:53:G:C2	56:v:54:G:C8	3.04	0.46
1:A:33:C:N4	1:A:446:G:O2'	2.36	0.45
1:A:848:C:H2'	1:A:849:A:C8	2.50	0.45
1:A:1463:C:H2'	1:A:1464:G:H8	1.80	0.45
35:a:757:U:OP1	35:a:822:U:O2'	2.31	0.45
43:i:12:ARG:HH11	43:i:13:LYS:HB2	1.79	0.45
50:p:77:GLU:O	50:p:81:ALA:HB2	2.15	0.45
56:v:20:A:C6	56:v:58:G:C2	3.04	0.45
1:A:948:C:O2	1:A:984:A:O2'	2.30	0.45
1:A:1069:A:O2'	1:A:1073:A:OP1	2.34	0.45
1:A:1324:G:O2'	1:A:1326:U:OP2	2.24	0.45
1:A:1862:G:H2'	1:A:1863:G:H8	1.81	0.45
17:R:68:ARG:HD3	17:R:90:ARG:HB3	1.98	0.45
20:U:52:LEU:O	20:U:54:GLN:NE2	2.49	0.45
35:a:87:C:O2'	35:a:88:U:O4'	2.34	0.45
36:b:66:LYS:NZ	36:b:154:MET:O	2.48	0.45
38:d:104:ARG:HB3	38:d:171:LEU:HD21	1.97	0.45
54:t:28:MET:HE2	54:t:28:MET:HB3	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:373:U:H2'	1:A:374:A:H8	1.81	0.45
1:A:2320:U:C2	1:A:2333:A:N6	2.84	0.45
41:g:4:ARG:HG2	41:g:5:ARG:HG3	1.97	0.45
1:A:598:U:H2'	1:A:599:A:C8	2.50	0.45
1:A:1250:G:OP2	11:L:21:ARG:NH1	2.48	0.45
2:B:112:G:N2	14:O:45:SER:O	2.48	0.45
23:X:7:VAL:O	23:X:74:ARG:NH2	2.49	0.45
23:X:68:LEU:HB3	23:X:72:ARG:HH12	1.81	0.45
39:e:82:GLN:HB2	39:e:83:HIS:HD2	1.80	0.45
39:e:133:PRO:HA	39:e:136:VAL:HG12	1.99	0.45
47:m:97:VAL:HG23	47:m:98:ARG:HG3	1.97	0.45
56:v:2:C:C2	56:v:3:A:C8	3.04	0.45
1:A:693:A:O2'	1:A:1353:A:N3	2.39	0.45
1:A:1550:C:H2'	1:A:1551:A:C8	2.52	0.45
1:A:1709:U:H2'	1:A:1710:G:C8	2.52	0.45
1:A:2452:C:N3	33:7:6:ARG:NH1	2.65	0.45
35:a:811:C:O2'	35:a:901:A:N1	2.49	0.45
38:d:87:GLY:HA3	38:d:197:GLU:HG3	1.97	0.45
50:p:75:ILE:O	50:p:79:ASN:HB2	2.16	0.45
54:t:57:ILE:HD13	54:t:60:ARG:HH22	1.82	0.45
56:v:28:C:C2	56:v:29:U:C5	3.04	0.45
1:A:639:U:H2'	1:A:640:C:H6	1.81	0.45
1:A:1219:U:OP2	16:Q:19:LYS:NZ	2.44	0.45
1:A:2639:A:N6	1:A:2775:G:O2'	2.50	0.45
4:D:2:ILE:HG21	4:D:48:ILE:HD11	1.98	0.45
35:a:501:C:OP1	46:l:114:ARG:NH2	2.34	0.45
35:a:744:C:H2'	35:a:745:G:H8	1.81	0.45
39:e:86:LYS:HD3	39:e:95:PHE:HD1	1.82	0.45
40:f:22:ILE:O	40:f:26:THR:N	2.41	0.45
40:f:39:LEU:HD23	40:f:39:LEU:HA	1.85	0.45
1:A:926:G:H2'	1:A:927:A:C8	2.51	0.45
1:A:1849:G:H2'	1:A:1850:G:H8	1.82	0.45
1:A:2591:C:N4	1:A:2592:G:O6	2.50	0.45
4:D:11:MET:HE2	4:D:11:MET:HB3	1.80	0.45
35:a:461:A:H2'	35:a:462:G:H8	1.81	0.45
46:l:56:ARG:HA	46:l:62:GLU:HA	1.98	0.45
1:A:287:G:H2'	1:A:288:U:C6	2.52	0.45
3:C:252:THR:OG1	3:C:253:LYS:N	2.50	0.45
15:P:92:VAL:HG11	15:P:97:LEU:HD11	1.98	0.45
35:a:459:A:H2'	35:a:460:A:C8	2.52	0.45
36:b:163:VAL:HG11	36:b:173:ILE:HD11	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
56:v:50:G:H2'	56:v:51:G:C8	2.52	0.45
56:v:52:A:H2'	56:v:53:G:C8	2.52	0.45
1:A:2813:A:H2'	1:A:2814:A:H8	1.82	0.45
1:A:2885:G:O6	26:0:40:ARG:NH2	2.50	0.45
31:5:11:GLU:HA	31:5:25:ARG:HA	1.99	0.45
41:g:123:GLU:O	41:g:127:ALA:N	2.49	0.45
1:A:987:C:O2'	1:A:1000:A:N3	2.43	0.45
1:A:2246:G:H2'	1:A:2247:A:H8	1.82	0.45
4:D:11:MET:HG2	4:D:25:THR:HG23	1.99	0.45
17:R:54:VAL:HG23	17:R:55:ASP:H	1.82	0.45
35:a:546:A:P	38:d:69:GLU:HB3	2.57	0.45
37:c:73:PRO:HG3	37:c:105:GLU:HB2	1.99	0.45
55:u:62:ARG:HD2	55:u:66:ARG:HD3	1.99	0.45
1:A:805:G:H5''	11:L:38:GLN:HG3	1.98	0.44
1:A:1351:C:O2'	1:A:1571:A:N3	2.42	0.44
4:D:27:ILE:HD12	4:D:187:LEU:HD23	1.99	0.44
10:K:71:ARG:HD3	10:K:75:SER:HB2	1.99	0.44
11:L:1:MET:HG3	11:L:6:LEU:HD21	2.00	0.44
35:a:1160:G:H1	35:a:1176:A:H61	1.65	0.44
35:a:1373:G:H4'	41:g:31:MET:HE1	1.99	0.44
35:a:1441:A:H62	35:a:1461:G:H21	1.65	0.44
47:m:54:ASP:HA	47:m:57:ARG:HB2	1.98	0.44
53:s:17:LYS:HE3	53:s:17:LYS:HB2	1.81	0.44
1:A:272:A:H2'	1:A:273:G:C8	2.52	0.44
1:A:624:C:O2'	1:A:657:U:OP1	2.35	0.44
22:W:37:ILE:HD11	22:W:82:ILE:HD11	1.97	0.44
35:a:406:G:N7	35:a:495:A:O2'	2.38	0.44
35:a:652:U:O4	35:a:752:G:O2'	2.31	0.44
35:a:1071:C:H2'	35:a:1072:G:H8	1.82	0.44
41:g:30:LEU:HD23	41:g:39:ALA:HB1	1.99	0.44
55:u:31:GLU:OE1	55:u:35:ARG:NE	2.50	0.44
6:F:123:ASP:OD2	6:F:127:ASN:ND2	2.45	0.44
35:a:257:G:H2'	35:a:258:G:H8	1.83	0.44
35:a:1001:C:H2'	35:a:1002:G:H8	1.81	0.44
1:A:596:U:H2'	1:A:597:G:H8	1.82	0.44
1:A:1463:C:H2'	1:A:1464:G:C8	2.52	0.44
1:A:1889:A:H2'	1:A:1890:A:C8	2.52	0.44
11:L:85:VAL:HG11	11:L:90:VAL:HG22	2.00	0.44
21:V:65:VAL:O	21:V:68:LYS:NZ	2.43	0.44
34:8:55:G:H2'	34:8:56:G:C8	2.52	0.44
35:a:1015:G:H2'	35:a:1016:A:C8	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:a:1077:G:N2	35:a:1080:A:OP2	2.43	0.44
56:v:52:A:H2'	56:v:53:G:H8	1.81	0.44
1:A:144:A:H5''	19:T:2:ILE:HD11	1.99	0.44
1:A:833:A:H2'	1:A:834:G:C8	2.53	0.44
4:D:37:VAL:HG22	4:D:48:ILE:HG22	1.99	0.44
50:p:20:VAL:HA	50:p:35:ARG:HA	1.98	0.44
53:s:21:LYS:HD2	53:s:21:LYS:HA	1.79	0.44
56:v:2:C:O2	56:v:2:C:C2'	2.62	0.44
1:A:813:U:H2'	1:A:814:C:H6	1.83	0.44
20:U:96:PHE:CE2	20:U:103:ILE:HG12	2.53	0.44
21:V:72:VAL:HB	21:V:91:PHE:HB3	2.00	0.44
27:1:10:LYS:HA	27:1:22:THR:HA	2.00	0.44
35:a:264:C:H4'	51:q:65:ARG:HD2	2.00	0.44
35:a:745:G:H2'	35:a:746:A:C8	2.53	0.44
35:a:1041:G:H2'	35:a:1042:A:C8	2.52	0.44
35:a:1342:C:H2'	35:a:1343:G:C8	2.53	0.44
56:v:67:C:H2'	56:v:68:G:H8	1.82	0.44
1:A:767:U:H2'	1:A:768:G:H8	1.82	0.44
6:F:134:GLU:OE1	6:F:135:GLN:N	2.49	0.44
15:P:13:MET:HG3	15:P:55:LEU:HD13	1.99	0.44
27:1:11:LEU:HA	27:1:50:LYS:O	2.18	0.44
35:a:198:G:O6	35:a:219:U:O4	2.36	0.44
35:a:1118:U:H2'	35:a:1119:C:H6	1.82	0.44
38:d:118:VAL:HG23	38:d:123:ILE:HD11	2.00	0.44
56:v:25:G:C2	56:v:26:U:C1'	2.98	0.44
1:A:1178:C:H2'	1:A:1179:G:C8	2.53	0.44
1:A:2087:G:H2'	1:A:2088:A:H8	1.83	0.44
1:A:2619:C:H5''	4:D:157:LYS:HA	2.00	0.44
1:A:2646:C:OP2	1:A:2732:G:O2'	2.36	0.44
5:E:128:ALA:HB3	5:E:133:LEU:HD12	1.99	0.44
8:H:84:ALA:HA	8:H:91:PHE:H	1.83	0.44
18:S:17:VAL:HG12	18:S:76:VAL:HG21	1.99	0.44
21:V:62:THR:HG23	21:V:69:GLU:HB2	2.00	0.44
57:7:101:ERY:H71	57:7:101:ERY:H4	1.72	0.44
35:a:765:G:N1	35:a:812:G:O2'	2.44	0.44
35:a:825:A:O2'	42:h:9:ASP:OD1	2.31	0.44
35:a:1159:U:O4'	35:a:1182:G:N2	2.50	0.44
56:v:20:A:N6	56:v:58:G:C6	2.86	0.44
1:A:993:G:OP2	16:Q:51:ARG:NH2	2.51	0.44
26:0:34:SER:HB3	26:0:36:GLU:HG2	2.00	0.44
35:a:261:U:OP2	54:t:74:ARG:NH2	2.47	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:a:837:U:H2'	35:a:838:G:C8	2.50	0.44
35:a:1314:C:H2'	35:a:1315:U:C6	2.53	0.44
1:A:155:A:H2'	1:A:156:A:C8	2.53	0.43
1:A:263:G:O2'	1:A:429:A:N3	2.49	0.43
1:A:302:C:H2'	1:A:303:G:H8	1.84	0.43
1:A:598:U:H2'	1:A:599:A:H8	1.81	0.43
1:A:1278:C:H2'	1:A:1279:G:H8	1.83	0.43
1:A:1716:U:H2'	1:A:1717:A:C8	2.53	0.43
1:A:2287:A:OP1	27:1:30:LYS:NZ	2.47	0.43
3:C:155:ALA:HB2	3:C:162:VAL:HG23	2.00	0.43
5:E:105:LEU:HD23	5:E:105:LEU:HA	1.83	0.43
6:F:115:ARG:HG3	47:m:71:ARG:HH12	1.83	0.43
23:X:37:ARG:HG2	23:X:46:PHE:HB3	1.99	0.43
35:a:198:G:H2'	35:a:199:A:H8	1.83	0.43
35:a:254:G:OP1	51:q:70:THR:OG1	2.27	0.43
48:n:6:MET:SD	48:n:9:ARG:NH2	2.83	0.43
50:p:6:LEU:HD22	50:p:17:TYR:HB3	2.00	0.43
1:A:2182:U:H2'	1:A:2183:A:C8	2.53	0.43
1:A:2339:C:H2'	1:A:2340:A:C8	2.52	0.43
3:C:105:LEU:HD23	3:C:105:LEU:HA	1.84	0.43
8:H:69:ALA:HA	8:H:72:ILE:HG13	2.00	0.43
9:J:17:VAL:HG23	9:J:137:PRO:HB2	1.99	0.43
35:a:1040:U:H2'	35:a:1041:G:C8	2.53	0.43
35:a:1219:A:H2'	35:a:1220:G:C8	2.52	0.43
36:b:161:LEU:HD23	36:b:181:ILE:HG21	2.01	0.43
37:c:131:ARG:NE	37:c:166:GLU:OE2	2.42	0.43
1:A:2335:A:H5'	14:O:13:ARG:HH21	1.83	0.43
3:C:10:SER:O	3:C:14:ARG:N	2.51	0.43
7:G:44:LYS:HG2	7:G:51:THR:HG22	2.00	0.43
8:H:86:ASP:OD1	8:H:86:ASP:N	2.50	0.43
37:c:40:ARG:HG2	37:c:55:ILE:HD11	2.00	0.43
38:d:90:LEU:HD22	38:d:200:ILE:HG21	2.00	0.43
56:v:14:A:C5	56:v:23:G:C2	3.06	0.43
1:A:713:G:H21	1:A:718:A:H62	1.66	0.43
1:A:2233:U:H2'	1:A:2234:G:C8	2.53	0.43
1:A:2308:G:H2'	1:A:2310:C:H5	1.82	0.43
5:E:1:MET:HG2	5:E:16:GLU:HG3	1.99	0.43
13:N:103:ARG:HB3	13:N:108:ALA:H	1.83	0.43
14:O:40:ILE:HG12	14:O:47:VAL:HG12	1.99	0.43
35:a:297:G:N2	35:a:301:G:N7	2.67	0.43
38:d:106:GLY:HA3	38:d:162:ALA:HB2	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:924:G:H2'	1:A:925:A:H8	1.84	0.43
1:A:2081:U:H2'	1:A:2082:A:H8	1.83	0.43
2:B:95:U:H2'	2:B:96:G:C8	2.53	0.43
3:C:145:GLU:HB2	3:C:188:CYS:HB3	1.99	0.43
3:C:166:ALA:HB3	3:C:173:THR:HB	2.00	0.43
12:M:67:VAL:HG11	12:M:96:ILE:HD11	1.99	0.43
14:O:25:ARG:HE	14:O:40:ILE:HD12	1.83	0.43
19:T:6:ARG:HE	19:T:42:GLU:HG2	1.83	0.43
33:7:4:SER:CB	57:7:101:ERY:H24	2.49	0.43
35:a:187:G:N2	35:a:190:A:OP2	2.36	0.43
38:d:78:GLU:HA	38:d:81:ARG:HG2	1.99	0.43
42:h:63:LEU:HD13	42:h:63:LEU:HA	1.91	0.43
1:A:419:U:H2'	1:A:420:C:C6	2.53	0.43
1:A:2310:C:H2'	6:F:77:PHE:HE2	1.82	0.43
4:D:7:LYS:HB2	4:D:7:LYS:HE3	1.77	0.43
10:K:110:GLU:N	10:K:110:GLU:OE1	2.50	0.43
30:4:1:MET:HE2	30:4:36:ARG:HB2	2.01	0.43
35:a:120:A:O2'	35:a:122:G:N7	2.42	0.43
35:a:1160:G:H1	35:a:1176:A:N6	2.17	0.43
46:l:108:LYS:HA	46:l:108:LYS:HD3	1.79	0.43
1:A:176:A:H3'	1:A:177:G:N2	2.34	0.43
1:A:463:G:N2	1:A:466:A:OP2	2.50	0.43
1:A:1548:A:H2'	1:A:1549:A:C8	2.54	0.43
1:A:2093:G:H21	1:A:2198:A:N6	2.17	0.43
4:D:199:SER:OG	4:D:200:ASP:N	2.50	0.43
5:E:48:THR:HB	5:E:86:ALA:HB2	2.01	0.43
6:F:38:MET:HE3	6:F:152:LEU:HB3	2.00	0.43
12:M:38:ARG:HG3	12:M:98:PRO:HD3	2.01	0.43
35:a:413:G:H4'	35:a:414:A:H5'	2.00	0.43
35:a:1011:C:H2'	35:a:1012:A:C8	2.53	0.43
35:a:1223:C:H5''	35:a:1224:U:H5''	2.00	0.43
36:b:113:ARG:HD2	36:b:113:ARG:HA	1.77	0.43
1:A:172:A:H2'	1:A:173:A:C8	2.54	0.43
1:A:976:G:O2'	1:A:1155:A:O2'	2.32	0.43
1:A:1636:U:H2'	1:A:1637:A:C8	2.53	0.43
1:A:2328:A:H2'	1:A:2329:U:C6	2.53	0.43
1:A:2335:A:OP1	14:O:13:ARG:NE	2.49	0.43
20:U:34:VAL:HG13	20:U:67:VAL:HG22	2.00	0.43
31:5:56:ARG:HH12	53:s:69:HIS:CE1	2.37	0.43
35:a:438:U:H3	35:a:496:A:H62	1.66	0.43
35:a:1308:U:H2'	35:a:1309:G:H8	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:d:160:GLU:HA	38:d:163:GLU:HG2	2.00	0.43
39:e:106:ILE:HD11	39:e:124:LEU:HD22	2.00	0.43
1:A:729:G:H5'	1:A:730:A:H5''	2.01	0.43
9:J:93:ILE:HD13	9:J:93:ILE:HA	1.90	0.43
16:Q:87:SER:O	16:Q:87:SER:OG	2.36	0.43
35:a:222:C:H2'	35:a:223:A:C8	2.54	0.43
1:A:1254:A:H5''	1:A:1255:U:H5''	2.01	0.43
1:A:1358:G:N1	1:A:1372:U:OP2	2.37	0.43
1:A:2079:U:O2'	23:X:23:ASN:OD1	2.37	0.43
1:A:2330:G:H21	22:W:42:GLY:HA2	1.84	0.43
4:D:51:THR:HB	4:D:79:LEU:HD23	2.00	0.43
6:F:128:TYR:HE2	6:F:130:MET:HB3	1.84	0.43
22:W:37:ILE:HG22	22:W:38:VAL:HG23	2.00	0.43
22:W:41:ARG:HA	22:W:41:ARG:HD3	1.81	0.43
25:Z:9:GLN:HB2	25:Z:29:LEU:HD13	2.00	0.43
35:a:554:A:H2'	35:a:555:U:C6	2.54	0.43
35:a:1222:G:OP1	53:s:78:ARG:NH1	2.52	0.43
35:a:1363:A:O2'	35:a:1365:G:N7	2.49	0.43
37:c:20:SER:HG	37:c:40:ARG:HH21	1.66	0.43
54:t:5:LYS:HB3	54:t:5:LYS:HE3	1.89	0.43
1:A:2698:U:H2'	1:A:2699:C:C6	2.54	0.42
1:A:2810:A:H4'	4:D:62:LYS:HD2	2.00	0.42
2:B:49:C:H2'	2:B:50:A:H8	1.84	0.42
4:D:5:VAL:HG22	4:D:32:ASN:HD21	1.84	0.42
20:U:89:ASP:O	20:U:91:LYS:N	2.51	0.42
21:V:71:LYS:HB3	21:V:71:LYS:HE3	1.75	0.42
35:a:137:U:H2'	35:a:138:G:H8	1.84	0.42
35:a:166:U:H2'	35:a:167:A:C8	2.53	0.42
4:D:157:LYS:HE3	4:D:157:LYS:HB2	1.87	0.42
5:E:131:THR:HA	5:E:160:ALA:HB1	2.01	0.42
8:H:5:LEU:HD23	8:H:5:LEU:HA	1.90	0.42
17:R:57:GLY:HA2	17:R:102:SER:HB3	2.02	0.42
35:a:505:G:H2'	35:a:506:G:H8	1.83	0.42
35:a:1178:G:O2'	35:a:1180:A:N7	2.45	0.42
44:j:7:ARG:HB3	44:j:101:SER:O	2.19	0.42
1:A:1019:U:OP1	1:A:1035:U:O2'	2.31	0.42
5:E:21:ARG:HD3	5:E:106:LYS:HB3	2.00	0.42
8:H:70:GLU:HB2	8:H:134:VAL:HG21	2.00	0.42
17:R:7:SER:OG	17:R:8:GLY:N	2.51	0.42
35:a:476:U:H2'	35:a:477:C:C6	2.54	0.42
35:a:1120:C:H2'	35:a:1121:U:H6	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:151:C:H2'	1:A:152:A:C8	2.55	0.42
1:A:171:U:H2'	1:A:172:A:C8	2.55	0.42
1:A:741:U:H2'	1:A:742:A:C8	2.55	0.42
1:A:1037:G:H2'	1:A:1038:G:C8	2.54	0.42
1:A:1044:C:O2'	1:A:1111:A:N6	2.36	0.42
1:A:1358:G:O2'	1:A:1373:A:N6	2.52	0.42
15:P:39:ARG:NH2	35:a:346:G:OP1	2.46	0.42
19:T:11:LEU:O	24:Y:29:ARG:NH1	2.48	0.42
21:V:63:ILE:O	21:V:69:GLU:HA	2.20	0.42
35:a:412:A:H62	35:a:431:A:H61	1.66	0.42
37:c:11:ARG:O	37:c:16:LYS:N	2.46	0.42
37:c:56:VAL:HB	37:c:67:THR:HB	2.01	0.42
1:A:296:U:H2'	1:A:297:G:C8	2.52	0.42
6:F:49:LEU:O	6:F:150:ARG:NH2	2.52	0.42
7:G:72:LEU:HD23	7:G:72:LEU:HA	1.90	0.42
19:T:72:GLN:OE1	19:T:73:ARG:NH2	2.53	0.42
23:X:55:GLY:O	23:X:59:ILE:HG12	2.19	0.42
29:3:31:HIS:O	29:3:33:LEU:N	2.53	0.42
35:a:322:C:H2'	35:a:323:U:C6	2.54	0.42
35:a:672:U:H2'	35:a:673:A:C8	2.55	0.42
36:b:54:LEU:HD22	36:b:220:THR:HG21	2.02	0.42
37:c:83:ASP:HA	37:c:86:LYS:HD2	2.00	0.42
46:l:53:CYS:HB3	46:l:67:ILE:HD11	2.01	0.42
56:v:1:G:C2'	56:v:2:C:H6	2.30	0.42
1:A:910:A:H62	12:M:12:MET:HA	1.84	0.42
1:A:1112:G:H2'	1:A:1113:U:C6	2.54	0.42
1:A:1759:A:HO2'	1:A:2714:G:HO2'	1.66	0.42
35:a:197:A:N1	35:a:220:G:O2'	2.40	0.42
35:a:971:G:OP2	35:a:1231:G:N2	2.47	0.42
38:d:159:LEU:HD23	38:d:159:LEU:HA	1.78	0.42
41:g:22:LEU:H	41:g:22:LEU:HG	1.68	0.42
1:A:219:A:N3	1:A:234:U:O2'	2.46	0.42
1:A:1201:U:H2'	1:A:1202:G:H8	1.84	0.42
2:B:81:G:O6	2:B:95:U:O2	2.38	0.42
5:E:145:ASP:HA	5:E:166:LYS:HB3	2.02	0.42
35:a:88:U:H2'	35:a:89:U:C6	2.55	0.42
35:a:202:G:H21	35:a:466:A:H61	1.68	0.42
39:e:137:VAL:HA	39:e:140:THR:HG22	2.02	0.42
44:j:12:ALA:HB2	44:j:96:VAL:HG13	2.01	0.42
1:A:807:U:H5	11:L:41:ARG:HH22	1.68	0.42
1:A:1799:G:N7	3:C:178:SER:OG	2.45	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2809:A:H2'	1:A:2810:A:C8	2.55	0.42
34:8:32:C:O2'	35:a:1340:A:O2'	2.24	0.42
35:a:166:U:H2'	35:a:167:A:H8	1.85	0.42
1:A:438:G:H2'	1:A:439:A:C8	2.55	0.42
1:A:639:U:H2'	1:A:640:C:C6	2.55	0.42
1:A:995:C:OP2	16:Q:54:LYS:NZ	2.40	0.42
1:A:2039:U:H2'	1:A:2040:G:C8	2.55	0.42
1:A:2304:G:H22	1:A:2312:U:H3	1.68	0.42
3:C:16:VAL:HG23	3:C:206:GLY:HA3	2.02	0.42
5:E:59:PRO:HG3	5:E:73:ILE:HG23	2.02	0.42
12:M:134:THR:OG1	21:V:79:ARG:NH2	2.53	0.42
13:N:107:ASN:OD1	18:S:40:ASN:ND2	2.53	0.42
20:U:12:ILE:HD11	20:U:80:ALA:HB2	2.01	0.42
22:W:18:ALA:O	22:W:20:ARG:NH1	2.53	0.42
35:a:499:A:O4'	35:a:547:A:N6	2.52	0.42
35:a:546:A:O2'	35:a:548:G:O2'	2.29	0.42
35:a:884:U:H4'	35:a:885:G:H5''	2.01	0.42
35:a:1279:G:H5''	44:j:9:ARG:NH1	2.34	0.42
37:c:94:ILE:HD12	37:c:94:ILE:HA	1.87	0.42
38:d:95:GLU:HA	38:d:100:ASN:HD22	1.84	0.42
42:h:79:SER:O	42:h:79:SER:OG	2.30	0.42
49:o:11:ILE:HD11	49:o:30:ALA:HB1	2.02	0.42
50:p:67:ILE:H	50:p:67:ILE:HG13	1.67	0.42
1:A:2144:G:O2'	1:A:2147:A:N1	2.43	0.42
2:B:1:U:H2'	2:B:2:G:C8	2.55	0.42
2:B:63:C:H2'	2:B:64:G:C8	2.55	0.42
6:F:114:PHE:HE1	6:F:117:LEU:HB3	1.84	0.42
7:G:35:ARG:HB2	7:G:75:MET:HE1	2.02	0.42
18:S:51:LEU:HD13	18:S:105:VAL:HG21	2.02	0.42
35:a:674:G:H2'	35:a:675:A:H8	1.85	0.42
35:a:1238:A:H62	35:a:1301:U:H3	1.66	0.42
40:f:18:VAL:HA	40:f:21:MET:HE2	2.01	0.42
43:i:84:THR:O	43:i:88:MET:HG2	2.19	0.42
56:v:1:G:C2	56:v:2:C:C4	3.08	0.42
1:A:873:C:H2'	1:A:874:G:C8	2.49	0.41
1:A:1432:G:H2'	1:A:1433:A:C8	2.55	0.41
1:A:1667:G:O2'	1:A:1991:U:O4	2.38	0.41
7:G:107:LEU:HD13	7:G:152:ARG:HB2	2.01	0.41
18:S:71:VAL:HG22	18:S:107:VAL:HG12	2.01	0.41
23:X:37:ARG:HA	23:X:47:VAL:O	2.19	0.41
35:a:878:A:H1'	42:h:4:GLN:HE21	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:d:116:GLN:HE21	38:d:120:HIS:CE1	2.38	0.41
38:d:166:GLU:H	38:d:166:GLU:HG3	1.71	0.41
44:j:53:ILE:HD11	44:j:61:ALA:HB1	2.02	0.41
50:p:80:LYS:HA	50:p:80:LYS:HD3	1.80	0.41
1:A:659:G:N2	5:E:30:GLN:OE1	2.45	0.41
1:A:2183:A:H2'	1:A:2184:A:C8	2.51	0.41
35:a:382:A:H2'	35:a:383:A:C8	2.55	0.41
36:b:117:LEU:HD22	36:b:141:LEU:HD13	2.02	0.41
41:g:111:ARG:HH22	41:g:122:ASN:HB3	1.84	0.41
48:n:46:LEU:HD23	48:n:46:LEU:HA	1.87	0.41
51:q:17:MET:HG3	51:q:18:GLU:H	1.84	0.41
56:v:62:C:H2'	56:v:63:C:H6	1.84	0.41
4:D:83:ARG:HA	4:D:83:ARG:HD2	1.86	0.41
5:E:112:LEU:HD23	5:E:112:LEU:HA	1.93	0.41
9:J:95:ARG:HG2	9:J:96:ARG:HG2	2.02	0.41
35:a:634:C:H2'	35:a:635:A:C8	2.55	0.41
35:a:1245:C:H2'	35:a:1246:A:H8	1.86	0.41
43:i:57:MET:HE2	43:i:61:LEU:HD22	2.02	0.41
44:j:82:LYS:HE2	44:j:82:LYS:HB2	1.79	0.41
1:A:121:G:H2'	1:A:122:G:H8	1.85	0.41
1:A:1013:C:H2'	1:A:1014:A:C8	2.56	0.41
1:A:1447:C:H2'	1:A:1448:G:H8	1.84	0.41
1:A:2316:G:H2'	1:A:2317:A:H8	1.85	0.41
6:F:115:ARG:HG3	47:m:71:ARG:NH1	2.35	0.41
9:J:59:ALA:HB3	9:J:126:ALA:HA	2.02	0.41
10:K:78:ARG:HH21	15:P:71:GLU:CD	2.28	0.41
12:M:76:LYS:NZ	12:M:83:GLY:O	2.51	0.41
17:R:36:ALA:HA	17:R:58:VAL:HG12	2.02	0.41
34:8:3:C:H2'	34:8:4:G:C8	2.54	0.41
34:8:29:U:H2'	34:8:30:A:C8	2.55	0.41
35:a:538:G:H2'	35:a:539:A:C8	2.54	0.41
45:k:23:ILE:HB	45:k:86:VAL:HG23	2.02	0.41
56:v:22:A:C4	56:v:47:G:C2	3.08	0.41
1:A:2515:C:H2'	1:A:2516:A:H8	1.85	0.41
1:A:2684:U:O4'	10:K:70:ARG:NH1	2.54	0.41
3:C:2:ALA:N	3:C:20:VAL:O	2.54	0.41
11:L:84:LYS:HA	11:L:84:LYS:HD3	1.82	0.41
15:P:24:ASP:OD2	15:P:90:GLY:N	2.49	0.41
16:Q:15:LYS:HB3	16:Q:15:LYS:HE3	1.90	0.41
18:S:76:VAL:HG22	18:S:103:ILE:HG23	2.02	0.41
28:2:10:LEU:HD12	28:2:10:LEU:HA	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:4:11:CYS:HB3	30:4:33:HIS:CE1	2.56	0.41
35:a:262:A:H2'	35:a:263:A:C8	2.55	0.41
35:a:1095:U:P	35:a:1108:G:H1	2.43	0.41
35:a:1352:C:H2'	35:a:1353:G:C8	2.55	0.41
43:i:21:ILE:HB	43:i:61:LEU:HD12	2.01	0.41
45:k:34:ILE:HD11	45:k:79:ILE:HG21	2.03	0.41
1:A:743:A:O2'	1:A:1659:G:OP1	2.39	0.41
1:A:1441:G:H2'	1:A:1442:U:C6	2.56	0.41
1:A:2291:U:H2'	1:A:2292:U:C6	2.56	0.41
2:B:55:U:H2'	2:B:56:G:C8	2.56	0.41
3:C:3:VAL:HG22	3:C:19:VAL:HG22	2.02	0.41
12:M:77:PRO:HD2	12:M:80:VAL:HG11	2.03	0.41
22:W:56:ASP:HB3	22:W:58:THR:HG23	2.02	0.41
35:a:979:C:H41	35:a:1360:A:H62	1.68	0.41
36:b:192:ASP:N	36:b:192:ASP:OD1	2.45	0.41
40:f:29:ILE:HB	40:f:34:GLY:HA3	2.02	0.41
41:g:70:ARG:HE	41:g:70:ARG:HB2	1.59	0.41
1:A:13:A:O4'	1:A:526:A:N6	2.53	0.41
1:A:833:A:H2'	1:A:834:G:H8	1.86	0.41
1:A:1112:G:H2'	1:A:1113:U:H6	1.85	0.41
1:A:1794:A:H2'	1:A:1795:C:C6	2.56	0.41
2:B:80:U:H2'	2:B:81:G:H8	1.85	0.41
35:a:72:A:H61	35:a:98:A:H2	1.67	0.41
35:a:236:A:H2'	35:a:237:G:C8	2.56	0.41
35:a:1052:U:O4	35:a:1206:G:O6	2.38	0.41
35:a:1149:C:H2'	35:a:1150:A:C8	2.55	0.41
35:a:1255:G:OP2	44:j:45:ARG:NH2	2.53	0.41
35:a:1464:U:H2'	35:a:1465:A:C8	2.53	0.41
52:r:33:ILE:HD13	52:r:68:LEU:HD23	2.01	0.41
1:A:528:A:H5''	9:J:113:PRO:HG3	2.03	0.41
1:A:903:C:H2'	1:A:904:G:C8	2.56	0.41
1:A:2011:U:OP2	18:S:16:LYS:NZ	2.48	0.41
1:A:2100:G:H2'	1:A:2101:A:C8	2.56	0.41
1:A:2688:G:N1	1:A:2720:U:OP2	2.38	0.41
1:A:2699:C:H2'	1:A:2700:A:H8	1.85	0.41
1:A:2818:U:H2'	1:A:2819:G:C8	2.56	0.41
4:D:85:ALA:N	4:D:88:GLU:OE2	2.54	0.41
7:G:89:LEU:HD23	7:G:94:TYR:HB3	2.02	0.41
18:S:109:ASP:N	18:S:109:ASP:OD1	2.52	0.41
33:7:1:MET:HB2	57:7:101:ERY:H213	2.02	0.41
35:a:1162:C:H2'	35:a:1163:A:C8	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:f:38:ARG:HD2	40:f:96:VAL:HG23	2.02	0.41
44:j:36:VAL:HG22	44:j:38:GLY:H	1.86	0.41
47:m:9:ILE:HG23	47:m:18:ALA:HB1	2.03	0.41
51:q:47:HIS:HA	51:q:71:LYS:HE3	2.01	0.41
1:A:592:A:H1'	29:3:3:LYS:HA	2.03	0.41
1:A:1509:A:H2'	1:A:1510:G:C8	2.56	0.41
2:B:19:C:H2'	2:B:20:G:C8	2.56	0.41
2:B:88:C:O2'	2:B:89:U:O5'	2.34	0.41
3:C:147:LYS:HB2	3:C:150:LYS:HB2	2.03	0.41
4:D:124:ARG:HG3	4:D:165:MET:HB2	2.03	0.41
9:J:45:THR:HG23	9:J:48:VAL:HB	2.02	0.41
11:L:134:ALA:O	11:L:138:ALA:HB2	2.21	0.41
15:P:52:ASN:O	15:P:53:ARG:NH1	2.43	0.41
17:R:102:SER:OG	17:R:103:ALA:N	2.53	0.41
20:U:42:VAL:HG23	20:U:61:LYS:HG3	2.02	0.41
26:O:40:ARG:HA	26:O:40:ARG:HD2	1.94	0.41
57:7:101:ERY:H312	57:7:101:ERY:H2	1.77	0.41
35:a:138:G:H2'	35:a:139:A:C8	2.56	0.41
35:a:198:G:H2'	35:a:199:A:C8	2.56	0.41
35:a:449:G:H2'	35:a:450:G:C8	2.55	0.41
35:a:599:C:H2'	35:a:600:A:C8	2.54	0.41
35:a:1261:A:H5''	35:a:1262:C:H5	1.86	0.41
35:a:1405:G:H21	35:a:1518:A:H8	1.67	0.41
36:b:66:LYS:HB2	36:b:158:PRO:HA	2.03	0.41
36:b:167:ASP:O	36:b:170:HIS:ND1	2.50	0.41
37:c:14:ILE:HG22	37:c:15:VAL:HG23	2.03	0.41
37:c:63:SER:OG	37:c:64:ILE:N	2.54	0.41
37:c:111:LEU:HA	37:c:111:LEU:HD12	1.84	0.41
39:e:141:ILE:HD13	39:e:141:ILE:HA	1.85	0.41
43:i:33:ARG:HB2	43:i:38:TYR:HD1	1.85	0.41
43:i:50:GLN:O	43:i:54:LEU:HB2	2.21	0.41
48:n:46:LEU:O	48:n:50:THR:HG23	2.21	0.41
1:A:1251:C:OP2	16:Q:6:ARG:NH2	2.54	0.41
1:A:2386:A:O2'	22:W:56:ASP:OD1	2.38	0.41
3:C:53:HIS:HA	3:C:217:ARG:HB2	2.02	0.41
8:H:39:ALA:O	8:H:41:LYS:N	2.54	0.41
15:P:89:ARG:HH21	15:P:113:ARG:NH2	2.19	0.41
15:P:115:ASN:OD1	15:P:115:ASN:N	2.54	0.41
18:S:72:THR:OG1	18:S:73:LYS:N	2.54	0.41
19:T:68:LYS:HD3	19:T:68:LYS:HA	1.78	0.41
28:2:3:ARG:HA	28:2:3:ARG:HD3	1.67	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:2:42:LEU:HD12	28:2:42:LEU:HA	1.87	0.41
32:6:26:U:OP1	35:a:1498:U:O2'	2.30	0.41
35:a:1410:A:H2'	35:a:1411:C:C6	2.56	0.41
1:A:1039:A:H2	1:A:1116:G:H1	1.65	0.40
1:A:1733:G:H2'	1:A:1734:G:C8	2.57	0.40
18:S:14:ALA:O	18:S:18:ARG:HB2	2.20	0.40
24:Y:7:ARG:HD2	24:Y:7:ARG:HA	1.80	0.40
35:a:150:U:H2'	35:a:151:A:H8	1.86	0.40
35:a:255:G:H2'	35:a:256:U:C6	2.55	0.40
35:a:456:A:H2'	35:a:457:G:C8	2.56	0.40
35:a:738:C:OP1	40:f:2:ARG:NH1	2.53	0.40
37:c:135:LYS:HA	37:c:135:LYS:HD2	1.95	0.40
38:d:115:ARG:HA	38:d:118:VAL:HG12	2.03	0.40
43:i:116:VAL:HG21	44:j:62:ARG:HB2	2.03	0.40
48:n:43:ASN:O	48:n:47:LYS:HB2	2.21	0.40
1:A:181:A:H2'	1:A:182:A:C8	2.56	0.40
1:A:1796:U:H2'	1:A:1797:G:C8	2.56	0.40
1:A:2615:U:C2	26:0:4:GLN:HA	2.56	0.40
4:D:179:ARG:HB3	4:D:188:LEU:HD12	2.03	0.40
11:L:91:ASP:OD1	11:L:91:ASP:N	2.53	0.40
30:4:10:LEU:HD12	30:4:33:HIS:HD2	1.86	0.40
35:a:398:U:H2'	35:a:399:G:C8	2.56	0.40
35:a:1218:C:H2'	35:a:1219:A:H8	1.86	0.40
37:c:175:LEU:HD13	37:c:175:LEU:HA	1.95	0.40
44:j:6:ILE:HB	44:j:76:ILE:HB	2.03	0.40
51:q:31:HIS:HA	51:q:32:PRO:HD3	1.88	0.40
1:A:1291:C:H2'	1:A:1292:G:H8	1.86	0.40
6:F:44:ILE:HG22	6:F:83:TYR:HD2	1.85	0.40
12:M:42:THR:HG22	12:M:44:ARG:H	1.86	0.40
15:P:60:THR:O	15:P:60:THR:OG1	2.39	0.40
18:S:19:LEU:HD23	18:S:19:LEU:HA	1.93	0.40
23:X:40:VAL:O	23:X:44:LYS:N	2.55	0.40
31:5:3:LYS:HD2	31:5:3:LYS:HA	1.84	0.40
41:g:114:LYS:HD3	41:g:114:LYS:HA	1.89	0.40
53:s:5:LEU:HD23	53:s:5:LEU:HA	1.93	0.40
1:A:376:G:H2'	1:A:377:G:H8	1.87	0.40
1:A:1570:A:H2'	1:A:1571:A:C8	2.57	0.40
1:A:1724:G:O6	1:A:1736:U:O4	2.39	0.40
1:A:1923:U:H2'	1:A:1924:C:C6	2.57	0.40
1:A:2641:G:H5''	9:J:78:THR:HB	2.04	0.40
4:D:110:THR:HG22	4:D:171:THR:HB	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:48:THR:OG1	5:E:49:ARG:N	2.53	0.40
6:F:114:PHE:HZ	6:F:117:LEU:HD22	1.87	0.40
7:G:15:VAL:HG13	7:G:16:ASP:H	1.87	0.40
11:L:126:ARG:HE	11:L:126:ARG:HB2	1.67	0.40
12:M:53:MET:HE1	12:M:103:TYR:CG	2.57	0.40
14:O:25:ARG:HG3	14:O:40:ILE:HB	2.03	0.40
24:Y:6:LEU:HA	24:Y:9:LYS:HG2	2.03	0.40
35:a:686:U:O4	35:a:703:G:O2'	2.25	0.40
35:a:744:C:H2'	35:a:745:G:C8	2.57	0.40
38:d:121:LYS:HE2	38:d:129:VAL:HG11	2.03	0.40
47:m:48:LEU:HG	47:m:52:GLN:HB2	2.02	0.40
54:t:32:ILE:HG23	54:t:79:LEU:HD21	2.03	0.40
1:A:37:C:H2'	1:A:38:A:C8	2.56	0.40
1:A:1510:G:H2'	1:A:1511:G:C8	2.57	0.40
21:V:63:ILE:HD12	21:V:72:VAL:HG11	2.03	0.40
35:a:1284:C:H3'	35:a:1285:A:H2'	2.03	0.40
51:q:46:VAL:HG21	51:q:61:ILE:HD13	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	C	269/271 (99%)	249 (93%)	19 (7%)	1 (0%)	30	62
4	D	207/209 (99%)	189 (91%)	18 (9%)	0	100	100
5	E	199/201 (99%)	187 (94%)	12 (6%)	0	100	100
6	F	175/177 (99%)	157 (90%)	18 (10%)	0	100	100
7	G	172/174 (99%)	157 (91%)	14 (8%)	1 (1%)	21	54
8	H	147/149 (99%)	128 (87%)	15 (10%)	4 (3%)	4	27
9	J	140/142 (99%)	133 (95%)	7 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
10	K	120/122 (98%)	109 (91%)	11 (9%)	0	100	100
11	L	142/144 (99%)	128 (90%)	14 (10%)	0	100	100
12	M	134/136 (98%)	126 (94%)	7 (5%)	1 (1%)	18	51
13	N	116/118 (98%)	108 (93%)	8 (7%)	0	100	100
14	O	114/116 (98%)	109 (96%)	5 (4%)	0	100	100
15	P	112/114 (98%)	105 (94%)	7 (6%)	0	100	100
16	Q	115/117 (98%)	108 (94%)	7 (6%)	0	100	100
17	R	101/103 (98%)	91 (90%)	9 (9%)	1 (1%)	12	44
18	S	108/110 (98%)	99 (92%)	9 (8%)	0	100	100
19	T	87/89 (98%)	75 (86%)	12 (14%)	0	100	100
20	U	100/102 (98%)	90 (90%)	9 (9%)	1 (1%)	12	44
21	V	92/94 (98%)	90 (98%)	2 (2%)	0	100	100
22	W	73/75 (97%)	69 (94%)	4 (6%)	0	100	100
23	X	75/77 (97%)	73 (97%)	2 (3%)	0	100	100
24	Y	61/63 (97%)	58 (95%)	3 (5%)	0	100	100
25	Z	56/58 (97%)	53 (95%)	3 (5%)	0	100	100
26	0	53/55 (96%)	50 (94%)	3 (6%)	0	100	100
27	1	48/50 (96%)	38 (79%)	10 (21%)	0	100	100
28	2	44/46 (96%)	41 (93%)	3 (7%)	0	100	100
29	3	62/64 (97%)	51 (82%)	9 (14%)	2 (3%)	3	24
30	4	36/38 (95%)	33 (92%)	3 (8%)	0	100	100
31	5	63/65 (97%)	54 (86%)	9 (14%)	0	100	100
33	7	5/7 (71%)	4 (80%)	0	1 (20%)	0	1
36	b	222/224 (99%)	201 (90%)	21 (10%)	0	100	100
37	c	204/206 (99%)	191 (94%)	13 (6%)	0	100	100
38	d	203/205 (99%)	176 (87%)	26 (13%)	1 (0%)	24	57
39	e	155/157 (99%)	143 (92%)	11 (7%)	1 (1%)	21	54
40	f	97/99 (98%)	89 (92%)	8 (8%)	0	100	100
41	g	149/151 (99%)	134 (90%)	15 (10%)	0	100	100
42	h	127/129 (98%)	121 (95%)	6 (5%)	0	100	100
43	i	125/127 (98%)	110 (88%)	15 (12%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
44	j	96/98 (98%)	90 (94%)	5 (5%)	1 (1%)	12	44
45	k	115/117 (98%)	105 (91%)	10 (9%)	0	100	100
46	l	121/123 (98%)	106 (88%)	15 (12%)	0	100	100
47	m	112/114 (98%)	102 (91%)	10 (9%)	0	100	100
48	n	98/100 (98%)	87 (89%)	10 (10%)	1 (1%)	12	44
49	o	86/88 (98%)	77 (90%)	8 (9%)	1 (1%)	10	41
50	p	80/82 (98%)	73 (91%)	7 (9%)	0	100	100
51	q	78/80 (98%)	69 (88%)	9 (12%)	0	100	100
52	r	64/66 (97%)	60 (94%)	4 (6%)	0	100	100
53	s	81/83 (98%)	76 (94%)	5 (6%)	0	100	100
54	t	84/86 (98%)	82 (98%)	2 (2%)	0	100	100
55	u	68/70 (97%)	66 (97%)	2 (3%)	0	100	100
All	All	5591/5691 (98%)	5120 (92%)	454 (8%)	17 (0%)	37	67

All (17) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
29	3	32	ILE
33	7	2	THR
8	H	40	THR
20	U	90	GLY
29	3	33	LEU
39	e	98	PRO
8	H	2	GLN
44	j	57	VAL
48	n	33	ASP
49	o	47	LYS
3	C	122	ALA
7	G	109	PHE
8	H	8	LYS
8	H	9	VAL
38	d	32	CYS
12	M	69	PRO
17	R	54	VAL

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	C	216/216 (100%)	215 (100%)	1 (0%)	81	80
4	D	164/164 (100%)	163 (99%)	1 (1%)	78	79
5	E	165/165 (100%)	165 (100%)	0	100	100
6	F	148/148 (100%)	147 (99%)	1 (1%)	76	78
7	G	135/135 (100%)	134 (99%)	1 (1%)	76	78
8	H	114/114 (100%)	113 (99%)	1 (1%)	70	76
9	J	116/116 (100%)	114 (98%)	2 (2%)	53	70
10	K	103/103 (100%)	102 (99%)	1 (1%)	68	75
11	L	103/103 (100%)	101 (98%)	2 (2%)	50	68
12	M	109/109 (100%)	108 (99%)	1 (1%)	70	76
13	N	98/98 (100%)	98 (100%)	0	100	100
14	O	86/86 (100%)	85 (99%)	1 (1%)	63	73
15	P	99/99 (100%)	98 (99%)	1 (1%)	68	75
16	Q	89/89 (100%)	89 (100%)	0	100	100
17	R	84/84 (100%)	84 (100%)	0	100	100
18	S	93/93 (100%)	92 (99%)	1 (1%)	65	74
19	T	77/77 (100%)	77 (100%)	0	100	100
20	U	83/83 (100%)	83 (100%)	0	100	100
21	V	78/78 (100%)	78 (100%)	0	100	100
22	W	57/57 (100%)	57 (100%)	0	100	100
23	X	67/67 (100%)	67 (100%)	0	100	100
24	Y	55/55 (100%)	54 (98%)	1 (2%)	51	69
25	Z	48/48 (100%)	48 (100%)	0	100	100
26	0	46/46 (100%)	46 (100%)	0	100	100
27	1	45/45 (100%)	44 (98%)	1 (2%)	45	65
28	2	38/38 (100%)	38 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
29	3	51/51 (100%)	51 (100%)	0	100	100
30	4	34/34 (100%)	33 (97%)	1 (3%)	37	60
31	5	58/58 (100%)	58 (100%)	0	100	100
33	7	7/7 (100%)	7 (100%)	0	100	100
36	b	186/186 (100%)	181 (97%)	5 (3%)	39	62
37	c	170/170 (100%)	170 (100%)	0	100	100
38	d	172/172 (100%)	169 (98%)	3 (2%)	53	70
39	e	119/119 (100%)	116 (98%)	3 (2%)	42	63
40	f	86/86 (100%)	84 (98%)	2 (2%)	44	64
41	g	124/124 (100%)	120 (97%)	4 (3%)	34	59
42	h	104/104 (100%)	104 (100%)	0	100	100
43	i	105/105 (100%)	104 (99%)	1 (1%)	68	75
44	j	86/86 (100%)	85 (99%)	1 (1%)	63	73
45	k	90/90 (100%)	90 (100%)	0	100	100
46	l	103/103 (100%)	101 (98%)	2 (2%)	50	68
47	m	92/92 (100%)	90 (98%)	2 (2%)	45	65
48	n	83/83 (100%)	82 (99%)	1 (1%)	63	73
49	o	76/76 (100%)	76 (100%)	0	100	100
50	p	65/65 (100%)	64 (98%)	1 (2%)	57	71
51	q	74/74 (100%)	73 (99%)	1 (1%)	59	71
52	r	57/57 (100%)	57 (100%)	0	100	100
53	s	72/72 (100%)	72 (100%)	0	100	100
54	t	65/65 (100%)	65 (100%)	0	100	100
55	u	60/60 (100%)	60 (100%)	0	100	100
All	All	4655/4655 (100%)	4612 (99%)	43 (1%)	68	76

All (43) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	C	228	VAL
4	D	202	ILE
6	F	40	VAL
7	G	15	VAL
8	H	19	VAL

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Mol	Chain	Res	Type
9	J	62	VAL
9	J	84	ILE
10	K	65	THR
11	L	27	LEU
11	L	95	LEU
12	M	135	VAL
14	O	90	VAL
15	P	73	VAL
18	S	69	LEU
24	Y	8	GLU
27	1	23	THR
30	4	14	CYS
36	b	40	ILE
36	b	47	VAL
36	b	140	GLU
36	b	186	ILE
36	b	196	VAL
38	d	94	LEU
38	d	125	VAL
38	d	191	LEU
39	e	56	VAL
39	e	76	LEU
39	e	105	ILE
40	f	10	VAL
40	f	55	HIS
41	g	6	VAL
41	g	7	ILE
41	g	22	LEU
41	g	49	THR
43	i	9	THR
44	j	52	LEU
46	l	52	VAL
46	l	104	CYS
47	m	73	ILE
47	m	89	LEU
48	n	58	SER
50	p	67	ILE
51	q	79	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (72) such sidechains are listed below:

Mol	Chain	Res	Type
3	C	37	ASN
3	C	53	HIS
3	C	86	ASN
3	C	117	GLN
3	C	142	HIS
3	C	163	GLN
4	D	32	ASN
4	D	36	GLN
4	D	49	GLN
4	D	130	GLN
5	E	41	GLN
5	E	90	GLN
5	E	94	GLN
6	F	52	ASN
7	G	111	HIS
7	G	139	GLN
8	H	2	GLN
8	H	43	ASN
8	H	145	ASN
9	J	40	HIS
9	J	58	ASN
9	J	130	HIS
10	K	5	GLN
12	M	97	GLN
13	N	31	HIS
13	N	107	ASN
15	P	41	GLN
15	P	77	HIS
16	Q	20	GLN
16	Q	44	GLN
18	S	7	HIS
18	S	40	ASN
18	S	61	ASN
19	T	48	GLN
20	U	69	ASN
21	V	75	GLN
23	X	16	ASN
23	X	36	HIS
24	Y	15	ASN
24	Y	20	ASN
26	0	19	HIS
28	2	16	HIS
30	4	35	GLN

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Mol	Chain	Res	Type
36	b	58	ASN
36	b	177	ASN
37	c	123	GLN
38	d	85	ASN
38	d	116	GLN
39	e	43	ASN
40	f	11	HIS
40	f	17	GLN
40	f	55	HIS
42	h	4	GLN
42	h	18	GLN
42	h	21	ASN
42	h	118	GLN
43	i	50	GLN
45	k	38	GLN
46	l	5	ASN
47	m	8	ASN
47	m	100	GLN
48	n	4	GLN
48	n	49	GLN
50	p	29	ASN
52	r	52	GLN
52	r	54	GLN
52	r	74	HIS
53	s	52	HIS
53	s	57	HIS
53	s	69	HIS
54	t	68	HIS
55	u	64	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	2902/2903 (99%)	677 (23%)	45 (1%)
2	B	119/120 (99%)	27 (22%)	3 (2%)
32	6	5/6 (83%)	2 (40%)	1 (20%)
34	8	86/87 (98%)	26 (30%)	1 (1%)
35	a	1539/1540 (99%)	338 (21%)	0
56	v	76/77 (98%)	32 (42%)	0
All	All	4727/4733 (99%)	1102 (23%)	50 (1%)

All (1102) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	2	G
1	A	10	A
1	A	13	A
1	A	15	G
1	A	23	G
1	A	27	G
1	A	34	U
1	A	35	G
1	A	46	G
1	A	50	U
1	A	51	G
1	A	55	G
1	A	60	G
1	A	61	C
1	A	62	U
1	A	63	A
1	A	71	A
1	A	74	A
1	A	75	G
1	A	82	U
1	A	84	A
1	A	88	G
1	A	93	G
1	A	98	G
1	A	103	A
1	A	110	G
1	A	118	A
1	A	119	A
1	A	120	U
1	A	135	U
1	A	136	G
1	A	137	U
1	A	138	U
1	A	139	U
1	A	140	C
1	A	141	G
1	A	144	A
1	A	149	A
1	A	158	U
1	A	160	A
1	A	163	C
1	A	164	C
1	A	165	A

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Mol	Chain	Res	Type
1	A	178	G
1	A	196	A
1	A	197	A
1	A	199	A
1	A	204	A
1	A	215	G
1	A	216	A
1	A	219	A
1	A	222	A
1	A	229	C
1	A	230	G
1	A	231	A
1	A	233	A
1	A	241	A
1	A	242	G
1	A	243	U
1	A	248	G
1	A	249	C
1	A	255	A
1	A	265	A
1	A	267	C
1	A	275	C
1	A	276	U
1	A	278	A
1	A	279	A
1	A	282	A
1	A	285	G
1	A	291	G
1	A	294	A
1	A	301	G
1	A	302	C
1	A	308	G
1	A	311	A
1	A	322	A
1	A	323	C
1	A	329	G
1	A	330	A
1	A	331	C
1	A	334	C
1	A	335	C
1	A	343	C
1	A	346	A

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Mol	Chain	Res	Type
1	A	354	A
1	A	358	U
1	A	359	G
1	A	361	G
1	A	367	G
1	A	371	A
1	A	372	G
1	A	377	G
1	A	386	G
1	A	387	U
1	A	391	A
1	A	396	G
1	A	403	U
1	A	405	U
1	A	406	G
1	A	411	G
1	A	412	A
1	A	413	C
1	A	424	G
1	A	431	U
1	A	435	C
1	A	448	U
1	A	456	C
1	A	457	A
1	A	459	U
1	A	467	G
1	A	473	G
1	A	477	A
1	A	480	A
1	A	481	G
1	A	489	G
1	A	491	G
1	A	496	G
1	A	501	A
1	A	505	A
1	A	508	A
1	A	526	A
1	A	527	C
1	A	529	A
1	A	530	G
1	A	531	C
1	A	532	A

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Mol	Chain	Res	Type
1	A	533	G
1	A	542	C
1	A	543	G
1	A	544	C
1	A	547	A
1	A	555	G
1	A	563	A
1	A	573	U
1	A	575	A
1	A	586	A
1	A	603	A
1	A	613	A
1	A	614	A
1	A	615	U
1	A	616	A
1	A	621	A
1	A	627	A
1	A	634	C
1	A	637	A
1	A	645	C
1	A	646	U
1	A	654	A
1	A	655	A
1	A	656	G
1	A	659	G
1	A	668	A
1	A	669	G
1	A	670	A
1	A	686	U
1	A	687	C
1	A	695	G
1	A	701	G
1	A	711	G
1	A	714	U
1	A	717	C
1	A	726	G
1	A	730	A
1	A	738	G
1	A	745	G
1	A	747	U
1	A	748	G
1	A	749	A

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Mol	Chain	Res	Type
1	A	752	A
1	A	753	A
1	A	764	A
1	A	775	G
1	A	776	G
1	A	777	G
1	A	782	A
1	A	784	G
1	A	785	G
1	A	792	A
1	A	799	G
1	A	800	A
1	A	801	G
1	A	805	G
1	A	812	C
1	A	819	A
1	A	822	G
1	A	827	U
1	A	830	G
1	A	845	A
1	A	846	U
1	A	847	U
1	A	858	G
1	A	859	G
1	A	860	U
1	A	866	A
1	A	869	G
1	A	878	A
1	A	881	G
1	A	882	G
1	A	883	G
1	A	884	U
1	A	885	C
1	A	887	U
1	A	890	C
1	A	891	G
1	A	892	A
1	A	895	U
1	A	896	A
1	A	897	C
1	A	899	A
1	A	901	C

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Mol	Chain	Res	Type
1	A	902	C
1	A	903	C
1	A	906	U
1	A	907	G
1	A	910	A
1	A	927	A
1	A	941	A
1	A	945	A
1	A	946	C
1	A	953	G
1	A	958	U
1	A	961	C
1	A	973	A
1	A	974	G
1	A	975	A
1	A	983	A
1	A	989	G
1	A	996	A
1	A	997	G
1	A	1005	C
1	A	1009	A
1	A	1012	U
1	A	1013	C
1	A	1021	A
1	A	1023	U
1	A	1025	G
1	A	1026	G
1	A	1033	U
1	A	1046	A
1	A	1059	G
1	A	1060	U
1	A	1061	U
1	A	1062	G
1	A	1063	G
1	A	1065	U
1	A	1066	U
1	A	1067	A
1	A	1068	G
1	A	1069	A
1	A	1070	A
1	A	1071	G
1	A	1072	C

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Mol	Chain	Res	Type
1	A	1073	A
1	A	1075	C
1	A	1076	C
1	A	1078	U
1	A	1079	C
1	A	1080	A
1	A	1081	U
1	A	1083	U
1	A	1087	G
1	A	1088	A
1	A	1089	A
1	A	1090	A
1	A	1096	A
1	A	1101	U
1	A	1103	A
1	A	1104	C
1	A	1111	A
1	A	1112	G
1	A	1114	C
1	A	1115	G
1	A	1116	G
1	A	1119	U
1	A	1131	G
1	A	1132	U
1	A	1133	A
1	A	1134	A
1	A	1135	C
1	A	1139	G
1	A	1142	A
1	A	1143	A
1	A	1156	A
1	A	1169	A
1	A	1172	C
1	A	1173	U
1	A	1174	U
1	A	1175	A
1	A	1176	U
1	A	1177	G
1	A	1178	C
1	A	1180	U
1	A	1186	G
1	A	1204	A

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Mol	Chain	Res	Type
1	A	1206	G
1	A	1211	C
1	A	1212	G
1	A	1218	G
1	A	1236	G
1	A	1247	A
1	A	1248	G
1	A	1251	C
1	A	1253	A
1	A	1256	G
1	A	1262	A
1	A	1265	A
1	A	1271	G
1	A	1272	A
1	A	1273	U
1	A	1300	G
1	A	1301	A
1	A	1302	A
1	A	1305	C
1	A	1306	C
1	A	1321	A
1	A	1324	G
1	A	1329	U
1	A	1330	C
1	A	1333	G
1	A	1341	G
1	A	1345	C
1	A	1352	U
1	A	1360	G
1	A	1365	A
1	A	1368	G
1	A	1378	A
1	A	1379	U
1	A	1383	A
1	A	1385	A
1	A	1386	C
1	A	1394	U
1	A	1395	A
1	A	1403	A
1	A	1406	U
1	A	1413	A
1	A	1414	C

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Mol	Chain	Res	Type
1	A	1415	U
1	A	1416	G
1	A	1419	A
1	A	1420	A
1	A	1421	G
1	A	1427	A
1	A	1428	C
1	A	1429	G
1	A	1437	C
1	A	1454	C
1	A	1456	G
1	A	1458	U
1	A	1460	U
1	A	1461	C
1	A	1476	U
1	A	1480	C
1	A	1482	G
1	A	1490	A
1	A	1493	C
1	A	1504	A
1	A	1508	A
1	A	1509	A
1	A	1515	A
1	A	1523	U
1	A	1524	G
1	A	1530	G
1	A	1531	C
1	A	1532	A
1	A	1533	C
1	A	1534	U
1	A	1535	A
1	A	1536	C
1	A	1537	G
1	A	1539	U
1	A	1542	U
1	A	1543	G
1	A	1544	A
1	A	1554	U
1	A	1558	C
1	A	1559	U
1	A	1560	G
1	A	1561	C

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Mol	Chain	Res	Type
1	A	1566	A
1	A	1567	G
1	A	1569	A
1	A	1578	U
1	A	1581	G
1	A	1583	A
1	A	1584	U
1	A	1585	C
1	A	1586	A
1	A	1587	G
1	A	1608	A
1	A	1610	A
1	A	1616	A
1	A	1627	G
1	A	1632	A
1	A	1646	C
1	A	1647	U
1	A	1648	U
1	A	1651	G
1	A	1672	A
1	A	1674	G
1	A	1675	C
1	A	1693	U
1	A	1694	C
1	A	1695	G
1	A	1698	A
1	A	1703	G
1	A	1706	C
1	A	1707	G
1	A	1713	A
1	A	1715	G
1	A	1721	G
1	A	1724	G
1	A	1726	C
1	A	1729	U
1	A	1730	C
1	A	1732	C
1	A	1738	G
1	A	1764	C
1	A	1773	A
1	A	1776	G
1	A	1780	A

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Mol	Chain	Res	Type
1	A	1781	U
1	A	1782	U
1	A	1784	A
1	A	1800	C
1	A	1801	A
1	A	1802	A
1	A	1808	A
1	A	1811	G
1	A	1815	A
1	A	1816	C
1	A	1820	U
1	A	1821	A
1	A	1826	G
1	A	1828	G
1	A	1829	A
1	A	1833	C
1	A	1834	U
1	A	1839	G
1	A	1848	A
1	A	1858	A
1	A	1870	C
1	A	1871	A
1	A	1873	G
1	A	1878	G
1	A	1884	G
1	A	1896	G
1	A	1901	A
1	A	1906	G
1	A	1910	G
1	A	1912	A
1	A	1913	A
1	A	1914	C
1	A	1917	U
1	A	1918	A
1	A	1927	A
1	A	1929	G
1	A	1930	G
1	A	1931	U
1	A	1934	C
1	A	1936	A
1	A	1940	U
1	A	1941	C

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Mol	Chain	Res	Type
1	A	1955	U
1	A	1963	U
1	A	1966	A
1	A	1967	C
1	A	1970	A
1	A	1971	U
1	A	1972	G
1	A	1981	A
1	A	1982	U
1	A	1991	U
1	A	1992	G
1	A	1996	C
1	A	1997	C
1	A	2018	G
1	A	2020	A
1	A	2022	U
1	A	2023	C
1	A	2031	A
1	A	2033	A
1	A	2034	U
1	A	2035	G
1	A	2041	U
1	A	2043	C
1	A	2052	A
1	A	2055	C
1	A	2056	G
1	A	2060	A
1	A	2061	G
1	A	2062	A
1	A	2063	C
1	A	2068	U
1	A	2069	G
1	A	2077	A
1	A	2080	A
1	A	2092	U
1	A	2093	G
1	A	2096	C
1	A	2098	U
1	A	2099	U
1	A	2100	G
1	A	2102	G
1	A	2104	C

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Mol	Chain	Res	Type
1	A	2107	G
1	A	2108	A
1	A	2110	G
1	A	2111	U
1	A	2112	G
1	A	2113	U
1	A	2115	G
1	A	2117	A
1	A	2118	U
1	A	2119	A
1	A	2125	G
1	A	2127	G
1	A	2131	U
1	A	2132	U
1	A	2133	G
1	A	2134	A
1	A	2137	U
1	A	2146	C
1	A	2148	G
1	A	2149	U
1	A	2157	G
1	A	2162	G
1	A	2164	C
1	A	2167	U
1	A	2170	A
1	A	2171	A
1	A	2172	U
1	A	2173	A
1	A	2175	C
1	A	2178	C
1	A	2180	U
1	A	2181	U
1	A	2186	G
1	A	2187	U
1	A	2188	U
1	A	2189	U
1	A	2191	A
1	A	2198	A
1	A	2199	A
1	A	2203	U
1	A	2204	G
1	A	2211	A

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Mol	Chain	Res	Type
1	A	2212	A
1	A	2219	U
1	A	2223	G
1	A	2225	A
1	A	2239	G
1	A	2250	G
1	A	2252	G
1	A	2266	A
1	A	2278	A
1	A	2279	G
1	A	2283	C
1	A	2287	A
1	A	2288	A
1	A	2305	U
1	A	2307	G
1	A	2308	G
1	A	2309	A
1	A	2317	A
1	A	2320	U
1	A	2325	G
1	A	2327	A
1	A	2333	A
1	A	2344	U
1	A	2347	C
1	A	2350	C
1	A	2354	C
1	A	2357	G
1	A	2361	G
1	A	2367	G
1	A	2382	G
1	A	2383	G
1	A	2384	U
1	A	2385	C
1	A	2389	G
1	A	2392	A
1	A	2402	U
1	A	2403	C
1	A	2406	A
1	A	2422	C
1	A	2423	U
1	A	2425	A
1	A	2429	G

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Mol	Chain	Res	Type
1	A	2430	A
1	A	2435	A
1	A	2440	C
1	A	2441	U
1	A	2445	G
1	A	2448	A
1	A	2476	A
1	A	2481	G
1	A	2491	U
1	A	2494	G
1	A	2498	C
1	A	2502	G
1	A	2503	A
1	A	2504	U
1	A	2505	G
1	A	2513	A
1	A	2518	A
1	A	2519	U
1	A	2520	C
1	A	2529	G
1	A	2542	A
1	A	2554	U
1	A	2556	C
1	A	2564	A
1	A	2567	G
1	A	2572	A
1	A	2573	C
1	A	2586	U
1	A	2602	A
1	A	2603	G
1	A	2609	U
1	A	2613	U
1	A	2615	U
1	A	2629	U
1	A	2630	G
1	A	2646	C
1	A	2654	A
1	A	2655	G
1	A	2656	U
1	A	2661	G
1	A	2673	G
1	A	2682	A

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Mol	Chain	Res	Type
1	A	2689	U
1	A	2690	U
1	A	2714	G
1	A	2718	G
1	A	2726	A
1	A	2731	G
1	A	2732	G
1	A	2733	A
1	A	2739	U
1	A	2744	G
1	A	2748	A
1	A	2764	A
1	A	2765	A
1	A	2776	A
1	A	2778	A
1	A	2779	U
1	A	2789	C
1	A	2790	U
1	A	2793	C
1	A	2794	C
1	A	2798	U
1	A	2799	A
1	A	2800	A
1	A	2801	G
1	A	2807	U
1	A	2808	G
1	A	2809	A
1	A	2818	U
1	A	2820	A
1	A	2821	A
1	A	2824	C
1	A	2826	A
1	A	2833	U
1	A	2834	G
1	A	2849	U
1	A	2861	U
1	A	2867	G
1	A	2868	A
1	A	2869	G
1	A	2873	A
1	A	2879	A
1	A	2880	C

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Mol	Chain	Res	Type
1	A	2892	G
1	A	2893	A
1	A	2902	C
1	A	2903	U
2	B	4	C
2	B	12	C
2	B	13	G
2	B	18	G
2	B	21	G
2	B	24	G
2	B	25	U
2	B	34	A
2	B	35	C
2	B	40	U
2	B	41	G
2	B	42	C
2	B	44	G
2	B	45	A
2	B	52	A
2	B	58	A
2	B	66	A
2	B	67	G
2	B	75	G
2	B	87	U
2	B	88	C
2	B	89	U
2	B	98	G
2	B	108	A
2	B	109	A
2	B	118	C
2	B	119	A
32	6	27	U
32	6	28	C
34	8	8	U
34	8	9	G
34	8	17	U
34	8	19	G
34	8	20	U
34	8	21	A
34	8	24	C
34	8	25	A
34	8	26	C

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Mol	Chain	Res	Type
34	8	37	G
34	8	47	C
34	8	48	C
34	8	49	C
34	8	50	A
34	8	51	A
34	8	54	G
34	8	58	U
34	8	59	U
34	8	64	G
34	8	67	C
34	8	68	A
34	8	69	A
34	8	72	C
34	8	80	C
34	8	86	C
34	8	87	A
35	a	5	U
35	a	6	G
35	a	7	A
35	a	8	A
35	a	9	G
35	a	14	U
35	a	22	G
35	a	31	G
35	a	32	A
35	a	37	U
35	a	39	G
35	a	47	C
35	a	48	C
35	a	50	A
35	a	51	A
35	a	57	G
35	a	58	C
35	a	71	A
35	a	73	C
35	a	75	G
35	a	80	A
35	a	81	A
35	a	82	G
35	a	83	C
35	a	84	U

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Mol	Chain	Res	Type
35	a	85	U
35	a	86	G
35	a	87	C
35	a	89	U
35	a	91	U
35	a	92	U
35	a	94	G
35	a	96	U
35	a	97	G
35	a	98	A
35	a	101	A
35	a	108	G
35	a	120	A
35	a	130	A
35	a	131	A
35	a	132	C
35	a	141	G
35	a	144	G
35	a	149	A
35	a	154	U
35	a	159	G
35	a	160	A
35	a	163	C
35	a	168	G
35	a	173	U
35	a	181	A
35	a	183	C
35	a	184	G
35	a	192	A
35	a	197	A
35	a	203	G
35	a	209	U
35	a	210	C
35	a	211	G
35	a	212	G
35	a	217	C
35	a	226	G
35	a	238	A
35	a	240	G
35	a	244	U
35	a	245	U
35	a	247	G

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Mol	Chain	Res	Type
35	a	251	G
35	a	258	G
35	a	262	A
35	a	265	G
35	a	266	G
35	a	267	C
35	a	280	C
35	a	281	G
35	a	282	A
35	a	283	U
35	a	289	G
35	a	299	G
35	a	303	A
35	a	306	A
35	a	321	A
35	a	328	C
35	a	329	A
35	a	330	C
35	a	342	C
35	a	344	A
35	a	345	C
35	a	347	G
35	a	351	G
35	a	352	C
35	a	354	G
35	a	367	U
35	a	372	C
35	a	375	U
35	a	384	G
35	a	390	U
35	a	397	A
35	a	406	G
35	a	412	A
35	a	423	G
35	a	424	G
35	a	429	U
35	a	438	U
35	a	439	U
35	a	446	G
35	a	458	U
35	a	462	G
35	a	465	A

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Mol	Chain	Res	Type
35	a	467	U
35	a	474	G
35	a	476	U
35	a	478	A
35	a	484	G
35	a	485	U
35	a	486	U
35	a	496	A
35	a	497	G
35	a	499	A
35	a	511	C
35	a	518	C
35	a	524	G
35	a	527	G
35	a	531	U
35	a	533	A
35	a	535	A
35	a	547	A
35	a	559	A
35	a	562	U
35	a	564	C
35	a	572	A
35	a	573	A
35	a	575	G
35	a	576	C
35	a	577	G
35	a	579	A
35	a	616	G
35	a	618	C
35	a	633	G
35	a	642	A
35	a	650	G
35	a	653	U
35	a	661	G
35	a	665	A
35	a	687	A
35	a	695	A
35	a	702	A
35	a	703	G
35	a	713	G
35	a	717	U
35	a	721	G

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Mol	Chain	Res	Type
35	a	731	G
35	a	734	G
35	a	736	C
35	a	753	A
35	a	754	C
35	a	755	G
35	a	777	A
35	a	781	A
35	a	782	A
35	a	790	A
35	a	802	A
35	a	815	A
35	a	817	C
35	a	818	G
35	a	819	A
35	a	820	U
35	a	821	G
35	a	829	G
35	a	832	G
35	a	836	G
35	a	841	C
35	a	842	U
35	a	843	U
35	a	844	G
35	a	845	A
35	a	846	G
35	a	851	G
35	a	859	G
35	a	871	U
35	a	872	A
35	a	876	C
35	a	885	G
35	a	889	A
35	a	890	G
35	a	900	A
35	a	902	G
35	a	918	A
35	a	919	A
35	a	926	G
35	a	931	C
35	a	933	G
35	a	934	C

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Mol	Chain	Res	Type
35	a	935	A
35	a	942	G
35	a	960	U
35	a	961	U
35	a	965	U
35	a	966	G
35	a	969	A
35	a	971	G
35	a	975	A
35	a	976	G
35	a	977	A
35	a	989	U
35	a	992	U
35	a	993	G
35	a	994	A
35	a	1003	G
35	a	1004	A
35	a	1006	G
35	a	1022	A
35	a	1027	C
35	a	1028	C
35	a	1031	C
35	a	1032	G
35	a	1033	G
35	a	1034	G
35	a	1035	A
35	a	1036	A
35	a	1037	C
35	a	1050	G
35	a	1053	G
35	a	1064	G
35	a	1065	U
35	a	1085	U
35	a	1089	G
35	a	1092	A
35	a	1094	G
35	a	1095	U
35	a	1099	G
35	a	1101	A
35	a	1108	G
35	a	1117	A
35	a	1124	G

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Mol	Chain	Res	Type
35	a	1125	U
35	a	1130	A
35	a	1131	G
35	a	1133	G
35	a	1134	G
35	a	1137	C
35	a	1138	G
35	a	1139	G
35	a	1143	G
35	a	1144	G
35	a	1151	A
35	a	1152	A
35	a	1158	C
35	a	1159	U
35	a	1166	G
35	a	1167	A
35	a	1169	A
35	a	1171	A
35	a	1179	A
35	a	1182	G
35	a	1183	U
35	a	1184	G
35	a	1191	A
35	a	1196	A
35	a	1201	A
35	a	1202	U
35	a	1213	A
35	a	1214	C
35	a	1227	A
35	a	1228	C
35	a	1236	A
35	a	1238	A
35	a	1239	A
35	a	1250	A
35	a	1253	G
35	a	1256	A
35	a	1257	A
35	a	1262	C
35	a	1269	A
35	a	1273	C
35	a	1275	A
35	a	1280	A

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Mol	Chain	Res	Type
35	a	1282	C
35	a	1285	A
35	a	1287	A
35	a	1294	G
35	a	1297	G
35	a	1298	U
35	a	1300	G
35	a	1301	U
35	a	1302	C
35	a	1305	G
35	a	1317	C
35	a	1320	C
35	a	1322	C
35	a	1323	G
35	a	1335	U
35	a	1336	C
35	a	1338	G
35	a	1340	A
35	a	1346	A
35	a	1363	A
35	a	1368	A
35	a	1370	G
35	a	1380	U
35	a	1383	C
35	a	1394	A
35	a	1395	C
35	a	1397	C
35	a	1398	A
35	a	1399	C
35	a	1400	C
35	a	1402	C
35	a	1403	C
35	a	1419	G
35	a	1429	A
35	a	1441	A
35	a	1446	A
35	a	1447	A
35	a	1448	C
35	a	1451	U
35	a	1452	C
35	a	1453	G
35	a	1470	U

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Mol	Chain	Res	Type
35	a	1471	U
35	a	1473	G
35	a	1475	G
35	a	1478	U
35	a	1487	G
35	a	1492	A
35	a	1493	A
35	a	1494	G
35	a	1502	A
35	a	1503	A
35	a	1506	U
35	a	1517	G
35	a	1520	C
35	a	1529	G
35	a	1530	G
35	a	1534	A
35	a	1535	C
35	a	1536	C
35	a	1540	U
56	v	2	C
56	v	3	A
56	v	7	G
56	v	8	U
56	v	9	A
56	v	13	C
56	v	15	G
56	v	17	U
56	v	18	G
56	v	19	G
56	v	20	A
56	v	21	U
56	v	22	A
56	v	34	U
56	v	37	G
56	v	43	A
56	v	47	G
56	v	48	U
56	v	49	C
56	v	51	G
56	v	54	G
56	v	55	U
56	v	58	G

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Mol	Chain	Res	Type
56	v	59	A
56	v	60	A
56	v	61	U
56	v	62	C
56	v	63	C
56	v	74	A
56	v	75	C
56	v	76	C
56	v	77	A

All (50) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	4	U
1	A	134	G
1	A	242	G
1	A	277	G
1	A	281	C
1	A	358	U
1	A	404	A
1	A	479	A
1	A	490	C
1	A	546	U
1	A	655	A
1	A	752	A
1	A	827	U
1	A	858	G
1	A	859	G
1	A	890	C
1	A	1020	A
1	A	1022	G
1	A	1062	G
1	A	1064	C
1	A	1074	G
1	A	1111	A
1	A	1130	U
1	A	1171	G
1	A	1173	U
1	A	1179	G
1	A	1182	G
1	A	1190	G
1	A	1300	G

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Mol	Chain	Res	Type
1	A	1378	A
1	A	1399	C
1	A	1420	A
1	A	1508	A
1	A	1530	G
1	A	1541	C
1	A	1729	U
1	A	1913	A
1	A	1930	G
1	A	1940	U
1	A	2326	C
1	A	2391	G
1	A	2566	A
1	A	2655	G
1	A	2808	G
1	A	2901	C
2	B	66	A
2	B	86	G
2	B	88	C
32	6	27	U
34	8	63	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](#)

1 ligand is modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
57	ERY	7	101	-	53,53,53	1.60	5 (9%)	82,82,82	1.80	20 (24%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
57	ERY	7	101	-	-	14/72/107/107	0/3/3/3

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
57	7	101	ERY	C10-C9	-7.22	1.41	1.52
57	7	101	ERY	C2-C1	-5.90	1.39	1.51
57	7	101	ERY	C8-C9	-3.03	1.42	1.52
57	7	101	ERY	O7-C22	2.28	1.48	1.41
57	7	101	ERY	O3-C14	2.04	1.47	1.41

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
57	7	101	ERY	O5-C16-C17	6.09	112.68	103.86
57	7	101	ERY	O7-C5-C6	4.56	111.84	106.40
57	7	101	ERY	C6-C5-C4	-3.84	108.31	113.89
57	7	101	ERY	C32-C6-C5	3.47	116.06	110.13
57	7	101	ERY	C36-C13-C12	-3.28	109.20	115.20
57	7	101	ERY	C13-O2-C1	-2.95	113.05	118.20
57	7	101	ERY	O2-C13-C36	2.84	112.64	107.36
57	7	101	ERY	C8-C9-C10	2.79	123.83	119.13
57	7	101	ERY	C27-C26-C25	-2.58	109.37	113.27
57	7	101	ERY	C31-C4-C3	-2.45	107.08	111.40
57	7	101	ERY	C22-O9-C26	2.35	116.54	112.91
57	7	101	ERY	C19-C16-C15	-2.34	106.56	110.64
57	7	101	ERY	C14-O3-C3	-2.29	110.15	114.72
57	7	101	ERY	C7-C6-C5	-2.23	106.16	110.38
57	7	101	ERY	C32-C6-C7	-2.16	107.58	111.09
57	7	101	ERY	C16-C17-C18	-2.16	107.97	111.12
57	7	101	ERY	C35-C12-C11	-2.08	109.53	113.14
57	7	101	ERY	O10-C6-C7	2.08	113.54	108.34
57	7	101	ERY	O3-C14-O4	2.00	116.44	109.97
57	7	101	ERY	C16-C15-C14	-2.00	111.61	114.99

There are no chirality outliers.

All (14) torsion outliers are listed below:

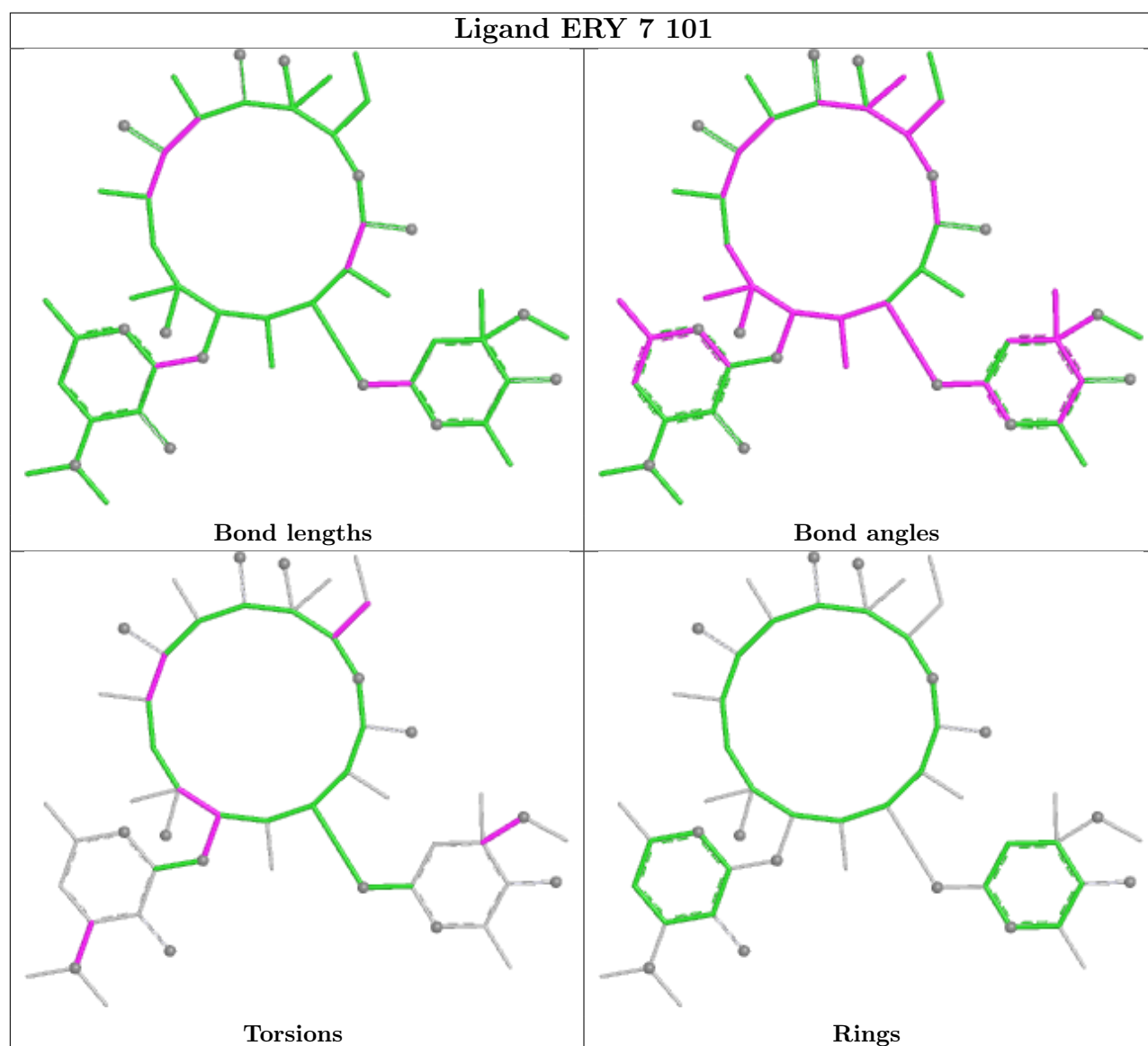
Mol	Chain	Res	Type	Atoms
57	7	101	ERY	C12-C13-C36-C37
57	7	101	ERY	C25-C24-N1-C28
57	7	101	ERY	C19-C16-O5-C20
57	7	101	ERY	O2-C13-C36-C37
57	7	101	ERY	C4-C5-C6-O10
57	7	101	ERY	C15-C16-O5-C20
57	7	101	ERY	C17-C16-O5-C20
57	7	101	ERY	C33-C8-C9-O11
57	7	101	ERY	C4-C5-C6-C32
57	7	101	ERY	C23-C24-N1-C29
57	7	101	ERY	C33-C8-C9-C10
57	7	101	ERY	C7-C8-C9-O11
57	7	101	ERY	C25-C24-N1-C29
57	7	101	ERY	C4-C5-O7-C22

There are no ring outliers.

1 monomer is involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
57	7	101	ERY	11	0

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



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

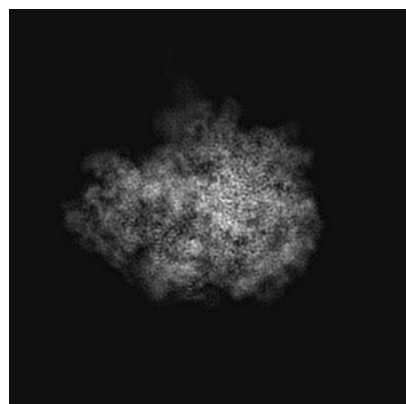
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-12574. These allow visual inspection of the internal detail of the map and identification of artifacts.

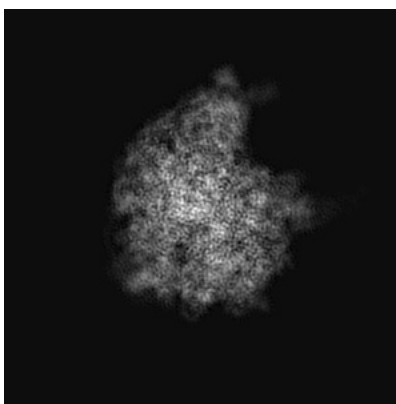
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

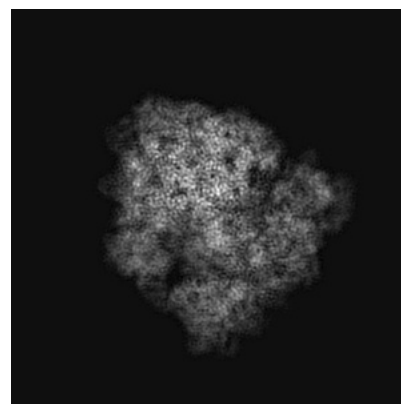
6.1.1 Primary map



X

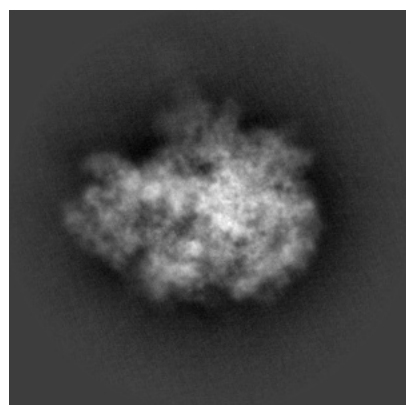


Y

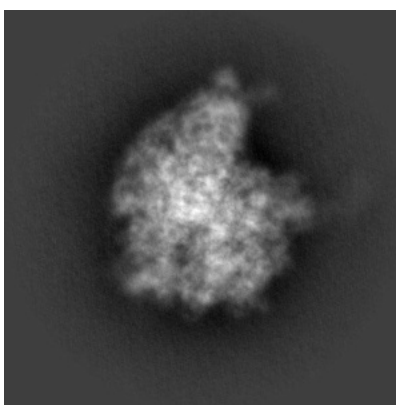


Z

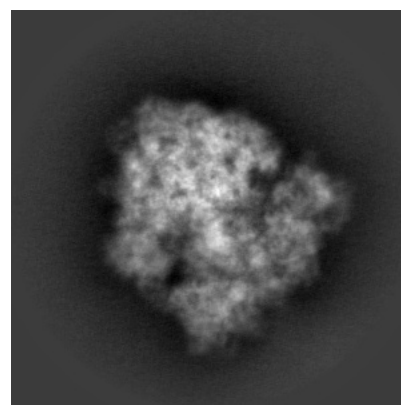
6.1.2 Raw map



X



Y

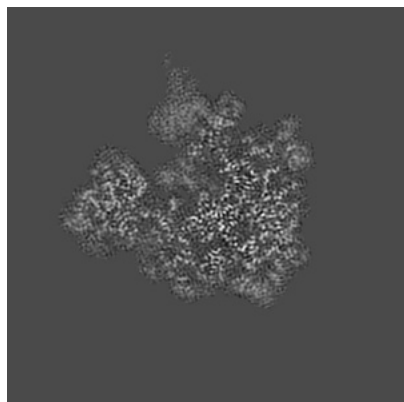


Z

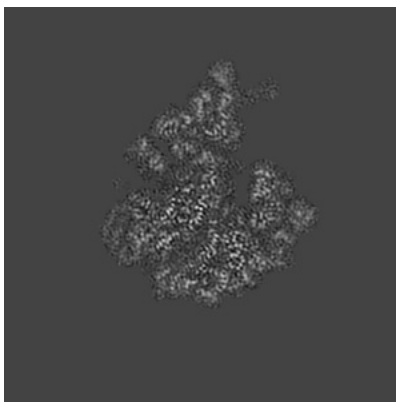
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

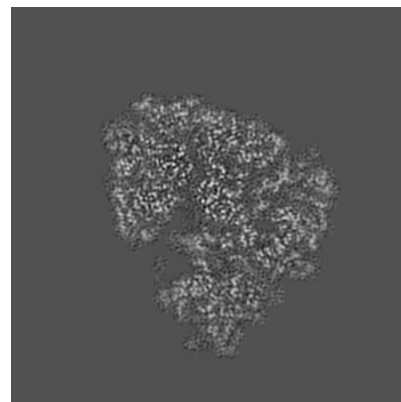
6.2.1 Primary map



X Index: 180

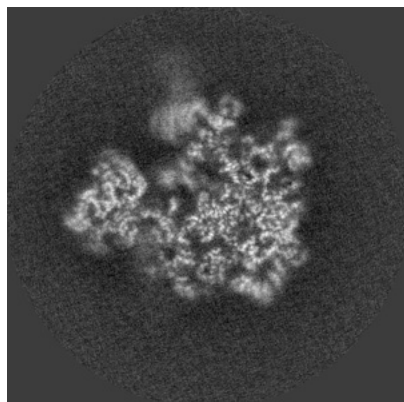


Y Index: 180

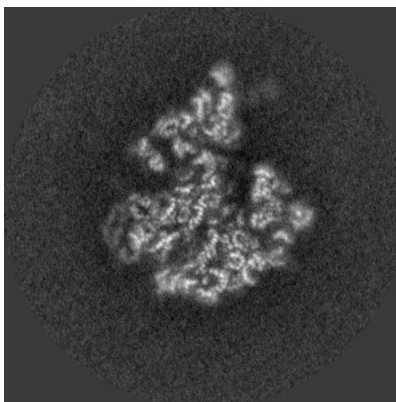


Z Index: 180

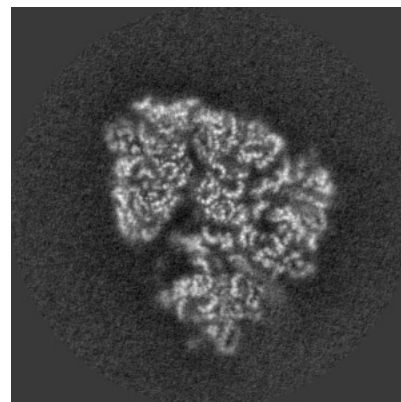
6.2.2 Raw map



X Index: 180



Y Index: 180

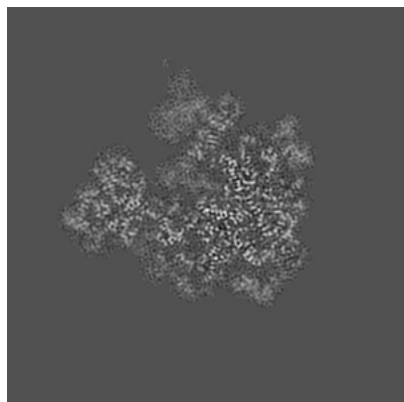


Z Index: 180

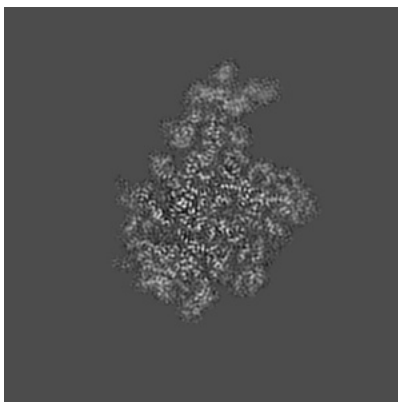
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

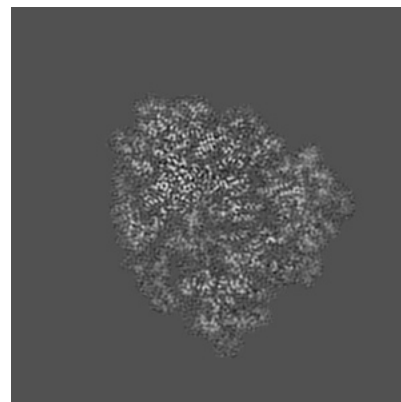
6.3.1 Primary map



X Index: 178

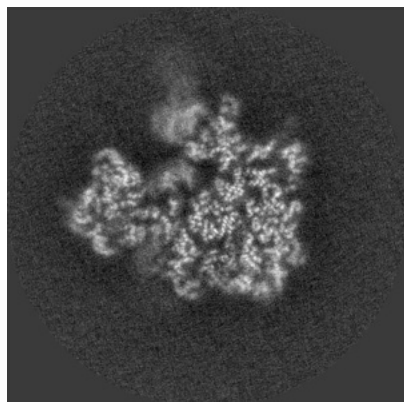


Y Index: 194

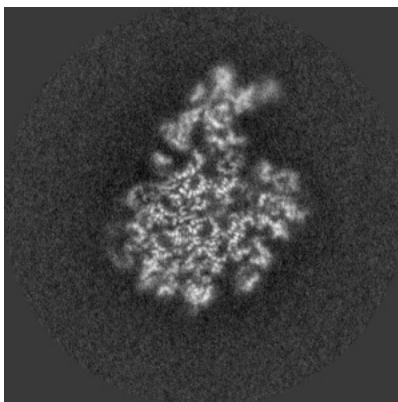


Z Index: 187

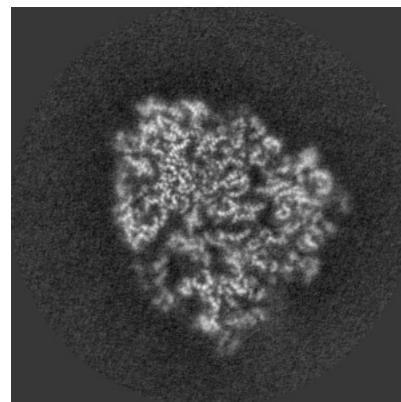
6.3.2 Raw map



X Index: 184



Y Index: 189

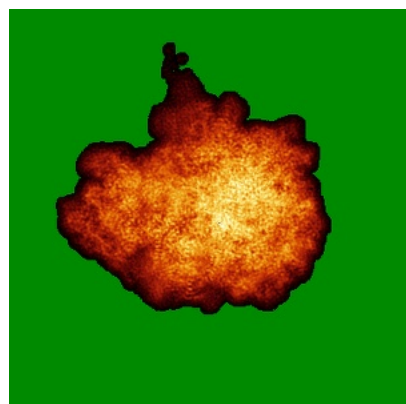


Z Index: 186

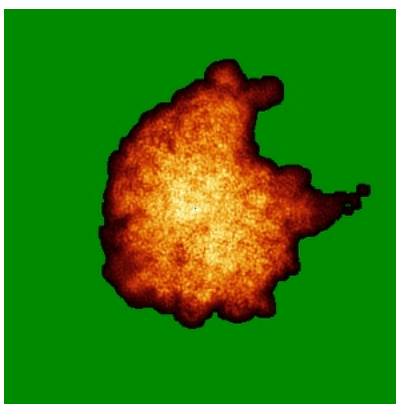
The images above show the largest variance slices of the map in three orthogonal directions.

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

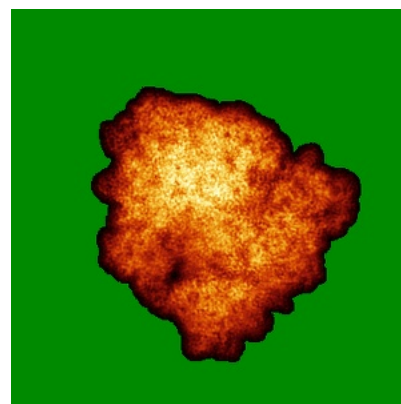
6.4.1 Primary map



X

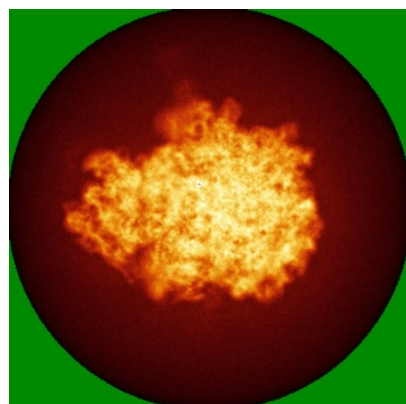


Y

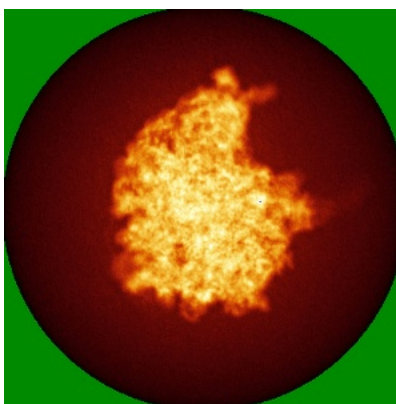


Z

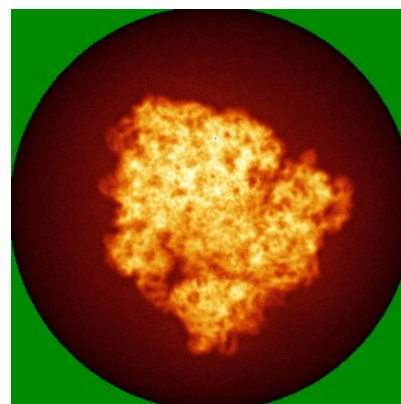
6.4.2 Raw map



X



Y

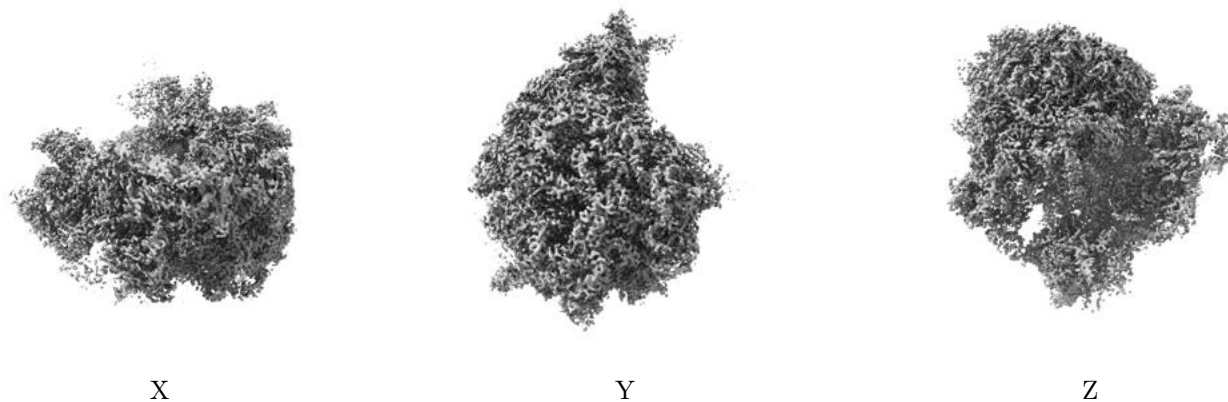


Z

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

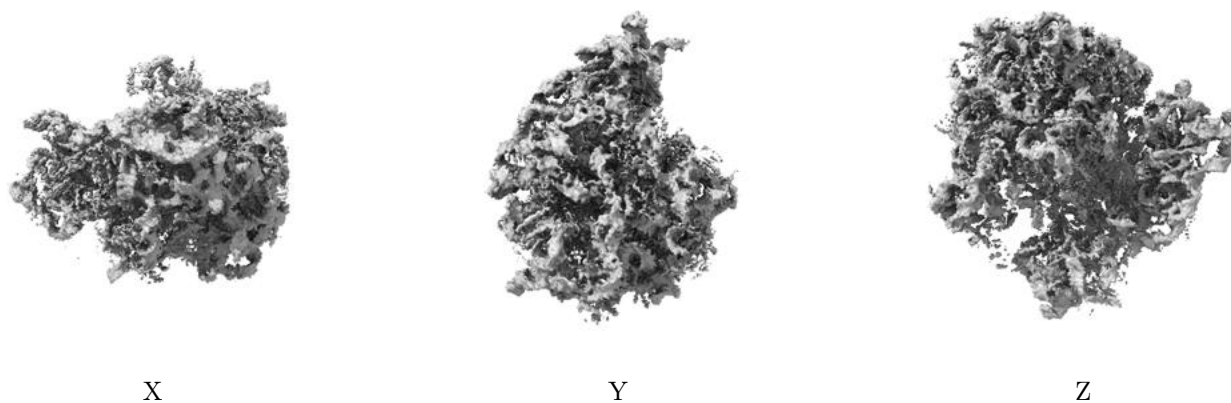
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.07. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

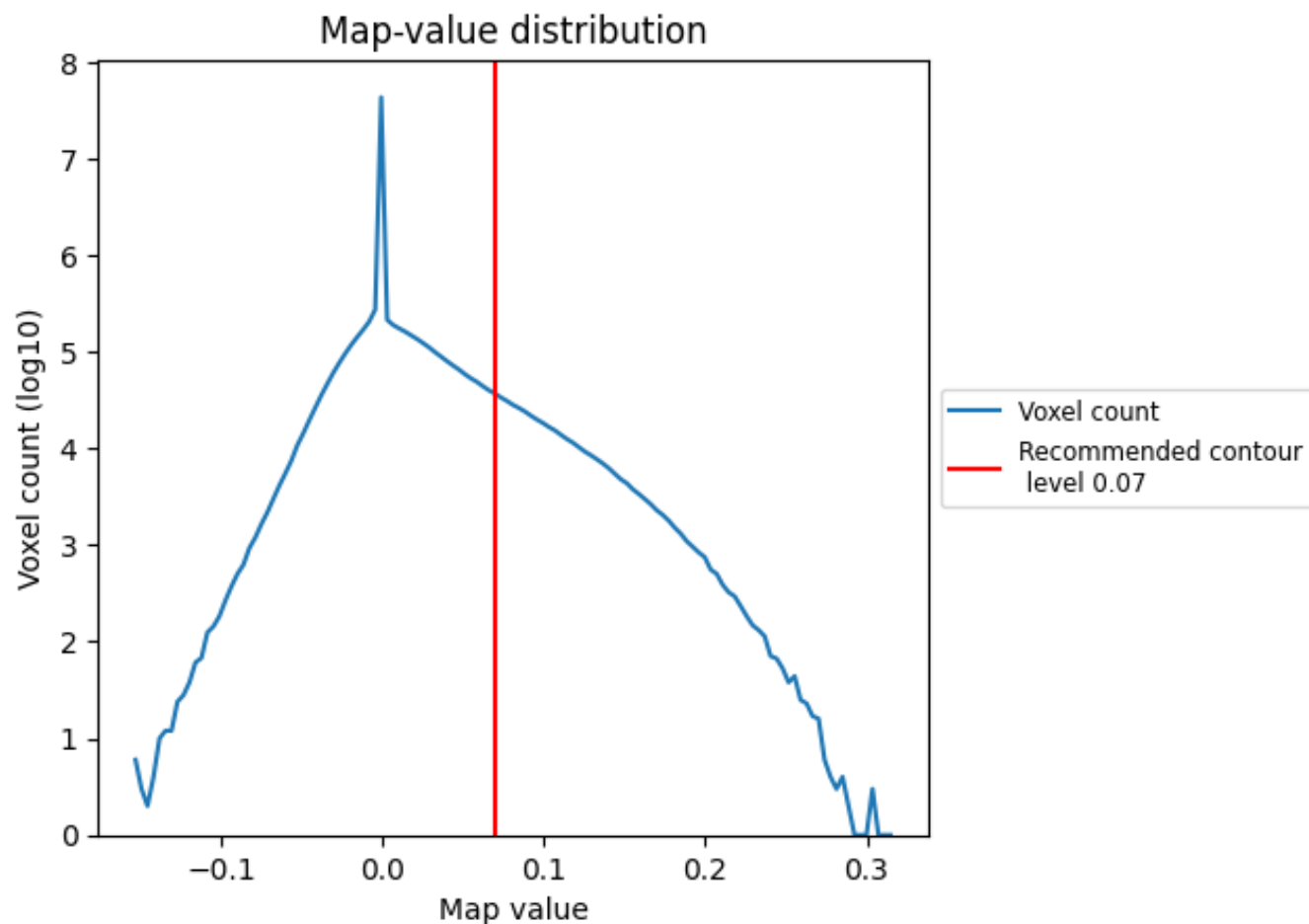
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

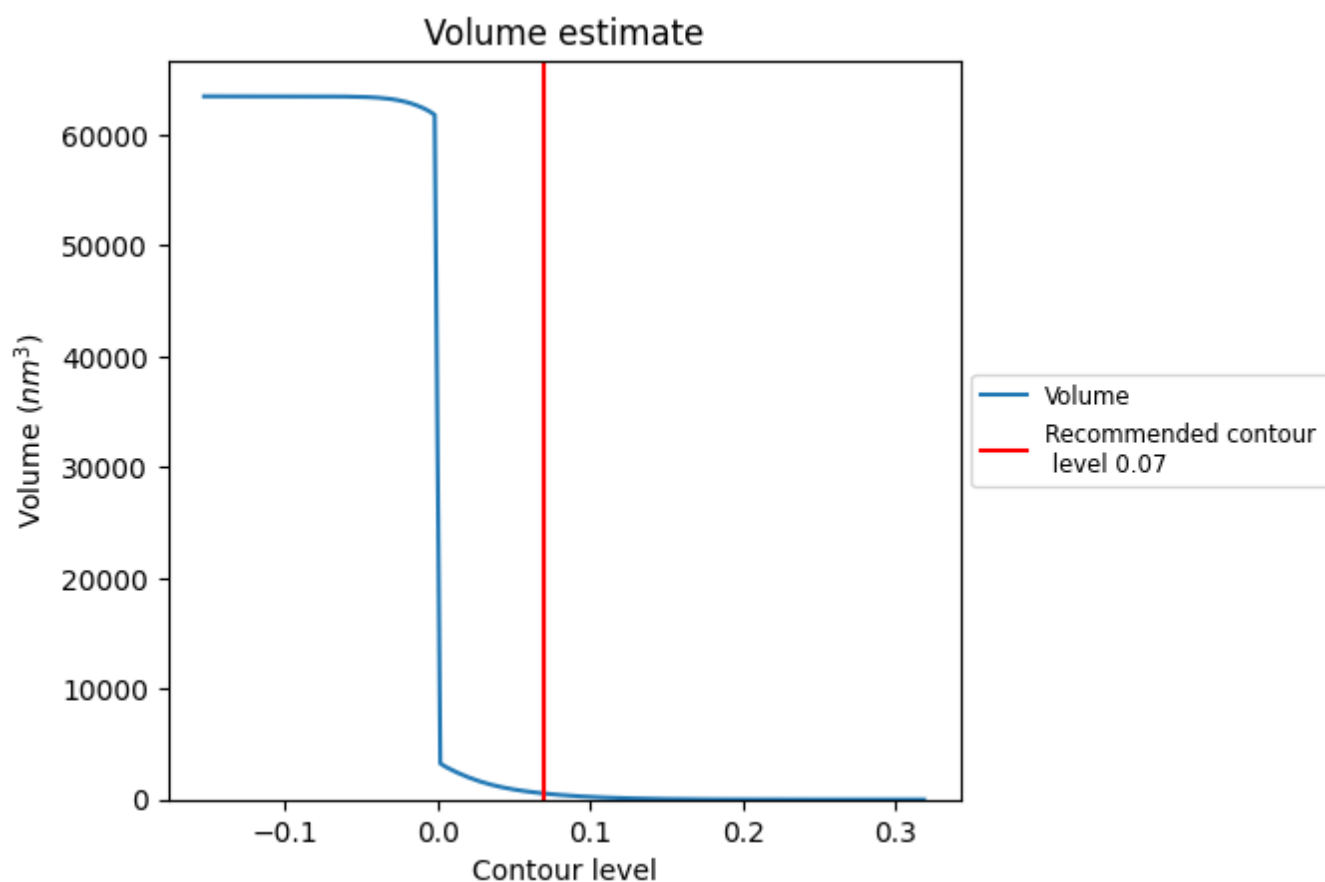
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

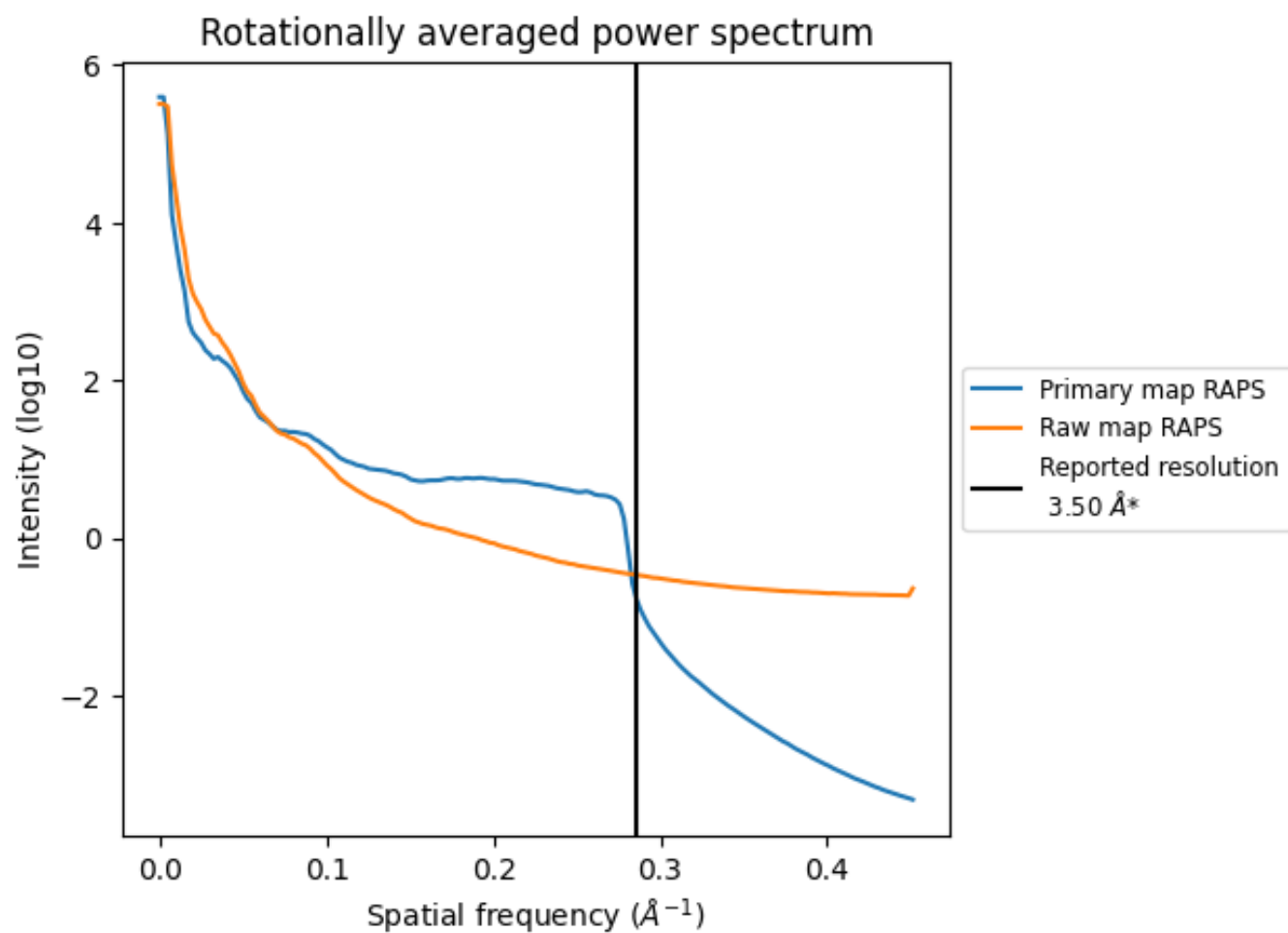
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 543 nm³; this corresponds to an approximate mass of 490 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 ⓘ

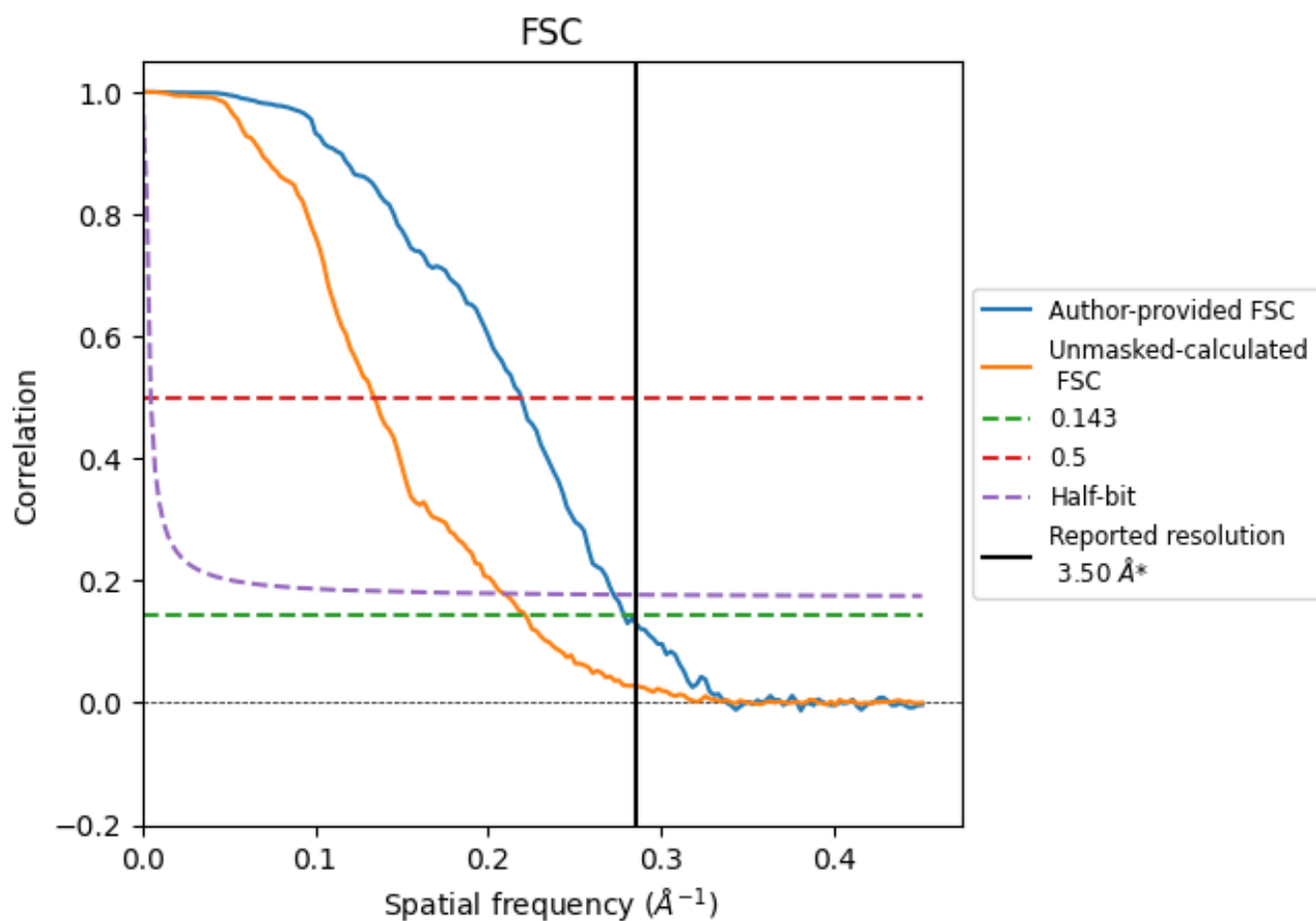


*Reported resolution corresponds to spatial frequency of 0.286 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.286 Å⁻¹

8.2 Resolution estimates [i](#)

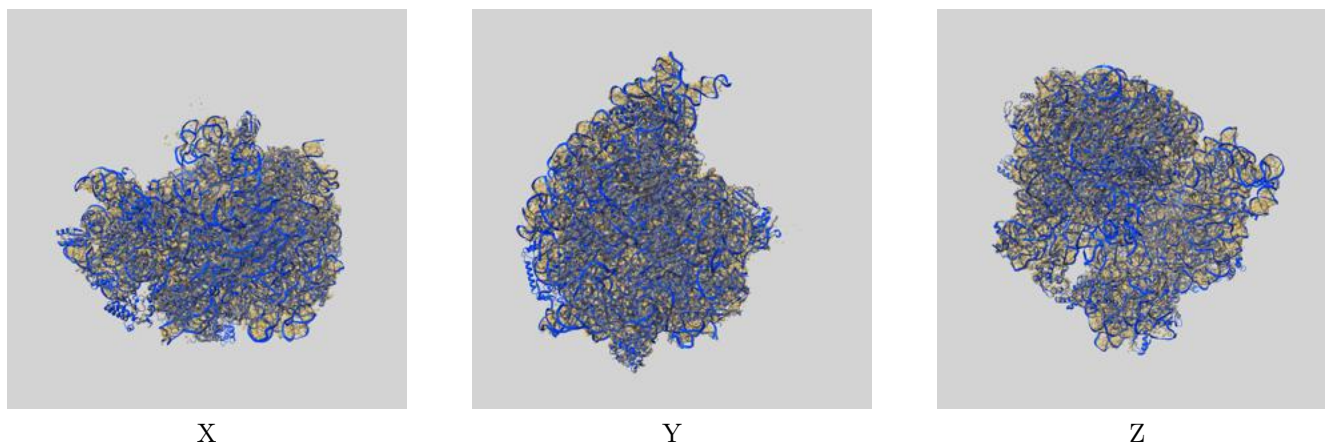
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.50	-	-
Author-provided FSC curve	3.59	4.56	3.67
Unmasked-calculated*	4.51	7.45	4.78

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.51 differs from the reported value 3.5 by more than 10 %

9 Map-model fit [i](#)

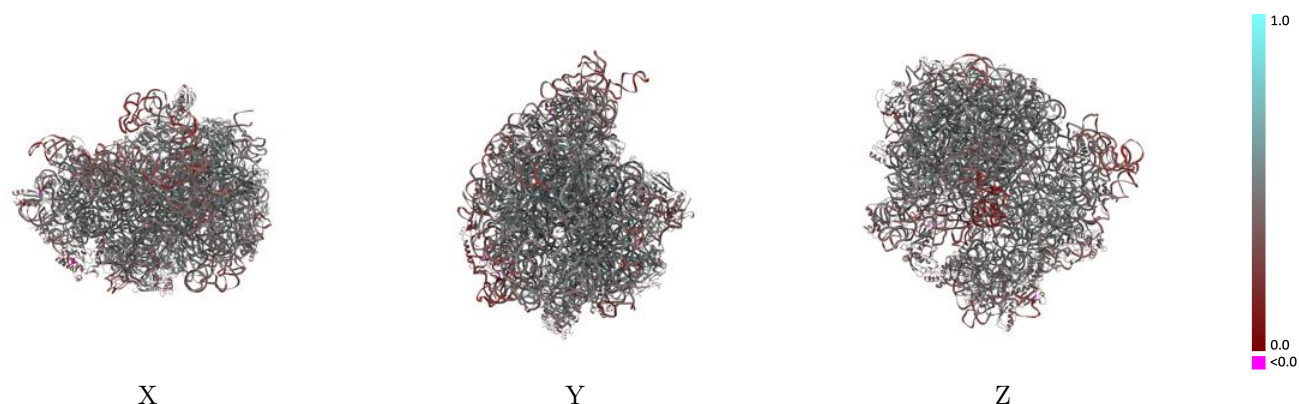
This section contains information regarding the fit between EMDB map EMD-12574 and PDB model 7NSP. Per-residue inclusion information can be found in section [3](#) on page [15](#).

9.1 Map-model overlay [i](#)



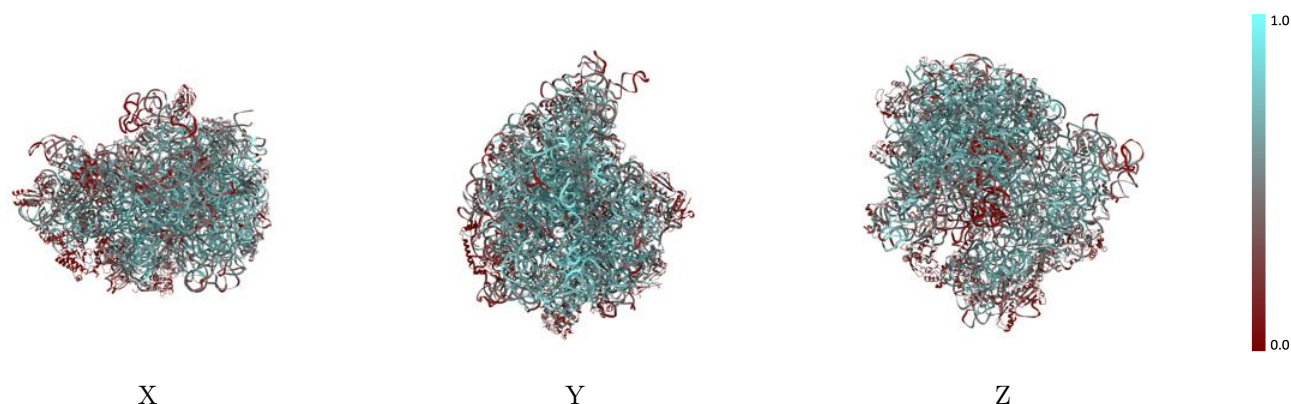
The images above show the 3D surface view of the map at the recommended contour level 0.07 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



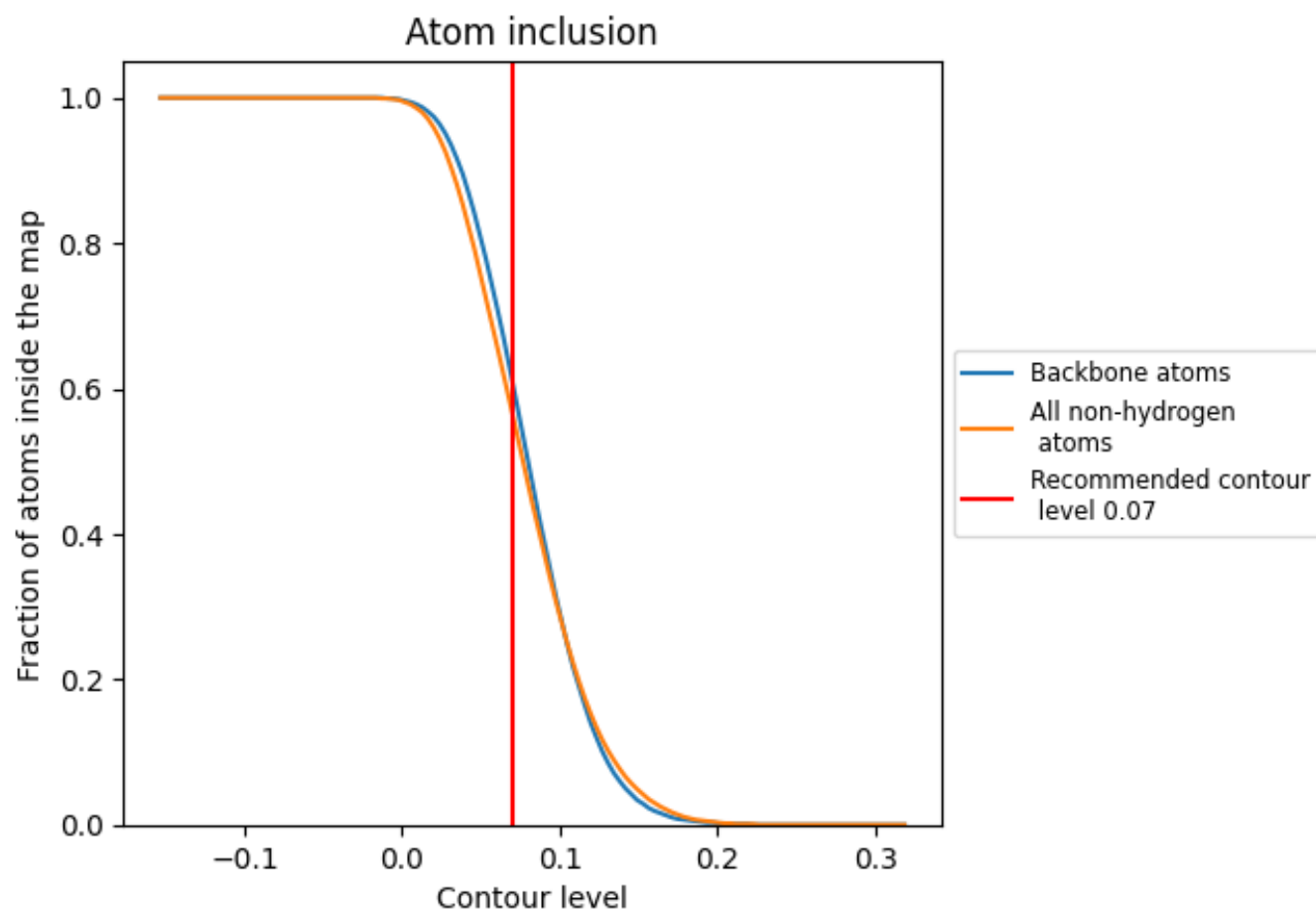
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.07).

9.4 Atom inclusion [i](#)



At the recommended contour level, 61% of all backbone atoms, 56% 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 (0.07) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.5650	 0.4480
0	 0.4880	 0.4810
1	 0.0650	 0.4140
2	 0.6140	 0.5250
3	 0.5340	 0.5130
4	 0.4760	 0.5040
5	 0.1370	 0.3740
6	 0.6750	 0.4740
7	 0.3830	 0.4550
8	 0.4440	 0.4000
A	 0.6700	 0.4520
B	 0.6070	 0.4120
C	 0.5440	 0.5170
D	 0.4790	 0.4870
E	 0.4000	 0.4700
F	 0.2740	 0.4040
G	 0.2280	 0.4160
H	 0.0270	 0.3200
J	 0.5010	 0.4960
K	 0.4340	 0.4880
L	 0.4380	 0.4770
M	 0.4690	 0.4980
N	 0.5520	 0.4920
O	 0.3460	 0.4240
P	 0.4450	 0.4880
Q	 0.5840	 0.5040
R	 0.4470	 0.4800
S	 0.4900	 0.4950
T	 0.4230	 0.4670
U	 0.3420	 0.4570
V	 0.3880	 0.4570
W	 0.5080	 0.5160
X	 0.4490	 0.4830
Y	 0.3520	 0.4150
Z	 0.4690	 0.4690



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Chain	Atom inclusion	Q-score
a	 0.6420	 0.4420
b	 0.1030	 0.4020
c	 0.3670	 0.4540
d	 0.2260	 0.4190
e	 0.4310	 0.4780
f	 0.3460	 0.4420
g	 0.2140	 0.4110
h	 0.4310	 0.4740
i	 0.3290	 0.4270
j	 0.2810	 0.4400
k	 0.3680	 0.4610
l	 0.4090	 0.4880
m	 0.3410	 0.4280
n	 0.4200	 0.4630
o	 0.4060	 0.4520
p	 0.3650	 0.4480
q	 0.3540	 0.4520
r	 0.3610	 0.4780
s	 0.3660	 0.4580
t	 0.3970	 0.4400
u	 0.0520	 0.4060
v	 0.1990	 0.3210