



Full wwPDB EM Validation Report ⓘ

Mar 8, 2026 – 01:47 AM UTC

PDB ID : 7QV2 / pdb_00007qv2
EMDB ID : EMD-14158
Title : Bacillus subtilis collided disome (Collided 70S)
Authors : Filbeck, S.; Pfeffer, S.
Deposited on : 2022-01-19
Resolution : 3.50 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

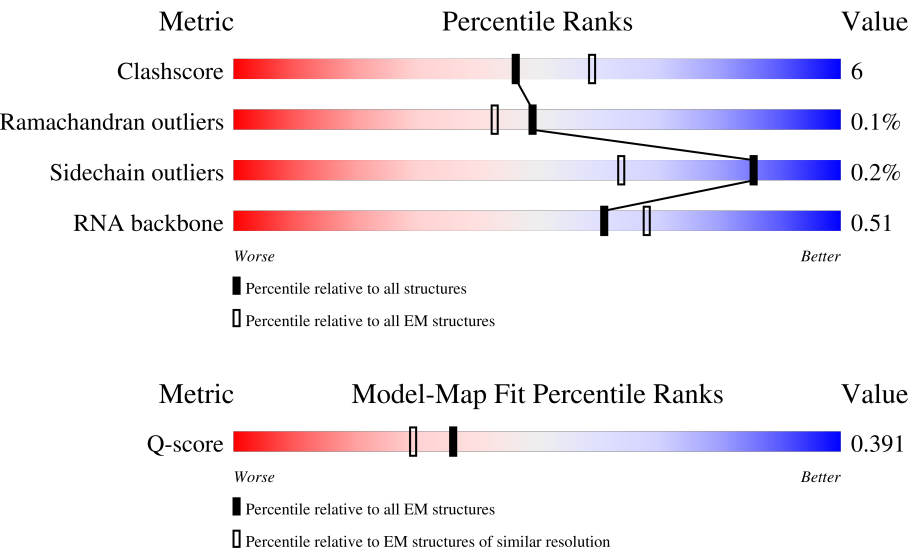
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDb archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & 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 3.50 Å.

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



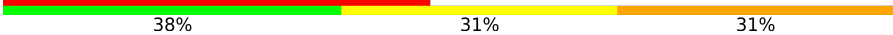
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	13950 (3.00 - 4.00)

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

Mol	Chain	Length	Quality of chain
1	0	59	
2	1	49	
3	2	44	

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Mol	Chain	Length	Quality of chain
4	3	66	
5	4	37	
6	6	66	
7	A	29	
8	B	112	
9	C	277	
10	D	209	
11	E	207	
12	F	179	
13	G	179	
14	H	77	
15	I	24	
16	J	145	
17	K	122	
18	L	146	
19	M	144	
20	N	120	
21	O	120	
22	P	115	
23	Q	119	
24	R	102	
25	S	113	
26	T	95	
27	U	103	
28	V	2928	

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Mol	Chain	Length	Quality of chain
29	W	94	
30	Y	66	
31	Z	59	
32	a	1545	
33	b	246	
34	c	218	
35	d	200	
36	e	166	
37	f	95	
38	g	156	
39	h	132	
40	i	130	
41	j	102	
42	k	131	
43	l	138	
44	m	121	
45	n	61	
46	o	89	
47	p	90	
48	q	87	
49	r	79	
50	s	92	
51	t	88	
52	u	62	
53	x	76	

2 Entry composition

There are 53 unique types of molecules in this entry. The entry contains 142856 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	0	54	Total	C	N	O	S	0	0
			426	262	86	71	7		

- Molecule 2 is a protein called 50S ribosomal protein L33 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	1	48	Total	C	N	O	S	0	0
			401	244	80	73	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	2	44	Total	C	N	O	S	0	0
			368	222	89	55	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	3	64	Total	C	N	O	S	0	0
			512	321	107	82	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
5	4	37	Total	C	N	O	S	0	0
			297	186	60	46	5		

- Molecule 6 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	6	54	Total	C	N	O	S	0	0
			413	257	73	78	5		

- Molecule 7 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	A	29	Total	C	N	O	P	0	0
			630	282	124	195	29		

- Molecule 8 is a RNA chain called 5S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	B	112	Total	C	N	O	P	0	0
			2392	1068	435	778	111		

- Molecule 9 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	C	272	Total	C	N	O	S	0	0
			2083	1296	408	373	6		

- Molecule 10 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	D	206	Total	C	N	O	S	0	0
			1569	985	289	290	5		

- Molecule 11 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	E	205	Total	C	N	O	S	0	0
			1561	980	289	290	2		

- Molecule 12 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	F	176	Total	C	N	O	S	0	0
			1386	882	241	256	7		

- Molecule 13 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	G	175	Total	C	N	O	S	0	0
			1342	835	248	257	2		

- Molecule 14 is a RNA chain called A/P-site tRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	H	77	Total	C	N	O	P	0	0
			1643	731	290	545	77		

- Molecule 15 is a protein called Nascent chain.

Mol	Chain	Residues	Atoms				AltConf	Trace
15	I	24	Total	C	N	O	0	0
			121	72	24	25		

- Molecule 16 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	J	142	Total	C	N	O	S	0	0
			1124	710	206	203	5		

- Molecule 17 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	K	122	Total	C	N	O	S	0	0
			921	571	173	173	4		

- Molecule 18 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	L	146	Total	C	N	O	S	0	0
			1082	671	207	202	2		

- Molecule 19 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	M	135	Total	C	N	O	S	0	0
			1076	690	205	176	5		

- Molecule 20 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	N	119	Total	C	N	O	S	0	0
			954	583	186	181	4		

- Molecule 21 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	O	120	Total	C	N	O	S	0	0
			913	564	176	172	1		

- Molecule 22 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	P	115	Total	C	N	O	S	0	0
			945	600	185	159	1		

- Molecule 23 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	Q	117	Total	C	N	O	S	0	0
			940	591	189	156	4		

- Molecule 24 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	R	101	Total	C	N	O		0	0
			787	501	139	147			

- Molecule 25 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	S	109	Total	C	N	O	S	0	0
			842	525	164	150	3		

- Molecule 26 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	T	90	Total	C	N	O	S	0	0
			725	452	134	136	3		

- Molecule 27 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	U	101	Total	C	N	O	S	0	0
			762	478	142	138	4		

- Molecule 28 is a RNA chain called 23S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	V	2887	Total	C	N	O	P	0	0
			61999	27661	11460	19994	2884		

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
V	243	G	A	conflict	GB 1491848961
V	325	A	-	insertion	GB 1491848961
V	326	A	-	insertion	GB 1491848961
V	327	G	-	insertion	GB 1491848961
V	328	G	-	insertion	GB 1491848961
V	640	U	C	conflict	GB 1491848961

- Molecule 29 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms				AltConf	Trace
29	W	82	Total	C	N	O	0	0
			630	390	123	117		

- Molecule 30 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	Y	65	Total	C	N	O	S	0	0
			530	328	102	98	2		

- Molecule 31 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	Z	58	Total	C	N	O	S	0	0
			456	281	89	85	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
32	a	1545	Total	C	N	O	P	0	0
			33138	14778	6072	10743	1545		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
a	1541	G	-	insertion	GB 225184640

- Molecule 33 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	b	218	Total	C	N	O	S	0	0
			1757	1119	309	323	6		

- Molecule 34 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	c	206	Total	C	N	O	S	0	0
			1619	1011	304	301	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
35	d	195	Total	C	N	O	S	0	0
			1569	991	291	285	2		

- Molecule 36 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	e	164	Total	C	N	O	S	0	0
			1219	767	225	225	2		

- Molecule 37 is a protein called 30S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	f	92	Total	C	N	O	S	0	0
			755	476	132	146	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
38	g	149	Total	C	N	O	S	0	0
			1181	740	220	215	6		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
39	h	131	Total	C	N	O	S	0	0
			1037	655	191	188	3		

- Molecule 40 is a protein called 30S ribosomal protein S9.

Mol	Chain	Residues	Atoms				AltConf	Trace
40	i	103	Total	C	N	O	0	0
			784	485	151	148		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
41	j	95	Total	C	N	O	S	0
			761	479	139	141	2	0

- Molecule 42 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms				AltConf	Trace
42	k	114	Total	C	N	O	S	0
			839	516	164	157	2	0

- Molecule 43 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues	Atoms				AltConf	Trace
43	l	136	Total	C	N	O	S	0
			1052	653	211	186	2	0

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

Mol	Chain	Residues	Atoms				AltConf	Trace
44	m	108	Total	C	N	O	0	0
			868	534	176	158		

- Molecule 45 is a protein called 30S ribosomal protein S14.

Mol	Chain	Residues	Atoms				AltConf	Trace
45	n	60	Total	C	N	O	S	0
			498	317	98	78	5	0

- Molecule 46 is a protein called 30S ribosomal protein S15.

Mol	Chain	Residues	Atoms				AltConf	Trace
46	o	85	Total	C	N	O	S	0
			710	436	144	129	1	0

- Molecule 47 is a protein called 30S ribosomal protein S16.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	p	88	Total	C	N	O	S	0	0
			695	441	128	124	2		

- Molecule 48 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	q	84	Total	C	N	O	S	0	0
			691	435	128	126	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
49	r	64	Total	C	N	O	S	0	0
			518	332	96	88	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
50	s	78	Total	C	N	O	S	0	0
			633	409	112	110	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
51	t	83	Total	C	N	O	S	0	0
			637	390	130	116	1		

- Molecule 52 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	u	58	Total	C	N	O	S	0	0
			444	275	92	75	2		

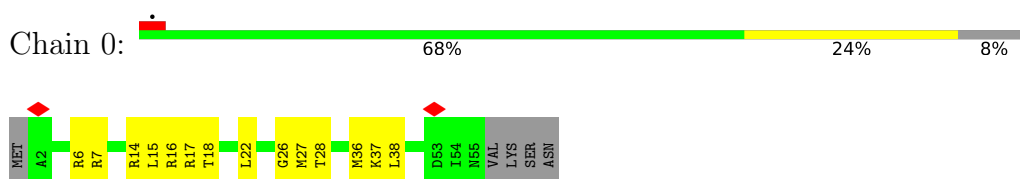
- Molecule 53 is a RNA chain called P/E-site tRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	x	76	Total	C	N	O	P	0	0
			1621	721	285	539	76		

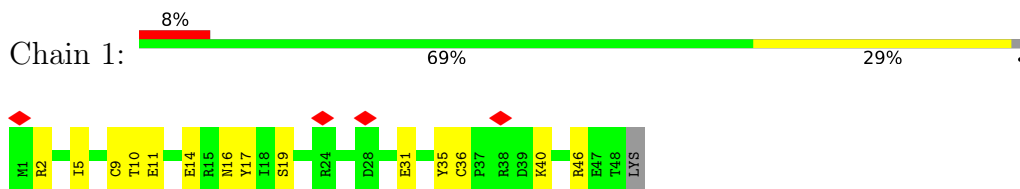
3 Residue-property plots [i](#)

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

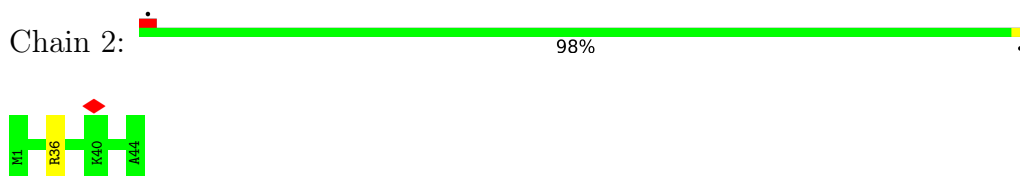
- Molecule 1: 50S ribosomal protein L32



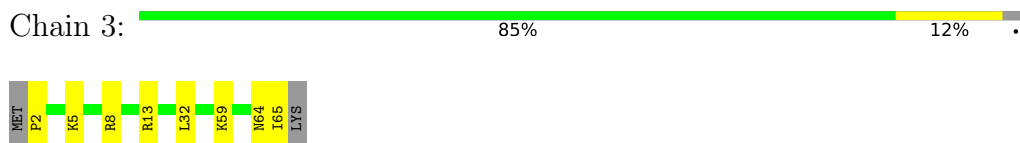
- Molecule 2: 50S ribosomal protein L33 1



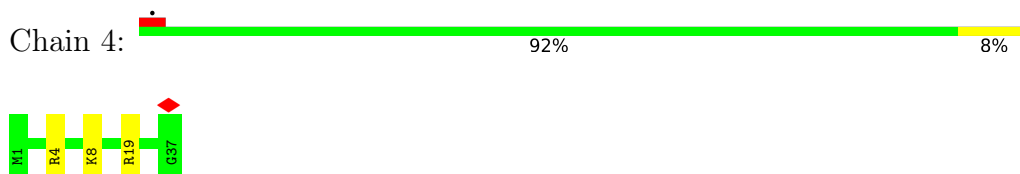
- Molecule 3: 50S ribosomal protein L34



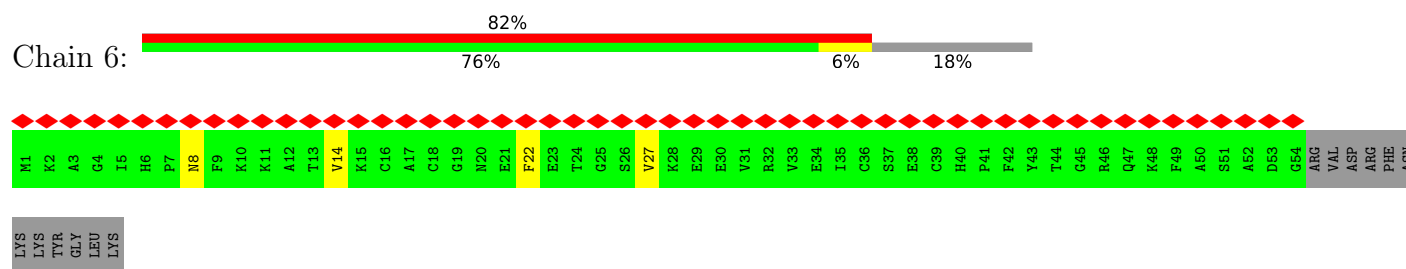
- Molecule 4: 50S ribosomal protein L35



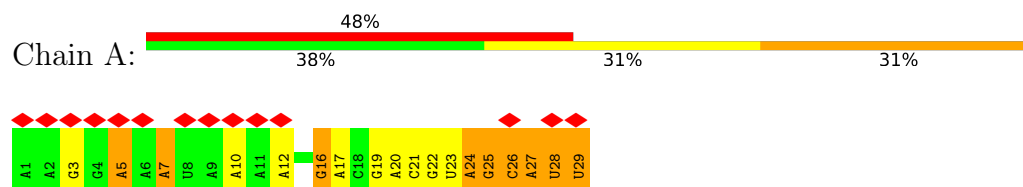
- Molecule 5: 50S ribosomal protein L36



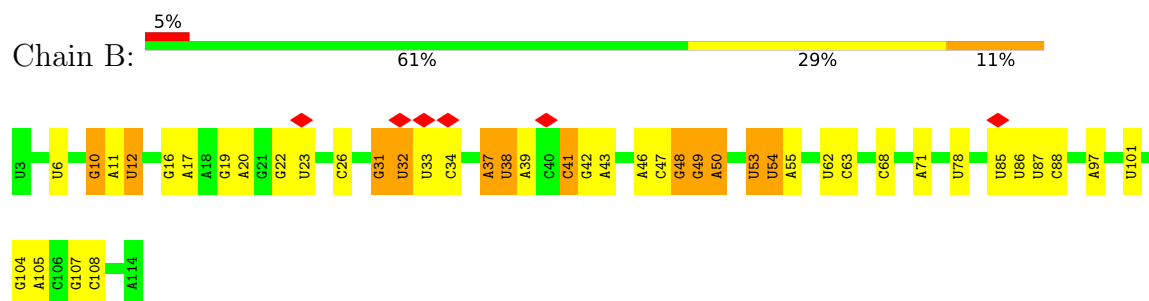
- Molecule 6: 50S ribosomal protein L31



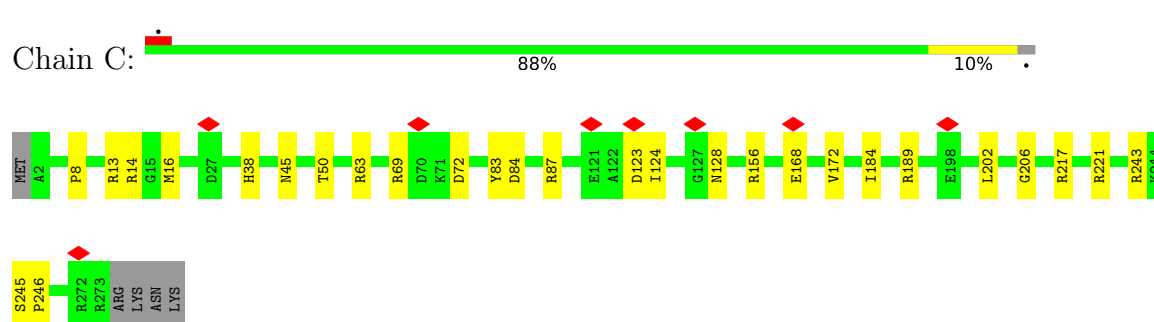
- Molecule 7: mRNA



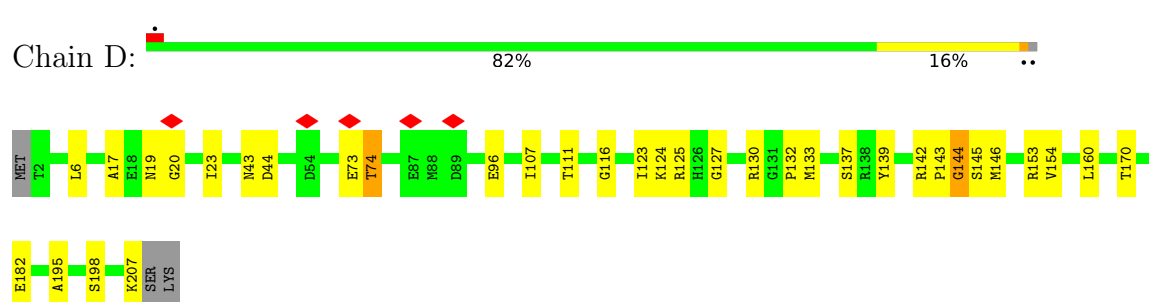
- Molecule 8: 5S ribosomal RNA



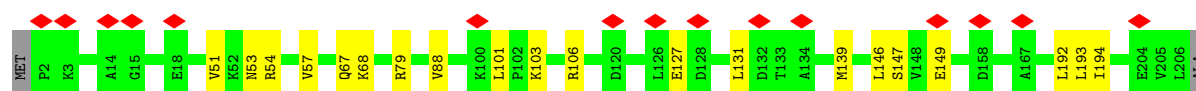
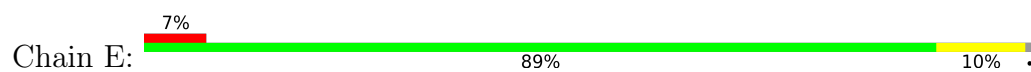
- Molecule 9: 50S ribosomal protein L2



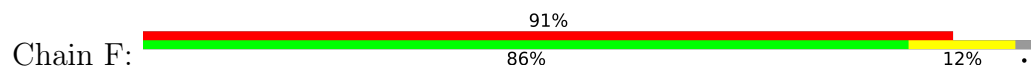
- Molecule 10: 50S ribosomal protein L3



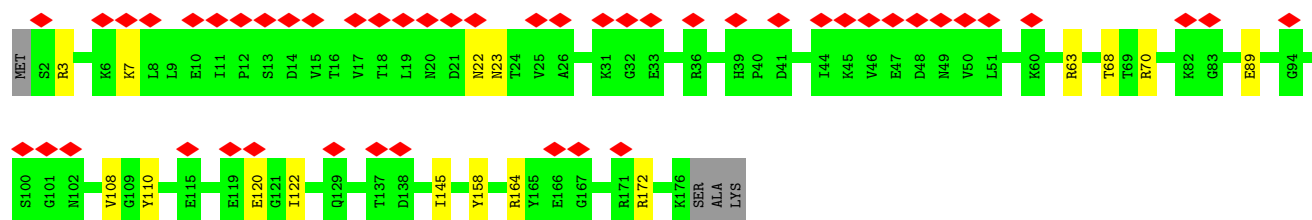
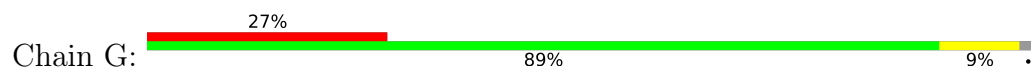
- Molecule 11: 50S ribosomal protein L4



• Molecule 12: 50S ribosomal protein L5



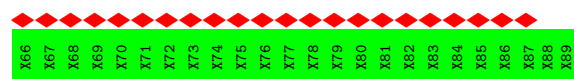
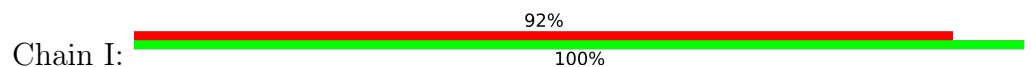
• Molecule 13: 50S ribosomal protein L6



• Molecule 14: A/P-site tRNA

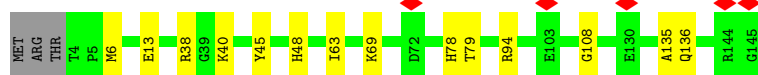


• Molecule 15: Nascent chain



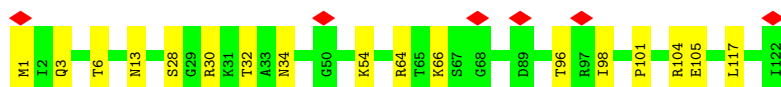
- Molecule 16: 50S ribosomal protein L13

Chain J:  88% 10%



- Molecule 17: 50S ribosomal protein L14

Chain K:  86% 14% 5%



- Molecule 18: 50S ribosomal protein L15

Chain L:  91% 9% 8%



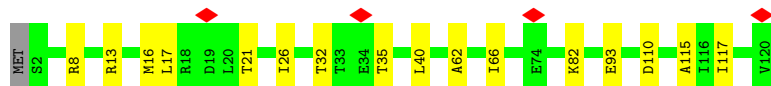
- Molecule 19: 50S ribosomal protein L16

Chain M:  87% 7% 6%



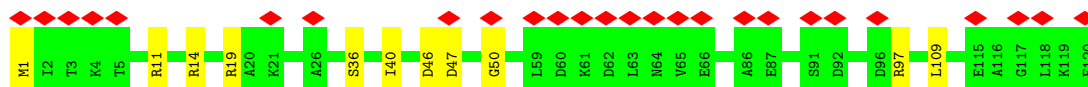
- Molecule 20: 50S ribosomal protein L17

Chain N:  86% 13%



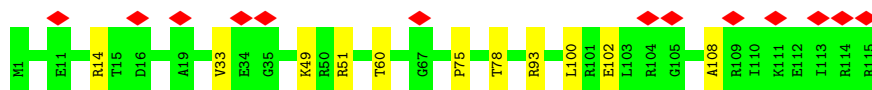
- Molecule 21: 50S ribosomal protein L18

Chain O:  91% 9% 22%

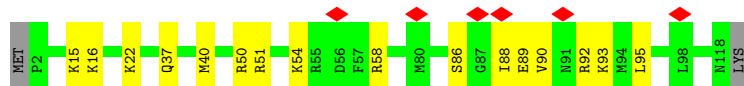
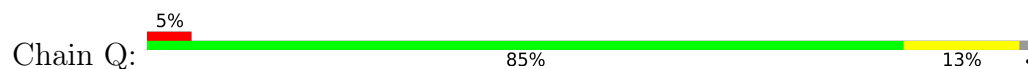


- Molecule 22: 50S ribosomal protein L19

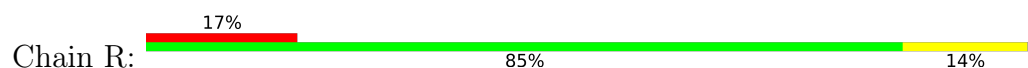
Chain P:  90% 10% 11%



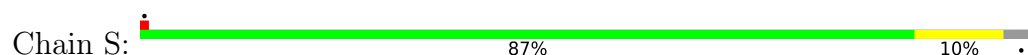
- Molecule 23: 50S ribosomal protein L20



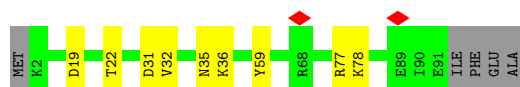
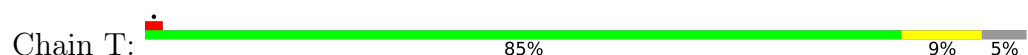
- Molecule 24: 50S ribosomal protein L21



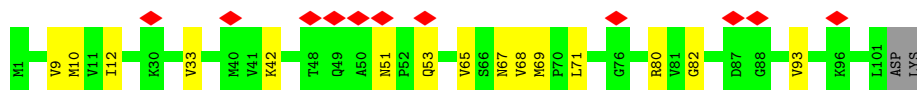
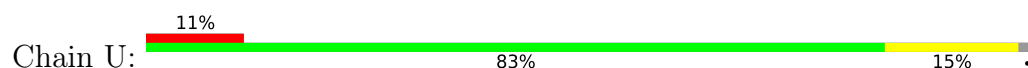
- Molecule 25: 50S ribosomal protein L22



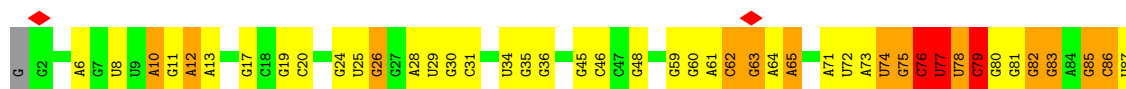
- Molecule 26: 50S ribosomal protein L23



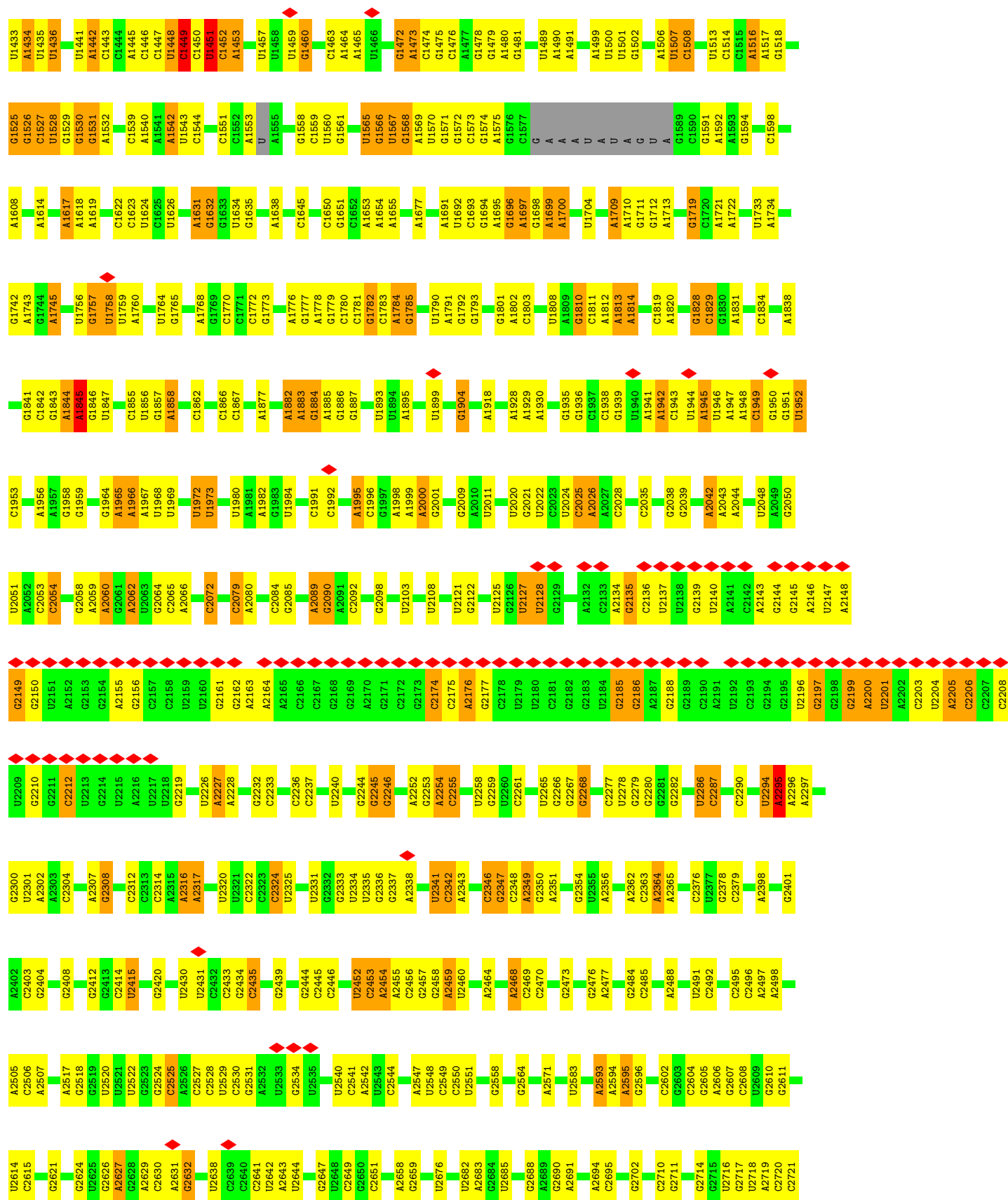
- Molecule 27: 50S ribosomal protein L24

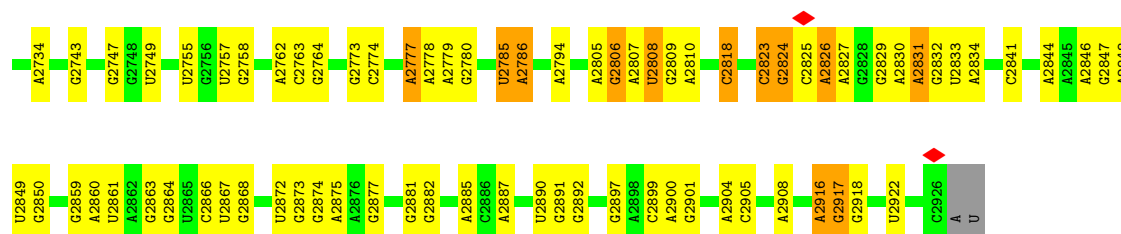


- Molecule 28: 23S ribosomal RNA

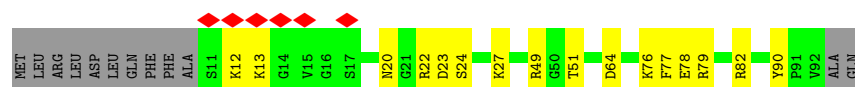




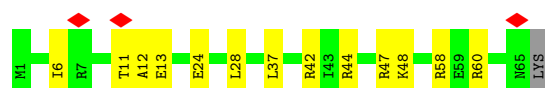
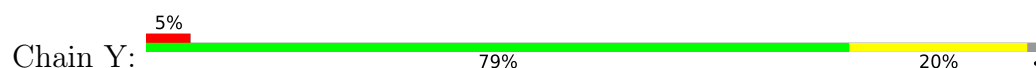




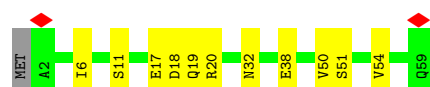
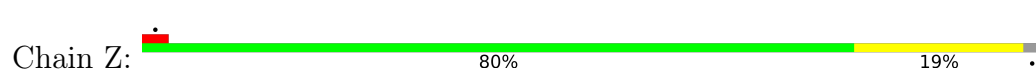
- Molecule 29: 50S ribosomal protein L27



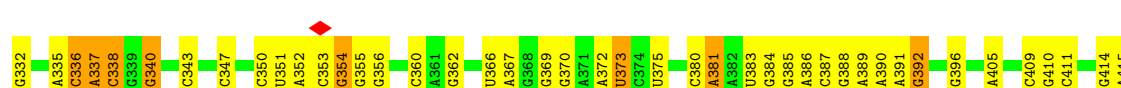
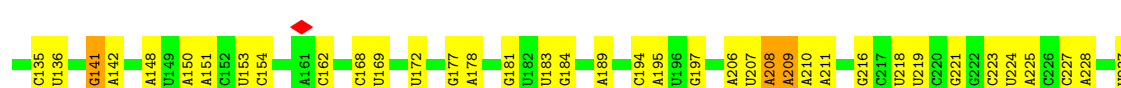
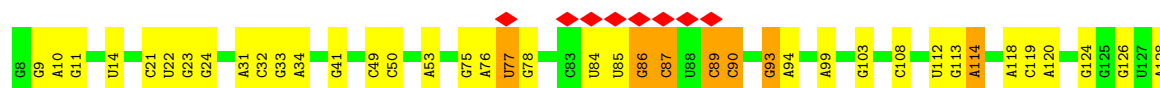
- Molecule 30: 50S ribosomal protein L29

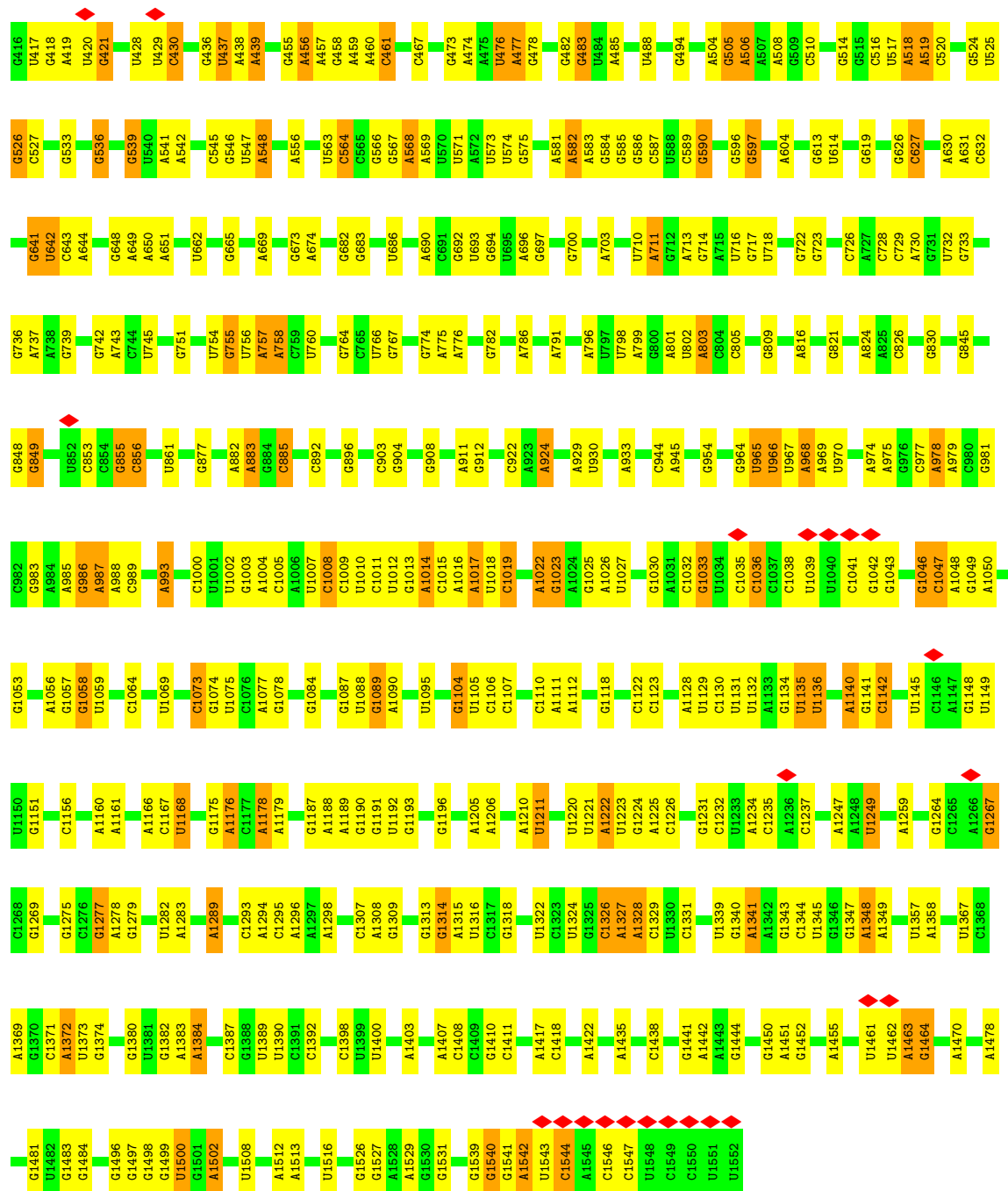


- Molecule 31: 50S ribosomal protein L30

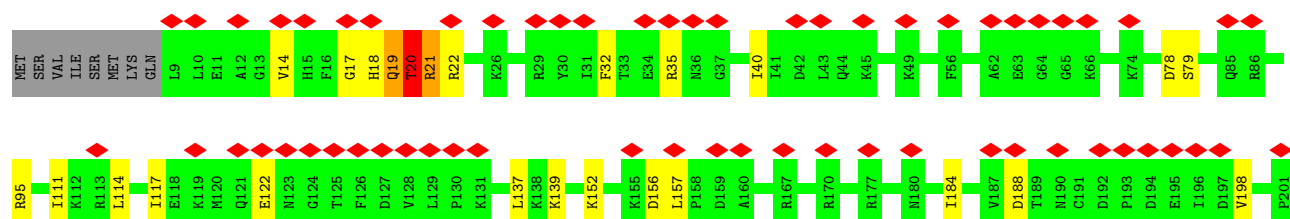
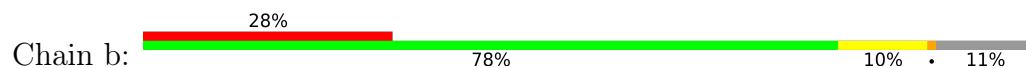


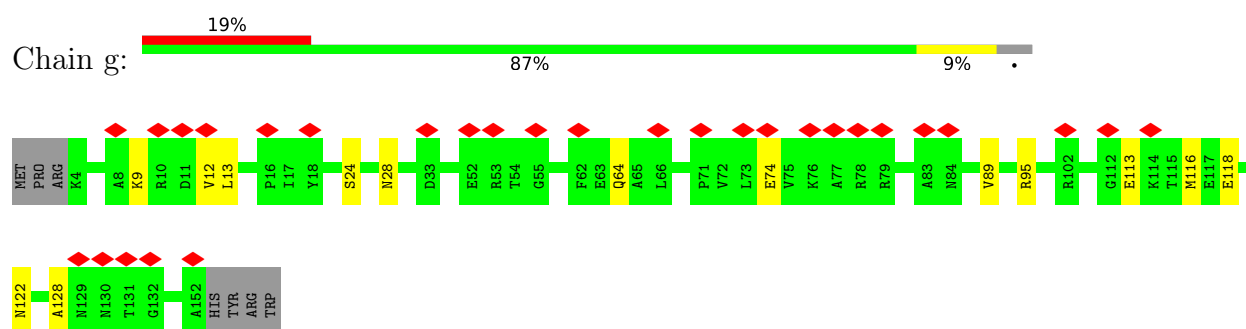
- Molecule 32: 16S ribosomal RNA



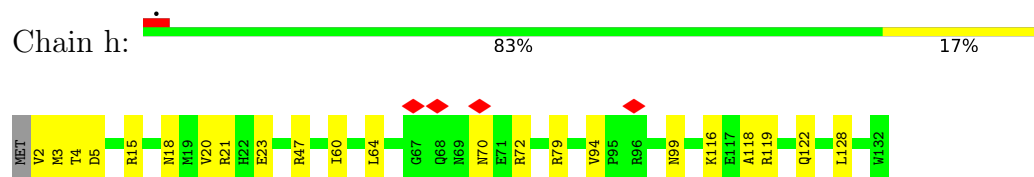


• Molecule 33: 30S ribosomal protein S2

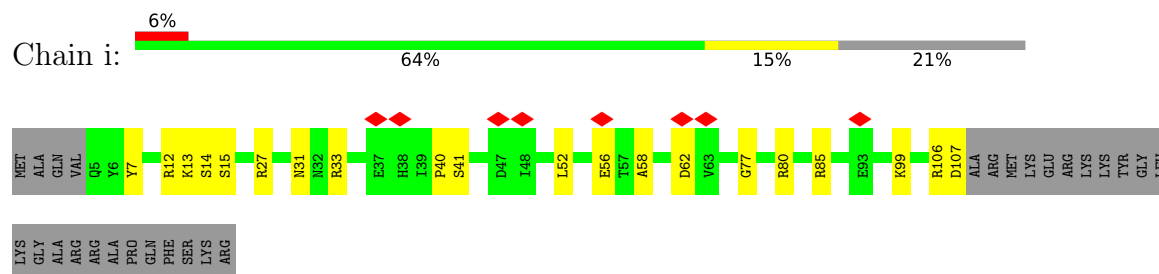




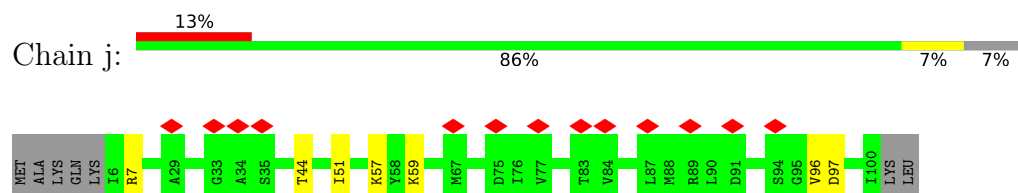
- Molecule 39: 30S ribosomal protein S8



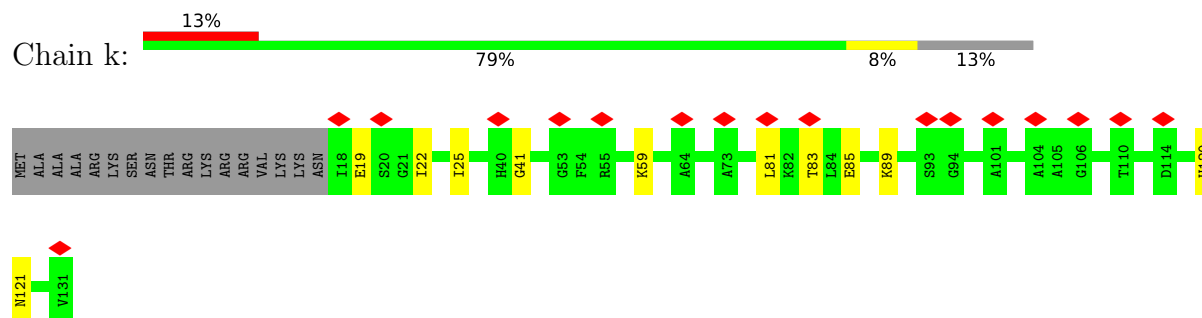
- Molecule 40: 30S ribosomal protein S9



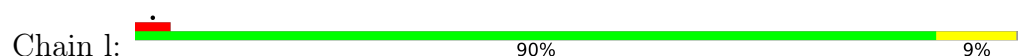
- Molecule 41: 30S ribosomal protein S10

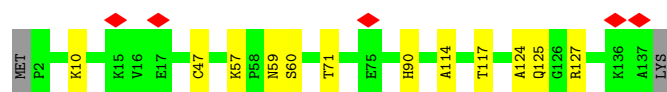


- Molecule 42: 30S ribosomal protein S11



- Molecule 43: 30S ribosomal protein S12





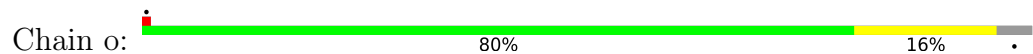
- Molecule 44: 30S ribosomal protein S13



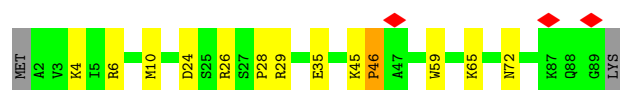
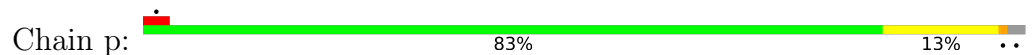
- Molecule 45: 30S ribosomal protein S14



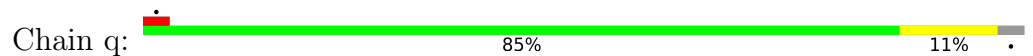
- Molecule 46: 30S ribosomal protein S15



- Molecule 47: 30S ribosomal protein S16

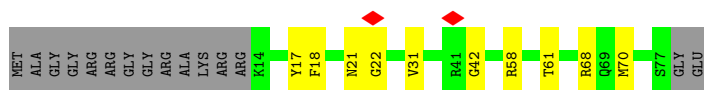


- Molecule 48: 30S ribosomal protein S17

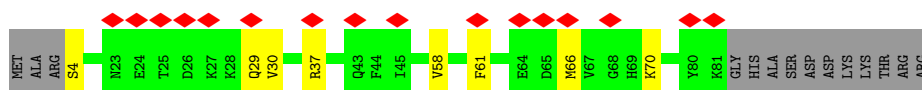
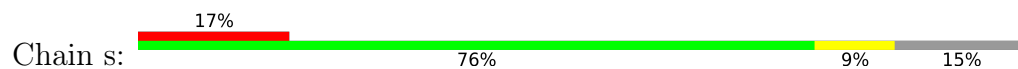


- Molecule 49: 30S ribosomal protein S18

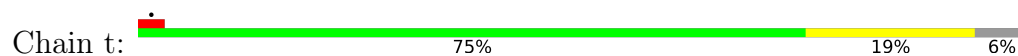




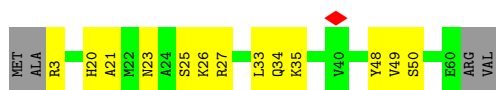
- Molecule 50: 30S ribosomal protein S19



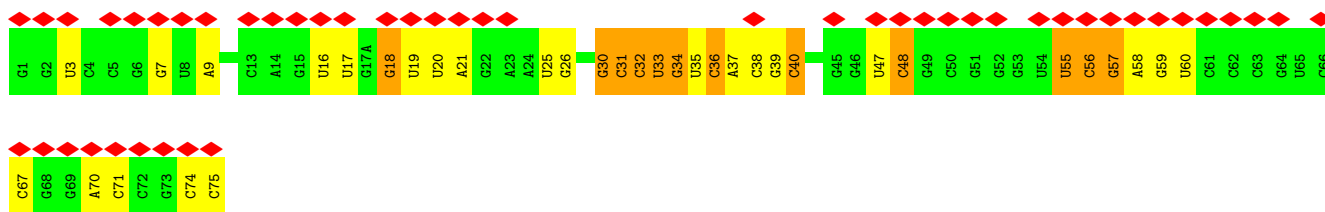
- Molecule 51: 30S ribosomal protein S20



- Molecule 52: 50S ribosomal protein L28



- Molecule 53: P/E-site tRNA



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	27833	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 ($e^-/\text{\AA}^2$)	46.5	Depositor
Minimum defocus (nm)	750	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	43.238	Depositor
Minimum map value	-15.141	Depositor
Average map value	-0.028	Depositor
Map value standard deviation	1.347	Depositor
Recommended contour level	5	Depositor
Map size ($\text{\AA}$)	590.64, 590.64, 590.64	wwPDB
Map dimensions	368, 368, 368	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.605, 1.605, 1.605	Depositor

5 Model quality

5.1 Standard geometry

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	0	0.13	0/433	0.27	0/574
2	1	0.13	0/406	0.25	0/540
3	2	0.17	0/371	0.30	0/483
4	3	0.13	0/519	0.33	0/680
5	4	0.14	0/300	0.26	0/393
6	6	0.13	0/421	0.26	0/562
7	A	0.44	0/708	0.79	3/1103 (0.3%)
8	B	0.08	0/2675	0.24	0/4170
9	C	0.12	0/2120	0.29	0/2845
10	D	0.26	0/1591	0.38	1/2132 (0.0%)
11	E	0.12	0/1580	0.28	0/2132
12	F	0.13	0/1405	0.31	0/1887
13	G	0.10	0/1360	0.25	0/1832
14	H	0.11	0/1834	0.30	0/2858
16	J	0.12	0/1147	0.28	0/1542
17	K	0.14	0/928	0.28	0/1245
18	L	0.13	0/1094	0.27	0/1457
19	M	0.13	0/1099	0.25	0/1468
20	N	0.13	0/961	0.29	0/1284
21	O	0.11	0/922	0.25	0/1236
22	P	0.15	0/958	0.31	0/1279
23	Q	0.14	0/952	0.31	0/1266
24	R	0.12	0/798	0.30	0/1070
25	S	0.13	0/851	0.30	0/1146
26	T	0.13	0/731	0.27	0/974
27	U	0.13	0/772	0.27	0/1032
28	V	0.12	0/69445	0.27	24/108336 (0.0%)
29	W	0.29	0/638	0.53	0/847
30	Y	0.14	0/531	0.28	0/707
31	Z	0.11	0/458	0.28	0/613
32	a	0.09	0/37100	0.22	0/57875
33	b	0.14	0/1782	0.36	0/2392
34	c	0.13	0/1641	0.27	0/2208
35	d	0.12	0/1599	0.31	0/2147

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
36	e	0.13	0/1231	0.29	0/1655
37	f	0.09	0/766	0.25	0/1031
38	g	0.11	0/1196	0.28	0/1604
39	h	0.13	0/1049	0.29	0/1407
40	i	0.13	0/794	0.30	0/1074
41	j	0.12	0/773	0.29	0/1044
42	k	0.11	0/853	0.32	0/1153
43	l	0.13	0/1069	0.31	0/1435
44	m	0.14	0/873	0.36	0/1166
45	n	0.15	0/508	0.37	0/672
46	o	0.12	0/718	0.26	0/960
47	p	0.12	0/708	0.30	0/950
48	q	0.11	0/699	0.26	0/933
49	r	0.12	0/526	0.32	0/705
50	s	0.10	0/649	0.23	0/872
51	t	0.12	0/639	0.28	0/852
52	u	0.13	0/448	0.31	0/596
53	x	0.09	0/1809	0.24	0/2819
All	All	0.12	0/155438	0.27	28/233243 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
33	b	0	1

There are no bond length outliers.

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A	21	C	P-O3'-C3'	-10.06	105.11	120.20
28	V	181	G	P-O3'-C3'	-8.13	108.00	120.20
28	V	76	C	P-O3'-C3'	-8.07	108.10	120.20
7	A	27	A	P-O3'-C3'	-7.39	109.12	120.20
28	V	1842	C	P-O3'-C3'	-7.34	109.19	120.20
28	V	1844	A	P-O3'-C3'	-6.94	109.79	120.20
28	V	1449	C	P-O3'-C3'	-6.64	110.25	120.20
28	V	182	C	P-O3'-C3'	-6.49	110.47	120.20
28	V	1452	C	P-O3'-C3'	-6.37	110.64	120.20
28	V	74	U	P-O3'-C3'	-6.10	111.05	120.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	V	79	C	P-O3'-C3'	-6.05	111.12	120.20
10	D	144	GLY	CA-C-O	-6.04	118.11	122.45
28	V	78	U	P-O3'-C3'	-5.89	111.37	120.20
28	V	1845	A	P-O3'-C3'	-5.86	111.41	120.20
7	A	25	G	P-O3'-C3'	-5.84	111.43	120.20
28	V	254	A	P-O3'-C3'	-5.73	111.61	120.20
28	V	183	A	P-O3'-C3'	-5.72	111.62	120.20
28	V	958	A	P-O3'-C3'	-5.54	111.90	120.20
28	V	2295	A	C4'-C3'-O3'	5.53	117.70	109.40
28	V	184	G	P-O3'-C3'	-5.48	111.98	120.20
28	V	1450	C	P-O3'-C3'	-5.45	112.02	120.20
28	V	955	C	P-O3'-C3'	-5.43	112.05	120.20
28	V	125	A	P-O3'-C3'	-5.30	112.25	120.20
28	V	77	U	P-O3'-C3'	-5.28	112.28	120.20
28	V	2294	U	P-O3'-C3'	-5.27	112.30	120.20
28	V	956	A	P-O3'-C3'	-5.18	112.43	120.20
28	V	1451	U	P-O3'-C3'	-5.13	112.51	120.20
28	V	253	G	P-O3'-C3'	-5.02	112.67	120.20

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
33	b	20	THR	Peptide

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	0	426	0	445	11	0
2	1	401	0	413	9	0
3	2	368	0	410	1	0
4	3	512	0	564	8	0
5	4	297	0	342	3	0
6	6	413	0	402	4	0
7	A	630	0	315	10	0
8	B	2392	0	1213	23	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	C	2083	0	2168	28	0
10	D	1569	0	1637	30	0
11	E	1561	0	1647	17	0
12	F	1386	0	1446	20	0
13	G	1342	0	1388	12	0
14	H	1643	0	831	29	0
15	I	121	0	26	0	0
16	J	1124	0	1162	11	0
17	K	921	0	977	14	0
18	L	1082	0	1132	11	0
19	M	1076	0	1145	9	0
20	N	954	0	983	10	0
21	O	913	0	947	9	0
22	P	945	0	1020	9	0
23	Q	940	0	1005	18	0
24	R	787	0	826	9	0
25	S	842	0	899	9	0
26	T	725	0	770	6	0
27	U	762	0	821	16	0
28	V	61999	0	31209	623	0
29	W	630	0	644	17	0
30	Y	530	0	568	9	0
31	Z	456	0	491	6	0
32	a	33138	0	16687	342	0
33	b	1757	0	1830	18	0
34	c	1619	0	1658	17	0
35	d	1569	0	1604	20	0
36	e	1219	0	1300	19	0
37	f	755	0	746	7	0
38	g	1181	0	1235	9	0
39	h	1037	0	1095	15	0
40	i	784	0	803	13	0
41	j	761	0	795	7	0
42	k	839	0	854	8	0
43	l	1052	0	1112	10	0
44	m	868	0	925	19	0
45	n	498	0	533	11	0
46	o	710	0	735	10	0
47	p	695	0	721	9	0
48	q	691	0	728	11	0
49	r	518	0	555	7	0
50	s	633	0	649	8	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
51	t	637	0	696	13	0
52	u	444	0	487	10	0
53	x	1621	0	820	20	0
All	All	142856	0	94414	1366	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 6.

All (1366) 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)
28:V:1243:A:O2'	28:V:1244:A:OP1	1.83	0.94
32:a:1175:G:O2'	32:a:1176:A:OP1	1.85	0.93
28:V:310:C:O2	28:V:406:G:N2	2.02	0.93
28:V:688:G:H21	28:V:692:A:H62	1.13	0.92
28:V:688:G:O2'	28:V:2378:G:O2'	1.90	0.90
32:a:455:G:O2'	32:a:456:A:O5'	1.91	0.89
51:t:61:ALA:O	51:t:64:THR:OG1	1.90	0.89
32:a:1038:C:O2	32:a:1043:G:N2	2.07	0.88
32:a:582:A:O2'	32:a:583:A:O4'	1.92	0.88
32:a:1156:C:HO2'	40:i:7:TYR:HH	1.16	0.88
8:B:37:A:O2'	8:B:38:U:O5'	1.92	0.86
32:a:1348:A:N6	53:x:31:C:OP1	2.07	0.86
32:a:518:A:O2'	32:a:519:A:O5'	1.92	0.86
32:a:1543:U:O2'	32:a:1544:C:OP1	1.92	0.86
28:V:2144:G:N2	28:V:2148:A:OP1	2.09	0.86
32:a:968:A:O2'	32:a:969:A:O4'	1.93	0.85
32:a:1032:C:O2'	32:a:1033:G:OP1	1.94	0.85
28:V:2072:C:OP1	28:V:2806:G:O2'	1.95	0.85
28:V:2825:C:N3	28:V:2826:A:N6	2.25	0.85
14:H:41:A:O2'	14:H:42:G:O4'	1.95	0.84
28:V:1866:C:O2'	28:V:1956:A:N3	2.10	0.84
14:H:8:U:O2'	14:H:21:A:N1	2.10	0.84
32:a:207:U:O2'	32:a:208:A:OP1	1.94	0.83
8:B:47:C:N4	8:B:48:G:O6	2.12	0.83
49:r:42:GLY:O	49:r:68:ARG:NH2	2.12	0.83
32:a:1348:A:O2'	53:x:40:C:O2	1.95	0.82
32:a:547:U:O2'	32:a:548:A:OP1	1.96	0.82
28:V:2261:C:OP2	52:u:27:ARG:NH2	2.12	0.82
28:V:2092:C:N4	28:V:2530:C:O2	2.12	0.82
14:H:17(A):G:O2'	14:H:18:G:OP1	1.97	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:a:10:A:N6	35:d:196:GLU:O	2.13	0.81
32:a:1005:C:N3	32:a:1056:A:O2'	2.13	0.81
28:V:458:G:OP2	28:V:2435:C:O2'	1.98	0.81
32:a:641:G:O2'	32:a:642:U:OP1	1.96	0.81
32:a:1275:G:N2	32:a:1278:A:OP2	2.13	0.81
32:a:1542:A:O2'	32:a:1543:U:O4'	1.98	0.81
29:W:78:GLU:HG2	29:W:79:ARG:H	1.45	0.81
32:a:1089:G:O2'	32:a:1090:A:O4'	1.97	0.81
28:V:1216:C:O2	28:V:1220:G:N2	2.10	0.81
28:V:280:G:N2	28:V:291:C:O2	2.09	0.81
23:Q:92:ARG:NH2	28:V:1042:A:O3'	2.13	0.80
28:V:2540:U:O4	28:V:2604:C:N3	2.14	0.80
14:H:40:C:O2'	14:H:41:A:OP1	1.98	0.80
28:V:1171:G:OP2	28:V:1172:A:O2'	1.98	0.80
5:4:19:ARG:NE	28:V:2785:U:OP2	2.15	0.80
18:L:38:GLN:OE1	28:V:878:G:O2'	1.99	0.80
18:L:55:MET:O	18:L:60:ARG:NH2	2.15	0.80
28:V:2890:U:OP2	28:V:2891:G:O2'	2.00	0.80
53:x:18:G:O2'	53:x:57:G:N2	2.14	0.80
53:x:33:U:O2'	53:x:34:G:OP1	2.00	0.80
28:V:2135:G:N2	28:V:2212:C:O2	2.15	0.79
32:a:1187:G:OP2	40:i:99:LYS:NZ	2.15	0.79
32:a:1142:C:O2	32:a:1151:G:N2	2.15	0.79
32:a:516:C:OP2	32:a:517:U:O2'	1.99	0.79
28:V:1036:A:O2'	28:V:1037:C:OP1	1.99	0.79
28:V:2060:A:N3	28:V:2484:G:O2'	2.15	0.79
44:m:85:SER:O	44:m:88:GLY:N	2.15	0.79
19:M:80:GLU:O	29:W:13:LYS:NZ	2.16	0.79
32:a:1056:A:N6	32:a:1220:U:O2	2.16	0.78
32:a:22:U:O2'	32:a:582:A:N6	2.16	0.78
14:H:16:U:O2'	14:H:60:U:O3'	2.00	0.78
32:a:1541:G:O2'	32:a:1542:A:O5'	2.02	0.78
32:a:1462:U:O2'	32:a:1463:A:OP1	2.02	0.78
53:x:30:G:O6	53:x:40:C:N4	2.14	0.78
28:V:1177:G:O2'	28:V:2054:C:O2'	2.02	0.78
9:C:72:ASP:OD2	9:C:189:ARG:NH2	2.17	0.77
39:h:47:ARG:NH1	39:h:64:LEU:O	2.17	0.77
28:V:619:A:OP2	28:V:2528:C:O2'	2.01	0.77
28:V:1027:A:HO2'	28:V:2065:C:HO2'	1.33	0.77
32:a:757:A:O2'	32:a:758:A:O5'	2.02	0.77
32:a:567:G:OP2	32:a:568:A:O2'	2.03	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:V:2874:G:O3'	28:V:2891:G:N2	2.18	0.77
32:a:729:C:O2'	49:r:61:THR:HG21	1.85	0.76
9:C:69:ARG:O	9:C:189:ARG:NH1	2.19	0.76
28:V:2287:C:O2'	28:V:2456:C:OP2	2.02	0.76
33:b:17:GLY:O	33:b:18:HIS:ND1	2.18	0.76
28:V:2605:G:O2'	28:V:2608:C:OP2	2.04	0.76
32:a:1122:C:O2'	34:c:178:ARG:NH1	2.18	0.76
14:H:75:C:O2'	14:H:76:A:O4'	2.01	0.76
28:V:689:A:O2'	28:V:690:A:OP1	2.04	0.75
28:V:1542:A:O2'	28:V:1544:C:N4	2.19	0.75
9:C:217:ARG:NH1	28:V:828:A:OP1	2.18	0.75
28:V:419:G:N2	28:V:448:A:OP2	2.19	0.75
28:V:1380:U:OP2	28:V:1433:U:O2'	2.02	0.75
28:V:1938:C:O2'	28:V:1939:G:O4'	2.03	0.75
28:V:1882:A:O2'	28:V:1883:A:OP1	2.04	0.75
28:V:310:C:N3	28:V:406:G:N1	2.35	0.75
28:V:2551:U:O2'	28:V:2676:U:OP1	2.01	0.75
32:a:409:C:O2'	32:a:630:A:N3	2.19	0.75
28:V:160:G:O2'	28:V:168:A:N6	2.20	0.75
47:p:6:ARG:NH2	47:p:28:PRO:O	2.20	0.75
28:V:31:C:O2'	28:V:1278:G:OP1	2.04	0.75
28:V:131:C:O2	28:V:148:G:N2	2.16	0.75
9:C:13:ARG:NH1	9:C:16:MET:SD	2.59	0.74
28:V:2785:U:O2'	28:V:2786:A:O5'	2.03	0.74
28:V:2349:A:O2'	28:V:2362:A:N6	2.20	0.74
7:A:5:A:N6	32:a:1547:C:O2	2.17	0.74
14:H:47:U:O2'	14:H:48:C:OP2	2.03	0.74
32:a:1142:C:N3	32:a:1151:G:N1	2.35	0.74
4:3:8:ARG:NH2	28:V:246:U:OP2	2.21	0.74
33:b:19:GLN:NE2	33:b:188:ASP:OD2	2.20	0.74
22:P:14:ARG:NH1	22:P:78:THR:O	2.21	0.74
26:T:77:ARG:NH1	28:V:1645:C:OP1	2.20	0.74
27:U:42:LYS:O	28:V:527:A:O2'	2.06	0.74
32:a:267:G:OP1	51:t:78:ARG:NE	2.20	0.74
28:V:810:G:O2'	28:V:811:A:OP1	2.05	0.74
28:V:1784:A:O2'	28:V:1785:G:OP1	2.06	0.73
28:V:140:A:O2'	28:V:1447:C:O2'	2.06	0.73
28:V:1027:A:O2'	28:V:2065:C:O2'	2.06	0.73
10:D:132:PRO:O	10:D:137:SER:OG	2.06	0.73
1:0:6:ARG:NH1	28:V:2048:U:OP2	2.22	0.73
26:T:19:ASP:O	26:T:22:THR:OG1	2.06	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:V:88:G:O2'	28:V:89:U:OP1	2.06	0.73
28:V:1139:G:N2	28:V:1145:G:O6	2.21	0.73
28:V:2135:G:N1	28:V:2212:C:N3	2.37	0.73
32:a:1057:G:OP1	45:n:4:LYS:NZ	2.19	0.73
53:x:39:G:O2'	53:x:40:C:O5'	2.06	0.73
32:a:692:G:N2	42:k:41:GLY:O	2.22	0.72
31:Z:17:GLU:OE1	31:Z:20:ARG:NH1	2.22	0.72
28:V:1371:G:N7	28:V:1654:A:O2'	2.21	0.72
28:V:1893:U:OP1	28:V:2439:G:O2'	2.08	0.72
32:a:1106:C:O2	32:a:1179:A:O2'	2.06	0.72
28:V:500:A:N3	28:V:504:A:O2'	2.22	0.72
17:K:1:MET:N	17:K:34:ASN:OD1	2.18	0.72
23:Q:89:GLU:N	23:Q:89:GLU:OE1	2.22	0.72
32:a:124:G:OP1	32:a:614:U:O2'	2.03	0.72
32:a:421:G:N2	32:a:436:G:O2'	2.23	0.72
28:V:1116:A:O2'	28:V:1117:G:OP1	2.03	0.72
28:V:1695:A:O2'	28:V:1696:G:O5'	2.08	0.71
32:a:409:C:OP2	35:d:66:ARG:NH1	2.23	0.71
28:V:1402:C:O2'	28:V:1838:A:N3	2.21	0.71
32:a:331:U:OP1	51:t:21:ASN:ND2	2.23	0.71
32:a:510:C:OP1	43:l:127:ARG:NH1	2.23	0.71
28:V:675:C:O2	28:V:685:U:O2'	2.09	0.71
28:V:1474:C:O2'	28:V:1617:A:OP2	2.04	0.71
16:J:136:GLN:NE2	28:V:6:A:N3	2.39	0.71
28:V:342:A:O2'	28:V:343:A:O4'	2.05	0.71
9:C:13:ARG:HH21	28:V:775:G:H4'	1.54	0.71
28:V:482:C:O2'	28:V:483:C:O5'	2.07	0.71
32:a:574:U:OP2	32:a:575:G:O2'	2.06	0.71
28:V:443:G:O2'	28:V:444:U:OP1	2.09	0.71
28:V:2847:G:O2'	28:V:2849:U:OP2	2.04	0.71
32:a:1541:G:HO2'	32:a:1542:A:P	2.13	0.71
28:V:1772:C:N4	28:V:1773:G:O6	2.23	0.71
40:i:106:ARG:NH2	40:i:107:ASP:O	2.24	0.71
45:n:23:ARG:NH1	45:n:28:GLY:O	2.24	0.71
36:e:20:ARG:HD2	36:e:31:PHE:CD2	2.25	0.70
32:a:14:U:O2'	32:a:924:A:OP2	2.10	0.70
32:a:526:G:N2	32:a:539:G:OP1	2.23	0.70
32:a:563:U:O2'	32:a:564:C:OP1	2.08	0.70
32:a:892:C:OP2	43:l:10:LYS:NZ	2.24	0.70
35:d:81:LYS:NZ	36:e:101:GLU:O	2.22	0.70
27:U:9:VAL:HG21	27:U:68:VAL:CG1	2.21	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:V:2734:A:O2'	28:V:2877:G:OP1	2.08	0.70
32:a:21:C:OP1	36:e:135:ASN:ND2	2.24	0.70
8:B:16:G:O6	8:B:17:A:N6	2.24	0.70
10:D:145:SER:HB3	28:V:2604:C:O2	1.91	0.70
32:a:383:U:O2	47:p:29:ARG:NH2	2.24	0.70
28:V:2290:C:OP1	29:W:27:LYS:NZ	2.25	0.70
28:V:2148:A:N6	28:V:2199:G:N7	2.40	0.69
40:i:31:ASN:O	40:i:33:ARG:NH1	2.25	0.69
28:V:688:G:N2	28:V:692:A:H62	1.90	0.69
32:a:1036:C:N4	32:a:1046:G:O6	2.25	0.69
28:V:1116:A:HO2'	28:V:1117:G:P	2.16	0.69
28:V:2226:U:O2	28:V:2227:A:O2'	2.09	0.69
32:a:1107:C:OP1	33:b:139:LYS:NZ	2.26	0.69
18:L:71:ARG:NH2	28:V:680:G:O6	2.25	0.69
28:V:177:G:O2'	28:V:178:A:O5'	2.11	0.69
28:V:1135:G:N2	28:V:1136:U:O4	2.26	0.69
29:W:78:GLU:HG2	29:W:79:ARG:N	2.06	0.69
32:a:302:C:OP1	32:a:619:G:O2'	2.08	0.69
32:a:775:A:OP2	32:a:821:G:N2	2.26	0.69
23:Q:51:ARG:NH1	28:V:1202:A:O4'	2.26	0.69
28:V:1474:C:N4	28:V:1618:A:OP2	2.18	0.69
32:a:343:C:O2'	32:a:1442:A:N3	2.25	0.69
28:V:1122:C:O2'	28:V:1123:A:N7	2.25	0.68
28:V:1886:G:OP2	28:V:1886:G:N2	2.23	0.68
32:a:254:A:N1	32:a:286:G:O2'	2.25	0.68
32:a:1463:A:O2'	32:a:1464:G:O5'	2.08	0.68
14:H:42:G:O2'	14:H:43:G:OP1	2.11	0.68
8:B:41:C:O2'	8:B:43:A:N7	2.25	0.68
28:V:2841:C:O2	28:V:2908:A:O2'	2.10	0.68
28:V:1941:A:N6	32:a:1417:A:O2'	2.24	0.68
32:a:757:A:HO2'	32:a:758:A:P	2.17	0.68
28:V:273:A:OP2	28:V:297:G:N1	2.26	0.68
28:V:2143:A:N3	28:V:2196:U:O2'	2.24	0.68
32:a:150:A:OP2	32:a:168:C:N4	2.26	0.68
9:C:168:GLU:OE2	32:a:690:A:O2'	2.10	0.67
28:V:74:U:OP1	30:Y:47:ARG:NH2	2.25	0.67
32:a:1088:U:O2'	32:a:1089:G:OP1	2.11	0.67
10:D:111:THR:HB	10:D:170:THR:HG22	1.76	0.67
28:V:1065:U:H5'	28:V:1166:G:H22	1.60	0.67
32:a:774:G:N1	32:a:821:G:O2'	2.25	0.67
8:B:48:G:O2'	8:B:49:G:O5'	2.12	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:V:347:G:O2'	28:V:348:U:OP1	2.11	0.67
28:V:732:A:O2'	28:V:820:U:O4	2.08	0.67
28:V:1895:A:N6	28:V:1904:G:O2'	2.27	0.67
10:D:146:MET:HE1	10:D:160:LEU:HD11	1.77	0.67
28:V:290:U:O2'	28:V:291:C:O5'	2.10	0.67
4:3:8:ARG:NH1	28:V:247:A:OP2	2.28	0.67
32:a:596:G:O2'	32:a:597:G:OP2	2.12	0.67
32:a:372:A:O2'	32:a:373:U:O5'	2.10	0.67
32:a:458:G:OP2	32:a:459:A:O2'	2.13	0.67
32:a:987:A:O2'	32:a:989:C:OP2	2.13	0.67
32:a:1087:G:N2	32:a:1090:A:OP2	2.25	0.66
32:a:1318:G:N7	44:m:98:ARG:NH2	2.42	0.66
16:J:78:HIS:ND1	16:J:79:THR:O	2.29	0.66
32:a:536:G:N7	43:l:57:LYS:NZ	2.44	0.66
16:J:63:ILE:O	16:J:94:ARG:NH1	2.29	0.66
28:V:676:G:N2	28:V:679:A:OP2	2.24	0.66
28:V:1104:U:N3	28:V:1105:G:O6	2.28	0.66
32:a:305:G:N2	32:a:308:A:OP2	2.24	0.66
33:b:122:GLU:N	33:b:122:GLU:OE1	2.29	0.66
32:a:1013:G:N2	32:a:1014:A:O2'	2.29	0.66
28:V:2320:U:O2'	28:V:2403:C:O2	2.14	0.66
37:f:11:ARG:NH2	37:f:13:ASN:O	2.28	0.66
39:h:94:VAL:O	39:h:119:ARG:NH1	2.29	0.66
12:F:51:ASP:OD1	12:F:52:SER:N	2.30	0.65
32:a:1438:C:O2	32:a:1481:G:N2	2.20	0.65
14:H:31:C:O2'	14:H:32:C:OP2	2.12	0.65
29:W:76:LYS:HD2	29:W:90:TYR:CE2	2.31	0.65
32:a:262:G:O4'	48:q:19:MET:HE3	1.97	0.65
32:a:1077:A:N1	32:a:1118:G:O2'	2.28	0.65
10:D:145:SER:OG	28:V:2541:C:O2	2.15	0.65
13:G:3:ARG:NE	28:V:2778:A:OP1	2.29	0.65
28:V:1265:A:O2'	28:V:1266:A:O4'	2.05	0.65
35:d:58:ARG:O	35:d:62:GLY:N	2.29	0.65
28:V:1035:G:OP2	31:Z:11:SER:OG	2.09	0.65
28:V:2149:G:O2'	28:V:2150:G:O4'	2.11	0.65
25:S:92:ARG:O	25:S:92:ARG:NE	2.27	0.65
32:a:261:U:O2'	48:q:19:MET:HE1	1.96	0.65
28:V:83:G:O2'	28:V:101:G:N2	2.30	0.65
49:r:18:PHE:O	49:r:22:GLY:N	2.29	0.65
28:V:1530:G:O2'	28:V:1531:G:OP1	2.14	0.65
28:V:1995:A:N3	28:V:2621:G:O2'	2.24	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:V:747:G:O2'	28:V:1677:A:N3	2.29	0.65
28:V:1944:U:O2'	28:V:1945:A:O4'	2.15	0.65
53:x:16:U:O4'	53:x:59:G:N2	2.30	0.65
16:J:40:LYS:NZ	28:V:1055:A:OP2	2.17	0.65
2:1:17:TYR:OH	2:1:35:TYR:O	2.06	0.64
28:V:2341:U:O2'	28:V:2342:C:OP1	2.15	0.64
32:a:986:G:N2	32:a:1372:A:OP2	2.25	0.64
16:J:108:GLY:O	28:V:1183:G:N2	2.24	0.64
22:P:93:ARG:NH2	28:V:1782:G:OP1	2.31	0.64
28:V:2593:A:O2'	28:V:2594:A:O4'	2.09	0.64
32:a:1231:G:OP2	32:a:1331:C:N4	2.31	0.64
28:V:1965:A:OP2	28:V:1991:C:N4	2.30	0.64
27:U:9:VAL:CG2	27:U:68:VAL:CG1	2.76	0.64
22:P:75:PRO:HB2	22:P:78:THR:HG23	1.79	0.64
34:c:37:LYS:NZ	34:c:37:LYS:O	2.29	0.64
32:a:1400:U:O2'	32:a:1542:A:OP2	2.14	0.64
3:2:36:ARG:NH2	28:V:184:G:C4	2.66	0.64
28:V:1423:A:O2'	28:V:1443:C:O2	2.15	0.64
8:B:53:U:O2'	8:B:54:U:O4'	2.10	0.64
43:l:114:ALA:N	43:l:117:THR:OG1	2.31	0.64
19:M:83:MET:HE1	28:V:2279:G:C6	2.33	0.63
28:V:753:A:H62	28:V:772:G:H21	1.46	0.63
28:V:977:U:O4	28:V:978:A:N6	2.31	0.63
28:V:2200:A:O2'	28:V:2201:U:OP2	2.14	0.63
28:V:199:A:H61	28:V:878:G:H21	1.46	0.63
28:V:1855:C:O2'	28:V:2000:A:OP2	2.15	0.63
32:a:649:A:O2'	32:a:650:A:O4'	2.16	0.63
32:a:1175:G:HO2'	32:a:1176:A:P	2.19	0.63
20:N:8:ARG:NH1	20:N:16:MET:SD	2.72	0.63
38:g:64:GLN:NE2	38:g:128:ALA:O	2.30	0.63
53:x:56:C:O2'	53:x:57:G:O4'	2.16	0.63
21:O:14:ARG:NH2	28:V:2324:C:OP1	2.31	0.63
29:W:76:LYS:HD2	29:W:90:TYR:CD2	2.34	0.63
11:E:67:GLN:NE2	28:V:721:G:O2'	2.32	0.63
28:V:2624:G:N2	28:V:2627:A:OP2	2.31	0.63
29:W:49:ARG:NH2	29:W:64:ASP:OD1	2.31	0.62
35:d:15:LEU:O	35:d:56:LYS:NZ	2.32	0.62
11:E:101:LEU:O	11:E:106:ARG:NH2	2.32	0.62
28:V:1427:G:O2'	28:V:1572:G:O2'	2.09	0.62
28:V:1784:A:HO2'	28:V:1785:G:P	2.23	0.62
8:B:34:C:N3	8:B:47:C:O2'	2.30	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:A:16:G:N2	53:x:36:C:O2	2.31	0.62
32:a:237:U:O2'	47:p:24:ASP:OD2	2.17	0.62
29:W:76:LYS:O	29:W:77:PHE:C	2.42	0.62
32:a:885:C:O2'	39:h:15:ARG:NH1	2.33	0.62
9:C:221:ARG:NH2	28:V:1856:U:OP2	2.33	0.61
28:V:2881:G:O6	28:V:2887:A:N6	2.33	0.61
28:V:1941:A:N6	32:a:1417:A:HO2'	1.96	0.61
28:V:1022:G:O2'	28:V:1201:A:O2'	2.14	0.61
28:V:1243:A:HO2'	28:V:1244:A:P	2.17	0.61
28:V:2830:A:O2'	28:V:2831:A:OP2	2.16	0.61
4:3:5:LYS:NZ	28:V:256:C:OP2	2.24	0.61
28:V:1598:C:OP1	28:V:1764:U:O2'	2.13	0.61
32:a:1123:C:C1'	34:c:177:LEU:HD13	2.30	0.61
6:6:8:ASN:O	6:6:27:VAL:HG13	2.00	0.61
32:a:385:G:O6	32:a:386:A:N6	2.33	0.61
28:V:1269:A:O2'	28:V:1270:C:OP1	2.17	0.61
32:a:584:G:O2'	32:a:830:G:OP2	2.14	0.61
28:V:1944:U:O2'	28:V:1945:A:O5'	2.11	0.61
32:a:977:C:OP2	32:a:978:A:O2'	2.05	0.61
46:o:16:LYS:NZ	46:o:19:GLU:O	2.22	0.61
28:V:1565:U:O2'	28:V:1566:G:OP1	2.15	0.61
28:V:2721:C:O2	28:V:2872:U:O2'	2.19	0.61
32:a:209:A:O2'	32:a:210:A:O4'	2.17	0.61
28:V:975:C:O2'	31:Z:38:GLU:OE2	2.19	0.61
32:a:751:G:OP1	46:o:59:MET:HE2	2.00	0.60
23:Q:15:LYS:NZ	28:V:1257:C:OP2	2.23	0.60
28:V:2875:A:P	28:V:2891:G:H22	2.24	0.60
13:G:7:LYS:O	13:G:70:ARG:NH2	2.34	0.60
28:V:1403:G:OP1	52:u:3:ARG:NH1	2.33	0.60
28:V:1867:C:N4	28:V:1928:A:O4'	2.34	0.60
36:e:20:ARG:HD2	36:e:31:PHE:HD2	1.67	0.60
28:V:1033:C:O2'	28:V:1046:A:N3	2.29	0.60
12:F:37:ASN:ND2	28:V:2341:U:O2	2.35	0.60
23:Q:92:ARG:O	23:Q:95:LEU:N	2.34	0.60
28:V:2127:U:O2'	28:V:2128:U:OP1	2.17	0.60
28:V:645:C:O2'	28:V:649:G:OP1	2.13	0.60
28:V:2307:A:OP2	29:W:20:ASN:ND2	2.34	0.60
28:V:1526:G:HO2'	28:V:1608:A:HO2'	1.50	0.60
28:V:1757:G:O2'	28:V:1758:U:O3'	2.19	0.60
28:V:1109:G:O2'	28:V:1110:C:O5'	2.19	0.60
28:V:2468:A:O2'	28:V:2629:A:OP1	2.19	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:V:1093:G:N2	28:V:1157:A:OP2	2.34	0.60
28:V:2135:G:N2	28:V:2212:C:C2	2.70	0.60
43:l:124:ALA:O	43:l:127:ARG:NH2	2.34	0.60
32:a:482:G:O2'	32:a:483:G:OP1	2.16	0.59
25:S:88:ARG:NH2	28:V:795:G:OP1	2.34	0.59
28:V:1074:A:N6	28:V:1172:A:OP1	2.35	0.59
28:V:1383:U:O2'	28:V:1424:A:O2'	2.19	0.59
17:K:64:ARG:NH1	17:K:101:PRO:O	2.35	0.59
28:V:310:C:C2	28:V:406:G:N2	2.69	0.59
28:V:628:C:N4	28:V:629:G:O6	2.35	0.59
28:V:1175:A:O2'	28:V:2544:C:O2	2.16	0.59
32:a:1110:C:OP2	33:b:95:ARG:NH1	2.36	0.59
34:c:47:SER:O	34:c:121:ARG:NH2	2.35	0.59
18:L:21:ARG:NH2	28:V:858:U:O4	2.36	0.59
27:U:80:ARG:NH1	28:V:343:A:OP2	2.35	0.59
28:V:745:C:O2'	28:V:781:A:N6	2.35	0.59
32:a:989:C:OP1	32:a:1232:C:N4	2.35	0.59
36:e:164:LEU:O	39:h:116:LYS:NZ	2.35	0.59
28:V:2244:G:O2'	28:V:2245:G:OP2	2.14	0.59
28:V:2607:G:OP1	28:V:2643:A:N6	2.36	0.59
32:a:569:A:C6	36:e:128:LEU:HD13	2.37	0.59
28:V:529:C:O2'	28:V:543:A:N1	2.32	0.59
32:a:370:G:H5''	43:l:71:THR:HG21	1.84	0.59
27:U:33:VAL:HG23	27:U:65:VAL:HG22	1.83	0.59
28:V:1075:A:N6	28:V:1171:G:O2'	2.35	0.59
32:a:710:U:OP1	32:a:711:A:O2'	2.18	0.59
32:a:436:G:O2'	32:a:437:U:OP2	2.19	0.59
32:a:1450:G:O2'	32:a:1470:A:N6	2.33	0.59
4:3:59:LYS:NZ	28:V:985:G:OP1	2.36	0.59
8:B:31:G:O2'	8:B:32:U:OP1	2.19	0.59
11:E:127:GLU:OE1	11:E:127:GLU:N	2.33	0.58
28:V:88:G:HO2'	28:V:89:U:P	2.26	0.58
28:V:1302:A:C2	28:V:1303:U:C5	2.90	0.58
2:1:31:GLU:OE1	2:1:46:ARG:NH1	2.36	0.58
10:D:96:GLU:N	10:D:96:GLU:OE1	2.35	0.58
20:N:35:THR:HG21	28:V:1696:G:H3'	1.85	0.58
32:a:473:G:N1	32:a:476:U:OP2	2.35	0.58
32:a:1384:A:OP2	38:g:9:LYS:NZ	2.35	0.58
28:V:1623:C:C2	28:V:1624:U:C6	2.91	0.58
32:a:184:G:O6	32:a:206:A:N6	2.37	0.58
28:V:116:G:OP2	28:V:118:A:O2'	2.21	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:V:648:G:O2'	28:V:649:G:OP2	2.19	0.58
28:V:2122:G:O2'	28:V:2227:A:N1	2.30	0.58
28:V:2833:U:N3	28:V:2917:G:O6	2.36	0.58
32:a:1324:U:O2'	32:a:1369:A:N3	2.22	0.58
40:i:40:PRO:O	40:i:41:SER:OG	2.17	0.58
28:V:688:G:H21	28:V:692:A:N6	1.94	0.58
28:V:1813:A:O2'	28:V:1814:A:OP2	2.15	0.58
2:1:2:ARG:NH2	28:V:2314:C:OP2	2.35	0.58
28:V:1964:G:N2	28:V:1991:C:O2'	2.37	0.58
32:a:855:G:O2'	32:a:856:C:OP1	2.19	0.58
28:V:438:A:O2'	28:V:457:G:OP1	2.22	0.58
28:V:1391:U:O2'	28:V:1618:A:N3	2.35	0.58
8:B:6:U:OP1	21:O:11:ARG:NH1	2.36	0.58
11:E:146:LEU:O	11:E:147:SER:OG	2.19	0.58
17:K:66:LYS:NZ	28:V:1710:A:O3'	2.37	0.58
24:R:89:ARG:NH2	28:V:1263:G:OP2	2.37	0.58
28:V:1565:U:HO2'	28:V:1566:G:P	2.25	0.58
32:a:986:G:OP2	32:a:1367:U:O2'	2.22	0.58
50:s:37:ARG:O	50:s:70:LYS:NZ	2.37	0.58
8:B:34:C:N4	8:B:47:C:O2	2.36	0.57
26:T:35:ASN:OD1	26:T:36:LYS:N	2.37	0.57
28:V:689:A:N1	28:V:2398:A:O2'	2.34	0.57
28:V:1448:U:H4'	28:V:1449:C:OP1	2.04	0.57
9:C:13:ARG:HH21	28:V:775:G:C5'	2.17	0.57
28:V:1026:A:O2'	28:V:2066:A:O2'	2.03	0.57
28:V:1305:A:O2'	28:V:1306:G:OP2	2.18	0.57
28:V:1575:A:OP2	28:V:1591:G:N2	2.37	0.57
28:V:1765:G:N2	28:V:1768:A:OP2	2.37	0.57
32:a:1293:C:OP2	32:a:1294:A:O2'	2.16	0.57
36:e:78:GLY:O	36:e:79:THR:OG1	2.20	0.57
10:D:73:GLU:O	10:D:74:THR:HG23	2.05	0.57
28:V:1513:U:O3'	28:V:1594:G:O2'	2.22	0.57
28:V:2295:A:C2	28:V:2301:U:C5	2.91	0.57
32:a:1142:C:C2	32:a:1151:G:N2	2.72	0.57
32:a:1247:A:OP1	32:a:1344:C:O2'	2.16	0.57
28:V:80:G:C2	28:V:106:G:C2	2.92	0.57
28:V:2364:A:O2'	28:V:2365:A:O5'	2.22	0.57
26:T:59:TYR:OH	28:V:1379:U:OP2	2.22	0.57
32:a:1383:A:O3'	38:g:28:ASN:ND2	2.37	0.57
33:b:35:ARG:O	33:b:35:ARG:HG2	2.04	0.57
28:V:1103:A:N6	28:V:1133:G:OP2	2.37	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:V:2058:G:N1	28:V:2062:A:OP2	2.36	0.57
35:d:54:LYS:NZ	35:d:65:GLU:OE2	2.33	0.57
12:F:38:MET:HG3	12:F:40:VAL:HG13	1.87	0.57
28:V:226:A:O2'	28:V:467:C:O2	2.20	0.57
33:b:20:THR:O	33:b:22:ARG:N	2.38	0.57
44:m:83:ILE:HD12	50:s:66:MET:HG2	1.86	0.57
7:A:26:C:H42	36:e:20:ARG:NH2	2.03	0.57
28:V:2021:G:N2	28:V:2025:C:O2'	2.38	0.57
32:a:1387:C:O4'	38:g:95:ARG:NH2	2.38	0.57
17:K:13:ASN:ND2	32:a:347:C:OP1	2.38	0.57
28:V:1699:A:N6	28:V:2035:C:O4'	2.38	0.57
32:a:505:G:H21	32:a:506:A:H3'	1.70	0.57
32:a:954:G:N1	32:a:1347:G:OP2	2.36	0.57
1:O:17:ARG:NH2	28:V:1306:G:OP2	2.34	0.56
10:D:142:ARG:HB3	10:D:143:PRO:HD2	1.86	0.56
23:Q:90:VAL:HG23	23:Q:90:VAL:O	2.05	0.56
28:V:276:C:O4'	28:V:305:A:O2'	2.22	0.56
51:t:68:HIS:O	51:t:70:ASN:N	2.37	0.56
28:V:432:C:O2'	28:V:435:G:N2	2.38	0.56
28:V:1473:A:N6	28:V:1619:A:OP2	2.38	0.56
28:V:2688:G:N2	28:V:2691:A:OP2	2.36	0.56
28:V:2806:G:OP1	28:V:2810:A:O2'	2.18	0.56
33:b:32:PHE:N	33:b:40:ILE:O	2.32	0.56
34:c:16:ARG:NH2	34:c:182:ASP:OD1	2.37	0.56
4:3:13:ARG:NH1	18:L:61:LEU:O	2.34	0.56
13:G:158:TYR:O	13:G:172:ARG:NH2	2.37	0.56
28:V:1453:A:C2	28:V:1635:G:C6	2.93	0.56
32:a:1168:U:O4'	32:a:1191:G:N2	2.38	0.56
32:a:1277:G:O2'	32:a:1278:A:O4'	2.16	0.56
39:h:18:ASN:O	39:h:72:ARG:NE	2.36	0.56
6:6:27:VAL:HG12	6:6:27:VAL:O	2.04	0.56
28:V:698:C:O2'	28:V:699:A:O4'	2.24	0.56
32:a:518:A:HO2'	32:a:519:A:P	2.29	0.56
32:a:1441:G:N2	32:a:1478:A:OP2	2.36	0.56
53:x:17:U:OP1	53:x:60:U:O2'	2.19	0.56
32:a:877:G:O2'	32:a:883:A:N1	2.28	0.56
39:h:23:GLU:N	39:h:23:GLU:OE1	2.38	0.56
28:V:1964:G:O2'	28:V:1966:A:N1	2.37	0.56
11:E:51:VAL:HG11	11:E:88:VAL:HG21	1.87	0.56
23:Q:37:GLN:NE2	28:V:608:C:O4'	2.37	0.56
28:V:45:G:H21	28:V:183:A:N6	2.04	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:K:96:THR:OG1	32:a:347:C:OP1	2.24	0.56
28:V:194:A:HO2'	28:V:725:C:HO2'	1.54	0.56
28:V:1036:A:HO2'	28:V:1037:C:P	2.28	0.56
30:Y:24:GLU:OE2	30:Y:42:ARG:NH2	2.39	0.56
52:u:33:LEU:HD13	52:u:48:TYR:CD1	2.40	0.56
28:V:280:G:N1	28:V:291:C:N3	2.43	0.55
32:a:113:G:H4'	32:a:114:A:O5'	2.06	0.55
32:a:1135:U:O2	32:a:1136:U:O2'	2.11	0.55
11:E:54:ARG:NH1	28:V:720:C:OP1	2.39	0.55
23:Q:16:LYS:NZ	28:V:1267:G:N7	2.52	0.55
46:o:26:GLU:OE2	46:o:77:ARG:NH2	2.40	0.55
2:1:11:GLU:OE1	2:1:11:GLU:N	2.39	0.55
12:F:135:GLN:HG2	12:F:136:LEU:HD12	1.87	0.55
28:V:28:A:HO2'	28:V:626:G:HO2'	1.55	0.55
28:V:222:A:N3	28:V:237:U:O2'	2.32	0.55
1:0:26:GLY:O	1:0:38:LEU:HD12	2.07	0.55
12:F:48:LYS:NZ	12:F:51:ASP:OD2	2.37	0.55
28:V:1883:A:O2'	28:V:1884:G:OP1	2.24	0.55
10:D:107:ILE:HD12	10:D:207:LYS:HE2	1.88	0.55
14:H:42:G:HO2'	14:H:43:G:P	2.29	0.55
23:Q:88:ILE:HG22	23:Q:88:ILE:O	2.06	0.55
28:V:59:G:O2'	28:V:74:U:OP2	2.17	0.55
32:a:526:G:H21	32:a:539:G:P	2.29	0.55
32:a:1275:G:O2'	32:a:1277:G:O6	2.22	0.55
32:a:1499:G:O2'	32:a:1500:U:OP1	2.23	0.55
28:V:307:A:N6	28:V:410:G:O6	2.40	0.55
36:e:39:VAL:O	36:e:47:GLY:N	2.39	0.55
23:Q:40:MET:HE3	24:R:76:TYR:CD1	2.41	0.55
24:R:88:HIS:NE2	24:R:90:GLN:OE1	2.38	0.55
10:D:139:TYR:CE2	10:D:142:ARG:HB2	2.42	0.55
28:V:1574:G:N1	28:V:1592:A:OP2	2.40	0.55
30:Y:6:ILE:O	30:Y:60:ARG:NH2	2.40	0.55
12:F:91:LEU:HD22	12:F:96:MET:HG2	1.89	0.54
23:Q:92:ARG:NH1	28:V:1042:A:O2'	2.38	0.54
28:V:389:A:N3	28:V:391:A:N6	2.55	0.54
28:V:1116:A:O2'	28:V:1118:C:N4	2.36	0.54
32:a:848:G:O2'	32:a:849:G:P	2.64	0.54
32:a:1175:G:N1	32:a:1178:A:OP2	2.40	0.54
32:a:1462:U:HO2'	32:a:1463:A:P	2.29	0.54
32:a:1499:G:O2'	32:a:1500:U:P	2.66	0.54
9:C:13:ARG:HH21	28:V:775:G:C4'	2.20	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:U:9:VAL:HG22	27:U:68:VAL:HG13	1.89	0.54
28:V:1308:A:H1'	28:V:2042:A:H61	1.71	0.54
18:L:41:ARG:NH2	28:V:854:U:OP2	2.41	0.54
28:V:30:G:O2'	28:V:1254:A:N3	2.40	0.54
28:V:1263:G:N2	28:V:1266:A:OP2	2.37	0.54
28:V:1340:A:O2'	28:V:1341:U:OP2	2.22	0.54
38:g:118:GLU:O	38:g:122:ASN:ND2	2.39	0.54
12:F:31:ILE:HG23	12:F:31:ILE:O	2.08	0.54
17:K:3:GLN:NE2	28:V:2024:U:O2	2.40	0.54
28:V:790:A:O2'	28:V:1704:U:OP1	2.24	0.54
28:V:2108:U:O2'	52:u:23:ASN:OD1	2.25	0.54
35:d:101:LEU:HD21	35:d:165:LEU:HD12	1.88	0.54
28:V:1010:C:O2'	28:V:2302:A:N3	2.37	0.54
28:V:1417:A:O2'	28:V:1418:U:OP2	2.23	0.54
32:a:1059:U:OP1	45:n:2:ALA:N	2.41	0.54
16:J:38:ARG:NH2	16:J:45:TYR:OH	2.40	0.54
22:P:100:LEU:HD11	22:P:108:ALA:HB1	1.89	0.54
28:V:1427:G:HO2'	28:V:1572:G:HO2'	1.39	0.54
9:C:243:ARG:NH2	28:V:2268:G:OP1	2.37	0.54
28:V:1426:A:OP1	28:V:1516:A:O2'	2.26	0.54
28:V:1441:U:O2'	28:V:1517:A:N1	2.36	0.54
31:Z:18:ASP:OD1	31:Z:19:GLN:N	2.40	0.54
32:a:9:G:O6	36:e:97:LYS:NZ	2.30	0.54
28:V:199:A:H61	28:V:878:G:N2	2.05	0.54
28:V:443:G:HO2'	28:V:444:U:P	2.31	0.54
32:a:387:C:N4	32:a:388:G:O6	2.40	0.54
8:B:12:U:OP2	8:B:68:C:O2'	2.27	0.54
10:D:146:MET:HE2	28:V:2079:C:O2	2.06	0.54
32:a:1298:A:N1	32:a:1380:G:O2'	2.40	0.54
28:V:1565:U:O2'	28:V:1566:G:P	2.66	0.53
32:a:604:A:N6	32:a:650:A:O2'	2.40	0.53
1:O:14:ARG:NH1	28:V:17:G:OP1	2.41	0.53
27:U:71:LEU:HD12	27:U:71:LEU:O	2.08	0.53
2:1:10:THR:OG1	2:1:11:GLU:OE1	2.26	0.53
32:a:103:G:OP2	51:t:17:ARG:NH2	2.41	0.53
6:6:14:VAL:O	6:6:22:PHE:N	2.40	0.53
28:V:2196:U:O3'	28:V:2197:G:O4'	2.26	0.53
9:C:245:SER:O	9:C:245:SER:OG	2.24	0.53
28:V:2277:C:H2'	28:V:2278:U:O4'	2.07	0.53
28:V:2286:U:O2'	28:V:2287:C:P	2.66	0.53
32:a:1018:U:O2'	32:a:1019:C:P	2.66	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:d:91:ASP:OD1	35:d:96:ASN:ND2	2.41	0.53
28:V:510:G:N2	28:V:513:A:OP2	2.37	0.53
28:V:1339:A:H4'	28:V:1340:A:H5'	1.91	0.53
32:a:686:U:O2	32:a:786:A:O2'	2.26	0.53
32:a:700:G:O6	42:k:59:LYS:NZ	2.40	0.53
33:b:117:ILE:HD11	33:b:137:LEU:CD1	2.39	0.53
39:h:3:MET:O	39:h:4:THR:OG1	2.26	0.53
32:a:428:U:N3	32:a:430:C:O2	2.41	0.53
39:h:5:ASP:OD2	39:h:79:ARG:NH1	2.42	0.53
28:V:181:G:C2	28:V:182:C:O2	2.62	0.53
28:V:1037:C:O2'	28:V:1038:C:OP1	2.26	0.53
28:V:2035:C:O2'	28:V:2848:A:N3	2.42	0.53
28:V:2164:A:O4'	28:V:2188:G:O2'	2.26	0.53
32:a:1038:C:N3	32:a:1043:G:N1	2.43	0.53
23:Q:86:SER:OG	23:Q:89:GLU:OE2	2.21	0.53
28:V:2279:G:N2	28:V:2304:C:O2'	2.42	0.53
32:a:135:C:O3'	47:p:65:LYS:NZ	2.31	0.53
32:a:177:G:C2	32:a:178:A:C8	2.97	0.53
32:a:728:C:OP2	32:a:729:C:N4	2.41	0.53
32:a:848:G:O2'	32:a:849:G:O5'	2.26	0.53
40:i:56:GLU:N	40:i:56:GLU:OE1	2.42	0.53
5:4:8:LYS:NZ	28:V:2496:C:OP1	2.41	0.53
9:C:38:HIS:NE2	28:V:739:C:O2'	2.33	0.53
26:T:78:LYS:NZ	28:V:1378:G:OP2	2.42	0.53
28:V:644:G:O6	28:V:705:A:N6	2.41	0.53
28:V:1966:A:O2'	28:V:1968:U:OP2	2.26	0.53
32:a:1135:U:O2'	32:a:1136:U:OP2	2.22	0.53
28:V:1403:G:N2	28:V:1406:A:OP2	2.38	0.52
28:V:1742:G:OP2	28:V:1743:A:O2'	2.20	0.52
28:V:837:U:OP1	28:V:1810:G:N1	2.42	0.52
10:D:153:ARG:NH1	28:V:2054:C:OP1	2.35	0.52
13:G:89:GLU:N	13:G:164:ARG:O	2.42	0.52
42:k:19:GLU:OE2	42:k:83:THR:N	2.42	0.52
28:V:1526:G:O2'	28:V:1608:A:O2'	2.21	0.52
28:V:2716:U:H2'	28:V:2717:G:O4'	2.09	0.52
32:a:547:U:HO2'	32:a:548:A:P	2.28	0.52
32:a:1032:C:O2'	32:a:1033:G:P	2.67	0.52
44:m:105:ASN:O	44:m:106:ALA:HB3	2.08	0.52
28:V:1525:G:O2'	28:V:1526:G:P	2.67	0.52
28:V:681:C:O2'	28:V:685:U:OP1	2.28	0.52
28:V:1269:A:HO2'	28:V:1270:C:P	2.32	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:a:1499:G:HO2'	32:a:1500:U:P	2.33	0.52
8:B:38:U:O2'	8:B:41:C:OP2	2.22	0.52
14:H:61:C:C2	14:H:62:C:C5	2.98	0.52
28:V:2497:A:HO2'	28:V:2498:A:C5'	2.22	0.52
32:a:323:A:O2'	32:a:338:C:O2'	2.21	0.52
32:a:736:G:N2	32:a:739:G:OP2	2.38	0.52
32:a:1016:A:O2'	32:a:1017:A:OP1	2.20	0.52
32:a:1540:G:O2'	32:a:1541:G:O5'	2.28	0.52
34:c:28:TYR:CE2	34:c:32:LEU:HD11	2.44	0.52
12:F:135:GLN:CG	12:F:136:LEU:HD12	2.40	0.51
17:K:30:ARG:NE	17:K:32:THR:O	2.42	0.51
28:V:186:C:O2	28:V:218:G:N2	2.43	0.51
28:V:482:C:O2'	28:V:483:C:C5'	2.58	0.51
28:V:933:C:O2'	28:V:934:U:OP1	2.28	0.51
33:b:111:ILE:HD12	33:b:114:LEU:HD23	1.91	0.51
2:1:36:CYS:O	2:1:40:LYS:N	2.42	0.51
27:U:82:GLY:N	27:U:93:VAL:O	2.40	0.51
28:V:689:A:O2'	28:V:690:A:P	2.67	0.51
28:V:2103:U:O2'	28:V:2626:G:O2'	1.91	0.51
32:a:141:G:O2'	32:a:210:A:N1	2.36	0.51
32:a:665:G:N1	32:a:760:U:O4	2.43	0.51
32:a:1136:U:OP1	41:j:7:ARG:NH2	2.36	0.51
28:V:1101:G:O2'	28:V:1131:A:N1	2.42	0.51
28:V:1808:U:OP2	28:V:1813:A:N6	2.43	0.51
32:a:547:U:O2'	32:a:548:A:P	2.68	0.51
9:C:50:THR:OG1	28:V:1834:C:O2	2.27	0.51
11:E:131:LEU:HD11	11:E:139:MET:HE3	1.92	0.51
28:V:1306:G:N2	28:V:2042:A:OP2	2.35	0.51
32:a:261:U:C2'	48:q:19:MET:HE1	2.40	0.51
32:a:1463:A:O2'	32:a:1464:G:P	2.68	0.51
50:s:29:GLN:NE2	50:s:30:VAL:O	2.44	0.51
14:H:61:C:N3	14:H:62:C:C5	2.79	0.51
20:N:32:THR:O	20:N:115:ALA:N	2.42	0.51
29:W:78:GLU:CG	29:W:79:ARG:H	2.17	0.51
35:d:125:ARG:NH1	35:d:127:ASP:OD2	2.43	0.51
11:E:57:VAL:HG11	11:E:79:ARG:HB3	1.92	0.51
28:V:1380:U:OP1	28:V:1436:U:N3	2.41	0.51
28:V:351:G:H21	28:V:374:A:H62	1.57	0.51
28:V:1567:U:C2'	28:V:1568:G:OP1	2.59	0.51
32:a:1018:U:O2'	32:a:1019:C:OP1	2.28	0.51
28:V:762:A:OP1	46:o:64:ARG:NH2	2.43	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:a:1073:C:OP2	32:a:1074:G:O2'	2.07	0.51
21:O:46:ASP:O	21:O:50:GLY:N	2.43	0.51
32:a:933:A:OP1	36:e:26:LYS:NZ	2.35	0.51
11:E:149:GLU:OE1	11:E:149:GLU:N	2.44	0.51
18:L:131:SER:OG	28:V:683:A:OP1	2.25	0.51
20:N:13:ARG:NH1	28:V:2719:A:OP2	2.44	0.51
28:V:1398:A:OP2	28:V:1410:G:N1	2.43	0.51
28:V:1948:A:O2'	28:V:1949:C:O5'	2.29	0.51
18:L:30:THR:OG1	28:V:1231:G:OP1	2.22	0.50
25:S:98:LYS:NZ	28:V:1362:G:OP1	2.44	0.50
27:U:9:VAL:HG21	27:U:68:VAL:HG12	1.93	0.50
28:V:24:G:H2'	28:V:25:U:C6	2.46	0.50
28:V:1394:G:O6	28:V:1416:G:N2	2.44	0.50
32:a:286:G:OP2	48:q:45:LYS:NZ	2.35	0.50
10:D:133:MET:SD	10:D:133:MET:N	2.76	0.50
22:P:51:ARG:NH2	28:V:2749:U:OP1	2.39	0.50
32:a:1316:U:O4	32:a:1340:G:N2	2.44	0.50
26:T:31:ASP:OD1	26:T:32:VAL:N	2.45	0.50
28:V:1359:G:OP2	28:V:1359:G:N2	2.25	0.50
9:C:202:LEU:HD13	32:a:782:G:H5''	1.93	0.50
20:N:62:ALA:O	20:N:66:ILE:N	2.41	0.50
24:R:48:VAL:HG21	24:R:53:VAL:HB	1.92	0.50
28:V:1090:U:O2'	28:V:1157:A:N6	2.43	0.50
32:a:1046:G:O2'	32:a:1047:C:O4'	2.30	0.50
28:V:2163:A:N6	28:V:2186:G:N3	2.60	0.50
1:O:27:MET:HB3	1:O:36:MET:HE2	1.94	0.50
28:V:2308:G:N7	29:W:22:ARG:NH2	2.60	0.50
32:a:754:U:OP1	32:a:861:U:O2'	2.15	0.50
32:a:855:G:O2'	32:a:856:C:P	2.69	0.50
53:x:58:A:O2'	53:x:60:U:OP2	2.18	0.50
9:C:8:PRO:HB2	9:C:14:ARG:HH11	1.76	0.50
10:D:125:ARG:NH2	10:D:160:LEU:O	2.42	0.50
28:V:1125:C:O2'	28:V:1126:A:O5'	2.30	0.50
28:V:2610:G:OP2	28:V:2610:G:N2	2.44	0.50
30:Y:13:GLU:N	30:Y:13:GLU:OE1	2.42	0.50
32:a:1160:A:H5''	41:j:44:THR:HG23	1.94	0.50
32:a:1526:G:N2	32:a:1529:A:OP2	2.33	0.50
7:A:24:A:C8	34:c:161:ILE:HG13	2.47	0.50
24:R:98:GLU:OE1	24:R:98:GLU:N	2.44	0.50
25:S:71:ILE:HG23	25:S:71:ILE:O	2.11	0.50
28:V:219:A:C8	28:V:479:A:N6	2.80	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:V:229:A:O2'	28:V:231:A:N1	2.39	0.50
28:V:916:G:C2	28:V:956:A:C2	3.00	0.50
28:V:2279:G:H21	28:V:2279:G:P	2.35	0.50
39:h:118:ALA:O	39:h:122:GLN:N	2.45	0.50
28:V:1451:U:H2'	28:V:1452:C:C6	2.47	0.50
28:V:1460:G:O2'	28:V:1631:A:N6	2.45	0.50
36:e:41:ASP:OD1	36:e:42:LYS:N	2.45	0.50
28:V:354:A:N6	28:V:1250:G:O2'	2.45	0.49
28:V:1757:G:O2'	28:V:1758:U:O5'	2.30	0.49
28:V:2630:C:N4	28:V:2632:G:O6	2.44	0.49
28:V:2818:C:O2'	28:V:2917:G:N2	2.45	0.49
32:a:216:G:HO2'	32:a:477:A:H8	1.59	0.49
42:k:120:HIS:O	42:k:121:ASN:ND2	2.45	0.49
1:O:16:ARG:NH2	28:V:1304:G:OP1	2.45	0.49
5:4:4:ARG:NH1	28:V:2506:C:O2	2.39	0.49
6:6:14:VAL:N	6:6:22:PHE:O	2.45	0.49
8:B:49:G:O2'	8:B:50:A:C8	2.65	0.49
20:N:26:ILE:O	20:N:82:LYS:NZ	2.45	0.49
28:V:865:G:N1	28:V:1229:U:OP2	2.36	0.49
34:c:91:ASN:OD1	34:c:98:VAL:N	2.45	0.49
19:M:3:LEU:HD22	19:M:93:TRP:CD1	2.47	0.49
19:M:83:MET:HE1	28:V:2279:G:C5	2.48	0.49
32:a:1225:A:C2	32:a:1226:C:C5	2.99	0.49
53:x:30:G:O2'	53:x:31:C:OP1	2.28	0.49
10:D:130:ARG:NH1	28:V:2026:A:OP2	2.39	0.49
28:V:2164:A:N6	28:V:2185:G:O2'	2.44	0.49
29:W:78:GLU:CG	29:W:79:ARG:N	2.76	0.49
32:a:682:G:H2'	32:a:683:G:C8	2.47	0.49
36:e:105:VAL:O	36:e:112:ARG:NH2	2.46	0.49
46:o:82:ILE:O	46:o:86:GLY:N	2.45	0.49
17:K:28:SER:OG	28:V:2595:A:N1	2.45	0.49
28:V:93:C:H2'	28:V:94:A:O4'	2.12	0.49
32:a:461:C:O3'	47:p:72:ASN:ND2	2.41	0.49
32:a:1023:G:N2	32:a:1026:A:OP2	2.42	0.49
28:V:1831:A:H2	28:V:1844:A:H62	1.60	0.49
28:V:2365:A:H61	29:W:51:THR:CG2	2.25	0.49
32:a:1129:U:OP1	40:i:85:ARG:NH1	2.46	0.49
13:G:89:GLU:N	13:G:89:GLU:OE1	2.45	0.49
28:V:2009:G:O2'	28:V:2011:U:OP2	2.23	0.49
32:a:673:G:OP1	49:r:58:ARG:NH1	2.43	0.49
32:a:1237:C:OP2	44:m:107:ARG:NH2	2.44	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:a:1307:C:N4	38:g:113:GLU:O	2.46	0.49
32:a:1463:A:HO2'	32:a:1464:G:C5'	2.23	0.49
8:B:38:U:O2	8:B:41:C:O2'	2.29	0.49
17:K:98:ILE:HD12	17:K:117:LEU:HB2	1.94	0.49
28:V:1711:G:H2'	28:V:1712:G:O4'	2.13	0.49
32:a:1326:C:O2	50:s:37:ARG:NH1	2.44	0.49
28:V:10:A:N6	28:V:2658:A:N1	2.61	0.49
28:V:698:C:O2'	28:V:699:A:O5'	2.29	0.49
28:V:2445:C:C2	28:V:2446:C:C5	3.01	0.49
28:V:2823:C:N4	28:V:2829:G:O6	2.46	0.49
32:a:545:C:N4	32:a:546:G:O6	2.46	0.49
47:p:45:LYS:HB2	47:p:46:PRO:HD3	1.95	0.49
28:V:1697:A:H2'	28:V:1698:G:O4'	2.13	0.49
46:o:67:LEU:HD11	46:o:87:LEU:CD2	2.43	0.49
20:N:17:LEU:O	20:N:21:THR:HG23	2.12	0.48
28:V:25:U:C2'	28:V:26:G:O5'	2.62	0.48
28:V:194:A:O2'	28:V:725:C:O2'	2.26	0.48
28:V:1623:C:N3	28:V:1624:U:C5	2.81	0.48
53:x:25:U:C2	53:x:26:G:C8	3.01	0.48
22:P:49:LYS:HB3	22:P:60:THR:HG22	1.95	0.48
28:V:2079:C:H2'	28:V:2080:A:O4'	2.13	0.48
28:V:2254:A:H4'	28:V:2255:C:O5'	2.12	0.48
32:a:272:C:O2'	48:q:68:PRO:O	2.30	0.48
32:a:1318:G:OP1	44:m:97:VAL:HG11	2.13	0.48
53:x:31:C:O2'	53:x:32:C:OP1	2.29	0.48
11:E:139:MET:HA	11:E:139:MET:HE2	1.94	0.48
11:E:192:LEU:C	11:E:193:LEU:HD12	2.38	0.48
28:V:82:G:H22	28:V:104:C:N4	2.11	0.48
28:V:1037:C:O2'	28:V:1038:C:P	2.70	0.48
28:V:1199:C:H2'	28:V:1200:G:O4'	2.14	0.48
28:V:1733:U:O2'	28:V:1745:A:N7	2.43	0.48
19:M:14:ARG:NH1	28:V:1001:U:OP2	2.46	0.48
27:U:9:VAL:HG22	27:U:10:MET:N	2.28	0.48
28:V:1713:A:O2'	28:V:1719:G:N7	2.32	0.48
28:V:2176:A:H2'	28:V:2177:G:O4'	2.13	0.48
28:V:2844:A:O2'	28:V:2846:A:N7	2.37	0.48
32:a:1222:A:O2'	32:a:1224:G:N7	2.34	0.48
32:a:1226:C:OP1	45:n:9:LYS:NZ	2.34	0.48
33:b:184:ILE:HG22	33:b:198:VAL:HB	1.95	0.48
37:f:29:VAL:O	37:f:33:ASN:ND2	2.46	0.48
52:u:25:SER:OG	52:u:26:LYS:N	2.46	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:7:ARG:NH2	28:V:1302:A:N3	2.61	0.48
28:V:482:C:O2'	28:V:483:C:O4'	2.31	0.48
28:V:971:A:H2'	28:V:972:U:C6	2.49	0.48
32:a:372:A:H4'	32:a:373:U:OP1	2.12	0.48
32:a:613:G:O6	32:a:644:A:N6	2.47	0.48
8:B:10:G:H1'	29:W:82:ARG:HD3	1.95	0.48
13:G:89:GLU:O	13:G:164:ARG:N	2.47	0.48
28:V:1304:G:OP2	28:V:1305:A:H2'	2.14	0.48
28:V:2882:G:N2	28:V:2885:A:OP2	2.43	0.48
32:a:1069:U:OP2	34:c:198:LYS:NZ	2.30	0.48
32:a:1249:U:O5'	38:g:116:MET:HE1	2.14	0.48
40:i:27:ARG:N	40:i:62:ASP:OD1	2.40	0.48
10:D:154:VAL:HG21	28:V:2647:G:H21	1.78	0.48
27:U:12:ILE:HD11	27:U:69:MET:HG3	1.95	0.48
28:V:177:G:HO2'	28:V:178:A:C5'	2.24	0.48
32:a:563:U:O2'	32:a:564:C:P	2.71	0.48
52:u:33:LEU:HD12	52:u:34:GLN:N	2.28	0.48
11:E:131:LEU:HD21	11:E:139:MET:HE3	1.95	0.48
28:V:206:A:OP2	28:V:207:A:O2'	2.26	0.48
28:V:1384:C:HO2'	28:V:1385:G:H8	1.60	0.48
37:f:7:MET:SD	49:r:70:MET:HE2	2.53	0.48
9:C:45:ASN:OD1	28:V:1841:G:O2'	2.24	0.48
28:V:250:G:C8	28:V:252:C:C5	3.01	0.48
28:V:441:C:O2'	28:V:442:C:OP1	2.27	0.48
28:V:1366:C:H2'	28:V:1367:G:O4'	2.14	0.48
28:V:2089:A:HO2'	28:V:2090:G:P	2.34	0.48
32:a:1078:G:N7	32:a:1104:G:O2'	2.40	0.48
28:V:181:G:C2	28:V:182:C:C2	3.02	0.48
28:V:1527:C:C2'	28:V:1528:U:OP1	2.61	0.48
28:V:1734:A:OP2	28:V:1743:A:N6	2.44	0.48
28:V:2685:U:O2	28:V:2694:A:N7	2.47	0.48
32:a:1032:C:HO2'	32:a:1033:G:P	2.30	0.48
27:U:69:MET:HE3	28:V:379:C:H4'	1.95	0.47
28:V:1269:A:O2'	28:V:1270:C:P	2.72	0.47
28:V:1326:A:N6	28:V:1694:G:O4'	2.47	0.47
32:a:150:A:N7	32:a:169:U:O2	2.47	0.47
32:a:965:U:O2'	32:a:966:U:P	2.72	0.47
44:m:43:THR:HG22	44:m:44:ARG:N	2.28	0.47
7:A:5:A:OP2	7:A:7:A:N6	2.47	0.47
10:D:6:LEU:HD23	10:D:6:LEU:H	1.79	0.47
25:S:11:ARG:NH1	25:S:99:ARG:O	2.46	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:V:1082:G:N1	28:V:1166:G:N7	2.62	0.47
28:V:2497:A:O2'	28:V:2498:A:O5'	2.26	0.47
28:V:2517:A:N6	28:V:2518:G:O6	2.47	0.47
32:a:23:G:H2'	32:a:24:G:C8	2.49	0.47
32:a:330:C:O2	51:t:14:ASN:ND2	2.47	0.47
32:a:417:U:H2'	32:a:418:G:O4'	2.14	0.47
32:a:1543:U:HO2'	32:a:1544:C:P	2.31	0.47
35:d:191:GLU:O	35:d:192:ALA:HB3	2.14	0.47
39:h:5:ASP:N	39:h:5:ASP:OD1	2.47	0.47
44:m:43:THR:HG22	44:m:44:ARG:H	1.78	0.47
45:n:4:LYS:HA	45:n:7:ILE:HD12	1.96	0.47
45:n:39:LEU:HD13	45:n:47:LEU:HD12	1.95	0.47
28:V:77:U:O4	28:V:109:G:C6	2.68	0.47
28:V:248:G:O2'	28:V:431:A:N1	2.47	0.47
32:a:587:C:O2'	32:a:737:A:N3	2.40	0.47
32:a:974:A:O2'	41:j:57:LYS:NZ	2.43	0.47
35:d:15:LEU:HD22	35:d:56:LYS:HG3	1.96	0.47
50:s:58:VAL:HG23	50:s:58:VAL:O	2.14	0.47
13:G:63:ARG:NH1	28:V:2779:A:OP2	2.47	0.47
14:H:42:G:O2'	14:H:43:G:P	2.72	0.47
20:N:110:ASP:OD2	28:V:1694:G:O2'	2.26	0.47
28:V:614:G:H1'	28:V:1029:A:H61	1.78	0.47
32:a:328:G:O2'	32:a:1444:G:O2'	2.24	0.47
32:a:1339:U:H2'	32:a:1340:G:O4'	2.15	0.47
45:n:24:CYS:SG	45:n:40:CYS:N	2.83	0.47
10:D:17:ALA:HB2	10:D:23:ILE:HD12	1.97	0.47
10:D:124:LYS:NZ	28:V:2028:C:OP1	2.38	0.47
21:O:19:ARG:NH1	21:O:47:ASP:OD2	2.39	0.47
7:A:20:A:O2'	32:a:1502:A:N3	2.41	0.47
8:B:37:A:H4'	8:B:38:U:OP1	2.15	0.47
8:B:48:G:H4'	8:B:49:G:OP1	2.15	0.47
9:C:123:ASP:OD2	9:C:124:ILE:N	2.48	0.47
14:H:26:G:N2	14:H:44:A:N1	2.59	0.47
28:V:349:C:N4	28:V:357:G:O6	2.48	0.47
28:V:497:G:N1	28:V:501:A:OP2	2.42	0.47
28:V:1820:A:N1	28:V:1858:A:H4'	2.30	0.47
34:c:28:TYR:CZ	34:c:32:LEU:HD11	2.50	0.47
34:c:109:ASP:OD1	34:c:139:ARG:NH2	2.47	0.47
17:K:6:THR:HG22	28:V:1711:G:O2'	2.14	0.47
21:O:40:ILE:HD11	21:O:109:LEU:HD11	1.96	0.47
28:V:1030:G:OP1	28:V:1031:C:N4	2.46	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:V:1829:C:H42	28:V:1846:G:H22	1.62	0.47
32:a:411:C:OP2	35:d:67:GLN:NE2	2.47	0.47
32:a:726:C:O2'	32:a:743:A:O4'	2.22	0.47
39:h:60:ILE:HG23	39:h:60:ILE:O	2.15	0.47
32:a:269:U:OP2	51:t:74:ARG:NH2	2.48	0.47
37:f:52:ILE:HG21	37:f:86:ILE:CG2	2.44	0.47
44:m:25:ILE:HD11	44:m:60:ILE:HD12	1.97	0.47
14:H:40:C:H1'	14:H:41:A:P	2.55	0.47
23:Q:50:ARG:O	23:Q:54:LYS:NZ	2.47	0.47
28:V:591:U:OP1	28:V:1259:G:O2'	2.26	0.47
28:V:2286:U:O2'	28:V:2287:C:O5'	2.33	0.47
28:V:2717:G:N1	28:V:2749:U:OP2	2.34	0.47
32:a:1140:A:H2'	32:a:1141:G:N9	2.30	0.47
32:a:1382:G:N7	40:i:13:LYS:NZ	2.63	0.47
38:g:74:GLU:O	38:g:89:VAL:N	2.38	0.47
1:O:22:LEU:HD23	1:O:22:LEU:H	1.80	0.46
19:M:11:ARG:O	28:V:957:A:N6	2.48	0.46
28:V:2459:A:N3	28:V:2459:A:H2'	2.30	0.46
32:a:335:A:O2'	32:a:336:C:O4'	2.25	0.46
40:i:12:ARG:O	40:i:15:SER:OG	2.29	0.46
9:C:123:ASP:O	9:C:128:ASN:ND2	2.49	0.46
13:G:22:ASN:OD1	13:G:23:ASN:N	2.46	0.46
19:M:77:LYS:NZ	19:M:84:GLY:O	2.45	0.46
32:a:258:A:N6	32:a:283:G:O6	2.48	0.46
32:a:388:G:N2	32:a:391:A:OP2	2.44	0.46
32:a:669:A:C6	32:a:755:G:O6	2.68	0.46
7:A:19:G:C4	7:A:20:A:C8	3.03	0.46
31:Z:6:ILE:HG23	31:Z:54:VAL:HG13	1.97	0.46
32:a:1128:A:H2'	32:a:1129:U:O4'	2.15	0.46
32:a:1196:G:N3	45:n:60:SER:OG	2.47	0.46
10:D:142:ARG:HB3	10:D:143:PRO:CD	2.45	0.46
19:M:116:GLU:OE2	19:M:119:ARG:NH1	2.48	0.46
28:V:677:A:N3	28:V:2444:G:O2'	2.43	0.46
28:V:1139:G:C2	28:V:1145:G:O6	2.67	0.46
28:V:1820:A:C2	28:V:1858:A:H4'	2.50	0.46
32:a:1358:A:C4	32:a:1383:A:N6	2.84	0.46
42:k:25:ILE:HG23	42:k:25:ILE:O	2.15	0.46
28:V:29:U:C2	28:V:30:G:C8	3.04	0.46
28:V:1065:U:OP1	28:V:1081:U:O2'	2.23	0.46
28:V:1160:G:O2'	28:V:1161:A:P	2.74	0.46
28:V:1947:A:O2'	28:V:1949:C:N4	2.38	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:W:23:ASP:OD1	29:W:24:SER:N	2.44	0.46
32:a:239:G:C2	32:a:240:A:C8	3.04	0.46
32:a:1022:A:H3'	32:a:1023:G:O4'	2.14	0.46
32:a:1210:A:H1'	32:a:1211:U:OP2	2.16	0.46
52:u:33:LEU:HD12	52:u:35:LYS:H	1.80	0.46
9:C:63:ARG:NH1	9:C:83:TYR:O	2.45	0.46
32:a:908:G:N2	32:a:911:A:OP2	2.47	0.46
32:a:1327:A:O4'	50:s:37:ARG:NH2	2.47	0.46
12:F:141:ILE:HG22	12:F:141:ILE:O	2.16	0.46
28:V:613:U:H2'	28:V:614:G:O4'	2.16	0.46
32:a:1023:G:H2'	32:a:1025:G:N7	2.30	0.46
28:V:2043:A:O2'	28:V:2044:A:O4'	2.27	0.46
32:a:988:A:C2	32:a:1328:A:C4	3.04	0.46
32:a:1313:G:N2	32:a:1343:G:C6	2.83	0.46
32:a:1410:G:H2'	32:a:1411:C:O4'	2.16	0.46
28:V:80:G:N1	28:V:106:G:C6	2.84	0.46
28:V:1421:A:C2'	28:V:1422:C:O5'	2.63	0.46
28:V:1845:A:O2'	28:V:1846:G:P	2.73	0.46
32:a:271:A:OP1	51:t:74:ARG:NE	2.49	0.46
35:d:7:PRO:O	35:d:8:SER:OG	2.28	0.46
44:m:77:ILE:HG22	44:m:81:ILE:HD12	1.97	0.46
17:K:54:LYS:NZ	28:V:1980:U:OP1	2.45	0.46
28:V:80:G:N2	28:V:106:G:C4	2.84	0.46
28:V:1417:A:C4	28:V:1419:G:C8	3.04	0.46
36:e:82:PRO:O	39:h:99:ASN:ND2	2.44	0.46
38:g:12:VAL:O	38:g:24:SER:OG	2.28	0.46
7:A:17:A:OP1	32:a:1508:U:O2'	2.29	0.45
27:U:67:ASN:ND2	28:V:373:A:OP2	2.44	0.45
28:V:492:C:H2'	28:V:493:G:O4'	2.16	0.45
28:V:573:C:N4	28:V:2808:U:OP2	2.49	0.45
28:V:1631:A:C4'	28:V:1632:G:OP1	2.64	0.45
28:V:2280:G:N7	29:W:12:LYS:NZ	2.64	0.45
28:V:2823:C:H2'	28:V:2824:G:H8	1.81	0.45
32:a:262:G:O6	32:a:281:A:N6	2.50	0.45
32:a:1058:G:O5'	45:n:2:ALA:N	2.49	0.45
9:C:13:ARG:NH2	28:V:775:G:H4'	2.28	0.45
11:E:68:LYS:NZ	28:V:2473:G:OP2	2.49	0.45
28:V:340:U:H2'	28:V:341:G:O4'	2.15	0.45
28:V:648:G:O2'	28:V:649:G:P	2.73	0.45
32:a:631:A:OP2	32:a:632:C:N4	2.48	0.45
9:C:156:ARG:NH2	28:V:1847:U:OP2	2.43	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:G:68:THR:HG21	28:V:2786:A:H61	1.81	0.45
14:H:58:A:C4	14:H:61:C:C5	3.04	0.45
27:U:51:ASN:O	27:U:53:GLN:N	2.45	0.45
28:V:1622:C:C2	28:V:1623:C:C5	3.04	0.45
28:V:2695:C:O2	28:V:2695:C:O4'	2.35	0.45
32:a:223:C:H2'	32:a:224:U:O4'	2.16	0.45
32:a:693:U:H2'	32:a:694:G:O4'	2.16	0.45
32:a:801:A:O2'	32:a:803:A:N7	2.48	0.45
32:a:1235:C:O2'	44:m:102:SER:O	2.14	0.45
28:V:2080:A:N6	28:V:2643:A:O2'	2.49	0.45
28:V:2651:C:O2'	28:V:2850:G:N7	2.47	0.45
32:a:369:G:H2'	32:a:370:G:O4'	2.17	0.45
32:a:1328:A:OP1	50:s:4:SER:N	2.48	0.45
14:H:29:U:HO2'	14:H:30:G:P	2.40	0.45
21:O:97:ARG:NH1	28:V:2322:C:OP1	2.46	0.45
23:Q:58:ARG:NE	28:V:1043:G:OP2	2.49	0.45
28:V:183:A:N3	28:V:183:A:H2'	2.30	0.45
28:V:715:A:H2'	28:V:717:A:H62	1.81	0.45
32:a:745:U:O2'	37:f:90:VAL:O	2.33	0.45
32:a:1188:A:H2'	32:a:1189:A:O4'	2.16	0.45
20:N:93:GLU:OE1	20:N:93:GLU:N	2.48	0.45
28:V:234:C:H2'	28:V:235:G:O4'	2.16	0.45
28:V:1273:G:C2	28:V:1274:U:C4	3.05	0.45
32:a:983:G:OP1	41:j:59:LYS:NZ	2.47	0.45
32:a:1176:A:O2'	32:a:1178:A:N7	2.41	0.45
44:m:3:ARG:O	44:m:57:ARG:NE	2.50	0.45
10:D:19:ASN:OD1	10:D:20:GLY:N	2.46	0.45
13:G:120:GLU:HB3	13:G:122:ILE:HD11	1.99	0.45
22:P:102:GLU:N	22:P:102:GLU:OE1	2.50	0.45
28:V:278:A:N6	28:V:294:G:O6	2.50	0.45
48:q:16:SER:OG	48:q:24:THR:HG22	2.16	0.45
23:Q:54:LYS:NZ	28:V:1040:C:OP2	2.50	0.45
28:V:1126:A:O2'	28:V:1127:U:OP2	2.20	0.45
33:b:17:GLY:C	33:b:18:HIS:CG	2.94	0.45
36:e:25:VAL:HG12	36:e:26:LYS:N	2.31	0.45
21:O:14:ARG:HD3	21:O:14:ARG:N	2.32	0.45
28:V:753:A:H62	28:V:772:G:N2	2.11	0.45
28:V:1938:C:C2'	28:V:1939:G:O4'	2.64	0.45
28:V:2258:U:O2	28:V:2259:G:C8	2.70	0.45
28:V:2778:A:OP2	28:V:2779:A:O2'	2.26	0.45
32:a:259:G:O6	32:a:280:C:N4	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:a:332:G:OP2	51:t:66:LEU:HD11	2.17	0.45
32:a:351:U:O2'	32:a:354:G:O6	2.32	0.45
32:a:385:G:OP2	47:p:4:LYS:NZ	2.40	0.45
34:c:21:LYS:NZ	34:c:55:GLU:OE1	2.50	0.45
35:d:118:HIS:HD1	35:d:145:SER:HG	1.63	0.45
8:B:26:C:OP1	21:O:36:SER:OG	2.35	0.45
28:V:278:A:C6	28:V:294:G:C6	3.05	0.45
28:V:1421:A:O2'	28:V:1422:C:O5'	2.31	0.45
34:c:109:ASP:O	34:c:140:THR:HG22	2.17	0.45
35:d:178:ARG:O	35:d:179:LEU:HG	2.17	0.45
43:l:59:ASN:OD1	43:l:60:SER:N	2.50	0.45
28:V:48:G:N2	28:V:179:A:OP2	2.41	0.44
28:V:567:U:H2'	28:V:568:G:C8	2.53	0.44
32:a:372:A:HO2'	32:a:373:U:C5'	2.23	0.44
32:a:482:G:O2'	32:a:483:G:P	2.75	0.44
12:F:50:ILE:HG22	12:F:50:ILE:O	2.16	0.44
12:F:125:ARG:O	21:O:1:MET:N	2.41	0.44
17:K:104:ARG:NH2	22:P:33:VAL:O	2.47	0.44
28:V:139:A:N3	28:V:1449:C:O4'	2.51	0.44
28:V:1442:A:O2'	28:V:1518:G:O2'	2.24	0.44
28:V:2053:C:HO2'	28:V:2054:C:H6	1.63	0.44
28:V:2780:G:OP1	28:V:2780:G:N2	2.51	0.44
32:a:1088:U:HO2'	32:a:1089:G:P	2.40	0.44
41:j:51:ILE:HG23	45:n:41:ARG:CG	2.47	0.44
16:J:6:MET:SD	16:J:6:MET:N	2.77	0.44
28:V:309:U:H3'	28:V:310:C:H5''	1.98	0.44
28:V:907:U:C2	28:V:2297:A:C8	3.05	0.44
32:a:372:A:HO2'	32:a:373:U:P	2.37	0.44
32:a:415:A:O4'	35:d:112:GLN:NE2	2.51	0.44
32:a:547:U:H2'	32:a:548:A:C8	2.51	0.44
32:a:1008:C:O2	32:a:1008:C:H2'	2.17	0.44
32:a:1016:A:HO2'	32:a:1017:A:P	2.37	0.44
32:a:1314:G:O2'	32:a:1315:A:O4'	2.36	0.44
25:S:27:LYS:O	25:S:71:ILE:HG22	2.17	0.44
28:V:183:A:C4	28:V:185:A:N6	2.86	0.44
28:V:2593:A:C2	28:V:2676:U:H4'	2.52	0.44
32:a:340:G:OP2	51:t:4:ILE:N	2.51	0.44
32:a:388:G:N1	32:a:392:G:C6	2.85	0.44
32:a:1358:A:N3	32:a:1383:A:N6	2.66	0.44
32:a:1422:A:N6	32:a:1498:G:O6	2.50	0.44
36:e:29:ARG:O	36:e:30:ARG:NH1	2.45	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:B:78:U:O2'	28:V:965:A:N3	2.51	0.44
10:D:116:GLY:N	28:V:2846:A:OP1	2.41	0.44
14:H:37:A:O2'	14:H:38:C:P	2.75	0.44
25:S:78:GLU:O	28:V:24:G:O2'	2.35	0.44
28:V:199:A:N6	28:V:878:G:H21	2.14	0.44
28:V:1479:G:H2'	28:V:1480:A:O4'	2.17	0.44
28:V:1801:G:N2	28:V:1803:C:H5''	2.33	0.44
28:V:2316:A:O2'	28:V:2317:A:O5'	2.33	0.44
28:V:2415:U:O2'	29:W:64:ASP:OD1	2.35	0.44
32:a:224:U:H2'	32:a:225:A:C8	2.53	0.44
44:m:32:GLN:OE1	44:m:35:LYS:NZ	2.35	0.44
48:q:2:SER:OG	48:q:3:GLU:N	2.51	0.44
10:D:125:ARG:NH2	28:V:2649:C:O2'	2.42	0.44
28:V:617:G:N2	28:V:2060:A:OP1	2.50	0.44
28:V:1158:G:O2'	28:V:1159:U:OP2	2.27	0.44
32:a:227:C:C2	32:a:228:A:C8	3.06	0.44
32:a:330:C:H42	32:a:337:A:H62	1.66	0.44
32:a:409:C:C2	32:a:410:G:C8	3.06	0.44
32:a:547:U:OP2	43:l:125:GLN:NE2	2.42	0.44
32:a:929:A:C2	32:a:930:U:C5	3.05	0.44
41:j:51:ILE:HG23	45:n:41:ARG:HG3	2.00	0.44
18:L:86:ALA:O	18:L:89:THR:HG22	2.18	0.44
28:V:1429:U:O2	28:V:1434:A:N7	2.50	0.44
28:V:1650:C:H2'	28:V:1651:G:O4'	2.18	0.44
32:a:1264:G:H2'	32:a:1267:G:H21	1.83	0.44
10:D:43:ASN:OD1	10:D:44:ASP:N	2.51	0.44
14:H:37:A:C4	14:H:38:C:C6	3.06	0.44
28:V:92:G:O2'	28:V:93:C:C6	2.61	0.44
28:V:545:U:H2'	28:V:546:G:O4'	2.18	0.44
32:a:277:C:H2'	32:a:278:A:H8	1.83	0.44
32:a:648:G:C6	32:a:649:A:N6	2.86	0.44
34:c:136:GLN:OE1	34:c:139:ARG:NH1	2.51	0.44
37:f:54:ASP:O	37:f:56:ARG:NH1	2.50	0.44
8:B:48:G:O2'	8:B:49:G:P	2.76	0.44
16:J:13:GLU:N	16:J:13:GLU:OE1	2.51	0.44
28:V:560:A:N3	28:V:625:C:O2'	2.41	0.44
28:V:623:A:C2	28:V:1302:A:C5	3.06	0.44
28:V:2548:U:O4'	28:V:2571:A:N6	2.51	0.44
28:V:2824:G:N2	28:V:2827:A:C5	2.86	0.44
32:a:194:C:N3	48:q:7:ARG:NE	2.64	0.44
51:t:45:ASP:OD1	51:t:46:LYS:N	2.49	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:1:5:ILE:N	2:1:19:SER:O	2.43	0.43
4:3:64:ASN:C	4:3:65:ILE:HD12	2.43	0.43
14:H:36:C:H3'	14:H:37:A:H5''	2.00	0.43
28:V:88:G:O2'	28:V:89:U:P	2.74	0.43
28:V:250:G:C8	28:V:252:C:C6	3.06	0.43
28:V:524:A:H2'	28:V:525:A:O4'	2.18	0.43
28:V:810:G:O2'	28:V:811:A:P	2.75	0.43
28:V:872:C:H2'	28:V:873:U:O4'	2.17	0.43
28:V:1819:C:H2'	28:V:1820:A:C8	2.53	0.43
28:V:2316:A:HO2'	28:V:2317:A:C5'	2.31	0.43
32:a:209:A:H2'	32:a:210:A:C4	2.52	0.43
53:x:35:U:H2'	53:x:36:C:O4'	2.18	0.43
53:x:47:U:H1'	53:x:48:C:OP2	2.17	0.43
9:C:13:ARG:HH21	28:V:775:G:H5'	1.82	0.43
9:C:206:GLY:N	28:V:1820:A:O2'	2.39	0.43
12:F:136:LEU:HD11	12:F:146:VAL:CG1	2.48	0.43
17:K:105:GLU:OE1	17:K:105:GLU:N	2.51	0.43
28:V:1024:G:O6	28:V:1032:C:N4	2.50	0.43
28:V:1171:G:P	28:V:1172:A:HO2'	2.30	0.43
28:V:2606:A:O4'	28:V:2641:C:N4	2.51	0.43
28:V:2874:G:H1'	28:V:2891:G:H21	1.83	0.43
32:a:717:G:H2'	32:a:718:U:C6	2.52	0.43
32:a:903:C:C2	32:a:904:G:C8	3.06	0.43
42:k:81:LEU:HD23	42:k:81:LEU:H	1.83	0.43
28:V:556:C:N3	28:V:557:U:C5	2.86	0.43
28:V:2139:G:O2'	28:V:2149:G:OP1	2.37	0.43
30:Y:28:LEU:HD12	30:Y:37:LEU:HD11	1.99	0.43
32:a:108:C:O2'	47:p:26:ARG:O	2.36	0.43
32:a:124:G:C6	32:a:244:G:O6	2.70	0.43
32:a:993:A:N3	32:a:993:A:H2'	2.33	0.43
36:e:23:LYS:O	36:e:30:ARG:N	2.50	0.43
12:F:136:LEU:HD11	12:F:146:VAL:HG11	2.01	0.43
28:V:1929:A:O2'	28:V:1930:A:OP1	2.33	0.43
33:b:203:ASN:ND2	33:b:205:ASP:OD1	2.45	0.43
28:V:1036:A:O2'	28:V:1037:C:P	2.75	0.43
28:V:1699:A:N3	28:V:1700:A:C8	2.86	0.43
28:V:2294:U:C4	28:V:2295:A:C5	3.06	0.43
32:a:589:C:H2'	32:a:590:G:O4'	2.18	0.43
35:d:181:GLU:N	35:d:181:GLU:OE1	2.51	0.43
46:o:40:ASN:O	46:o:44:ARG:NH1	2.51	0.43
52:u:49:VAL:HG22	52:u:50:SER:H	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:1:9:CYS:SG	2:1:10:THR:N	2.92	0.43
10:D:139:TYR:CZ	10:D:142:ARG:HB2	2.54	0.43
28:V:75:G:O2'	28:V:76:C:P	2.76	0.43
28:V:75:G:C2	28:V:76:C:C5	3.07	0.43
28:V:441:C:C2'	28:V:442:C:OP1	2.67	0.43
28:V:1323:A:H2'	28:V:1324:G:O4'	2.19	0.43
28:V:1882:A:C6	28:V:1918:A:C6	3.07	0.43
28:V:2265:U:H2'	28:V:2266:G:O4'	2.19	0.43
32:a:332:G:N2	32:a:335:A:OP2	2.52	0.43
32:a:1340:G:HO2'	32:a:1341:A:H8	1.64	0.43
44:m:105:ASN:O	44:m:106:ALA:CB	2.67	0.43
53:x:33:U:O2	53:x:33:U:O4'	2.36	0.43
7:A:16:G:O3'	32:a:1508:U:H2'	2.18	0.43
12:F:37:ASN:OD1	12:F:38:MET:N	2.52	0.43
28:V:79:C:N3	28:V:107:G:C6	2.86	0.43
28:V:996:G:O6	28:V:1014:A:C6	2.72	0.43
28:V:1337:C:H2'	28:V:1338:G:O4'	2.17	0.43
32:a:436:G:O2'	35:d:29:ARG:NH1	2.52	0.43
32:a:455:G:H4'	32:a:456:A:OP1	2.19	0.43
32:a:739:G:O2'	32:a:775:A:O4'	2.31	0.43
10:D:144:GLY:O	10:D:145:SER:C	2.62	0.43
11:E:53:ASN:ND2	28:V:716:G:O6	2.52	0.43
14:H:40:C:H1'	14:H:41:A:OP1	2.19	0.43
23:Q:92:ARG:O	23:Q:93:LYS:C	2.61	0.43
28:V:45:G:H21	28:V:183:A:H62	1.65	0.43
28:V:1351:U:H1'	28:V:1352:U:OP2	2.19	0.43
32:a:77:U:O4'	32:a:93:G:N2	2.52	0.43
32:a:641:G:HO2'	32:a:642:U:P	2.32	0.43
32:a:713:A:C4	32:a:714:G:C8	3.06	0.43
32:a:798:U:N3	32:a:801:A:OP2	2.52	0.43
33:b:156:ASP:OD1	33:b:157:LEU:N	2.50	0.43
44:m:85:SER:O	44:m:86:TYR:C	2.62	0.43
49:r:31:VAL:HG22	49:r:31:VAL:O	2.18	0.43
53:x:18:G:H22	53:x:55:U:H3	1.67	0.43
53:x:47:U:O2'	53:x:48:C:OP2	2.32	0.43
10:D:182:GLU:OE1	10:D:182:GLU:N	2.50	0.43
14:H:41:A:O2'	14:H:42:G:O5'	2.37	0.43
25:S:71:ILE:HD11	25:S:74:ALA:HB2	2.00	0.43
28:V:199:A:O2'	28:V:200:A:H5''	2.19	0.43
28:V:787:C:H5'	28:V:1813:A:C2'	2.49	0.43
28:V:1424:A:C4	28:V:1425:C:C5	3.06	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:V:2252:A:H2'	28:V:2253:G:O4'	2.18	0.43
32:a:1023:G:N1	32:a:1026:A:OP2	2.49	0.43
16:J:135:ALA:O	28:V:2922:U:O2'	2.21	0.43
19:M:83:MET:HE1	28:V:2279:G:O6	2.19	0.43
24:R:14:VAL:HG13	24:R:97:ILE:HD13	2.01	0.43
27:U:67:ASN:ND2	28:V:372:U:O2'	2.51	0.43
28:V:12:A:O2'	28:V:572:A:N6	2.50	0.43
28:V:1972:U:O2'	28:V:1973:U:P	2.76	0.43
28:V:2863:G:C4	28:V:2864:G:C8	3.07	0.43
8:B:71:A:N7	8:B:101:U:O2	2.52	0.42
28:V:750:U:H2'	28:V:751:G:O4'	2.19	0.42
28:V:1012:G:H4'	28:V:2300:G:H22	1.84	0.42
28:V:1053:C:H5''	28:V:1054:A:H2'	2.01	0.42
28:V:1187:U:H4'	28:V:1188:A:O4'	2.19	0.42
28:V:1623:C:C2	28:V:1624:U:C5	3.07	0.42
28:V:2497:A:HO2'	28:V:2498:A:H8	1.67	0.42
28:V:2834:A:C8	28:V:2916:A:N6	2.87	0.42
32:a:113:G:H1'	32:a:114:A:OP2	2.19	0.42
11:E:57:VAL:HG11	11:E:79:ARG:CB	2.49	0.42
28:V:35:G:H2'	28:V:36:G:O4'	2.19	0.42
28:V:879:G:H2'	28:V:880:C:C6	2.54	0.42
28:V:1116:A:HO2'	28:V:1118:C:H41	1.63	0.42
28:V:1525:G:O2'	28:V:1526:G:OP1	2.37	0.42
28:V:1945:A:H61	32:a:1418:C:H4'	1.83	0.42
28:V:1949:C:O2'	28:V:1950:G:O5'	2.32	0.42
28:V:2830:A:O2'	28:V:2831:A:H5'	2.19	0.42
32:a:1408:C:O2	32:a:1512:A:N6	2.52	0.42
32:a:1540:G:HO2'	32:a:1541:G:C5'	2.32	0.42
40:i:52:LEU:HD21	40:i:58:ALA:HA	2.01	0.42
44:m:67:GLY:O	44:m:71:ARG:NH1	2.52	0.42
46:o:39:LEU:HD21	46:o:52:SER:HB2	2.01	0.42
9:C:245:SER:O	9:C:246:PRO:C	2.62	0.42
12:F:68:THR:OG1	12:F:85:ILE:O	2.32	0.42
28:V:1478:G:H2'	28:V:1479:G:C8	2.54	0.42
28:V:1862:C:O2'	28:V:1998:A:N1	2.42	0.42
28:V:2254:A:H1'	28:V:2255:C:OP2	2.18	0.42
28:V:2824:G:H22	28:V:2826:A:H3'	1.85	0.42
32:a:782:G:C6	32:a:816:A:N6	2.87	0.42
32:a:1314:G:HO2'	32:a:1315:A:C5'	2.32	0.42
32:a:1316:U:O2'	44:m:109:ARG:NH1	2.52	0.42
34:c:5:VAL:HG12	34:c:6:ASN:N	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
44:m:11:ARG:O	44:m:46:ARG:NE	2.52	0.42
28:V:177:G:HO2'	28:V:178:A:P	2.39	0.42
28:V:310:C:O2	28:V:406:G:C2	2.69	0.42
28:V:1054:A:N6	28:V:1182:G:O6	2.53	0.42
28:V:1243:A:C2'	28:V:1244:A:OP1	2.65	0.42
28:V:2433:C:H2'	28:V:2434:G:O4'	2.20	0.42
32:a:350:C:N4	32:a:356:G:O6	2.53	0.42
32:a:1142:C:O2	32:a:1151:G:C2	2.71	0.42
32:a:1357:U:H2'	32:a:1358:A:O4'	2.19	0.42
14:H:72:C:N4	14:H:73:G:O6	2.52	0.42
28:V:2139:G:N1	28:V:2149:G:O6	2.53	0.42
32:a:245:C:O3'	48:q:31:LYS:NZ	2.39	0.42
32:a:1084:G:OP1	36:e:69:LYS:NZ	2.44	0.42
33:b:20:THR:OG1	33:b:21:ARG:N	2.51	0.42
44:m:33:VAL:HG13	44:m:59:ILE:HG21	2.02	0.42
10:D:123:ILE:O	10:D:127:GLY:N	2.44	0.42
17:K:1:MET:HE1	28:V:1709:A:H2	1.84	0.42
28:V:181:G:O2'	28:V:182:C:C6	2.67	0.42
28:V:763:A:H3'	28:V:764:C:H5''	2.02	0.42
28:V:2676:U:O2	28:V:2702:G:O6	2.38	0.42
28:V:2777:A:H2'	28:V:2778:A:O4'	2.20	0.42
32:a:1123:C:O4'	34:c:177:LEU:HD13	2.18	0.42
32:a:1372:A:H1'	32:a:1374:G:N7	2.34	0.42
32:a:1543:U:O2'	32:a:1544:C:P	2.75	0.42
46:o:67:LEU:HD11	46:o:87:LEU:HD21	2.01	0.42
7:A:28:U:O3'	7:A:29:U:C6	2.73	0.42
14:H:40:C:C2'	14:H:41:A:OP1	2.67	0.42
28:V:1303:U:C4	28:V:1304:G:C6	3.08	0.42
28:V:1721:A:H2'	28:V:1722:A:O4'	2.19	0.42
33:b:78:ASP:OD1	33:b:79:SER:N	2.51	0.42
39:h:21:ARG:NH1	39:h:70:ASN:OD1	2.52	0.42
51:t:62:VAL:N	51:t:67:VAL:HG21	2.35	0.42
9:C:84:ASP:OD2	9:C:87:ARG:NE	2.48	0.42
11:E:103:LYS:O	11:E:106:ARG:HG2	2.20	0.42
14:H:47:U:H1'	14:H:48:C:OP2	2.20	0.42
16:J:69:LYS:NZ	28:V:1186:C:OP2	2.52	0.42
22:P:49:LYS:NZ	28:V:2714:G:OP1	2.48	0.42
28:V:716:G:N3	28:V:716:G:H2'	2.35	0.42
28:V:1244:A:H3'	28:V:1245:G:H5''	2.02	0.42
28:V:1419:G:C2	28:V:1420:G:N7	2.88	0.42
28:V:1756:U:C5'	28:V:1757:G:H5''	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:V:2028:C:O2	28:V:2716:U:O2'	2.35	0.42
28:V:2228:A:N6	28:V:2253:G:O2'	2.49	0.42
31:Z:50:VAL:O	31:Z:51:SER:OG	2.29	0.42
32:a:896:G:O6	32:a:922:C:N4	2.51	0.42
32:a:1048:A:H2'	32:a:1049:G:O4'	2.19	0.42
39:h:2:VAL:HG12	39:h:3:MET:H	1.84	0.42
43:l:47:CYS:O	43:l:90:HIS:N	2.45	0.42
28:V:575:A:H4'	28:V:576:G:OP2	2.20	0.42
28:V:1463:C:H2'	28:V:1464:A:O4'	2.20	0.42
32:a:547:U:OP1	43:l:125:GLN:N	2.41	0.42
32:a:566:G:H2'	32:a:567:G:O4'	2.19	0.42
46:o:39:LEU:HD23	46:o:39:LEU:O	2.20	0.42
52:u:20:HIS:O	52:u:21:ALA:HB3	2.20	0.42
12:F:144:ASP:OD1	12:F:144:ASP:N	2.52	0.42
13:G:108:VAL:O	13:G:110:TYR:N	2.48	0.42
28:V:181:G:O2'	28:V:182:C:P	2.78	0.42
28:V:1948:A:O2'	28:V:1949:C:H6	2.02	0.42
28:V:2495:C:N3	28:V:2496:C:N4	2.67	0.42
32:a:93:G:O2'	32:a:94:A:O4'	2.35	0.42
32:a:855:G:HO2'	32:a:856:C:P	2.41	0.42
41:j:96:VAL:HG23	41:j:97:ASP:N	2.35	0.42
1:0:28:THR:O	1:0:37:LYS:N	2.42	0.41
16:J:48:HIS:O	28:V:601:U:O2'	2.35	0.41
24:R:29:ALA:HA	24:R:62:VAL:HG11	2.01	0.41
28:V:189:G:C6	28:V:214:G:O6	2.73	0.41
28:V:582:A:H2'	28:V:583:G:O4'	2.20	0.41
28:V:1037:C:C5	28:V:1226:U:C4	3.08	0.41
28:V:1275:G:H4'	28:V:1276:G:OP1	2.20	0.41
28:V:1280:G:N7	28:V:1281:C:C5	2.88	0.41
28:V:2404:G:N1	28:V:2408:G:O6	2.53	0.41
28:V:2682:U:OP2	28:V:2683:A:O2'	2.36	0.41
32:a:716:U:OP1	42:k:89:LYS:NZ	2.40	0.41
32:a:791:A:OP1	32:a:1531:G:N2	2.45	0.41
39:h:20:VAL:HG12	39:h:20:VAL:O	2.20	0.41
1:0:16:ARG:NH2	28:V:1305:A:O2'	2.54	0.41
9:C:172:VAL:N	9:C:184:ILE:O	2.48	0.41
14:H:75:C:H3'	14:H:75:C:O2	2.20	0.41
28:V:163:U:C2	28:V:166:A:N6	2.88	0.41
28:V:567:U:H2'	28:V:568:G:N7	2.35	0.41
28:V:1304:G:OP2	28:V:1304:G:H8	2.03	0.41
28:V:2364:A:HO2'	28:V:2365:A:P	2.43	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:a:756:U:O3'	32:a:757:A:O4'	2.39	0.41
14:H:29:U:H2'	14:H:30:G:O5'	2.21	0.41
25:S:12:ILE:HG22	25:S:13:ALA:N	2.35	0.41
28:V:111:U:OP1	30:Y:58:ARG:NH2	2.49	0.41
28:V:252:C:H4'	28:V:253:G:O5'	2.21	0.41
28:V:1029:A:H2'	28:V:1030:G:O4'	2.20	0.41
28:V:1936:G:O6	28:V:1952:U:C4	2.73	0.41
32:a:262:G:OP1	48:q:72:THR:OG1	2.38	0.41
32:a:482:G:H4'	32:a:483:G:OP1	2.20	0.41
32:a:722:G:H2'	32:a:723:G:C8	2.56	0.41
32:a:766:U:H2'	32:a:767:G:O4'	2.20	0.41
32:a:1131:U:C2	32:a:1132:U:C5	3.08	0.41
14:H:28:C:HO2'	14:H:29:U:C5'	2.33	0.41
28:V:215:G:H2'	28:V:216:A:C8	2.56	0.41
30:Y:44:ARG:O	30:Y:48:LYS:HG3	2.21	0.41
32:a:775:A:C2	32:a:776:A:H1'	2.55	0.41
32:a:1032:C:N4	32:a:1033:G:O6	2.53	0.41
32:a:1496:G:H2'	32:a:1497:G:C8	2.54	0.41
4:3:2:PRO:O	28:V:713:G:N2	2.54	0.41
12:F:135:GLN:OE1	12:F:150:ARG:N	2.53	0.41
13:G:122:ILE:HD13	13:G:145:ILE:HD11	2.01	0.41
27:U:9:VAL:HG22	27:U:10:MET:H	1.86	0.41
28:V:81:G:C2'	28:V:82:G:O5'	2.69	0.41
28:V:482:C:O2'	28:V:483:C:P	2.79	0.41
28:V:616:A:H61	28:V:2058:G:H21	1.67	0.41
28:V:2295:A:N3	28:V:2301:U:C4	2.88	0.41
28:V:2757:U:H2'	28:V:2758:G:H8	1.84	0.41
32:a:112:U:O2'	32:a:113:G:H5'	2.21	0.41
32:a:206:A:H2'	32:a:207:U:O4'	2.21	0.41
32:a:265:G:C6	32:a:278:A:N6	2.88	0.41
32:a:1380:G:OP1	40:i:14:SER:OG	2.38	0.41
12:F:149:VAL:O	12:F:149:VAL:HG13	2.20	0.41
20:N:40:LEU:HD23	20:N:117:ILE:HD13	2.03	0.41
28:V:461:C:O2	28:V:1893:U:O2'	2.31	0.41
28:V:633:U:H2'	28:V:634:A:H8	1.86	0.41
28:V:1017:C:C2'	28:V:1018:G:O5'	2.69	0.41
28:V:1070:G:OP2	28:V:1071:G:O2'	2.29	0.41
28:V:2038:G:C2	28:V:2039:G:C8	3.08	0.41
28:V:2236:C:H2'	28:V:2237:C:C6	2.56	0.41
28:V:2444:G:C4	28:V:2445:C:C5	3.08	0.41
32:a:1166:A:H4'	32:a:1167:C:O4'	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:a:1282:U:H2'	32:a:1283:A:O4'	2.21	0.41
35:d:114:VAL:HG11	35:d:129:PRO:HA	2.02	0.41
12:F:113:ASP:OD2	12:F:113:ASP:N	2.51	0.41
28:V:62:C:H5'	28:V:63:G:O5'	2.21	0.41
28:V:85:G:O2'	28:V:86:C:H5'	2.21	0.41
28:V:942:U:H3'	28:V:943:A:H4'	2.03	0.41
28:V:1828:G:H1'	28:V:1829:C:OP2	2.19	0.41
32:a:1166:A:N7	32:a:1189:A:N6	2.69	0.41
33:b:14:VAL:O	33:b:14:VAL:HG13	2.20	0.41
33:b:111:ILE:HD11	33:b:152:LYS:HA	2.03	0.41
52:u:33:LEU:HD13	52:u:48:TYR:HD1	1.86	0.41
28:V:65:A:N1	28:V:90:A:N6	2.69	0.41
28:V:475:A:C2'	28:V:476:A:O5'	2.69	0.41
28:V:1321:U:H3	28:V:1325:A:H62	1.67	0.41
28:V:1972:U:O2'	28:V:1973:U:OP2	2.38	0.41
28:V:2524:G:H2'	28:V:2525:C:H5'	2.03	0.41
32:a:328:G:H2'	32:a:329:A:C8	2.56	0.41
32:a:703:A:N1	32:a:796:A:O2'	2.52	0.41
8:B:19:G:O6	8:B:20:A:N6	2.54	0.41
8:B:104:G:H2'	8:B:105:A:O4'	2.21	0.41
28:V:19:G:C6	28:V:568:G:O6	2.73	0.41
28:V:162:A:H62	28:V:166:A:N6	2.19	0.41
28:V:443:G:O2'	28:V:444:U:P	2.77	0.41
28:V:623:A:C5	28:V:1302:A:N6	2.89	0.41
28:V:854:U:O2'	28:V:2089:A:N1	2.47	0.41
28:V:1445:A:H2'	28:V:1446:C:O4'	2.20	0.41
28:V:1831:A:H2	28:V:1844:A:N6	2.18	0.41
28:V:2205:A:H4'	28:V:2206:C:OP1	2.20	0.41
28:V:2452:U:O2	28:V:2454:A:O2'	2.31	0.41
28:V:2484:G:C6	28:V:2485:C:N4	2.89	0.41
28:V:2491:U:H2'	28:V:2492:C:O4'	2.21	0.41
30:Y:24:GLU:O	30:Y:28:LEU:HD23	2.20	0.41
32:a:89:C:O2'	32:a:90:C:O5'	2.31	0.41
32:a:329:A:H2'	32:a:330:C:H6	1.86	0.41
32:a:1129:U:O2	32:a:1130:C:C5	2.74	0.41
32:a:1279:G:O2'	32:a:1322:U:O2'	2.37	0.41
36:e:20:ARG:HD2	36:e:31:PHE:CE2	2.55	0.41
37:f:51:GLU:OE1	37:f:56:ARG:NH2	2.54	0.41
42:k:22:ILE:HG22	42:k:85:GLU:CG	2.51	0.41
1:0:15:LEU:O	1:0:18:THR:HG23	2.20	0.41
11:E:54:ARG:O	11:E:57:VAL:HG12	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:R:40:PHE:O	24:R:41:VAL:C	2.64	0.41
28:V:1507:U:C5'	28:V:1508:C:O5'	2.69	0.41
28:V:1856:U:H2'	28:V:1857:G:O4'	2.21	0.41
28:V:2245:G:C2	28:V:2246:G:C5	3.09	0.41
32:a:366:U:H2'	32:a:367:A:H8	1.84	0.41
32:a:381:A:O2'	32:a:459:A:N7	2.54	0.41
34:c:115:VAL:HG13	34:c:136:GLN:HG2	2.01	0.41
47:p:35:GLU:OE1	47:p:59:TRP:NE1	2.51	0.41
50:s:61:PHE:O	50:s:66:MET:HE1	2.21	0.41
53:x:25:U:N3	53:x:26:G:N7	2.68	0.41
2:1:14:GLU:OE1	2:1:16:ASN:ND2	2.51	0.40
28:V:223:G:N1	28:V:475:A:OP2	2.52	0.40
28:V:1362:G:O2'	28:V:1363:G:H5'	2.21	0.40
30:Y:11:THR:OG1	30:Y:12:ALA:N	2.54	0.40
4:3:32:LEU:HD23	28:V:2420:G:H5'	2.02	0.40
18:L:103:SER:OG	28:V:671:G:O6	2.31	0.40
28:V:753:A:N6	28:V:772:G:H21	2.18	0.40
28:V:1472:G:OP2	28:V:1473:A:H2'	2.21	0.40
28:V:1886:G:H21	28:V:1886:G:P	2.39	0.40
28:V:2346:C:H2'	28:V:2347:G:C1'	2.52	0.40
28:V:2476:G:C2'	28:V:2529:U:OP2	2.69	0.40
32:a:86:G:H2'	32:a:87:C:O4'	2.21	0.40
32:a:183:U:O2'	51:t:76:LYS:NZ	2.44	0.40
32:a:439:A:N3	32:a:439:A:H2'	2.35	0.40
32:a:1483:G:H2'	32:a:1484:G:C8	2.56	0.40
9:C:168:GLU:N	9:C:168:GLU:OE1	2.54	0.40
14:H:16:U:H3'	14:H:17:U:C5'	2.51	0.40
23:Q:92:ARG:HG2	23:Q:95:LEU:HD12	2.03	0.40
28:V:62:C:H4'	28:V:63:G:OP2	2.22	0.40
28:V:1275:G:O3'	28:V:1276:G:O4'	2.38	0.40
28:V:2140:U:OP2	28:V:2174:C:N4	2.36	0.40
28:V:2452:U:O2'	28:V:2453:C:O5'	2.38	0.40
32:a:682:G:C6	32:a:743:A:C6	3.09	0.40
32:a:1167:C:H3'	32:a:1167:C:O2	2.21	0.40
9:C:124:ILE:O	9:C:124:ILE:HG23	2.21	0.40
10:D:195:ALA:O	10:D:198:SER:OG	2.32	0.40
18:L:6:LEU:O	28:V:1283:U:O2'	2.33	0.40
28:V:185:A:C2	28:V:186:C:C2	3.09	0.40
28:V:749:G:C2	28:V:778:C:C2	3.10	0.40
28:V:1093:G:O2'	28:V:1094:A:O5'	2.38	0.40
28:V:1948:A:HO2'	28:V:1949:C:C5'	2.33	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:V:2524:G:C2'	28:V:2525:C:H5'	2.51	0.40
32:a:99:A:N7	32:a:151:A:O2'	2.43	0.40
32:a:389:A:H2'	32:a:390:A:O4'	2.22	0.40
35:d:139:ILE:HD12	35:d:139:ILE:N	2.37	0.40
40:i:77:GLY:O	40:i:80:ARG:HG2	2.20	0.40
10:D:146:MET:HE3	10:D:146:MET:HB3	1.97	0.40
12:F:136:LEU:HG	12:F:141:ILE:HG21	2.04	0.40
23:Q:22:LYS:NZ	28:V:20:C:OP1	2.42	0.40
24:R:68:ALA:O	24:R:89:ARG:NE	2.50	0.40
28:V:85:G:H1'	28:V:86:C:H5'	2.04	0.40
28:V:280:G:O6	28:V:281:A:N6	2.54	0.40
28:V:526:A:H1'	28:V:528:G:H5''	2.03	0.40
28:V:1340:A:O2'	28:V:1341:U:P	2.80	0.40
28:V:1783:C:H2'	28:V:1784:A:O4'	2.21	0.40
28:V:1843:G:C6	28:V:1844:A:C6	3.09	0.40
28:V:1941:A:N7	28:V:1948:A:C6	2.89	0.40
28:V:1941:A:O2'	28:V:1942:A:H2'	2.21	0.40
28:V:2550:C:H2'	28:V:2551:U:O4'	2.22	0.40
32:a:126:G:O2'	48:q:7:ARG:NH1	2.55	0.40
32:a:524:G:H2'	32:a:525:U:O4'	2.21	0.40
32:a:626:G:H2'	32:a:627:C:O4'	2.22	0.40
32:a:1130:C:C2	32:a:1131:U:C5	3.10	0.40
32:a:1136:U:N3	32:a:1289:A:OP1	2.49	0.40
49:r:17:TYR:CE1	49:r:21:ASN:ND2	2.88	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	0	52/59 (88%)	51 (98%)	1 (2%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	1	46/49 (94%)	45 (98%)	1 (2%)	0	100	100
3	2	42/44 (96%)	41 (98%)	1 (2%)	0	100	100
4	3	62/66 (94%)	58 (94%)	4 (6%)	0	100	100
5	4	35/37 (95%)	34 (97%)	1 (3%)	0	100	100
6	6	52/66 (79%)	49 (94%)	3 (6%)	0	100	100
9	C	270/277 (98%)	258 (96%)	12 (4%)	0	100	100
10	D	204/209 (98%)	198 (97%)	6 (3%)	0	100	100
11	E	203/207 (98%)	192 (95%)	11 (5%)	0	100	100
12	F	174/179 (97%)	163 (94%)	11 (6%)	0	100	100
13	G	173/179 (97%)	170 (98%)	3 (2%)	0	100	100
16	J	140/145 (97%)	136 (97%)	4 (3%)	0	100	100
17	K	120/122 (98%)	118 (98%)	2 (2%)	0	100	100
18	L	144/146 (99%)	142 (99%)	2 (1%)	0	100	100
19	M	133/144 (92%)	128 (96%)	5 (4%)	0	100	100
20	N	117/120 (98%)	112 (96%)	5 (4%)	0	100	100
21	O	118/120 (98%)	116 (98%)	2 (2%)	0	100	100
22	P	113/115 (98%)	108 (96%)	5 (4%)	0	100	100
23	Q	115/119 (97%)	107 (93%)	8 (7%)	0	100	100
24	R	99/102 (97%)	90 (91%)	9 (9%)	0	100	100
25	S	107/113 (95%)	99 (92%)	8 (8%)	0	100	100
26	T	88/95 (93%)	85 (97%)	3 (3%)	0	100	100
27	U	99/103 (96%)	93 (94%)	6 (6%)	0	100	100
29	W	80/94 (85%)	75 (94%)	5 (6%)	0	100	100
30	Y	63/66 (96%)	62 (98%)	1 (2%)	0	100	100
31	Z	56/59 (95%)	53 (95%)	3 (5%)	0	100	100
33	b	216/246 (88%)	195 (90%)	18 (8%)	3 (1%)	9	38
34	c	204/218 (94%)	191 (94%)	13 (6%)	0	100	100
35	d	193/200 (96%)	188 (97%)	5 (3%)	0	100	100
36	e	162/166 (98%)	156 (96%)	6 (4%)	0	100	100
37	f	90/95 (95%)	87 (97%)	3 (3%)	0	100	100
38	g	147/156 (94%)	146 (99%)	1 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
39	h	129/132 (98%)	118 (92%)	11 (8%)	0	100	100
40	i	101/130 (78%)	97 (96%)	4 (4%)	0	100	100
41	j	93/102 (91%)	85 (91%)	8 (9%)	0	100	100
42	k	112/131 (86%)	108 (96%)	4 (4%)	0	100	100
43	l	134/138 (97%)	125 (93%)	9 (7%)	0	100	100
44	m	106/121 (88%)	98 (92%)	8 (8%)	0	100	100
45	n	58/61 (95%)	51 (88%)	6 (10%)	1 (2%)	7	35
46	o	83/89 (93%)	83 (100%)	0	0	100	100
47	p	86/90 (96%)	79 (92%)	6 (7%)	1 (1%)	10	41
48	q	82/87 (94%)	77 (94%)	5 (6%)	0	100	100
49	r	62/79 (78%)	58 (94%)	4 (6%)	0	100	100
50	s	76/92 (83%)	75 (99%)	1 (1%)	0	100	100
51	t	81/88 (92%)	78 (96%)	2 (2%)	1 (1%)	10	41
52	u	56/62 (90%)	51 (91%)	5 (9%)	0	100	100
All	All	5176/5518 (94%)	4929 (95%)	241 (5%)	6 (0%)	49	79

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
33	b	20	THR
51	t	69	LYS
33	b	21	ARG
47	p	46	PRO
33	b	19	GLN
45	n	32	SER

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	0	48/53 (91%)	48 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	1	46/47 (98%)	46 (100%)	0	100	100
3	2	39/39 (100%)	39 (100%)	0	100	100
4	3	54/56 (96%)	54 (100%)	0	100	100
5	4	35/35 (100%)	35 (100%)	0	100	100
6	6	44/55 (80%)	44 (100%)	0	100	100
9	C	220/225 (98%)	220 (100%)	0	100	100
10	D	167/170 (98%)	166 (99%)	1 (1%)	78	79
11	E	169/170 (99%)	168 (99%)	1 (1%)	78	79
12	F	151/154 (98%)	150 (99%)	1 (1%)	76	78
13	G	148/151 (98%)	148 (100%)	0	100	100
16	J	120/123 (98%)	120 (100%)	0	100	100
17	K	101/101 (100%)	101 (100%)	0	100	100
18	L	110/110 (100%)	110 (100%)	0	100	100
19	M	109/116 (94%)	109 (100%)	0	100	100
20	N	99/100 (99%)	99 (100%)	0	100	100
21	O	93/93 (100%)	93 (100%)	0	100	100
22	P	100/100 (100%)	100 (100%)	0	100	100
23	Q	96/98 (98%)	96 (100%)	0	100	100
24	R	83/84 (99%)	83 (100%)	0	100	100
25	S	90/93 (97%)	90 (100%)	0	100	100
26	T	81/85 (95%)	81 (100%)	0	100	100
27	U	85/87 (98%)	85 (100%)	0	100	100
29	W	64/74 (86%)	64 (100%)	0	100	100
30	Y	56/57 (98%)	56 (100%)	0	100	100
31	Z	52/53 (98%)	51 (98%)	1 (2%)	50	68
33	b	189/212 (89%)	189 (100%)	0	100	100
34	c	168/178 (94%)	167 (99%)	1 (1%)	78	79
35	d	169/173 (98%)	167 (99%)	2 (1%)	63	73
36	e	128/130 (98%)	128 (100%)	0	100	100
37	f	81/84 (96%)	81 (100%)	0	100	100
38	g	125/132 (95%)	124 (99%)	1 (1%)	73	77

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
39	h	111/112 (99%)	110 (99%)	1 (1%)	70	76
40	i	81/102 (79%)	81 (100%)	0	100	100
41	j	86/92 (94%)	86 (100%)	0	100	100
42	k	86/100 (86%)	86 (100%)	0	100	100
43	l	114/116 (98%)	114 (100%)	0	100	100
44	m	94/104 (90%)	94 (100%)	0	100	100
45	n	53/54 (98%)	52 (98%)	1 (2%)	50	68
46	o	80/83 (96%)	80 (100%)	0	100	100
47	p	74/76 (97%)	73 (99%)	1 (1%)	59	71
48	q	77/80 (96%)	77 (100%)	0	100	100
49	r	56/64 (88%)	56 (100%)	0	100	100
50	s	70/81 (86%)	70 (100%)	0	100	100
51	t	66/70 (94%)	66 (100%)	0	100	100
52	u	47/50 (94%)	47 (100%)	0	100	100
All	All	4415/4622 (96%)	4404 (100%)	11 (0%)	85	85

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
10	D	74	THR
11	E	194	ILE
12	F	27	GLN
31	Z	32	ASN
34	c	37	LYS
35	d	57	LEU
35	d	165	LEU
38	g	13	LEU
39	h	128	LEU
45	n	53	ILE
47	p	10	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
3	2	9	ASN
9	C	142	HIS

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Mol	Chain	Res	Type
10	D	33	ASN
10	D	140	HIS
16	J	54	HIS
16	J	81	HIS
16	J	118	GLN
17	K	110	ASN
18	L	27	ASN
20	N	27	ASN
22	P	77	HIS
31	Z	19	GLN
34	c	101	ASN
35	d	109	GLN
40	i	68	HIS
40	i	81	HIS
41	j	20	GLN
46	o	50	HIS
46	o	51	HIS
50	s	29	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
14	H	76/77 (98%)	28 (36%)	4 (5%)
28	V	2881/2928 (98%)	627 (21%)	57 (1%)
32	a	1544/1545 (99%)	278 (18%)	0
53	x	75/76 (98%)	25 (33%)	0
7	A	28/29 (96%)	14 (50%)	5 (17%)
8	B	111/112 (99%)	27 (24%)	4 (3%)
All	All	4715/4767 (98%)	999 (21%)	70 (1%)

All (999) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
7	A	3	G
7	A	5	A
7	A	7	A
7	A	10	A
7	A	12	A
7	A	16	G
7	A	22	G
7	A	23	U

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Mol	Chain	Res	Type
7	A	24	A
7	A	25	G
7	A	26	C
7	A	27	A
7	A	28	U
7	A	29	U
8	B	10	G
8	B	11	A
8	B	12	U
8	B	22	G
8	B	23	U
8	B	32	U
8	B	33	U
8	B	38	U
8	B	39	A
8	B	41	C
8	B	42	G
8	B	46	A
8	B	48	G
8	B	49	G
8	B	50	A
8	B	53	U
8	B	54	U
8	B	55	A
8	B	62	U
8	B	63	C
8	B	85	U
8	B	86	U
8	B	87	U
8	B	88	C
8	B	97	A
8	B	107	G
8	B	108	C
14	H	9	A
14	H	13	C
14	H	16	U
14	H	17	U
14	H	18	G
14	H	19	U
14	H	23	A
14	H	29	U
14	H	30	G

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Mol	Chain	Res	Type
14	H	31	C
14	H	33	U
14	H	34	G
14	H	35	U
14	H	36	C
14	H	37	A
14	H	38	C
14	H	40	C
14	H	41	A
14	H	42	G
14	H	43	G
14	H	48	C
14	H	56	C
14	H	70	A
14	H	71	C
14	H	72	C
14	H	74	C
14	H	75	C
14	H	76	A
28	V	8	U
28	V	10	A
28	V	11	G
28	V	12	A
28	V	13	A
28	V	26	G
28	V	34	U
28	V	46	C
28	V	60	G
28	V	61	A
28	V	63	G
28	V	64	A
28	V	65	A
28	V	71	A
28	V	72	U
28	V	73	A
28	V	75	G
28	V	76	C
28	V	77	U
28	V	78	U
28	V	79	C
28	V	82	G
28	V	83	G

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Mol	Chain	Res	Type
28	V	85	G
28	V	86	C
28	V	87	U
28	V	89	U
28	V	90	A
28	V	92	G
28	V	93	C
28	V	99	U
28	V	101	G
28	V	113	U
28	V	117	A
28	V	119	U
28	V	124	A
28	V	125	A
28	V	126	A
28	V	141	U
28	V	162	A
28	V	164	U
28	V	175	G
28	V	176	A
28	V	177	G
28	V	178	A
28	V	179	A
28	V	182	C
28	V	183	A
28	V	184	G
28	V	188	C
28	V	199	A
28	V	200	A
28	V	202	A
28	V	207	A
28	V	215	G
28	V	216	A
28	V	218	G
28	V	219	A
28	V	225	A
28	V	226	A
28	V	231	A
28	V	232	U
28	V	233	G
28	V	234	C
28	V	251	G

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Mol	Chain	Res	Type
28	V	253	G
28	V	258	A
28	V	267	C
28	V	270	C
28	V	275	A
28	V	283	G
28	V	284	C
28	V	285	U
28	V	286	U
28	V	287	G
28	V	290	U
28	V	291	C
28	V	298	U
28	V	300	G
28	V	301	U
28	V	302	A
28	V	307	A
28	V	308	C
28	V	310	C
28	V	342	A
28	V	344	G
28	V	345	A
28	V	346	G
28	V	348	U
28	V	349	C
28	V	355	A
28	V	361	G
28	V	373	A
28	V	374	A
28	V	375	C
28	V	382	G
28	V	397	U
28	V	407	A
28	V	411	G
28	V	412	A
28	V	413	U
28	V	418	A
28	V	419	G
28	V	420	U
28	V	421	A
28	V	433	G
28	V	434	U

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Mol	Chain	Res	Type
28	V	442	C
28	V	444	U
28	V	445	C
28	V	458	G
28	V	459	A
28	V	471	G
28	V	476	A
28	V	482	C
28	V	483	C
28	V	491	C
28	V	502	C
28	V	503	C
28	V	504	A
28	V	508	C
28	V	512	G
28	V	527	A
28	V	528	G
28	V	537	A
28	V	548	A
28	V	550	G
28	V	551	A
28	V	554	U
28	V	555	C
28	V	556	C
28	V	559	A
28	V	573	C
28	V	574	A
28	V	575	A
28	V	576	G
28	V	577	U
28	V	578	A
28	V	579	G
28	V	592	A
28	V	594	C
28	V	595	G
28	V	599	G
28	V	607	G
28	V	616	A
28	V	617	G
28	V	619	A
28	V	647	A
28	V	648	G

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Mol	Chain	Res	Type
28	V	649	G
28	V	659	A
28	V	662	U
28	V	667	A
28	V	673	A
28	V	683	A
28	V	690	A
28	V	691	U
28	V	692	A
28	V	699	A
28	V	700	U
28	V	701	G
28	V	702	A
28	V	706	C
28	V	718	C
28	V	719	C
28	V	729	G
28	V	732	A
28	V	733	U
28	V	764	C
28	V	773	G
28	V	777	C
28	V	787	C
28	V	794	U
28	V	804	G
28	V	810	G
28	V	811	A
28	V	812	G
28	V	822	G
28	V	823	G
28	V	829	A
28	V	831	U
28	V	832	G
28	V	837	U
28	V	839	G
28	V	840	A
28	V	852	G
28	V	859	C
28	V	866	A
28	V	874	U
28	V	875	U
28	V	892	U

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Mol	Chain	Res	Type
28	V	906	G
28	V	913	A
28	V	933	C
28	V	934	U
28	V	935	A
28	V	936	C
28	V	937	C
28	V	939	G
28	V	940	G
28	V	941	U
28	V	942	U
28	V	943	A
28	V	957	A
28	V	959	C
28	V	961	C
28	V	962	C
28	V	964	A
28	V	973	G
28	V	980	C
28	V	987	A
28	V	990	C
28	V	992	G
28	V	1005	A
28	V	1007	G
28	V	1018	G
28	V	1019	A
28	V	1020	A
28	V	1026	A
28	V	1027	A
28	V	1031	C
28	V	1036	A
28	V	1037	C
28	V	1038	C
28	V	1042	A
28	V	1054	A
28	V	1055	A
28	V	1058	U
28	V	1059	A
28	V	1067	A
28	V	1068	G
28	V	1073	A
28	V	1079	U

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Mol	Chain	Res	Type
28	V	1091	U
28	V	1094	A
28	V	1101	G
28	V	1102	G
28	V	1103	A
28	V	1105	G
28	V	1106	U
28	V	1107	U
28	V	1110	C
28	V	1111	U
28	V	1116	A
28	V	1118	C
28	V	1119	A
28	V	1121	C
28	V	1124	C
28	V	1125	C
28	V	1126	A
28	V	1127	U
28	V	1128	U
28	V	1134	A
28	V	1140	U
28	V	1143	U
28	V	1146	C
28	V	1157	A
28	V	1158	G
28	V	1159	U
28	V	1160	G
28	V	1161	A
28	V	1173	A
28	V	1174	A
28	V	1176	U
28	V	1178	U
28	V	1179	A
28	V	1181	C
28	V	1182	G
28	V	1188	A
28	V	1203	G
28	V	1244	A
28	V	1245	G
28	V	1248	C
28	V	1249	U
28	V	1251	U

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Mol	Chain	Res	Type
28	V	1252	G
28	V	1256	C
28	V	1260	A
28	V	1270	C
28	V	1274	U
28	V	1275	G
28	V	1276	G
28	V	1278	G
28	V	1293	A
28	V	1295	U
28	V	1296	G
28	V	1304	G
28	V	1306	G
28	V	1312	A
28	V	1313	A
28	V	1314	A
28	V	1315	G
28	V	1339	A
28	V	1340	A
28	V	1341	U
28	V	1352	U
28	V	1357	A
28	V	1362	G
28	V	1364	C
28	V	1365	U
28	V	1368	U
28	V	1369	C
28	V	1371	G
28	V	1372	C
28	V	1384	C
28	V	1385	G
28	V	1389	C
28	V	1404	A
28	V	1415	C
28	V	1417	A
28	V	1418	U
28	V	1422	C
28	V	1423	A
28	V	1424	A
28	V	1425	C
28	V	1426	A
28	V	1427	G

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Mol	Chain	Res	Type
28	V	1428	G
28	V	1434	A
28	V	1435	U
28	V	1436	U
28	V	1442	A
28	V	1449	C
28	V	1451	U
28	V	1453	A
28	V	1457	U
28	V	1459	U
28	V	1460	G
28	V	1465	A
28	V	1472	G
28	V	1473	A
28	V	1475	G
28	V	1476	C
28	V	1481	G
28	V	1489	U
28	V	1490	A
28	V	1491	A
28	V	1499	A
28	V	1500	U
28	V	1501	U
28	V	1502	G
28	V	1506	A
28	V	1507	U
28	V	1508	C
28	V	1514	C
28	V	1516	A
28	V	1525	G
28	V	1526	G
28	V	1527	C
28	V	1528	U
28	V	1529	G
28	V	1530	G
28	V	1531	G
28	V	1532	A
28	V	1539	C
28	V	1540	A
28	V	1542	A
28	V	1543	U
28	V	1551	C

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Mol	Chain	Res	Type
28	V	1553	A
28	V	1558	G
28	V	1559	C
28	V	1560	U
28	V	1561	G
28	V	1566	G
28	V	1568	G
28	V	1569	A
28	V	1570	U
28	V	1571	G
28	V	1573	C
28	V	1614	A
28	V	1617	A
28	V	1626	U
28	V	1632	G
28	V	1634	U
28	V	1638	A
28	V	1653	A
28	V	1655	A
28	V	1691	A
28	V	1692	U
28	V	1693	C
28	V	1696	G
28	V	1697	A
28	V	1699	A
28	V	1700	A
28	V	1709	A
28	V	1719	G
28	V	1745	A
28	V	1757	G
28	V	1758	U
28	V	1759	U
28	V	1760	A
28	V	1770	C
28	V	1776	A
28	V	1777	G
28	V	1778	A
28	V	1779	G
28	V	1780	C
28	V	1781	C
28	V	1782	G
28	V	1785	G

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Mol	Chain	Res	Type
28	V	1790	U
28	V	1791	A
28	V	1792	G
28	V	1793	G
28	V	1802	A
28	V	1810	G
28	V	1811	C
28	V	1812	A
28	V	1813	A
28	V	1814	A
28	V	1829	C
28	V	1845	A
28	V	1858	A
28	V	1877	A
28	V	1882	A
28	V	1883	A
28	V	1884	G
28	V	1885	A
28	V	1887	G
28	V	1899	U
28	V	1904	G
28	V	1935	G
28	V	1942	A
28	V	1943	C
28	V	1945	A
28	V	1946	U
28	V	1949	C
28	V	1951	G
28	V	1952	U
28	V	1953	C
28	V	1958	G
28	V	1959	G
28	V	1965	A
28	V	1966	A
28	V	1967	A
28	V	1969	U
28	V	1972	U
28	V	1973	U
28	V	1982	A
28	V	1984	U
28	V	1992	C
28	V	1995	A

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Mol	Chain	Res	Type
28	V	1996	C
28	V	1999	A
28	V	2000	A
28	V	2001	G
28	V	2020	U
28	V	2022	U
28	V	2025	C
28	V	2026	A
28	V	2042	A
28	V	2050	G
28	V	2051	U
28	V	2054	C
28	V	2059	A
28	V	2060	A
28	V	2062	A
28	V	2064	G
28	V	2072	C
28	V	2079	C
28	V	2084	C
28	V	2085	G
28	V	2089	A
28	V	2090	G
28	V	2098	G
28	V	2121	U
28	V	2125	U
28	V	2128	U
28	V	2134	A
28	V	2135	G
28	V	2136	C
28	V	2137	U
28	V	2145	G
28	V	2146	A
28	V	2147	U
28	V	2149	G
28	V	2156	G
28	V	2161	G
28	V	2162	G
28	V	2174	C
28	V	2175	C
28	V	2176	A
28	V	2185	G
28	V	2186	G

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Mol	Chain	Res	Type
28	V	2197	G
28	V	2199	G
28	V	2200	A
28	V	2201	U
28	V	2203	C
28	V	2204	U
28	V	2205	A
28	V	2206	C
28	V	2208	C
28	V	2210	G
28	V	2212	C
28	V	2219	G
28	V	2227	A
28	V	2232	G
28	V	2233	C
28	V	2240	U
28	V	2245	G
28	V	2246	G
28	V	2255	C
28	V	2267	G
28	V	2268	G
28	V	2282	G
28	V	2287	C
28	V	2295	A
28	V	2296	A
28	V	2308	G
28	V	2312	C
28	V	2316	A
28	V	2317	A
28	V	2324	C
28	V	2325	U
28	V	2331	U
28	V	2333	G
28	V	2334	U
28	V	2335	U
28	V	2336	G
28	V	2337	G
28	V	2338	A
28	V	2341	U
28	V	2342	C
28	V	2343	A
28	V	2346	C

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Mol	Chain	Res	Type
28	V	2347	G
28	V	2348	C
28	V	2349	A
28	V	2350	G
28	V	2351	A
28	V	2354	G
28	V	2356	A
28	V	2363	C
28	V	2364	A
28	V	2376	C
28	V	2379	C
28	V	2401	G
28	V	2412	G
28	V	2414	C
28	V	2415	U
28	V	2431	U
28	V	2435	C
28	V	2452	U
28	V	2453	C
28	V	2454	A
28	V	2455	A
28	V	2457	G
28	V	2458	G
28	V	2459	A
28	V	2460	U
28	V	2464	A
28	V	2469	C
28	V	2470	C
28	V	2477	A
28	V	2488	A
28	V	2505	A
28	V	2507	A
28	V	2520	U
28	V	2522	U
28	V	2525	C
28	V	2527	C
28	V	2531	G
28	V	2534	G
28	V	2542	A
28	V	2547	A
28	V	2549	C
28	V	2558	G

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Mol	Chain	Res	Type
28	V	2564	G
28	V	2583	U
28	V	2593	A
28	V	2595	A
28	V	2596	G
28	V	2602	C
28	V	2611	G
28	V	2614	U
28	V	2615	C
28	V	2627	A
28	V	2631	A
28	V	2632	G
28	V	2638	U
28	V	2642	U
28	V	2644	U
28	V	2659	G
28	V	2690	G
28	V	2711	G
28	V	2718	U
28	V	2720	C
28	V	2743	G
28	V	2747	G
28	V	2755	U
28	V	2762	A
28	V	2763	C
28	V	2764	G
28	V	2773	G
28	V	2774	C
28	V	2777	A
28	V	2785	U
28	V	2786	A
28	V	2794	A
28	V	2806	G
28	V	2807	A
28	V	2808	U
28	V	2809	G
28	V	2818	C
28	V	2823	C
28	V	2824	G
28	V	2826	A
28	V	2831	A
28	V	2832	G

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Mol	Chain	Res	Type
28	V	2859	G
28	V	2860	A
28	V	2861	U
28	V	2866	C
28	V	2867	U
28	V	2868	G
28	V	2873	G
28	V	2892	G
28	V	2897	G
28	V	2899	C
28	V	2900	A
28	V	2901	G
28	V	2905	C
28	V	2916	A
28	V	2917	G
28	V	2918	G
32	a	11	G
32	a	31	A
32	a	32	C
32	a	33	G
32	a	34	A
32	a	41	G
32	a	49	C
32	a	50	C
32	a	53	A
32	a	75	G
32	a	76	A
32	a	77	U
32	a	78	G
32	a	84	U
32	a	85	U
32	a	86	G
32	a	87	C
32	a	89	C
32	a	90	C
32	a	93	G
32	a	114	A
32	a	118	A
32	a	119	C
32	a	120	A
32	a	128	A
32	a	136	U

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Mol	Chain	Res	Type
32	a	141	G
32	a	142	A
32	a	148	A
32	a	153	U
32	a	154	C
32	a	162	C
32	a	172	U
32	a	181	G
32	a	189	A
32	a	195	A
32	a	197	G
32	a	208	A
32	a	209	A
32	a	211	A
32	a	218	U
32	a	219	U
32	a	221	G
32	a	249	G
32	a	255	G
32	a	258	A
32	a	259	G
32	a	274	G
32	a	275	C
32	a	287	A
32	a	288	C
32	a	297	G
32	a	314	A
32	a	316	C
32	a	336	C
32	a	337	A
32	a	338	C
32	a	340	G
32	a	352	A
32	a	353	C
32	a	354	G
32	a	355	G
32	a	360	C
32	a	362	G
32	a	373	U
32	a	375	U
32	a	380	C
32	a	381	A

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Mol	Chain	Res	Type
32	a	384	G
32	a	392	G
32	a	396	G
32	a	405	A
32	a	414	G
32	a	419	A
32	a	420	U
32	a	421	G
32	a	429	U
32	a	430	C
32	a	437	U
32	a	438	A
32	a	439	A
32	a	456	A
32	a	457	A
32	a	460	A
32	a	461	C
32	a	467	C
32	a	474	A
32	a	476	U
32	a	477	A
32	a	478	G
32	a	483	G
32	a	485	A
32	a	488	U
32	a	494	G
32	a	504	A
32	a	505	G
32	a	506	A
32	a	508	A
32	a	514	G
32	a	518	A
32	a	519	A
32	a	520	C
32	a	526	G
32	a	527	C
32	a	533	G
32	a	536	G
32	a	539	G
32	a	541	A
32	a	542	A
32	a	548	A

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Mol	Chain	Res	Type
32	a	556	A
32	a	564	C
32	a	568	A
32	a	571	U
32	a	573	U
32	a	581	A
32	a	582	A
32	a	585	G
32	a	586	G
32	a	590	G
32	a	597	G
32	a	627	C
32	a	641	G
32	a	642	U
32	a	643	C
32	a	651	A
32	a	662	U
32	a	674	A
32	a	696	A
32	a	697	G
32	a	711	A
32	a	730	A
32	a	732	U
32	a	733	G
32	a	742	G
32	a	755	G
32	a	757	A
32	a	758	A
32	a	764	G
32	a	799	A
32	a	802	U
32	a	803	A
32	a	805	C
32	a	809	G
32	a	824	A
32	a	826	C
32	a	845	G
32	a	849	G
32	a	853	C
32	a	855	G
32	a	856	C
32	a	882	A

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Mol	Chain	Res	Type
32	a	883	A
32	a	885	C
32	a	912	G
32	a	924	A
32	a	944	C
32	a	945	A
32	a	964	G
32	a	965	U
32	a	966	U
32	a	967	U
32	a	968	A
32	a	970	U
32	a	975	A
32	a	978	A
32	a	979	A
32	a	981	G
32	a	985	A
32	a	986	G
32	a	987	A
32	a	993	A
32	a	1000	C
32	a	1002	U
32	a	1003	G
32	a	1004	A
32	a	1007	U
32	a	1008	C
32	a	1009	C
32	a	1010	U
32	a	1011	C
32	a	1012	U
32	a	1014	A
32	a	1015	C
32	a	1017	A
32	a	1019	C
32	a	1022	A
32	a	1023	G
32	a	1027	U
32	a	1030	G
32	a	1033	G
32	a	1035	C
32	a	1036	C
32	a	1039	U

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Mol	Chain	Res	Type
32	a	1041	C
32	a	1042	G
32	a	1046	G
32	a	1047	C
32	a	1050	A
32	a	1053	G
32	a	1058	G
32	a	1064	C
32	a	1073	C
32	a	1075	U
32	a	1089	G
32	a	1095	U
32	a	1104	G
32	a	1105	U
32	a	1111	A
32	a	1112	A
32	a	1134	G
32	a	1135	U
32	a	1136	U
32	a	1140	A
32	a	1142	C
32	a	1145	U
32	a	1148	G
32	a	1149	U
32	a	1161	A
32	a	1168	U
32	a	1176	A
32	a	1178	A
32	a	1190	G
32	a	1192	U
32	a	1193	G
32	a	1205	A
32	a	1206	A
32	a	1211	U
32	a	1221	U
32	a	1222	A
32	a	1223	U
32	a	1234	A
32	a	1249	U
32	a	1259	A
32	a	1267	G
32	a	1269	G

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Mol	Chain	Res	Type
32	a	1277	G
32	a	1289	A
32	a	1295	C
32	a	1296	A
32	a	1308	A
32	a	1309	G
32	a	1314	G
32	a	1326	C
32	a	1327	A
32	a	1328	A
32	a	1329	C
32	a	1341	A
32	a	1345	U
32	a	1348	A
32	a	1349	A
32	a	1371	C
32	a	1372	A
32	a	1373	U
32	a	1384	A
32	a	1389	U
32	a	1390	U
32	a	1392	C
32	a	1398	C
32	a	1403	A
32	a	1407	A
32	a	1435	A
32	a	1451	A
32	a	1452	G
32	a	1455	A
32	a	1461	U
32	a	1463	A
32	a	1464	G
32	a	1500	U
32	a	1502	A
32	a	1513	A
32	a	1516	U
32	a	1527	G
32	a	1539	G
32	a	1540	G
32	a	1542	A
32	a	1544	C
32	a	1546	C

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Mol	Chain	Res	Type
53	x	3	U
53	x	7	G
53	x	9	A
53	x	18	G
53	x	19	U
53	x	20	U
53	x	21	A
53	x	30	G
53	x	31	C
53	x	32	C
53	x	33	U
53	x	34	G
53	x	36	C
53	x	37	A
53	x	38	C
53	x	40	C
53	x	48	C
53	x	55	U
53	x	56	C
53	x	57	G
53	x	67	C
53	x	70	A
53	x	71	C
53	x	74	C
53	x	75	C

All (70) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
7	A	24	A
7	A	25	G
7	A	26	C
7	A	27	A
7	A	28	U
8	B	31	G
8	B	37	A
8	B	48	G
8	B	49	G
14	H	29	U
14	H	40	C
14	H	42	G
14	H	47	U

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Mol	Chain	Res	Type
28	V	62	C
28	V	88	G
28	V	124	A
28	V	125	A
28	V	224	A
28	V	252	C
28	V	347	G
28	V	411	G
28	V	441	C
28	V	443	G
28	V	549	A
28	V	554	U
28	V	689	A
28	V	772	G
28	V	810	G
28	V	933	C
28	V	1036	A
28	V	1037	C
28	V	1093	G
28	V	1172	A
28	V	1243	A
28	V	1250	G
28	V	1269	A
28	V	1275	G
28	V	1305	A
28	V	1351	U
28	V	1435	U
28	V	1448	U
28	V	1507	U
28	V	1525	G
28	V	1527	C
28	V	1530	G
28	V	1565	U
28	V	1567	U
28	V	1570	U
28	V	1631	A
28	V	1784	A
28	V	1813	A
28	V	1828	G
28	V	1882	A
28	V	1883	A
28	V	2127	U

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Mol	Chain	Res	Type
28	V	2155	A
28	V	2205	A
28	V	2254	A
28	V	2286	U
28	V	2295	A
28	V	2316	A
28	V	2341	U
28	V	2430	U
28	V	2452	U
28	V	2454	A
28	V	2468	A
28	V	2631	A
28	V	2710	C
28	V	2805	A
28	V	2904	A

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

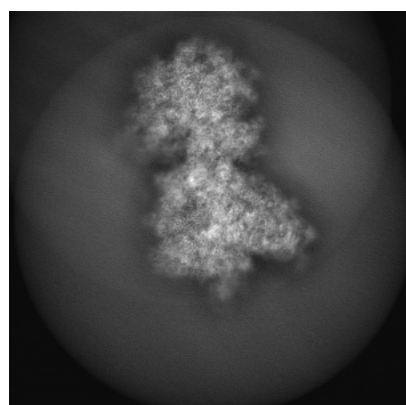
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-14158. These allow visual inspection of the internal detail of the map and identification of artifacts.

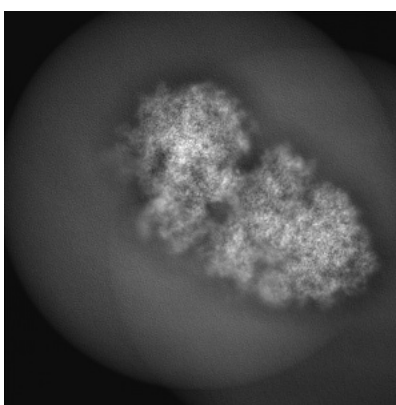
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

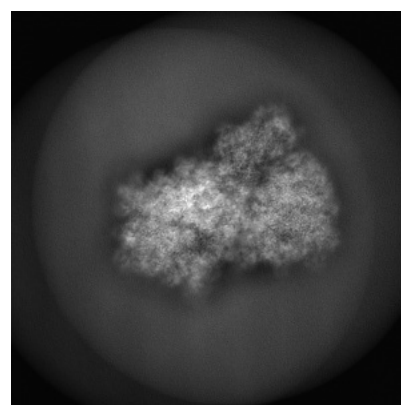
6.1.1 Primary map



X



Y

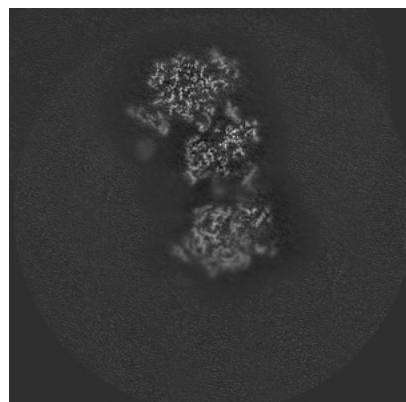


Z

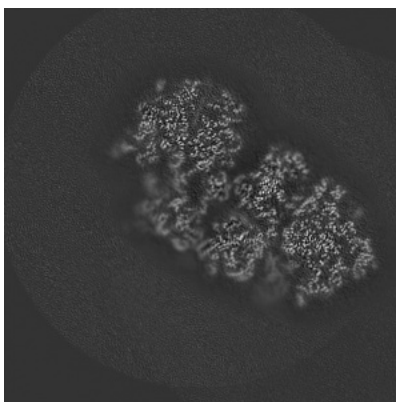
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

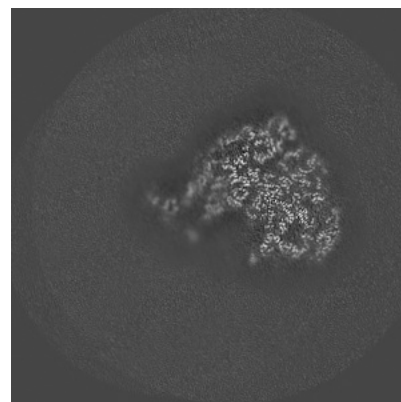
6.2.1 Primary map



X Index: 184



Y Index: 184

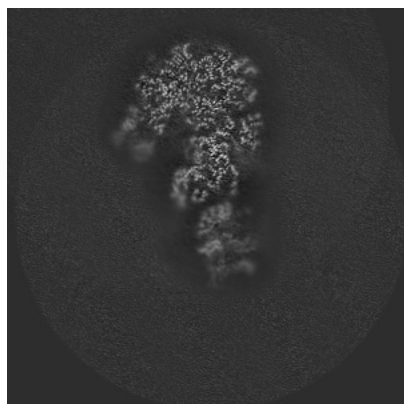


Z Index: 184

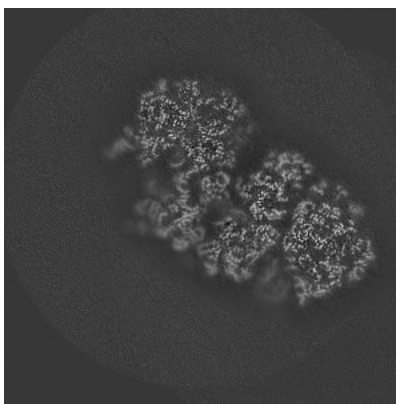
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

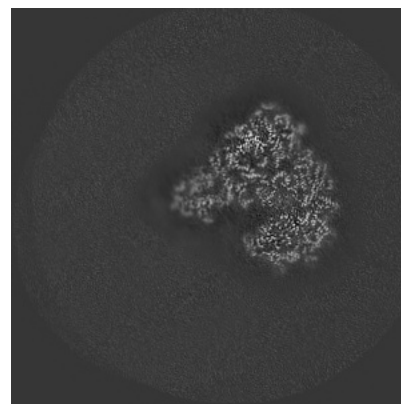
6.3.1 Primary map



X Index: 163



Y Index: 187

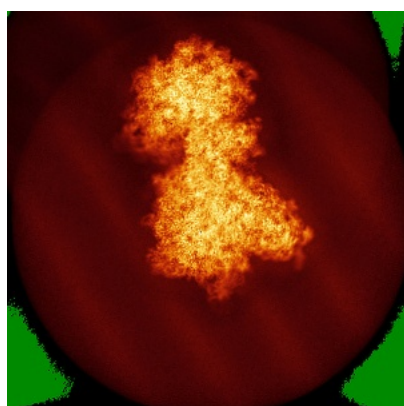


Z Index: 169

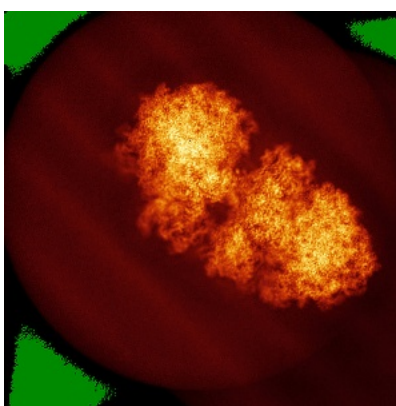
The images above show the largest variance slices of the map in three orthogonal directions.

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

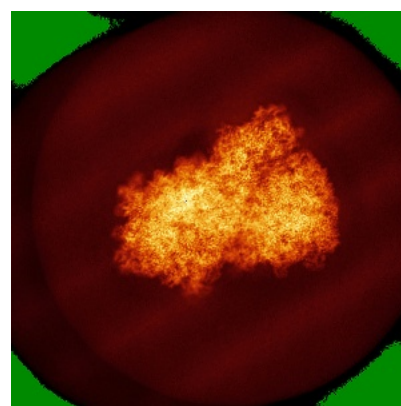
6.4.1 Primary map



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

This section was not generated.

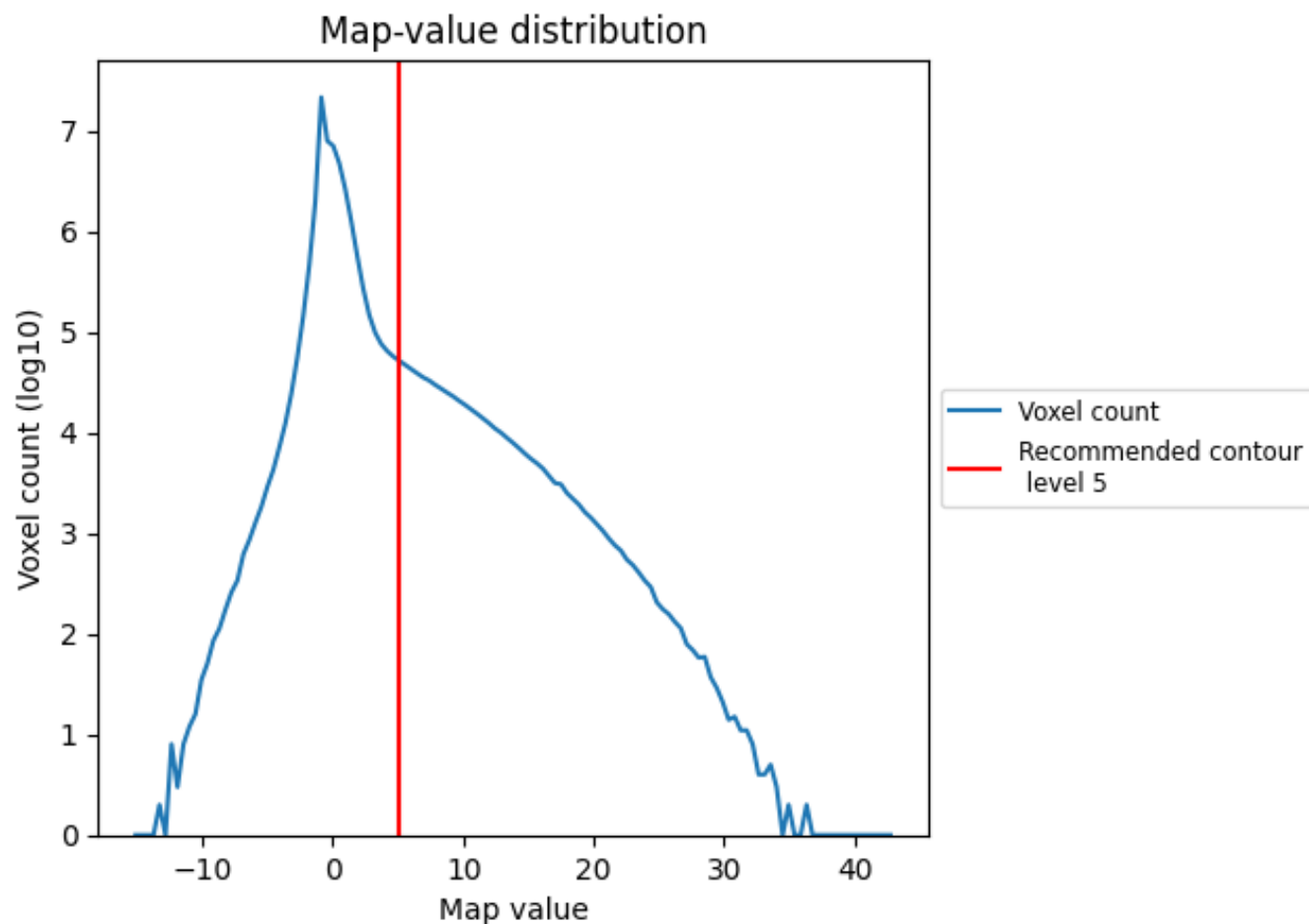
6.6 Mask visualisation

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

7 Map analysis [i](#)

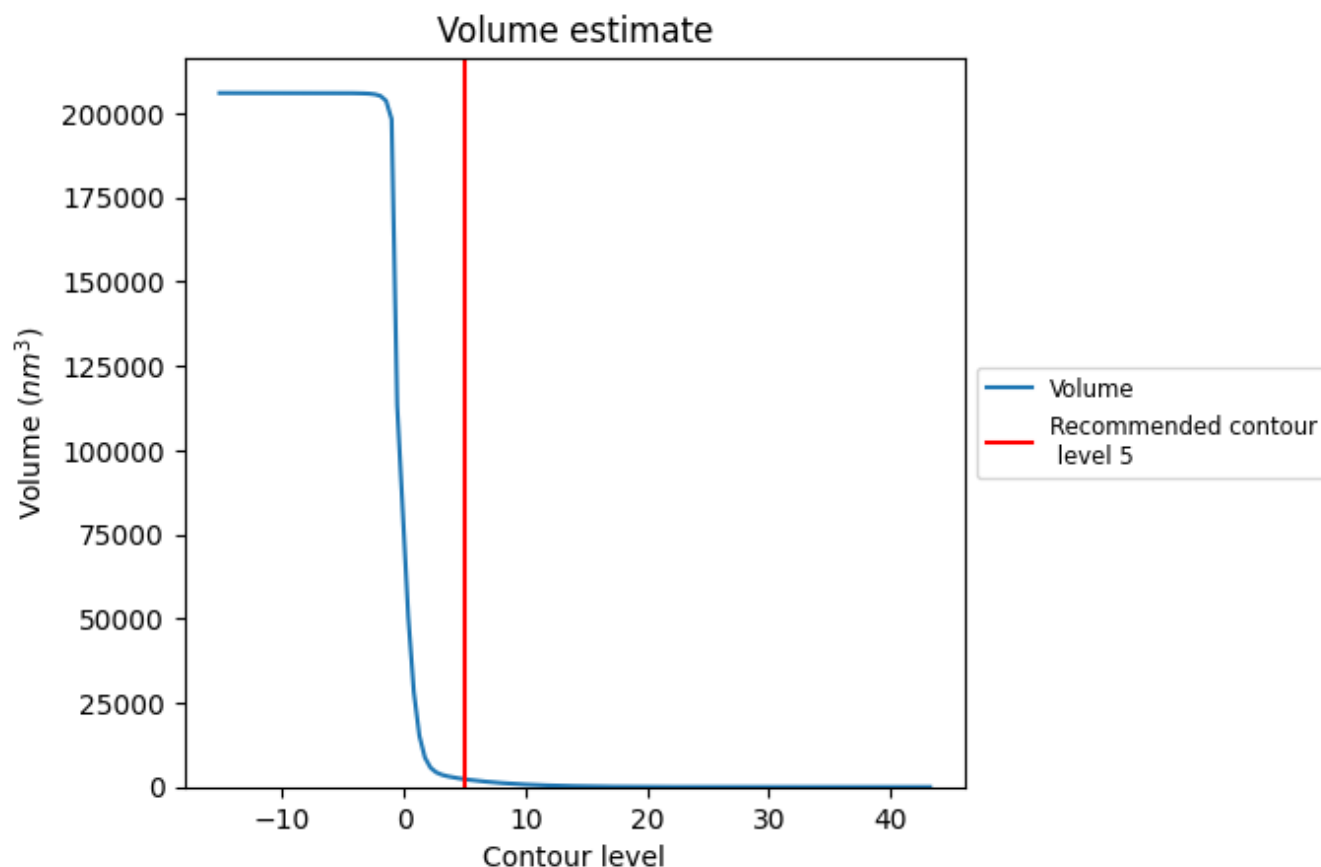
This section contains the results of statistical analysis of the map.

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.

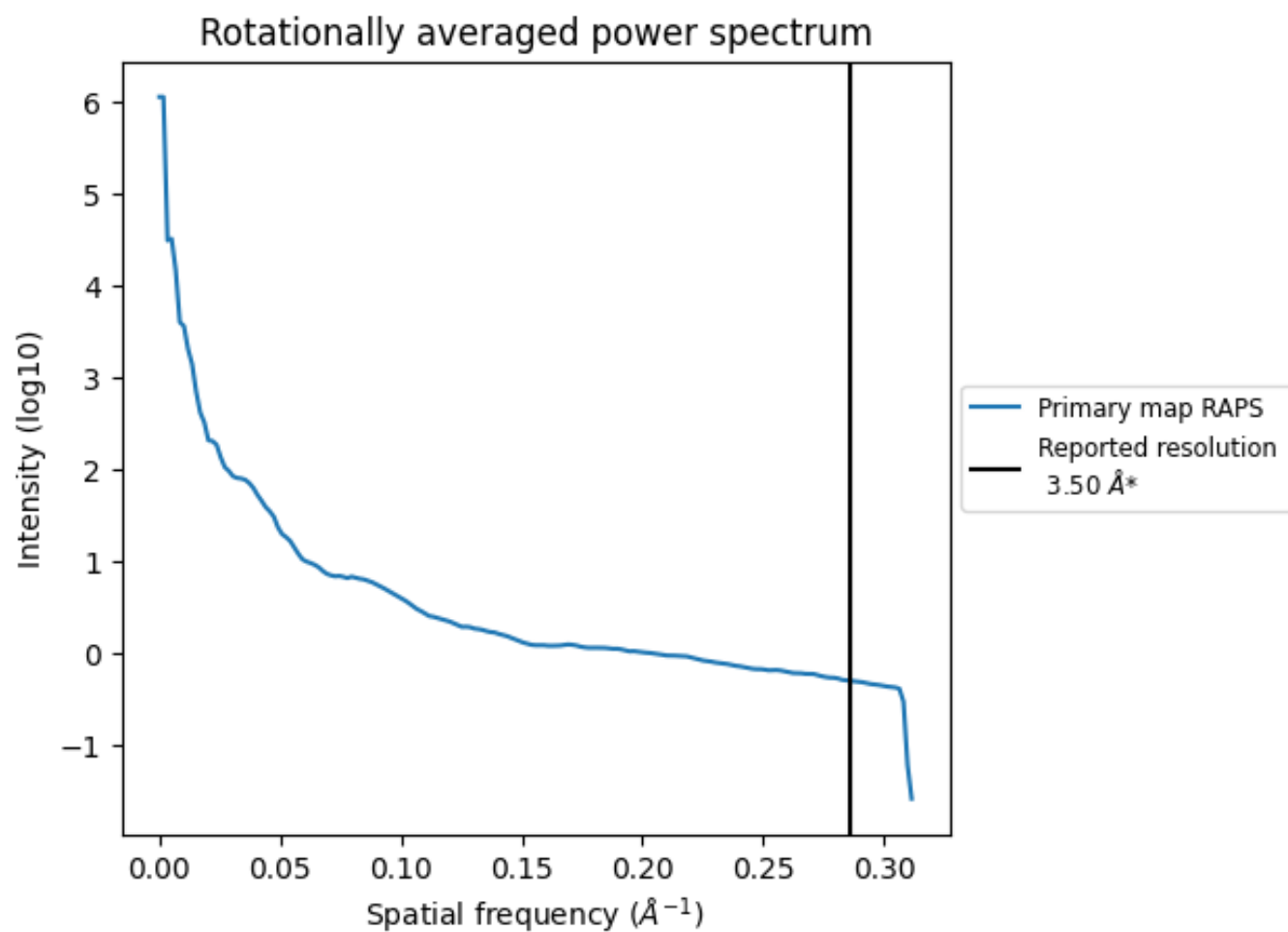
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 2302 nm^3 ; this corresponds to an approximate mass of 2079 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ



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

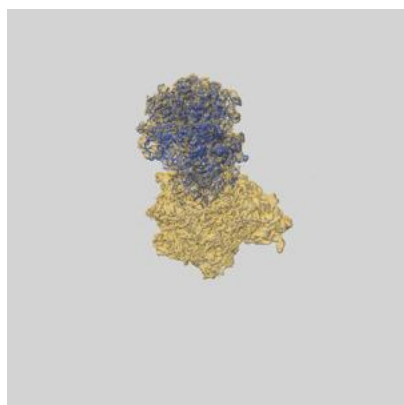
8 Fourier-Shell correlation

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

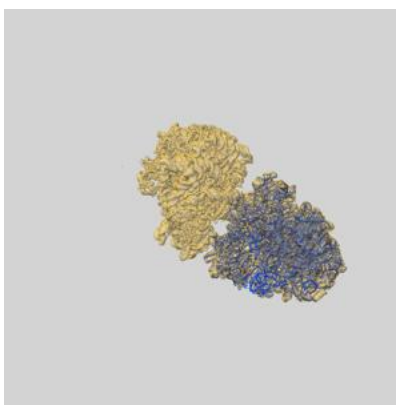
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-14158 and PDB model 7QV2. Per-residue inclusion information can be found in [section 3](#) on [page 13](#).

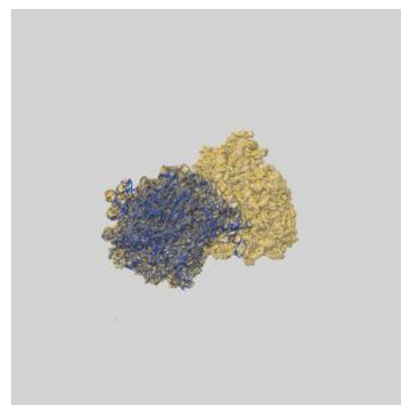
9.1 Map-model overlay [i](#)



X



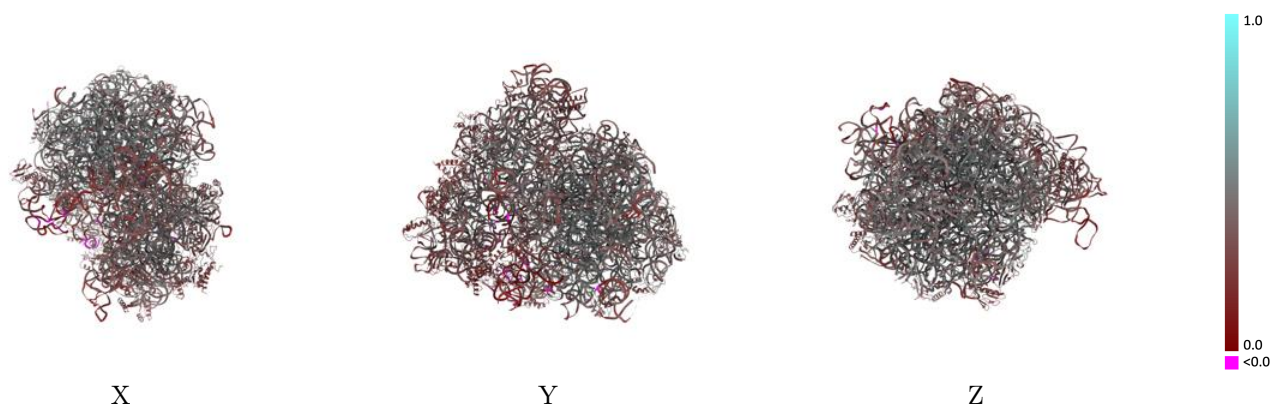
Y



Z

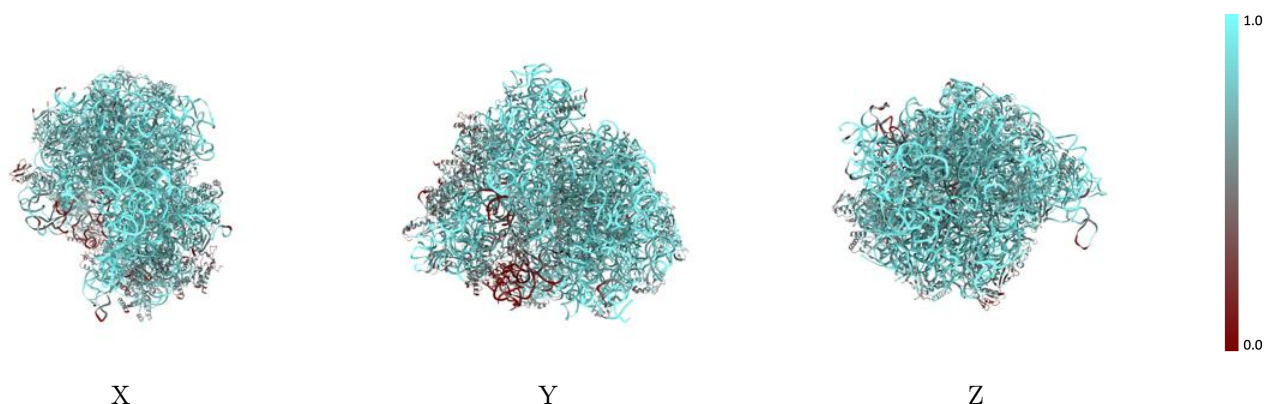
The images above show the 3D surface view of the map at the recommended contour level 5.0 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



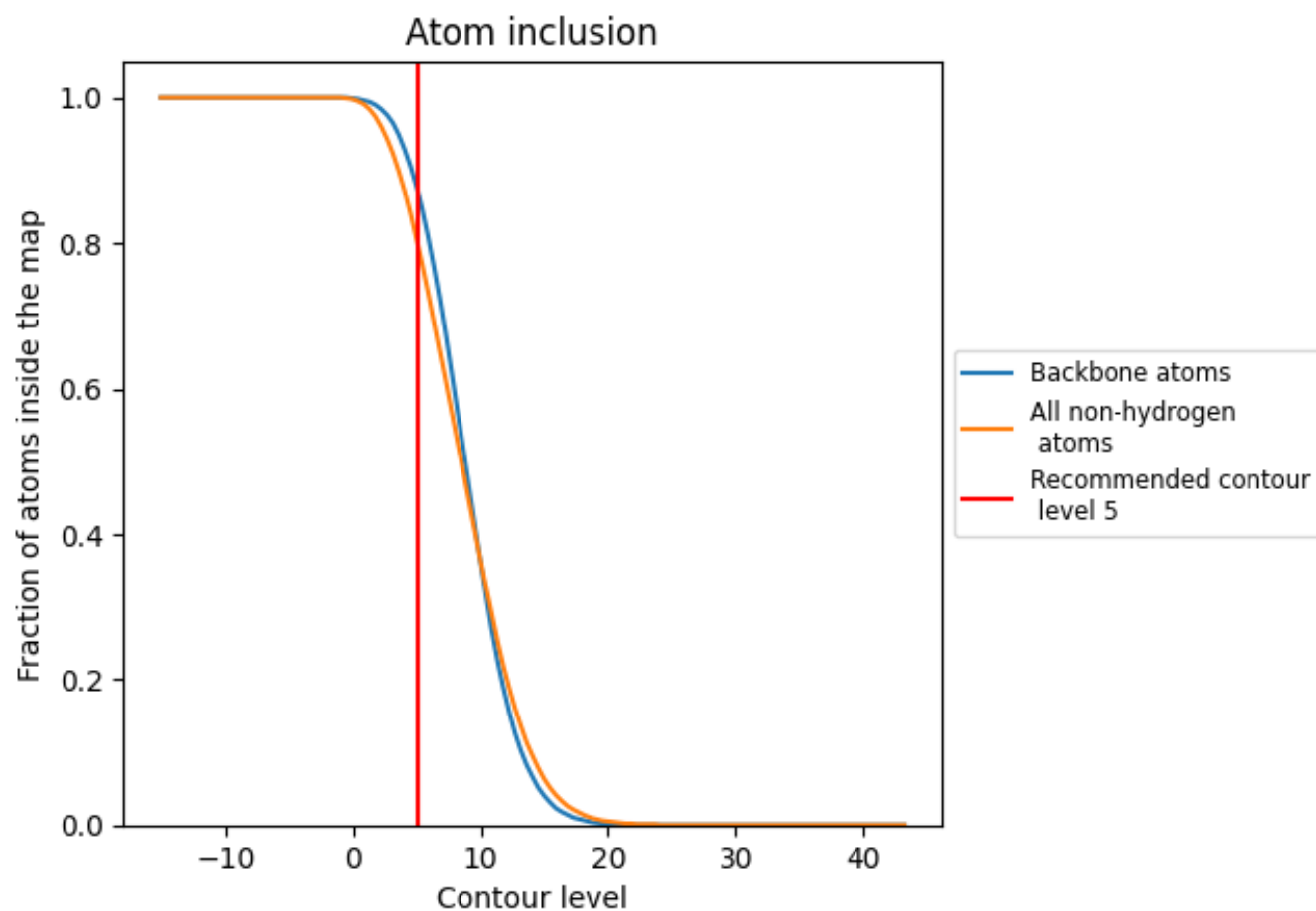
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (5).

9.4 Atom inclusion [i](#)



At the recommended contour level, 87% of all backbone atoms, 80% 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 (5) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8010	 0.3910
0	 0.7800	 0.4640
1	 0.6930	 0.4110
2	 0.8090	 0.4720
3	 0.8100	 0.5070
4	 0.6840	 0.4120
6	 0.0290	 0.1360
A	 0.4640	 0.2660
B	 0.8510	 0.3630
C	 0.7420	 0.4630
D	 0.7500	 0.4610
E	 0.6740	 0.4110
F	 0.1330	 0.2600
G	 0.5090	 0.3230
H	 0.3600	 0.2270
I	 0.1070	 0.2140
J	 0.7280	 0.4480
K	 0.6610	 0.4360
L	 0.6760	 0.4320
M	 0.7230	 0.4340
N	 0.7500	 0.4330
O	 0.5600	 0.3160
P	 0.6860	 0.4120
Q	 0.7340	 0.4250
R	 0.6230	 0.4130
S	 0.7130	 0.4500
T	 0.7200	 0.4200
U	 0.6750	 0.4180
V	 0.8730	 0.4170
W	 0.7370	 0.4550
Y	 0.6910	 0.3720
Z	 0.7040	 0.4170
a	 0.9170	 0.3820
b	 0.4780	 0.3030
c	 0.6430	 0.3500



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Chain	Atom inclusion	Q-score
d	 0.5440	 0.3310
e	 0.6190	 0.4060
f	 0.6010	 0.3470
g	 0.5540	 0.2530
h	 0.7030	 0.3920
i	 0.6530	 0.2940
j	 0.6350	 0.3340
k	 0.6250	 0.3180
l	 0.7400	 0.4270
m	 0.3640	 0.2180
n	 0.7630	 0.4090
o	 0.7460	 0.3550
p	 0.7260	 0.3870
q	 0.6800	 0.3630
r	 0.6910	 0.3790
s	 0.5590	 0.2940
t	 0.6750	 0.2750
u	 0.7320	 0.4380
x	 0.3710	 0.2120