



Full wwPDB EM Validation Report ⓘ

Mar 10, 2026 – 05:27 PM UTC

PDB ID : 6VWL / pdb_00006vwl
EMDB ID : EMD-21420
Title : 70S ribosome bound to HIV frameshifting stem-loop (FSS) and P/E tRNA (rotated conformation)
Authors : Loerch, S.; Bao, C.; Ling, C.; Korostelev, A.A.; Grigorieff, N.; Ermolenko, D.M.
Deposited on : 2020-02-20
Resolution : 3.10 Å(reported)

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

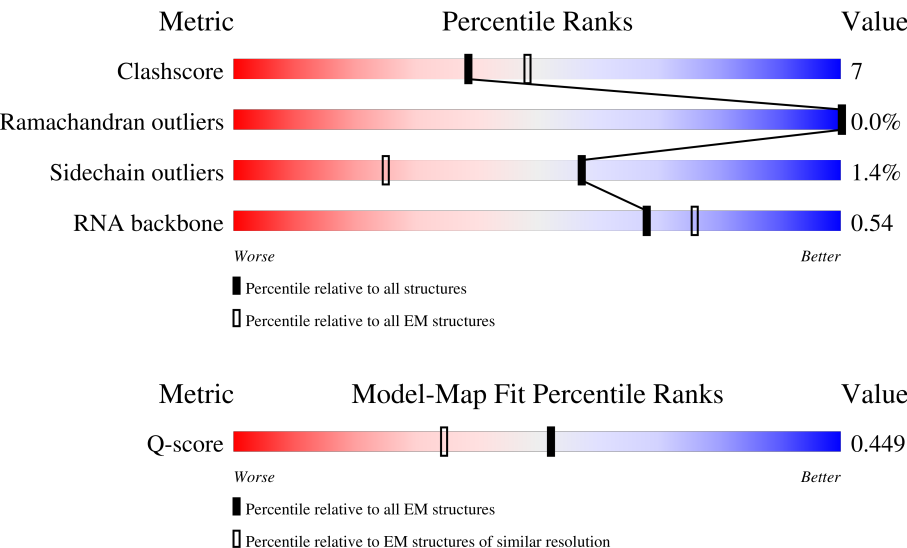
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh &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

1 Overall quality at a glance i

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

The reported resolution of this entry is 3.10 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	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	14724 (2.60 - 3.60)

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	273	79% 20%
2	B	209	83% 17%
3	C	201	9% 81% 19%

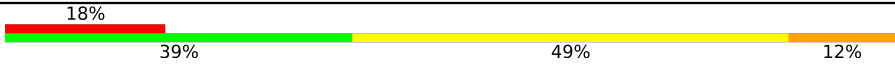
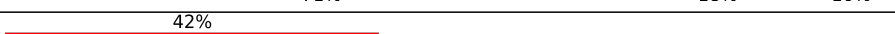
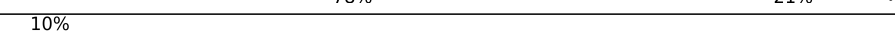
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Mol	Chain	Length	Quality of chain
4	D	179	
5	E	177	
6	F	149	
7	G	142	
8	I	123	
9	J	144	
10	K	136	
11	L	127	
12	M	117	
13	N	115	
14	O	118	
15	P	103	
16	Q	110	
17	R	100	
18	S	104	
19	T	94	
20	U	85	
21	V	78	
22	W	63	
23	X	59	
24	Y	57	
25	Z	55	
26	AA	46	
27	AB	65	
28	3	120	

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Mol	Chain	Length	Quality of chain
29	5	76	
30	AC	38	
31	2	2903	
32	a	241	
33	b	233	
34	c	206	
35	d	167	
36	e	135	
37	f	179	
38	g	130	
39	h	130	
40	i	103	
41	j	129	
42	k	124	
43	l	118	
44	m	101	
45	n	89	
46	o	82	
47	p	84	
48	q	75	
49	r	92	
50	s	87	
51	t	71	
52	1	1540	
53	4	93	

2 Entry composition

There are 54 unique types of molecules in this entry. The entry contains 140603 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called 50S ribosomal protein L2.

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

- Molecule 2 is a protein called 50S ribosomal protein L3.

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

- Molecule 3 is a protein called 50S ribosomal protein L4.

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

- Molecule 4 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	175	Total	C	N	O	S	0	0
			1396	890	246	254	6		

- Molecule 5 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	173	Total	C	N	O	S	0	0
			1298	817	238	241	2		

- Molecule 6 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	57	Total	C	N	O	S	0	0
			440	281	79	79	1		

- Molecule 7 is a protein called 50S ribosomal protein L13.

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

- Molecule 8 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	I	123	Total	C	N	O	S	0	0
			947	593	181	167	6		

- Molecule 9 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	J	143	Total	C	N	O	S	0	0
			1043	649	206	186	2		

- Molecule 10 is a protein called 50S ribosomal protein L16.

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

- Molecule 11 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	L	119	Total	C	N	O	S	0	0
			951	588	195	163	5		

- Molecule 12 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms				AltConf	Trace
12	M	114	Total	C	N	O	0	0
			875	542	175	158		

- Molecule 13 is a protein called 50S ribosomal protein L19.

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

- Molecule 14 is a protein called 50S ribosomal protein L20.

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

- Molecule 15 is a protein called 50S ribosomal protein L21.

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

- Molecule 16 is a protein called 50S ribosomal protein L22.

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

- Molecule 17 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	R	90	Total	C	N	O	S	0	0
			714	449	136	128	1		

- Molecule 18 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms				AltConf	Trace
18	S	96	Total	C	N	O	0	0
			735	464	138	133		

- Molecule 19 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	T	93	Total	C	N	O	S	0	0
			745	474	136	133	2		

- Molecule 20 is a protein called 50S ribosomal protein L27.

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

- Molecule 21 is a protein called 50S ribosomal protein L28.

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

- Molecule 22 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	W	60	Total	C	N	O	S	0	0
			491	303	96	91	1		

- Molecule 23 is a protein called 50S ribosomal protein L30.

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

- Molecule 24 is a protein called 50S ribosomal protein L32.

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

- Molecule 25 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms				AltConf	Trace
25	Z	48	Total	C	N	O	0	0
			396	255	72	69		

- Molecule 26 is a protein called 50S ribosomal protein L34.

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

- Molecule 27 is a protein called 50S ribosomal protein L35.

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

- Molecule 28 is a RNA chain called 5S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	3	120	Total	C	N	O	P	0	0
			2568	1145	471	833	119		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
3	120	A	U	conflict	GB 984297099

- Molecule 29 is a RNA chain called tRNAPhe.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	5	76	Total	C	N	O	P	0	0
			1625	724	292	533	76		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
5	47	G	U	conflict	GB 984297099
5	48	U	C	conflict	GB 984297099

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

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

- Molecule 31 is a RNA chain called 23S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	2	2833	Total	C	N	O	P	0	0
			60819	27131	11192	19664	2832		

There are 19 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
2	208	C	-	insertion	GB 984297099
2	284	U	C	conflict	GB 984297099
2	285	G	A	conflict	GB 984297099
2	356	G	A	conflict	GB 984297099
2	542	C	U	conflict	GB 984297099
2	747	C	U	conflict	GB 984297099
2	1174	U	G	conflict	GB 984297099

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Chain	Residue	Modelled	Actual	Comment	Reference
2	1211	C	U	conflict	GB 984297099
2	1513	U	C	conflict	GB 984297099
2	1723	G	A	conflict	GB 984297099
2	1730	C	U	conflict	GB 984297099
2	1865	U	C	conflict	GB 984297099
2	2163	A	G	conflict	GB 984297099
2	2712	C	U	conflict	GB 984297099
2	2794	C	U	conflict	GB 984297099
2	2796	U	C	conflict	GB 984297099
2	2797	U	C	conflict	GB 984297099
2	2799	A	G	conflict	GB 984297099
2	2802	G	A	conflict	GB 984297099

- Molecule 32 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	a	222	Total	C	N	O	S	0	0
			1689	1071	296	315	7		

- Molecule 33 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	b	197	Total	C	N	O	S	0	0
			1502	957	276	266	3		

- Molecule 34 is a protein called 30S ribosomal protein S4.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	c	158	Total	C	N	O	S	0	0
			1262	790	236	233	3		

- Molecule 35 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	d	156	Total	C	N	O	S	0	0
			1137	709	214	208	6		

- Molecule 36 is a protein called 30S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	e	102	Total	C	N	O	S	0	0
			832	525	150	150	7		

- Molecule 37 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	f	108	Total	C	N	O	S	0	0
			837	525	158	151	3		

- Molecule 38 is a protein called 30S ribosomal protein S8.

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

- Molecule 39 is a protein called 30S ribosomal protein S9.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	h	127	Total	C	N	O	S	0	0
			1006	626	200	178	2		

- Molecule 40 is a protein called 30S ribosomal protein S10.

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

- Molecule 41 is a protein called 30S ribosomal protein S11.

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

- Molecule 42 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	k	121	Total	C	N	O	S	0	0
			940	581	193	162	4		

- Molecule 43 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	l	106	Total	C	N	O	S	0	0
			806	500	156	147	3		

- Molecule 44 is a protein called 30S ribosomal protein S14.

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

- Molecule 45 is a protein called 30S ribosomal protein S15.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	n	87	Total	C	N	O	S	0	0
			702	433	140	128	1		

- Molecule 46 is a protein called 30S ribosomal protein S16.

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

- Molecule 47 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	p	79	Total	C	N	O	S	0	0
			641	406	120	112	3		

- Molecule 48 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms				AltConf	Trace
48	q	54	Total	C	N	O	0	0
			443	281	81	81		

- Molecule 49 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	r	80	Total	C	N	O	S	0	0
			644	413	121	108	2		

- Molecule 50 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	s	85	Total	C	N	O	S	0	0
			660	409	137	111	3		

- Molecule 51 is a protein called 30S ribosomal protein S21.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	t	68	Total	C	N	O	S	0	0
			566	351	120	94	1		

- Molecule 52 is a RNA chain called 16S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	1	1521	Total	C	N	O	P	0	0
			32632	14554	5986	10571	1521		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
1	1517	A	G	conflict	GB 1726036237

- Molecule 53 is a RNA chain called HIV frameshift stimulating sequence mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	4	43	Total	C	N	O	P	0	0
			926	413	174	296	43		

- Molecule 54 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

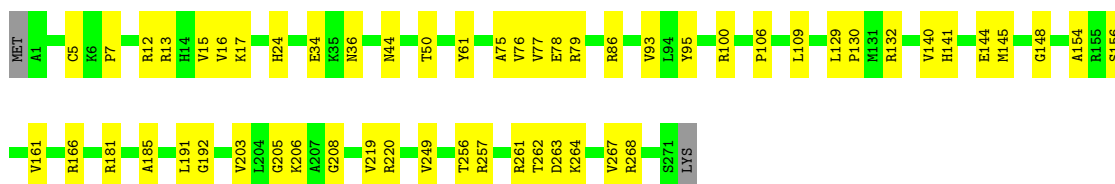
Mol	Chain	Residues	Atoms		AltConf
54	A	1	Total	Mg	0
			1	1	
54	B	1	Total	Mg	0
			1	1	
54	3	5	Total	Mg	0
			5	5	
54	2	26	Total	Mg	0
			26	26	
54	1	1	Total	Mg	0
			1	1	

3 Residue-property plots

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

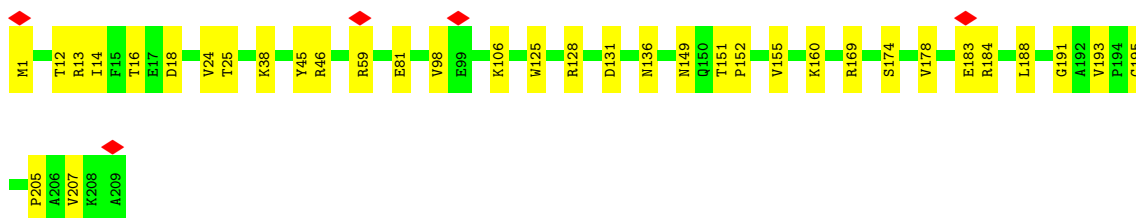
- Molecule 1: 50S ribosomal protein L2

Chain A: 



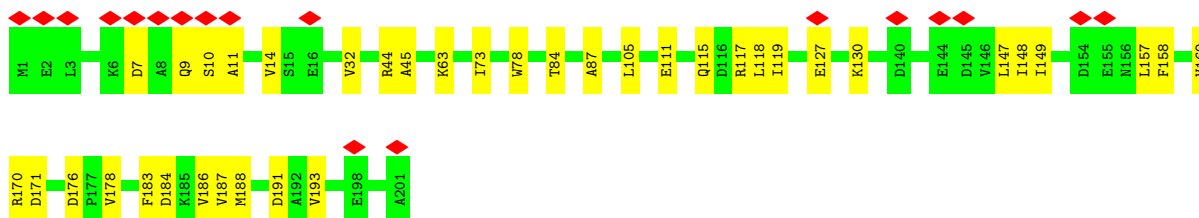
- Molecule 2: 50S ribosomal protein L3

Chain B: 



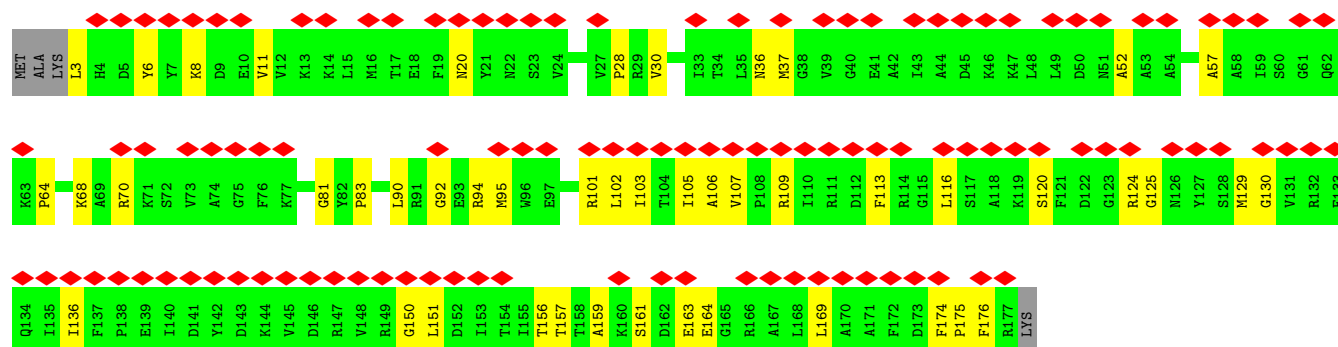
- Molecule 3: 50S ribosomal protein L4

Chain C: 

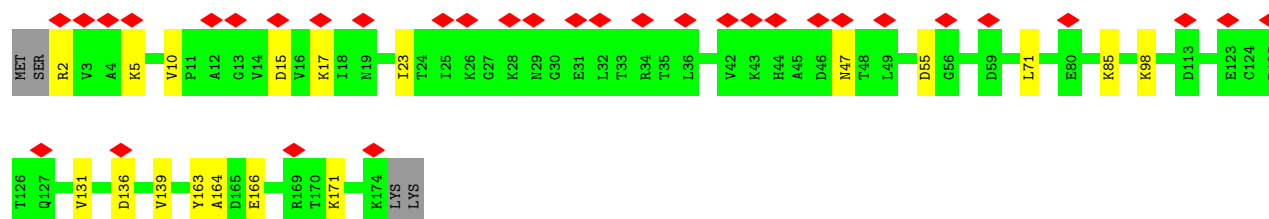
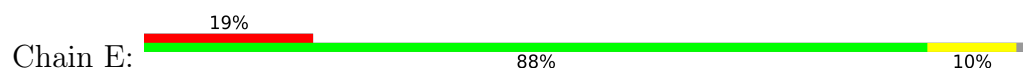


- Molecule 4: 50S ribosomal protein L5

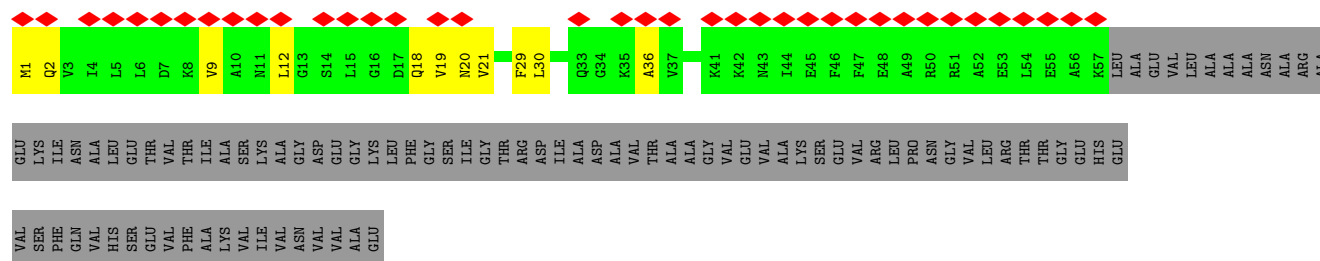
Chain D: 



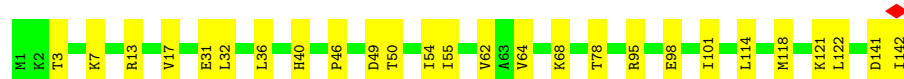
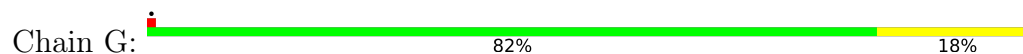
• Molecule 5: 50S ribosomal protein L6



• Molecule 6: 50S ribosomal protein L9



• Molecule 7: 50S ribosomal protein L13



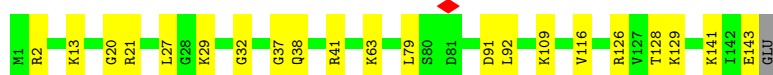
• Molecule 8: 50S ribosomal protein L14



L123

- Molecule 9: 50S ribosomal protein L15

Chain J:  85% 15%



- Molecule 10: 50S ribosomal protein L16

Chain K:  80% 20%



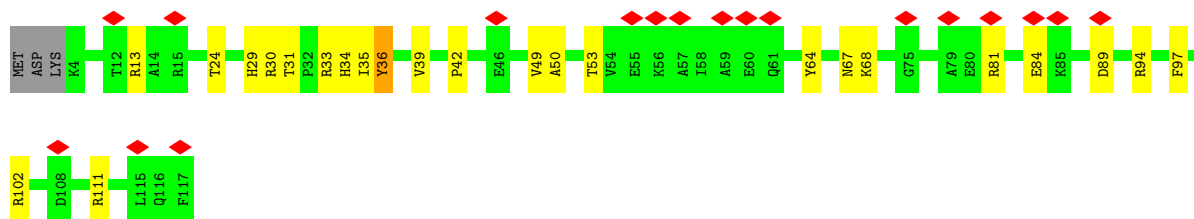
- Molecule 11: 50S ribosomal protein L17

Chain L:  77% 16% 6%



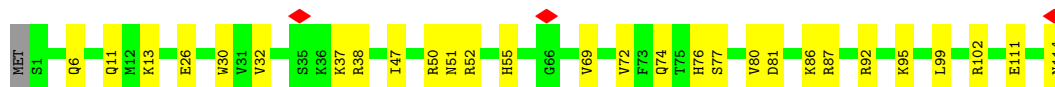
- Molecule 12: 50S ribosomal protein L18

Chain M:  15% 77% 20%



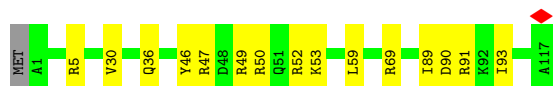
- Molecule 13: 50S ribosomal protein L19

Chain N:  75% 24%

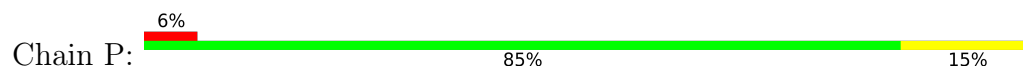


- Molecule 14: 50S ribosomal protein L20

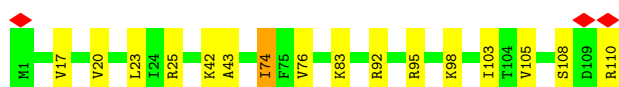
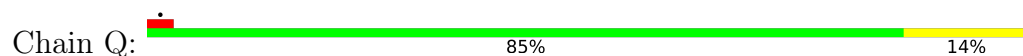
Chain O:  86% 13%



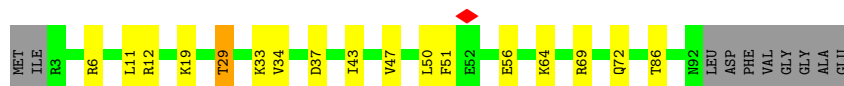
- Molecule 15: 50S ribosomal protein L21



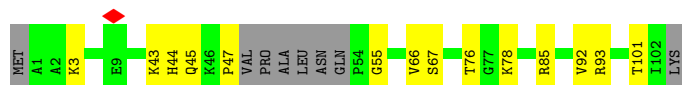
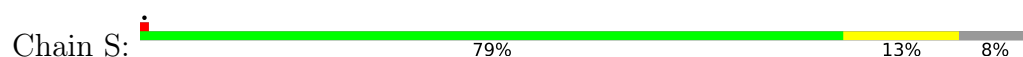
- Molecule 16: 50S ribosomal protein L22



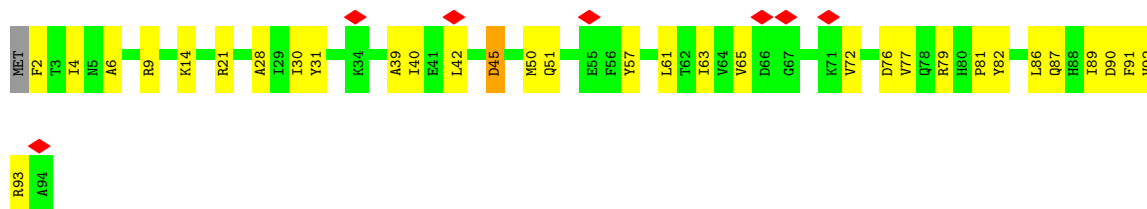
- Molecule 17: 50S ribosomal protein L23



- Molecule 18: 50S ribosomal protein L24



- Molecule 19: 50S ribosomal protein L25



- Molecule 20: 50S ribosomal protein L27



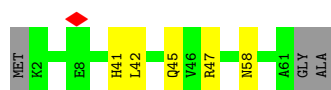
- Molecule 21: 50S ribosomal protein L28

Chain V:  81% 18% .



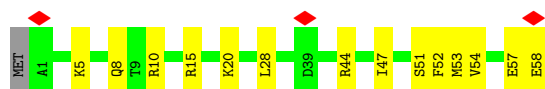
- Molecule 22: 50S ribosomal protein L29

Chain W:  87% 8% 5%



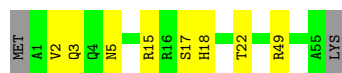
- Molecule 23: 50S ribosomal protein L30

Chain X:  5% 75% 24% .



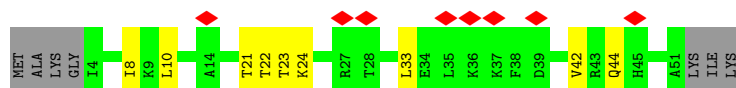
- Molecule 24: 50S ribosomal protein L32

Chain Y:  82% 14% .



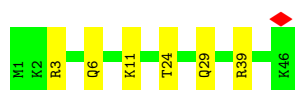
- Molecule 25: 50S ribosomal protein L33

Chain Z:  15% 71% 16% 13%



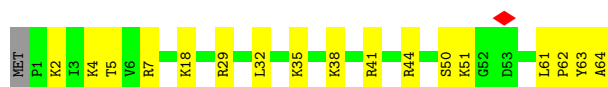
- Molecule 26: 50S ribosomal protein L34

Chain AA:  87% 13%

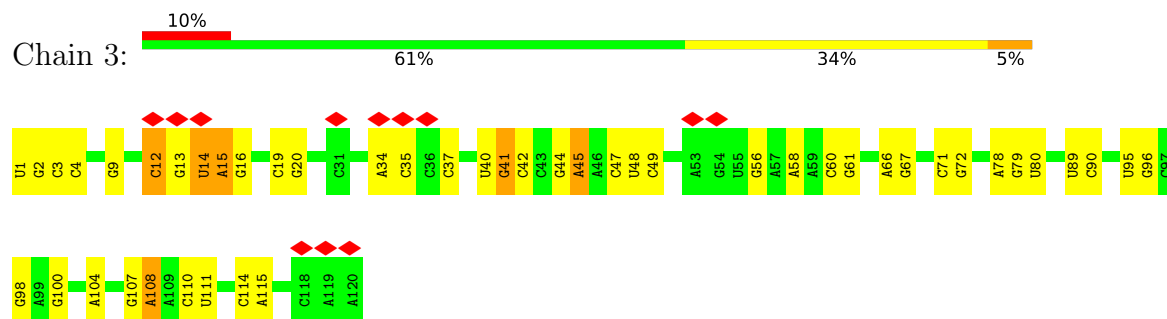


- Molecule 27: 50S ribosomal protein L35

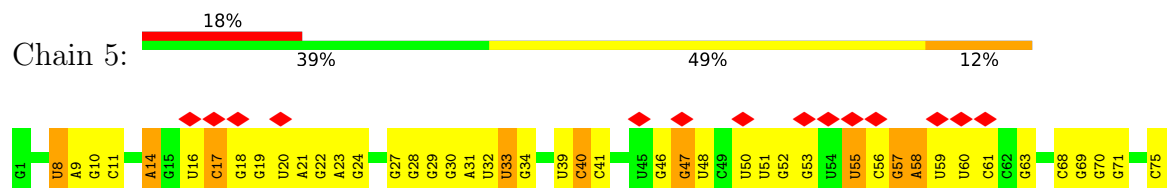
Chain AB:  72% 26% .



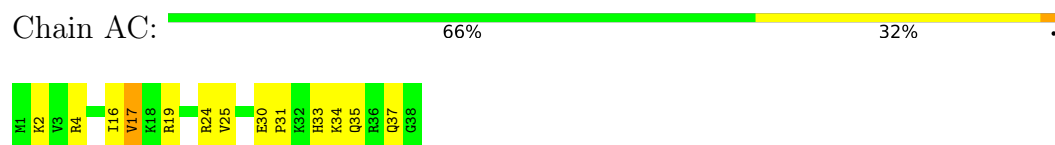
- Molecule 28: 5S ribosomal RNA



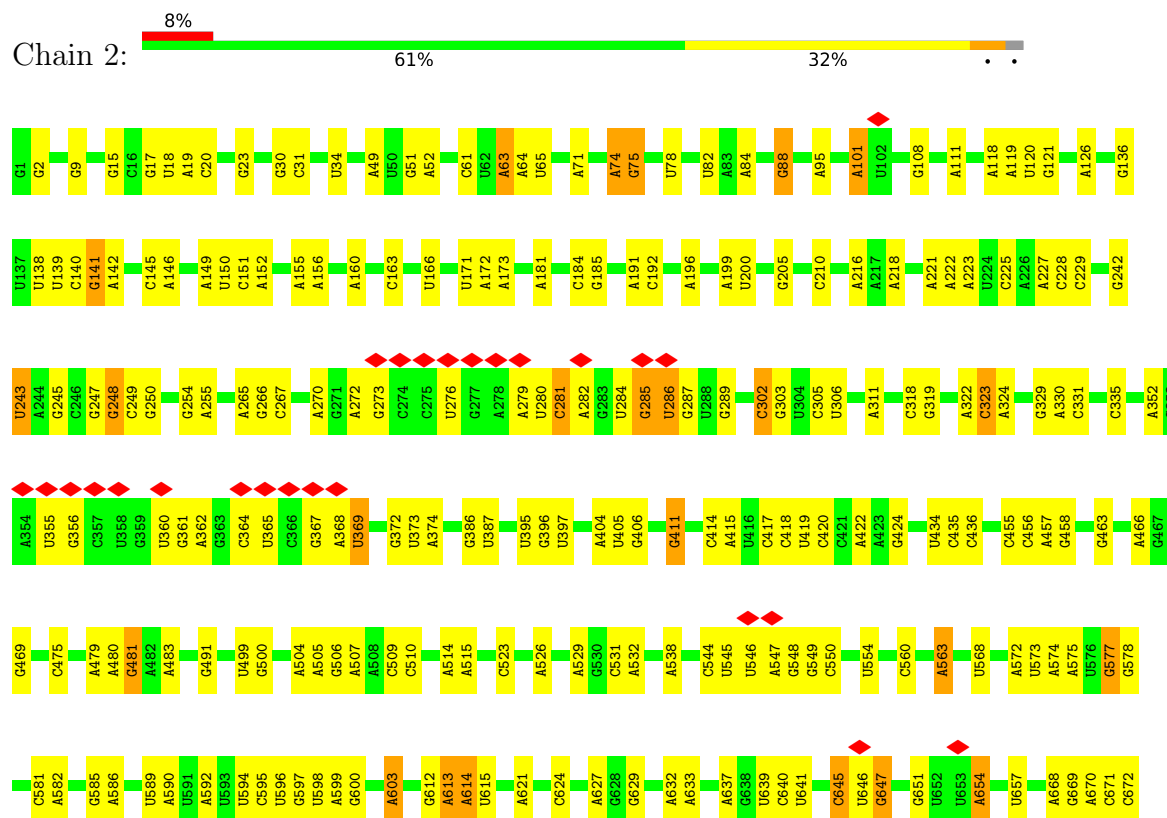
- Molecule 29: tRNA^{Phe}

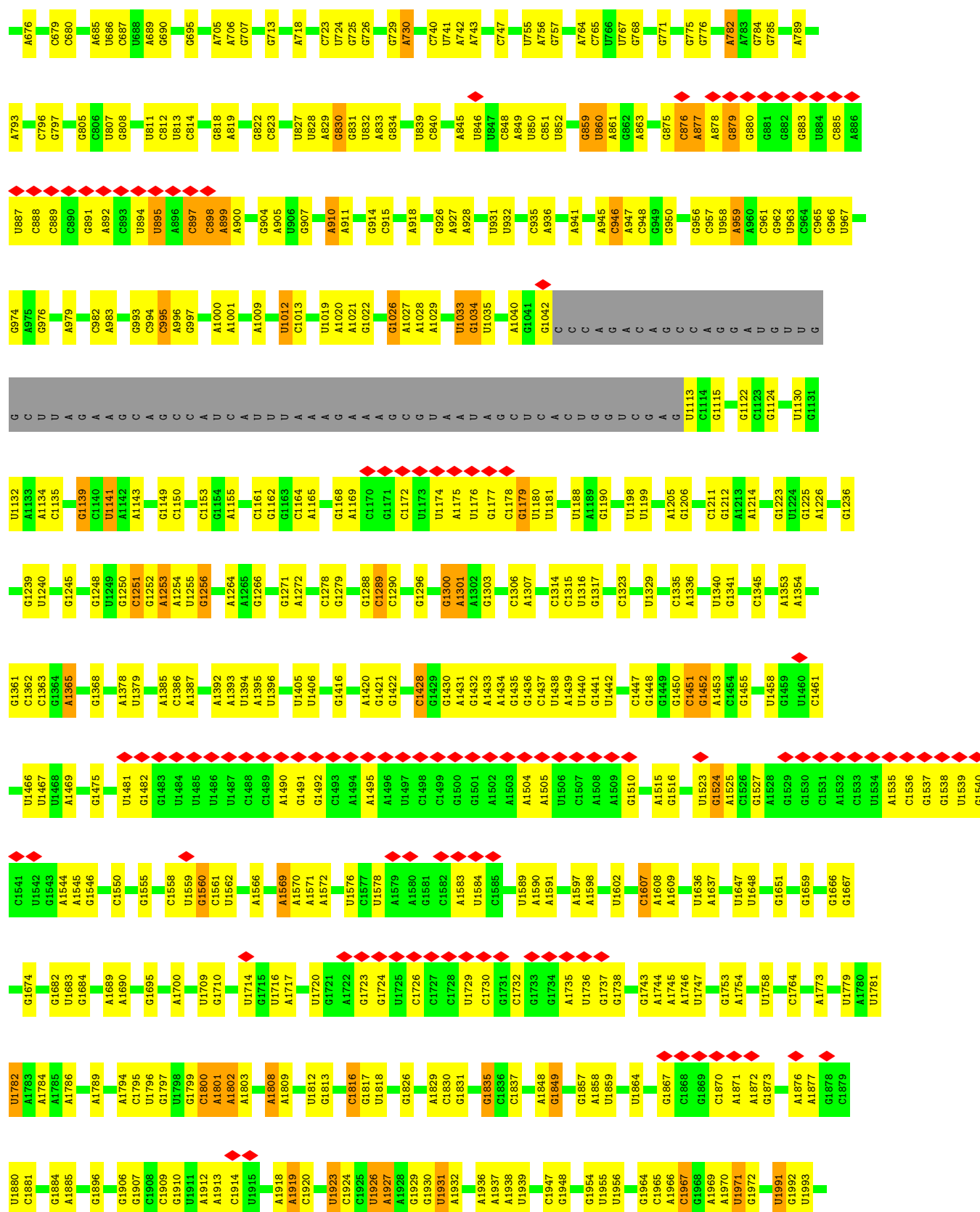


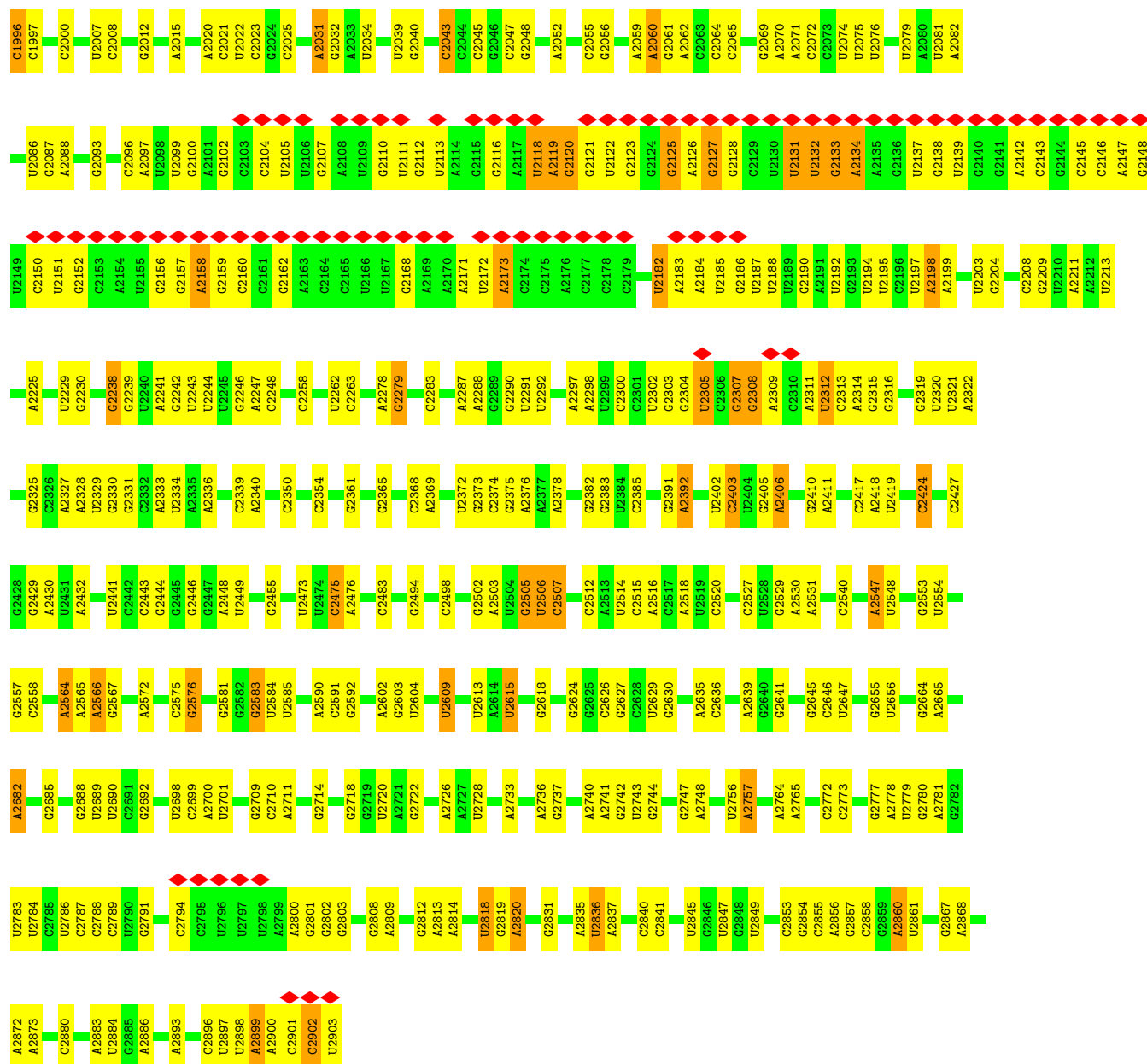
- Molecule 30: 50S ribosomal protein L36



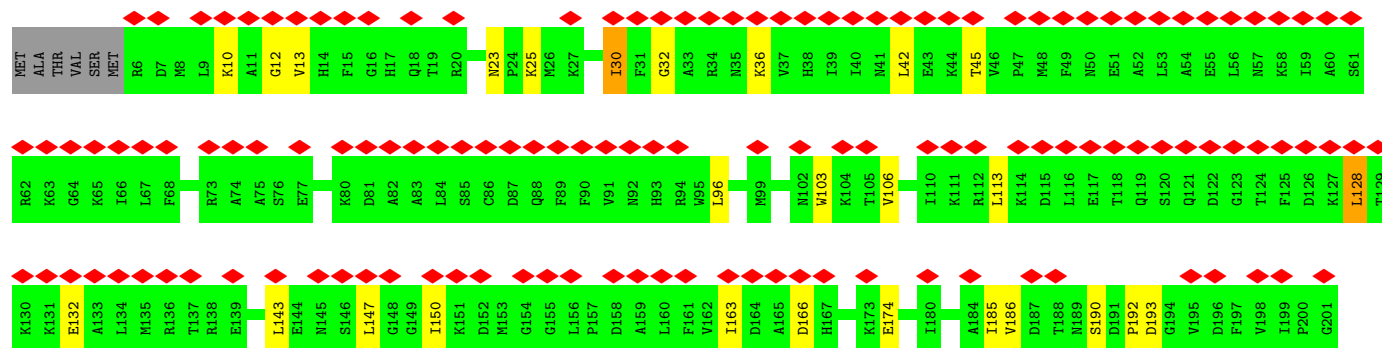
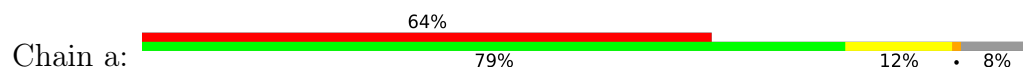
- Molecule 31: 23S ribosomal RNA

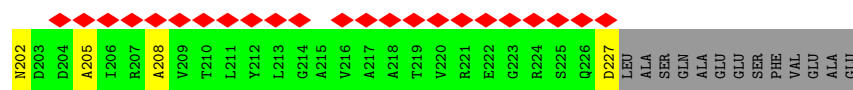




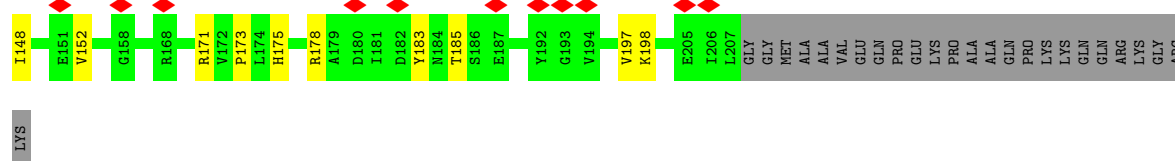
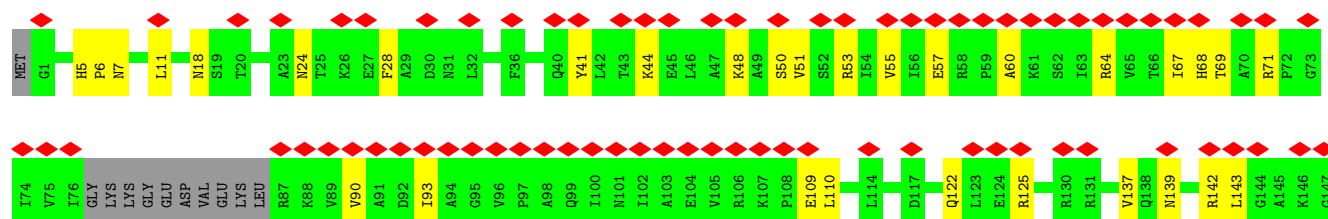


• Molecule 32: 30S ribosomal protein S2

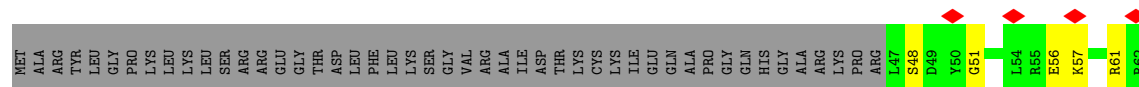




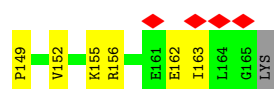
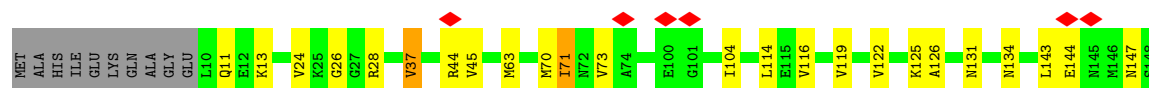
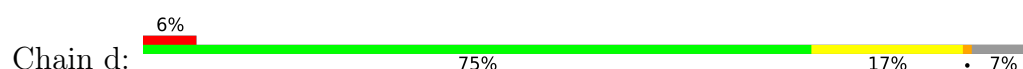
• Molecule 33: 30S ribosomal protein S3



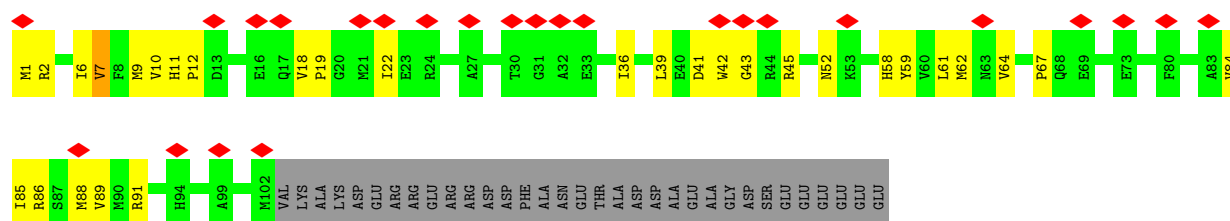
• Molecule 34: 30S ribosomal protein S4



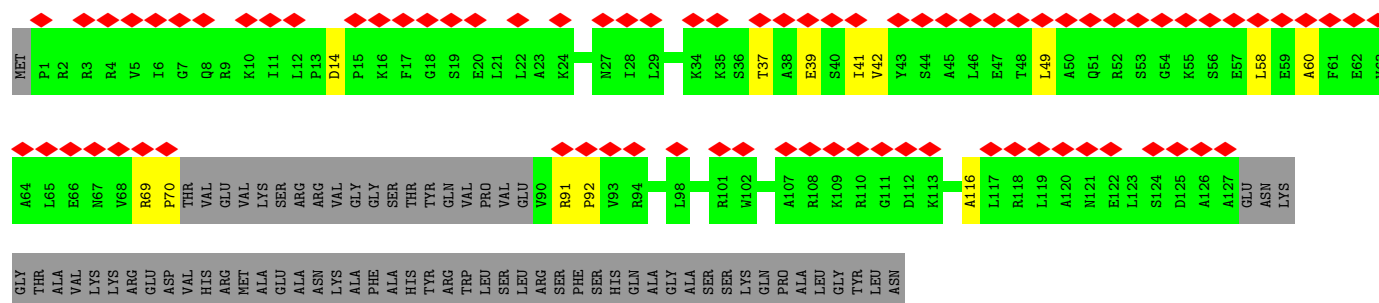
• Molecule 35: 30S ribosomal protein S5



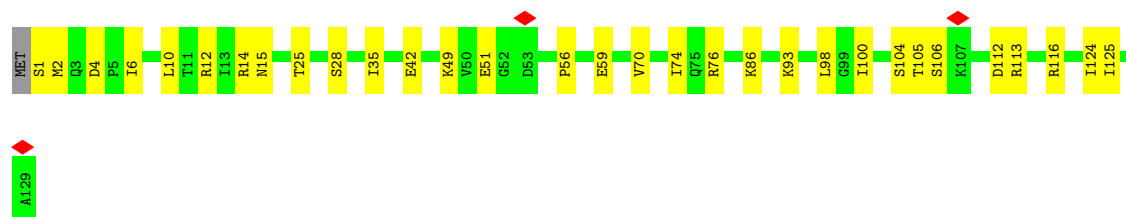
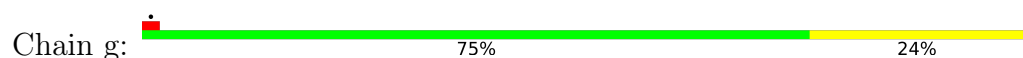
• Molecule 36: 30S ribosomal protein S6



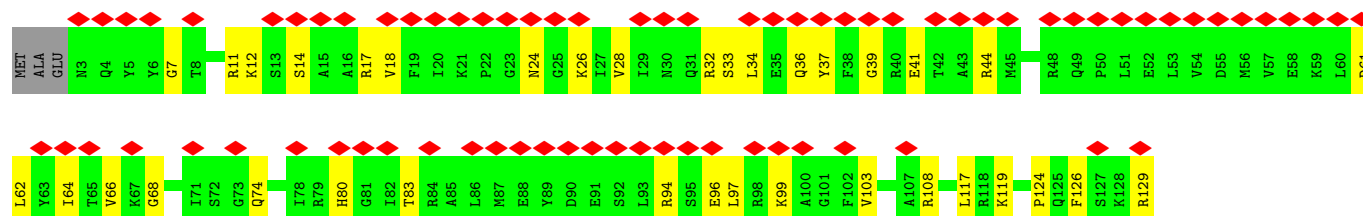
• Molecule 37: 30S ribosomal protein S7



• Molecule 38: 30S ribosomal protein S8



• Molecule 39: 30S ribosomal protein S9

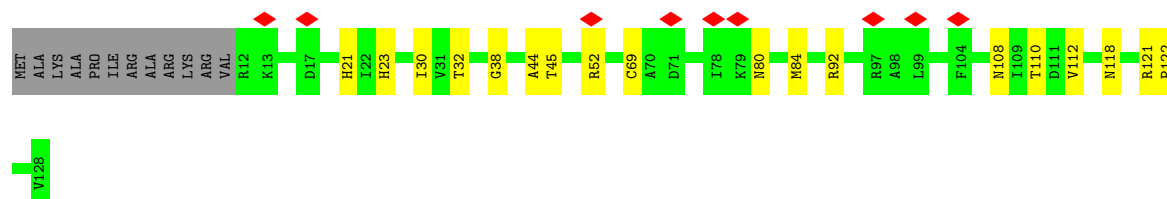
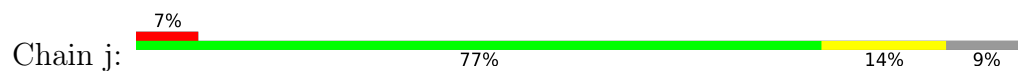


• Molecule 40: 30S ribosomal protein S10

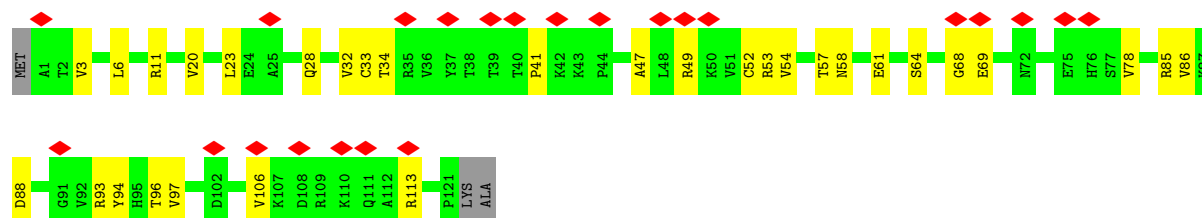
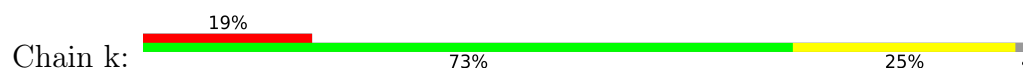




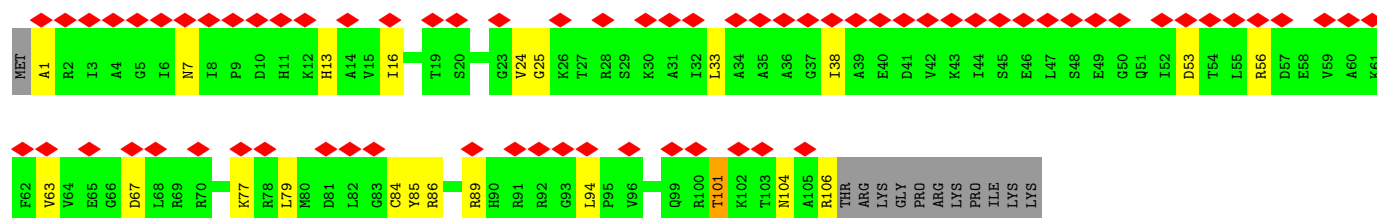
- Molecule 41: 30S ribosomal protein S11



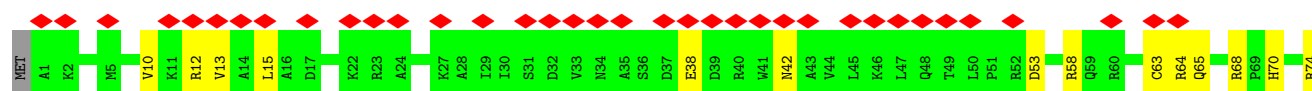
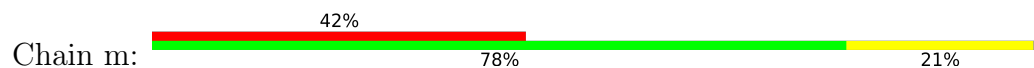
- Molecule 42: 30S ribosomal protein S12

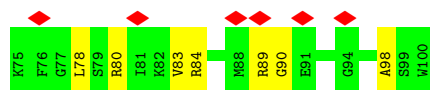


- Molecule 43: 30S ribosomal protein S13

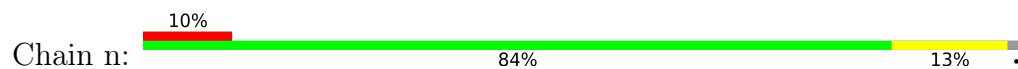


- Molecule 44: 30S ribosomal protein S14

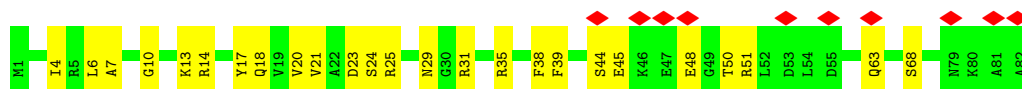




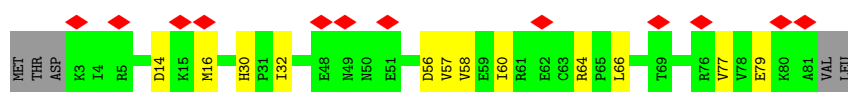
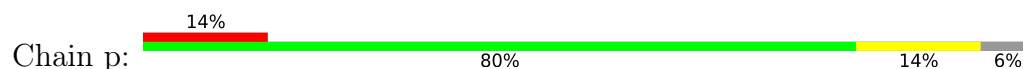
- Molecule 45: 30S ribosomal protein S15



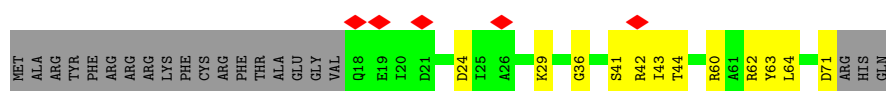
- Molecule 46: 30S ribosomal protein S16



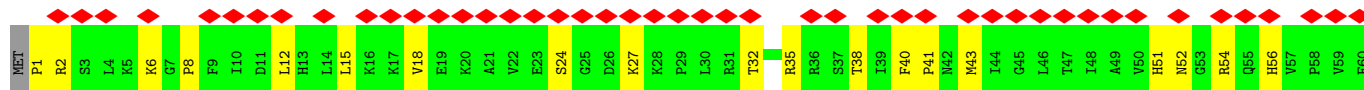
- Molecule 47: 30S ribosomal protein S17



- Molecule 48: 30S ribosomal protein S18

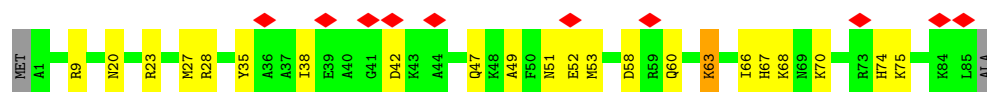


- Molecule 49: 30S ribosomal protein S19

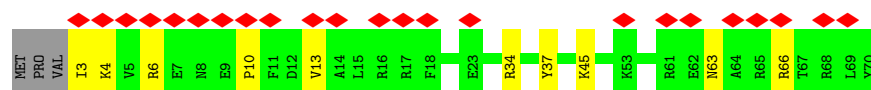
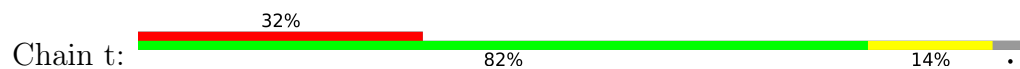


- Molecule 50: 30S ribosomal protein S20

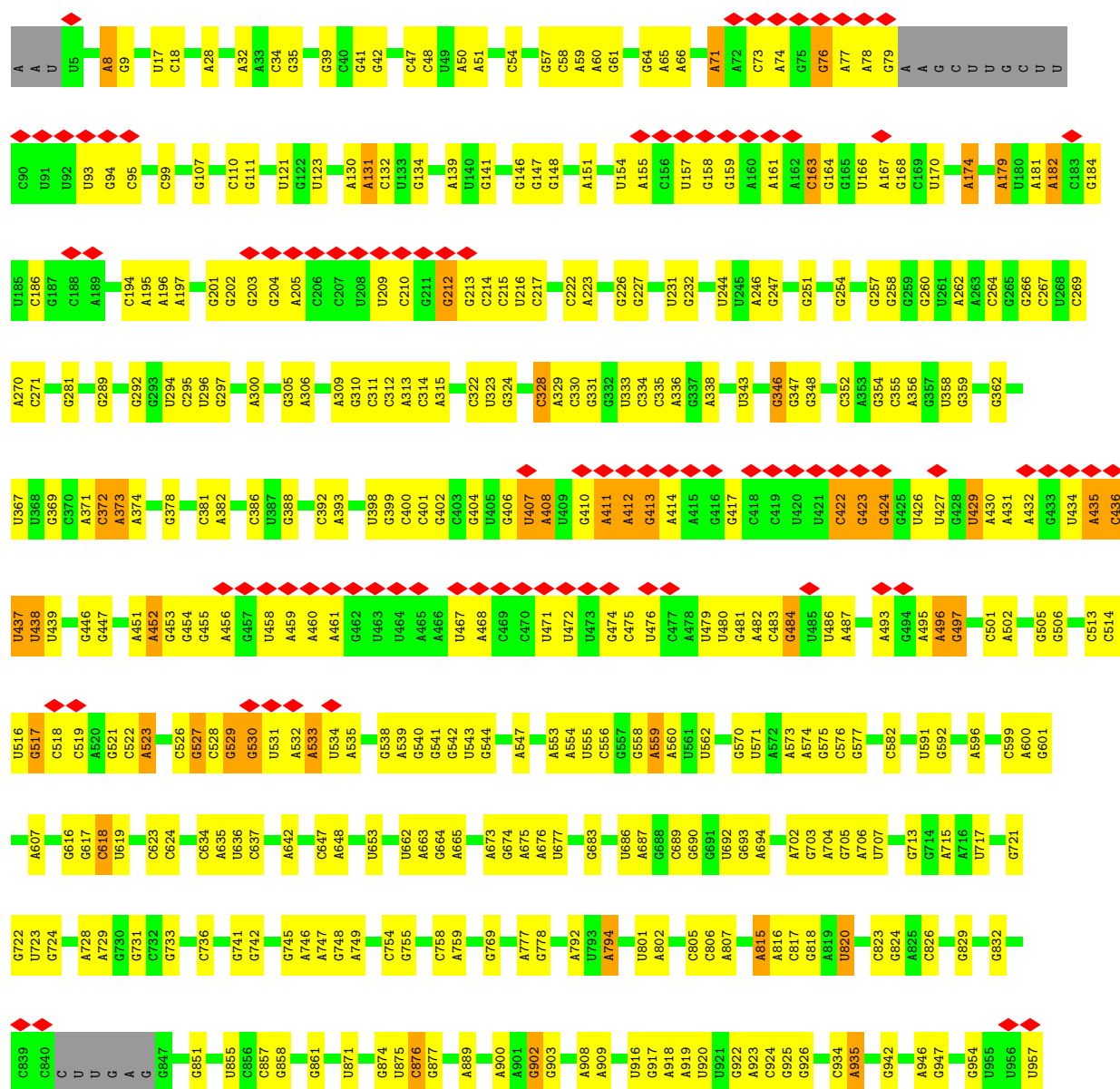


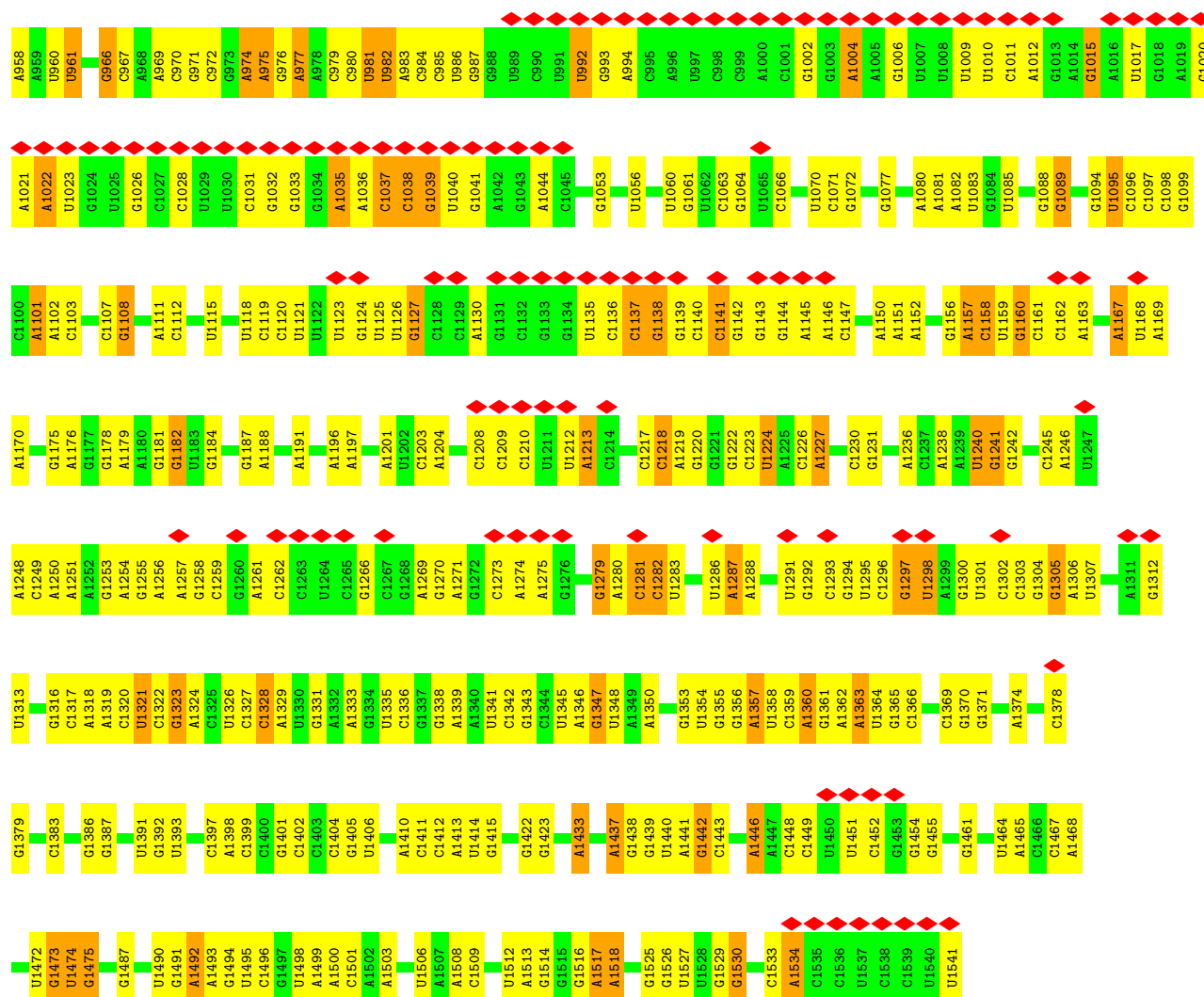


- Molecule 51: 30S ribosomal protein S21

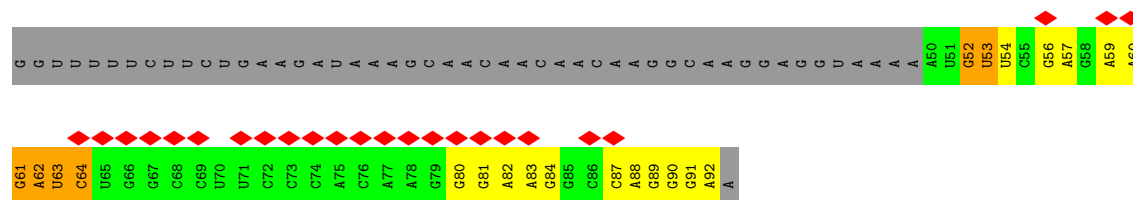
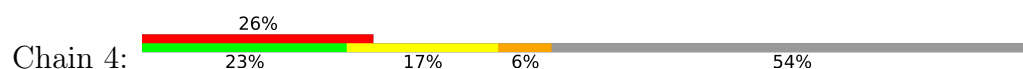


- Molecule 52: 16S ribosomal RNA





● Molecule 53: HIV frameshift stimulating sequence mRNA



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	640261	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 ($e^-/\text{\AA}^2$)	75	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	32.492	Depositor
Minimum map value	-11.578	Depositor
Average map value	0.189	Depositor
Map value standard deviation	1.179	Depositor
Recommended contour level	7	Depositor
Map size (Å)	654.48, 654.48, 654.48	wwPDB
Map dimensions	648, 648, 648	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.01, 1.01, 1.01	Depositor

5 Model quality

5.1 Standard geometry

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

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	0.31	0/2121	0.40	0/2852
2	B	0.33	1/1586 (0.1%)	0.40	0/2134
3	C	0.27	0/1571	0.35	0/2113
4	D	0.18	0/1420	0.37	0/1908
5	E	0.20	0/1318	0.36	0/1786
6	F	0.18	0/445	0.37	0/597
7	G	0.28	0/1152	0.36	0/1551
8	I	0.29	0/956	0.40	0/1279
9	J	0.28	0/1052	0.36	0/1401
10	K	0.28	0/1093	0.37	0/1460
11	L	0.30	0/964	0.45	0/1289
12	M	0.20	0/885	0.38	0/1187
13	N	0.27	0/929	0.43	0/1242
14	O	0.30	0/960	0.39	0/1278
15	P	0.33	0/829	0.42	0/1107
16	Q	0.30	0/864	0.43	0/1156
17	R	0.26	0/720	0.35	0/962
18	S	0.23	0/741	0.34	0/984
19	T	0.23	0/758	0.37	0/1015
20	U	0.29	0/582	0.37	0/769
21	V	0.28	0/635	0.40	0/848
22	W	0.22	0/492	0.31	0/655
23	X	0.27	0/453	0.34	0/605
24	Y	0.32	0/440	0.41	0/588
25	Z	0.18	0/403	0.28	0/538
26	AA	0.32	0/380	0.41	0/498
27	AB	0.28	0/513	0.39	0/676
28	3	0.21	0/2872	0.28	0/4479
29	5	0.21	1/1816 (0.1%)	0.34	0/2830
30	AC	0.25	0/303	0.42	0/397
31	2	0.30	1/68117 (0.0%)	0.30	0/106268
32	a	0.16	0/1720	0.33	0/2328

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	b	0.19	0/1528	0.36	0/2069
34	c	0.18	0/1278	0.39	0/1715
35	d	0.24	0/1150	0.34	0/1549
36	e	0.21	0/851	0.42	0/1150
37	f	0.18	0/846	0.38	0/1135
38	g	0.22	0/989	0.35	0/1326
39	h	0.18	0/1018	0.40	0/1358
40	i	0.20	0/796	0.41	0/1077
41	j	0.20	0/893	0.34	0/1205
42	k	0.25	0/954	0.48	0/1282
43	l	0.21	0/813	0.45	0/1090
44	m	0.17	0/817	0.38	0/1088
45	n	0.23	0/710	0.35	0/950
46	o	0.20	0/659	0.37	0/884
47	p	0.21	0/650	0.36	0/871
48	q	0.21	0/449	0.36	0/604
49	r	0.19	0/660	0.42	0/888
50	s	0.20	0/666	0.39	0/883
51	t	0.18	0/573	0.39	0/759
52	1	0.21	0/36536	0.29	0/56991
53	4	0.15	0/1037	0.27	0/1616
All	All	0.26	3/152963 (0.0%)	0.32	0/229270

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	2	887	U	C1'-N1	6.31	1.56	1.47
29	5	17	C	C1'-N1	5.57	1.55	1.47
2	B	195	GLY	C-O	-5.05	1.18	1.23

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	2082	0	2157	36	0
2	B	1565	0	1616	23	0
3	C	1552	0	1619	25	0
4	D	1396	0	1426	27	0
5	E	1298	0	1340	12	0
6	F	440	0	464	6	0
7	G	1129	0	1162	18	0
8	I	947	0	1023	23	0
9	J	1043	0	1123	13	0
10	K	1074	0	1157	18	0
11	L	951	0	994	13	0
12	M	875	0	906	16	0
13	N	917	0	965	20	0
14	O	947	0	1022	14	0
15	P	816	0	839	11	0
16	Q	857	0	922	10	0
17	R	714	0	773	10	0
18	S	735	0	788	8	0
19	T	745	0	768	20	0
20	U	575	0	592	11	0
21	V	625	0	655	9	0
22	W	491	0	523	4	0
23	X	449	0	491	8	0
24	Y	434	0	448	9	0
25	Z	396	0	424	5	0
26	AA	377	0	418	5	0
27	AB	504	0	574	13	0
28	3	2568	0	1303	30	0
29	5	1625	0	821	23	0
30	AC	302	0	343	11	0
31	2	60819	0	30591	580	0
32	a	1689	0	1661	19	0
33	b	1502	0	1534	25	0
34	c	1262	0	1291	24	0
35	d	1137	0	1178	19	0
36	e	832	0	824	20	0
37	f	837	0	877	10	0
38	g	979	0	1034	23	0
39	h	1006	0	1041	26	0
40	i	786	0	828	26	0
41	j	877	0	887	15	0
42	k	940	0	999	19	0
43	l	806	0	846	14	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
44	m	805	0	847	19	0
45	n	702	0	724	8	0
46	o	649	0	666	17	0
47	p	641	0	682	8	0
48	q	443	0	466	10	0
49	r	644	0	675	21	0
50	s	660	0	713	19	0
51	t	566	0	597	8	0
52	1	32632	0	16427	466	0
53	4	926	0	467	20	0
54	1	1	0	0	0	0
54	2	26	0	0	0	0
54	3	5	0	0	0	0
54	A	1	0	0	0	0
54	B	1	0	0	0	0
All	All	140603	0	93511	1631	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 7.

All (1631) 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)
53:4:62:A:N6	53:4:91:G:H1	1.47	1.11
52:1:447:G:N2	52:1:487:A:H62	1.54	1.04
31:2:2747:G:N2	31:2:2757:A:H62	1.56	1.03
31:2:706:A:H62	31:2:725:G:H21	1.04	1.02
52:1:447:G:H21	52:1:487:A:N6	1.56	1.02
52:1:76:G:H1	52:1:93:U:H3	1.02	1.00
31:2:284:U:H3	31:2:356:G:H1	1.04	1.00
29:5:51:U:H3	29:5:63:G:H1	1.00	0.99
31:2:2747:G:H21	31:2:2757:A:N6	1.61	0.98
52:1:1088:G:N2	52:1:1167:A:H61	1.62	0.98
52:1:1088:G:H21	52:1:1167:A:H61	0.96	0.95
52:1:942:G:H1	52:1:1341:U:H3	0.99	0.93
52:1:1088:G:H21	52:1:1167:A:N6	1.66	0.92
31:2:2107:G:H1	31:2:2182:U:H3	0.95	0.91
52:1:410:G:H21	52:1:432:A:H62	0.98	0.91
52:1:410:G:N2	52:1:432:A:H62	1.68	0.90
52:1:1009:U:H3	52:1:1020:G:H1	1.05	0.90
31:2:706:A:H62	31:2:725:G:N2	1.70	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
52:1:447:G:H21	52:1:487:A:H62	0.88	0.87
53:4:62:A:H62	53:4:91:G:H1	1.17	0.87
22:W:41:HIS:HD1	31:2:95:A:HO2'	1.20	0.85
52:1:417:G:H1	52:1:426:U:H3	1.25	0.84
52:1:683:G:H1	52:1:707:U:H3	1.21	0.84
53:4:62:A:N6	53:4:91:G:N1	2.24	0.84
31:2:1168:G:H1	31:2:1181:U:H3	1.25	0.83
52:1:410:G:H21	52:1:432:A:N6	1.76	0.82
31:2:706:A:N6	31:2:725:G:H21	1.76	0.82
47:p:57:VAL:HG12	47:p:79:GLU:HB2	1.63	0.81
49:r:8:PRO:HB2	49:r:38:THR:HG21	1.64	0.79
42:k:23:LEU:HG	42:k:58:ASN:HD22	1.48	0.78
31:2:1907:G:H1	31:2:1923:U:H3	1.31	0.77
31:2:2185:U:H2'	31:2:2186:G:H8	1.49	0.76
52:1:452:A:N6	52:1:480:U:C2	2.53	0.76
31:2:1433:A:N1	31:2:1560:G:O6	2.18	0.76
31:2:976:G:HO2'	31:2:1155:A:HO2'	1.32	0.76
31:2:1040:A:H2	31:2:1115:G:H1	1.34	0.76
31:2:1527:G:H21	31:2:1545:A:H62	1.34	0.76
36:e:42:TRP:HB2	36:e:59:TYR:HB2	1.68	0.73
31:2:200:U:H3	31:2:250:G:H1	1.33	0.73
31:2:270:A:N1	31:2:369:U:O2'	2.22	0.73
31:2:2857:G:N2	31:2:2860:A:OP2	2.21	0.73
31:2:2682:A:H61	31:2:2728:U:H1'	1.56	0.71
31:2:1434:A:H61	31:2:1558:C:H42	1.38	0.71
52:1:1304:G:H21	52:1:1333:A:N6	1.89	0.71
52:1:201:G:H1	52:1:216:U:H3	1.37	0.71
29:5:51:U:O2	29:5:63:G:N2	2.24	0.70
31:2:713:G:H21	31:2:718:A:H62	1.39	0.70
31:2:84:A:H62	31:2:101:A:H2	1.39	0.70
52:1:1011:C:H2'	52:1:1012:A:H8	1.57	0.70
52:1:722:G:H1	52:1:733:G:H1	1.40	0.69
31:2:1717:A:H62	31:2:1743:G:H21	1.40	0.69
48:q:60:ARG:NH2	52:1:736:C:OP1	2.25	0.69
52:1:1141:C:H2'	52:1:1142:G:H8	1.55	0.69
52:1:1304:G:N2	52:1:1333:A:N6	2.41	0.69
49:r:2:ARG:NH2	52:1:1318:A:OP1	2.26	0.69
31:2:1020:A:N1	31:2:1141:U:O2'	2.23	0.69
53:4:61:G:O6	53:4:92:A:N1	2.25	0.69
29:5:33:U:OP2	39:h:129:ARG:NH2	2.25	0.69
42:k:33:CYS:SG	42:k:34:THR:N	2.66	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:I:123:LEU:HD11	13:N:69:VAL:HG11	1.75	0.69
15:P:79:ARG:NH2	31:2:563:A:OP2	2.24	0.69
31:2:1779:U:OP2	31:2:1784:A:N6	2.26	0.69
52:1:454:G:N2	52:1:479:U:O2	2.26	0.69
1:A:77:VAL:HG12	1:A:93:VAL:HG12	1.74	0.69
31:2:1303:G:N7	31:2:1607:C:N4	2.41	0.69
27:AB:4:LYS:NZ	31:2:254:G:N7	2.40	0.68
52:1:1356:G:H2'	52:1:1357:A:H8	1.58	0.68
15:P:80:ARG:NH2	31:2:572:A:OP2	2.26	0.68
10:K:123:LYS:NZ	31:2:2483:C:N3	2.39	0.68
52:1:1393:U:HO2'	52:1:1501:C:HO2'	1.41	0.68
52:1:1440:U:O2	52:1:1461:G:N2	2.26	0.68
52:1:987:G:H21	52:1:1015:G:H21	1.41	0.67
52:1:1347:G:N2	52:1:1374:A:OP2	2.26	0.67
37:f:91:ARG:NH2	52:1:1378:C:N3	2.42	0.67
36:e:22:ILE:HD11	36:e:39:LEU:HD11	1.76	0.67
33:b:51:VAL:HA	33:b:69:THR:HG22	1.77	0.67
32:a:113:LEU:HD12	32:a:143:LEU:HB3	1.77	0.67
52:1:992:U:O2	52:1:1044:A:N7	2.27	0.67
24:Y:18:HIS:HE1	31:2:2624:G:H1'	1.58	0.67
31:2:475:C:O2	31:2:479:A:N6	2.27	0.67
12:M:50:ALA:O	12:M:81:ARG:NH2	2.28	0.67
52:1:1006:G:H1	52:1:1023:U:H3	1.43	0.67
21:V:2:ARG:NH1	31:2:1365:A:OP1	2.26	0.67
44:m:12:ARG:HH21	44:m:58:ARG:HH21	1.43	0.66
27:AB:7:ARG:NH1	31:2:243:U:OP1	2.29	0.66
52:1:1242:G:O6	52:1:1295:U:O4	2.14	0.66
52:1:1490:U:H2'	52:1:1491:G:H8	1.60	0.66
53:4:62:A:H61	53:4:91:G:H1	1.39	0.66
4:D:125:GLY:HA3	4:D:159:ALA:HB3	1.77	0.66
27:AB:61:LEU:HB3	27:AB:64:ALA:HB3	1.77	0.66
2:B:131:ASP:O	2:B:136:ASN:ND2	2.29	0.66
31:2:2107:G:O6	31:2:2182:U:O4	2.14	0.66
32:a:174:GLU:OE2	52:1:1101:A:N6	2.27	0.66
36:e:52:ASN:HD21	36:e:85:ILE:HD11	1.61	0.66
28:3:9:G:H1	28:3:111:U:H3	1.43	0.66
31:2:1835:G:C8	31:2:1969:A:H2	2.14	0.66
52:1:1413:A:H2	52:1:1487:G:H1	1.43	0.66
50:s:66:ILE:HG22	50:s:68:LYS:H	1.59	0.65
2:B:151:THR:OG1	31:2:2032:G:N2	2.30	0.65
27:AB:32:LEU:HD23	27:AB:35:LYS:HD2	1.78	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:3:78:A:H62	28:3:98:G:H21	1.44	0.65
32:a:186:VAL:HG13	32:a:190:SER:HB2	1.77	0.65
1:A:5:CYS:SG	1:A:17:LYS:NZ	2.70	0.65
31:2:2102:G:N2	31:2:2187:U:O2	2.27	0.65
31:2:2656:U:O2	31:2:2665:A:N7	2.30	0.65
8:I:65:THR:HG22	8:I:67:LYS:H	1.61	0.65
52:1:1291:U:H2'	52:1:1292:G:H8	1.62	0.65
9:J:63:LYS:O	27:AB:29:ARG:NH1	2.31	0.64
32:a:10:LYS:HE2	32:a:13:VAL:HG11	1.78	0.64
46:o:48:GLU:OE2	46:o:51:ARG:NH2	2.30	0.64
4:D:68:LYS:HA	4:D:83:PRO:HA	1.78	0.64
31:2:463:G:N2	31:2:466:A:OP2	2.27	0.64
39:h:68:GLY:HA2	52:1:1250:A:H4'	1.80	0.64
9:J:79:LEU:HB3	9:J:116:VAL:HG23	1.80	0.64
16:Q:98:LYS:NZ	31:2:1323:C:OP1	2.31	0.64
52:1:1413:A:N1	52:1:1487:G:O6	2.31	0.64
35:d:162:GLU:O	38:g:113:ARG:NH1	2.31	0.64
14:O:91:ARG:NH2	31:2:1153:C:OP1	2.24	0.63
23:X:47:ILE:O	23:X:51:SER:HB3	1.97	0.63
31:2:1040:A:N1	31:2:1115:G:O6	2.31	0.63
31:2:1422:G:O2'	31:2:1492:G:N3	2.29	0.63
52:1:148:G:O6	52:1:174:A:N1	2.31	0.63
1:A:208:GLY:HA2	31:2:764:A:H5''	1.79	0.63
10:K:20:LEU:HD13	19:T:81:PRO:HG2	1.79	0.63
31:2:2802:G:H2'	31:2:2803:G:H8	1.62	0.63
33:b:185:THR:HG22	33:b:198:LYS:HG2	1.80	0.63
52:1:1304:G:N2	52:1:1333:A:H62	1.96	0.63
34:c:120:LYS:HG2	34:c:130:ASN:HB3	1.79	0.63
52:1:297:G:N2	52:1:300:A:OP2	2.30	0.63
1:A:86:ARG:NH1	31:2:1817:G:OP1	2.29	0.63
31:2:2747:G:H21	31:2:2757:A:H62	0.78	0.63
52:1:372:C:N4	52:1:388:G:OP2	2.29	0.63
10:K:50:ARG:HG3	10:K:65:ILE:HD11	1.79	0.63
40:i:9:ARG:NH2	52:1:1279:G:OP1	2.31	0.63
49:r:52:ASN:ND2	49:r:75:PRO:O	2.31	0.63
52:1:1009:U:O2	52:1:1020:G:N2	2.24	0.63
52:1:1156:G:H21	52:1:1179:A:H61	1.46	0.63
31:2:1926:U:H2'	31:2:1927:A:C8	2.34	0.63
31:2:2405:G:O2'	31:2:2411:A:N6	2.32	0.63
33:b:53:ARG:HB2	33:b:68:HIS:HB2	1.80	0.63
52:1:412:A:H62	52:1:431:A:H61	1.47	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
52:1:1083:U:O2'	52:1:1102:A:OP2	2.15	0.63
52:1:527:G:O2'	52:1:535:A:N1	2.30	0.63
52:1:1026:G:O6	52:1:1035:A:N1	2.31	0.63
2:B:14:ILE:HD11	2:B:188:LEU:HD13	1.81	0.62
5:E:85:LYS:HG3	5:E:164:ALA:HB2	1.80	0.62
1:A:257:ARG:NH2	31:2:1799:G:OP1	2.33	0.62
20:U:10:ARG:NH2	31:2:2279:G:N7	2.47	0.62
34:c:48:SER:O	34:c:51:GLY:N	2.27	0.62
44:m:84:ARG:NH2	52:1:1060:U:OP1	2.31	0.62
49:r:54:ARG:NH2	52:1:957:U:O2'	2.32	0.62
16:Q:25:ARG:NH1	16:Q:74:ILE:O	2.31	0.62
28:3:12:C:O2'	28:3:15:A:N3	2.32	0.62
52:1:1386:G:H2'	52:1:1387:G:H8	1.62	0.62
13:N:32:VAL:HG12	13:N:37:LYS:HG2	1.82	0.62
38:g:4:ASP:OD2	38:g:76:ARG:NH1	2.33	0.62
40:i:19:ASP:OD1	40:i:72:ARG:NH1	2.30	0.62
37:f:41:ILE:HD11	37:f:116:ALA:HB2	1.82	0.62
52:1:1071:C:H2'	52:1:1072:G:H8	1.65	0.62
31:2:1700:A:N6	52:1:1475:G:OP1	2.31	0.62
38:g:42:GLU:HG2	38:g:100:ILE:HD13	1.80	0.62
44:m:15:LEU:HD23	44:m:53:ASP:HB2	1.81	0.61
49:r:54:ARG:NH2	52:1:958:A:N7	2.47	0.61
48:q:36:GLY:O	48:q:62:ARG:NH2	2.34	0.61
4:D:92:GLY:HA2	4:D:95:MET:HG2	1.83	0.61
31:2:151:C:H2'	31:2:152:A:H8	1.66	0.61
31:2:1433:A:H2'	31:2:1434:A:H8	1.66	0.61
52:1:961:U:OP2	52:1:1223:C:O2'	2.18	0.61
30:AC:37:GLN:O	31:2:1124:G:O2'	2.17	0.61
31:2:1438:U:H2'	31:2:1439:A:H8	1.66	0.61
31:2:2372:U:H2'	31:2:2373:G:H8	1.65	0.61
41:j:21:HIS:NE2	41:j:84:MET:SD	2.74	0.61
10:K:74:THR:HG21	10:K:86:LYS:HE2	1.83	0.61
31:2:2:G:O6	31:2:2902:C:N4	2.33	0.61
34:c:77:GLU:OE2	34:c:80:ARG:NH2	2.33	0.61
3:C:158:PHE:HA	3:C:169:VAL:HG21	1.83	0.61
31:2:2076:U:OP2	31:2:2238:G:N2	2.30	0.61
40:i:41:PRO:HA	40:i:72:ARG:HG2	1.82	0.61
52:1:664:G:H22	52:1:741:G:H1	1.48	0.61
31:2:2131:U:H5'	31:2:2132:U:H5''	1.81	0.61
37:f:69:ARG:HH11	37:f:70:PRO:HD2	1.66	0.61
46:o:31:ARG:HB2	52:1:310:G:H5''	1.83	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:2:247:G:O2'	31:2:250:G:O6	2.19	0.60
3:C:119:ILE:HB	3:C:187:VAL:HG12	1.81	0.60
8:I:76:VAL:H	13:N:72:VAL:HG22	1.66	0.60
34:c:61:ARG:HH11	34:c:67:LEU:HA	1.65	0.60
19:T:2:PHE:HB2	19:T:61:LEU:HD22	1.83	0.60
31:2:2507:C:H41	31:2:2581:G:H21	1.48	0.60
49:r:2:ARG:HH12	49:r:6:LYS:HB3	1.65	0.60
49:r:77:ARG:NH2	52:1:1321:U:O2'	2.35	0.60
52:1:182:A:N6	52:1:194:C:O2	2.34	0.60
52:1:618:C:H5'	52:1:619:U:H5''	1.83	0.60
52:1:1222:G:OP2	52:1:1322:C:N4	2.30	0.60
12:M:24:THR:HG22	12:M:42:PRO:HD3	1.83	0.60
15:P:1:MET:HA	15:P:42:ALA:O	2.00	0.60
44:m:68:ARG:NH1	52:1:974:A:OP1	2.31	0.60
1:A:34:GLU:OE2	31:2:1816:C:N4	2.32	0.60
52:1:1124:G:O2'	52:1:1127:G:O6	2.20	0.60
17:R:11:LEU:HD12	17:R:50:LEU:HD12	1.83	0.60
31:2:1802:A:H2'	31:2:1803:A:C8	2.36	0.60
33:b:24:ASN:O	33:b:28:PHE:N	2.32	0.60
33:b:139:ASN:OD1	33:b:142:ARG:NH2	2.34	0.60
2:B:128:ARG:NH2	31:2:2512:C:OP2	2.35	0.60
10:K:26:VAL:HG13	10:K:104:GLU:HG2	1.83	0.60
29:5:34:G:H5'	52:1:966:G:C2	2.37	0.60
31:2:1912:A:H1'	52:1:1494:G:H21	1.67	0.60
31:2:1434:A:N6	31:2:1558:C:H42	1.99	0.59
34:c:204:SER:OG	52:1:8:A:N6	2.35	0.59
39:h:129:ARG:O	52:1:970:C:N4	2.35	0.59
40:i:44:THR:HG22	40:i:70:HIS:HA	1.83	0.59
46:o:7:ALA:O	46:o:29:ASN:ND2	2.35	0.59
52:1:1089:G:O6	52:1:1097:C:N4	2.35	0.59
19:T:6:ALA:HB3	19:T:65:VAL:HG22	1.84	0.59
33:b:178:ARG:HD3	52:1:1112:C:H1'	1.85	0.59
52:1:437:U:H2'	52:1:438:U:H4'	1.82	0.59
52:1:222:C:H2'	52:1:223:A:H8	1.67	0.59
31:2:1864:U:OP1	31:2:2410:G:O2'	2.20	0.59
52:1:131:A:O2'	52:1:262:A:O2'	2.20	0.59
10:K:11:LYS:NZ	31:2:2278:A:OP1	2.35	0.59
49:r:18:VAL:HG21	49:r:43:MET:HE3	1.83	0.59
14:O:69:ARG:NH1	31:2:1012:U:OP2	2.36	0.59
31:2:950:G:H1	31:2:967:U:H3	1.51	0.59
31:2:1826:G:O2'	31:2:1971:U:OP2	2.21	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:O:46:TYR:O	14:O:50:ARG:NH1	2.32	0.59
50:s:9:ARG:NH2	52:1:107:G:N7	2.51	0.59
52:1:454:G:C2	52:1:479:U:O2	2.56	0.59
29:5:8:U:C4	29:5:14:A:C5	2.91	0.59
42:k:86:VAL:HG13	42:k:88:ASP:H	1.67	0.59
44:m:12:ARG:NH2	52:1:980:C:O2'	2.36	0.59
2:B:59:ARG:NH2	31:2:2831:G:OP2	2.35	0.59
21:V:36:ARG:NH2	31:2:2199:A:OP1	2.35	0.59
41:j:122:PRO:HD2	51:t:37:TYR:HB2	1.85	0.59
33:b:57:GLU:HB2	33:b:64:ARG:HB2	1.83	0.58
9:J:91:ASP:OD1	9:J:92:LEU:N	2.34	0.58
31:2:284:U:O4	31:2:356:G:O6	2.22	0.58
47:p:30:HIS:HD2	47:p:32:ILE:H	1.50	0.58
31:2:284:U:O2	31:2:356:G:N2	2.29	0.58
31:2:632:A:N3	31:2:2403:C:O2'	2.35	0.58
31:2:2813:A:H2'	31:2:2814:A:H8	1.67	0.58
40:i:29:ALA:HB1	40:i:36:VAL:HG21	1.85	0.58
40:i:70:HIS:NE2	52:1:1152:A:OP1	2.26	0.58
41:j:118:ASN:HD22	51:t:34:ARG:HH12	1.51	0.58
49:r:41:PRO:HG3	49:r:66:VAL:HG22	1.85	0.58
31:2:1801:A:H5''	31:2:2203:U:H2'	1.86	0.58
42:k:41:PRO:HB3	42:k:49:ARG:HH21	1.68	0.58
49:r:43:MET:SD	49:r:43:MET:N	2.77	0.58
2:B:169:ARG:NH2	31:2:2773:C:OP1	2.36	0.58
20:U:33:ILE:HG22	20:U:34:VAL:HG23	1.84	0.58
31:2:280:U:H3	31:2:360:U:H3	1.50	0.58
31:2:411:G:OP2	31:2:2406:A:O2'	2.17	0.58
52:1:1297:G:N2	52:1:1298:U:O4	2.32	0.58
40:i:43:PRO:HB3	52:1:1150:A:H4'	1.86	0.58
32:a:25:LYS:NZ	32:a:193:ASP:OD1	2.28	0.58
32:a:42:LEU:HA	32:a:45:THR:HG22	1.86	0.58
14:O:36:GLN:HE21	31:2:1252:G:H1	1.52	0.58
42:k:53:ARG:NH2	42:k:61:GLU:OE1	2.36	0.58
43:l:101:THR:HG21	52:1:1226:C:H2'	1.85	0.58
31:2:581:C:H2'	31:2:582:A:H8	1.68	0.58
17:R:6:ARG:NH2	17:R:37:ASP:O	2.37	0.57
31:2:742:A:H2'	31:2:743:A:C8	2.38	0.57
31:2:1315:C:O2'	31:2:1392:A:O2'	2.21	0.57
2:B:14:ILE:HG12	13:N:11:GLN:HE22	1.69	0.57
11:L:44:LEU:HD23	11:L:113:ILE:HD13	1.85	0.57
13:N:87:ARG:NE	13:N:111:GLU:OE2	2.37	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:2:2086:U:H2'	31:2:2087:G:C8	2.40	0.57
32:a:103:TRP:HA	32:a:106:VAL:HG22	1.86	0.57
43:l:84:CYS:SG	43:l:85:TYR:N	2.77	0.57
52:1:673:A:H2'	52:1:674:G:C8	2.40	0.57
52:1:1323:G:H2'	52:1:1324:A:C8	2.39	0.57
1:A:220:ARG:NH1	31:2:1789:A:OP2	2.38	0.57
28:3:1:U:H2'	28:3:2:G:H8	1.69	0.57
31:2:1341:G:OP2	31:2:1394:U:O2'	2.22	0.57
31:2:1724:G:H1	31:2:1736:U:H3	1.51	0.57
35:d:155:LYS:HG2	38:g:70:VAL:HG23	1.85	0.57
50:s:67:HIS:O	50:s:67:HIS:ND1	2.37	0.57
52:1:71:A:H61	52:1:99:C:H1'	1.68	0.57
5:E:23:ILE:HG21	5:E:71:LEU:HD11	1.86	0.57
12:M:35:ILE:HD11	12:M:102:ARG:HD2	1.85	0.57
31:2:1717:A:H62	31:2:1743:G:N2	2.03	0.57
52:1:1160:G:H1	52:1:1176:A:N6	2.01	0.57
21:V:9:LYS:NZ	31:2:397:U:OP2	2.32	0.57
23:X:10:ARG:NH2	23:X:52:PHE:O	2.37	0.57
31:2:523:C:O2	31:2:554:U:O2'	2.23	0.57
42:k:113:ARG:NH2	52:1:501:C:OP1	2.38	0.57
52:1:1356:G:H2'	52:1:1357:A:C8	2.39	0.57
1:A:181:ARG:NH2	31:2:1800:C:OP2	2.37	0.57
33:b:7:ASN:ND2	44:m:89:ARG:O	2.38	0.57
31:2:1300:G:H4'	31:2:1301:A:H5''	1.85	0.57
45:n:1:SER:OG	45:n:37:HIS:ND1	2.37	0.57
52:1:1328:C:H2'	52:1:1329:A:H8	1.68	0.57
8:I:3:GLN:NE2	31:2:1666:G:N3	2.53	0.57
11:L:72:ASP:HB3	11:L:75:ILE:HB	1.86	0.57
31:2:1918:A:H2	31:2:1919:A:H62	1.52	0.57
31:2:1434:A:H61	31:2:1558:C:N4	2.02	0.57
52:1:529:G:O2'	52:1:533:A:N6	2.36	0.57
52:1:1412:C:H2'	52:1:1413:A:C8	2.40	0.57
3:C:115:GLN:HE22	9:J:2:ARG:HD3	1.70	0.56
31:2:1796:U:H2'	31:2:1797:G:H8	1.70	0.56
31:2:1527:G:N2	31:2:1545:A:H62	2.01	0.56
34:c:125:ASN:HA	34:c:141:VAL:HG23	1.86	0.56
52:1:1281:C:H5''	52:1:1282:C:H5	1.70	0.56
52:1:1323:G:H2'	52:1:1324:A:H8	1.69	0.56
8:I:28:SER:OG	31:2:2566:A:N1	2.32	0.56
19:T:45:ASP:OD1	19:T:45:ASP:N	2.38	0.56
31:2:75:G:H22	31:2:111:A:H2	1.53	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:2:481:G:O2'	31:2:506:G:N2	2.38	0.56
31:2:2102:G:H1	31:2:2187:U:H3	1.53	0.56
31:2:2229:U:H2'	31:2:2230:G:H8	1.70	0.56
31:2:2515:C:H2'	31:2:2516:A:H8	1.69	0.56
34:c:100:VAL:HG21	34:c:136:VAL:HG21	1.87	0.56
38:g:14:ARG:NH1	52:1:875:U:O2'	2.37	0.56
44:m:38:GLU:O	44:m:42:ASN:ND2	2.39	0.56
52:1:309:A:H2'	52:1:310:G:H8	1.70	0.56
52:1:674:G:H2'	52:1:675:A:H8	1.70	0.56
29:5:57:G:H22	31:2:2168:G:H21	1.52	0.56
4:D:103:ILE:HD13	4:D:107:VAL:HG21	1.88	0.56
15:P:6:GLN:NE2	15:P:37:GLU:OE1	2.39	0.56
26:AA:3:ARG:O	26:AA:6:GLN:NE2	2.37	0.56
27:AB:41:ARG:HG2	27:AB:44:ARG:HH12	1.70	0.56
31:2:1539:U:H2'	31:2:1540:G:H8	1.71	0.56
52:1:1040:U:H2'	52:1:1041:G:C8	2.40	0.56
13:N:26:GLU:OE1	13:N:86:LYS:NZ	2.37	0.56
31:2:2692:G:H1'	31:2:2847:U:H1'	1.88	0.56
34:c:84:ASN:O	34:c:88:ASN:ND2	2.39	0.56
31:2:1278:C:H2'	31:2:1279:G:H8	1.69	0.56
38:g:104:SER:HB2	38:g:125:ILE:HD11	1.87	0.56
40:i:52:LEU:HD11	40:i:58:ASN:HB3	1.88	0.56
52:1:529:G:HO2'	52:1:533:A:N6	2.03	0.56
52:1:1137:C:O2'	52:1:1138:G:N2	2.39	0.56
18:S:76:THR:HG23	18:S:78:LYS:H	1.71	0.56
23:X:44:ARG:NH2	23:X:58:GLU:OE2	2.38	0.56
39:h:94:ARG:NH2	52:1:1178:G:OP1	2.39	0.56
7:G:7:LYS:HG2	31:2:538:A:H4'	1.87	0.56
17:R:69:ARG:HH11	17:R:72:GLN:HA	1.71	0.56
31:2:1033:U:H2'	31:2:1034:G:H8	1.71	0.56
40:i:9:ARG:HH12	52:1:1279:G:H5''	1.71	0.56
52:1:212:G:H2'	52:1:213:G:C8	2.40	0.56
15:P:68:ARG:NH2	31:2:1223:G:OP1	2.38	0.56
17:R:34:VAL:HG21	17:R:43:ILE:HD11	1.88	0.56
31:2:598:U:H2'	31:2:599:A:H8	1.71	0.56
31:2:818:G:N1	31:2:1188:U:OP2	2.30	0.56
31:2:1481:U:O2	31:2:1510:G:O6	2.23	0.56
50:s:67:HIS:NE2	52:1:132:C:O3'	2.39	0.56
52:1:1230:C:H2'	52:1:1231:G:H8	1.70	0.56
52:1:1266:G:N2	52:1:1269:A:OP2	2.36	0.56
4:D:70:ARG:NH2	31:2:2298:A:OP1	2.39	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:2:1909:C:H2'	31:2:1910:G:C8	2.41	0.55
37:f:37:THR:HB	52:1:1240:U:H4'	1.87	0.55
47:p:56:ASP:OD1	47:p:56:ASP:N	2.39	0.55
52:1:1210:C:O2'	52:1:1213:A:O2'	2.21	0.55
16:Q:92:ARG:HH22	31:2:2015:A:H5'	1.71	0.55
16:Q:74:ILE:HG22	16:Q:105:VAL:HG22	1.88	0.55
28:3:12:C:H1'	28:3:15:A:H1'	1.88	0.55
28:3:14:U:H1'	28:3:108:A:H1'	1.88	0.55
43:l:13:HIS:HB2	43:l:16:ILE:HG12	1.88	0.55
4:D:161:SER:OG	4:D:163:GLU:OE1	2.24	0.55
7:G:78:THR:HB	31:2:2641:G:H5''	1.87	0.55
31:2:2303:G:O6	31:2:2314:A:N6	2.39	0.55
52:1:582:C:OP2	52:1:758:C:N4	2.40	0.55
1:A:15:VAL:HG22	1:A:205:GLY:HA3	1.87	0.55
18:S:85:ARG:NH1	18:S:101:THR:OG1	2.31	0.55
48:q:41:SER:HA	48:q:44:THR:HG22	1.89	0.55
31:2:1802:A:H2'	31:2:1803:A:H8	1.71	0.55
52:1:977:A:O2'	52:1:979:C:OP2	2.25	0.55
3:C:111:GLU:OE2	3:C:115:GLN:NE2	2.39	0.55
50:s:63:LYS:NZ	52:1:196:A:OP1	2.39	0.55
19:T:14:LYS:NZ	28:3:79:G:N7	2.54	0.55
40:i:42:LEU:HD22	40:i:71:LEU:HD23	1.88	0.55
52:1:123:U:OP1	52:1:311:C:O2'	2.24	0.55
52:1:517:G:N3	52:1:519:C:N4	2.55	0.55
3:C:188:MET:HE3	3:C:193:VAL:HG22	1.89	0.55
30:AC:16:ILE:HG12	30:AC:25:VAL:HG22	1.89	0.55
33:b:7:ASN:O	33:b:11:LEU:HB2	2.07	0.55
39:h:117:LEU:HA	39:h:124:PRO:HD3	1.89	0.55
31:2:639:U:H2'	31:2:640:C:H6	1.70	0.55
36:e:6:ILE:HG12	36:e:89:VAL:HG12	1.89	0.55
50:s:42:ASP:OD1	50:s:42:ASP:N	2.40	0.55
50:s:47:GLN:HG3	50:s:51:ASN:HD21	1.72	0.55
52:1:582:C:O2	52:1:759:A:N6	2.40	0.55
52:1:1125:U:H2'	52:1:1126:U:H2'	1.89	0.55
25:Z:21:THR:HG21	31:2:2419:U:H4'	1.88	0.54
31:2:272:A:H2'	31:2:273:G:C8	2.42	0.54
31:2:629:G:N3	31:2:639:U:O2'	2.40	0.54
41:j:110:THR:HB	51:t:4:LYS:HG3	1.89	0.54
52:1:41:G:H2'	52:1:42:G:H8	1.73	0.54
26:AA:29:GLN:NE2	31:2:210:C:OP1	2.32	0.54
31:2:1683:U:H2'	31:2:1684:G:C8	2.42	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
52:1:212:G:H2'	52:1:213:G:H8	1.72	0.54
52:1:1255:G:H2'	52:1:1258:G:H21	1.73	0.54
52:1:1414:U:H2'	52:1:1415:G:H8	1.72	0.54
9:J:13:LYS:NZ	31:2:1245:G:OP1	2.33	0.54
31:2:1178:C:H2'	31:2:1179:G:H8	1.70	0.54
47:p:64:ARG:NH1	52:1:264:C:O2'	2.40	0.54
52:1:1391:U:H2'	52:1:1392:G:H8	1.72	0.54
1:A:206:LYS:HB2	31:2:729:G:C5	2.42	0.54
21:V:22:ASN:OD1	31:2:2079:U:O2'	2.25	0.54
31:2:1139:G:O2'	31:2:1143:A:N1	2.39	0.54
1:A:261:ARG:HG3	1:A:262:THR:HG23	1.89	0.54
19:T:30:ILE:HG12	19:T:91:PHE:HB2	1.90	0.54
30:AC:31:PRO:HB2	31:2:2527:C:H5''	1.90	0.54
31:2:279:A:N6	31:2:361:G:O2'	2.40	0.54
31:2:848:C:H2'	31:2:849:A:H8	1.72	0.54
39:h:119:LYS:NZ	52:1:1350:A:OP2	2.29	0.54
49:r:12:LEU:HD13	49:r:15:LEU:HD21	1.89	0.54
52:1:292:G:OP2	52:1:305:G:N2	2.35	0.54
52:1:1391:U:H2'	52:1:1392:G:C8	2.42	0.54
53:4:89:G:H2'	53:4:90:G:H8	1.73	0.54
1:A:36:ASN:HB2	1:A:61:TYR:HB2	1.90	0.54
31:2:191:A:H2'	31:2:192:C:H6	1.73	0.54
31:2:767:U:H2'	31:2:768:G:H8	1.73	0.54
4:D:3:LEU:HB2	4:D:6:TYR:HB3	1.89	0.54
5:E:85:LYS:HB3	5:E:131:VAL:HG22	1.89	0.54
32:a:23:ASN:ND2	32:a:190:SER:O	2.40	0.54
36:e:43:GLY:HA2	36:e:58:HIS:CE1	2.43	0.54
38:g:15:ASN:ND2	52:1:826:C:O2	2.41	0.54
42:k:41:PRO:HG3	42:k:47:ALA:H	1.72	0.54
52:1:1533:C:H5'	52:1:1534:A:H8	1.73	0.54
2:B:12:THR:OG1	2:B:13:ARG:N	2.41	0.54
6:F:9:VAL:HG21	6:F:12:LEU:HB2	1.90	0.54
31:2:742:A:H2'	31:2:743:A:H8	1.71	0.54
46:o:25:ARG:O	52:1:110:C:O2'	2.22	0.54
28:3:60:C:H2'	28:3:61:G:H8	1.73	0.54
34:c:57:LYS:HB3	34:c:199:ILE:HD12	1.89	0.54
44:m:65:GLN:HG3	44:m:78:LEU:HD22	1.88	0.54
19:T:51:GLN:NE2	19:T:57:TYR:OH	2.31	0.54
31:2:1939:U:OP1	31:2:2604:U:O2'	2.26	0.54
31:2:2246:G:H2'	31:2:2247:A:H8	1.73	0.54
46:o:25:ARG:NH1	52:1:134:G:O6	2.41	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
52:1:76:G:O6	52:1:93:U:O4	2.26	0.54
7:G:64:VAL:HB	7:G:68:LYS:HE2	1.88	0.53
8:I:63:VAL:HG12	8:I:107:LEU:HD21	1.90	0.53
16:Q:108:SER:OG	16:Q:110:ARG:OXT	2.25	0.53
20:U:39:THR:H	31:2:2331:G:H4'	1.74	0.53
41:j:30:ILE:HA	41:j:45:THR:HG22	1.90	0.53
43:l:33:LEU:HB2	43:l:38:ILE:HB	1.90	0.53
52:1:358:U:H2'	52:1:359:G:H8	1.73	0.53
18:S:45:GLN:O	18:S:55:GLY:HA3	2.08	0.53
31:2:2688:G:N1	31:2:2720:U:OP2	2.25	0.53
37:f:39:GLU:HA	37:f:42:VAL:HG12	1.90	0.53
42:k:28:GLN:HE22	52:1:34:C:H1'	1.74	0.53
52:1:179:A:H61	52:1:196:A:H62	1.57	0.53
52:1:1259:C:O2'	52:1:1283:U:O2	2.19	0.53
5:E:163:TYR:HB2	5:E:166:GLU:HB2	1.89	0.53
31:2:1683:U:H2'	31:2:1684:G:H8	1.73	0.53
40:i:52:LEU:HB3	44:m:80:ARG:HD2	1.90	0.53
41:j:38:GLY:O	52:1:683:G:N2	2.42	0.53
43:l:85:TYR:OH	43:l:89:ARG:NH2	2.41	0.53
52:1:309:A:O2'	52:1:607:A:N1	2.39	0.53
52:1:818:G:O2'	52:1:820:U:OP2	2.25	0.53
31:2:581:C:H2'	31:2:582:A:C8	2.42	0.53
32:a:166:ASP:OD2	32:a:190:SER:OG	2.27	0.53
48:q:24:ASP:OD1	48:q:24:ASP:N	2.33	0.53
52:1:792:A:O2'	52:1:794:A:N7	2.37	0.53
1:A:257:ARG:NH1	1:A:263:ASP:OD1	2.41	0.53
31:2:1387:A:H5'	31:2:1469:A:H1'	1.91	0.53
31:2:2375:G:N2	31:2:2378:A:OP2	2.32	0.53
34:c:130:ASN:OD1	52:1:619:U:N3	2.42	0.53
52:1:505:G:H2'	52:1:506:G:C8	2.44	0.53
1:A:129:LEU:HD12	1:A:130:PRO:HD2	1.90	0.53
31:2:2125:G:N2	31:2:2127:G:O2'	2.41	0.53
50:s:58:ASP:OD1	50:s:75:LYS:NZ	2.37	0.53
52:1:1335:U:H5''	52:1:1336:C:H5'	1.91	0.53
52:1:1500:A:H5''	52:1:1508:A:H5''	1.90	0.53
3:C:117:ARG:NH2	3:C:183:PHE:O	2.40	0.53
9:J:32:GLY:HA2	31:2:1190:G:H5''	1.91	0.53
52:1:1513:A:H2'	52:1:1514:G:C8	2.44	0.53
5:E:55:ASP:N	5:E:55:ASP:OD1	2.42	0.53
8:I:74:GLY:O	13:N:74:GLN:NE2	2.42	0.53
39:h:11:ARG:NH2	52:1:1347:G:O6	2.41	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
52:1:146:G:H2'	52:1:147:G:H8	1.73	0.53
5:E:10:VAL:HB	5:E:47:ASN:HA	1.90	0.53
31:2:18:U:H2'	31:2:19:A:H8	1.74	0.53
31:2:63:A:H2'	31:2:64:A:H8	1.73	0.53
31:2:1724:G:N7	31:2:1737:G:N2	2.57	0.53
52:1:747:A:H2'	52:1:748:G:H8	1.73	0.53
14:O:89:ILE:HA	15:P:11:GLN:HE22	1.74	0.53
31:2:1782:U:H1'	31:2:2609:U:H5''	1.91	0.53
35:d:131:ASN:ND2	35:d:134:ASN:OD1	2.37	0.53
52:1:411:A:H1'	52:1:413:G:H4'	1.90	0.52
31:2:879:G:H2'	31:2:880:G:H8	1.73	0.52
31:2:898:C:H2'	31:2:899:A:C8	2.44	0.52
33:b:90:VAL:HA	33:b:93:ILE:HG22	1.90	0.52
52:1:1359:C:H4'	52:1:1362:A:H62	1.74	0.52
52:1:1413:A:N1	52:1:1487:G:C6	2.77	0.52
3:C:149:ILE:HB	3:C:188:MET:HG2	1.91	0.52
13:N:50:ARG:HE	13:N:52:ARG:HG3	1.74	0.52
21:V:1:SER:O	21:V:49:ARG:NH1	2.42	0.52
28:3:1:U:H2'	28:3:2:G:C8	2.45	0.52
31:2:1495:A:N3	31:2:1578:U:O2'	2.35	0.52
31:2:2119:A:N6	31:2:2168:G:O6	2.43	0.52
35:d:114:LEU:HD13	35:d:122:VAL:HG21	1.91	0.52
40:i:51:VAL:HG11	44:m:84:ARG:HB2	1.91	0.52
52:1:1467:C:H2'	52:1:1468:A:H8	1.74	0.52
1:A:144:GLU:OE1	1:A:148:GLY:N	2.39	0.52
7:G:13:ARG:NH2	7:G:49:ASP:O	2.42	0.52
28:3:72:G:H21	28:3:104:A:H62	1.57	0.52
29:5:68:C:H2'	29:5:69:G:H8	1.74	0.52
38:g:12:ARG:NH1	38:g:25:THR:O	2.43	0.52
31:2:1796:U:H2'	31:2:1797:G:C8	2.44	0.52
33:b:18:ASN:OD1	33:b:53:ARG:NH2	2.42	0.52
42:k:57:THR:HG21	52:1:362:G:H5''	1.91	0.52
43:l:63:VAL:HG13	43:l:67:ASP:HB2	1.92	0.52
52:1:647:C:H2'	52:1:648:A:H8	1.73	0.52
29:5:8:U:C2	29:5:14:A:N6	2.77	0.52
31:2:2246:G:H2'	31:2:2247:A:C8	2.45	0.52
35:d:125:LYS:NZ	35:d:126:ALA:O	2.42	0.52
36:e:9:MET:HG2	36:e:86:ARG:HB3	1.92	0.52
51:t:63:ASN:OD1	51:t:66:ARG:NH2	2.43	0.52
52:1:151:A:N7	52:1:170:U:N3	2.57	0.52
53:4:90:G:H2'	53:4:91:G:C8	2.45	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:AA:39:ARG:NH2	31:2:468:G:N7	2.58	0.52
52:1:662:U:H2'	52:1:663:A:C8	2.45	0.52
9:J:141:LYS:NZ	9:J:143:GLU:OE1	2.42	0.52
27:AB:18:LYS:HG3	31:2:651:G:H5'	1.92	0.52
31:2:373:U:H2'	31:2:374:A:H8	1.75	0.52
45:n:7:THR:HG23	45:n:30:LEU:HD21	1.91	0.52
8:I:31:ARG:NH2	31:2:1996:C:OP1	2.43	0.52
18:S:67:SER:OG	31:2:335:C:O2	2.27	0.52
23:X:51:SER:HA	23:X:54:VAL:HG22	1.92	0.52
31:2:30:G:O2'	31:2:1214:A:N3	2.40	0.52
31:2:1926:U:H2'	31:2:1927:A:H8	1.74	0.52
36:e:19:PRO:HA	36:e:22:ILE:HG22	1.92	0.52
52:1:816:A:OP1	52:1:1526:G:O2'	2.27	0.52
52:1:1328:C:H2'	52:1:1329:A:C8	2.44	0.52
52:1:1355:G:H2'	52:1:1356:G:H8	1.75	0.52
9:J:38:GLN:OE1	31:2:831:G:O2'	2.27	0.52
27:AB:38:LYS:NZ	31:2:2365:G:N7	2.40	0.52
31:2:1451:C:H4'	31:2:1452:G:C5	2.45	0.52
2:B:25:THR:OG1	2:B:191:GLY:O	2.28	0.51
19:T:72:VAL:HG12	19:T:93:ARG:HA	1.92	0.51
31:2:860:U:H2'	31:2:861:A:H8	1.74	0.51
33:b:122:GLN:HA	33:b:125:ARG:HG2	1.91	0.51
38:g:10:LEU:HD22	38:g:74:ILE:HD11	1.92	0.51
39:h:96:GLU:HG2	39:h:99:LYS:HE2	1.91	0.51
40:i:66:GLU:HB2	44:m:98:ALA:HB2	1.92	0.51
52:1:1224:U:O2'	52:1:1322:C:OP1	2.28	0.51
52:1:1303:C:H2'	52:1:1304:G:C8	2.45	0.51
52:1:1533:C:H5'	52:1:1534:A:C8	2.45	0.51
49:r:51:HIS:HB2	49:r:56:HIS:CD2	2.45	0.51
12:M:111:ARG:NH2	31:2:2376:A:O2'	2.39	0.51
31:2:926:G:H2'	31:2:927:A:H8	1.76	0.51
31:2:1848:A:H4'	31:2:1849:G:H5'	1.92	0.51
31:2:1965:C:H5''	31:2:1966:A:H2'	1.92	0.51
47:p:16:MET:O	52:1:254:G:O2'	2.27	0.51
52:1:392:C:O2'	52:1:483:C:O2'	2.17	0.51
52:1:1454:G:H2'	52:1:1455:G:H8	1.75	0.51
4:D:116:LEU:H	4:D:175:PRO:HB2	1.75	0.51
12:M:89:ASP:OD1	12:M:89:ASP:N	2.41	0.51
14:O:5:ARG:NH1	31:2:585:G:N7	2.59	0.51
31:2:151:C:H2'	31:2:152:A:C8	2.44	0.51
31:2:612:G:C6	31:2:614:A:H8	2.29	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:2:2802:G:H2'	31:2:2803:G:C8	2.43	0.51
52:1:59:A:H3'	52:1:331:G:H22	1.74	0.51
12:M:35:ILE:HD11	12:M:102:ARG:HH21	1.76	0.51
13:N:38:ARG:NH2	52:1:346:G:O2'	2.43	0.51
14:O:93:ILE:HD12	15:P:13:ARG:HB2	1.91	0.51
24:Y:17:SER:HB2	31:2:15:G:H4'	1.93	0.51
31:2:160:A:N3	31:2:2208:C:O2'	2.40	0.51
31:2:639:U:H2'	31:2:640:C:C6	2.46	0.51
31:2:1539:U:H2'	31:2:1540:G:C8	2.45	0.51
31:2:2692:G:N3	31:2:2847:U:O2'	2.42	0.51
48:q:42:ARG:HG3	48:q:43:ILE:HG23	1.92	0.51
52:1:1472:U:HO2'	52:1:1473:G:H8	1.56	0.51
1:A:132:ARG:O	1:A:166:ARG:NH2	2.43	0.51
24:Y:5:ASN:ND2	31:2:2020:A:H62	2.09	0.51
31:2:1278:C:H2'	31:2:1279:G:C8	2.46	0.51
33:b:137:VAL:HG13	33:b:148:ILE:HD11	1.93	0.51
35:d:44:ARG:HE	35:d:70:MET:HE3	1.76	0.51
52:1:157:U:H3	52:1:164:G:H1	1.59	0.51
19:T:86:LEU:HD13	19:T:89:ILE:HD11	1.93	0.51
35:d:24:VAL:HG23	35:d:26:GLY:H	1.75	0.51
52:1:1156:G:H21	52:1:1179:A:N6	2.08	0.51
2:B:16:THR:OG1	2:B:18:ASP:OD1	2.27	0.51
10:K:36:VAL:HG12	19:T:82:TYR:HB2	1.93	0.51
28:3:66:A:N6	28:3:108:A:OP2	2.44	0.51
28:3:78:A:H62	28:3:98:G:N2	2.07	0.51
31:2:2327:A:H2'	31:2:2328:A:C8	2.46	0.51
52:1:34:C:H2'	52:1:35:G:H8	1.75	0.51
52:1:157:U:H2'	52:1:158:G:C8	2.46	0.51
52:1:401:C:H2'	52:1:402:G:H8	1.75	0.51
52:1:408:A:N6	52:1:435:A:H61	2.09	0.51
52:1:1077:G:N2	52:1:1080:A:OP2	2.29	0.51
1:A:156:SER:HB2	31:2:1818:U:H5'	1.93	0.51
3:C:148:ILE:HB	3:C:169:VAL:HG12	1.93	0.51
9:J:109:LYS:HG2	9:J:126:ARG:HB2	1.92	0.51
11:L:39:PRO:HG2	31:2:1651:G:H4'	1.93	0.51
31:2:2047:C:H2'	31:2:2048:G:H8	1.76	0.51
31:2:2591:C:H2'	31:2:2592:G:H8	1.75	0.51
31:2:2836:U:H2'	31:2:2837:A:H8	1.75	0.51
31:2:138:U:O2'	31:2:141:G:O6	2.26	0.51
31:2:2507:C:N4	31:2:2581:G:H21	2.09	0.51
36:e:41:ASP:OD1	36:e:58:HIS:NE2	2.44	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:f:49:LEU:HD21	37:f:60:ALA:HB3	1.93	0.51
52:1:147:G:H2'	52:1:148:G:H8	1.76	0.51
52:1:148:G:O2'	52:1:1446:A:N3	2.39	0.51
52:1:926:G:H22	53:4:52:G:H3'	1.75	0.51
2:B:1:MET:HB2	2:B:205:PRO:HG2	1.92	0.50
31:2:2328:A:H2'	31:2:2329:U:C6	2.46	0.50
45:n:57:ARG:HH11	52:1:742:G:H5''	1.76	0.50
50:s:47:GLN:O	50:s:51:ASN:ND2	2.45	0.50
51:t:45:LYS:NZ	52:1:1530:G:O6	2.40	0.50
52:1:1342:C:H2'	52:1:1343:G:C8	2.45	0.50
52:1:1495:U:H2'	52:1:1496:C:C6	2.46	0.50
18:S:47:PRO:HB3	18:S:55:GLY:H	1.77	0.50
31:2:434:U:O2	31:2:436:C:N4	2.44	0.50
31:2:1149:G:H2'	31:2:1150:C:C6	2.46	0.50
31:2:1931:U:H2'	31:2:1932:A:C8	2.45	0.50
31:2:2372:U:H2'	31:2:2373:G:C8	2.46	0.50
46:o:39:PHE:HD1	46:o:50:THR:HG22	1.75	0.50
49:r:32:THR:HG21	49:r:70:LEU:HD21	1.93	0.50
31:2:2506:U:OP2	31:2:2576:G:N1	2.44	0.50
44:m:74:ARG:NH2	52:1:1360:A:OP2	2.44	0.50
52:1:935:A:O2'	52:1:1383:C:N3	2.40	0.50
52:1:946:A:H2'	52:1:947:G:H8	1.75	0.50
50:s:28:ARG:NH2	52:1:1437:A:OP1	2.44	0.50
52:1:1218:C:H2'	52:1:1219:A:C8	2.46	0.50
14:O:49:ARG:O	14:O:53:LYS:NZ	2.42	0.50
41:j:121:ARG:HD3	52:1:778:G:H21	1.77	0.50
52:1:922:G:H2'	52:1:923:A:H8	1.76	0.50
22:W:42:LEU:HA	22:W:45:GLN:HG2	1.94	0.50
31:2:832:U:H2'	31:2:833:A:C8	2.46	0.50
31:2:2258:C:O2'	31:2:2427:C:OP2	2.26	0.50
7:G:3:THR:OG1	31:2:995:C:O2	2.29	0.50
31:2:598:U:H2'	31:2:599:A:C8	2.46	0.50
31:2:1857:G:N2	31:2:1884:G:O2'	2.43	0.50
31:2:2553:G:N3	31:2:2583:G:H1'	2.26	0.50
35:d:11:GLN:HG2	35:d:116:VAL:HG23	1.94	0.50
7:G:141:ASP:OD1	7:G:141:ASP:N	2.38	0.50
18:S:3:LYS:O	18:S:93:ARG:NH2	2.45	0.50
32:a:128:LEU:HD12	32:a:132:GLU:HB3	1.92	0.50
37:f:91:ARG:HG2	52:1:1378:C:H42	1.77	0.50
13:N:95:LYS:NZ	31:2:2847:U:OP1	2.40	0.50
16:Q:83:LYS:HG2	16:Q:95:ARG:HD3	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:T:4:ILE:HB	19:T:63:ILE:HG12	1.93	0.50
31:2:414:C:H2'	31:2:415:A:C8	2.47	0.50
31:2:2368:C:H2'	31:2:2369:A:H8	1.77	0.50
38:g:112:ASP:OD1	38:g:112:ASP:N	2.45	0.50
41:j:23:HIS:HB3	41:j:30:ILE:HB	1.93	0.50
46:o:14:ARG:NH1	52:1:618:C:O2'	2.45	0.50
52:1:374:A:O2'	52:1:451:A:OP2	2.25	0.50
52:1:616:G:H2'	52:1:617:G:C8	2.47	0.50
4:D:36:ASN:ND2	31:2:2312:U:O2	2.45	0.49
15:P:71:LYS:NZ	31:2:1225:G:OP1	2.39	0.49
31:2:318:C:H2'	31:2:319:G:H8	1.76	0.49
31:2:1255:U:H5''	31:2:1256:G:H5''	1.93	0.49
31:2:1386:C:H2'	31:2:1387:A:H8	1.77	0.49
31:2:1432:G:H2'	31:2:1433:A:C8	2.47	0.49
31:2:2120:G:N2	31:2:2121:G:O6	2.45	0.49
18:S:43:LYS:NZ	31:2:480:A:OP2	2.45	0.49
20:U:22:PHE:N	20:U:25:GLU:OE2	2.42	0.49
31:2:160:A:H62	31:2:166:U:H3	1.60	0.49
31:2:191:A:H2'	31:2:192:C:C6	2.47	0.49
31:2:285:G:H3'	31:2:286:U:H5''	1.94	0.49
31:2:813:U:H2'	31:2:814:C:H6	1.77	0.49
31:2:1913:A:N7	52:1:1492:A:N6	2.58	0.49
31:2:2898:U:H2'	31:2:2899:A:C8	2.47	0.49
52:1:1412:C:H2'	52:1:1413:A:H8	1.76	0.49
53:4:87:C:H2'	53:4:88:A:H8	1.77	0.49
29:5:8:U:C4	29:5:14:A:N7	2.80	0.49
31:2:514:A:H2'	31:2:515:A:C8	2.47	0.49
31:2:743:A:O2'	31:2:1659:G:OP1	2.25	0.49
32:a:147:LEU:HD22	32:a:150:ILE:HD11	1.94	0.49
33:b:152:VAL:HG22	33:b:197:VAL:HG22	1.94	0.49
52:1:257:G:H2'	52:1:258:G:H8	1.77	0.49
52:1:922:G:H2'	52:1:923:A:C8	2.47	0.49
52:1:1370:G:H2'	52:1:1371:G:H8	1.77	0.49
5:E:2:ARG:O	5:E:5:LYS:NZ	2.43	0.49
19:T:28:ALA:HA	19:T:89:ILE:O	2.11	0.49
31:2:2099:U:H2'	31:2:2100:G:H8	1.78	0.49
31:2:2813:A:H2'	31:2:2814:A:C8	2.47	0.49
52:1:1156:G:N2	52:1:1179:A:H61	2.10	0.49
52:1:1181:G:H1'	52:1:1182:G:C4	2.47	0.49
44:m:63:CYS:SG	44:m:64:ARG:N	2.85	0.49
46:o:63:GLN:OE1	52:1:227:G:O2'	2.28	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
52:1:1095:U:P	52:1:1108:G:H1	2.35	0.49
11:L:4:ARG:HD2	31:2:2820:A:N3	2.28	0.49
28:3:19:C:H2'	28:3:20:G:C8	2.47	0.49
28:3:95:U:H2'	28:3:96:G:H8	1.78	0.49
29:5:23:A:H2'	29:5:24:G:C8	2.48	0.49
31:2:910:A:H2'	31:2:911:A:C8	2.47	0.49
31:2:1251:C:O2'	31:2:1253:A:OP2	2.30	0.49
31:2:1794:A:H2'	31:2:1795:C:C6	2.48	0.49
42:k:64:SER:HG	42:k:96:THR:HG1	1.57	0.49
52:1:981:U:H5''	52:1:982:U:H2'	1.93	0.49
6:F:30:LEU:HB3	6:F:36:ALA:HB3	1.94	0.49
31:2:514:A:H2'	31:2:515:A:H8	1.78	0.49
31:2:574:A:N6	31:2:2034:U:OP1	2.46	0.49
31:2:1385:A:O2'	31:2:1396:U:O2	2.23	0.49
31:2:2836:U:H2'	31:2:2837:A:C8	2.48	0.49
50:s:75:LYS:HG3	52:1:186:C:H4'	1.94	0.49
1:A:267:VAL:HG12	1:A:268:ARG:HG3	1.94	0.49
8:I:40:LYS:HD2	8:I:57:VAL:HG12	1.93	0.49
26:AA:11:LYS:NZ	31:2:771:G:OP2	2.45	0.49
32:a:96:LEU:HD13	52:1:1103:C:H4'	1.95	0.49
40:i:51:VAL:HG13	44:m:80:ARG:HB2	1.93	0.49
52:1:333:U:H2'	52:1:334:C:H6	1.77	0.49
52:1:407:U:O2'	52:1:408:A:OP1	2.25	0.49
52:1:1162:C:H2'	52:1:1163:A:H8	1.78	0.49
28:3:114:C:H2'	28:3:115:A:C8	2.48	0.49
29:5:8:U:N3	29:5:14:A:C6	2.81	0.49
29:5:40:C:H2'	29:5:41:C:C6	2.48	0.49
31:2:1042:G:O6	31:2:1113:U:O4	2.31	0.49
31:2:2070:A:H2'	31:2:2071:A:H8	1.77	0.49
31:2:2128:G:H1	31:2:2160:C:H42	1.60	0.49
47:p:14:ASP:N	47:p:14:ASP:OD1	2.46	0.49
52:1:41:G:H2'	52:1:42:G:C8	2.48	0.49
52:1:1021:A:H2'	52:1:1022:A:C8	2.48	0.49
39:h:80:HIS:NE2	39:h:103:VAL:O	2.46	0.49
52:1:270:A:H2'	52:1:271:C:C6	2.48	0.49
2:B:81:GLU:OE1	31:2:2635:A:O2'	2.20	0.48
31:2:1909:C:H2'	31:2:1910:G:H8	1.77	0.48
37:f:91:ARG:HD2	37:f:92:PRO:HD2	1.95	0.48
40:i:38:GLY:HA3	52:1:1123:U:H4'	1.94	0.48
44:m:53:ASP:OD1	44:m:58:ARG:NH1	2.39	0.48
52:1:496:A:H2'	52:1:497:G:H8	1.78	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
52:1:634:C:H2'	52:1:635:A:H8	1.78	0.48
31:2:514:A:N3	31:2:581:C:O2'	2.44	0.48
43:l:79:LEU:HD11	43:l:86:ARG:HB2	1.94	0.48
52:1:147:G:H2'	52:1:148:G:C8	2.48	0.48
52:1:312:C:H2'	52:1:313:A:C8	2.49	0.48
28:3:14:U:O2	28:3:107:G:O2'	2.30	0.48
31:2:832:U:H2'	31:2:833:A:H8	1.78	0.48
51:t:10:PRO:HB2	51:t:13:VAL:HB	1.95	0.48
52:1:312:C:H2'	52:1:313:A:H8	1.78	0.48
52:1:1291:U:H2'	52:1:1292:G:C8	2.47	0.48
1:A:141:HIS:ND1	1:A:192:GLY:O	2.41	0.48
8:I:107:LEU:HB2	8:I:116:ILE:HD12	1.95	0.48
31:2:9:G:H21	31:2:2800:A:H61	1.61	0.48
31:2:1954:G:O2'	31:2:1956:U:O4	2.26	0.48
52:1:358:U:H2'	52:1:359:G:C8	2.47	0.48
52:1:1251:A:N3	52:1:1369:C:O2'	2.35	0.48
4:D:57:ALA:HB2	4:D:64:PRO:HD3	1.96	0.48
31:2:833:A:H2'	31:2:834:G:C8	2.49	0.48
31:2:1353:A:H2'	31:2:1354:A:C8	2.49	0.48
31:2:2229:U:H2'	31:2:2230:G:C8	2.49	0.48
31:2:2443:C:H2'	31:2:2444:G:H8	1.77	0.48
52:1:422:C:O2'	52:1:424:G:N7	2.46	0.48
52:1:453:G:H2'	52:1:454:G:C8	2.48	0.48
4:D:68:LYS:HD3	4:D:81:GLY:HA2	1.95	0.48
31:2:63:A:H2'	31:2:64:A:C8	2.48	0.48
31:2:1964:G:O2'	31:2:1967:C:OP2	2.24	0.48
31:2:2118:U:H5''	31:2:2148:G:H4'	1.96	0.48
31:2:2591:C:H2'	31:2:2592:G:C8	2.49	0.48
31:2:2898:U:H2'	31:2:2899:A:H8	1.79	0.48
35:d:73:VAL:HG11	35:d:143:LEU:HB3	1.95	0.48
39:h:126:PHE:HE1	52:1:967:C:H4'	1.78	0.48
24:Y:18:HIS:CE1	31:2:2624:G:H1'	2.46	0.48
28:3:60:C:H2'	28:3:61:G:C8	2.48	0.48
31:2:1386:C:H2'	31:2:1387:A:C8	2.48	0.48
31:2:2329:U:H2'	31:2:2330:G:C8	2.48	0.48
52:1:538:G:H2'	52:1:539:A:H8	1.78	0.48
52:1:1250:A:H2'	52:1:1251:A:C8	2.49	0.48
52:1:1410:A:H2'	52:1:1411:C:H6	1.79	0.48
17:R:56:GLU:HB3	17:R:86:THR:HG23	1.95	0.48
31:2:1363:C:O2'	31:2:1809:A:N3	2.41	0.48
52:1:355:C:H1'	52:1:388:G:H1'	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
52:1:454:G:N1	52:1:479:U:N3	2.61	0.48
52:1:1269:A:H1'	52:1:1326:U:H1'	1.95	0.48
53:4:81:G:H2'	53:4:82:A:H8	1.79	0.48
3:C:45:ALA:HA	3:C:87:ALA:O	2.14	0.48
24:Y:15:ARG:NH1	31:2:1264:A:OP1	2.47	0.48
31:2:723:C:H2'	31:2:724:U:C6	2.48	0.48
31:2:2185:U:H2'	31:2:2186:G:C8	2.39	0.48
46:o:6:LEU:HG	46:o:17:TYR:HB3	1.95	0.48
52:1:204:G:H2'	52:1:205:A:H8	1.78	0.48
52:1:513:C:H2'	52:1:514:C:C6	2.49	0.48
52:1:975:A:N1	52:1:1366:C:O2'	2.36	0.48
4:D:37:MET:HE3	4:D:52:ALA:HB1	1.96	0.48
31:2:1435:G:H2'	31:2:1436:G:H8	1.79	0.48
31:2:1570:A:H2'	31:2:1571:A:C8	2.48	0.48
31:2:2241:A:H2'	31:2:2242:G:C8	2.49	0.48
34:c:151:GLN:HE22	52:1:436:C:H4'	1.79	0.48
49:r:77:ARG:HH11	52:1:1222:G:H5''	1.79	0.48
52:1:977:A:O2'	52:1:982:U:O4	2.21	0.48
52:1:992:U:C2	52:1:1044:A:N7	2.81	0.48
52:1:1040:U:H2'	52:1:1041:G:H8	1.79	0.48
53:4:63:U:H2'	53:4:64:C:C6	2.48	0.48
11:L:8:ARG:NH2	11:L:43:GLU:OE2	2.45	0.47
12:M:68:LYS:HE3	28:3:49:C:H4'	1.96	0.47
13:N:47:ILE:HG22	13:N:99:LEU:HD12	1.94	0.47
28:3:2:G:H2'	28:3:3:C:C6	2.49	0.47
31:2:1019:U:OP1	31:2:1035:U:O2'	2.26	0.47
31:2:2070:A:H2'	31:2:2071:A:C8	2.48	0.47
33:b:175:HIS:O	52:1:1111:A:N6	2.47	0.47
52:1:392:C:H2'	52:1:393:A:H8	1.79	0.47
52:1:958:A:N3	52:1:985:C:O2'	2.43	0.47
10:K:75:GLU:HB3	10:K:90:GLU:HG3	1.96	0.47
12:M:30:ARG:NH2	28:3:48:U:OP2	2.47	0.47
16:Q:20:VAL:HG21	16:Q:43:ALA:HB3	1.96	0.47
29:5:69:G:H2'	29:5:70:G:H8	1.79	0.47
31:2:18:U:H2'	31:2:19:A:C8	2.49	0.47
31:2:318:C:H2'	31:2:319:G:C8	2.50	0.47
31:2:926:G:H2'	31:2:927:A:C8	2.49	0.47
31:2:1794:A:H2'	31:2:1795:C:H6	1.79	0.47
31:2:2071:A:H2'	31:2:2072:C:C6	2.49	0.47
5:E:136:ASP:HB3	5:E:139:VAL:HB	1.96	0.47
10:K:47:GLU:OE2	10:K:50:ARG:NH1	2.47	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:U:62:LYS:HG3	20:U:81:GLU:HG3	1.97	0.47
31:2:64:A:H2'	31:2:65:U:C6	2.48	0.47
31:2:1447:C:H2'	31:2:1448:G:C8	2.50	0.47
33:b:171:ARG:HG2	33:b:173:PRO:HD3	1.96	0.47
52:1:1060:U:H2'	52:1:1061:G:H8	1.79	0.47
53:4:89:G:H2'	53:4:90:G:C8	2.50	0.47
13:N:13:LYS:HE3	13:N:76:HIS:HA	1.95	0.47
31:2:64:A:H2'	31:2:65:U:H6	1.80	0.47
31:2:395:U:H2'	31:2:396:G:C8	2.49	0.47
31:2:1040:A:N1	31:2:1115:G:C6	2.82	0.47
31:2:1726:C:O2	31:2:1735:A:N6	2.47	0.47
31:2:2584:U:H2'	31:2:2585:U:H2'	1.96	0.47
31:2:2698:U:H2'	31:2:2699:C:C6	2.49	0.47
34:c:84:ASN:HB3	34:c:87:GLU:HG2	1.97	0.47
52:1:516:U:H2'	52:1:517:G:C4	2.50	0.47
4:D:150:GLY:HA3	31:2:2305:U:H3	1.79	0.47
31:2:2514:U:H2'	31:2:2515:C:C6	2.50	0.47
31:2:2855:C:H2'	31:2:2856:A:H8	1.80	0.47
32:a:30:ILE:HG13	32:a:32:GLY:H	1.78	0.47
52:1:920:U:HO2'	52:1:1081:A:HO2'	1.56	0.47
52:1:1157:A:H5'	52:1:1158:C:C2	2.49	0.47
52:1:1342:C:H2'	52:1:1343:G:H8	1.78	0.47
52:1:1454:G:H2'	52:1:1455:G:C8	2.50	0.47
7:G:17:VAL:HG22	7:G:55:ILE:HB	1.96	0.47
28:3:56:G:H21	28:3:58:A:H61	1.62	0.47
31:2:1440:U:H2'	31:2:1441:G:H8	1.79	0.47
42:k:69:GLU:H	42:k:106:VAL:HG11	1.80	0.47
46:o:18:GLN:HA	46:o:38:PHE:HA	1.97	0.47
52:1:64:G:H4'	52:1:65:A:H3'	1.97	0.47
52:1:454:G:N1	52:1:479:U:C2	2.82	0.47
52:1:529:G:H5''	52:1:530:G:H21	1.79	0.47
4:D:102:LEU:HD13	4:D:106:ALA:HB3	1.96	0.47
13:N:102:ARG:NH1	31:2:1754:A:O3'	2.48	0.47
25:Z:8:ILE:HD13	25:Z:24:LYS:HD2	1.96	0.47
29:5:55:U:H3	29:5:58:A:H2	1.63	0.47
31:2:419:U:H2'	31:2:420:C:C6	2.50	0.47
31:2:458:G:O2'	31:2:469:G:O6	2.30	0.47
42:k:53:ARG:HH21	42:k:61:GLU:HB3	1.80	0.47
49:r:35:ARG:NH2	49:r:71:GLY:O	2.48	0.47
52:1:902:G:H2'	52:1:903:G:H8	1.78	0.47
52:1:1326:U:H2'	52:1:1327:C:H6	1.80	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:25:THR:HG21	2:B:193:VAL:HG22	1.97	0.47
5:E:171:LYS:NZ	31:2:2530:A:N7	2.56	0.47
20:U:42:HIS:CE1	20:U:73:ARG:HH21	2.33	0.47
31:2:2039:U:H2'	31:2:2040:G:H8	1.80	0.47
43:l:104:ASN:HB2	43:l:106:ARG:HG2	1.97	0.47
52:1:1096:C:O2	52:1:1170:A:O2'	2.28	0.47
52:1:1203:C:H2'	52:1:1204:A:C8	2.50	0.47
5:E:15:ASP:HB2	5:E:17:LYS:HE2	1.96	0.47
9:J:20:GLY:O	9:J:21:ARG:NH1	2.40	0.47
19:T:21:ARG:HE	19:T:87:GLN:HA	1.80	0.47
25:Z:22:THR:OG1	25:Z:23:THR:N	2.48	0.47
52:1:946:A:H2'	52:1:947:G:C8	2.50	0.47
52:1:1098:C:H2'	52:1:1099:G:C8	2.49	0.47
52:1:1410:A:N6	52:1:1491:G:O6	2.48	0.47
20:U:55:LEU:HD12	20:U:76:ILE:HD12	1.97	0.47
30:AC:19:ARG:NE	31:2:2756:U:OP2	2.40	0.47
31:2:2788:C:H2'	31:2:2789:C:C6	2.50	0.47
35:d:28:ARG:NH2	52:1:1397:C:OP2	2.47	0.47
52:1:979:C:H41	52:1:1360:A:H62	1.63	0.47
3:C:10:SER:OG	3:C:11:ALA:N	2.47	0.46
4:D:151:LEU:N	31:2:2305:U:O4	2.49	0.46
28:3:40:U:H1'	28:3:45:A:H61	1.80	0.46
30:AC:2:LYS:HG2	30:AC:4:ARG:HG3	1.98	0.46
31:2:947:A:H2'	31:2:948:C:C6	2.50	0.46
31:2:2247:A:H2'	31:2:2248:C:H6	1.79	0.46
31:2:2313:C:H2'	31:2:2314:A:H8	1.79	0.46
32:a:25:LYS:HE3	32:a:192:PRO:HD2	1.97	0.46
39:h:17:ARG:NH1	52:1:1147:C:O2	2.46	0.46
52:1:555:U:H2'	52:1:556:C:C6	2.50	0.46
9:J:128:THR:OG1	9:J:129:LYS:N	2.49	0.46
29:5:29:G:H2'	29:5:30:G:C8	2.50	0.46
31:2:713:G:N2	31:2:718:A:H62	2.10	0.46
31:2:1689:A:H2'	31:2:1690:A:C8	2.50	0.46
31:2:1872:A:H2'	31:2:1873:G:O4'	2.16	0.46
36:e:88:MET:HG2	48:q:64:LEU:HD21	1.97	0.46
43:l:25:GLY:H	52:1:1329:A:H5''	1.80	0.46
52:1:1261:A:H5''	52:1:1262:C:H5	1.80	0.46
52:1:1287:A:H2'	52:1:1288:A:H8	1.80	0.46
52:1:1512:U:H2'	52:1:1513:A:C8	2.50	0.46
3:C:44:ARG:NH1	31:2:1248:G:OP1	2.30	0.46
27:AB:2:LYS:HA	31:2:592:A:H1'	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:5:29:G:H2'	29:5:30:G:H8	1.81	0.46
31:2:707:G:H1	31:2:724:U:H3	1.63	0.46
31:2:1405:U:H2'	31:2:1406:U:C6	2.49	0.46
31:2:2417:C:H2'	31:2:2418:A:H8	1.80	0.46
33:b:5:HIS:CE1	33:b:7:ASN:HB3	2.50	0.46
36:e:7:VAL:HG23	36:e:88:MET:HG3	1.97	0.46
38:g:51:GLU:O	38:g:56:PRO:HA	2.15	0.46
52:1:182:A:N6	52:1:194:C:C2	2.83	0.46
52:1:269:C:H2'	52:1:270:A:C8	2.50	0.46
4:D:28:PRO:HG2	4:D:164:GLU:HB3	1.97	0.46
22:W:47:ARG:NH1	31:2:61:C:OP2	2.40	0.46
31:2:1589:U:H2'	31:2:1590:A:H8	1.79	0.46
32:a:202:ASN:OD1	32:a:205:ALA:N	2.45	0.46
34:c:143:SER:HB2	34:c:178:GLU:HG2	1.98	0.46
40:i:24:GLU:O	40:i:27:GLU:HG3	2.14	0.46
41:j:32:THR:HG21	52:1:706:A:H1'	1.97	0.46
52:1:923:A:O2'	52:1:1399:C:OP2	2.32	0.46
52:1:1006:G:O6	52:1:1023:U:O4	2.34	0.46
4:D:120:SER:HA	31:2:2303:G:H4'	1.97	0.46
5:E:23:ILE:HD12	5:E:71:LEU:HD21	1.97	0.46
31:2:74:A:O2'	31:2:88:G:OP2	2.30	0.46
31:2:723:C:H2'	31:2:724:U:H6	1.81	0.46
52:1:475:C:H2'	52:1:476:U:C6	2.50	0.46
52:1:1010:U:H2'	52:1:1011:C:C6	2.51	0.46
9:J:37:GLY:O	9:J:41:ARG:HG2	2.16	0.46
31:2:849:A:H2'	31:2:850:U:C6	2.50	0.46
31:2:1000:A:H2'	31:2:1001:A:C8	2.51	0.46
31:2:1447:C:H2'	31:2:1448:G:H8	1.80	0.46
52:1:154:U:O4	52:1:155:A:N6	2.49	0.46
52:1:202:G:H2'	52:1:203:G:C8	2.50	0.46
52:1:458:U:H3	52:1:474:G:H1	1.62	0.46
52:1:460:A:H2'	52:1:461:A:H8	1.81	0.46
52:1:496:A:H2'	52:1:497:G:C8	2.50	0.46
24:Y:18:HIS:NE2	31:2:2045:C:O2	2.48	0.46
31:2:171:U:H2'	31:2:172:A:H8	1.81	0.46
31:2:848:C:H2'	31:2:849:A:C8	2.51	0.46
31:2:876:C:H3'	31:2:877:A:C5	2.50	0.46
31:2:1438:U:H2'	31:2:1439:A:C8	2.47	0.46
31:2:2540:C:O2'	31:2:2740:A:N3	2.42	0.46
31:2:2700:A:H2'	31:2:2701:U:C6	2.51	0.46
34:c:67:LEU:HB2	34:c:70:GLN:HE22	1.81	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:c:114:ARG:NH2	52:1:404:G:OP2	2.39	0.46
39:h:33:SER:H	39:h:36:GLN:HE21	1.64	0.46
52:1:131:A:H2'	52:1:132:C:C6	2.50	0.46
52:1:335:C:H2'	52:1:336:A:H8	1.80	0.46
52:1:728:A:H2'	52:1:729:A:C8	2.50	0.46
19:T:31:TYR:OH	19:T:90:ASP:OD2	2.25	0.46
30:AC:24:ARG:NH1	31:2:2742:G:OP2	2.44	0.46
31:2:632:A:H2'	31:2:633:A:C8	2.51	0.46
31:2:2626:C:H2'	31:2:2627:G:H8	1.81	0.46
47:p:30:HIS:CD2	47:p:32:ILE:HG22	2.51	0.46
52:1:378:G:O6	52:1:386:C:N4	2.49	0.46
52:1:501:C:H2'	52:1:502:A:C8	2.51	0.46
52:1:635:A:H2'	52:1:636:U:C6	2.51	0.46
52:1:728:A:H2'	52:1:729:A:H8	1.81	0.46
2:B:45:TYR:OH	31:2:2636:C:O2'	2.33	0.46
31:2:741:U:H2'	31:2:742:A:C8	2.50	0.46
31:2:1042:G:N1	31:2:1113:U:N3	2.58	0.46
31:2:1435:G:H2'	31:2:1436:G:C8	2.51	0.46
31:2:2290:G:H2'	31:2:2291:U:C6	2.51	0.46
1:A:7:PRO:HB3	1:A:13:ARG:HG3	1.97	0.46
23:X:5:LYS:HB2	23:X:57:GLU:HG3	1.98	0.46
27:AB:50:SER:OG	27:AB:51:LYS:N	2.49	0.46
31:2:689:A:H2'	31:2:690:G:C8	2.51	0.46
31:2:813:U:H2'	31:2:814:C:C6	2.51	0.46
31:2:2081:U:H2'	31:2:2082:A:H8	1.81	0.46
34:c:123:MET:HG3	34:c:145:ARG:HG2	1.96	0.46
45:n:28:VAL:HG11	45:n:66:LEU:HD21	1.97	0.46
52:1:1270:G:H2'	52:1:1271:A:C8	2.51	0.46
52:1:1448:C:H2'	52:1:1449:C:C6	2.50	0.46
10:K:134:THR:HG1	19:T:79:ARG:HH12	1.62	0.45
23:X:8:GLN:HB2	23:X:28:LEU:HD13	1.97	0.45
31:2:248:G:O2'	31:2:2432:A:OP1	2.31	0.45
31:2:1590:A:H2'	31:2:1591:A:H8	1.80	0.45
31:2:2116:G:H22	31:2:2171:A:H61	1.63	0.45
31:2:2700:A:H2'	31:2:2701:U:H6	1.80	0.45
31:2:807:U:O2'	31:2:2060:A:N1	2.50	0.45
31:2:1440:U:H2'	31:2:1441:G:C8	2.51	0.45
31:2:2074:U:H2'	31:2:2075:U:C6	2.52	0.45
34:c:75:TYR:CE2	34:c:203:TYR:HB3	2.51	0.45
35:d:163:ILE:O	38:g:113:ARG:NH2	2.46	0.45
40:i:91:ASP:OD1	40:i:92:LEU:N	2.38	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
50:s:35:TYR:HA	50:s:38:ILE:HG22	1.97	0.45
52:1:517:G:N2	52:1:529:G:O2'	2.44	0.45
2:B:106:LYS:HE2	2:B:174:SER:HB3	1.98	0.45
13:N:114:ASN:OD1	13:N:114:ASN:N	2.49	0.45
31:2:78:U:H3	31:2:108:G:H1	1.64	0.45
31:2:1544:A:H2'	31:2:1545:A:C8	2.51	0.45
39:h:18:VAL:HA	39:h:64:ILE:HG22	1.99	0.45
52:1:146:G:H2'	52:1:147:G:C8	2.51	0.45
52:1:399:G:H2'	52:1:400:C:C6	2.51	0.45
2:B:155:VAL:HG21	31:2:2618:G:H21	1.82	0.45
4:D:129:MET:SD	4:D:130:GLY:N	2.89	0.45
7:G:114:LEU:HG	7:G:118:MET:HE3	1.98	0.45
31:2:1709:U:H2'	31:2:1710:G:H8	1.82	0.45
31:2:2710:C:H2'	31:2:2711:A:C8	2.52	0.45
33:b:41:TYR:HA	33:b:44:LYS:HG2	1.97	0.45
35:d:63:MET:HB3	35:d:63:MET:HE3	1.74	0.45
37:f:14:ASP:OD1	37:f:14:ASP:N	2.43	0.45
45:n:35:ILE:HD11	45:n:58:MET:HG3	1.99	0.45
52:1:514:C:H2'	52:1:515:G:C8	2.51	0.45
52:1:543:U:H2'	52:1:544:G:C8	2.51	0.45
52:1:558:G:OP2	52:1:559:A:O2'	2.31	0.45
52:1:636:U:H2'	52:1:637:C:C6	2.52	0.45
52:1:686:U:H2'	52:1:687:A:C8	2.51	0.45
52:1:1097:C:H2'	52:1:1098:C:C6	2.51	0.45
52:1:1526:G:H2'	52:1:1527:U:C6	2.52	0.45
1:A:256:THR:OG1	31:2:1797:G:O2'	2.33	0.45
10:K:12:MET:HA	31:2:910:A:H62	1.81	0.45
31:2:2303:G:H2'	31:2:2304:G:C8	2.52	0.45
31:2:2339:C:H2'	31:2:2340:A:C8	2.51	0.45
31:2:2626:C:H2'	31:2:2627:G:C8	2.51	0.45
52:1:392:C:H2'	52:1:393:A:C8	2.51	0.45
52:1:647:C:H2'	52:1:648:A:C8	2.50	0.45
52:1:1245:C:H2'	52:1:1246:A:C8	2.52	0.45
1:A:78:GLU:OE2	1:A:100:ARG:NE	2.43	0.45
3:C:118:LEU:HD11	3:C:188:MET:HE2	1.98	0.45
21:V:15:ASN:HD22	21:V:23:ALA:HB1	1.81	0.45
31:2:1597:A:H5''	31:2:1598:A:H5'	1.99	0.45
34:c:143:SER:OG	34:c:144:ILE:N	2.49	0.45
36:e:10:VAL:HG12	36:e:84:VAL:HG12	1.97	0.45
50:s:66:ILE:HG23	50:s:70:LYS:HB3	1.97	0.45
52:1:1162:C:H2'	52:1:1163:A:C8	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
52:1:1437:A:H2'	52:1:1438:G:H8	1.82	0.45
53:4:53:U:H2'	53:4:54:U:C6	2.52	0.45
31:2:1716:U:H2'	31:2:1717:A:H8	1.82	0.45
31:2:2564:A:H2'	31:2:2565:A:C8	2.52	0.45
31:2:2812:G:H2'	31:2:2813:A:H8	1.81	0.45
39:h:83:THR:HG23	39:h:97:LEU:HD11	1.99	0.45
40:i:68:ARG:HH22	52:1:1115:U:H5'	1.81	0.45
52:1:34:C:H2'	52:1:35:G:C8	2.50	0.45
11:L:86:ARG:NH1	11:L:117:ASP:OD1	2.49	0.45
17:R:64:LYS:NZ	31:2:1602:U:OP2	2.50	0.45
20:U:14:ALA:O	20:U:16:ARG:NH1	2.46	0.45
31:2:1026:G:H2'	31:2:1027:A:H8	1.82	0.45
31:2:1636:U:H2'	31:2:1637:A:C8	2.52	0.45
31:2:1717:A:N6	31:2:1743:G:H21	2.10	0.45
31:2:2291:U:H2'	31:2:2292:U:C6	2.52	0.45
31:2:2302:U:H2'	31:2:2303:G:C8	2.52	0.45
31:2:2443:C:H2'	31:2:2444:G:C8	2.51	0.45
36:e:1:MET:HE3	36:e:67:PRO:HD3	1.99	0.45
40:i:9:ARG:NH1	52:1:1279:G:H5''	2.31	0.45
48:q:71:ASP:OD2	51:t:3:ILE:N	2.49	0.45
50:s:20:ASN:HD22	52:1:323:U:H5''	1.82	0.45
52:1:455:G:H2'	52:1:456:A:H8	1.81	0.45
52:1:554:A:H2'	52:1:555:U:C6	2.51	0.45
52:1:1338:G:H2'	52:1:1339:A:C8	2.52	0.45
52:1:1386:G:H2'	52:1:1387:G:C8	2.47	0.45
28:3:80:U:O2'	31:2:918:A:N3	2.49	0.45
31:2:904:G:H2'	31:2:905:A:H8	1.81	0.45
31:2:2039:U:H2'	31:2:2040:G:C8	2.51	0.45
31:2:2127:G:H21	31:2:2173:A:H1'	1.82	0.45
31:2:2812:G:H2'	31:2:2813:A:C8	2.52	0.45
35:d:156:ARG:NH2	38:g:98:LEU:O	2.50	0.45
52:1:748:G:H2'	52:1:749:A:H8	1.81	0.45
52:1:1354:U:H2'	52:1:1355:G:H8	1.82	0.45
1:A:145:MET:HE1	31:2:1800:C:H5'	1.98	0.45
10:K:29:GLY:HA2	10:K:106:ASP:HB2	1.99	0.45
10:K:35:ALA:HB2	10:K:102:LEU:HD11	1.98	0.45
31:2:796:C:H2'	31:2:797:G:H8	1.82	0.45
31:2:1550:C:OP1	31:2:1720:U:O2'	2.23	0.45
31:2:1837:C:O2'	31:2:1927:A:N3	2.41	0.45
31:2:2194:U:H2'	31:2:2195:U:H6	1.81	0.45
2:B:184:ARG:NH2	13:N:6:GLN:OE1	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:K:35:ALA:HA	10:K:128:THR:HG22	2.00	0.44
29:5:27:G:H2'	29:5:28:G:H8	1.81	0.44
31:2:962:G:H2'	31:2:963:U:C6	2.52	0.44
35:d:13:LYS:HB2	35:d:37:VAL:HG23	1.99	0.44
40:i:42:LEU:HG	40:i:43:PRO:HD2	1.99	0.44
46:o:44:SER:OG	46:o:45:GLU:N	2.50	0.44
52:1:1160:G:H1	52:1:1176:A:H61	1.64	0.44
52:1:1160:G:O6	52:1:1182:G:O6	2.34	0.44
4:D:109:ARG:HD3	4:D:136:ILE:HA	1.99	0.44
11:L:13:ASN:OD1	11:L:13:ASN:N	2.47	0.44
23:X:15:ARG:HG3	23:X:53:MET:HE1	1.99	0.44
31:2:935:C:H2'	31:2:936:A:H8	1.81	0.44
31:2:1524:G:H2'	31:2:1525:A:H8	1.82	0.44
31:2:1746:A:H2'	31:2:1747:U:C6	2.53	0.44
31:2:2139:U:O2	31:2:2152:G:O6	2.36	0.44
39:h:24:ASN:N	39:h:61:ASP:OD1	2.50	0.44
52:1:539:A:H2'	52:1:540:G:C8	2.53	0.44
52:1:747:A:H2'	52:1:748:G:C8	2.51	0.44
2:B:13:ARG:HH11	13:N:55:HIS:HA	1.83	0.44
31:2:859:G:H1'	31:2:860:U:H5	1.81	0.44
31:2:2392:A:OP2	31:2:2424:C:N4	2.50	0.44
31:2:2627:G:N2	31:2:2777:G:OP2	2.49	0.44
32:a:227:ASP:OD1	32:a:227:ASP:N	2.51	0.44
52:1:543:U:H2'	52:1:544:G:H8	1.82	0.44
52:1:801:U:H2'	52:1:802:A:H8	1.82	0.44
52:1:942:G:N2	52:1:1341:U:O2	2.35	0.44
52:1:983:A:H2	52:1:984:C:C6	2.35	0.44
4:D:101:ARG:O	4:D:105:ILE:HG22	2.18	0.44
8:I:49:ARG:NH2	52:1:1423:G:OP1	2.50	0.44
31:2:895:U:O4	31:2:897:C:N4	2.50	0.44
31:2:1130:U:C2	31:2:2025:C:H5''	2.53	0.44
31:2:1306:C:H2'	31:2:1307:A:H8	1.82	0.44
31:2:2146:C:O2'	31:2:2147:A:N7	2.50	0.44
31:2:2553:G:C2	31:2:2583:G:H1'	2.51	0.44
52:1:1433:A:N6	52:1:1467:C:O2	2.51	0.44
10:K:13:HIS:O	10:K:71:LYS:NZ	2.50	0.44
13:N:30:TRP:NE1	13:N:81:ASP:OD2	2.50	0.44
28:3:114:C:H2'	28:3:115:A:H8	1.81	0.44
31:2:172:A:H2'	31:2:173:A:C8	2.53	0.44
31:2:281:C:H2'	31:2:282:A:C8	2.53	0.44
31:2:1475:G:N2	31:2:1516:G:N7	2.66	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:2:1830:C:H2'	31:2:1831:G:H8	1.82	0.44
31:2:2557:G:H2'	31:2:2558:C:C6	2.52	0.44
31:2:2786:U:H2'	31:2:2787:C:H6	1.83	0.44
38:g:6:ILE:HD12	38:g:35:ILE:HD12	2.00	0.44
38:g:86:LYS:HB2	38:g:124:ILE:HD11	2.00	0.44
43:l:1:ALA:O	43:l:7:ASN:ND2	2.50	0.44
52:1:73:C:H2'	52:1:74:A:H8	1.82	0.44
52:1:78:A:H2'	52:1:79:G:C8	2.52	0.44
52:1:381:C:H2'	52:1:382:A:O4'	2.18	0.44
52:1:806:C:H2'	52:1:807:A:H8	1.82	0.44
52:1:954:G:H21	52:1:1227:A:N6	2.16	0.44
52:1:1253:G:H2'	52:1:1254:A:C8	2.53	0.44
14:O:50:ARG:NH2	31:2:993:G:OP2	2.50	0.44
31:2:603:A:H8	31:2:654:A:H2	1.66	0.44
31:2:1466:U:O3'	31:2:1546:G:O2'	2.36	0.44
33:b:6:PRO:HD2	33:b:183:TYR:CD2	2.53	0.44
38:g:1:SER:N	52:1:823:C:O2'	2.51	0.44
41:j:44:ALA:HB3	41:j:69:CYS:HB2	1.99	0.44
44:m:78:LEU:HB2	44:m:83:VAL:HG13	1.99	0.44
46:o:10:GLY:HA2	52:1:624:C:H4'	1.98	0.44
52:1:270:A:H2'	52:1:271:C:H6	1.83	0.44
52:1:635:A:H2'	52:1:636:U:H6	1.83	0.44
52:1:1175:G:H2'	52:1:1176:A:H8	1.83	0.44
52:1:1363:A:H2'	52:1:1365:G:N7	2.33	0.44
7:G:62:VAL:HG21	7:G:101:ILE:HD11	1.98	0.44
11:L:5:LYS:NZ	31:2:2000:C:OP1	2.39	0.44
16:Q:42:LYS:HE3	16:Q:42:LYS:HB3	1.91	0.44
31:2:1744:A:H3'	31:2:1745:A:H8	1.83	0.44
31:2:2064:C:H2'	31:2:2065:C:C6	2.53	0.44
31:2:2307:G:H5'	31:2:2308:G:N3	2.33	0.44
34:c:187:ARG:NE	34:c:196:GLU:OE2	2.48	0.44
41:j:84:MET:HE2	41:j:112:VAL:HG11	2.00	0.44
52:1:823:C:H2'	52:1:824:G:H8	1.82	0.44
52:1:1004:A:O2'	52:1:1036:A:N1	2.51	0.44
52:1:1242:G:N1	52:1:1295:U:N3	2.66	0.44
52:1:1464:U:H2'	52:1:1465:A:H8	1.83	0.44
1:A:140:VAL:HG12	1:A:191:LEU:HD23	1.99	0.44
19:T:9:ARG:HD3	19:T:39:ALA:HB1	2.00	0.44
7:G:31:GLU:HG2	7:G:142:ILE:HB	1.99	0.44
8:I:26:GLY:HA3	8:I:30:ARG:HH11	1.81	0.44
12:M:29:HIS:HB3	12:M:36:TYR:HD2	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:V:6:VAL:HG23	21:V:7:THR:HG23	2.00	0.44
31:2:121:G:H4'	31:2:149:A:H5'	1.99	0.44
31:2:589:U:H2'	31:2:590:A:H8	1.83	0.44
31:2:1913:A:C4	52:1:1492:A:N7	2.85	0.44
31:2:2064:C:H2'	31:2:2065:C:H6	1.82	0.44
52:1:246:A:H62	52:1:281:G:N2	2.15	0.44
52:1:1120:C:H2'	52:1:1121:U:H6	1.82	0.44
52:1:1242:G:O6	52:1:1295:U:C4	2.70	0.44
1:A:44:ASN:N	31:2:1812:U:O2'	2.44	0.43
7:G:50:THR:O	7:G:50:THR:OG1	2.34	0.43
31:2:1523:U:H5''	31:2:1524:G:C8	2.53	0.43
31:2:2137:U:H2'	31:2:2138:G:C8	2.53	0.43
31:2:2506:U:O2'	31:2:2507:C:OP1	2.29	0.43
32:a:36:LYS:HE2	32:a:36:LYS:HB2	1.91	0.43
33:b:18:ASN:O	33:b:55:VAL:HA	2.18	0.43
49:r:24:SER:OG	49:r:27:LYS:NZ	2.42	0.43
52:1:214:C:H2'	52:1:215:C:H6	1.83	0.43
52:1:422:C:H4'	52:1:423:G:H21	1.82	0.43
4:D:90:LEU:HD23	4:D:94:ARG:HB3	1.99	0.43
7:G:36:LEU:HD11	7:G:122:LEU:HB2	2.00	0.43
31:2:965:C:H2'	31:2:966:G:H8	1.83	0.43
31:2:1251:C:O2'	31:2:1252:G:H3'	2.18	0.43
31:2:1289:C:H2'	31:2:1290:C:C6	2.53	0.43
31:2:2150:C:H2'	31:2:2151:U:C6	2.52	0.43
33:b:50:SER:HB3	33:b:71:ARG:HH11	1.82	0.43
39:h:33:SER:OG	39:h:34:LEU:N	2.50	0.43
40:i:5:ARG:NH1	40:i:77:VAL:O	2.51	0.43
41:j:108:ASN:HB3	51:t:6:ARG:HD2	2.00	0.43
52:1:516:U:O2'	52:1:519:C:N3	2.51	0.43
52:1:861:G:HO2'	52:1:874:G:HO2'	1.60	0.43
52:1:1187:G:H2'	52:1:1188:A:C8	2.53	0.43
52:1:1241:G:H1	52:1:1296:C:H42	1.66	0.43
52:1:1250:A:C2	52:1:1370:G:H1'	2.54	0.43
52:1:1287:A:H2'	52:1:1288:A:C8	2.53	0.43
52:1:1355:G:H2'	52:1:1356:G:C8	2.53	0.43
6:F:1:MET:N	6:F:20:ASN:OD1	2.42	0.43
8:I:17:ARG:HB3	8:I:45:GLU:HB2	2.01	0.43
10:K:34:LYS:HA	10:K:101:VAL:HA	1.98	0.43
25:Z:10:LEU:HD21	25:Z:33:LEU:HD23	2.01	0.43
25:Z:42:VAL:HG23	25:Z:44:GLN:HG2	1.99	0.43
31:2:149:A:H2'	31:2:150:U:C6	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:2:171:U:H2'	31:2:172:A:C8	2.54	0.43
31:2:594:U:H2'	31:2:595:C:C6	2.53	0.43
49:r:15:LEU:HA	49:r:18:VAL:HG12	1.98	0.43
50:s:27:MET:SD	50:s:66:ILE:HD11	2.58	0.43
52:1:1307:U:O4	52:1:1331:G:N2	2.52	0.43
1:A:50:THR:HG23	31:2:1813:G:H21	1.83	0.43
10:K:33:LEU:O	10:K:102:LEU:N	2.51	0.43
31:2:19:A:H2'	31:2:20:C:C6	2.54	0.43
31:2:577:G:H2'	31:2:578:G:C8	2.54	0.43
31:2:1947:C:H2'	31:2:1948:G:H8	1.83	0.43
31:2:2655:G:O2'	31:2:2664:G:O6	2.31	0.43
33:b:11:LEU:HD21	44:m:90:GLY:HA2	2.01	0.43
52:1:483:C:H3'	52:1:484:G:H8	1.82	0.43
52:1:1219:A:H2'	52:1:1220:G:H8	1.83	0.43
52:1:1525:G:H2'	52:1:1526:G:H8	1.82	0.43
7:G:95:ARG:HA	7:G:95:ARG:HD3	1.77	0.43
8:I:98:ARG:NH1	52:1:338:A:OP2	2.50	0.43
19:T:28:ALA:HB3	19:T:40:ILE:HG13	2.01	0.43
31:2:793:A:OP2	31:2:2071:A:O2'	2.37	0.43
31:2:829:A:N7	31:2:2247:A:O2'	2.51	0.43
31:2:956:G:H22	31:2:959:A:H3'	1.84	0.43
31:2:1296:G:OP1	31:2:2709:G:O2'	2.24	0.43
31:2:2475:C:H42	31:2:2529:G:N2	2.17	0.43
42:k:85:ARG:HA	42:k:93:ARG:HA	2.01	0.43
52:1:591:U:H2'	52:1:592:G:H8	1.83	0.43
52:1:689:C:H2'	52:1:690:G:C8	2.53	0.43
52:1:924:C:H2'	52:1:925:G:H8	1.84	0.43
52:1:926:G:N2	53:4:52:G:H3'	2.34	0.43
53:4:87:C:H2'	53:4:88:A:C8	2.54	0.43
2:B:38:LYS:O	2:B:46:ARG:HA	2.19	0.43
3:C:7:ASP:O	3:C:9:GLN:NE2	2.51	0.43
12:M:31:THR:OG1	12:M:33:ARG:O	2.26	0.43
31:2:1028:A:H2'	31:2:1029:A:C8	2.53	0.43
31:2:1353:A:H2'	31:2:1354:A:H8	1.83	0.43
31:2:2243:U:H2'	31:2:2244:U:C6	2.54	0.43
31:2:2547:A:H2'	31:2:2548:U:C6	2.53	0.43
35:d:149:PRO:HA	35:d:152:VAL:HG12	2.00	0.43
36:e:36:ILE:HG23	36:e:64:VAL:HG12	2.00	0.43
38:g:93:LYS:HG2	38:g:116:ARG:NH2	2.34	0.43
7:G:49:ASP:OD1	7:G:121:LYS:NZ	2.38	0.43
17:R:19:LYS:NZ	31:2:1340:U:OP1	2.50	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:AC:30:GLU:OE2	30:AC:33:HIS:ND1	2.51	0.43
31:2:2853:C:H2'	31:2:2854:G:H8	1.83	0.43
33:b:67:ILE:HG22	33:b:69:THR:HG23	1.99	0.43
38:g:28:SER:HB3	38:g:56:PRO:HB2	2.01	0.43
46:o:13:LYS:N	52:1:392:C:OP1	2.42	0.43
52:1:920:U:O2'	52:1:1081:A:O2'	2.27	0.43
52:1:1021:A:H2'	52:1:1022:A:H8	1.84	0.43
52:1:1442:G:H2'	52:1:1443:C:C6	2.54	0.43
52:1:1473:G:H2'	52:1:1474:U:C6	2.54	0.43
1:A:16:VAL:HB	1:A:203:VAL:HB	2.01	0.43
4:D:169:LEU:HG	4:D:174:PHE:CD2	2.53	0.43
8:I:66:LYS:HE3	8:I:66:LYS:HB3	1.88	0.43
21:V:6:VAL:HG11	21:V:58:ILE:HD11	2.00	0.43
27:AB:5:THR:HG22	27:AB:62:PRO:HD2	2.01	0.43
29:5:27:G:H2'	29:5:28:G:C8	2.54	0.43
31:2:1168:G:H2'	31:2:1169:A:C8	2.54	0.43
31:2:1441:G:H2'	31:2:1442:U:C6	2.54	0.43
34:c:57:LYS:HB2	34:c:57:LYS:HE2	1.86	0.43
38:g:105:THR:OG1	38:g:106:SER:N	2.52	0.43
52:1:553:A:H2'	52:1:554:A:H8	1.82	0.43
52:1:1098:C:H2'	52:1:1099:G:H8	1.84	0.43
52:1:1250:A:H2	52:1:1370:G:H1'	1.84	0.43
1:A:132:ARG:HB3	1:A:185:ALA:HB1	1.99	0.43
2:B:24:VAL:HG12	2:B:178:VAL:HG21	2.01	0.43
2:B:125:TRP:CG	2:B:160:LYS:HB3	2.54	0.43
2:B:151:THR:HB	2:B:152:PRO:HD3	2.01	0.43
3:C:147:LEU:HB3	3:C:186:VAL:HG22	2.00	0.43
28:3:2:G:H2'	28:3:3:C:H6	1.83	0.43
31:2:414:C:H2'	31:2:415:A:H8	1.83	0.43
31:2:679:C:H2'	31:2:680:C:H6	1.84	0.43
39:h:119:LYS:HB2	39:h:119:LYS:HE3	1.81	0.43
46:o:17:TYR:HB2	46:o:39:PHE:HD2	1.84	0.43
46:o:20:VAL:HG23	46:o:35:ARG:HA	2.01	0.43
52:1:398:U:H2'	52:1:399:G:H8	1.83	0.43
52:1:600:A:H2'	52:1:601:G:H8	1.84	0.43
52:1:769:G:H4'	52:1:1513:A:H4'	2.00	0.43
52:1:1405:G:H2'	52:1:1406:U:C6	2.54	0.43
1:A:5:CYS:SG	1:A:12:ARG:NH2	2.92	0.43
3:C:170:ARG:NH2	3:C:176:ASP:OD2	2.52	0.43
18:S:44:HIS:HD2	31:2:483:A:C8	2.36	0.43
31:2:577:G:O2'	31:2:1254:A:OP1	2.37	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:2:596:U:H2'	31:2:597:G:H8	1.83	0.43
31:2:962:G:H2'	31:2:963:U:H6	1.83	0.43
31:2:2313:C:H2'	31:2:2314:A:C8	2.54	0.43
36:e:18:VAL:HG11	36:e:58:HIS:CD2	2.53	0.43
42:k:32:VAL:HG12	42:k:78:VAL:HG22	2.01	0.43
52:1:745:G:H2'	52:1:746:A:C8	2.53	0.43
7:G:32:LEU:HD22	7:G:54:ILE:HG21	2.01	0.42
7:G:98:GLU:OE1	7:G:98:GLU:N	2.50	0.42
30:AC:25:VAL:HB	30:AC:35:GLN:HB2	2.01	0.42
31:2:526:A:O2'	31:2:2043:C:O2	2.34	0.42
31:2:645:C:H2'	31:2:647:G:C8	2.54	0.42
31:2:946:C:H2'	31:2:947:A:H8	1.83	0.42
31:2:1168:G:O6	31:2:1181:U:O4	2.37	0.42
31:2:1223:G:N2	31:2:1226:A:OP2	2.47	0.42
31:2:1858:A:H2'	31:2:1859:U:O4'	2.19	0.42
36:e:88:MET:HB3	48:q:63:TYR:HE2	1.84	0.42
52:1:861:G:O2'	52:1:874:G:O2'	2.28	0.42
52:1:1158:C:OP2	52:1:1181:G:N2	2.51	0.42
4:D:113:PHE:HZ	4:D:175:PRO:HG2	1.84	0.42
8:I:111:LYS:HB3	8:I:111:LYS:HE2	1.82	0.42
31:2:323:C:H2'	31:2:1205:A:N1	2.34	0.42
31:2:671:C:H2'	31:2:672:C:C6	2.54	0.42
31:2:1428:C:C5	31:2:1569:A:H5''	2.55	0.42
31:2:1561:C:H2'	31:2:1562:U:C6	2.54	0.42
49:r:69:LYS:HA	49:r:69:LYS:HD3	1.84	0.42
52:1:130:A:O2'	52:1:131:A:O5'	2.35	0.42
52:1:417:G:O6	52:1:426:U:O4	2.37	0.42
52:1:908:A:H2'	52:1:909:A:H8	1.83	0.42
52:1:1063:C:OP2	52:1:1064:G:O2'	2.34	0.42
52:1:1144:G:H21	52:1:1146:A:H61	1.67	0.42
52:1:1410:A:H2'	52:1:1411:C:C6	2.53	0.42
3:C:73:ILE:HG13	3:C:78:TRP:CZ3	2.54	0.42
3:C:105:LEU:HD23	3:C:105:LEU:HA	1.88	0.42
8:I:7:MET:HB3	8:I:18:ARG:HH21	1.84	0.42
29:5:8:U:N3	29:5:14:A:C5	2.87	0.42
30:AC:17:VAL:HG22	30:AC:19:ARG:HG3	2.01	0.42
31:2:2515:C:H2'	31:2:2516:A:C8	2.52	0.42
31:2:2801:G:H2'	31:2:2802:G:C8	2.55	0.42
43:l:53:ASP:HA	43:l:56:ARG:HB2	2.00	0.42
52:1:1144:G:N2	52:1:1146:A:H61	2.17	0.42
3:C:32:VAL:HG13	3:C:178:VAL:HG12	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:N:92:ARG:HD3	31:2:1753:G:H5''	2.01	0.42
14:O:90:ASP:OD1	14:O:90:ASP:N	2.52	0.42
31:2:1178:C:H2'	31:2:1179:G:C8	2.53	0.42
31:2:1198:U:H2'	31:2:1199:U:C6	2.54	0.42
31:2:1198:U:H2'	31:2:1199:U:H6	1.84	0.42
31:2:2087:G:H2'	31:2:2088:A:H8	1.85	0.42
31:2:2182:U:H2'	31:2:2183:A:C8	2.54	0.42
31:2:2783:U:H2'	31:2:2784:U:H6	1.83	0.42
32:a:163:ILE:HA	32:a:185:ILE:HD13	2.01	0.42
52:1:216:U:H2'	52:1:217:C:C6	2.54	0.42
52:1:371:A:N3	52:1:373:A:N6	2.67	0.42
52:1:1095:U:OP1	52:1:1108:G:N2	2.43	0.42
52:1:1208:C:H2'	52:1:1209:C:H6	1.85	0.42
1:A:24:HIS:CG	1:A:79:ARG:HD2	2.55	0.42
4:D:8:LYS:HA	4:D:11:VAL:HG22	2.00	0.42
8:I:4:GLU:OE1	31:2:2548:U:O2'	2.37	0.42
8:I:10:VAL:HG12	8:I:12:ASP:H	1.84	0.42
10:K:66:ARG:NH1	10:K:104:GLU:OE2	2.50	0.42
13:N:51:ASN:O	31:2:2845:U:H5''	2.19	0.42
27:AB:63:TYR:OH	31:2:592:A:O2'	2.34	0.42
28:3:100:G:N2	31:2:863:A:O3'	2.51	0.42
31:2:302:C:H2'	31:2:303:G:H8	1.84	0.42
31:2:729:G:H5'	31:2:730:A:H5''	2.02	0.42
31:2:1504:A:H2'	31:2:1505:A:C8	2.54	0.42
31:2:2291:U:O2'	31:2:2374:C:O2	2.37	0.42
40:i:9:ARG:HG2	40:i:71:LEU:HD11	2.00	0.42
42:k:11:ARG:HD2	52:1:562:U:H1'	2.00	0.42
45:n:31:LEU:HD22	45:n:58:MET:HB2	2.00	0.42
52:1:17:U:H2'	52:1:18:C:C6	2.54	0.42
52:1:323:U:H2'	52:1:324:G:O4'	2.19	0.42
52:1:599:C:H2'	52:1:600:A:H8	1.84	0.42
52:1:1118:U:H2'	52:1:1119:C:H6	1.84	0.42
52:1:1270:G:H2'	52:1:1271:A:H8	1.83	0.42
20:U:12:SER:OG	20:U:13:GLU:N	2.52	0.42
29:5:30:G:H5''	52:1:1230:C:H5'	2.02	0.42
31:2:172:A:H2'	31:2:173:A:H8	1.84	0.42
31:2:851:C:H2'	31:2:852:U:C6	2.55	0.42
31:2:2197:U:H1'	31:2:2198:A:C8	2.55	0.42
31:2:2840:C:H2'	31:2:2841:C:H6	1.85	0.42
39:h:41:GLU:HA	39:h:44:ARG:HD2	2.00	0.42
42:k:113:ARG:N	52:1:502:A:OP1	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
52:1:294:U:H2'	52:1:295:C:C6	2.55	0.42
52:1:505:G:H2'	52:1:506:G:H8	1.83	0.42
52:1:676:A:H2'	52:1:677:U:H6	1.84	0.42
3:C:84:THR:HG21	31:2:586:A:H5'	2.01	0.42
4:D:124:ARG:NH2	31:2:2316:G:O2'	2.42	0.42
7:G:40:HIS:CD2	7:G:40:HIS:H	2.38	0.42
8:I:104:THR:OG1	8:I:105:ARG:N	2.53	0.42
12:M:64:TYR:HD2	12:M:67:ASN:HD22	1.67	0.42
31:2:395:U:H2'	31:2:396:G:H8	1.85	0.42
31:2:741:U:H2'	31:2:742:A:H8	1.84	0.42
31:2:839:U:H2'	31:2:840:C:C6	2.55	0.42
31:2:2853:C:H2'	31:2:2854:G:C8	2.54	0.42
31:2:2896:C:H2'	31:2:2897:U:C6	2.55	0.42
35:d:155:LYS:HD2	38:g:70:VAL:HA	1.99	0.42
40:i:44:THR:HG23	52:1:1151:A:H4'	2.02	0.42
45:n:73:ASP:OD2	45:n:76:ARG:NH1	2.52	0.42
52:1:451:A:H4'	52:1:452:A:O4'	2.18	0.42
52:1:459:A:H2'	52:1:460:A:H8	1.85	0.42
52:1:1071:C:H2'	52:1:1072:G:C8	2.50	0.42
1:A:86:ARG:HE	31:2:1817:G:H5''	1.84	0.42
3:C:157:LEU:HG	3:C:169:VAL:HG11	2.00	0.42
11:L:51:LEU:HB3	11:L:79:LEU:HD21	2.02	0.42
31:2:150:U:H2'	31:2:151:C:C6	2.54	0.42
31:2:613:A:C2	31:2:614:A:H4'	2.55	0.42
31:2:2142:A:H2'	31:2:2143:C:C6	2.55	0.42
31:2:2262:U:H2'	31:2:2263:C:H6	1.85	0.42
31:2:2328:A:H2'	31:2:2329:U:H6	1.84	0.42
31:2:2783:U:H2'	31:2:2784:U:C6	2.55	0.42
34:c:187:ARG:NH1	34:c:194:ILE:O	2.53	0.42
39:h:11:ARG:NH2	39:h:108:ARG:HH21	2.17	0.42
41:j:52:ARG:NH2	52:1:690:G:O6	2.49	0.42
2:B:149:ASN:O	2:B:152:PRO:HD2	2.19	0.42
12:M:94:ARG:NH1	12:M:97:PHE:O	2.49	0.42
29:5:47:G:OP1	29:5:47:G:N2	2.53	0.42
31:2:624:C:O2'	31:2:657:U:OP1	2.38	0.42
31:2:927:A:H2'	31:2:928:A:C8	2.54	0.42
31:2:979:A:H2'	31:2:982:C:H42	1.85	0.42
31:2:1430:G:H2'	31:2:1431:A:H8	1.85	0.42
31:2:2208:C:H2'	31:2:2209:G:C8	2.54	0.42
39:h:32:ARG:HH21	39:h:37:TYR:HE1	1.67	0.42
42:k:6:LEU:HD21	42:k:11:ARG:HH21	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
52:1:985:C:H2'	52:1:986:U:C6	2.55	0.42
52:1:1273:C:H2'	52:1:1274:A:O4'	2.20	0.42
11:L:30:ARG:HB2	11:L:75:ILE:HD11	2.02	0.42
15:P:86:GLN:HE21	15:P:86:GLN:HB3	1.70	0.42
19:T:76:ASP:OD1	19:T:77:VAL:N	2.53	0.42
20:U:38:GLY:HA2	31:2:2330:G:H21	1.85	0.42
30:AC:34:LYS:NZ	31:2:2743:U:OP1	2.38	0.42
31:2:184:C:H2'	31:2:185:G:C8	2.55	0.42
31:2:481:G:H2'	31:2:507:A:N1	2.35	0.42
31:2:1682:G:H2'	31:2:1683:U:H6	1.84	0.42
31:2:1709:U:H2'	31:2:1710:G:C8	2.55	0.42
31:2:2446:G:N2	31:2:2449:U:O2	2.51	0.42
31:2:2475:C:N4	31:2:2529:G:H22	2.18	0.42
36:e:45:ARG:HB2	36:e:59:TYR:HE1	1.85	0.42
52:1:522:C:H2'	52:1:523:A:C8	2.55	0.42
52:1:623:C:H2'	52:1:624:C:C6	2.55	0.42
52:1:1245:C:H2'	52:1:1246:A:H8	1.85	0.42
1:A:154:ALA:HB2	1:A:161:VAL:HG13	2.02	0.41
8:I:6:THR:HG23	31:2:1666:G:H4'	2.01	0.41
19:T:50:MET:HB3	19:T:50:MET:HE2	1.75	0.41
31:2:30:G:H2'	31:2:31:C:C6	2.55	0.41
31:2:355:U:H2'	31:2:356:G:H8	1.85	0.41
31:2:599:A:H2'	31:2:600:G:H8	1.85	0.41
31:2:1786:A:H1'	31:2:1938:A:N6	2.34	0.41
31:2:1808:A:H3'	31:2:1809:A:C8	2.55	0.41
31:2:1880:U:H2'	31:2:1881:C:C6	2.55	0.41
39:h:7:GLY:HA3	39:h:18:VAL:HG22	2.01	0.41
39:h:11:ARG:HH11	39:h:12:LYS:HB2	1.85	0.41
52:1:328:C:H4'	52:1:329:A:H5'	2.02	0.41
14:O:52:ARG:NH1	31:2:994:C:OP1	2.53	0.41
31:2:418:C:H2'	31:2:419:U:C6	2.55	0.41
31:2:1361:G:H2'	31:2:1362:C:C6	2.55	0.41
39:h:39:GLY:H	39:h:44:ARG:HH21	1.69	0.41
41:j:80:ASN:N	41:j:80:ASN:OD1	2.53	0.41
52:1:455:G:H2'	52:1:456:A:C8	2.54	0.41
1:A:75:ALA:HB2	1:A:95:TYR:CD1	2.56	0.41
16:Q:17:VAL:HB	16:Q:76:VAL:HG11	2.02	0.41
31:2:155:A:H2'	31:2:156:A:C8	2.56	0.41
31:2:499:U:H2'	31:2:500:G:O4'	2.21	0.41
31:2:807:U:OP1	31:2:830:G:N2	2.51	0.41
31:2:833:A:H2'	31:2:834:G:H8	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:2:1433:A:H2'	31:2:1434:A:C8	2.50	0.41
31:2:1434:A:H2'	31:2:1435:G:C8	2.55	0.41
31:2:2007:U:H2'	31:2:2008:C:H6	1.85	0.41
31:2:2736:A:H2'	31:2:2737:G:H8	1.85	0.41
35:d:71:ILE:HD12	35:d:71:ILE:HA	1.82	0.41
36:e:11:HIS:ND1	36:e:12:PRO:HD2	2.36	0.41
40:i:53:ILE:HG23	52:1:1060:U:H4'	2.02	0.41
45:n:31:LEU:O	45:n:35:ILE:HG12	2.20	0.41
47:p:58:VAL:HG23	47:p:77:VAL:HG22	2.03	0.41
50:s:53:MET:HE2	50:s:53:MET:HB2	1.90	0.41
50:s:74:HIS:NE2	52:1:260:G:OP1	2.53	0.41
52:1:322:C:H2'	52:1:323:U:C6	2.55	0.41
9:J:29:LYS:HE2	9:J:29:LYS:HB3	1.85	0.41
17:R:12:ARG:HB2	17:R:33:LYS:O	2.21	0.41
31:2:305:C:H2'	31:2:306:U:C6	2.55	0.41
31:2:475:C:N3	31:2:479:A:N7	2.67	0.41
31:2:2590:A:H2'	31:2:2591:C:H6	1.85	0.41
31:2:2818:U:H2'	31:2:2819:G:C8	2.56	0.41
50:s:49:ALA:HA	50:s:52:GLU:HG2	2.02	0.41
52:1:554:A:H2'	52:1:555:U:H6	1.85	0.41
52:1:1208:C:H2'	52:1:1209:C:C6	2.56	0.41
52:1:1305:G:O2'	52:1:1331:G:N2	2.54	0.41
15:P:3:ALA:HA	15:P:40:MET:O	2.21	0.41
17:R:29:THR:HA	17:R:86:THR:HA	2.02	0.41
28:3:71:C:H2'	28:3:72:G:O4'	2.20	0.41
31:2:145:C:H2'	31:2:146:A:H8	1.85	0.41
31:2:1239:G:H2'	31:2:1240:U:O4'	2.21	0.41
31:2:2329:U:H2'	31:2:2330:G:H8	1.85	0.41
31:2:2855:C:H2'	31:2:2856:A:C8	2.55	0.41
33:b:110:LEU:HD21	33:b:143:LEU:HB2	2.02	0.41
52:1:313:A:H2'	52:1:314:C:C6	2.56	0.41
52:1:570:G:H2'	52:1:571:U:C6	2.55	0.41
52:1:801:U:H2'	52:1:802:A:C8	2.56	0.41
52:1:1020:G:H2'	52:1:1021:A:C8	2.55	0.41
52:1:1107:C:C4	52:1:1108:G:C8	3.09	0.41
52:1:1181:G:H1'	52:1:1182:G:C5	2.55	0.41
6:F:29:PHE:HB2	31:2:2198:A:C2	2.56	0.41
11:L:103:ARG:HD2	11:L:106:ASP:OD1	2.21	0.41
16:Q:17:VAL:HG11	16:Q:103:ILE:HG12	2.03	0.41
21:V:14:GLY:HA3	21:V:28:PHE:HE1	1.86	0.41
26:AA:3:ARG:HA	26:AA:3:ARG:HD3	1.77	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:2:364:C:H2'	31:2:365:U:H6	1.84	0.41
31:2:679:C:H2'	31:2:680:C:C6	2.56	0.41
34:c:56:GLU:HG2	34:c:198:LEU:HD21	2.03	0.41
43:l:94:LEU:HD21	52:1:1226:C:H5''	2.03	0.41
44:m:68:ARG:NH1	44:m:70:HIS:O	2.53	0.41
52:1:855:U:OP2	52:1:871:U:N3	2.43	0.41
52:1:857:C:H2'	52:1:858:G:O4'	2.21	0.41
52:1:1513:A:H2'	52:1:1514:G:H8	1.84	0.41
3:C:63:LYS:HD2	31:2:2444:G:P	2.60	0.41
12:M:34:HIS:HA	12:M:53:THR:OG1	2.20	0.41
23:X:15:ARG:O	23:X:20:LYS:NZ	2.54	0.41
31:2:796:C:H2'	31:2:797:G:C8	2.56	0.41
31:2:1335:C:H2'	31:2:1336:A:C8	2.56	0.41
31:2:2122:U:H2'	31:2:2123:G:C8	2.55	0.41
31:2:2475:C:H42	31:2:2529:G:H22	1.69	0.41
52:1:28:A:O2'	52:1:296:U:OP1	2.36	0.41
52:1:110:C:H2'	52:1:111:G:O4'	2.20	0.41
52:1:257:G:H2'	52:1:258:G:C8	2.55	0.41
52:1:453:G:H2'	52:1:454:G:H8	1.86	0.41
52:1:555:U:H2'	52:1:556:C:H6	1.86	0.41
52:1:704:A:C4	52:1:705:G:C8	3.08	0.41
52:1:1442:G:H2'	52:1:1443:C:H6	1.86	0.41
1:A:264:LYS:HE2	1:A:264:LYS:HB3	1.82	0.41
4:D:30:VAL:HA	4:D:157:THR:HG22	2.02	0.41
19:T:40:ILE:HD12	19:T:42:LEU:HD21	2.02	0.41
28:3:79:G:O2'	31:2:861:A:N3	2.54	0.41
31:2:1316:U:H2'	31:2:1317:G:H8	1.85	0.41
31:2:1430:G:H2'	31:2:1431:A:C8	2.55	0.41
31:2:1527:G:H21	31:2:1545:A:N6	2.10	0.41
31:2:1571:A:H2'	31:2:1572:A:C8	2.55	0.41
31:2:1716:U:H2'	31:2:1717:A:C8	2.55	0.41
31:2:1779:U:H5	31:2:1784:A:N7	2.19	0.41
31:2:2118:U:O5'	31:2:2147:A:O2'	2.35	0.41
31:2:2184:A:H2'	31:2:2185:U:C6	2.56	0.41
34:c:63:ILE:HD13	34:c:63:ILE:HA	1.90	0.41
38:g:2:MET:HE2	38:g:2:MET:HB3	1.87	0.41
39:h:74:GLN:NE2	52:1:1249:C:O2'	2.54	0.41
44:m:10:VAL:HA	44:m:13:VAL:HG12	2.02	0.41
52:1:513:C:H2'	52:1:514:C:H6	1.85	0.41
52:1:876:C:H2'	52:1:877:G:H8	1.85	0.41
52:1:1414:U:H2'	52:1:1415:G:C8	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:219:VAL:HG21	31:2:782:A:N7	2.36	0.41
3:C:117:ARG:NE	3:C:184:ASP:O	2.53	0.41
3:C:171:ASP:OD1	3:C:171:ASP:N	2.51	0.41
7:G:46:PRO:HD3	14:O:59:LEU:HD13	2.03	0.41
11:L:46:ARG:HE	11:L:46:ARG:HB3	1.74	0.41
22:W:58:ASN:ND2	31:2:111:A:O2'	2.53	0.41
24:Y:3:GLN:HA	31:2:2615:U:C2	2.56	0.41
27:AB:18:LYS:HB3	27:AB:18:LYS:HE2	1.89	0.41
28:3:41:G:N2	31:2:2340:A:OP1	2.54	0.41
28:3:95:U:H2'	28:3:96:G:C8	2.55	0.41
31:2:155:A:H2'	31:2:156:A:H8	1.86	0.41
31:2:822:G:H2'	31:2:823:C:C6	2.56	0.41
31:2:1266:G:O2'	31:2:2012:G:O6	2.30	0.41
31:2:1386:C:O2'	31:2:1469:A:N3	2.47	0.41
31:2:1452:G:H2'	31:2:1453:A:C2	2.56	0.41
31:2:1590:A:H2'	31:2:1591:A:C8	2.56	0.41
31:2:2071:A:H2'	31:2:2072:C:H6	1.86	0.41
31:2:2187:U:H2'	31:2:2188:U:C6	2.55	0.41
31:2:2736:A:H2'	31:2:2737:G:C8	2.56	0.41
34:c:152:SER:HA	34:c:155:LYS:HG2	2.03	0.41
35:d:44:ARG:HH21	35:d:70:MET:HE3	1.86	0.41
39:h:11:ARG:O	39:h:14:SER:OG	2.29	0.41
42:k:20:VAL:HG13	42:k:94:TYR:CE1	2.56	0.41
42:k:68:GLY:N	52:1:522:C:OP1	2.54	0.41
52:1:916:U:H2'	52:1:917:G:H8	1.86	0.41
52:1:918:A:H2'	52:1:919:A:C8	2.55	0.41
52:1:1026:G:C6	52:1:1035:A:N1	2.89	0.41
52:1:1070:U:H2'	52:1:1071:C:C6	2.56	0.41
52:1:1081:A:H2'	52:1:1082:A:H8	1.86	0.41
52:1:1353:G:H2'	52:1:1354:U:H6	1.86	0.41
52:1:1361:G:H2'	52:1:1362:A:C8	2.55	0.41
8:I:23:LYS:HB3	8:I:40:LYS:HB3	2.03	0.41
12:M:81:ARG:O	12:M:84:GLU:HG3	2.21	0.41
13:N:74:GLN:HB2	13:N:77:SER:HB2	2.03	0.41
14:O:47:ARG:NH2	31:2:560:C:O2'	2.54	0.41
24:Y:49:ARG:HG2	31:2:2884:U:C6	2.56	0.41
31:2:1161:C:H2'	31:2:1162:G:H8	1.86	0.41
31:2:1746:A:H2'	31:2:1747:U:H6	1.86	0.41
31:2:2031:A:N3	31:2:2455:G:O2'	2.41	0.41
31:2:2104:C:H2'	31:2:2105:U:C6	2.55	0.41
31:2:2134:A:N6	31:2:2158:A:O2'	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:b:48:LYS:HE3	33:b:48:LYS:HB3	1.93	0.41
37:f:58:LEU:H	37:f:58:LEU:HD23	1.86	0.41
38:g:42:GLU:HG2	38:g:100:ILE:HG21	2.03	0.41
43:l:77:LYS:HA	43:l:77:LYS:HD3	1.90	0.41
48:q:29:LYS:HB3	48:q:29:LYS:HE2	1.86	0.41
48:q:64:LEU:HD23	48:q:64:LEU:HA	1.93	0.41
52:1:71:A:N6	52:1:99:C:O2	2.53	0.41
52:1:231:U:H2'	52:1:232:G:H8	1.86	0.41
52:1:315:A:O2'	52:1:330:C:O2'	2.31	0.41
52:1:541:G:H2'	52:1:542:G:C8	2.56	0.41
52:1:674:G:N2	52:1:717:U:O2	2.53	0.41
52:1:1316:G:N2	52:1:1318:A:H3'	2.36	0.41
52:1:1404:C:H2'	52:1:1405:G:C8	2.56	0.41
53:4:53:U:H2'	53:4:54:U:H6	1.86	0.41
53:4:80:G:H2'	53:4:81:G:H8	1.86	0.41
5:E:98:LYS:HE3	5:E:98:LYS:HB3	1.90	0.40
6:F:2:GLN:HB3	6:F:18:GLN:HE21	1.85	0.40
8:I:34:GLY:N	8:I:37:ASP:OD2	2.54	0.40
12:M:39:VAL:HG12	12:M:49:VAL:H	1.86	0.40
31:2:1288:G:H2'	31:2:1288:G:N3	2.36	0.40
31:2:2133:G:H2'	31:2:2157:G:C8	2.56	0.40
31:2:2247:A:H2'	31:2:2248:C:C6	2.56	0.40
36:e:6:ILE:HB	36:e:62:MET:HG3	2.03	0.40
40:i:8:ILE:HB	40:i:74:VAL:HG12	2.02	0.40
41:j:92:ARG:HE	41:j:92:ARG:HB2	1.67	0.40
46:o:23:ASP:OD1	46:o:24:SER:N	2.54	0.40
50:s:23:ARG:HD2	50:s:60:GLN:HE22	1.86	0.40
52:1:815:A:N7	52:1:1509:C:O2'	2.50	0.40
53:4:81:G:H2'	53:4:82:A:C8	2.56	0.40
31:2:145:C:H2'	31:2:146:A:C8	2.56	0.40
31:2:807:U:H2'	31:2:808:G:H8	1.86	0.40
31:2:1667:G:O2'	31:2:1991:U:O4	2.37	0.40
31:2:1689:A:H2'	31:2:1690:A:H8	1.86	0.40
31:2:2243:U:H2'	31:2:2244:U:H6	1.86	0.40
31:2:2772:C:H2'	31:2:2773:C:H6	1.85	0.40
32:a:12:GLY:O	32:a:208:ALA:HB2	2.21	0.40
52:1:163:C:H2'	52:1:164:G:C8	2.56	0.40
52:1:909:A:N3	52:1:1413:A:O2'	2.51	0.40
52:1:1037:C:H2'	52:1:1038:C:C6	2.57	0.40
52:1:1038:C:H2'	52:1:1039:G:C8	2.56	0.40
52:1:1219:A:H2'	52:1:1220:G:C8	2.57	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:106:PRO:HD2	1:A:109:LEU:HD22	2.04	0.40
3:C:130:LYS:HD3	3:C:130:LYS:HA	1.87	0.40
12:M:13:ARG:HG3	31:2:2334:U:O3'	2.21	0.40
15:P:68:ARG:HB3	15:P:90:ARG:HB3	2.03	0.40
31:2:19:A:H2'	31:2:20:C:H6	1.87	0.40
31:2:1028:A:H2'	31:2:1029:A:H8	1.86	0.40
31:2:1168:G:H2'	31:2:1169:A:H8	1.86	0.40
31:2:2059:A:H61	31:2:2505:G:H22	1.69	0.40
31:2:2740:A:H2'	31:2:2741:A:C8	2.56	0.40
39:h:26:LYS:N	39:h:61:ASP:OD2	2.37	0.40
40:i:41:PRO:HB2	52:1:1151:A:H1'	2.03	0.40
43:l:84:CYS:HA	49:r:73:PHE:HA	2.02	0.40
46:o:4:ILE:HG12	46:o:21:VAL:HB	2.04	0.40
49:r:1:PRO:HB3	52:1:1312:G:N7	2.36	0.40
49:r:35:ARG:HB2	49:r:71:GLY:HA3	2.04	0.40
52:1:57:G:H2'	52:1:58:C:C6	2.56	0.40
52:1:216:U:H2'	52:1:217:C:H6	1.86	0.40
52:1:398:U:H2'	52:1:399:G:C8	2.56	0.40
52:1:1010:U:H2'	52:1:1011:C:H6	1.86	0.40
52:1:1217:C:H2'	52:1:1218:C:C6	2.56	0.40
52:1:1517:A:O2'	52:1:1518:A:O4'	2.39	0.40
17:R:47:VAL:HG13	17:R:51:PHE:HD2	1.86	0.40
24:Y:2:VAL:HG23	31:2:2015:A:C6	2.57	0.40
29:5:70:G:H2'	29:5:71:G:H8	1.87	0.40
30:AC:2:LYS:HE2	30:AC:2:LYS:HB2	1.90	0.40
31:2:594:U:H2'	31:2:595:C:H6	1.86	0.40
31:2:640:C:H2'	31:2:641:U:C6	2.56	0.40
31:2:755:U:H2'	31:2:756:A:C8	2.56	0.40
31:2:1405:U:H2'	31:2:1406:U:H6	1.86	0.40
31:2:2315:G:H2'	31:2:2316:G:H8	1.86	0.40
36:e:2:ARG:HD3	36:e:91:ARG:NE	2.37	0.40
38:g:49:LYS:NZ	38:g:59:GLU:OE1	2.54	0.40
52:1:471:U:H2'	52:1:472:U:C6	2.57	0.40
52:1:1261:A:H5''	52:1:1262:C:C5	2.55	0.40
52:1:1293:C:C2	52:1:1294:G:C8	3.09	0.40
52:1:1294:G:C2	52:1:1295:U:C5	3.10	0.40
3:C:191:ASP:N	3:C:191:ASP:OD1	2.55	0.40
4:D:169:LEU:HD23	4:D:176:PHE:HE2	1.87	0.40
6:F:19:VAL:HG13	6:F:21:VAL:HG13	2.03	0.40
11:L:28:LEU:HD23	11:L:48:VAL:HG11	2.02	0.40
14:O:91:ARG:HD3	31:2:997:G:OP1	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:U:19:VAL:HG22	20:U:34:VAL:HG22	2.03	0.40
29:5:52:G:H2'	29:5:53:G:H8	1.86	0.40
31:2:17:G:H2'	31:2:18:U:H6	1.86	0.40
31:2:849:A:H2'	31:2:850:U:H6	1.86	0.40
31:2:1042:G:H1	31:2:1113:U:H3	1.53	0.40
31:2:1164:C:H2'	31:2:1165:A:H8	1.85	0.40
31:2:2627:G:O2'	31:2:2781:A:N1	2.45	0.40
35:d:114:LEU:HD22	35:d:119:VAL:HG21	2.04	0.40
36:e:45:ARG:HB2	36:e:59:TYR:CE1	2.56	0.40
52:1:181:A:H2'	52:1:182:A:C8	2.56	0.40
52:1:429:U:H5	52:1:430:A:H62	1.68	0.40
52:1:715:A:OP1	52:1:805:C:O2'	2.32	0.40
53:4:83:A:H2'	53:4:84:G:H8	1.86	0.40
53:4:88:A:H2'	53:4:89:G:H8	1.86	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	269/273 (98%)	263 (98%)	6 (2%)	0	100	100
2	B	207/209 (99%)	201 (97%)	6 (3%)	0	100	100
3	C	199/201 (99%)	192 (96%)	7 (4%)	0	100	100
4	D	173/179 (97%)	164 (95%)	9 (5%)	0	100	100
5	E	171/177 (97%)	166 (97%)	5 (3%)	0	100	100
6	F	55/149 (37%)	54 (98%)	1 (2%)	0	100	100
7	G	140/142 (99%)	137 (98%)	3 (2%)	0	100	100
8	I	121/123 (98%)	118 (98%)	3 (2%)	0	100	100
9	J	141/144 (98%)	134 (95%)	7 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
10	K	134/136 (98%)	129 (96%)	5 (4%)	0	100	100
11	L	117/127 (92%)	110 (94%)	7 (6%)	0	100	100
12	M	112/117 (96%)	106 (95%)	6 (5%)	0	100	100
13	N	112/115 (97%)	105 (94%)	7 (6%)	0	100	100
14	O	115/118 (98%)	114 (99%)	1 (1%)	0	100	100
15	P	101/103 (98%)	93 (92%)	8 (8%)	0	100	100
16	Q	108/110 (98%)	104 (96%)	4 (4%)	0	100	100
17	R	88/100 (88%)	86 (98%)	2 (2%)	0	100	100
18	S	92/104 (88%)	91 (99%)	1 (1%)	0	100	100
19	T	91/94 (97%)	89 (98%)	2 (2%)	0	100	100
20	U	73/85 (86%)	70 (96%)	3 (4%)	0	100	100
21	V	75/78 (96%)	74 (99%)	1 (1%)	0	100	100
22	W	58/63 (92%)	58 (100%)	0	0	100	100
23	X	56/59 (95%)	55 (98%)	1 (2%)	0	100	100
24	Y	53/57 (93%)	53 (100%)	0	0	100	100
25	Z	46/55 (84%)	46 (100%)	0	0	100	100
26	AA	44/46 (96%)	42 (96%)	2 (4%)	0	100	100
27	AB	62/65 (95%)	57 (92%)	5 (8%)	0	100	100
30	AC	36/38 (95%)	35 (97%)	1 (3%)	0	100	100
32	a	220/241 (91%)	206 (94%)	14 (6%)	0	100	100
33	b	193/233 (83%)	187 (97%)	5 (3%)	1 (0%)	24	57
34	c	156/206 (76%)	147 (94%)	9 (6%)	0	100	100
35	d	154/167 (92%)	149 (97%)	5 (3%)	0	100	100
36	e	100/135 (74%)	96 (96%)	4 (4%)	0	100	100
37	f	104/179 (58%)	101 (97%)	3 (3%)	0	100	100
38	g	127/130 (98%)	125 (98%)	2 (2%)	0	100	100
39	h	125/130 (96%)	114 (91%)	11 (9%)	0	100	100
40	i	96/103 (93%)	88 (92%)	8 (8%)	0	100	100
41	j	115/129 (89%)	111 (96%)	4 (4%)	0	100	100
42	k	119/124 (96%)	109 (92%)	10 (8%)	0	100	100
43	l	104/118 (88%)	95 (91%)	9 (9%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
44	m	98/101 (97%)	91 (93%)	7 (7%)	0	100	100
45	n	85/89 (96%)	83 (98%)	2 (2%)	0	100	100
46	o	80/82 (98%)	77 (96%)	3 (4%)	0	100	100
47	p	77/84 (92%)	72 (94%)	5 (6%)	0	100	100
48	q	52/75 (69%)	51 (98%)	1 (2%)	0	100	100
49	r	78/92 (85%)	67 (86%)	10 (13%)	1 (1%)	9	35
50	s	83/87 (95%)	80 (96%)	3 (4%)	0	100	100
51	t	66/71 (93%)	61 (92%)	5 (8%)	0	100	100
All	All	5281/5843 (90%)	5056 (96%)	223 (4%)	2 (0%)	100	100

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
33	b	60	ALA
49	r	40	PHE

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	216/218 (99%)	214 (99%)	2 (1%)	70	80
2	B	164/164 (100%)	161 (98%)	3 (2%)	51	73
3	C	165/165 (100%)	163 (99%)	2 (1%)	63	78
4	D	147/150 (98%)	145 (99%)	2 (1%)	59	76
5	E	134/138 (97%)	134 (100%)	0	100	100
6	F	45/114 (40%)	45 (100%)	0	100	100
7	G	116/116 (100%)	116 (100%)	0	100	100
8	I	104/104 (100%)	99 (95%)	5 (5%)	23	54
9	J	102/103 (99%)	101 (99%)	1 (1%)	68	79
10	K	109/109 (100%)	108 (99%)	1 (1%)	70	80

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
11	L	99/103 (96%)	97 (98%)	2 (2%)	48	72
12	M	84/87 (97%)	83 (99%)	1 (1%)	63	78
13	N	99/100 (99%)	98 (99%)	1 (1%)	68	79
14	O	89/90 (99%)	88 (99%)	1 (1%)	65	78
15	P	84/84 (100%)	83 (99%)	1 (1%)	63	78
16	Q	93/93 (100%)	91 (98%)	2 (2%)	45	71
17	R	77/84 (92%)	76 (99%)	1 (1%)	61	77
18	S	78/85 (92%)	76 (97%)	2 (3%)	40	68
19	T	77/78 (99%)	75 (97%)	2 (3%)	40	68
20	U	57/63 (90%)	57 (100%)	0	100	100
21	V	67/68 (98%)	66 (98%)	1 (2%)	57	75
22	W	54/55 (98%)	54 (100%)	0	100	100
23	X	48/49 (98%)	48 (100%)	0	100	100
24	Y	46/48 (96%)	45 (98%)	1 (2%)	45	71
25	Z	44/49 (90%)	44 (100%)	0	100	100
26	AA	38/38 (100%)	37 (97%)	1 (3%)	40	68
27	AB	51/52 (98%)	51 (100%)	0	100	100
30	AC	34/34 (100%)	33 (97%)	1 (3%)	37	66
32	a	173/199 (87%)	171 (99%)	2 (1%)	63	78
33	b	152/190 (80%)	151 (99%)	1 (1%)	76	82
34	c	132/173 (76%)	128 (97%)	4 (3%)	36	65
35	d	116/126 (92%)	110 (95%)	6 (5%)	21	51
36	e	89/116 (77%)	87 (98%)	2 (2%)	45	71
37	f	87/147 (59%)	87 (100%)	0	100	100
38	g	104/105 (99%)	104 (100%)	0	100	100
39	h	102/107 (95%)	99 (97%)	3 (3%)	37	66
40	i	86/90 (96%)	85 (99%)	1 (1%)	63	78
41	j	90/99 (91%)	90 (100%)	0	100	100
42	k	102/104 (98%)	98 (96%)	4 (4%)	28	60
43	l	83/96 (86%)	81 (98%)	2 (2%)	43	69
44	m	83/84 (99%)	83 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
45	n	75/77 (97%)	75 (100%)	0	100	100
46	o	65/65 (100%)	64 (98%)	1 (2%)	57	75
47	p	73/78 (94%)	71 (97%)	2 (3%)	39	67
48	q	47/65 (72%)	47 (100%)	0	100	100
49	r	71/79 (90%)	71 (100%)	0	100	100
50	s	64/66 (97%)	63 (98%)	1 (2%)	55	75
51	t	56/61 (92%)	56 (100%)	0	100	100
All	All	4371/4768 (92%)	4309 (99%)	62 (1%)	57	76

All (62) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	76	VAL
1	A	249	VAL
2	B	98	VAL
2	B	183	GLU
2	B	207	VAL
3	C	14	VAL
3	C	127	GLU
4	D	20	ASN
4	D	156	THR
8	I	5	GLN
8	I	31	ARG
8	I	38	ILE
8	I	61	VAL
8	I	76	VAL
9	J	27	LEU
10	K	93	VAL
11	L	48	VAL
11	L	70	THR
12	M	36	TYR
13	N	80	VAL
14	O	30	VAL
15	P	20	VAL
16	Q	23	LEU
16	Q	74	ILE
17	R	29	THR
18	S	66	VAL
18	S	92	VAL
19	T	45	ASP

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Mol	Chain	Res	Type
19	T	92	VAL
21	V	59	ASP
24	Y	22	THR
26	AA	24	THR
30	AC	17	VAL
32	a	30	ILE
32	a	128	LEU
33	b	109	GLU
34	c	89	LEU
34	c	141	VAL
34	c	172	VAL
34	c	193	ASP
35	d	37	VAL
35	d	45	VAL
35	d	71	ILE
35	d	104	ILE
35	d	144	GLU
35	d	147	ASN
36	e	7	VAL
36	e	61	LEU
39	h	28	VAL
39	h	62	LEU
39	h	66	VAL
40	i	78	GLU
42	k	3	VAL
42	k	52	CYS
42	k	54	VAL
42	k	97	VAL
43	l	24	VAL
43	l	101	THR
46	o	68	SER
47	p	60	ILE
47	p	66	LEU
50	s	63	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (75) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	45	ASN
1	A	85	ASN
1	A	133	ASN
1	A	242	HIS

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Mol	Chain	Res	Type
2	B	49	GLN
2	B	164	GLN
2	B	173	GLN
3	C	9	GLN
3	C	115	GLN
3	C	136	GLN
4	D	51	ASN
4	D	134	GLN
5	E	63	GLN
5	E	114	HIS
6	F	18	GLN
7	G	40	HIS
7	G	76	HIS
7	G	86	GLN
9	J	104	GLN
11	L	18	GLN
11	L	81	ASN
12	M	38	GLN
12	M	98	GLN
13	N	11	GLN
13	N	51	ASN
14	O	36	GLN
14	O	43	GLN
14	O	71	ASN
15	P	11	GLN
15	P	66	HIS
15	P	86	GLN
15	P	89	HIS
16	Q	7	HIS
16	Q	9	HIS
16	Q	31	GLN
17	R	15	HIS
17	R	70	HIS
18	S	65	GLN
18	S	73	ASN
19	T	44	HIS
20	U	42	HIS
21	V	5	GLN
21	V	15	ASN
24	Y	5	ASN
26	AA	16	HIS
32	a	38	HIS

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Mol	Chain	Res	Type
34	c	70	GLN
34	c	73	ASN
34	c	151	GLN
35	d	81	GLN
35	d	145	ASN
36	e	14	GLN
36	e	52	ASN
39	h	30	ASN
39	h	36	GLN
39	h	74	GLN
40	i	15	HIS
41	j	23	HIS
41	j	118	ASN
42	k	4	ASN
42	k	28	GLN
42	k	45	ASN
43	l	7	ASN
43	l	99	GLN
44	m	42	ASN
45	n	27	GLN
45	n	49	HIS
46	o	59	HIS
47	p	30	HIS
48	q	53	GLN
49	r	42	ASN
49	r	55	GLN
50	s	51	ASN
50	s	60	GLN
50	s	83	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
28	3	119/120 (99%)	19 (15%)	0
29	5	75/76 (98%)	28 (37%)	5 (6%)
31	2	2831/2903 (97%)	454 (16%)	9 (0%)
52	1	1518/1540 (98%)	268 (17%)	6 (0%)
53	4	42/93 (45%)	10 (23%)	0
All	All	4585/4732 (96%)	779 (16%)	20 (0%)

All (779) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
28	3	4	C
28	3	12	C
28	3	13	G
28	3	14	U
28	3	15	A
28	3	16	G
28	3	34	A
28	3	35	C
28	3	37	C
28	3	41	G
28	3	42	C
28	3	44	G
28	3	45	A
28	3	47	C
28	3	67	G
28	3	89	U
28	3	90	C
28	3	108	A
28	3	110	C
29	5	8	U
29	5	10	G
29	5	11	C
29	5	14	A
29	5	16	U
29	5	17	C
29	5	18	G
29	5	19	G
29	5	20	U
29	5	21	A
29	5	22	G
29	5	31	A
29	5	32	U
29	5	33	U
29	5	40	C
29	5	46	G
29	5	47	G
29	5	48	U
29	5	50	U
29	5	55	U
29	5	56	C
29	5	57	G
29	5	58	A
29	5	59	U

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Mol	Chain	Res	Type
29	5	60	U
29	5	61	C
29	5	75	C
29	5	76	A
31	2	23	G
31	2	34	U
31	2	49	A
31	2	51	G
31	2	52	A
31	2	63	A
31	2	71	A
31	2	74	A
31	2	75	G
31	2	82	U
31	2	88	G
31	2	101	A
31	2	118	A
31	2	119	A
31	2	120	U
31	2	126	A
31	2	136	G
31	2	139	U
31	2	140	C
31	2	141	G
31	2	142	A
31	2	163	C
31	2	181	A
31	2	196	A
31	2	199	A
31	2	205	G
31	2	216	A
31	2	218	A
31	2	221	A
31	2	222	A
31	2	223	A
31	2	225	C
31	2	228	C
31	2	229	C
31	2	242	G
31	2	243	U
31	2	245	G
31	2	248	G

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Mol	Chain	Res	Type
31	2	249	C
31	2	255	A
31	2	265	A
31	2	266	G
31	2	267	C
31	2	276	U
31	2	281	C
31	2	285	G
31	2	286	U
31	2	287	G
31	2	289	G
31	2	302	C
31	2	311	A
31	2	322	A
31	2	323	C
31	2	324	A
31	2	329	G
31	2	330	A
31	2	331	C
31	2	352	A
31	2	362	A
31	2	367	G
31	2	368	A
31	2	369	U
31	2	372	G
31	2	386	G
31	2	387	U
31	2	404	A
31	2	405	U
31	2	406	G
31	2	411	G
31	2	417	C
31	2	422	A
31	2	424	G
31	2	435	C
31	2	455	C
31	2	456	C
31	2	457	A
31	2	481	G
31	2	491	G
31	2	504	A
31	2	505	A

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Mol	Chain	Res	Type
31	2	509	C
31	2	510	C
31	2	529	A
31	2	531	C
31	2	532	A
31	2	545	U
31	2	546	U
31	2	548	G
31	2	549	G
31	2	550	C
31	2	563	A
31	2	568	U
31	2	573	U
31	2	575	A
31	2	577	G
31	2	603	A
31	2	613	A
31	2	614	A
31	2	615	U
31	2	621	A
31	2	627	A
31	2	637	A
31	2	645	C
31	2	646	U
31	2	647	G
31	2	654	A
31	2	668	A
31	2	669	G
31	2	670	A
31	2	676	A
31	2	685	A
31	2	686	U
31	2	687	C
31	2	695	G
31	2	705	A
31	2	726	G
31	2	730	A
31	2	740	C
31	2	747	C
31	2	757	G
31	2	765	C
31	2	775	G

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Mol	Chain	Res	Type
31	2	776	G
31	2	782	A
31	2	784	G
31	2	785	G
31	2	789	A
31	2	805	G
31	2	811	U
31	2	812	C
31	2	819	A
31	2	827	U
31	2	828	U
31	2	830	G
31	2	845	A
31	2	846	U
31	2	860	U
31	2	875	G
31	2	876	C
31	2	877	A
31	2	878	A
31	2	879	G
31	2	883	G
31	2	885	C
31	2	888	C
31	2	889	C
31	2	891	G
31	2	892	A
31	2	894	U
31	2	895	U
31	2	897	C
31	2	898	C
31	2	899	A
31	2	900	A
31	2	907	G
31	2	910	A
31	2	914	G
31	2	915	C
31	2	931	U
31	2	932	U
31	2	941	A
31	2	945	A
31	2	946	C
31	2	957	C

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Mol	Chain	Res	Type
31	2	958	U
31	2	959	A
31	2	961	C
31	2	974	G
31	2	983	A
31	2	995	C
31	2	996	A
31	2	1009	A
31	2	1012	U
31	2	1013	C
31	2	1021	A
31	2	1022	G
31	2	1026	G
31	2	1033	U
31	2	1034	G
31	2	1122	G
31	2	1132	U
31	2	1134	A
31	2	1135	C
31	2	1139	G
31	2	1141	U
31	2	1172	C
31	2	1174	U
31	2	1175	A
31	2	1176	U
31	2	1177	G
31	2	1179	G
31	2	1180	U
31	2	1206	G
31	2	1211	C
31	2	1212	G
31	2	1236	G
31	2	1250	G
31	2	1251	C
31	2	1253	A
31	2	1256	G
31	2	1271	G
31	2	1272	A
31	2	1289	C
31	2	1300	G
31	2	1301	A
31	2	1314	C

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Mol	Chain	Res	Type
31	2	1329	U
31	2	1345	C
31	2	1365	A
31	2	1368	G
31	2	1378	A
31	2	1379	U
31	2	1393	A
31	2	1395	A
31	2	1416	G
31	2	1420	A
31	2	1421	G
31	2	1428	C
31	2	1437	C
31	2	1450	G
31	2	1451	C
31	2	1452	G
31	2	1455	G
31	2	1458	U
31	2	1461	C
31	2	1467	U
31	2	1482	G
31	2	1490	A
31	2	1491	G
31	2	1515	A
31	2	1524	G
31	2	1535	A
31	2	1536	C
31	2	1537	G
31	2	1538	G
31	2	1555	G
31	2	1559	U
31	2	1560	G
31	2	1566	A
31	2	1569	A
31	2	1576	U
31	2	1583	A
31	2	1584	U
31	2	1607	C
31	2	1608	A
31	2	1609	A
31	2	1647	U
31	2	1648	U

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Mol	Chain	Res	Type
31	2	1674	G
31	2	1695	G
31	2	1714	U
31	2	1723	G
31	2	1729	U
31	2	1730	C
31	2	1732	C
31	2	1738	G
31	2	1758	U
31	2	1764	C
31	2	1773	A
31	2	1781	U
31	2	1782	U
31	2	1800	C
31	2	1801	A
31	2	1802	A
31	2	1808	A
31	2	1816	C
31	2	1829	A
31	2	1835	G
31	2	1849	G
31	2	1867	G
31	2	1870	C
31	2	1871	A
31	2	1876	A
31	2	1877	A
31	2	1885	A
31	2	1896	G
31	2	1906	G
31	2	1914	C
31	2	1919	A
31	2	1920	C
31	2	1923	U
31	2	1924	C
31	2	1926	U
31	2	1927	A
31	2	1929	G
31	2	1930	G
31	2	1931	U
31	2	1936	A
31	2	1937	A
31	2	1955	U

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Mol	Chain	Res	Type
31	2	1967	C
31	2	1970	A
31	2	1971	U
31	2	1972	G
31	2	1991	U
31	2	1992	G
31	2	1993	U
31	2	1996	C
31	2	1997	C
31	2	2021	C
31	2	2022	U
31	2	2023	C
31	2	2031	A
31	2	2043	C
31	2	2052	A
31	2	2055	C
31	2	2056	G
31	2	2060	A
31	2	2061	G
31	2	2062	A
31	2	2069	G
31	2	2093	G
31	2	2096	C
31	2	2097	A
31	2	2110	G
31	2	2111	U
31	2	2112	G
31	2	2113	U
31	2	2118	U
31	2	2119	A
31	2	2120	G
31	2	2125	G
31	2	2126	A
31	2	2127	G
31	2	2131	U
31	2	2132	U
31	2	2133	G
31	2	2134	A
31	2	2145	C
31	2	2156	G
31	2	2158	A
31	2	2159	G

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Mol	Chain	Res	Type
31	2	2162	G
31	2	2172	U
31	2	2173	A
31	2	2182	U
31	2	2190	G
31	2	2192	U
31	2	2198	A
31	2	2204	G
31	2	2211	A
31	2	2213	U
31	2	2225	A
31	2	2238	G
31	2	2239	G
31	2	2279	G
31	2	2283	C
31	2	2287	A
31	2	2288	A
31	2	2297	A
31	2	2300	C
31	2	2305	U
31	2	2307	G
31	2	2308	G
31	2	2309	A
31	2	2311	A
31	2	2312	U
31	2	2319	G
31	2	2320	U
31	2	2321	U
31	2	2322	A
31	2	2325	G
31	2	2333	A
31	2	2336	A
31	2	2350	C
31	2	2354	C
31	2	2361	G
31	2	2382	G
31	2	2383	G
31	2	2385	C
31	2	2391	G
31	2	2392	A
31	2	2402	U
31	2	2403	C

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Mol	Chain	Res	Type
31	2	2406	A
31	2	2424	C
31	2	2429	G
31	2	2430	A
31	2	2441	U
31	2	2448	A
31	2	2473	U
31	2	2475	C
31	2	2476	A
31	2	2494	G
31	2	2498	C
31	2	2502	G
31	2	2503	A
31	2	2505	G
31	2	2506	U
31	2	2507	C
31	2	2518	A
31	2	2520	C
31	2	2531	A
31	2	2547	A
31	2	2554	U
31	2	2564	A
31	2	2566	A
31	2	2567	G
31	2	2572	A
31	2	2576	G
31	2	2583	G
31	2	2602	A
31	2	2603	G
31	2	2609	U
31	2	2613	U
31	2	2615	U
31	2	2629	U
31	2	2630	G
31	2	2639	A
31	2	2645	G
31	2	2646	C
31	2	2647	U
31	2	2682	A
31	2	2685	G
31	2	2689	U
31	2	2690	U

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Mol	Chain	Res	Type
31	2	2714	G
31	2	2718	G
31	2	2722	G
31	2	2726	A
31	2	2733	A
31	2	2744	G
31	2	2748	A
31	2	2757	A
31	2	2764	A
31	2	2765	A
31	2	2778	A
31	2	2779	U
31	2	2780	G
31	2	2791	G
31	2	2794	C
31	2	2808	G
31	2	2809	A
31	2	2818	U
31	2	2820	A
31	2	2835	A
31	2	2836	U
31	2	2849	U
31	2	2858	C
31	2	2860	A
31	2	2861	U
31	2	2867	G
31	2	2868	A
31	2	2872	A
31	2	2873	A
31	2	2880	C
31	2	2883	A
31	2	2886	A
31	2	2893	A
31	2	2899	A
31	2	2900	A
31	2	2901	C
31	2	2902	C
31	2	2903	U
52	1	8	A
52	1	9	G
52	1	32	A
52	1	39	G

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Mol	Chain	Res	Type
52	1	47	C
52	1	48	C
52	1	50	A
52	1	51	A
52	1	54	C
52	1	60	A
52	1	61	G
52	1	66	A
52	1	71	A
52	1	76	G
52	1	77	A
52	1	94	G
52	1	95	C
52	1	121	U
52	1	131	A
52	1	139	A
52	1	141	G
52	1	159	G
52	1	161	A
52	1	163	C
52	1	166	U
52	1	167	A
52	1	168	G
52	1	174	A
52	1	179	A
52	1	182	A
52	1	184	G
52	1	195	A
52	1	197	A
52	1	209	U
52	1	210	C
52	1	212	G
52	1	226	G
52	1	244	U
52	1	247	G
52	1	251	G
52	1	266	G
52	1	267	C
52	1	289	G
52	1	306	A
52	1	328	C
52	1	343	U

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Mol	Chain	Res	Type
52	1	346	G
52	1	347	G
52	1	348	G
52	1	352	C
52	1	354	G
52	1	356	A
52	1	367	U
52	1	369	G
52	1	372	C
52	1	373	A
52	1	406	G
52	1	408	A
52	1	411	A
52	1	412	A
52	1	413	G
52	1	414	A
52	1	422	C
52	1	423	G
52	1	424	G
52	1	427	U
52	1	429	U
52	1	434	U
52	1	435	A
52	1	436	C
52	1	437	U
52	1	438	U
52	1	439	U
52	1	446	G
52	1	452	A
52	1	467	U
52	1	468	A
52	1	481	G
52	1	482	A
52	1	484	G
52	1	486	U
52	1	493	A
52	1	495	A
52	1	496	A
52	1	497	G
52	1	517	G
52	1	518	C
52	1	521	G

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Mol	Chain	Res	Type
52	1	523	A
52	1	526	C
52	1	527	G
52	1	528	C
52	1	529	G
52	1	530	G
52	1	531	U
52	1	532	A
52	1	533	A
52	1	534	U
52	1	547	A
52	1	559	A
52	1	560	A
52	1	573	A
52	1	574	A
52	1	575	G
52	1	576	C
52	1	577	G
52	1	596	A
52	1	618	C
52	1	642	A
52	1	653	U
52	1	665	A
52	1	692	U
52	1	693	G
52	1	694	A
52	1	702	A
52	1	703	G
52	1	713	G
52	1	721	G
52	1	723	U
52	1	724	G
52	1	731	G
52	1	754	C
52	1	755	G
52	1	777	A
52	1	794	A
52	1	815	A
52	1	817	C
52	1	820	U
52	1	829	G
52	1	832	G

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Mol	Chain	Res	Type
52	1	851	G
52	1	876	C
52	1	889	A
52	1	900	A
52	1	902	G
52	1	934	C
52	1	935	A
52	1	960	U
52	1	961	U
52	1	966	G
52	1	969	A
52	1	971	G
52	1	972	C
52	1	974	A
52	1	975	A
52	1	976	G
52	1	977	A
52	1	981	U
52	1	982	U
52	1	992	U
52	1	993	G
52	1	994	A
52	1	1002	G
52	1	1004	A
52	1	1015	G
52	1	1017	U
52	1	1022	A
52	1	1028	C
52	1	1031	C
52	1	1032	G
52	1	1033	G
52	1	1035	A
52	1	1037	C
52	1	1038	C
52	1	1039	G
52	1	1053	G
52	1	1056	U
52	1	1066	C
52	1	1085	U
52	1	1089	G
52	1	1094	G
52	1	1095	U

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Mol	Chain	Res	Type
52	1	1101	A
52	1	1108	G
52	1	1127	G
52	1	1130	A
52	1	1135	U
52	1	1136	C
52	1	1137	C
52	1	1138	G
52	1	1139	G
52	1	1140	C
52	1	1141	C
52	1	1143	G
52	1	1145	A
52	1	1157	A
52	1	1158	C
52	1	1159	U
52	1	1160	G
52	1	1161	C
52	1	1168	U
52	1	1169	A
52	1	1182	G
52	1	1184	G
52	1	1191	A
52	1	1196	A
52	1	1197	A
52	1	1201	A
52	1	1212	U
52	1	1213	A
52	1	1218	C
52	1	1224	U
52	1	1227	A
52	1	1236	A
52	1	1238	A
52	1	1240	U
52	1	1241	G
52	1	1248	A
52	1	1256	A
52	1	1257	A
52	1	1275	A
52	1	1279	G
52	1	1280	A
52	1	1281	C

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Mol	Chain	Res	Type
52	1	1282	C
52	1	1286	U
52	1	1287	A
52	1	1297	G
52	1	1298	U
52	1	1300	G
52	1	1301	U
52	1	1302	C
52	1	1305	G
52	1	1306	A
52	1	1313	U
52	1	1317	C
52	1	1319	A
52	1	1320	C
52	1	1321	U
52	1	1323	G
52	1	1328	C
52	1	1345	U
52	1	1346	A
52	1	1347	G
52	1	1348	U
52	1	1357	A
52	1	1358	U
52	1	1360	A
52	1	1363	A
52	1	1364	U
52	1	1379	G
52	1	1398	A
52	1	1401	G
52	1	1402	C
52	1	1422	G
52	1	1433	A
52	1	1437	A
52	1	1439	G
52	1	1441	A
52	1	1442	G
52	1	1446	A
52	1	1451	U
52	1	1452	C
52	1	1473	G
52	1	1475	G
52	1	1492	A

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Mol	Chain	Res	Type
52	1	1493	A
52	1	1498	U
52	1	1499	A
52	1	1503	A
52	1	1506	U
52	1	1516	G
52	1	1517	A
52	1	1518	A
52	1	1529	G
52	1	1530	G
52	1	1534	A
52	1	1541	U
53	4	52	G
53	4	53	U
53	4	56	G
53	4	57	A
53	4	59	A
53	4	60	A
53	4	61	G
53	4	62	A
53	4	63	U
53	4	64	C

All (20) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
29	5	9	A
29	5	10	G
29	5	21	A
29	5	39	U
29	5	58	A
31	2	227	A
31	2	242	G
31	2	404	A
31	2	544	C
31	2	547	A
31	2	784	G
31	2	859	G
31	2	2506	U
31	2	2575	C
52	1	407	U
52	1	1037	C

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Mol	Chain	Res	Type
52	1	1157	A
52	1	1167	A
52	1	1347	G
52	1	1474	U

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 34 ligands modelled in this entry, 34 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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.

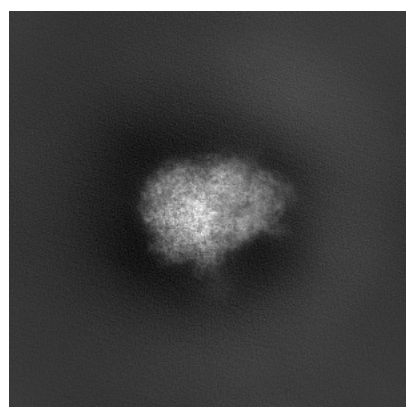
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-21420. These allow visual inspection of the internal detail of the map and identification of artifacts.

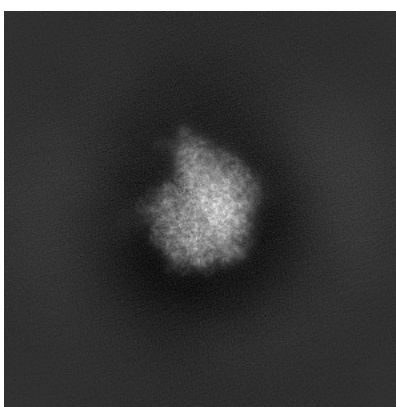
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

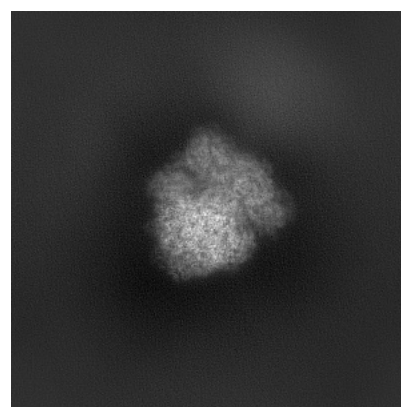
6.1.1 Primary map



X



Y

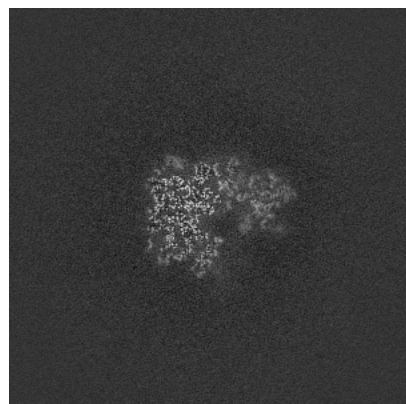


Z

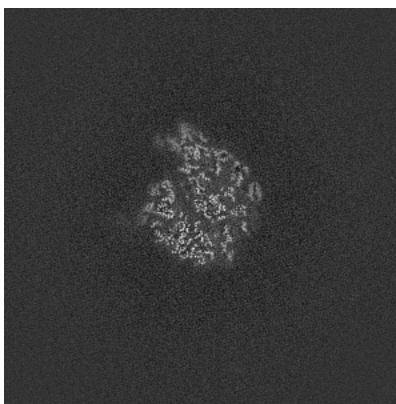
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

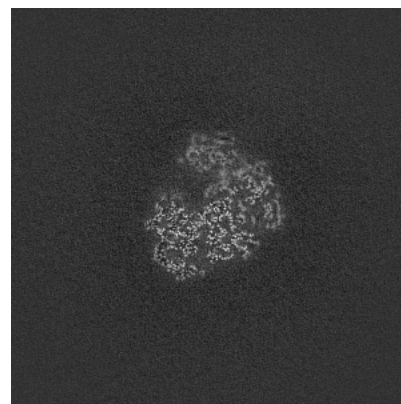
6.2.1 Primary map



X Index: 324



Y Index: 324

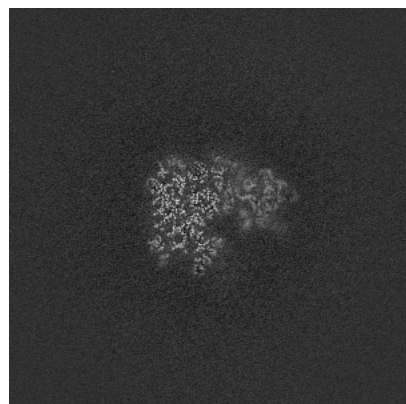


Z Index: 324

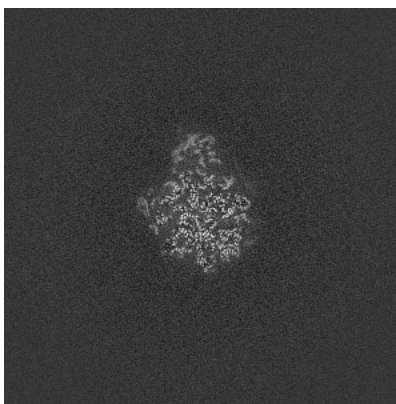
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

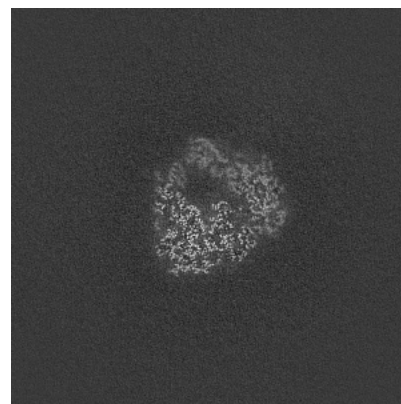
6.3.1 Primary map



X Index: 330



Y Index: 302

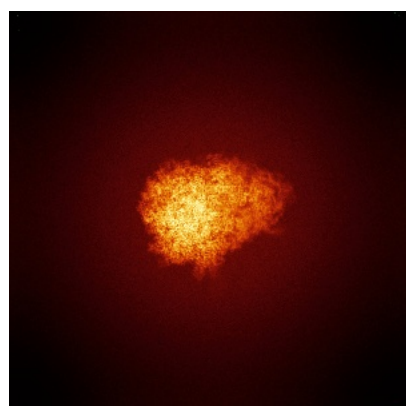


Z Index: 310

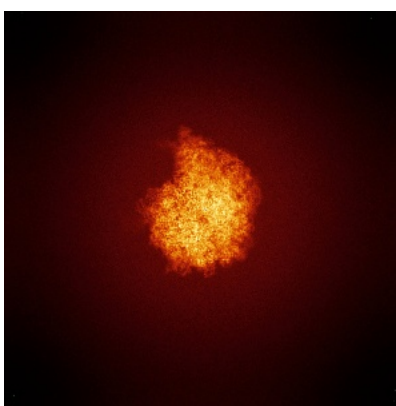
The images above show the largest variance slices of the map in three orthogonal directions.

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

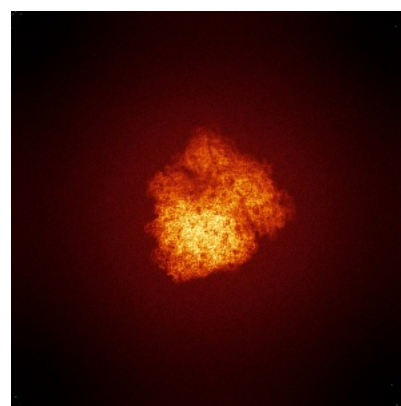
6.4.1 Primary map



X



Y

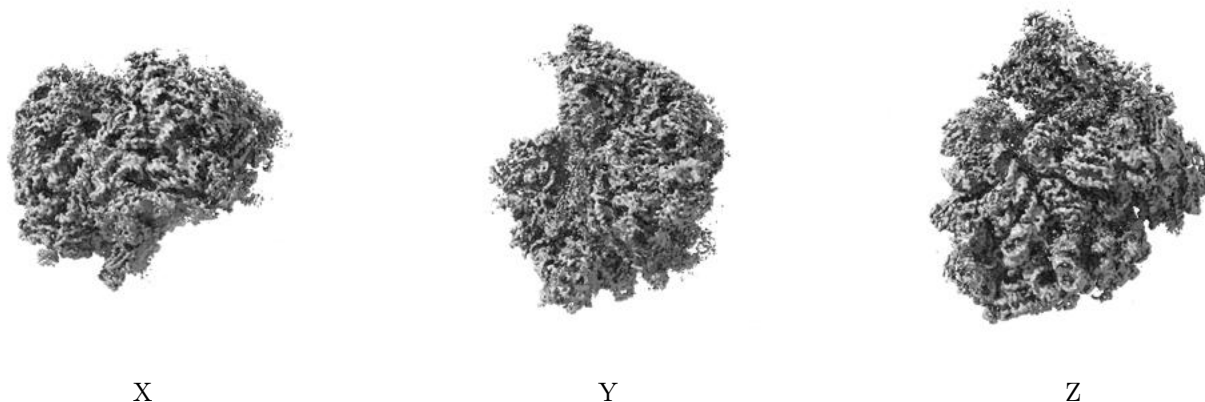


Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 7.0. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

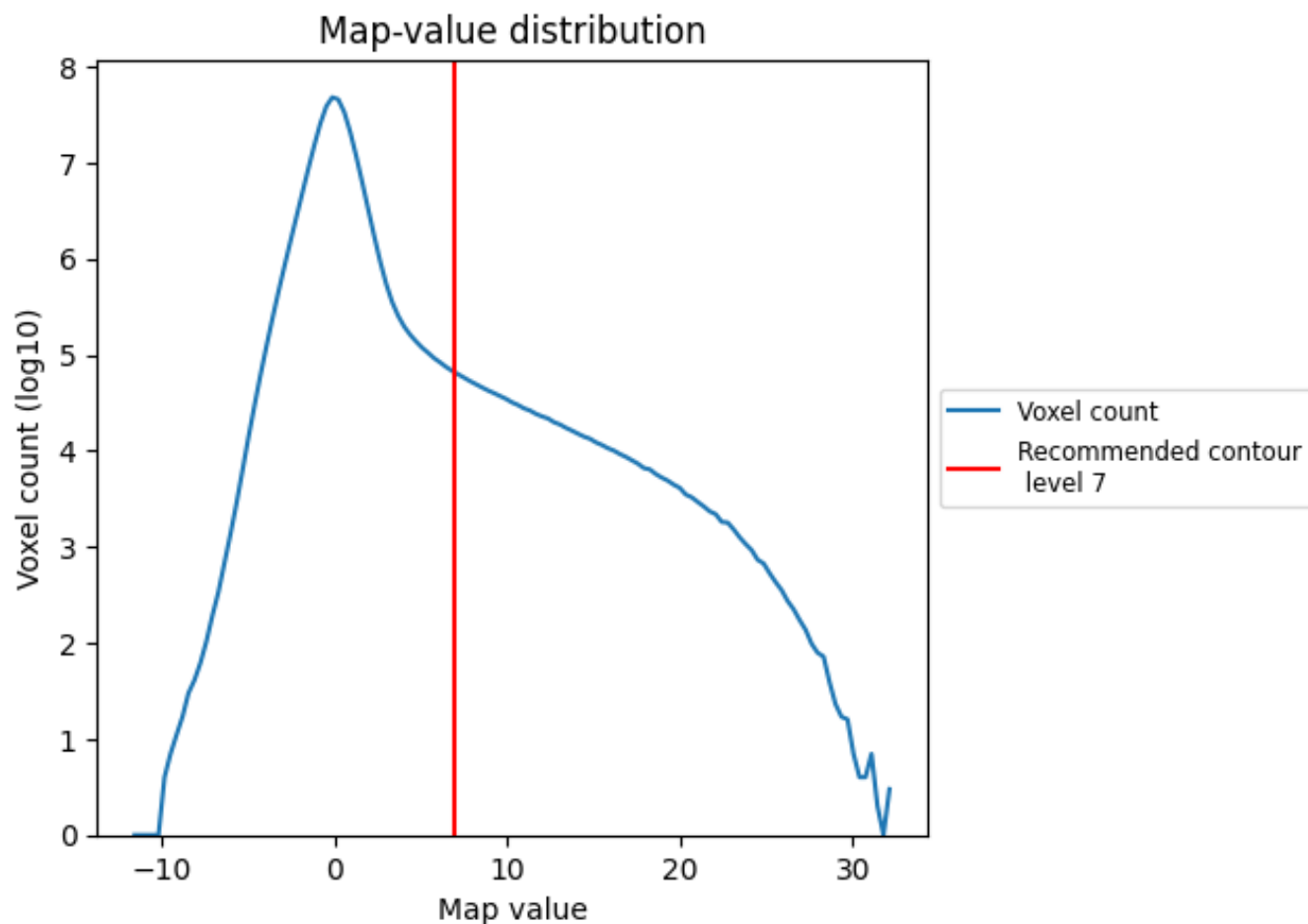
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

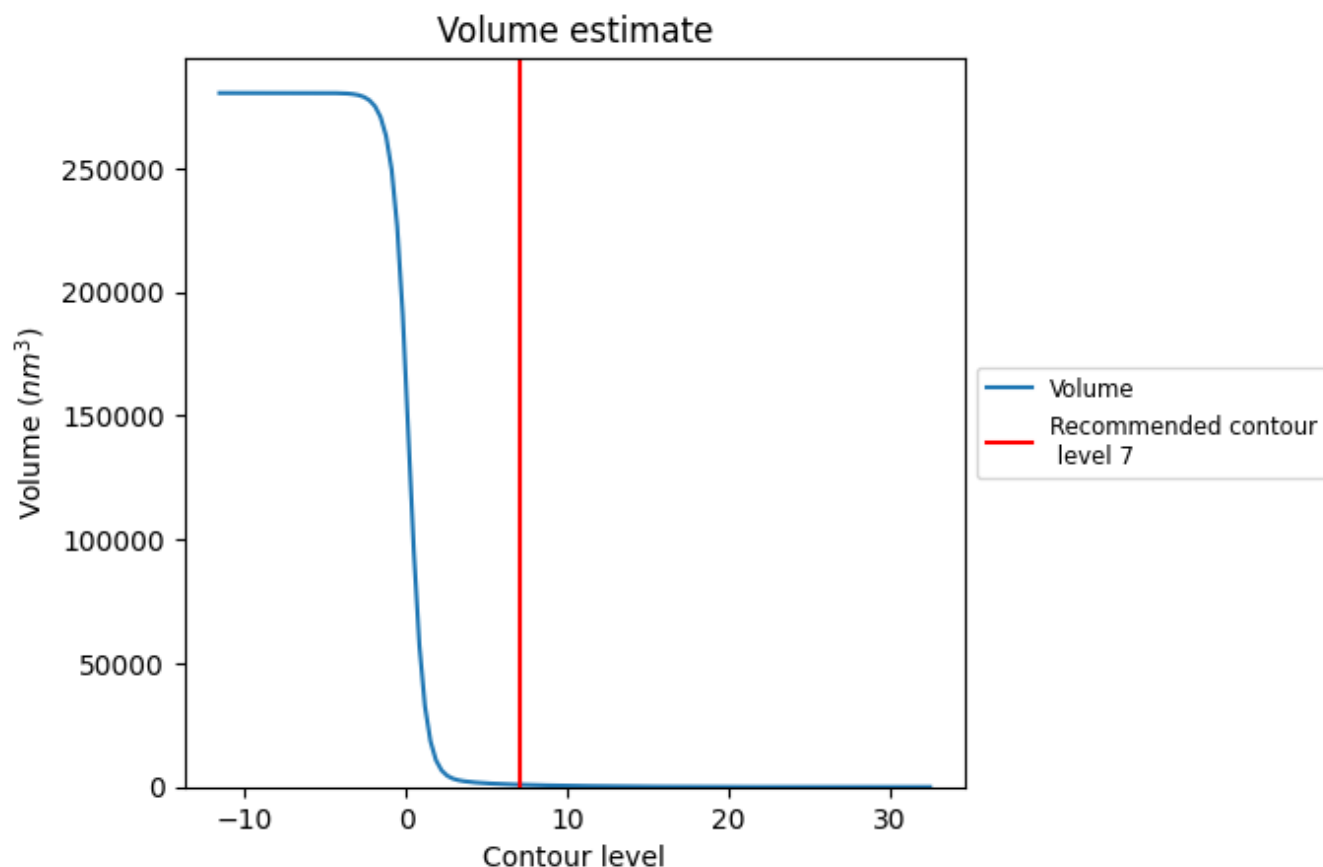
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

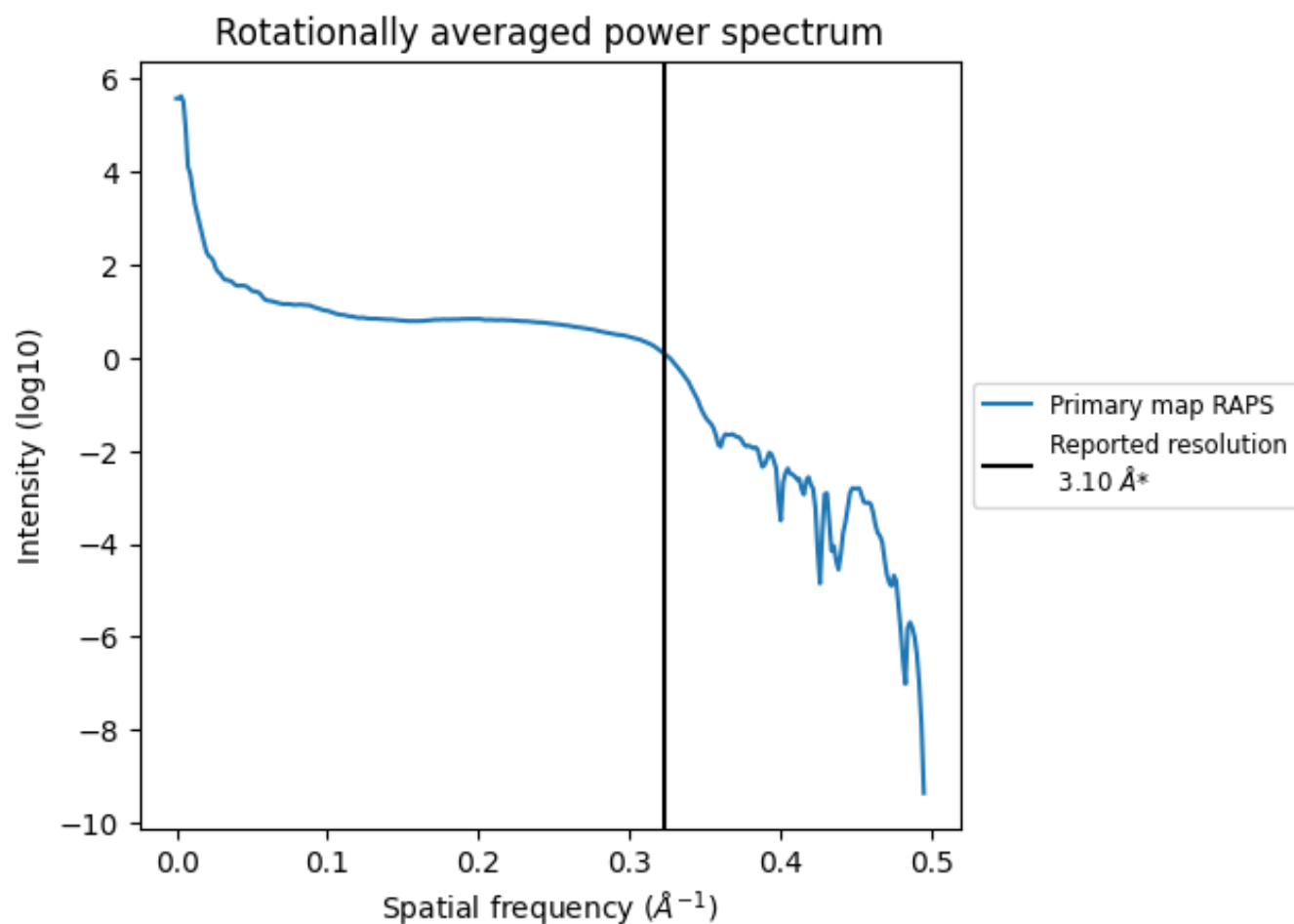
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 922 nm³; this corresponds to an approximate mass of 833 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum ⓘ

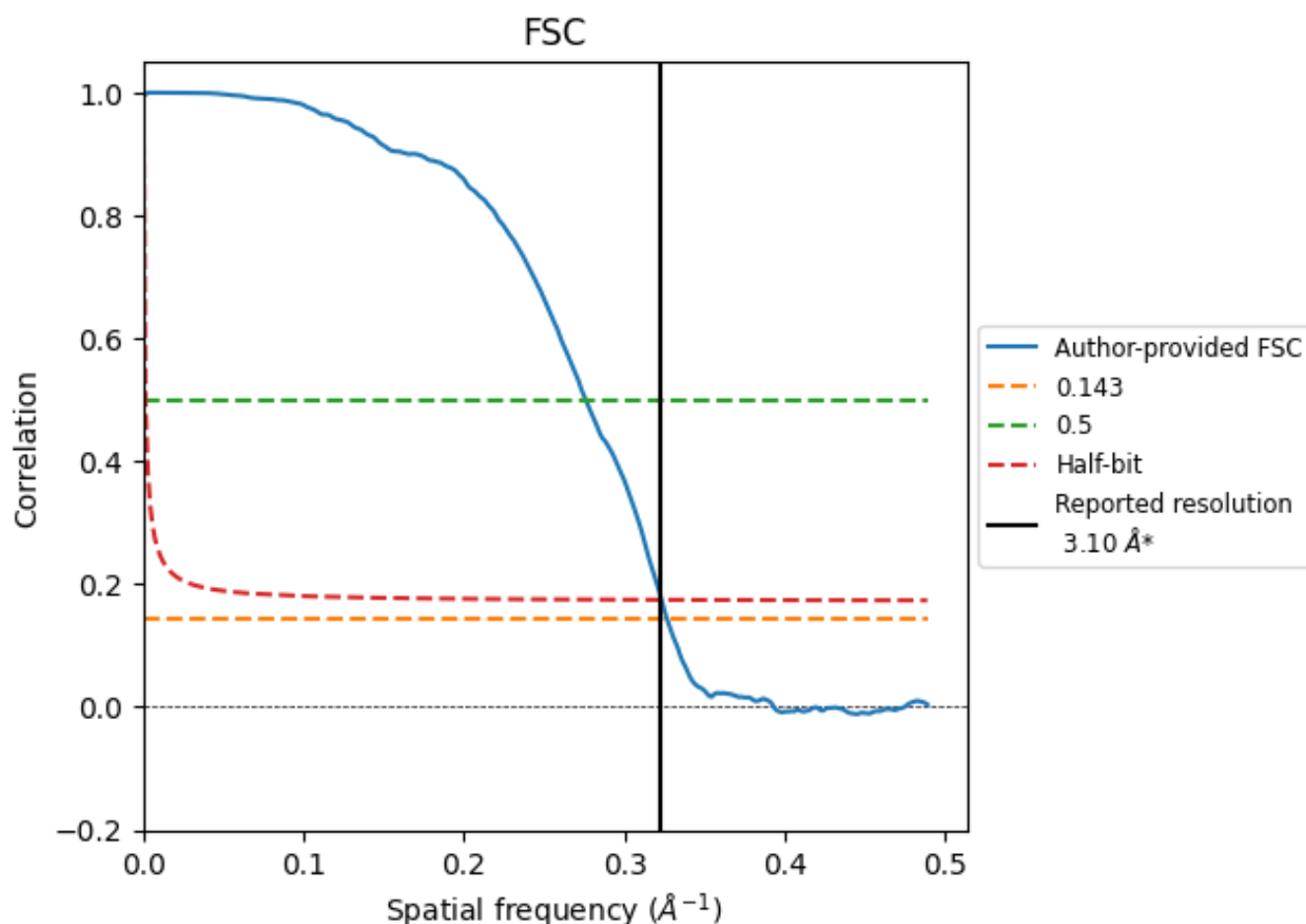


*Reported resolution corresponds to spatial frequency of 0.323 Å⁻¹

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 0.323 Å⁻¹

8.2 Resolution estimates [i](#)

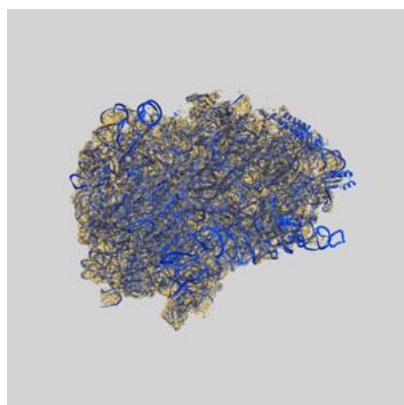
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.10	-	-
Author-provided FSC curve	3.06	3.63	3.10
Unmasked-calculated*	-	-	-

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

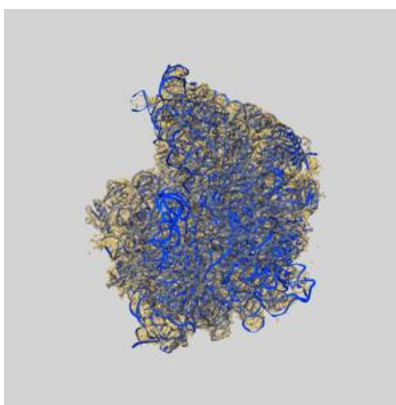
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-21420 and PDB model 6VWL. Per-residue inclusion information can be found in section [3](#) on page [14](#).

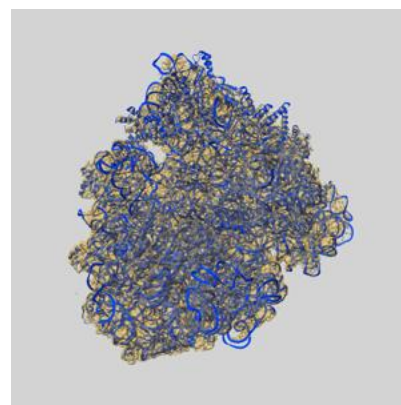
9.1 Map-model overlay [i](#)



X



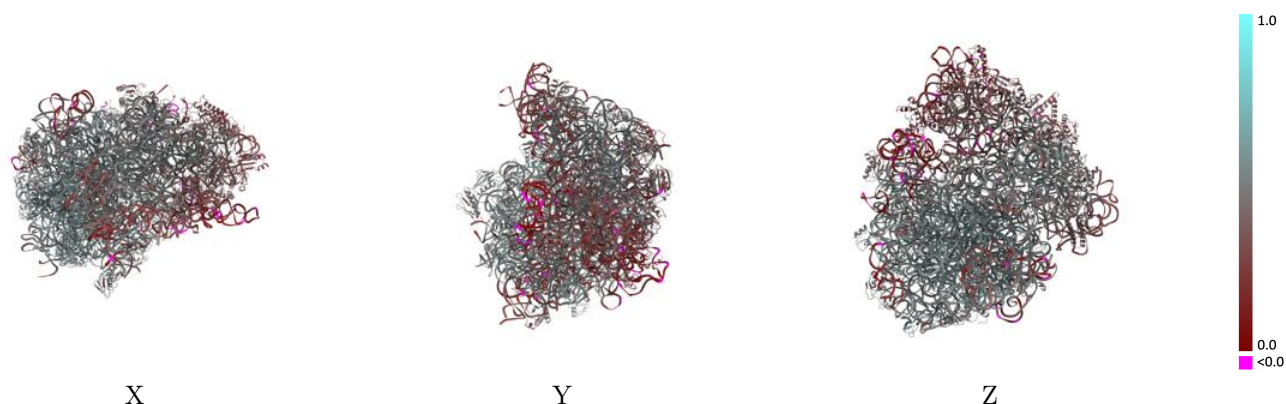
Y



Z

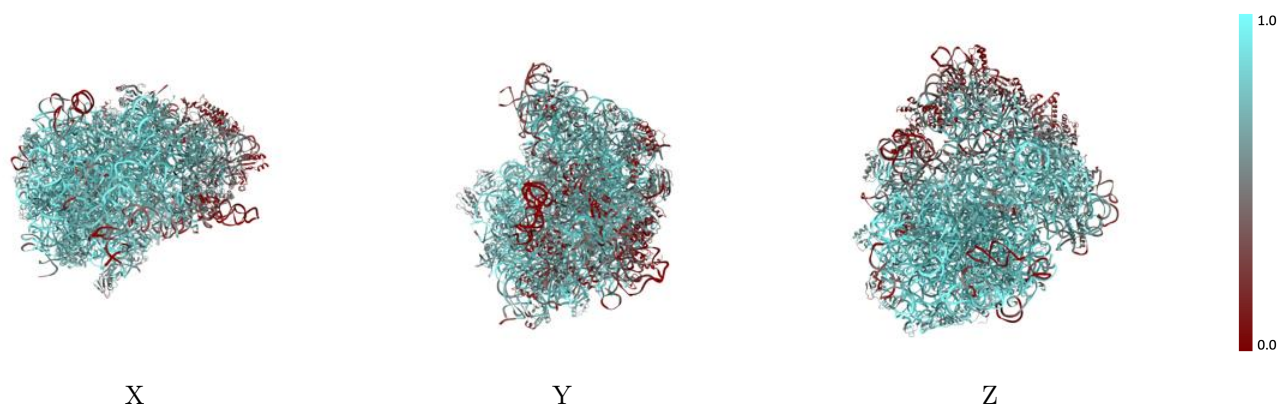
The images above show the 3D surface view of the map at the recommended contour level 7.0 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



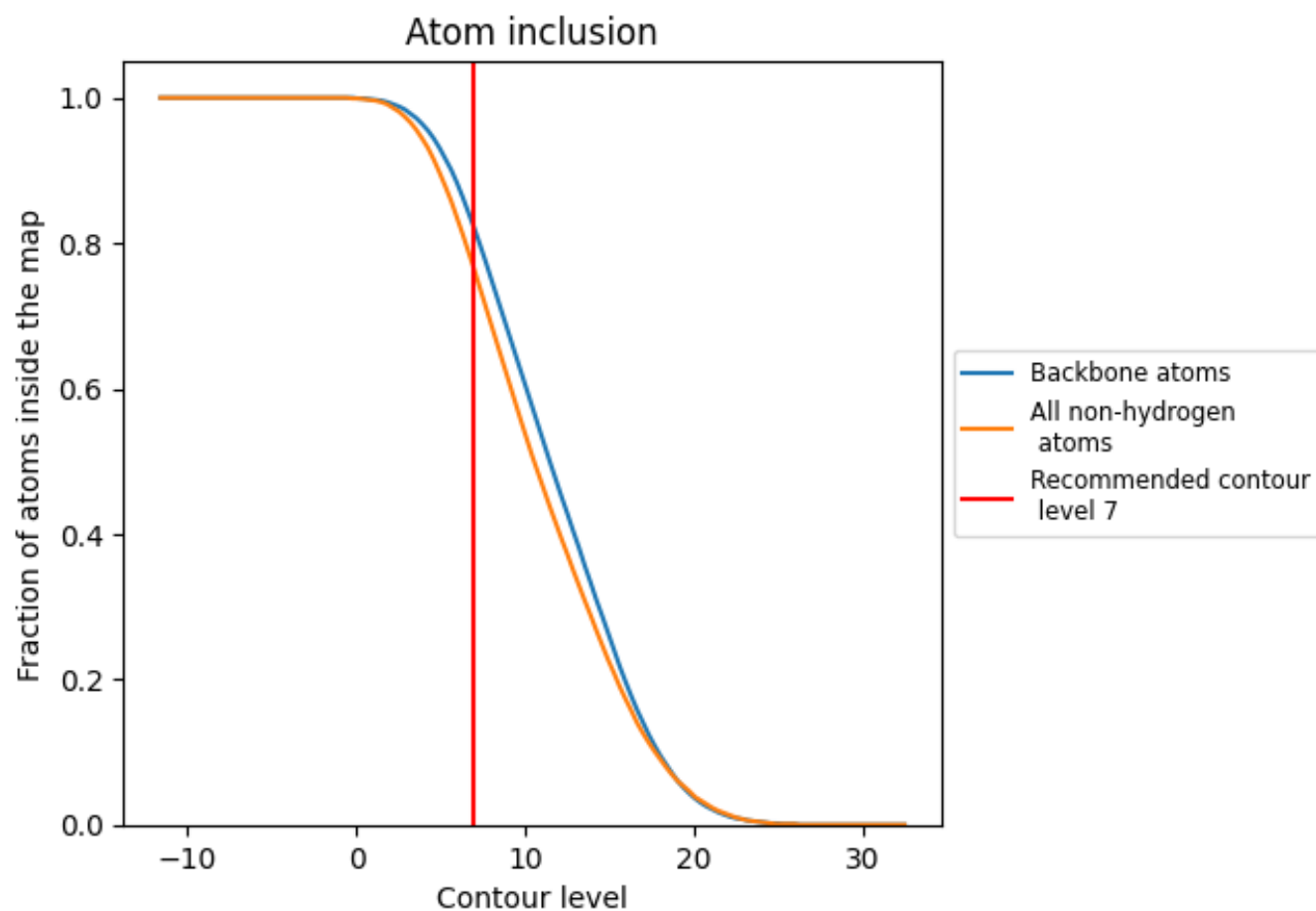
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (7).

9.4 Atom inclusion [i](#)



At the recommended contour level, 82% of all backbone atoms, 76% 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 (7) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7640	 0.4490
1	 0.7570	 0.3940
2	 0.8650	 0.4870
3	 0.7350	 0.3720
4	 0.3730	 0.1650
5	 0.6140	 0.2950
A	 0.8620	 0.5500
AA	 0.9150	 0.5670
AB	 0.9040	 0.5410
AC	 0.7940	 0.5170
B	 0.8120	 0.5450
C	 0.7380	 0.5150
D	 0.3150	 0.2980
E	 0.5810	 0.4500
F	 0.3050	 0.3900
G	 0.8290	 0.5390
I	 0.8410	 0.5410
J	 0.8110	 0.5330
K	 0.8230	 0.5240
L	 0.8680	 0.5420
M	 0.5840	 0.4020
N	 0.7800	 0.5170
O	 0.8460	 0.5440
P	 0.7380	 0.5240
Q	 0.8130	 0.5340
R	 0.7810	 0.5260
S	 0.7220	 0.5230
T	 0.6850	 0.4830
U	 0.8250	 0.5440
V	 0.8340	 0.5180
W	 0.6990	 0.4730
X	 0.7870	 0.5370
Y	 0.8250	 0.5350
Z	 0.5490	 0.4900
a	 0.3130	 0.3800



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Chain	Atom inclusion	Q-score
b	 0.4410	 0.3600
c	 0.3920	 0.3170
d	 0.6920	 0.4700
e	 0.5230	 0.4020
f	 0.2550	 0.2790
g	 0.6970	 0.4970
h	 0.3340	 0.3140
i	 0.2540	 0.3010
j	 0.6730	 0.4580
k	 0.6030	 0.4140
l	 0.3130	 0.2810
m	 0.4700	 0.3420
n	 0.6790	 0.4450
o	 0.6620	 0.4500
p	 0.6590	 0.4640
q	 0.6480	 0.4530
r	 0.2870	 0.2730
s	 0.6190	 0.3750
t	 0.5330	 0.3880