



Full wwPDB EM Validation Report ⓘ

Mar 9, 2026 – 04:08 PM UTC

PDB ID : 5ND9 / pdb_00005nd9
EMDB ID : EMD-3625
Title : Hibernating ribosome from Staphylococcus aureus (Rotated state)
Authors : Khusainov, I.; Vicens, Q.; Ayupov, R.; Usachev, K.; Myasnikov, A.; Simonetti, A.; Validov, S.; Kieffer, B.; Yusupova, G.; Yusupov, M.; Hashem, Y.
Deposited on : 2017-03-07
Resolution : 3.70 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

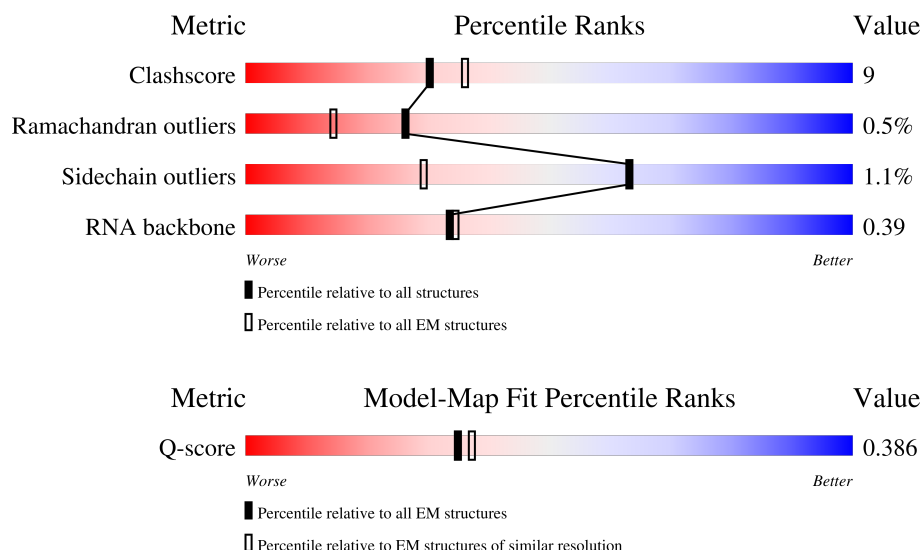
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.70 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	11569 (3.20 - 4.20)

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

Mol	Chain	Length	Quality of chain
1	a	1556	5% 56% 34% 9% •
2	b	255	63% 62% 25% 13% •
3	c	217	74% 71% 21% 6% •

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Mol	Chain	Length	Quality of chain
4	d	200	
5	e	166	
6	f	98	
7	g	156	
8	h	132	
9	i	132	
10	j	102	
11	k	129	
12	l	137	
13	m	121	
14	n	61	
15	o	89	
16	p	91	
17	q	87	
18	r	80	
19	s	92	
20	t	83	
21	u	58	
22	v	190	
23	A	2923	
24	B	114	
25	D	277	
26	E	220	
27	F	207	
28	G	179	

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Mol	Chain	Length	Quality of chain
29	H	178	
30	M	145	
31	N	122	
32	O	146	
33	P	144	
34	Q	122	
35	R	119	
36	S	116	
37	T	118	
38	U	102	
39	V	117	
40	W	91	
41	X	105	
42	Y	217	
43	Z	94	
44	0	62	
45	1	69	
46	2	59	
47	3	84	
48	4	58	
49	5	49	
50	6	45	
51	7	66	
52	8	37	

2 Entry composition

There are 52 unique types of molecules in this entry. The entry contains 141051 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a RNA chain called 16S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	a	1541	Total	C	N	O	P	0	0
			33006	14736	6021	10708	1541		

- Molecule 2 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	b	222	Total	C	N	O	S	0	0
			1788	1139	313	330	6		

- Molecule 3 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	c	203	Total	C	N	O	S	0	0
			1600	1007	301	290	2		

- Molecule 4 is a protein called 30S ribosomal protein S4.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	d	197	Total	C	N	O	S	0	0
			1600	1009	300	289	2		

- Molecule 5 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	e	160	Total	C	N	O	S	0	0
			1194	750	218	224	2		

- Molecule 6 is a protein called 30S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	f	94	Total	C	N	O	S	0	0
			781	494	137	147	3		

- Molecule 7 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	g	143	Total	C	N	O	S	0	0
			1142	712	216	210	4		

- Molecule 8 is a protein called 30S ribosomal protein S8.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	h	131	Total	C	N	O	S	0	0
			1032	652	183	193	4		

- Molecule 9 is a protein called 30S ribosomal protein S9.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	i	128	Total	C	N	O	S	0	0
			1017	629	203	184	1		

- Molecule 10 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	j	99	Total	C	N	O	S	0	0
			791	498	144	147	2		

- Molecule 11 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	k	115	Total	C	N	O	S	0	0
			851	526	160	162	3		

- Molecule 12 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	l	135	Total	C	N	O	S	0	0
			1058	658	214	184	2		

- Molecule 13 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	m	110	Total	C	N	O	S	0	0
			877	537	175	164	1		

- Molecule 14 is a protein called 30S ribosomal protein S14 type Z.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	n	60	Total	C	N	O	S	0	0
			502	317	100	80	5		

- Molecule 15 is a protein called 30S ribosomal protein S15.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	o	88	Total	C	N	O	S	0	0
			738	454	153	130	1		

- Molecule 16 is a protein called 30S ribosomal protein S16.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	p	90	Total	C	N	O	S	0	0
			712	448	132	131	1		

- Molecule 17 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	q	85	Total	C	N	O	S	0	0
			698	441	125	131	1		

- Molecule 18 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	r	56	Total	C	N	O	S	0	0
			466	295	88	81	2		

- Molecule 19 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	s	84	Total	C	N	O	S	0	0
			677	434	120	121	2		

- Molecule 20 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	t	80	Total	C	N	O	S	0	0
			606	367	119	118	2		

- Molecule 21 is a protein called 30S ribosomal protein S21.

Mol	Chain	Residues	Atoms				AltConf	Trace
21	u	45	Total	C	N	O	0	0
			377	233	76	68		

- Molecule 22 is a protein called Ribosome hibernation promotion factor.

Mol	Chain	Residues	Atoms				AltConf	Trace
22	v	101	Total	C	N	O	0	0
			831	518	156	157		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
23	A	2914	Total	C	N	O	P	0	0
			62480	27894	11427	20245	2914		

- Molecule 24 is a RNA chain called 5S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	B	114	Total	C	N	O	P	0	0
			2430	1086	436	794	114		

- Molecule 25 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	D	275	Total	C	N	O	S	0	0
			2103	1309	417	372	5		

- Molecule 26 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	E	218	Total	C	N	O	S	0	0
			1649	1030	304	310	5		

- Molecule 27 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	F	199	Total	C	N	O	S	0	0
			1524	955	281	286	2		

- Molecule 28 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	G	166	Total	C	N	O	S	0	0
			1311	832	223	250	6		

- Molecule 29 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	H	164	Total	C	N	O	S	0	0
			1284	799	232	250	3		

- Molecule 30 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	M	145	Total	C	N	O	S	0	0
			1151	717	211	220	3		

- Molecule 31 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	N	122	Total	C	N	O	S	0	0
			920	572	174	170	4		

- Molecule 32 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	O	131	Total	C	N	O	S	0	0
			997	618	197	181	1		

- Molecule 33 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	P	133	Total	C	N	O	S	0	0
			1065	681	203	178	3		

- Molecule 34 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	Q	117	Total	C	N	O	S	0	0
			924	564	179	180	1		

- Molecule 35 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	R	119	Total	C	N	O	S	0	0
			922	574	174	173	1		

- Molecule 36 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	S	107	Total	C	N	O	S	0	0
			862	544	173	145			

- Molecule 37 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	T	116	Total	C	N	O	S	0	0
			943	593	189	157	4		

- Molecule 38 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	U	102	Total	C	N	O	S	0	0
			799	506	142	150	1		

- Molecule 39 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	V	112	Total	C	N	O	S	0	0
			862	537	164	158	3		

- Molecule 40 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	W	89	Total	C	N	O	S	0	0
			725	457	130	134	4		

- Molecule 41 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	X	87	Total	C	N	O	S	0	0
			668	423	122	122	1		

- Molecule 42 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	Y	94	Total	C	N	O	S	0	0
			738	471	131	134	2		

- Molecule 43 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	Z	77	Total	C	N	O		0	0
			591	364	115	112			

- Molecule 44 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	0	46	Total	C	N	O		0	0
			373	231	83	59			

- Molecule 45 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	1	65	Total	C	N	O		0	0
			536	330	101	105			

- Molecule 46 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	2	57	Total	C	N	O		0	0
			441	274	83	84			

- Molecule 47 is a protein called 50S ribosomal protein L31 type B.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	3	81	Total	C	N	O	S	0	0
			663	423	113	124	3		

- Molecule 48 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	4	44	Total	C	N	O	S	0	0
			360	220	78	58	4		

- Molecule 49 is a protein called 50S ribosomal protein L33 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	5	28	Total	C	N	O	S	0	0
			229	137	45	43	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
50	6	44	Total	C	N	O	S	0	0
			373	228	90	54	1		

- Molecule 51 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	7	60	Total	C	N	O	S	0	0
			487	300	108	77	2		

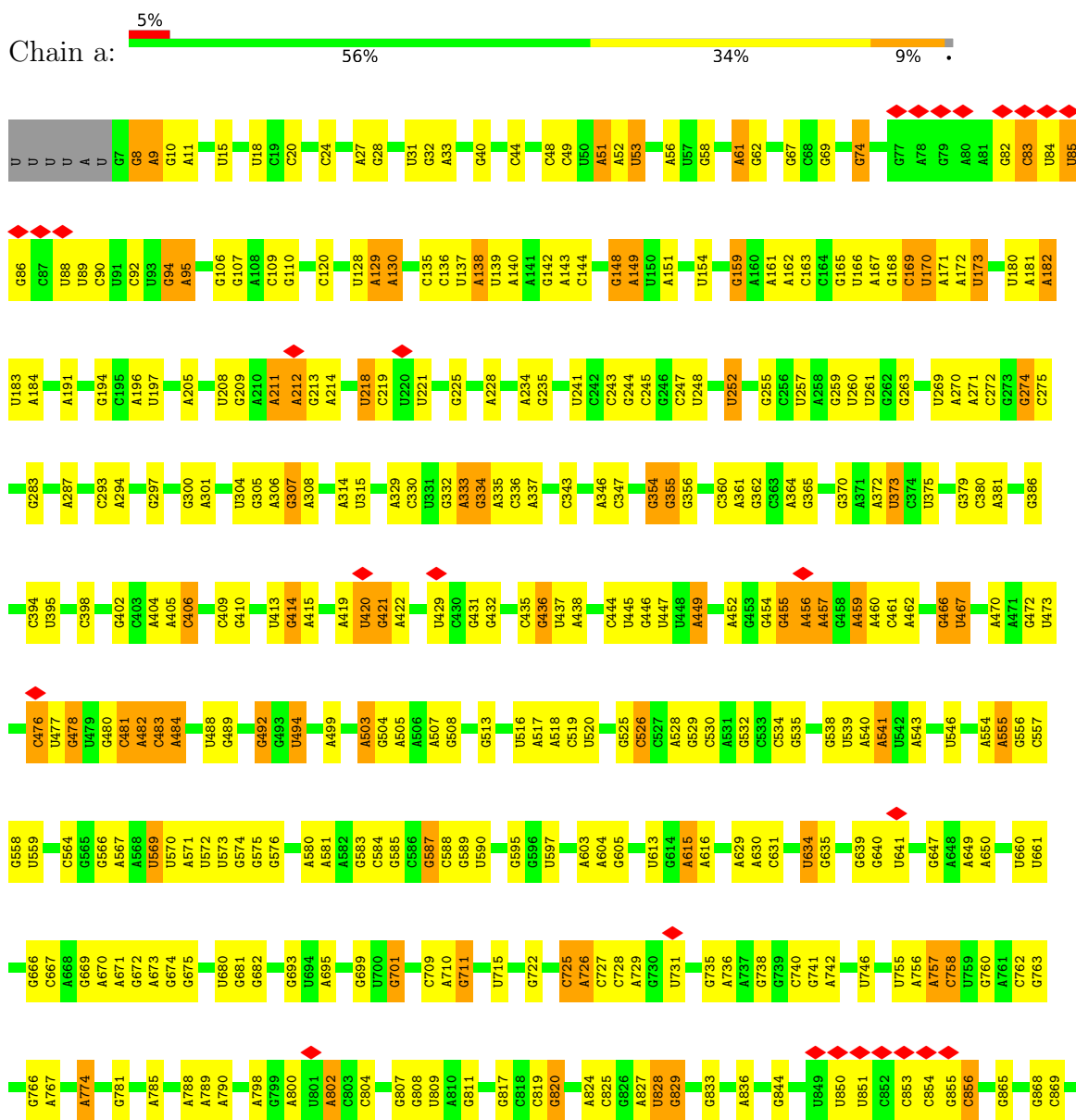
- Molecule 52 is a protein called 50S ribosomal protein L36.

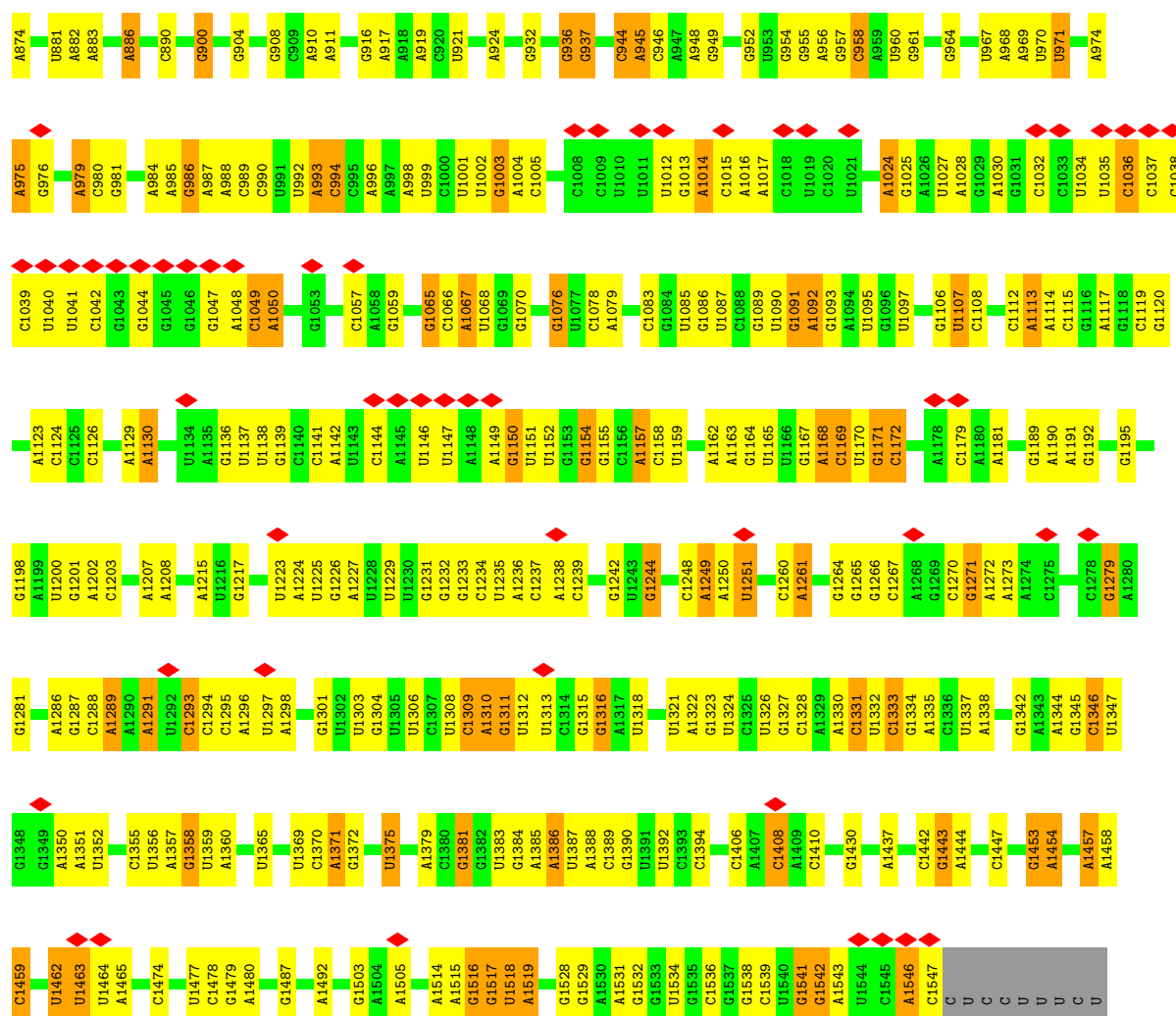
Mol	Chain	Residues	Atoms					AltConf	Trace
52	8	37	Total	C	N	O	S	0	0
			297	186	60	46	5		

3 Residue-property plots

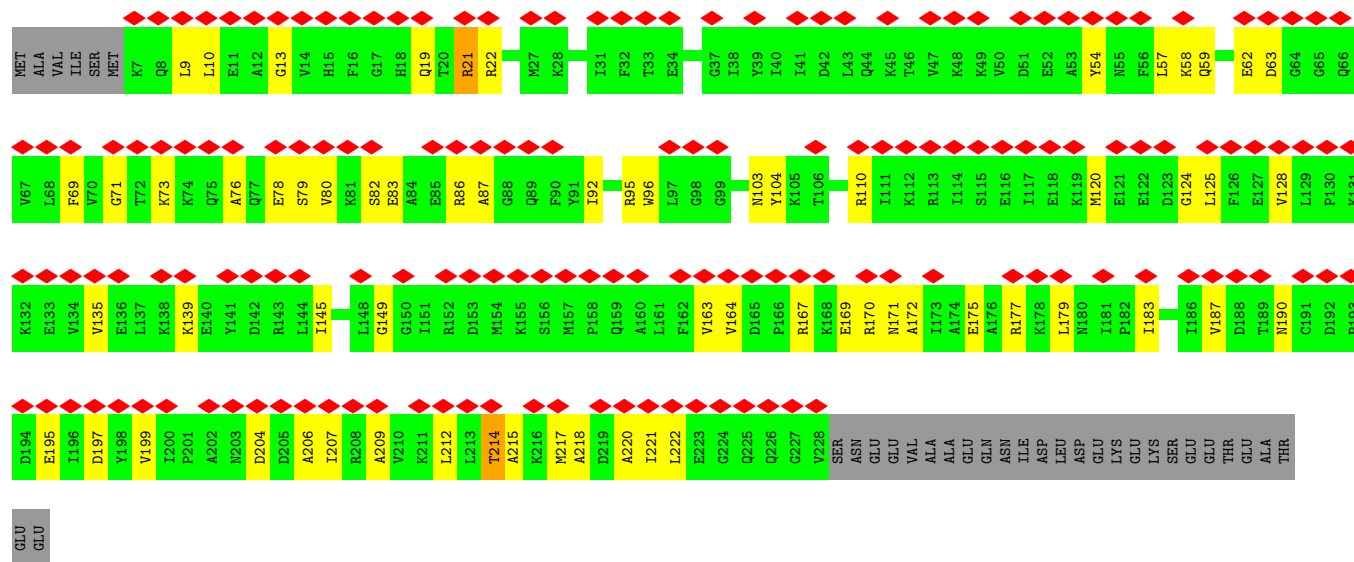
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

• Molecule 1: 16S ribosomal RNA

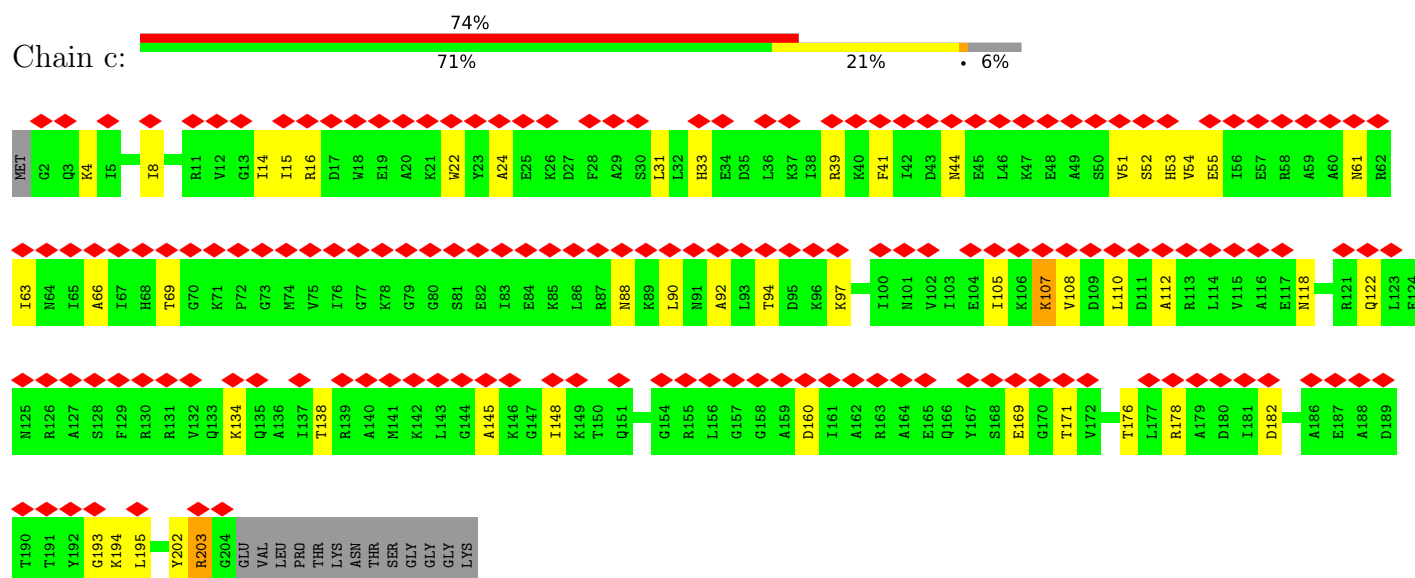




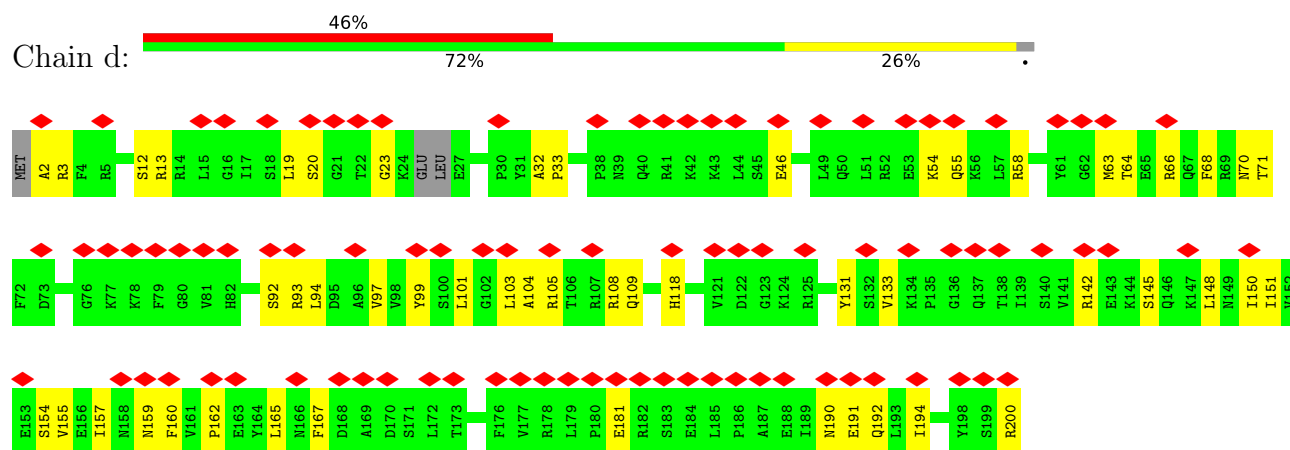
• Molecule 2: 30S ribosomal protein S2



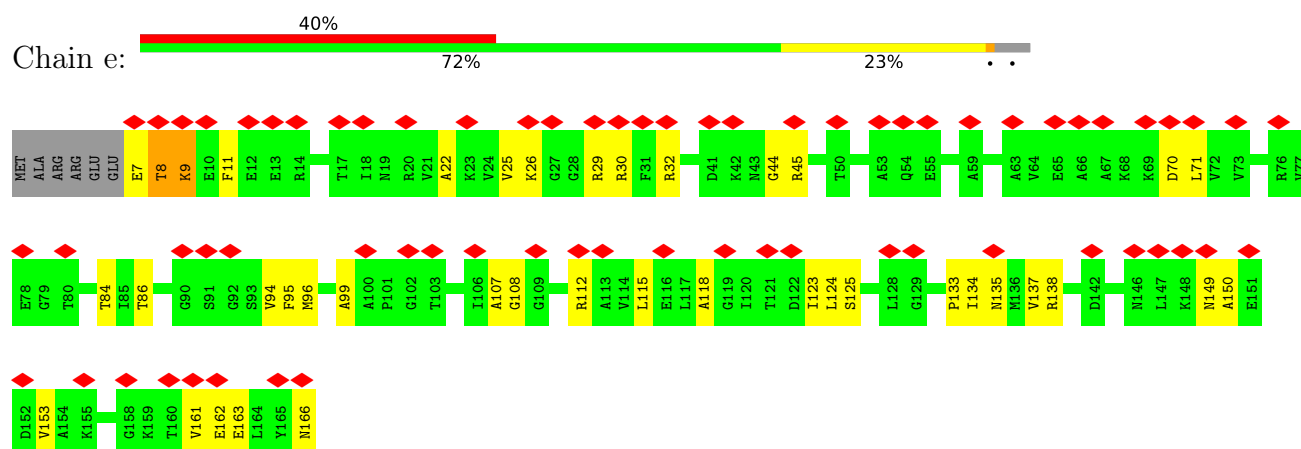
- Molecule 3: 30S ribosomal protein S3



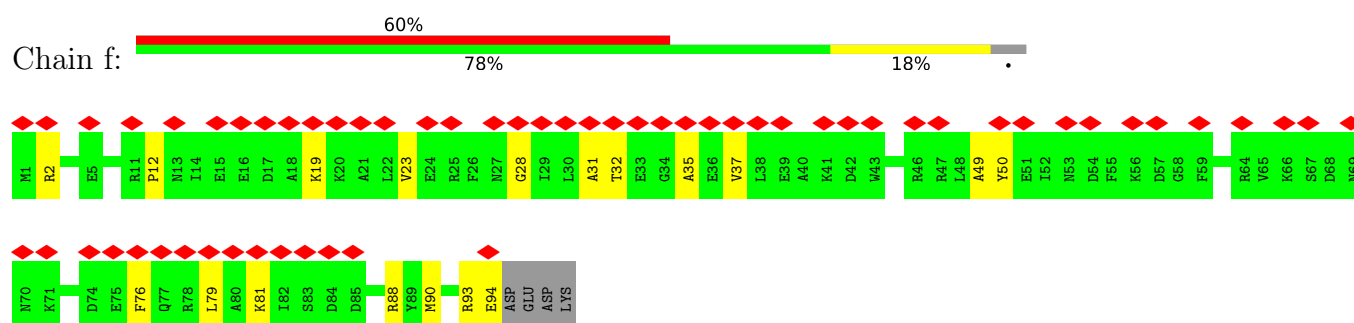
- Molecule 4: 30S ribosomal protein S4



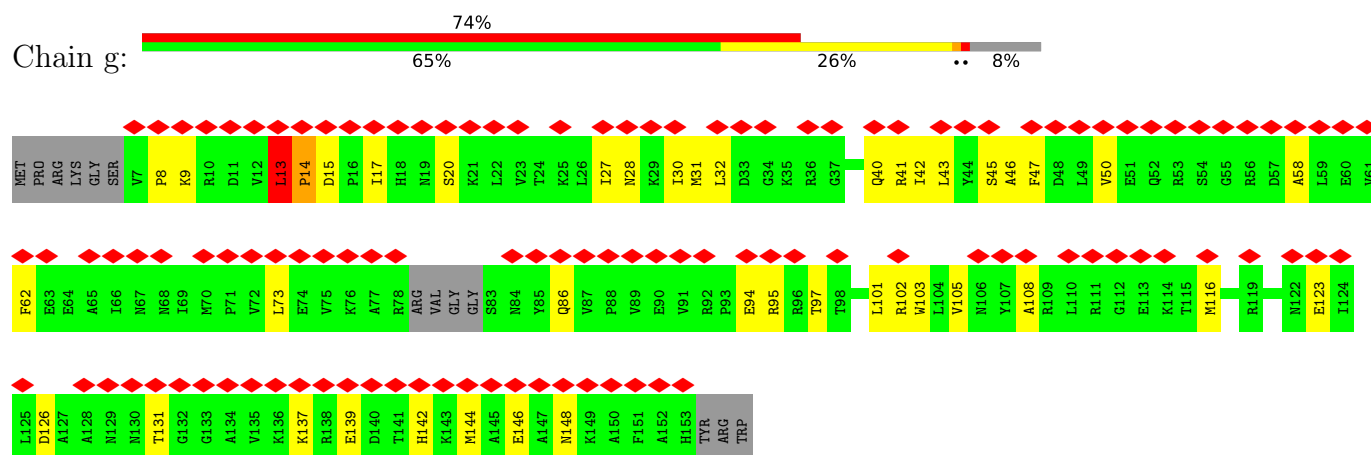
- Molecule 5: 30S ribosomal protein S5



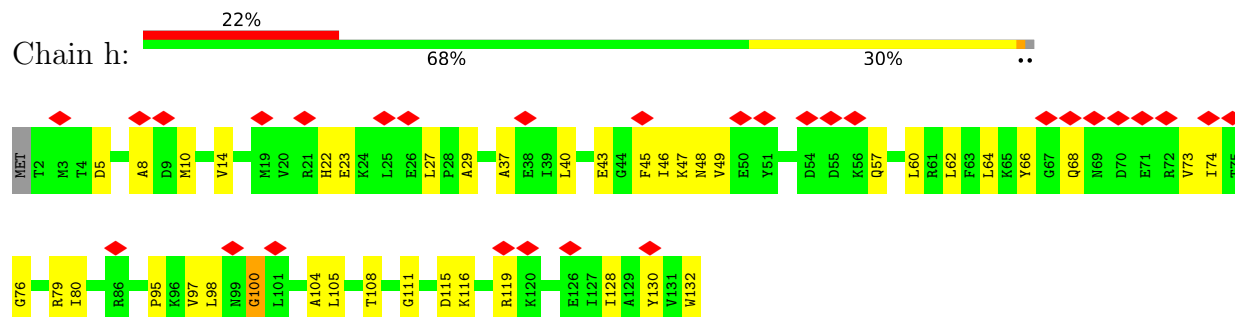
- Molecule 6: 30S ribosomal protein S6



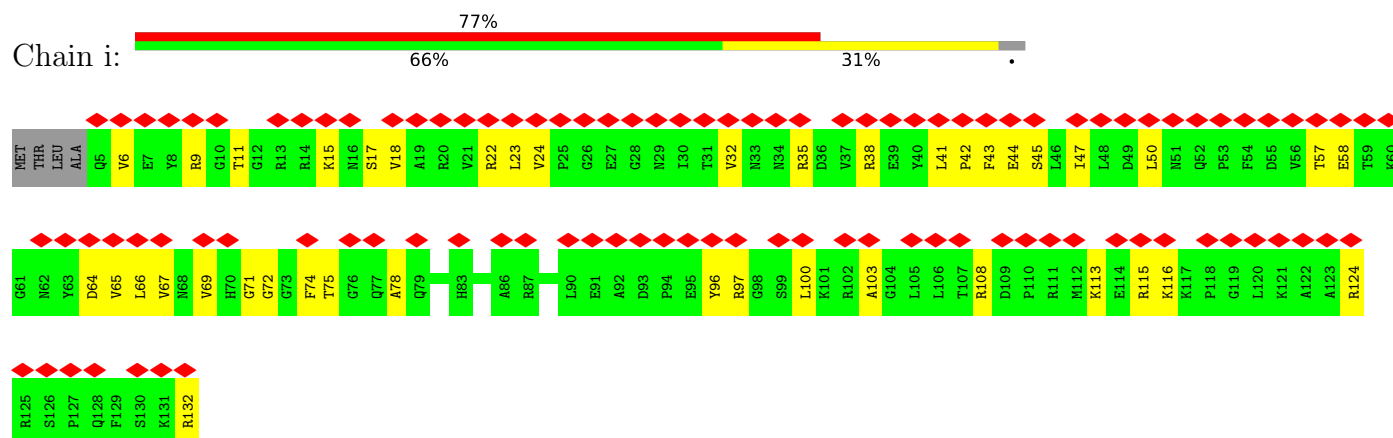
• Molecule 7: 30S ribosomal protein S7



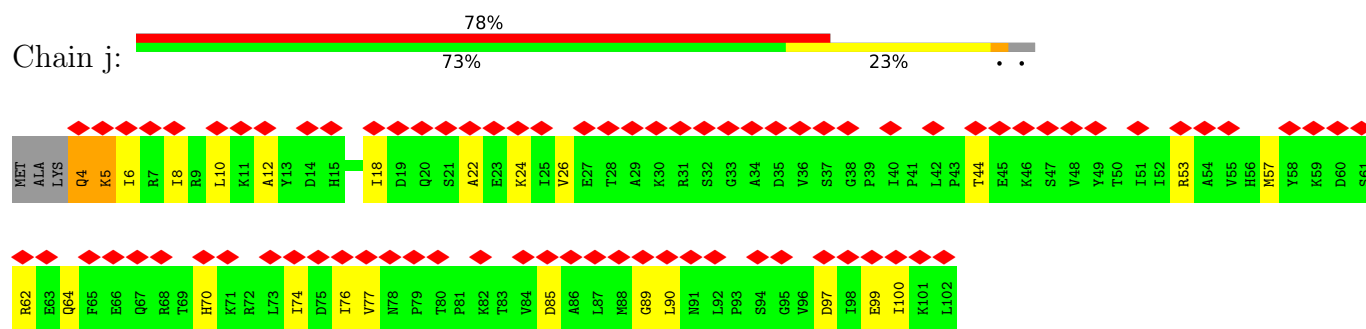
• Molecule 8: 30S ribosomal protein S8



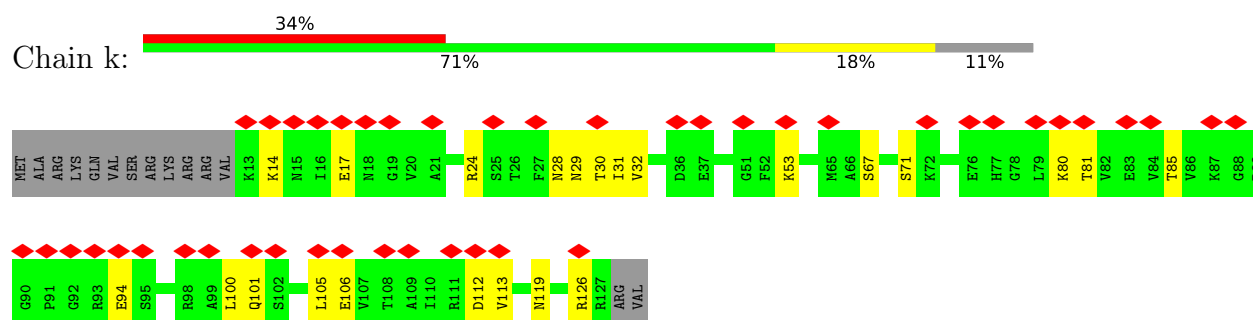
• Molecule 9: 30S ribosomal protein S9



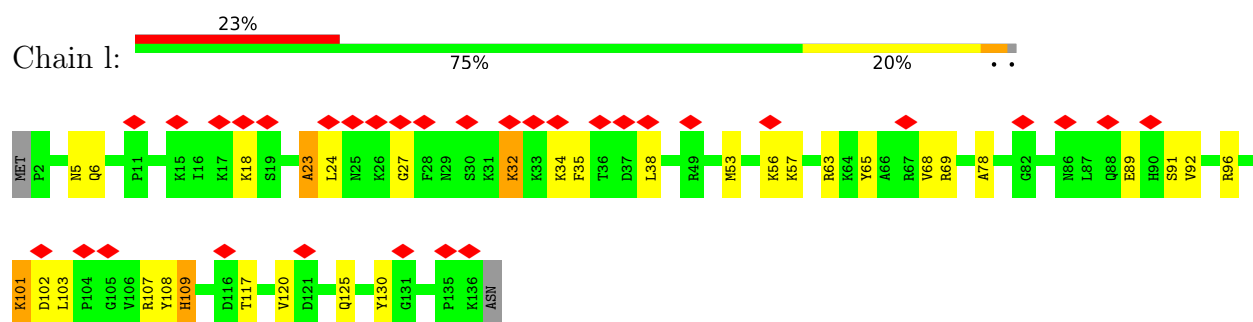
- Molecule 10: 30S ribosomal protein S10



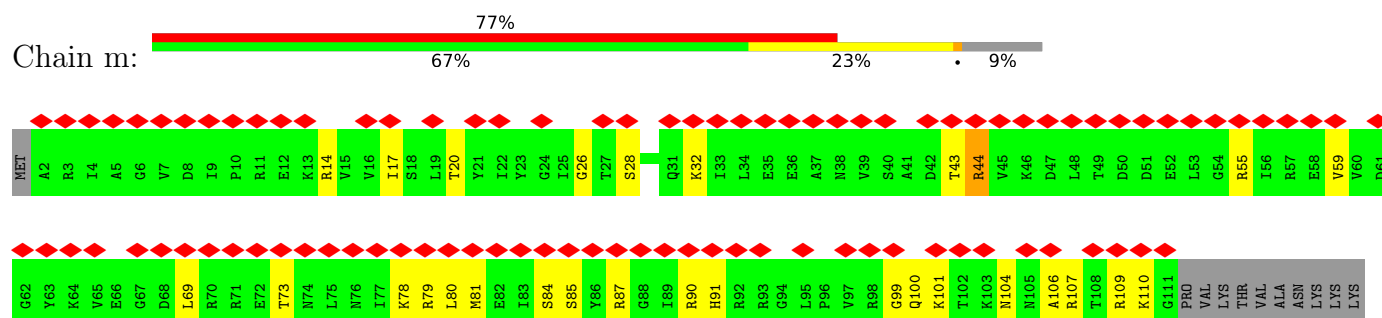
- Molecule 11: 30S ribosomal protein S11



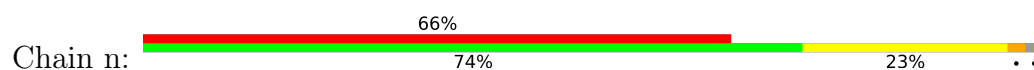
- Molecule 12: 30S ribosomal protein S12

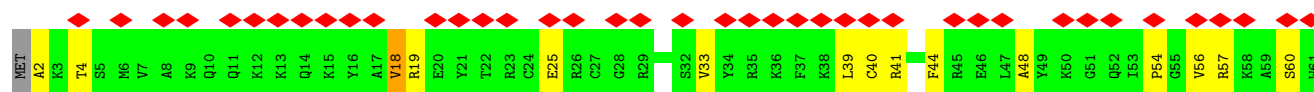


- Molecule 13: 30S ribosomal protein S13

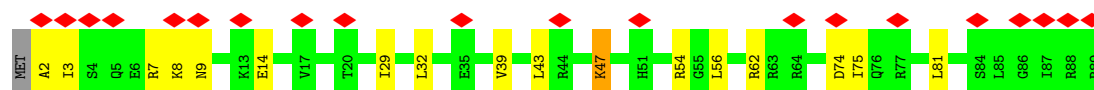
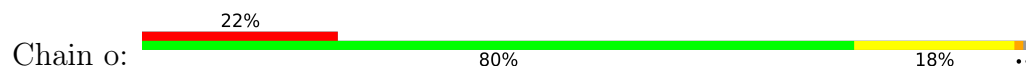


- Molecule 14: 30S ribosomal protein S14 type Z

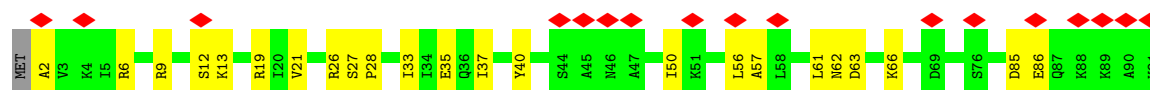
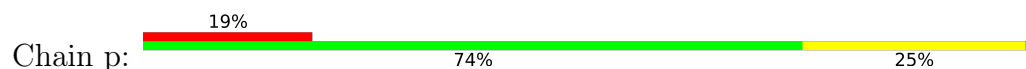




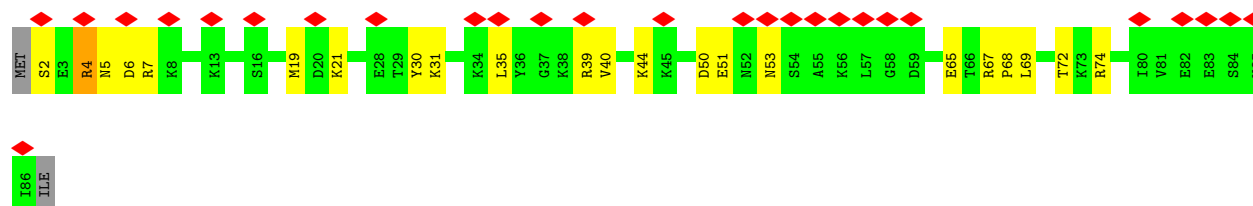
- Molecule 15: 30S ribosomal protein S15



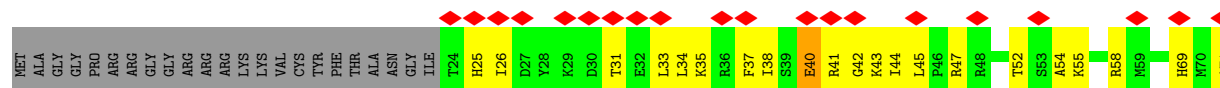
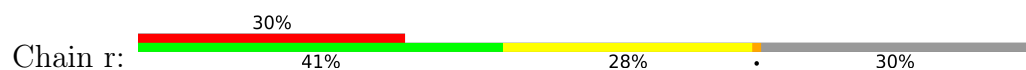
- Molecule 16: 30S ribosomal protein S16



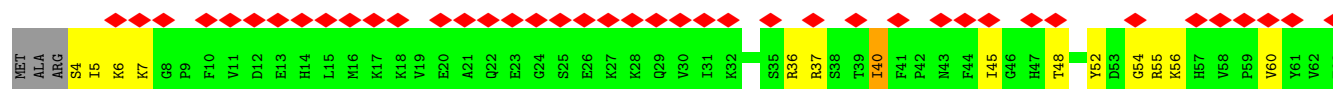
- Molecule 17: 30S ribosomal protein S17



- Molecule 18: 30S ribosomal protein S18

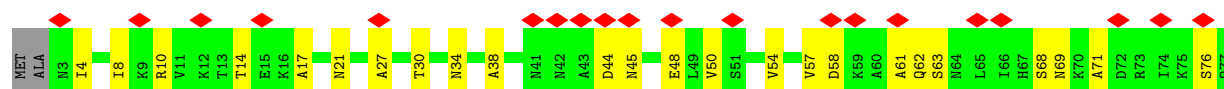


- Molecule 19: 30S ribosomal protein S19

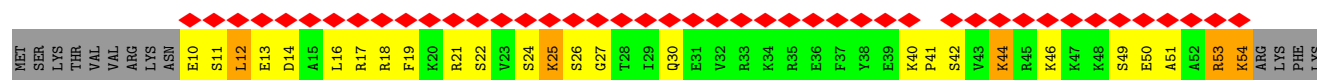
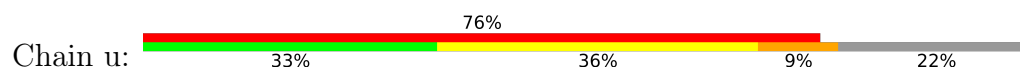




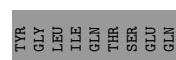
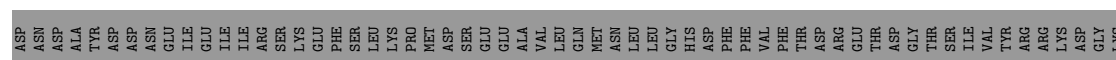
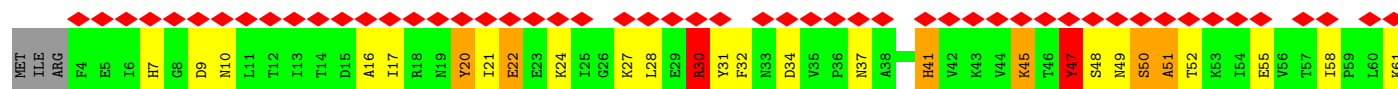
• Molecule 20: 30S ribosomal protein S20



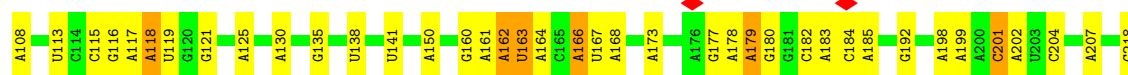
• Molecule 21: 30S ribosomal protein S21



• Molecule 22: Ribosome hibernation promotion factor



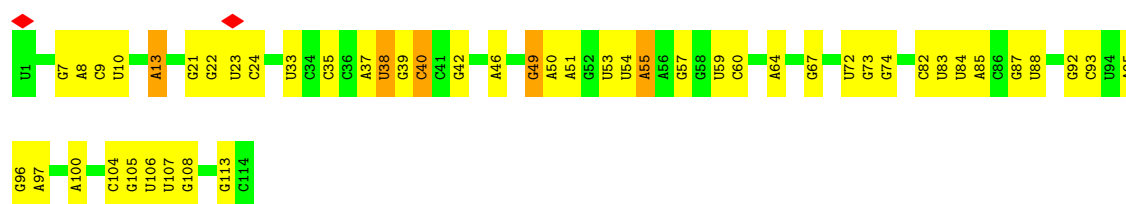
• Molecule 23: 23S ribosomal RNA





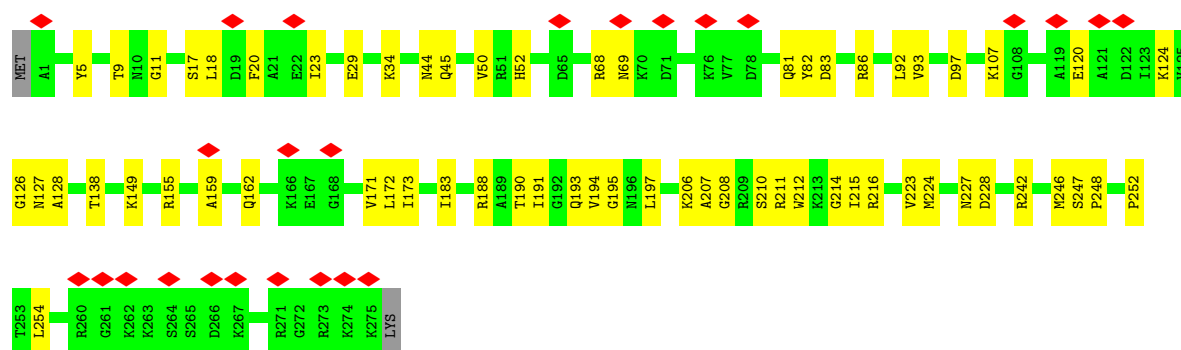


Chain B: 



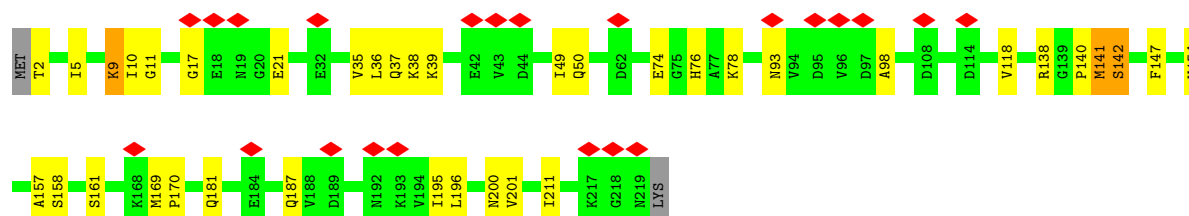
- Molecule 25: 50S ribosomal protein L2

Chain D: 



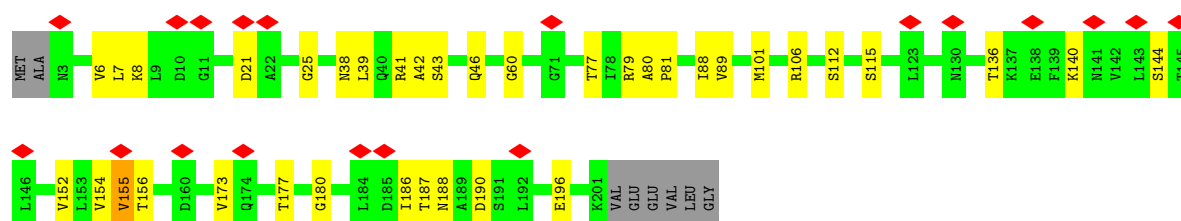
- Molecule 26: 50S ribosomal protein L3

Chain E: 



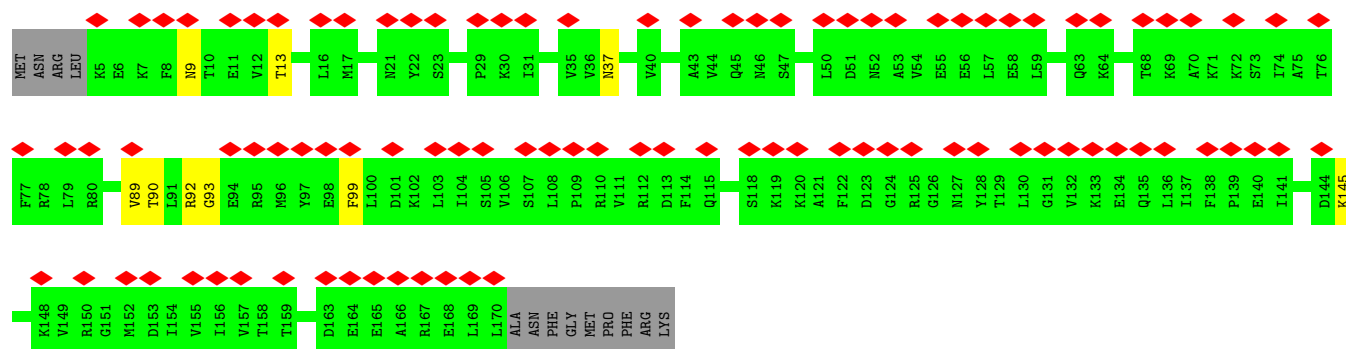
- Molecule 27: 50S ribosomal protein L4

Chain F: 

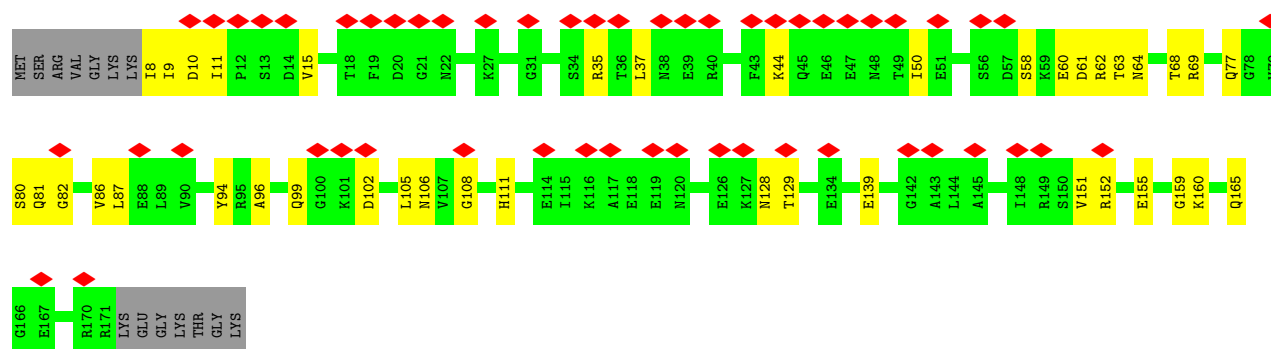


- Molecule 28: 50S ribosomal protein L5

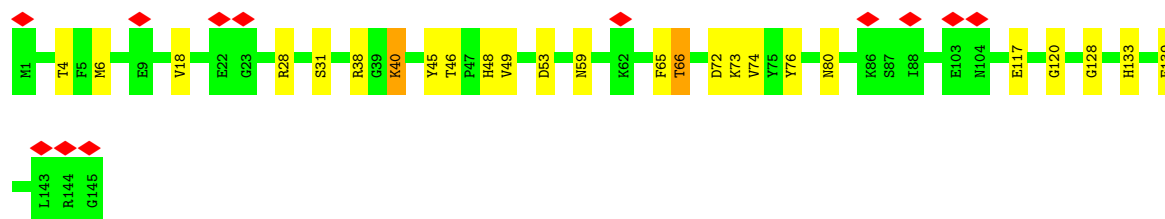
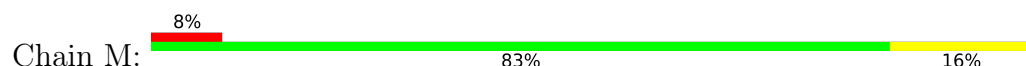
Chain G: 



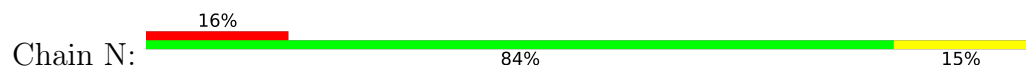
• Molecule 29: 50S ribosomal protein L6



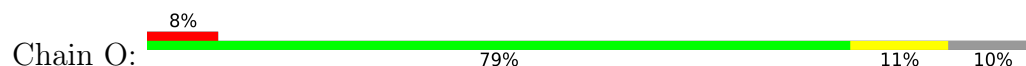
• Molecule 30: 50S ribosomal protein L13

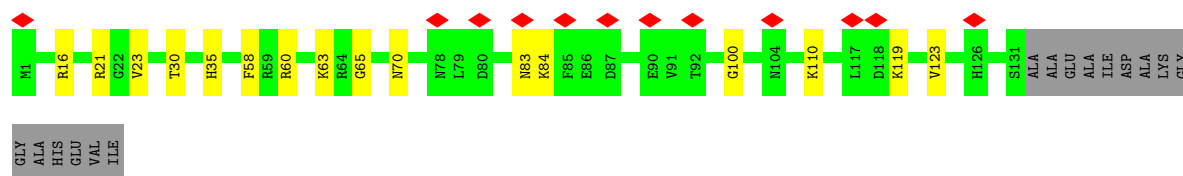


• Molecule 31: 50S ribosomal protein L14

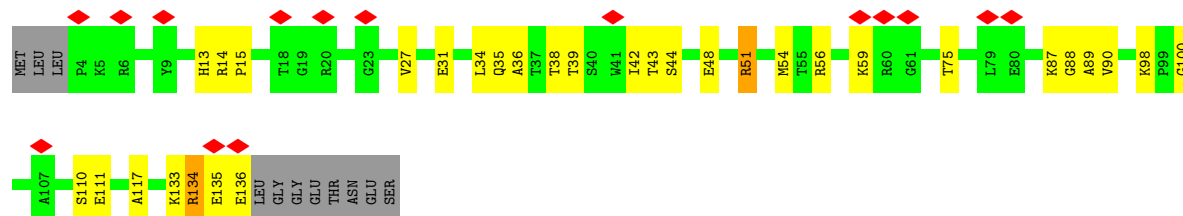


• Molecule 32: 50S ribosomal protein L15

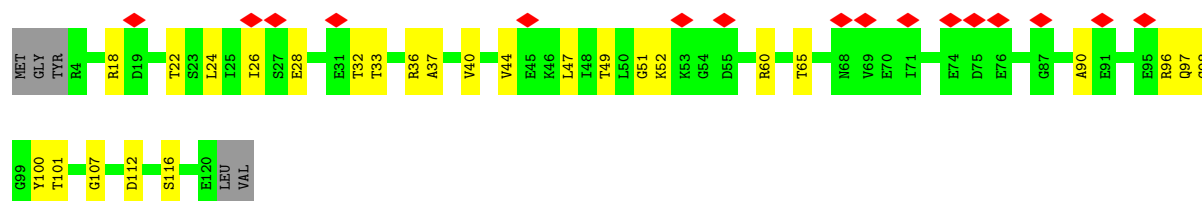
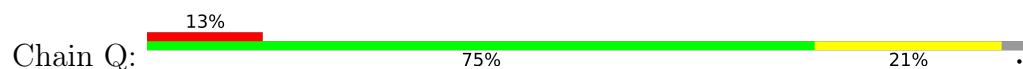




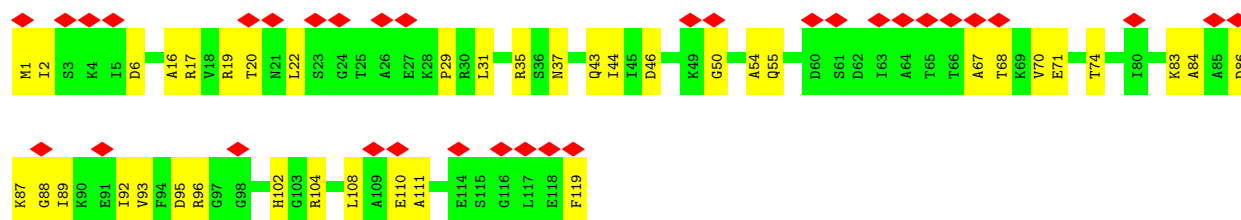
• Molecule 33: 50S ribosomal protein L16



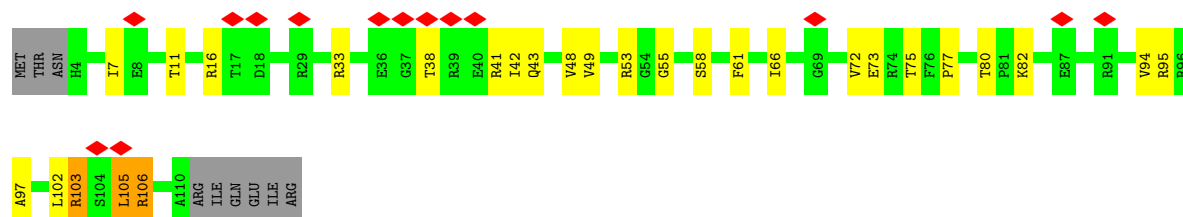
• Molecule 34: 50S ribosomal protein L17



• Molecule 35: 50S ribosomal protein L18



• Molecule 36: 50S ribosomal protein L19



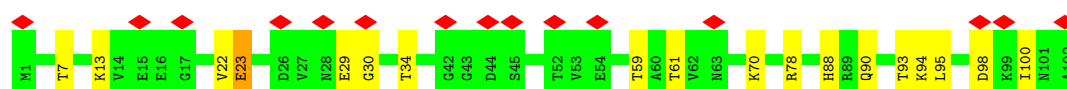
- Molecule 37: 50S ribosomal protein L20

Chain T: 



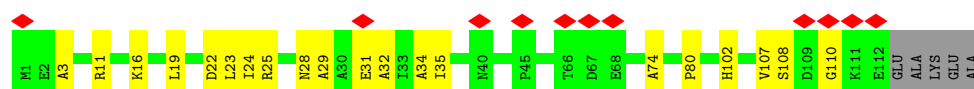
- Molecule 38: 50S ribosomal protein L21

Chain U: 



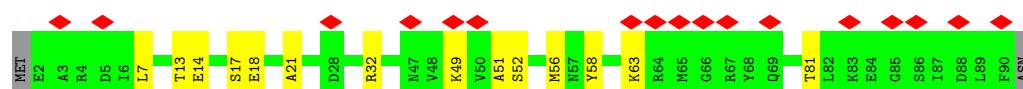
- Molecule 39: 50S ribosomal protein L22

Chain V: 



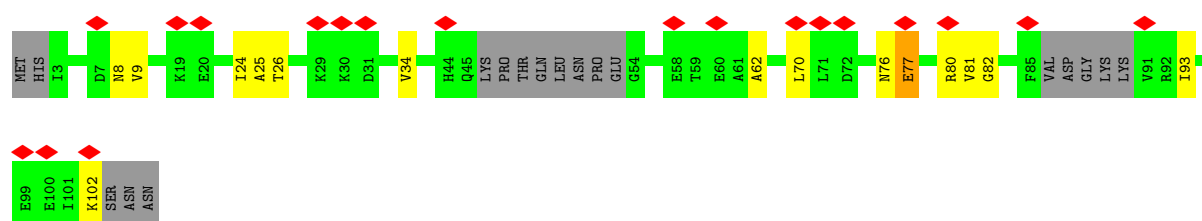
- Molecule 40: 50S ribosomal protein L23

Chain W: 



- Molecule 41: 50S ribosomal protein L24

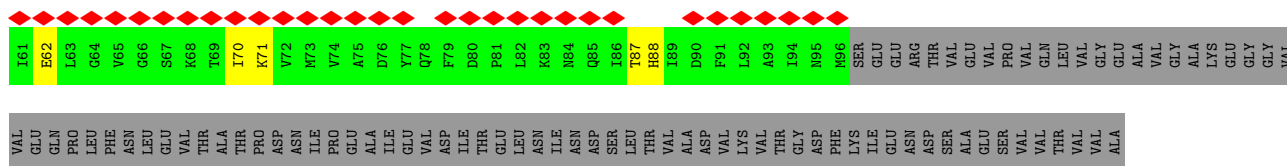
Chain X: 



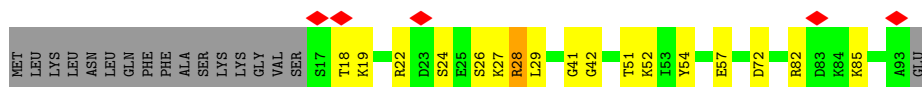
- Molecule 42: 50S ribosomal protein L25

Chain Y: 

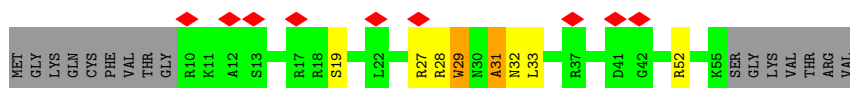




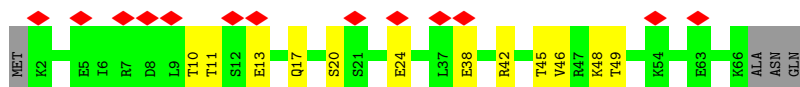
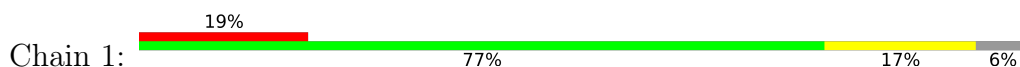
- Molecule 43: 50S ribosomal protein L27



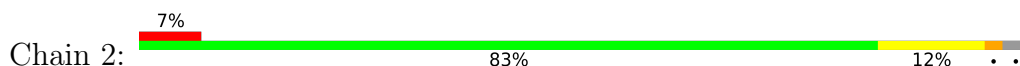
- Molecule 44: 50S ribosomal protein L28



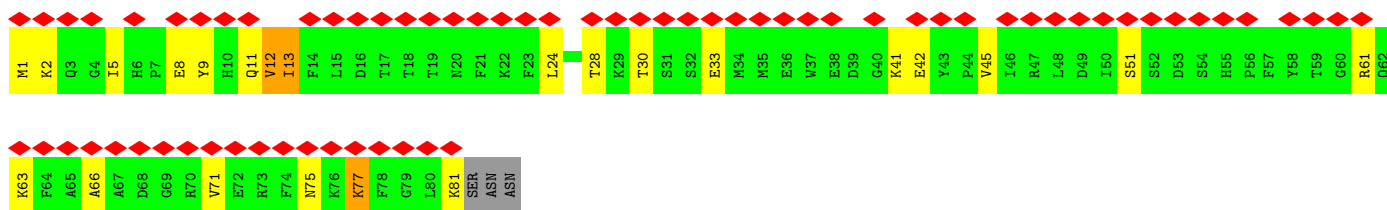
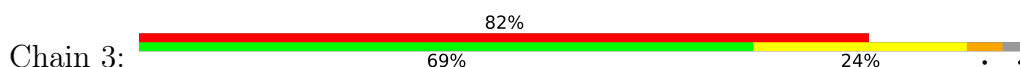
- Molecule 45: 50S ribosomal protein L29



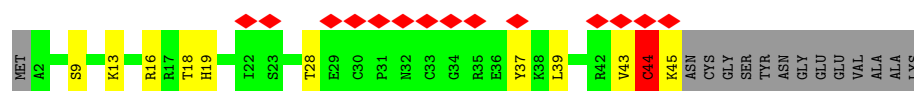
- Molecule 46: 50S ribosomal protein L30



- Molecule 47: 50S ribosomal protein L31 type B



- Molecule 48: 50S ribosomal protein L32



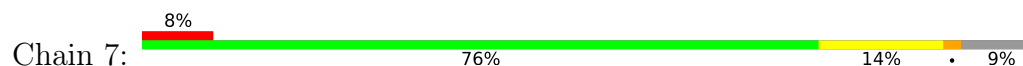
- Molecule 49: 50S ribosomal protein L33 2



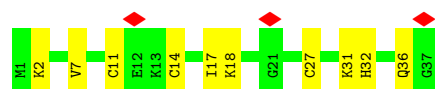
- Molecule 50: 50S ribosomal protein L34



- Molecule 51: 50S ribosomal protein L35



- Molecule 52: 50S ribosomal protein L36



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	83000	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 ($e^-/\text{\AA}^2$)	60	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	FEI FALCON II (4k x 4k)	Depositor
Maximum map value	0.299	Depositor
Minimum map value	-0.132	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.017	Depositor
Recommended contour level	0.05	Depositor
Map size (Å)	374.0, 374.0, 374.0	wwPDB
Map dimensions	340, 340, 340	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.1, 1.1, 1.1	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	a	0.44	0/36954	0.48	1/57629 (0.0%)
2	b	0.46	0/1815	0.76	2/2436 (0.1%)
3	c	0.40	0/1622	0.69	2/2178 (0.1%)
4	d	0.42	0/1629	0.72	0/2185
5	e	0.52	0/1208	0.71	0/1628
6	f	0.48	0/792	0.60	0/1062
7	g	0.43	0/1157	0.73	0/1557
8	h	0.59	0/1044	0.74	0/1401
9	i	0.39	0/1033	0.73	0/1386
10	j	0.40	0/803	0.65	0/1082
11	k	0.47	0/866	0.67	0/1169
12	l	0.60	0/1075	0.84	0/1439
13	m	0.40	0/883	0.77	0/1182
14	n	0.42	0/512	0.86	3/678 (0.4%)
15	o	0.54	0/747	0.82	0/996
16	p	0.56	0/723	0.67	0/971
17	q	0.51	0/706	0.73	0/944
18	r	0.54	0/473	0.79	0/632
19	s	0.39	0/695	0.74	0/934
20	t	0.46	0/606	0.76	2/810 (0.2%)
21	u	0.32	0/380	0.60	0/498
22	v	0.41	0/841	0.86	4/1131 (0.4%)
23	A	0.60	0/69971	0.55	5/109124 (0.0%)
24	B	0.42	0/2717	0.47	0/4232
25	D	0.87	1/2138 (0.0%)	0.79	0/2869
26	E	0.76	1/1673 (0.1%)	0.72	0/2243
27	F	0.70	0/1547	0.75	0/2088
28	G	0.39	0/1326	0.75	0/1780
29	H	0.50	1/1302 (0.1%)	0.63	0/1757
30	M	0.67	0/1173	0.70	0/1578
31	N	0.78	0/927	0.78	0/1243
32	O	0.71	0/1010	0.91	2/1344 (0.1%)
33	P	0.73	0/1089	0.83	0/1460
34	Q	0.67	0/927	0.78	1/1238 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
35	R	0.48	0/931	0.74	1/1244 (0.1%)
36	S	0.66	0/874	0.82	2/1168 (0.2%)
37	T	0.79	0/955	0.76	0/1265
38	U	0.69	0/809	0.68	0/1080
39	V	0.72	0/870	0.71	0/1171
40	W	0.68	1/733 (0.1%)	0.78	0/978
41	X	0.49	0/672	0.72	1/893 (0.1%)
42	Y	1.10	1/746 (0.1%)	1.82	3/1000 (0.3%)
43	Z	0.69	0/597	0.68	0/793
44	0	0.60	0/378	1.04	3/504 (0.6%)
45	1	0.56	0/537	0.74	0/714
46	2	0.66	0/443	0.78	0/597
47	3	0.43	0/680	0.87	0/911
48	4	0.72	0/366	0.74	0/485
49	5	0.39	0/230	0.84	0/303
50	6	0.89	0/377	0.83	0/491
51	7	0.82	1/491 (0.2%)	0.97	0/643
52	8	0.65	0/300	0.84	0/393
All	All	0.56	6/153353 (0.0%)	0.61	32/229517 (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
2	b	0	2
3	c	0	1
4	d	0	2
5	e	0	1
6	f	0	1
7	g	0	6
11	k	0	1
12	l	0	3
13	m	0	1
14	n	0	2
17	q	0	2
19	s	0	1
22	v	0	7
25	D	0	2
26	E	0	5
27	F	0	2

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Mol	Chain	#Chirality outliers	#Planarity outliers
30	M	0	1
31	N	0	1
32	O	0	4
33	P	0	3
35	R	0	3
36	S	0	2
37	T	0	1
38	U	0	1
41	X	0	1
43	Z	0	1
46	2	0	1
47	3	0	3
50	6	0	2
51	7	0	2
All	All	0	65

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
42	Y	25	GLY	C-N	28.26	1.74	1.33
29	H	87	LEU	CA-CB	-7.34	1.42	1.53
51	7	10	ALA	CA-C	-7.27	1.42	1.52
26	E	147	PHE	CA-CB	-6.82	1.36	1.53
40	W	7	LEU	CA-CB	-5.73	1.45	1.52
25	D	5	TYR	C-N	-5.12	1.17	1.33

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
42	Y	25	GLY	O-C-N	31.33	163.44	122.70
42	Y	25	GLY	CA-C-N	-29.23	63.28	122.03
42	Y	25	GLY	C-N-CA	-29.23	63.28	122.03
23	A	260	A	C5'-C4'-C3'	-15.84	92.23	116.00
32	O	100	GLY	N-CA-C	-8.71	103.28	112.08
44	0	31	ALA	CA-C-N	8.37	132.62	120.82
44	0	31	ALA	C-N-CA	8.37	132.62	120.82
23	A	260	A	C2'-C3'-O3'	-7.97	101.75	113.70
22	v	50	SER	N-CA-C	7.19	124.44	113.51
34	Q	98	GLY	N-CA-C	-6.73	104.92	112.33
14	n	56	VAL	CA-C-N	6.44	133.29	121.70
14	n	56	VAL	C-N-CA	6.44	133.29	121.70
44	0	29	TRP	N-CA-C	-6.31	100.07	108.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	b	214	THR	OG1-CB-CG2	6.19	121.69	109.30
23	A	260	A	C5'-C4'-O4'	6.17	119.06	109.80
32	O	100	GLY	CA-C-O	-6.16	117.87	122.37
22	v	50	SER	N-CA-CB	-6.09	108.01	114.10
41	X	77	GLU	N-CA-C	6.03	113.56	108.13
3	c	107	LYS	CA-C-N	5.75	132.04	121.70
3	c	107	LYS	C-N-CA	5.75	132.04	121.70
23	A	260	A	O4'-C4'-C3'	-5.61	98.39	104.00
35	R	22	LEU	N-CA-C	5.56	116.60	108.14
2	b	214	THR	CA-CB-CG2	5.34	119.58	110.50
20	t	44	ASP	CA-C-N	5.34	131.30	121.70
20	t	44	ASP	C-N-CA	5.34	131.30	121.70
36	S	94	VAL	CG1-CB-CG2	5.31	122.49	110.80
23	A	260	A	O4'-C1'-C2'	-5.22	102.38	107.60
36	S	94	VAL	CA-CB-CG2	5.07	119.01	110.40
14	n	57	ARG	CA-CB-CG	5.06	124.22	114.10
1	a	1474	C	C2'-C3'-O3'	5.04	121.26	113.70
22	v	50	SER	CB-CA-C	-5.03	104.85	109.83
22	v	30	ARG	N-CA-C	-5.01	105.27	111.33

There are no chirality outliers.

All (65) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
46	2	17	GLU	Peptide
47	3	11	GLN	Peptide
47	3	13	ILE	Peptide
47	3	42	GLU	Peptide
50	6	15	LYS	Peptide
50	6	7	GLN	Peptide
51	7	28	PHE	Peptide
51	7	33	PHE	Peptide
25	D	120	GLU	Peptide
25	D	214	GLY	Peptide
26	E	140	PRO	Peptide
26	E	141	MET	Peptide
26	E	142	SER	Peptide
26	E	200	ASN	Peptide
26	E	9	LYS	Peptide
27	F	154	VAL	Peptide
27	F	155	VAL	Peptide
30	M	40	LYS	Peptide

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Mol	Chain	Res	Type	Group
31	N	23	LYS	Peptide
32	O	110	LYS	Peptide
32	O	35	HIS	Peptide
32	O	58	PHE	Peptide
32	O	65	GLY	Peptide
33	P	134	ARG	Sidechain
33	P	90	VAL	Peptide
33	P	98	LYS	Peptide
35	R	110	GLU	Peptide
35	R	29	PRO	Peptide
35	R	89	ILE	Peptide
36	S	103	ARG	Peptide
36	S	105	LEU	Peptide
37	T	85	LYS	Peptide
38	U	100	ILE	Peptide
41	X	77	GLU	Peptide
43	Z	82	ARG	Peptide
2	b	19	GLN	Peptide
2	b	21	ARG	Peptide
3	c	160	ASP	Peptide
4	d	160	PHE	Peptide
4	d	93	ARG	Peptide
5	e	108	GLY	Peptide
6	f	81	LYS	Peptide
7	g	13	LEU	Peptide
7	g	14	PRO	Peptide
7	g	146	GLU	Peptide
7	g	73	LEU	Peptide
7	g	8	PRO	Peptide
7	g	9	LYS	Peptide
11	k	53	LYS	Peptide
12	l	109	HIS	Peptide
12	l	23	ALA	Peptide
12	l	32	LYS	Peptide
13	m	44	ARG	Peptide
14	n	18	VAL	Peptide
14	n	54	PRO	Peptide
17	q	4	ARG	Peptide
17	q	72	THR	Peptide
19	s	40	ILE	Peptide
22	v	47	TYR	Peptide
22	v	49	ASN	Peptide

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Mol	Chain	Res	Type	Group
22	v	50	SER	Peptide
22	v	51	ALA	Peptide
22	v	66	ARG	Sidechain
22	v	87	ARG	Sidechain
22	v	98	ARG	Sidechain

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	a	33006	0	16615	408	0
2	b	1788	0	1847	47	0
3	c	1600	0	1662	41	0
4	d	1600	0	1628	36	0
5	e	1194	0	1255	33	0
6	f	781	0	784	13	0
7	g	1142	0	1171	27	0
8	h	1032	0	1082	25	0
9	i	1017	0	1039	34	0
10	j	791	0	829	53	0
11	k	851	0	864	17	0
12	l	1058	0	1130	27	0
13	m	877	0	919	23	0
14	n	502	0	527	12	0
15	o	738	0	769	14	0
16	p	712	0	744	17	0
17	q	698	0	738	20	0
18	r	466	0	496	47	0
19	s	677	0	672	21	0
20	t	606	0	650	15	0
21	u	377	0	404	57	0
22	v	831	0	846	193	0
23	A	62480	0	31402	529	0
24	B	2430	0	1229	26	0
25	D	2103	0	2221	38	0
26	E	1649	0	1689	27	0
27	F	1524	0	1570	25	0
28	G	1311	0	1366	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
29	H	1284	0	1301	24	0
30	M	1151	0	1145	16	0
31	N	920	0	981	14	0
32	O	997	0	1044	10	0
33	P	1065	0	1122	26	0
34	Q	924	0	970	20	0
35	R	922	0	968	26	0
36	S	862	0	932	21	0
37	T	943	0	1014	18	0
38	U	799	0	836	13	0
39	V	862	0	920	11	0
40	W	725	0	761	11	0
41	X	668	0	725	8	0
42	Y	738	0	785	45	0
43	Z	591	0	602	29	0
44	0	373	0	407	5	0
45	1	536	0	567	9	0
46	2	441	0	478	5	0
47	3	663	0	644	23	0
48	4	360	0	385	11	0
49	5	229	0	224	12	0
50	6	373	0	420	13	0
51	7	487	0	548	9	0
52	8	297	0	342	8	0
All	All	141051	0	94269	1911	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 9.

All (1911) 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)
10:j:5:LYS:CG	10:j:77:VAL:HG22	1.16	1.57
10:j:5:LYS:HG2	10:j:77:VAL:CB	1.18	1.56
10:j:5:LYS:HG2	10:j:77:VAL:CG2	1.08	1.53
33:P:48:GLU:HG3	33:P:51:ARG:NH1	1.22	1.50
1:a:701:G:H4'	22:v:100:SER:CB	1.45	1.44
22:v:82:ASN:CA	22:v:85:LEU:HD21	1.50	1.41
1:a:1547:C:O3'	21:u:54:LYS:CG	1.67	1.40
10:j:5:LYS:CG	10:j:77:VAL:CB	1.97	1.35
10:j:5:LYS:CD	10:j:77:VAL:HG22	1.56	1.34

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:r:33:LEU:O	18:r:37:PHE:CD2	1.79	1.32
23:A:373:A:N7	23:A:1248:U:C4	2.00	1.30
42:Y:21:LEU:CD1	42:Y:42:LYS:HE3	1.60	1.28
22:v:81:ILE:O	22:v:85:LEU:HD22	1.21	1.26
22:v:20:TYR:OH	22:v:78:ILE:HG21	1.25	1.26
42:Y:21:LEU:HD12	42:Y:42:LYS:CE	1.64	1.26
22:v:82:ASN:O	22:v:85:LEU:HD23	1.24	1.25
10:j:5:LYS:CG	10:j:77:VAL:CG2	1.77	1.23
1:a:936:G:N2	22:v:91:LYS:HB2	1.52	1.22
10:j:5:LYS:CD	10:j:77:VAL:CG2	2.15	1.22
33:P:48:GLU:CG	33:P:51:ARG:NH1	2.01	1.22
42:Y:21:LEU:CD1	42:Y:42:LYS:CE	2.17	1.22
22:v:82:ASN:HA	22:v:85:LEU:CD2	1.70	1.21
1:a:534:C:OP2	12:l:101:LYS:NZ	1.70	1.20
18:r:33:LEU:HB3	18:r:37:PHE:CE2	1.76	1.20
10:j:5:LYS:HG2	10:j:77:VAL:CA	1.72	1.19
1:a:1547:C:O3'	21:u:54:LYS:HG2	1.26	1.19
1:a:1547:C:O3'	21:u:54:LYS:CB	1.90	1.19
22:v:82:ASN:O	22:v:85:LEU:CD2	1.90	1.19
22:v:80:LEU:O	22:v:84:LYS:HG2	1.40	1.17
22:v:98:ARG:O	22:v:100:SER:N	1.79	1.16
18:r:43:LYS:O	18:r:44:ILE:HG13	1.41	1.16
10:j:5:LYS:HB3	10:j:76:ILE:O	1.47	1.15
42:Y:22:ARG:NH2	42:Y:87:THR:HG23	1.60	1.15
10:j:5:LYS:CG	10:j:77:VAL:CG1	2.25	1.14
10:j:5:LYS:HG3	10:j:77:VAL:HG13	1.26	1.13
22:v:45:LYS:NZ	22:v:45:LYS:HB3	1.60	1.12
10:j:5:LYS:CG	10:j:77:VAL:CA	2.28	1.11
10:j:5:LYS:CG	10:j:77:VAL:HG13	1.82	1.09
22:v:82:ASN:CA	22:v:85:LEU:CD2	2.29	1.09
33:P:48:GLU:CG	33:P:51:ARG:HH11	1.60	1.09
1:a:701:G:H4'	22:v:100:SER:HB3	1.32	1.08
1:a:1547:C:H5'	21:u:54:LYS:HG3	1.31	1.08
18:r:33:LEU:C	18:r:37:PHE:CE2	2.31	1.08
23:A:2287:C:N4	43:Z:22:ARG:HD3	1.68	1.08
42:Y:21:LEU:CD1	42:Y:42:LYS:CD	2.32	1.08
18:r:41:ARG:HG3	18:r:78:GLU:OE1	1.54	1.07
23:A:275:A:N6	23:A:296:G:C2	2.22	1.07
18:r:41:ARG:CG	18:r:78:GLU:OE1	2.03	1.06
22:v:73:ASP:OD1	22:v:74:LEU:HD23	1.52	1.06
1:a:1547:C:C5'	21:u:54:LYS:HG3	1.86	1.06

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:r:25:HIS:HB3	18:r:26:ILE:HD13	1.06	1.05
23:A:1583:G:OP1	23:A:1584:A:C8	2.09	1.05
18:r:25:HIS:CB	18:r:26:ILE:HD13	1.87	1.05
10:j:5:LYS:CB	10:j:77:VAL:HG22	1.86	1.04
49:5:35:PHE:CD1	49:5:36:CYS:N	2.25	1.04
1:a:701:G:H4'	22:v:100:SER:HB2	1.04	1.04
10:j:5:LYS:CG	10:j:77:VAL:HA	1.84	1.04
18:r:25:HIS:HB3	18:r:26:ILE:CD1	1.88	1.03
23:A:1496:G:N7	23:A:1501:G:N1	2.06	1.03
22:v:81:ILE:O	22:v:85:LEU:CD2	2.07	1.02
23:A:1584:A:P	23:A:1585:G:H8	1.82	1.02
42:Y:21:LEU:HD11	42:Y:42:LYS:CD	1.87	1.02
22:v:74:LEU:HD23	22:v:74:LEU:H	1.19	1.02
18:r:33:LEU:HB3	18:r:37:PHE:HE2	0.89	1.02
22:v:21:ILE:HG13	22:v:78:ILE:HD11	1.36	1.02
22:v:20:TYR:OH	22:v:78:ILE:CG2	2.08	1.01
43:Z:27:LYS:HG3	43:Z:29:LEU:HD11	1.43	1.01
42:Y:21:LEU:HD13	42:Y:42:LYS:HE3	1.38	1.01
3:c:110:LEU:HD23	3:c:203:ARG:NH1	1.74	1.01
3:c:110:LEU:HD23	3:c:203:ARG:HH12	1.23	1.01
18:r:33:LEU:CB	18:r:37:PHE:HE2	1.73	1.00
42:Y:21:LEU:HD11	42:Y:42:LYS:CG	1.90	1.00
1:a:1547:C:C4'	21:u:54:LYS:HG3	1.92	1.00
22:v:31:TYR:CE2	22:v:89:VAL:HB	1.97	1.00
22:v:82:ASN:C	22:v:85:LEU:CD2	2.35	0.99
42:Y:25:GLY:O	42:Y:44:ASP:HA	1.62	0.99
42:Y:21:LEU:HD11	42:Y:42:LYS:HG2	1.42	0.99
22:v:88:GLN:HA	22:v:91:LYS:HE2	1.44	0.98
1:a:701:G:C4'	22:v:100:SER:CB	2.40	0.98
18:r:33:LEU:C	18:r:37:PHE:CD2	2.40	0.98
1:a:936:G:H21	22:v:91:LYS:HB2	1.11	0.98
18:r:33:LEU:O	18:r:37:PHE:CE2	2.15	0.98
1:a:701:G:C4'	22:v:100:SER:HB2	1.94	0.97
22:v:90:ARG:HG3	22:v:91:LYS:N	1.79	0.97
10:j:5:LYS:CE	10:j:77:VAL:HG22	1.94	0.97
1:a:936:G:N2	22:v:91:LYS:CB	2.27	0.96
1:a:1547:C:O3'	21:u:54:LYS:HB2	1.65	0.96
10:j:5:LYS:HG3	10:j:77:VAL:CG1	1.91	0.94
22:v:95:ARG:HB3	22:v:96:ILE:CG2	1.97	0.94
1:a:954:G:H21	1:a:1350:A:H62	0.99	0.93
22:v:45:LYS:HB3	22:v:45:LYS:HZ2	1.22	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:v:82:ASN:C	22:v:85:LEU:HD21	1.94	0.93
22:v:90:ARG:HG3	22:v:91:LYS:H	1.32	0.93
49:5:35:PHE:HD1	49:5:36:CYS:H	0.99	0.93
22:v:27:LYS:O	22:v:30:ARG:HD2	1.69	0.92
33:P:48:GLU:HG3	33:P:51:ARG:HH11	1.12	0.92
23:A:1307:G:H1	23:A:2038:U:H3	1.15	0.92
1:a:1547:C:C3'	21:u:54:LYS:CG	2.47	0.92
22:v:32:PHE:CD2	22:v:34:ASP:HB2	2.03	0.91
22:v:95:ARG:CZ	22:v:96:ILE:HG22	2.01	0.91
23:A:1584:A:OP1	23:A:1585:G:H8	1.55	0.90
23:A:2288:C:OP2	43:Z:24:SER:OG	1.86	0.90
1:a:445:U:C2	1:a:503:A:N7	2.39	0.90
22:v:92:TYR:O	22:v:95:ARG:HG3	1.71	0.90
1:a:954:G:N2	1:a:1350:A:H62	1.69	0.90
23:A:1584:A:OP1	23:A:1585:G:C8	2.25	0.90
43:Z:27:LYS:HG3	43:Z:29:LEU:CD1	2.02	0.89
1:a:1271:G:N2	1:a:1286:A:N7	2.19	0.89
33:P:48:GLU:HG3	33:P:51:ARG:HH12	1.31	0.89
22:v:45:LYS:NZ	22:v:45:LYS:CB	2.26	0.89
18:r:33:LEU:CB	18:r:37:PHE:CE2	2.51	0.89
22:v:82:ASN:C	22:v:85:LEU:HD23	1.98	0.88
23:A:1086:G:O6	23:A:1157:U:C4	2.28	0.87
23:A:1584:A:O5'	23:A:1585:G:C8	2.26	0.87
22:v:32:PHE:HD2	22:v:34:ASP:HB2	1.39	0.87
1:a:420:U:O2'	1:a:421:G:O4'	1.92	0.87
21:u:14:ASP:OD1	21:u:17:ARG:NH2	2.08	0.86
23:A:1121:A:O2'	23:A:1122:U:O4'	1.92	0.86
42:Y:21:LEU:HD12	42:Y:42:LYS:CD	2.02	0.86
1:a:615:A:OP1	1:a:639:G:N2	2.09	0.86
21:u:12:LEU:O	21:u:13:GLU:HB2	1.73	0.86
1:a:1547:C:H5'	21:u:54:LYS:CG	2.06	0.86
3:c:110:LEU:CD2	3:c:203:ARG:HH12	1.88	0.86
1:a:1547:C:C3'	21:u:54:LYS:HG2	2.05	0.85
21:u:46:LYS:HD2	21:u:50:GLU:CD	2.01	0.85
22:v:31:TYR:CE2	22:v:90:ARG:N	2.45	0.84
23:A:373:A:N7	23:A:1248:U:O4	2.08	0.84
42:Y:21:LEU:HD12	42:Y:42:LYS:HE2	1.59	0.84
22:v:95:ARG:HB3	22:v:96:ILE:HG23	1.55	0.84
10:j:5:LYS:HD2	10:j:77:VAL:CG2	2.06	0.84
42:Y:21:LEU:CD1	42:Y:42:LYS:HD3	2.06	0.84
1:a:300:G:H21	1:a:616:A:H61	1.23	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:v:101:ARG:HD2	22:v:101:ARG:O	1.76	0.84
18:r:33:LEU:CA	18:r:37:PHE:CE2	2.61	0.83
22:v:99:LYS:O	22:v:100:SER:O	1.94	0.83
23:A:1302:G:OP1	48:4:16:ARG:NH1	2.11	0.83
23:A:2287:C:H42	43:Z:22:ARG:HD3	1.36	0.83
23:A:1584:A:O5'	23:A:1585:G:H8	1.59	0.83
49:5:35:PHE:CE1	49:5:37:SER:N	2.46	0.83
24:B:64:A:N6	24:B:105:G:O4'	2.11	0.83
1:a:701:G:C4'	22:v:100:SER:HB3	2.06	0.83
22:v:45:LYS:HZ2	22:v:45:LYS:CB	1.91	0.83
1:a:587:G:O2'	15:o:54:ARG:NH1	2.11	0.83
10:j:5:LYS:HG3	10:j:77:VAL:HA	1.61	0.83
22:v:91:LYS:HG2	22:v:92:TYR:N	1.94	0.82
23:A:1851:G:OP2	25:D:52:HIS:NE2	2.11	0.82
22:v:45:LYS:HB3	22:v:45:LYS:HZ3	1.42	0.82
23:A:2581:U:O2'	23:A:2582:U:O4'	1.97	0.82
1:a:971:U:OP2	1:a:1234:C:O2'	1.97	0.82
23:A:263:G:C2	23:A:264:G:H1'	2.15	0.82
1:a:472:G:N2	1:a:478:G:O6	2.11	0.82
22:v:58:ILE:HD13	22:v:85:LEU:HB3	1.61	0.82
22:v:85:LEU:O	22:v:89:VAL:HG23	1.78	0.82
1:a:844:G:OP2	18:r:55:LYS:NZ	2.12	0.81
1:a:1358:G:N2	1:a:1385:A:OP2	2.12	0.81
23:A:1591:G:O2'	23:A:1592:A:O4'	1.98	0.81
23:A:2868:G:H21	23:A:2888:A:H62	1.24	0.81
3:c:110:LEU:CD2	3:c:203:ARG:NH1	2.43	0.81
1:a:1249:A:N7	1:a:1312:U:O2	2.13	0.81
21:u:53:ARG:O	21:u:54:LYS:HD3	1.80	0.81
22:v:71:ASN:ND2	22:v:77:GLY:N	2.28	0.81
47:3:9:TYR:OH	47:3:24:LEU:O	1.99	0.81
1:a:954:G:H21	1:a:1350:A:N6	1.79	0.81
22:v:88:GLN:HA	22:v:91:LYS:CE	2.11	0.81
22:v:97:ASN:ND2	22:v:99:LYS:HE2	1.96	0.81
22:v:80:LEU:O	22:v:84:LYS:CG	2.27	0.80
1:a:990:C:O2'	14:n:19:ARG:O	1.99	0.80
21:u:18:ARG:O	21:u:21:ARG:N	2.15	0.80
1:a:1126:C:O2'	14:n:60:SER:OG	1.98	0.80
23:A:1491:C:O2	23:A:1574:G:N2	2.14	0.80
1:a:1090:U:O2'	5:e:138:ARG:NH1	2.15	0.80
10:j:5:LYS:HB3	10:j:76:ILE:C	2.06	0.80
23:A:1583:G:OP1	23:A:1584:A:H8	1.64	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:a:1025:G:N3	1:a:1229:U:O2'	2.15	0.80
23:A:2332:U:O2'	23:A:2333:U:O4'	1.99	0.80
1:a:445:U:O2	1:a:503:A:N7	2.15	0.80
23:A:1806:U:OP2	23:A:1811:A:N6	2.15	0.80
23:A:1584:A:P	23:A:1585:G:C8	2.73	0.79
10:j:5:LYS:CD	10:j:77:VAL:CG1	2.60	0.79
23:A:84:A:N6	23:A:99:U:O4'	2.15	0.79
23:A:373:A:N7	23:A:1248:U:N3	2.31	0.79
18:r:41:ARG:HA	18:r:78:GLU:HB3	1.64	0.79
22:v:65:LEU:HD21	22:v:88:GLN:HE21	1.46	0.79
23:A:198:A:N6	23:A:201:C:OP2	2.16	0.79
23:A:955:A:N3	23:A:2291:C:O2'	2.15	0.79
23:A:1323:A:O2'	23:A:1325:U:OP2	2.01	0.79
24:B:7:G:OP1	35:R:19:ARG:NH1	2.15	0.79
23:A:1490:G:O6	23:A:1595:C:N4	2.15	0.79
23:A:1533:A:O2'	25:D:97:ASP:OD1	2.01	0.79
23:A:1652:A:O2'	23:A:1654:A:OP2	1.99	0.79
23:A:2260:A:N6	23:A:2261:G:O6	2.16	0.79
22:v:71:ASN:HD22	22:v:77:GLY:CA	1.95	0.79
23:A:2127:G:O6	23:A:2216:U:O2	2.00	0.79
1:a:996:A:N3	19:s:52:TYR:OH	2.15	0.79
22:v:20:TYR:CZ	22:v:78:ILE:HD12	2.18	0.79
23:A:2060:A:O2'	23:A:2062:G:OP2	1.99	0.78
23:A:2260:A:H2'	23:A:2261:G:C8	2.18	0.78
23:A:674:C:O2	23:A:684:U:O2'	2.01	0.78
22:v:71:ASN:HD22	22:v:77:GLY:N	1.79	0.78
1:a:18:U:HO2'	1:a:1091:G:HO2'	1.28	0.78
1:a:1115:C:O2'	2:b:110:ARG:NH2	2.16	0.78
22:v:31:TYR:CD2	22:v:89:VAL:HB	2.19	0.78
22:v:82:ASN:HA	22:v:85:LEU:HD21	0.80	0.78
23:A:2442:G:O2'	32:O:60:ARG:NH1	2.17	0.78
42:Y:14:THR:O	42:Y:18:LEU:CD2	2.32	0.78
1:a:300:G:N2	1:a:616:A:H61	1.81	0.78
10:j:5:LYS:HE3	10:j:77:VAL:HG22	1.65	0.78
1:a:1014:A:OP1	1:a:1035:U:O2'	2.01	0.77
1:a:1265:G:N2	1:a:1270:C:O2'	2.17	0.77
24:B:72:U:O2	42:Y:38:ASN:ND2	2.17	0.77
1:a:774:A:OP2	1:a:820:G:N2	2.18	0.77
1:a:996:A:O2'	19:s:55:ARG:O	2.01	0.77
22:v:17:ILE:HA	22:v:20:TYR:HD2	1.49	0.77
24:B:57:G:O2'	35:R:6:ASP:OD1	2.01	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:E:9:LYS:NZ	26:E:201:VAL:O	2.16	0.77
23:A:1499:U:O4	23:A:2731:C:N4	2.17	0.77
23:A:2682:G:O2'	23:A:2691:G:O6	2.03	0.77
1:a:800:A:O2'	1:a:802:A:N7	2.17	0.77
21:u:14:ASP:OD2	21:u:18:ARG:CG	2.32	0.77
43:Z:27:LYS:O	43:Z:28:ARG:HB2	1.83	0.77
1:a:919:A:OP1	12:l:18:LYS:NZ	2.17	0.77
22:v:95:ARG:NH2	22:v:96:ILE:HG22	1.99	0.77
23:A:1116:C:O2'	23:A:1138:U:O2	2.02	0.77
26:E:187:GLN:HB2	26:E:196:LEU:HD12	1.67	0.77
1:a:1408:C:OP2	5:e:29:ARG:NH2	2.18	0.77
8:h:29:ALA:O	8:h:57:GLN:NE2	2.17	0.77
23:A:1051:C:OP1	30:M:38:ARG:NH1	2.18	0.77
22:v:93:LYS:C	22:v:95:ARG:HB2	2.09	0.76
1:a:130:A:N6	1:a:241:U:O2	2.18	0.76
1:a:300:G:H21	1:a:616:A:N6	1.82	0.76
22:v:21:ILE:HG23	22:v:22:GLU:OE1	1.85	0.76
23:A:273:A:OP2	23:A:297:G:N2	2.19	0.76
23:A:1843:U:O4	25:D:34:LYS:NZ	2.18	0.76
1:a:51:A:OP2	12:l:34:LYS:NZ	2.19	0.76
18:r:43:LYS:O	18:r:44:ILE:CG1	2.29	0.76
22:v:20:TYR:CE1	22:v:78:ILE:HD13	2.21	0.76
23:A:59:U:O2'	23:A:74:U:OP2	2.02	0.76
23:A:2649:U:O2'	23:A:2845:G:N2	2.16	0.76
1:a:263:G:O6	1:a:274:G:O6	2.03	0.76
24:B:53:U:O2	24:B:55:A:N6	2.18	0.76
24:B:100:A:HO2'	42:Y:32:TYR:HH	1.31	0.76
1:a:245:C:O3'	17:q:31:LYS:NZ	2.19	0.76
23:A:1079:U:N3	23:A:1164:G:O6	2.18	0.76
23:A:2287:C:N4	43:Z:22:ARG:CD	2.48	0.76
1:a:1384:G:O6	9:i:113:LYS:NZ	2.18	0.76
1:a:682:G:O3'	6:f:50:TYR:OH	2.02	0.76
1:a:1085:U:O2	2:b:103:ASN:ND2	2.18	0.76
10:j:5:LYS:CD	10:j:77:VAL:HG13	2.14	0.76
23:A:275:A:C6	23:A:296:G:N2	2.54	0.76
43:Z:27:LYS:CG	43:Z:29:LEU:HD11	2.16	0.76
22:v:73:ASP:OD1	22:v:74:LEU:CD2	2.33	0.76
23:A:2102:U:OP2	23:A:2265:G:O2'	2.04	0.76
23:A:2550:G:O2'	23:A:2791:A:O2'	2.04	0.76
24:B:9:C:O2'	24:B:13:A:N6	2.18	0.76
1:a:1047:G:O2'	1:a:1048:A:O4'	2.04	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:u:12:LEU:O	21:u:13:GLU:CB	2.33	0.76
23:A:614:U:O5'	23:A:2057:A:N6	2.18	0.76
23:A:2146:A:N6	23:A:2197:G:O6	2.19	0.76
27:F:21:ASP:O	27:F:25:GLY:N	2.19	0.76
15:o:43:LEU:O	15:o:47:LYS:HA	1.86	0.75
23:A:269:G:N2	23:A:323:C:O2	2.18	0.75
23:A:923:A:O2'	23:A:924:G:OP2	2.04	0.75
1:a:969:A:N6	19:s:77:THR:O	2.19	0.75
22:v:78:ILE:C	22:v:80:LEU:H	1.94	0.75
23:A:2187:G:N2	23:A:2200:A:O2'	2.19	0.75
18:r:33:LEU:O	18:r:37:PHE:CG	2.38	0.75
23:A:328:G:N1	23:A:399:U:O2	2.18	0.75
23:A:373:A:C5	23:A:1248:U:C4	2.74	0.75
23:A:2404:A:O2'	35:R:119:PHE:OXT	2.03	0.75
23:A:373:A:C5	23:A:1248:U:N3	2.54	0.75
35:R:71:GLU:O	35:R:74:THR:OG1	2.04	0.75
23:A:815:G:OP1	50:6:9:ASN:ND2	2.19	0.75
23:A:2033:C:O2'	23:A:2843:A:N3	2.20	0.75
1:a:410:G:OP2	4:d:66:ARG:NH1	2.19	0.75
23:A:922:G:N2	23:A:945:A:N7	2.31	0.75
23:A:1265:G:N7	37:T:16:LYS:NZ	2.35	0.75
23:A:1379:A:O2'	23:A:1381:U:OP2	2.03	0.75
52:8:2:LYS:NZ	52:8:31:LYS:O	2.20	0.75
1:a:1233:G:OP2	1:a:1333:C:N4	2.19	0.75
1:a:1331:C:O2'	13:m:90:ARG:NH2	2.20	0.75
1:a:1244:G:N2	1:a:1375:U:O2	2.19	0.75
7:g:126:ASP:OD1	7:g:131:THR:OG1	2.01	0.75
23:A:2673:C:OP2	23:A:2759:G:O2'	2.05	0.75
1:a:1303:U:OP1	7:g:41:ARG:NH2	2.20	0.74
21:u:46:LYS:O	21:u:46:LYS:HD3	1.87	0.74
18:r:43:LYS:C	18:r:44:ILE:HG13	2.12	0.74
21:u:14:ASP:OD2	21:u:18:ARG:HG3	1.87	0.74
23:A:1880:A:N6	23:A:1916:A:N7	2.36	0.74
22:v:20:TYR:CZ	22:v:78:ILE:HG21	2.22	0.74
23:A:263:G:H5''	23:A:666:A:H1'	1.68	0.74
23:A:1423:C:O2'	23:A:1512:U:O2	2.04	0.74
33:P:35:GLN:NE2	33:P:36:ALA:O	2.20	0.74
23:A:512:A:OP1	50:6:35:ARG:NH1	2.20	0.74
10:j:5:LYS:CD	10:j:77:VAL:HG21	2.15	0.74
23:A:1101:A:N6	23:A:1131:G:OP2	2.21	0.74
23:A:1711:G:O2'	23:A:2018:U:O4	2.05	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:a:20:C:OP1	5:e:135:ASN:ND2	2.20	0.74
23:A:363:A:O2'	23:A:365:A:OP2	2.06	0.74
1:a:921:U:OP2	12:l:107:ARG:NH2	2.20	0.74
23:A:2124:U:O4	23:A:2219:C:N4	2.17	0.74
24:B:64:A:O2'	24:B:104:C:N4	2.20	0.74
20:t:62:GLN:NE2	20:t:63:SER:OG	2.20	0.74
23:A:608:C:N4	23:A:619:U:O4	2.20	0.74
23:A:2127:G:O6	23:A:2216:U:C2	2.41	0.74
22:v:31:TYR:HE2	22:v:89:VAL:HB	1.50	0.73
23:A:1963:A:OP2	23:A:1989:C:N4	2.21	0.73
23:A:2530:A:O2'	23:A:2532:G:OP2	2.06	0.73
23:A:2821:U:OP2	23:A:2824:G:N2	2.21	0.73
47:3:30:THR:OG1	47:3:33:GLU:O	2.06	0.73
23:A:116:G:OP2	23:A:118:A:O2'	2.04	0.73
23:A:865:A:N3	23:A:987:U:O2'	2.21	0.73
23:A:1520:A:N6	23:A:1562:C:O2	2.20	0.73
23:A:2277:G:O2'	23:A:2523:C:OP1	2.06	0.73
1:a:413:U:OP1	1:a:414:G:O2'	2.02	0.73
1:a:1231:G:N2	19:s:54:GLY:O	2.18	0.73
1:a:1546:A:O2'	1:a:1547:C:O4'	2.07	0.73
18:r:41:ARG:HG2	18:r:78:GLU:OE1	1.88	0.73
20:t:10:ARG:O	20:t:14:THR:OG1	2.05	0.73
1:a:605:G:O3'	17:q:39:ARG:NH2	2.21	0.73
1:a:1547:C:H5'	21:u:54:LYS:NZ	2.03	0.73
10:j:5:LYS:CB	10:j:77:VAL:HA	2.19	0.73
13:m:28:SER:OG	13:m:32:LYS:NZ	2.21	0.73
22:v:91:LYS:HG2	22:v:92:TYR:H	1.50	0.73
22:v:100:SER:C	22:v:101:ARG:HG3	2.13	0.73
4:d:66:ARG:O	4:d:70:ASN:ND2	2.22	0.73
10:j:5:LYS:HD2	10:j:77:VAL:HG21	1.69	0.73
23:A:1306:C:O2	23:A:2040:A:C6	2.41	0.73
1:a:1124:C:O2'	3:c:178:ARG:NE	2.22	0.73
5:e:86:THR:OG1	5:e:94:VAL:O	2.07	0.73
24:B:53:U:O2'	24:B:55:A:N7	2.21	0.73
1:a:1004:A:O4'	1:a:1227:A:O2'	2.06	0.73
3:c:118:ASN:OD1	3:c:122:GLN:NE2	2.22	0.73
17:q:19:MET:O	17:q:53:ASN:ND2	2.22	0.73
36:S:16:ARG:NH2	36:S:80:THR:O	2.22	0.73
36:S:61:PHE:O	36:S:75:THR:OG1	2.05	0.73
1:a:347:C:OP1	31:N:13:ASN:ND2	2.22	0.72
8:h:5:ASP:OD2	8:h:8:ALA:N	2.22	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:a:948:A:N3	1:a:1387:U:O2'	2.18	0.72
1:a:1113:A:OP1	2:b:95:ARG:NH2	2.22	0.72
23:A:2261:G:O2'	23:A:2262:G:H5'	1.88	0.72
23:A:2465:U:O2'	23:A:2467:C:OP1	2.06	0.72
23:A:2038:U:OP2	39:V:16:LYS:NZ	2.16	0.72
1:a:481:C:O2'	1:a:482:A:O5'	2.06	0.72
1:a:1013:G:OP2	1:a:1036:C:N4	2.22	0.72
1:a:1086:G:O2'	1:a:1113:A:N1	2.21	0.72
1:a:1462:U:O2'	1:a:1463:U:O4'	2.05	0.72
23:A:1215:U:O2'	23:A:1217:U:O5'	2.08	0.72
23:A:1306:C:C2	23:A:2040:A:C6	2.77	0.72
29:H:60:GLU:O	29:H:63:THR:OG1	2.06	0.72
23:A:418:G:O2'	23:A:446:G:O6	2.04	0.72
10:j:5:LYS:CE	10:j:77:VAL:CG2	2.62	0.72
22:v:74:LEU:H	22:v:74:LEU:CD2	1.96	0.72
45:1:46:VAL:O	45:1:49:THR:OG1	2.08	0.72
47:3:33:GLU:O	47:3:51:SER:OG	2.07	0.72
1:a:182:A:O2'	1:a:184:A:N7	2.23	0.72
1:a:261:U:O4'	1:a:283:G:N2	2.22	0.72
22:v:85:LEU:HD23	22:v:85:LEU:H	1.53	0.71
23:A:1891:U:OP1	23:A:2437:G:O2'	2.03	0.71
43:Z:41:GLY:N	43:Z:72:ASP:OD1	2.22	0.71
8:h:95:PRO:O	8:h:119:ARG:NH2	2.23	0.71
21:u:49:SER:O	21:u:51:ALA:N	2.23	0.71
1:a:208:U:O2'	20:t:58:ASP:OD2	2.04	0.71
1:a:413:U:O4	4:d:2:ALA:N	2.23	0.71
7:g:86:GLN:O	7:g:148:ASN:ND2	2.18	0.71
26:E:158:SER:O	26:E:161:SER:OG	2.07	0.71
23:A:327:G:N7	23:A:400:C:O2'	2.23	0.71
8:h:5:ASP:OD2	8:h:79:ARG:NH2	2.22	0.71
22:v:65:LEU:HD21	22:v:88:GLN:NE2	2.04	0.71
23:A:1067:U:OP2	23:A:1069:G:O2'	2.08	0.71
23:A:1088:C:O2'	23:A:1155:A:N6	2.22	0.71
1:a:1547:C:C3'	21:u:54:LYS:HG3	2.19	0.71
27:F:6:VAL:O	27:F:8:LYS:NZ	2.17	0.71
11:k:17:GLU:O	11:k:81:THR:OG1	2.04	0.71
23:A:1131:G:N2	23:A:1134:U:O4'	2.24	0.71
1:a:526:C:OP2	1:a:538:G:O2'	2.05	0.71
22:v:92:TYR:C	22:v:95:ARG:HG3	2.16	0.71
24:B:40:C:OP2	47:3:2:LYS:NZ	2.23	0.71
1:a:445:U:O2	1:a:503:A:C5	2.44	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
42:Y:15:ARG:O	42:Y:18:LEU:HD23	1.91	0.71
1:a:457:A:OP2	1:a:492:G:N2	2.23	0.71
1:a:1123:A:H61	3:c:176:THR:HG22	1.56	0.71
23:A:2647:C:O2'	26:E:170:PRO:O	2.09	0.71
42:Y:27:VAL:N	42:Y:43:VAL:O	2.23	0.71
51:7:34:ALA:O	51:7:38:THR:OG1	2.05	0.71
1:a:1324:U:OP1	19:s:7:LYS:NZ	2.23	0.70
23:A:1089:C:OP1	23:A:1090:A:O2'	2.05	0.70
42:Y:21:LEU:HD11	42:Y:42:LYS:HD3	1.68	0.70
9:i:24:VAL:O	9:i:64:ASP:N	2.24	0.70
23:A:1550:G:O2'	23:A:1551:U:O4'	2.09	0.70
23:A:2357:G:O3'	43:Z:52:LYS:NZ	2.24	0.70
42:Y:14:THR:HB	42:Y:18:LEU:HD22	1.72	0.70
3:c:118:ASN:O	3:c:122:GLN:NE2	2.24	0.70
22:v:95:ARG:HB3	22:v:96:ILE:HG22	1.72	0.70
1:a:9:A:N6	4:d:200:ARG:O	2.24	0.70
1:a:1359:U:OP1	9:i:124:ARG:NH1	2.24	0.70
3:c:134:LYS:O	3:c:138:THR:OG1	2.03	0.70
23:A:1377:U:OP2	40:W:58:TYR:OH	2.08	0.70
23:A:2695:G:O2'	29:H:111:HIS:NE2	2.16	0.70
23:A:1450:A:N6	23:A:1634:A:O2'	2.24	0.70
23:A:575:G:O2'	23:A:577:A:N7	2.22	0.70
14:n:44:PHE:O	14:n:48:ALA:N	2.24	0.70
19:s:45:ILE:HG21	47:3:71:VAL:HG22	1.73	0.70
1:a:1215:A:N3	3:c:194:LYS:NZ	2.40	0.70
17:q:31:LYS:N	17:q:40:VAL:O	2.25	0.70
21:u:14:ASP:OD1	21:u:17:ARG:CZ	2.40	0.70
23:A:1064:A:N1	23:A:1185:U:O2'	2.20	0.70
23:A:1357:G:N2	23:A:1357:G:OP2	2.20	0.70
23:A:2560:U:OP1	23:A:2692:A:O2'	2.09	0.70
1:a:1383:U:OP2	9:i:15:LYS:NZ	2.15	0.69
23:A:263:G:N2	23:A:652:A:N3	2.38	0.69
23:A:1945:A:O2'	23:A:1946:A:OP2	2.07	0.69
30:M:28:ARG:O	30:M:31:SER:OG	2.10	0.69
49:5:35:PHE:CZ	49:5:37:SER:HA	2.27	0.69
1:a:1203:C:OP2	3:c:4:LYS:NZ	2.23	0.69
23:A:722:A:O2'	23:A:2097:G:O2'	2.05	0.69
23:A:1168:C:O2	52:8:36:GLN:NE2	2.25	0.69
23:A:1844:G:OP2	25:D:155:ARG:NH2	2.24	0.69
23:A:1306:C:C2	23:A:2040:A:N6	2.61	0.69
26:E:37:GLN:OE1	26:E:76:HIS:NE2	2.26	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
42:Y:25:GLY:C	42:Y:44:ASP:OD1	2.36	0.69
7:g:94:GLU:O	7:g:97:THR:OG1	2.09	0.69
10:j:5:LYS:HG3	10:j:77:VAL:CA	2.20	0.69
23:A:229:A:O2'	23:A:231:A:N1	2.23	0.69
23:A:790:G:O2'	23:A:793:G:O2'	2.08	0.69
23:A:1567:A:OP2	23:A:1568:U:O2'	2.07	0.69
23:A:1740:G:N2	23:A:2004:A:O2'	2.25	0.69
23:A:1835:U:O2'	23:A:1836:A:O5'	2.11	0.69
37:T:48:ARG:NH2	37:T:49:ASP:OD1	2.24	0.69
1:a:989:C:OP1	1:a:1234:C:N4	2.26	0.69
25:D:68:ARG:O	25:D:188:ARG:NH1	2.26	0.69
1:a:828:U:O2'	1:a:829:G:OP1	2.11	0.69
23:A:1892:U:O2'	23:A:1902:G:N2	2.26	0.68
1:a:457:A:N7	1:a:494:U:O2	2.27	0.68
23:A:163:U:O2'	23:A:166:A:N6	2.26	0.68
23:A:1110:U:O2'	23:A:1113:A:N7	2.23	0.68
23:A:2589:U:O2'	31:N:23:LYS:NZ	2.25	0.68
37:T:26:GLY:O	37:T:29:HIS:ND1	2.27	0.68
22:v:84:LYS:O	22:v:88:GLN:HG2	1.93	0.68
22:v:21:ILE:CG1	22:v:78:ILE:HD11	2.17	0.68
23:A:672:A:O4'	23:A:682:A:N6	2.27	0.68
38:U:22:VAL:O	38:U:93:THR:N	2.26	0.68
1:a:1379:A:N7	9:i:116:LYS:NZ	2.32	0.68
1:a:143:A:O2'	1:a:212:A:OP1	2.04	0.68
1:a:936:G:H22	22:v:91:LYS:CB	2.06	0.68
1:a:554:A:OP2	4:d:58:ARG:NH2	2.26	0.68
1:a:1235:U:O2	13:m:101:LYS:NZ	2.23	0.68
23:A:1134:U:O4	23:A:1145:U:O2'	2.11	0.68
1:a:459:A:OP2	1:a:460:A:O2'	2.06	0.68
22:v:9:ASP:OD1	22:v:10:ASN:N	2.27	0.68
23:A:263:G:C2'	23:A:264:G:O5'	2.41	0.68
23:A:1491:C:C2	23:A:1574:G:N2	2.60	0.68
23:A:2229:C:O2'	23:A:2231:C:OP1	2.11	0.68
23:A:2287:C:H41	43:Z:22:ARG:HD3	1.57	0.68
23:A:373:A:C8	23:A:1248:U:C4	2.79	0.68
23:A:643:G:N2	23:A:648:G:O2'	2.26	0.68
34:Q:24:LEU:O	34:Q:28:GLU:HA	1.92	0.68
1:a:379:G:O2'	1:a:381:A:N7	2.26	0.68
1:a:398:C:O3'	16:p:9:ARG:NH2	2.27	0.68
21:u:50:GLU:O	21:u:51:ALA:HB2	1.93	0.68
23:A:1135:G:N2	23:A:1143:G:O2'	2.20	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:a:1539:C:OP2	21:u:42:SER:OG	2.11	0.67
23:A:242:U:O2'	23:A:667:G:O2'	2.12	0.67
23:A:572:C:O2'	23:A:573:A:OP2	2.10	0.67
23:A:1885:G:O2'	23:A:1911:A:N6	2.27	0.67
1:a:137:U:O2'	16:p:62:ASN:O	2.12	0.67
23:A:275:A:N6	23:A:296:G:N2	2.41	0.67
23:A:606:G:OP1	38:U:78:ARG:NH2	2.27	0.67
23:A:2302:C:O2	43:Z:18:THR:HG22	1.94	0.67
23:A:2333:U:OP2	23:A:2334:G:N1	2.27	0.67
33:P:27:VAL:CG1	33:P:134:ARG:HD2	2.24	0.67
42:Y:3:SER:O	42:Y:62:GLU:N	2.27	0.67
23:A:1053:A:OP2	30:M:40:LYS:NZ	2.27	0.67
1:a:660:U:O4	1:a:760:G:O2'	2.11	0.67
22:v:94:THR:HA	22:v:95:ARG:O	1.95	0.67
23:A:1631:G:O2'	23:A:1632:A:N1	2.26	0.67
27:F:152:VAL:HG12	27:F:190:ASP:OD2	1.95	0.67
1:a:148:G:O2'	1:a:1457:A:N3	2.21	0.67
23:A:246:U:OP2	51:7:8:ARG:NH1	2.28	0.67
23:A:2260:A:C6	23:A:2261:G:O6	2.48	0.67
23:A:2362:A:O2'	23:A:2364:G:N7	2.22	0.67
39:V:25:ARG:NH2	39:V:74:ALA:O	2.27	0.67
1:a:986:G:OP2	1:a:1369:U:O2'	2.12	0.67
9:i:32:VAL:N	9:i:35:ARG:O	2.27	0.67
23:A:729:G:O6	23:A:819:A:O2'	2.06	0.67
42:Y:10:GLN:HE21	42:Y:14:THR:HG21	1.59	0.67
16:p:21:VAL:HG23	16:p:33:ILE:HG23	1.75	0.67
34:Q:32:THR:OG1	34:Q:33:THR:O	2.11	0.67
1:a:305:G:N2	1:a:308:A:OP2	2.25	0.67
1:a:824:A:OP1	1:a:1538:G:O2'	2.11	0.67
1:a:1279:G:N3	1:a:1337:U:O2'	2.23	0.67
1:a:1547:C:H5'	21:u:54:LYS:HZ3	1.57	0.67
23:A:1452:C:H42	23:A:1632:A:H62	1.43	0.67
1:a:332:G:N1	1:a:335:A:OP2	2.27	0.66
35:R:84:ALA:O	35:R:88:GLY:N	2.27	0.66
1:a:381:A:O2'	1:a:489:G:N3	2.26	0.66
10:j:5:LYS:HD2	10:j:77:VAL:CG1	2.25	0.66
15:o:29:ILE:HD11	15:o:81:LEU:HD11	1.76	0.66
21:u:46:LYS:HD3	21:u:46:LYS:C	2.20	0.66
22:v:65:LEU:O	22:v:66:ARG:NH2	2.27	0.66
23:A:99:U:OP1	23:A:100:U:O2'	2.13	0.66
49:5:35:PHE:HD1	49:5:36:CYS:N	1.72	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:v:94:THR:N	22:v:95:ARG:HB2	2.09	0.66
23:A:1086:G:O6	23:A:1157:U:O4	2.14	0.66
49:5:32:MET:SD	49:5:46:ARG:NH1	2.68	0.66
22:v:20:TYR:CZ	22:v:78:ILE:CD1	2.79	0.66
23:A:1518:G:O2'	23:A:1519:U:O5'	2.13	0.66
49:5:36:CYS:SG	49:5:43:THR:OG1	2.51	0.66
4:d:105:ARG:N	4:d:109:GLN:OE1	2.28	0.66
45:1:42:ARG:O	45:1:45:THR:OG1	2.12	0.66
1:a:597:U:O2'	8:h:57:GLN:OE1	2.13	0.66
9:i:57:THR:HG22	9:i:58:GLU:OE1	1.95	0.66
1:a:184:A:N1	1:a:208:U:C5	2.63	0.66
1:a:675:G:OP1	1:a:740:C:O2'	2.14	0.66
4:d:162:PRO:HG2	4:d:165:LEU:HD12	1.77	0.66
23:A:2550:G:HO2'	23:A:2791:A:HO2'	1.43	0.66
23:A:224:A:N1	23:A:268:A:O2'	2.27	0.66
23:A:1018:A:O4'	23:A:1225:G:N2	2.29	0.66
1:a:908:G:O2'	1:a:910:A:N6	2.28	0.66
22:v:85:LEU:HA	22:v:88:GLN:HG3	1.78	0.66
23:A:731:U:O5'	50:6:12:LYS:NZ	2.29	0.66
23:A:263:G:N2	23:A:264:G:H1'	2.11	0.66
1:a:1003:G:N7	1:a:1224:A:N6	2.44	0.65
22:v:78:ILE:C	22:v:80:LEU:N	2.54	0.65
1:a:952:G:N2	1:a:1352:U:O2	2.28	0.65
1:a:1076:G:O2'	1:a:1201:G:N2	2.29	0.65
22:v:20:TYR:CE1	22:v:78:ILE:CD1	2.79	0.65
45:1:17:GLN:O	45:1:20:SER:OG	2.10	0.65
1:a:1138:U:N3	1:a:1291:A:OP1	2.29	0.65
7:g:144:MET:O	7:g:148:ASN:N	2.30	0.65
16:p:6:ARG:NH2	16:p:28:PRO:O	2.28	0.65
1:a:667:C:OP2	15:o:8:LYS:NZ	2.30	0.65
1:a:1235:U:O2'	19:s:78:ARG:NH2	2.29	0.65
22:v:71:ASN:ND2	22:v:77:GLY:CA	2.59	0.65
23:A:590:U:OP1	23:A:1257:G:O2'	2.13	0.65
48:4:28:THR:N	48:4:37:TYR:O	2.28	0.65
9:i:74:PHE:O	9:i:78:ALA:N	2.30	0.65
33:P:48:GLU:HG2	33:P:51:ARG:HH11	1.54	0.65
4:d:92:SER:OG	4:d:133:VAL:O	2.13	0.65
21:u:46:LYS:HD2	21:u:50:GLU:OE2	1.96	0.65
23:A:2260:A:H2'	23:A:2261:G:H8	1.62	0.65
23:A:2869:G:OP1	36:S:95:ARG:NH2	2.29	0.65
41:X:24:ILE:HG22	41:X:25:ALA:H	1.61	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:d:12:SER:OG	4:d:20:SER:O	2.14	0.65
37:T:18:ILE:O	37:T:21:ALA:N	2.30	0.65
40:W:13:THR:O	40:W:17:SER:OG	2.06	0.65
1:a:874:A:O2'	1:a:1090:U:O4	2.15	0.65
23:A:2161:A:N6	23:A:2184:G:C2	2.65	0.65
42:Y:14:THR:C	42:Y:18:LEU:HD23	2.22	0.65
7:g:139:GLU:O	7:g:142:HIS:N	2.29	0.65
23:A:2822:C:O2'	23:A:2823:G:O4'	2.15	0.65
1:a:243:C:OP1	17:q:74:ARG:NH1	2.30	0.65
1:a:421:G:O2'	1:a:436:G:N2	2.29	0.65
2:b:76:ALA:O	2:b:79:SER:OG	2.12	0.65
9:i:11:THR:O	9:i:108:ARG:NH2	2.30	0.65
22:v:20:TYR:OH	22:v:78:ILE:HD12	1.97	0.65
23:A:1039:C:O2'	37:T:93:LYS:NZ	2.30	0.65
23:A:1583:G:P	23:A:1584:A:H8	2.19	0.65
23:A:1651:C:N4	23:A:1666:A:OP2	2.30	0.65
23:A:1767:G:O2'	23:A:1768:C:O5'	2.14	0.65
1:a:670:A:O2'	1:a:844:G:OP1	2.15	0.64
1:a:1227:A:OP1	14:n:2:ALA:N	2.30	0.64
2:b:73:LYS:NZ	2:b:204:ASP:OD2	2.29	0.64
22:v:31:TYR:HD2	22:v:89:VAL:HG12	1.63	0.64
23:A:614:U:O2'	23:A:616:G:OP2	2.10	0.64
42:Y:25:GLY:O	42:Y:44:ASP:CA	2.42	0.64
1:a:83:C:O2'	1:a:85:U:OP2	2.14	0.64
23:A:319:G:N2	23:A:400:C:O2	2.30	0.64
23:A:1360:G:O2'	23:A:1361:G:O5'	2.13	0.64
42:Y:14:THR:O	42:Y:18:LEU:HD23	1.96	0.64
23:A:250:G:OP2	23:A:252:C:N4	2.29	0.64
23:A:312:A:O2'	23:A:313:U:O4'	2.11	0.64
23:A:1135:G:O2'	23:A:1146:C:N3	2.30	0.64
23:A:2058:A:O2'	23:A:2481:G:N2	2.31	0.64
1:a:415:A:OP1	4:d:108:ARG:NH2	2.29	0.64
1:a:746:U:OP2	6:f:93:ARG:NH1	2.30	0.64
1:a:964:G:H21	1:a:1238:A:H62	1.45	0.64
45:1:10:THR:O	45:1:11:THR:OG1	2.12	0.64
23:A:616:G:N2	23:A:2058:A:OP1	2.28	0.64
23:A:618:A:OP2	23:A:2526:C:O2'	2.15	0.64
23:A:1492:G:N3	23:A:1574:G:N2	2.46	0.64
23:A:2715:G:OP1	23:A:2740:A:N6	2.31	0.64
42:Y:21:LEU:HD12	42:Y:42:LYS:HD3	1.73	0.64
1:a:61:A:OP1	1:a:110:G:N2	2.30	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:a:343:C:O2'	1:a:1444:A:N3	2.26	0.64
31:N:24:VAL:CG1	31:N:33:ALA:HB2	2.26	0.64
23:A:1288:G:OP2	32:O:21:ARG:NH1	2.30	0.64
22:v:91:LYS:O	22:v:94:THR:N	2.21	0.64
23:A:1305:U:H5''	23:A:1306:C:OP2	1.98	0.64
23:A:1450:A:OP2	23:A:1634:A:N6	2.30	0.64
34:Q:18:ARG:NE	34:Q:65:THR:O	2.28	0.64
1:a:727:C:H1'	18:r:43:LYS:HG2	1.80	0.64
23:A:925:G:N2	23:A:926:G:N7	2.46	0.64
23:A:1733:A:OP2	23:A:1742:A:N6	2.31	0.64
1:a:107:G:N2	1:a:107:G:OP2	2.31	0.64
1:a:1013:G:N2	1:a:1014:A:O2'	2.29	0.64
18:r:47:ARG:NH1	18:r:52:THR:O	2.30	0.64
23:A:674:C:O3'	23:A:694:G:N2	2.31	0.64
23:A:1018:A:O5'	23:A:1225:G:N2	2.31	0.64
1:a:666:G:O6	1:a:755:U:N3	2.31	0.63
21:u:53:ARG:C	21:u:54:LYS:HD3	2.23	0.63
23:A:1320:G:N2	23:A:1366:U:O4	2.28	0.63
22:v:74:LEU:HD23	22:v:74:LEU:N	2.02	0.63
23:A:325:A:N6	23:A:402:C:O4'	2.31	0.63
23:A:562:C:OP1	48:4:13:LYS:NZ	2.30	0.63
1:a:1189:G:OP1	9:i:97:ARG:NH1	2.32	0.63
26:E:38:LYS:NZ	26:E:98:ALA:O	2.25	0.63
1:a:573:U:OP2	1:a:574:G:O2'	2.15	0.63
1:a:1233:G:OP1	19:s:77:THR:OG1	2.16	0.63
1:a:1547:C:C4'	21:u:54:LYS:CG	2.72	0.63
23:A:1453:G:O3'	23:A:1455:U:N3	2.31	0.63
2:b:187:VAL:HG21	2:b:199:VAL:HG13	1.81	0.63
22:v:96:ILE:O	22:v:97:ASN:CB	2.47	0.63
23:A:1128:A:N3	23:A:1149:U:O2'	2.23	0.63
23:A:2811:U:O2'	26:E:39:LYS:NZ	2.32	0.63
5:e:7:GLU:HA	5:e:11:PHE:HZ	1.63	0.63
22:v:96:ILE:O	22:v:97:ASN:HB2	1.99	0.63
23:A:1153:C:O2'	23:A:1154:G:O4'	2.15	0.63
50:6:20:ARG:O	50:6:24:SER:OG	2.16	0.63
2:b:58:LYS:O	2:b:62:GLU:N	2.31	0.63
23:A:2527:U:O2'	23:A:2531:U:OP1	2.12	0.63
7:g:46:ALA:O	7:g:50:VAL:HG12	1.99	0.63
22:v:95:ARG:CB	22:v:96:ILE:HG23	2.28	0.63
22:v:97:ASN:ND2	22:v:99:LYS:CE	2.62	0.63
23:A:1472:C:N4	23:A:1617:A:OP2	2.27	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:a:1198:G:O2'	9:i:115:ARG:NH1	2.32	0.62
1:a:1316:G:O2'	1:a:1342:G:N2	2.31	0.62
12:l:78:ALA:HB1	12:l:109:HIS:HA	1.79	0.62
5:e:149:ASN:O	5:e:153:VAL:HG23	1.98	0.62
22:v:85:LEU:HD23	22:v:85:LEU:N	2.13	0.62
23:A:582:G:O2'	23:A:599:A:N6	2.31	0.62
23:A:904:G:N2	23:A:962:A:OP2	2.32	0.62
29:H:99:GLN:O	29:H:102:ASP:N	2.31	0.62
50:6:3:LYS:NZ	50:6:7:GLN:OE1	2.32	0.62
1:a:1168:A:OP1	1:a:1169:C:N4	2.32	0.62
22:v:99:LYS:O	22:v:99:LYS:HG2	1.99	0.62
23:A:315:C:N4	23:A:404:U:OP2	2.33	0.62
25:D:81:GLN:NE2	25:D:82:TYR:O	2.31	0.62
33:P:31:GLU:HA	33:P:134:ARG:HD3	1.80	0.62
34:Q:47:LEU:O	34:Q:51:GLY:N	2.31	0.62
1:a:1235:U:HO2'	19:s:78:ARG:HH21	1.47	0.62
27:F:112:SER:O	27:F:115:SER:OG	2.12	0.62
1:a:1017:A:N1	1:a:1032:C:O2'	2.26	0.62
18:r:33:LEU:HD22	18:r:37:PHE:HZ	1.65	0.62
23:A:1938:U:O2'	23:A:1946:A:N6	2.32	0.62
23:A:2349:A:N6	23:A:2360:A:N7	2.47	0.62
1:a:1516:G:OP2	1:a:1519:A:O2'	2.15	0.62
23:A:287:G:N2	23:A:288:C:O3'	2.33	0.62
23:A:2024:A:OP2	26:E:138:ARG:NH1	2.33	0.62
42:Y:25:GLY:HA3	42:Y:44:ASP:OD1	2.00	0.62
1:a:1385:A:O2'	7:g:28:ASN:O	2.17	0.62
23:A:275:A:C5	23:A:296:G:N2	2.68	0.62
1:a:129:A:O5'	17:q:2:SER:N	2.33	0.62
1:a:701:G:C5'	22:v:100:SER:HB3	2.30	0.62
23:A:863:G:O2'	23:A:864:A:O5'	2.17	0.62
23:A:1810:A:O2'	23:A:2634:G:O2'	2.16	0.62
23:A:2372:G:O6	23:A:2398:G:N2	2.29	0.62
26:E:2:THR:OG1	26:E:93:ASN:O	2.18	0.62
1:a:1066:C:O2'	1:a:1067:A:OP2	2.13	0.62
1:a:1119:C:OP1	3:c:171:THR:OG1	2.18	0.62
25:D:29:GLU:OE1	25:D:29:GLU:N	2.33	0.62
23:A:160:G:N2	23:A:167:U:OP2	2.33	0.61
39:V:31:GLU:O	39:V:34:ALA:N	2.33	0.61
1:a:1065:G:N2	1:a:1070:G:O6	2.33	0.61
22:v:27:LYS:O	22:v:30:ARG:CD	2.47	0.61
23:A:263:G:H2'	23:A:264:G:O5'	1.99	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:A:545:G:N1	23:A:548:A:OP2	2.33	0.61
23:A:927:G:O6	23:A:939:U:N3	2.32	0.61
23:A:2272:U:O2'	23:A:2463:G:OP2	2.18	0.61
1:a:184:A:N1	1:a:208:U:C4	2.68	0.61
4:d:150:ILE:O	4:d:154:SER:OG	2.11	0.61
13:m:104:ASN:O	13:m:107:ARG:NH2	2.33	0.61
22:v:58:ILE:CD1	22:v:85:LEU:CB	2.78	0.61
22:v:75:TYR:O	22:v:78:ILE:HG22	1.99	0.61
23:A:1979:A:N3	23:A:2587:C:O2'	2.24	0.61
2:b:167:ARG:O	2:b:170:ARG:NH1	2.33	0.61
23:A:1145:U:O2'	23:A:1147:A:OP2	2.19	0.61
1:a:958:C:O2'	1:a:1375:U:O4	2.09	0.61
7:g:17:ILE:HD11	7:g:40:GLN:HE21	1.65	0.61
13:m:91:HIS:O	13:m:109:ARG:NH2	2.34	0.61
18:r:25:HIS:CG	18:r:26:ILE:HD13	2.36	0.61
18:r:47:ARG:CZ	18:r:54:ALA:HB2	2.30	0.61
22:v:58:ILE:CD1	22:v:85:LEU:HB3	2.30	0.61
22:v:78:ILE:O	22:v:80:LEU:N	2.33	0.61
23:A:661:U:OP1	27:F:106:ARG:NE	2.34	0.61
33:P:48:GLU:HG2	33:P:51:ARG:NH1	2.08	0.61
23:A:1401:G:N2	23:A:1404:A:OP2	2.33	0.61
23:A:2703:C:O2	23:A:2759:G:N2	2.33	0.61
1:a:1200:U:OP1	10:j:53:ARG:NH2	2.33	0.61
2:b:83:GLU:O	2:b:87:ALA:N	2.34	0.61
6:f:28:GLY:O	6:f:32:THR:N	2.34	0.61
22:v:101:ARG:O	22:v:102:ASP:O	2.18	0.61
23:A:1135:G:H21	23:A:1146:C:H41	1.49	0.61
23:A:2039:G:O2'	23:A:2040:A:O5'	2.14	0.61
23:A:1777:G:O2'	23:A:2880:A:N6	2.33	0.61
33:P:34:LEU:HD23	33:P:35:GLN:N	2.16	0.61
23:A:234:C:O2'	23:A:235:G:O4'	2.19	0.61
23:A:797:A:OP1	50:6:4:ARG:NH2	2.33	0.61
1:a:1091:G:OP1	5:e:138:ARG:NH1	2.34	0.61
1:a:1130:A:OP1	9:i:108:ARG:NH1	2.33	0.61
22:v:96:ILE:HG13	22:v:97:ASN:H	1.66	0.61
23:A:614:U:O4'	23:A:2057:A:N6	2.34	0.61
23:A:1091:G:N2	23:A:1154:G:O2'	2.33	0.61
50:6:19:PHE:O	50:6:22:ARG:N	2.34	0.61
1:a:1079:A:N1	1:a:1120:G:O2'	2.34	0.60
1:a:634:U:OP1	16:p:19:ARG:NH2	2.34	0.60
22:v:99:LYS:HD3	22:v:99:LYS:N	2.16	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:A:1952:C:O2'	23:A:1953:U:O4'	2.17	0.60
1:a:853:C:O2'	1:a:856:C:N4	2.34	0.60
1:a:1249:A:OP1	1:a:1346:C:O2'	2.19	0.60
1:a:1443:G:N2	1:a:1480:A:OP2	2.30	0.60
4:d:97:VAL:O	4:d:101:LEU:N	2.34	0.60
22:v:31:TYR:HE2	22:v:90:ARG:N	1.97	0.60
36:S:55:GLY:N	36:S:58:SER:OG	2.34	0.60
3:c:8:ILE:HG22	3:c:16:ARG:HH12	1.67	0.60
47:3:28:THR:HG22	47:3:30:THR:HG23	1.84	0.60
1:a:715:U:OP1	11:k:24:ARG:NH2	2.34	0.60
21:u:10:GLU:HA	21:u:10:GLU:OE1	2.02	0.60
22:v:20:TYR:OH	22:v:78:ILE:CD1	2.49	0.60
33:P:75:THR:OG1	33:P:89:ALA:O	2.09	0.60
30:M:38:ARG:NH2	30:M:45:TYR:OH	2.35	0.60
30:M:65:PHE:O	30:M:66:THR:OG1	2.17	0.60
4:d:118:HIS:NE2	4:d:148:LEU:HD12	2.17	0.60
22:v:92:TYR:O	22:v:95:ARG:NH1	2.31	0.60
23:A:902:A:OP1	43:Z:85:LYS:NZ	2.25	0.60
10:j:5:LYS:HE3	10:j:77:VAL:CG2	2.31	0.60
27:F:60:GLY:O	27:F:77:THR:OG1	2.19	0.60
1:a:1322:A:O3'	47:3:81:LYS:NZ	2.32	0.60
23:A:1487:G:N2	23:A:1597:U:O2	2.35	0.60
33:P:48:GLU:CG	33:P:51:ARG:HH12	1.98	0.60
22:v:17:ILE:HA	22:v:20:TYR:CD2	2.35	0.59
25:D:44:ASN:OD1	25:D:45:GLN:N	2.35	0.59
31:N:24:VAL:HG13	31:N:33:ALA:HB2	1.84	0.59
1:a:603:A:O2'	1:a:649:A:N6	2.34	0.59
1:a:1547:C:H4'	21:u:54:LYS:HG3	1.81	0.59
12:l:102:ASP:OD1	12:l:103:LEU:N	2.35	0.59
23:A:1306:C:O2	23:A:2040:A:N1	2.34	0.59
1:a:161:A:N1	1:a:355:G:O2'	2.29	0.59
1:a:546:U:OP2	12:l:125:GLN:NE2	2.35	0.59
15:o:39:VAL:HB	15:o:56:LEU:HD21	1.84	0.59
23:A:115:C:O2'	23:A:125:A:N3	2.32	0.59
1:a:936:G:H21	22:v:91:LYS:CB	1.99	0.59
5:e:133:PRO:O	5:e:137:VAL:HG23	2.01	0.59
23:A:1462:G:H21	23:A:1626:A:H62	1.48	0.59
1:a:1189:G:O2'	1:a:1191:A:N7	2.24	0.59
2:b:71:GLY:N	2:b:92:ILE:O	2.36	0.59
3:c:51:VAL:HG12	3:c:69:THR:OG1	2.00	0.59
7:g:27:ILE:O	7:g:31:MET:N	2.35	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:s:36:ARG:NH1	19:s:73:GLU:OE1	2.36	0.59
1:a:129:A:OP1	17:q:2:SER:OG	2.17	0.59
2:b:124:GLY:CA	2:b:128:VAL:HG21	2.32	0.59
2:b:177:ARG:NH2	2:b:195:GLU:O	2.35	0.59
4:d:68:PHE:O	4:d:71:THR:OG1	2.20	0.59
23:A:313:U:O2'	23:A:314:A:O4'	2.16	0.59
23:A:1896:U:N3	23:A:1898:C:OP2	2.35	0.59
23:A:2260:A:C6	23:A:2261:G:C6	2.91	0.59
34:Q:18:ARG:O	34:Q:22:THR:HG22	2.03	0.59
50:6:25:THR:O	50:6:28:GLY:N	2.35	0.59
1:a:151:A:OP2	1:a:169:C:N4	2.35	0.59
21:u:14:ASP:OD2	21:u:18:ARG:HG2	2.02	0.59
23:A:1578:A:N6	23:A:1591:G:O6	2.34	0.59
1:a:1158:C:O2'	9:i:9:ARG:NH2	2.35	0.59
1:a:1159:U:O2'	9:i:18:VAL:HG21	2.02	0.59
20:t:17:ALA:O	20:t:21:ASN:ND2	2.36	0.59
1:a:173:U:O2	1:a:211:A:N6	2.36	0.59
10:j:22:ALA:O	10:j:26:VAL:HG23	2.03	0.59
18:r:37:PHE:O	18:r:45:LEU:HB2	2.02	0.59
23:A:1109:U:O2'	23:A:1117:A:N6	2.30	0.59
24:B:82:C:O2'	24:B:83:U:O5'	2.20	0.59
5:e:7:GLU:HA	5:e:11:PHE:CZ	2.38	0.58
22:v:58:ILE:HD13	22:v:85:LEU:CB	2.32	0.58
22:v:94:THR:CA	22:v:95:ARG:HB2	2.32	0.58
23:A:588:G:N2	23:A:589:U:O4	2.35	0.58
23:A:2868:G:H8	36:S:97:ALA:HB2	1.68	0.58
26:E:17:GLY:N	26:E:21:GLU:O	2.36	0.58
29:H:94:TYR:OH	29:H:160:LYS:O	2.21	0.58
35:R:55:GLN:O	35:R:83:LYS:NZ	2.21	0.58
1:a:1310:A:O2'	1:a:1312:U:O4'	2.14	0.58
23:A:1038:C:OP2	37:T:54:LYS:NZ	2.36	0.58
36:S:7:ILE:O	36:S:11:THR:HG23	2.04	0.58
43:Z:51:THR:HG21	43:Z:54:TYR:CD1	2.38	0.58
47:3:1:MET:SD	47:3:2:LYS:N	2.77	0.58
18:r:41:ARG:NE	21:u:26:SER:HB3	2.18	0.58
23:A:1250:G:O2'	23:A:1274:G:N1	2.35	0.58
1:a:1351:A:O3'	22:v:61:LYS:NZ	2.36	0.58
22:v:71:ASN:HD22	22:v:77:GLY:HA3	1.68	0.58
23:A:1183:G:O2'	23:A:1187:A:N1	2.36	0.58
1:a:1016:A:N6	1:a:1032:C:N3	2.48	0.58
1:a:1107:U:OP1	1:a:1120:G:N2	2.35	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:A:675:G:N2	23:A:678:A:OP2	2.30	0.58
7:g:15:ASP:N	7:g:20:SER:O	2.35	0.58
22:v:31:TYR:HD2	22:v:89:VAL:CG1	2.17	0.58
23:A:138:U:N3	23:A:141:U:OP2	2.35	0.58
1:a:1136:G:N2	1:a:1137:U:O4	2.35	0.58
22:v:17:ILE:O	22:v:21:ILE:HG22	2.04	0.58
1:a:1090:U:O2'	1:a:1091:G:OP1	2.19	0.58
21:u:18:ARG:O	21:u:19:PHE:C	2.46	0.58
1:a:330:C:H42	1:a:337:A:H62	1.51	0.58
10:j:12:ALA:HB3	10:j:18:ILE:HG23	1.85	0.58
18:r:25:HIS:HB3	18:r:26:ILE:HA	1.86	0.57
22:v:88:GLN:CA	22:v:91:LYS:HE2	2.29	0.57
1:a:709:C:O2	1:a:711:G:N1	2.37	0.57
21:u:27:GLY:HA3	21:u:30:GLN:NE2	2.19	0.57
29:H:58:SER:O	29:H:62:ARG:NH1	2.37	0.57
31:N:71:ARG:NH1	31:N:72:ASN:OD1	2.37	0.57
38:U:88:HIS:NE2	38:U:90:GLN:OE1	2.34	0.57
40:W:51:ALA:HB1	40:W:81:THR:HG23	1.87	0.57
1:a:445:U:N3	1:a:503:A:C8	2.72	0.57
17:q:21:LYS:O	17:q:50:ASP:N	2.36	0.57
30:M:6:MET:SD	30:M:48:HIS:NE2	2.71	0.57
1:a:211:A:N1	1:a:228:A:O2'	2.36	0.57
1:a:555:A:OP2	4:d:3:ARG:NH1	2.36	0.57
1:a:900:G:O2'	1:a:916:G:O6	2.22	0.57
23:A:1397:G:N2	23:A:2241:C:H42	2.03	0.57
23:A:2693:C:N4	29:H:108:GLY:O	2.37	0.57
1:a:988:A:N6	1:a:1327:G:H21	2.02	0.57
4:d:190:ASN:OD1	4:d:192:GLN:N	2.36	0.57
22:v:71:ASN:HD22	22:v:77:GLY:H	1.52	0.57
1:a:726:A:N1	18:r:42:GLY:O	2.38	0.57
1:a:1326:U:O2'	1:a:1371:A:N3	2.28	0.57
3:c:14:ILE:HG22	3:c:15:ILE:HG23	1.86	0.57
23:A:2112:C:H42	23:A:2261:G:H1	1.51	0.57
34:Q:100:TYR:O	34:Q:101:THR:OG1	2.21	0.57
5:e:163:GLU:N	5:e:163:GLU:OE1	2.37	0.57
23:A:925:G:N1	23:A:941:A:C2	2.73	0.57
24:B:82:C:O2'	24:B:83:U:O4'	2.20	0.57
1:a:1547:C:C5'	21:u:54:LYS:NZ	2.66	0.57
23:A:677:A:O4'	32:O:60:ARG:NH2	2.37	0.57
42:Y:22:ARG:HH22	42:Y:87:THR:HG23	1.63	0.57
23:A:2683:U:O2	23:A:2692:A:N7	2.38	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:Q:52:LYS:NZ	34:Q:96:ARG:O	2.37	0.56
1:a:304:U:O2'	1:a:564:C:O2	2.22	0.56
1:a:944:C:O2'	1:a:1355:C:OP2	2.20	0.56
22:v:85:LEU:CD2	22:v:85:LEU:H	2.18	0.56
23:A:592:A:O2'	23:A:593:U:O5'	2.23	0.56
23:A:2302:C:O2	43:Z:18:THR:CG2	2.53	0.56
7:g:17:ILE:HG21	7:g:47:PHE:HE2	1.70	0.56
10:j:4:GLN:C	10:j:5:LYS:HD3	2.30	0.56
18:r:34:LEU:O	18:r:38:ILE:N	2.34	0.56
22:v:20:TYR:HE1	22:v:78:ILE:HD13	1.69	0.56
23:A:510:U:O2'	23:A:511:G:O5'	2.23	0.56
23:A:1518:G:HO2'	23:A:1519:U:P	2.28	0.56
33:P:54:MET:HG3	33:P:117:ALA:HB1	1.86	0.56
1:a:1547:C:C5'	21:u:54:LYS:HZ3	2.18	0.56
21:u:40:LYS:HB3	21:u:41:PRO:HD2	1.87	0.56
1:a:1261:A:N3	1:a:1381:G:O2'	2.30	0.56
13:m:106:ALA:HB3	13:m:107:ARG:HA	1.87	0.56
23:A:1927:A:O2'	23:A:1928:A:OP1	2.21	0.56
24:B:95:A:O2'	24:B:96:G:O4'	2.17	0.56
1:a:272:C:O2'	17:q:67:ARG:NH1	2.39	0.56
1:a:1171:G:O2'	1:a:1172:C:O5'	2.24	0.56
1:a:1248:C:O2'	1:a:1311:G:N2	2.29	0.56
20:t:50:VAL:HG23	20:t:78:LEU:CD1	2.35	0.56
22:v:20:TYR:C	22:v:20:TYR:CD1	2.83	0.56
26:E:9:LYS:O	26:E:11:GLY:N	2.39	0.56
1:a:329:A:O2'	1:a:330:C:O4'	2.22	0.56
1:a:1388:A:OP1	7:g:95:ARG:NH2	2.38	0.56
1:a:1458:A:OP1	1:a:1459:C:N4	2.39	0.56
5:e:149:ASN:HD22	5:e:150:ALA:N	2.03	0.56
10:j:5:LYS:HB2	10:j:77:VAL:HG22	1.85	0.56
16:p:85:ASP:OD1	16:p:86:GLU:N	2.38	0.56
17:q:5:ASN:OD1	17:q:6:ASP:N	2.39	0.56
22:v:65:LEU:HD23	22:v:66:ARG:N	2.21	0.56
22:v:81:ILE:C	22:v:85:LEU:HD22	2.19	0.56
23:A:2347:A:N6	23:A:2360:A:O2'	2.39	0.56
23:A:2860:U:H5''	34:Q:49:THR:HG21	1.88	0.56
36:S:77:PRO:O	36:S:80:THR:OG1	2.17	0.56
23:A:2261:G:H8	23:A:2261:G:O5'	1.89	0.56
23:A:2777:A:O2'	23:A:2780:A:N6	2.39	0.56
47:3:12:VAL:HG22	47:3:13:ILE:H	1.70	0.56
18:r:41:ARG:NH2	21:u:22:SER:O	2.38	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:v:20:TYR:HH	22:v:78:ILE:HG21	1.60	0.56
23:A:373:A:N6	23:A:1248:U:O4	2.38	0.56
23:A:510:U:O4	23:A:729:G:O2'	2.23	0.56
23:A:528:C:O2'	23:A:542:A:N1	2.39	0.56
23:A:1003:A:N3	23:A:2484:U:O2'	2.29	0.56
23:A:1885:G:H2'	23:A:1910:G:H22	1.71	0.56
24:B:49:G:H5'	35:R:67:ALA:HB1	1.87	0.56
25:D:124:LYS:HB2	25:D:127:ASN:HD22	1.70	0.56
1:a:1095:U:O2'	1:a:1114:A:OP2	2.23	0.56
1:a:1318:U:OP1	13:m:100:GLN:NE2	2.39	0.56
9:i:66:LEU:HD13	9:i:67:VAL:N	2.20	0.56
2:b:145:ILE:O	2:b:149:GLY:N	2.38	0.55
3:c:39:ARG:NH1	3:c:54:VAL:O	2.32	0.55
3:c:54:VAL:HG23	3:c:66:ALA:O	2.06	0.55
33:P:13:HIS:NE2	33:P:88:GLY:O	2.39	0.55
40:W:49:LYS:HD3	40:W:51:ALA:HB2	1.87	0.55
1:a:1231:G:OP1	19:s:37:ARG:NH1	2.37	0.55
1:a:1306:U:O3'	13:m:43:THR:OG1	2.24	0.55
12:l:23:ALA:N	12:l:108:TYR:OH	2.40	0.55
23:A:27:G:O2'	23:A:557:G:N2	2.38	0.55
23:A:1306:C:H2'	23:A:1307:G:H5'	1.88	0.55
23:A:1307:G:H8	23:A:1307:G:O5'	1.88	0.55
23:A:1450:A:HO2'	23:A:1451:U:C4'	2.18	0.55
23:A:2362:A:OP1	35:R:17:ARG:NH1	2.40	0.55
23:A:2905:C:H42	48:4:39:LEU:HD22	1.72	0.55
25:D:208:GLY:O	25:D:212:TRP:N	2.39	0.55
1:a:788:A:N6	1:a:809:U:OP2	2.34	0.55
23:A:192:G:OP2	44:0:28:ARG:NH1	2.39	0.55
23:A:1479:G:O2'	23:A:1480:G:OP2	2.18	0.55
23:A:2137:G:O2'	23:A:2138:U:O5'	2.25	0.55
23:A:2142:G:N2	23:A:2189:G:OP1	2.39	0.55
24:B:46:A:OP1	35:R:35:ARG:NH2	2.40	0.55
1:a:61:A:OP2	1:a:395:U:O2'	2.23	0.55
12:l:125:GLN:OE1	12:l:125:GLN:N	2.39	0.55
23:A:241:C:C4	23:A:263:G:O6	2.59	0.55
23:A:437:A:O2'	23:A:438:U:OP1	2.23	0.55
23:A:1865:C:N4	23:A:1926:A:O4'	2.39	0.55
35:R:68:THR:OG1	35:R:104:ARG:NH1	2.39	0.55
1:a:346:A:OP2	31:N:97:ARG:NH2	2.39	0.55
1:a:1534:U:O3'	11:k:126:ARG:NH2	2.39	0.55
3:c:194:LYS:C	3:c:195:LEU:HD12	2.32	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:e:70:ASP:C	5:e:71:LEU:HD12	2.32	0.55
7:g:42:ILE:O	7:g:45:SER:OG	2.24	0.55
23:A:659:A:O2'	27:F:43:SER:OG	2.22	0.55
23:A:1452:C:N4	23:A:1632:A:N7	2.55	0.55
23:A:1583:G:OP1	23:A:1584:A:N7	2.39	0.55
24:B:50:A:N6	35:R:37:ASN:O	2.38	0.55
1:a:671:A:O3'	18:r:58:ARG:NH1	2.40	0.55
1:a:261:U:C1'	1:a:283:G:H21	2.20	0.55
1:a:1360:A:H62	1:a:1384:G:H21	1.55	0.55
12:l:53:MET:HE3	12:l:65:TYR:CE1	2.41	0.55
22:v:91:LYS:CG	22:v:92:TYR:N	2.68	0.55
7:g:42:ILE:HG22	7:g:116:MET:SD	2.47	0.55
10:j:5:LYS:HB3	10:j:77:VAL:HA	1.88	0.55
23:A:1845:U:OP2	25:D:155:ARG:NE	2.40	0.55
48:4:43:VAL:O	48:4:44:CYS:HB2	2.06	0.55
18:r:41:ARG:CA	18:r:78:GLU:HB3	2.36	0.55
7:g:108:ALA:HB2	7:g:123:GLU:OE1	2.06	0.54
13:m:69:LEU:O	13:m:69:LEU:HD23	2.08	0.54
22:v:90:ARG:CG	22:v:91:LYS:N	2.63	0.54
48:4:18:THR:OG1	48:4:19:HIS:ND1	2.37	0.54
1:a:988:A:H61	1:a:1327:G:H21	1.54	0.54
22:v:76:ALA:O	22:v:80:LEU:HD23	2.08	0.54
22:v:94:THR:CA	22:v:95:ARG:CB	2.85	0.54
23:A:1400:C:O2'	23:A:1836:A:O2'	2.12	0.54
47:3:24:LEU:O	47:3:24:LEU:HD13	2.06	0.54
23:A:1063:U:O2'	23:A:1065:A:N7	2.35	0.54
23:A:1306:C:OP1	23:A:2033:C:OP1	2.25	0.54
28:G:89:VAL:O	28:G:92:ARG:N	2.40	0.54
36:S:33:ARG:N	36:S:82:LYS:O	2.34	0.54
1:a:137:U:O4	1:a:138:A:N6	2.41	0.54
17:q:50:ASP:OD1	17:q:51:GLU:N	2.40	0.54
23:A:1033:G:O2'	23:A:1034:A:OP2	2.23	0.54
28:G:90:THR:O	28:G:93:GLY:N	2.40	0.54
22:v:31:TYR:CD2	22:v:89:VAL:CB	2.91	0.54
23:A:49:A:H61	23:A:179:A:H2'	1.73	0.54
23:A:275:A:C6	23:A:296:G:C2	2.94	0.54
23:A:1597:U:O2'	23:A:1598:U:O4'	2.18	0.54
23:A:2112:C:N4	23:A:2261:G:H1	2.06	0.54
28:G:37:ASN:N	28:G:145:LYS:O	2.41	0.54
1:a:980:C:O2'	1:a:1242:G:N2	2.41	0.54
2:b:69:PHE:O	2:b:92:ILE:N	2.41	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:e:107:ALA:HB2	5:e:125:SER:HB2	1.90	0.54
23:A:1397:G:H22	23:A:2241:C:H42	1.56	0.54
1:a:409:C:O2'	1:a:629:A:N3	2.40	0.54
22:v:71:ASN:ND2	22:v:77:GLY:H	2.05	0.54
23:A:162:A:O2'	23:A:163:U:OP1	2.20	0.54
23:A:632:U:OP1	32:O:16:ARG:NH1	2.41	0.54
23:A:1037:A:OP2	37:T:51:ARG:NH1	2.39	0.54
11:k:67:SER:O	11:k:71:SER:OG	2.24	0.54
22:v:81:ILE:C	22:v:85:LEU:CD2	2.80	0.54
23:A:1124:A:O2'	23:A:1125:U:O5'	2.25	0.54
23:A:1582:U:O2'	23:A:1585:G:O6	2.17	0.54
23:A:2418:G:N2	23:A:2449:C:N3	2.55	0.54
42:Y:14:THR:O	42:Y:18:LEU:HD21	2.05	0.54
51:7:34:ALA:HB3	51:7:37:SER:HB2	1.89	0.54
1:a:1444:A:OP2	1:a:1479:G:N1	2.41	0.54
8:h:105:LEU:O	8:h:128:ILE:N	2.41	0.54
10:j:85:ASP:O	10:j:89:GLY:N	2.40	0.54
12:l:56:LYS:O	12:l:57:LYS:C	2.50	0.54
23:A:1306:C:C5	23:A:2039:G:N2	2.76	0.54
1:a:109:C:O2'	16:p:26:ARG:O	2.25	0.54
8:h:115:ASP:OD1	8:h:116:LYS:N	2.39	0.54
19:s:48:THR:HG23	19:s:60:VAL:O	2.08	0.54
23:A:178:A:OP2	23:A:179:A:N6	2.41	0.54
23:A:373:A:C8	23:A:1248:U:N3	2.75	0.54
32:O:83:ASN:OD1	32:O:84:LYS:N	2.41	0.54
1:a:181:A:H61	1:a:208:U:H3'	1.72	0.53
1:a:306:A:O2'	1:a:307:G:OP1	2.25	0.53
1:a:667:C:OP1	15:o:9:ASN:ND2	2.37	0.53
8:h:108:THR:OG1	8:h:111:GLY:N	2.39	0.53
1:a:993:A:O2'	1:a:994:C:O5'	2.17	0.53
6:f:2:ARG:NH2	6:f:94:GLU:O	2.41	0.53
26:E:74:GLU:O	26:E:78:LYS:N	2.40	0.53
1:a:975:A:O2'	1:a:979:A:N7	2.39	0.53
1:a:1238:A:OP1	13:m:110:LYS:NZ	2.24	0.53
5:e:25:VAL:HG22	5:e:26:LYS:H	1.72	0.53
1:a:1386:A:O2'	7:g:102:ARG:NH2	2.41	0.53
18:r:40:GLU:HG2	18:r:40:GLU:O	2.06	0.53
22:v:99:LYS:C	22:v:100:SER:O	2.50	0.53
22:v:94:THR:HA	22:v:95:ARG:C	2.32	0.53
23:A:1953:U:O2'	23:A:1954:A:N7	2.39	0.53
23:A:2869:G:H22	23:A:2887:G:P	2.31	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
47:3:30:THR:HG1	47:3:51:SER:HG	1.48	0.53
1:a:435:C:OP1	4:d:13:ARG:NH1	2.39	0.53
13:m:14:ARG:NH2	13:m:17:ILE:HG21	2.23	0.53
47:3:8:GLU:OE1	47:3:24:LEU:HD11	2.08	0.53
2:b:21:ARG:O	2:b:22:ARG:NH1	2.42	0.53
8:h:10:MET:O	8:h:14:VAL:HG23	2.09	0.53
22:v:71:ASN:ND2	22:v:73:ASP:O	2.41	0.53
22:v:98:ARG:C	22:v:100:SER:N	2.62	0.53
23:A:1397:G:H22	23:A:2241:C:N4	2.07	0.53
23:A:2161:A:C6	23:A:2184:G:C2	2.97	0.53
36:S:102:LEU:O	36:S:103:ARG:NE	2.41	0.53
1:a:180:U:N3	1:a:209:G:N7	2.57	0.53
1:a:184:A:N6	1:a:208:U:O4	2.42	0.53
23:A:687:G:N2	23:A:690:U:OP2	2.32	0.53
5:e:45:ARG:HB3	5:e:71:LEU:HD23	1.90	0.53
15:o:3:ILE:HD12	15:o:7:ARG:HB2	1.92	0.52
16:p:37:ILE:HG22	16:p:56:LEU:HD21	1.90	0.52
23:A:2860:U:O2'	34:Q:97:GLN:OE1	2.19	0.52
42:Y:25:GLY:CA	42:Y:44:ASP:OD1	2.57	0.52
50:6:15:LYS:O	50:6:17:HIS:N	2.42	0.52
1:a:1308:U:OP2	13:m:44:ARG:NE	2.42	0.52
6:f:50:TYR:HB3	18:r:71:ALA:HB1	1.90	0.52
23:A:2419:A:N6	23:A:2456:G:O2'	2.42	0.52
52:8:27:CYS:SG	52:8:32:HIS:ND1	2.75	0.52
2:b:171:ASN:OD1	2:b:172:ALA:N	2.42	0.52
3:c:41:PHE:O	3:c:44:ASN:ND2	2.43	0.52
4:d:63:MET:HE2	4:d:68:PHE:HA	1.91	0.52
7:g:103:TRP:CD1	7:g:137:LYS:HZ3	2.27	0.52
23:A:516:A:OP1	27:F:79:ARG:NH2	2.42	0.52
42:Y:25:GLY:C	42:Y:44:ASP:HA	2.33	0.52
1:a:1108:C:O2	1:a:1181:A:O2'	2.26	0.52
23:A:319:G:N2	23:A:321:U:O4	2.41	0.52
23:A:961:G:O2'	23:A:962:A:O5'	2.19	0.52
1:a:74:G:O2'	1:a:95:A:N6	2.42	0.52
1:a:166:U:O4	1:a:167:A:N6	2.42	0.52
1:a:354:G:OP1	36:S:41:ARG:NH1	2.43	0.52
23:A:488:G:O4'	27:F:46:GLN:NE2	2.42	0.52
23:A:522:G:N1	23:A:525:A:OP2	2.42	0.52
23:A:2119:U:N3	23:A:2253:C:OP2	2.39	0.52
23:A:2287:C:H41	43:Z:22:ARG:CG	2.23	0.52
42:Y:21:LEU:CD1	42:Y:42:LYS:CG	2.74	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:a:135:C:O2	16:p:2:ALA:HB2	2.09	0.52
1:a:151:A:N7	1:a:170:U:C4	2.77	0.52
21:u:50:GLU:O	21:u:51:ALA:CB	2.58	0.52
22:v:31:TYR:O	22:v:89:VAL:HG11	2.09	0.52
23:A:955:A:H62	33:P:15:PRO:HD3	1.73	0.52
1:a:987:A:N6	1:a:1235:U:O4'	2.42	0.52
3:c:24:ALA:HB3	10:j:97:ASP:OD1	2.09	0.52
4:d:101:LEU:HD23	4:d:103:LEU:HD11	1.92	0.52
10:j:8:ILE:HG22	10:j:100:ILE:HA	1.92	0.52
22:v:74:LEU:O	22:v:78:ILE:HG22	2.09	0.52
22:v:94:THR:HA	22:v:95:ARG:HB2	1.91	0.52
22:v:103:ARG:CG	22:v:104:GLY:N	2.70	0.52
23:A:419:U:OP2	44:0:52:ARG:NH1	2.41	0.52
35:R:31:LEU:HD12	35:R:43:GLN:O	2.10	0.52
45:1:24:GLU:OE2	45:1:42:ARG:NH2	2.40	0.52
1:a:945:A:O2'	1:a:1394:C:N3	2.38	0.52
1:a:1250:A:H62	1:a:1310:A:H62	1.58	0.52
1:a:1270:C:O2'	1:a:1294:C:O2	2.21	0.52
8:h:48:ASN:OD1	8:h:49:VAL:N	2.43	0.52
23:A:825:G:N1	25:D:228:ASP:OD2	2.40	0.52
23:A:2806:U:OP1	23:A:2807:G:N2	2.43	0.52
33:P:31:GLU:OE1	33:P:31:GLU:N	2.42	0.52
44:0:29:TRP:CZ2	44:0:31:ALA:HB2	2.43	0.52
1:a:263:G:O6	1:a:274:G:C6	2.61	0.52
1:a:421:G:N2	1:a:436:G:O3'	2.39	0.52
23:A:923:A:HO2'	23:A:924:G:P	2.30	0.52
23:A:2495:A:N1	23:A:2508:G:O2'	2.39	0.52
23:A:2772:C:O2'	29:H:139:GLU:O	2.16	0.52
42:Y:25:GLY:O	42:Y:45:GLU:N	2.42	0.52
1:a:1093:G:OP2	5:e:32:ARG:NH2	2.43	0.52
22:v:91:LYS:C	22:v:93:LYS:N	2.67	0.52
23:A:349:U:H3	23:A:353:A:H62	1.58	0.52
23:A:527:G:O2'	23:A:552:A:N6	2.43	0.52
23:A:1708:A:H61	23:A:2023:C:H42	1.57	0.52
23:A:1991:G:O2'	23:A:1994:C:OP1	2.19	0.52
23:A:2683:U:C2	23:A:2692:A:N7	2.77	0.52
24:B:100:A:O2'	42:Y:32:TYR:OH	2.09	0.52
36:S:42:ILE:HD12	36:S:43:GLN:N	2.25	0.52
1:a:74:G:N2	1:a:95:A:C8	2.75	0.51
1:a:1267:C:N4	1:a:1289:A:OP2	2.43	0.51
23:A:1008:C:O2'	23:A:2300:A:N3	2.33	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:A:2842:G:O2'	23:A:2844:U:OP2	2.14	0.51
3:c:61:ASN:O	3:c:61:ASN:ND2	2.42	0.51
18:r:25:HIS:CB	18:r:26:ILE:HA	2.38	0.51
22:v:20:TYR:OH	22:v:78:ILE:CB	2.58	0.51
23:A:1712:A:H61	23:A:1720:A:H61	1.58	0.51
23:A:2711:U:OP2	36:S:53:ARG:NH1	2.42	0.51
25:D:172:LEU:O	25:D:173:ILE:HD13	2.08	0.51
27:F:173:VAL:HG21	27:F:196:GLU:OE2	2.10	0.51
1:a:235:G:N2	16:p:63:ASP:O	2.43	0.51
1:a:701:G:H5''	22:v:100:SER:HB3	1.92	0.51
9:i:38:ARG:NH2	9:i:45:SER:OG	2.42	0.51
23:A:2361:U:H3	35:R:16:ALA:HB1	1.75	0.51
1:a:379:G:N3	1:a:381:A:N6	2.58	0.51
1:a:555:A:OP1	4:d:66:ARG:NE	2.43	0.51
1:a:559:U:O2'	12:l:96:ARG:NH2	2.41	0.51
1:a:1458:A:P	1:a:1459:C:H41	2.34	0.51
2:b:83:GLU:OE1	2:b:214:THR:HB	2.10	0.51
3:c:8:ILE:HG22	3:c:16:ARG:NH1	2.25	0.51
10:j:44:THR:HG1	10:j:70:HIS:HD1	1.52	0.51
23:A:275:A:N6	23:A:297:G:N3	2.58	0.51
23:A:1031:C:O2'	23:A:1044:A:N3	2.40	0.51
3:c:69:THR:O	3:c:105:ILE:HG22	2.11	0.51
22:v:94:THR:N	22:v:95:ARG:CB	2.73	0.51
22:v:95:ARG:NH2	22:v:96:ILE:CG2	2.73	0.51
22:v:95:ARG:NE	22:v:96:ILE:HG22	2.25	0.51
23:A:375:A:O2'	23:A:377:U:OP2	2.24	0.51
23:A:1583:G:P	23:A:1584:A:C8	2.99	0.51
23:A:1968:C:N4	23:A:1992:C:O4'	2.43	0.51
27:F:177:THR:O	27:F:180:GLY:N	2.44	0.51
35:R:70:VAL:HG12	35:R:104:ARG:HB3	1.93	0.51
1:a:988:A:H61	1:a:1327:G:N2	2.08	0.51
1:a:1249:A:N7	1:a:1312:U:C2	2.78	0.51
4:d:142:ARG:HE	4:d:145:SER:HB2	1.76	0.51
13:m:69:LEU:O	13:m:73:THR:OG1	2.24	0.51
23:A:1520:A:HO2'	23:A:1561:G:H22	1.59	0.51
23:A:2287:C:H42	43:Z:22:ARG:CD	2.15	0.51
33:P:35:GLN:HE21	33:P:100:GLY:HA2	1.75	0.51
43:Z:27:LYS:CG	43:Z:29:LEU:CD1	2.80	0.51
11:k:112:ASP:OD1	11:k:113:VAL:N	2.44	0.51
23:A:2192:G:OP1	23:A:2193:G:N2	2.43	0.51
23:A:2649:U:C2'	23:A:2845:G:H22	2.23	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:a:94:G:O2'	1:a:95:A:O5'	2.25	0.51
22:v:88:GLN:HA	22:v:91:LYS:CD	2.41	0.51
47:3:63:LYS:HD2	47:3:66:ALA:HB3	1.93	0.51
1:a:129:A:N3	17:q:2:SER:N	2.59	0.51
23:A:2152:G:N2	23:A:2200:A:H62	2.08	0.51
1:a:1189:G:N2	1:a:1192:G:OP2	2.40	0.51
22:v:88:GLN:HA	22:v:91:LYS:HD3	1.93	0.51
23:A:1825:U:O2'	23:A:1829:A:N3	2.43	0.51
43:Z:18:THR:O	43:Z:18:THR:HG23	2.10	0.51
7:g:148:ASN:ND2	7:g:148:ASN:O	2.41	0.50
19:s:66:MET:O	47:3:77:LYS:NZ	2.44	0.50
23:A:1320:G:N1	23:A:1323:A:OP2	2.43	0.50
23:A:1360:G:HO2'	23:A:1361:G:P	2.34	0.50
26:E:35:VAL:C	26:E:36:LEU:HD12	2.37	0.50
49:5:35:PHE:CZ	49:5:40:ASN:HA	2.46	0.50
2:b:217:MET:O	2:b:220:ALA:HB3	2.11	0.50
6:f:76:PHE:O	6:f:79:LEU:N	2.43	0.50
22:v:88:GLN:O	22:v:91:LYS:HG2	2.11	0.50
35:R:44:ILE:HD12	35:R:54:ALA:HB3	1.93	0.50
1:a:53:U:OP1	12:l:32:LYS:NZ	2.45	0.50
1:a:245:C:P	17:q:44:LYS:HZ3	2.34	0.50
1:a:790:A:H62	1:a:808:G:H21	1.58	0.50
1:a:1047:G:OP2	1:a:1048:A:N6	2.43	0.50
8:h:66:TYR:O	8:h:68:GLN:NE2	2.44	0.50
22:v:17:ILE:HG23	22:v:20:TYR:CE2	2.47	0.50
36:S:55:GLY:O	36:S:58:SER:OG	2.22	0.50
1:a:481:C:O2'	1:a:481:C:O2	2.28	0.50
1:a:722:G:O2'	1:a:785:A:N7	2.43	0.50
1:a:1136:G:O2'	1:a:1137:U:OP2	2.27	0.50
1:a:1231:G:O2'	19:s:36:ARG:NH2	2.44	0.50
12:l:89:GLU:OE1	12:l:89:GLU:N	2.45	0.50
22:v:16:ALA:O	22:v:20:TYR:HB3	2.11	0.50
23:A:1092:A:OP2	23:A:1154:G:N2	2.39	0.50
33:P:27:VAL:HG11	33:P:134:ARG:HD2	1.94	0.50
1:a:257:U:O2	1:a:283:G:O6	2.30	0.50
7:g:126:ASP:O	7:g:131:THR:OG1	2.30	0.50
18:r:25:HIS:HB3	18:r:26:ILE:CG1	2.41	0.50
22:v:91:LYS:O	22:v:95:ARG:HG2	2.11	0.50
23:A:321:U:O2'	23:A:322:A:OP1	2.28	0.50
4:d:103:LEU:HD21	4:d:167:PHE:CZ	2.47	0.50
8:h:22:HIS:O	8:h:66:TYR:OH	2.25	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:A:63:U:O3'	40:W:63:LYS:NZ	2.35	0.50
23:A:788:A:O2'	23:A:1703:U:OP1	2.28	0.50
23:A:1306:C:O2	23:A:2040:A:N6	2.43	0.50
23:A:2287:C:N4	43:Z:22:ARG:CG	2.75	0.50
1:a:252:U:O2	1:a:904:G:N2	2.45	0.50
23:A:460:C:O2	23:A:1891:U:O2'	2.27	0.50
23:A:677:A:O2'	23:A:678:A:O4'	2.18	0.50
29:H:10:ASP:OD1	29:H:11:ILE:N	2.44	0.50
1:a:1261:A:H61	1:a:1365:U:C1'	2.25	0.50
23:A:2432:G:N2	23:A:2439:A:H62	2.10	0.50
25:D:227:ASN:OD1	25:D:228:ASP:N	2.45	0.50
1:a:517:A:N6	1:a:518:A:N1	2.60	0.50
1:a:1155:G:N2	1:a:1157:A:H62	2.10	0.50
2:b:9:LEU:O	2:b:13:GLY:N	2.44	0.50
2:b:10:LEU:O	2:b:10:LEU:HD13	2.11	0.50
3:c:33:HIS:ND1	14:n:25:GLU:OE1	2.45	0.50
18:r:34:LEU:HA	18:r:37:PHE:HD2	1.75	0.50
23:A:1884:G:N2	23:A:1913:U:O4	2.44	0.50
23:A:2603:G:OP2	23:A:2603:G:N2	2.39	0.50
25:D:9:THR:HG23	25:D:11:GLY:H	1.76	0.50
33:P:14:ARG:O	33:P:87:LYS:NZ	2.45	0.50
43:Z:27:LYS:O	43:Z:28:ARG:CB	2.56	0.50
1:a:1049:C:N3	1:a:1050:A:N6	2.60	0.49
1:a:1327:G:O6	19:s:6:LYS:NZ	2.45	0.49
22:v:99:LYS:O	22:v:100:SER:C	2.53	0.49
23:A:1290:G:OP2	37:T:13:ARG:NH2	2.45	0.49
23:A:2432:G:OP1	32:O:63:LYS:NZ	2.44	0.49
29:H:155:GLU:O	29:H:159:GLY:N	2.44	0.49
1:a:728:C:OP2	1:a:729:A:O2'	2.29	0.49
23:A:227:G:O6	23:A:465:C:O2'	2.30	0.49
23:A:2231:C:OP2	25:D:149:LYS:NZ	2.45	0.49
13:m:20:THR:OG1	13:m:26:GLY:O	2.21	0.49
16:p:21:VAL:CG2	16:p:33:ILE:HG23	2.41	0.49
25:D:83:ASP:OD2	25:D:86:ARG:NH2	2.46	0.49
2:b:206:ALA:HB3	2:b:209:ALA:HB3	1.94	0.49
23:A:1805:U:H3	23:A:1812:A:H62	1.60	0.49
23:A:2039:G:OP1	39:V:11:ARG:NH1	2.45	0.49
23:A:2467:C:O2'	23:A:2468:C:O4'	2.29	0.49
29:H:44:LYS:O	29:H:50:ILE:HG23	2.11	0.49
1:a:151:A:N7	1:a:170:U:N3	2.60	0.49
2:b:207:ILE:HD12	2:b:207:ILE:H	1.77	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:e:8:THR:HG23	5:e:9:LYS:HD3	1.94	0.49
23:A:994:A:H4'	24:B:85:A:H61	1.77	0.49
23:A:1123:C:O2'	23:A:1124:A:O4'	2.26	0.49
23:A:2289:U:O2'	23:A:2355:A:N3	2.44	0.49
1:a:590:U:OP2	1:a:766:G:N1	2.45	0.49
1:a:833:G:O6	1:a:886:A:N6	2.46	0.49
15:o:43:LEU:O	15:o:47:LYS:CA	2.59	0.49
21:u:53:ARG:CZ	21:u:53:ARG:HB3	2.43	0.49
23:A:1496:G:N7	23:A:1501:G:C6	2.80	0.49
23:A:2516:G:O2'	23:A:2545:A:N6	2.40	0.49
40:W:49:LYS:CD	40:W:51:ALA:HB2	2.42	0.49
13:m:55:ARG:O	13:m:59:VAL:HG23	2.13	0.49
25:D:69:ASN:O	25:D:69:ASN:ND2	2.43	0.49
27:F:173:VAL:HG11	27:F:196:GLU:OE2	2.13	0.49
31:N:114:ILE:O	31:N:118:ALA:HB2	2.13	0.49
36:S:38:THR:O	36:S:38:THR:HG22	2.13	0.49
44:O:19:SER:N	44:O:27:ARG:O	2.38	0.49
1:a:446:G:O2'	1:a:449:A:N6	2.46	0.49
23:A:1303:A:C1'	23:A:1305:U:C4	2.96	0.49
23:A:1496:G:H22	23:A:2729:G:H3'	1.77	0.49
24:B:73:G:N3	42:Y:88:HIS:NE2	2.61	0.49
23:A:2868:G:N2	23:A:2888:A:H62	2.03	0.49
27:F:39:LEU:O	27:F:42:ALA:N	2.45	0.49
31:N:14:SER:O	31:N:51:VAL:N	2.46	0.49
6:f:2:ARG:HE	6:f:93:ARG:HE	1.61	0.49
9:i:100:LEU:O	9:i:103:ALA:N	2.46	0.49
23:A:1726:A:OP2	23:A:1743:G:N2	2.30	0.49
23:A:2302:C:C2	43:Z:18:THR:HG21	2.47	0.49
26:E:49:ILE:HG22	26:E:50:GLN:N	2.28	0.49
23:A:113:U:O2'	40:W:32:ARG:NH1	2.46	0.48
35:R:1:MET:HE3	35:R:2:ILE:HG12	1.95	0.48
36:S:66:ILE:HG22	36:S:66:ILE:O	2.13	0.48
48:4:18:THR:HG1	48:4:19:HIS:HD1	1.57	0.48
1:a:571:A:HO2'	1:a:574:G:HO2'	1.60	0.48
2:b:21:ARG:O	2:b:22:ARG:HG2	2.14	0.48
22:v:31:TYR:HH	22:v:90:ARG:HB3	1.78	0.48
23:A:260:A:N6	23:A:261:U:N3	2.61	0.48
23:A:1515:G:N2	23:A:1565:U:O2	2.45	0.48
25:D:171:VAL:O	25:D:183:ILE:N	2.45	0.48
1:a:149:A:H61	1:a:172:A:H62	1.61	0.48
1:a:996:A:O3'	19:s:56:LYS:NZ	2.46	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:b:71:GLY:HA3	2:b:80:VAL:HG21	1.95	0.48
8:h:76:GLY:N	8:h:132:TRP:O	2.46	0.48
9:i:22:ARG:HD3	9:i:66:LEU:HD12	1.95	0.48
11:k:85:THR:HG22	11:k:113:VAL:HG11	1.95	0.48
12:l:24:LEU:O	12:l:24:LEU:HD13	2.13	0.48
23:A:904:G:O2'	23:A:961:G:O6	2.31	0.48
23:A:1319:U:H3	23:A:1323:A:H62	1.60	0.48
23:A:1458:A:N6	23:A:1459:A:H62	2.11	0.48
28:G:9:ASN:O	28:G:13:THR:CB	2.62	0.48
38:U:34:THR:HG22	38:U:59:THR:HG22	1.94	0.48
1:a:460:A:N6	1:a:489:G:O5'	2.46	0.48
7:g:97:THR:O	7:g:101:LEU:HD23	2.12	0.48
8:h:80:ILE:HD11	8:h:130:TYR:CD1	2.47	0.48
29:H:99:GLN:N	29:H:102:ASP:O	2.47	0.48
1:a:541:A:O2'	1:a:543:A:OP2	2.22	0.48
2:b:71:GLY:CA	2:b:80:VAL:HG21	2.43	0.48
2:b:76:ALA:O	2:b:80:VAL:HG23	2.14	0.48
6:f:19:LYS:O	6:f:23:VAL:HG23	2.14	0.48
22:v:100:SER:O	22:v:101:ARG:HG3	2.14	0.48
23:A:342:A:OP1	41:X:80:ARG:NH1	2.46	0.48
23:A:373:A:C5	23:A:1248:U:O4	2.62	0.48
23:A:1290:G:H21	37:T:33:LYS:HB3	1.77	0.48
27:F:80:ALA:HB1	27:F:81:PRO:HD2	1.94	0.48
32:O:119:LYS:O	32:O:123:VAL:HG12	2.14	0.48
41:X:93:ILE:HD13	41:X:102:LYS:HB2	1.96	0.48
45:1:45:THR:O	45:1:49:THR:HG23	2.14	0.48
49:5:35:PHE:O	49:5:45:HIS:ND1	2.46	0.48
1:a:372:A:H61	12:l:38:LEU:HD11	1.78	0.48
4:d:109:GLN:HE21	4:d:150:ILE:CG2	2.27	0.48
22:v:87:ARG:O	22:v:91:LYS:HD3	2.14	0.48
23:A:2662:U:O2'	26:E:50:GLN:NE2	2.46	0.48
36:S:80:THR:HG22	36:S:82:LYS:H	1.79	0.48
43:Z:26:SER:OG	43:Z:28:ARG:NH1	2.38	0.48
1:a:525:G:N2	1:a:538:G:OP1	2.39	0.48
1:a:936:G:O2'	1:a:937:G:OP1	2.24	0.48
1:a:974:A:O2'	10:j:57:MET:SD	2.72	0.48
1:a:1048:A:O2'	1:a:1049:C:O4'	2.27	0.48
23:A:263:G:H5''	23:A:666:A:Cl'	2.41	0.48
23:A:1261:G:N2	23:A:1264:A:OP2	2.39	0.48
23:A:1261:G:N7	38:U:70:LYS:NZ	2.61	0.48
38:U:94:LYS:C	38:U:95:LEU:HD12	2.39	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
44:0:32:ASN:HD22	44:0:33:LEU:N	2.11	0.48
10:j:10:LEU:HD13	10:j:74:ILE:HD12	1.96	0.48
22:v:94:THR:N	22:v:95:ARG:CG	2.77	0.48
23:A:2502:C:O2'	23:A:2504:C:OP2	2.29	0.48
23:A:2505:A:OP2	52:8:2:LYS:NZ	2.43	0.48
24:B:107:U:H3'	24:B:108:G:H21	1.79	0.48
21:u:41:PRO:HA	21:u:44:LYS:HE2	1.95	0.48
23:A:2287:C:H41	43:Z:22:ARG:CD	2.20	0.48
23:A:2452:A:N3	23:A:2454:C:N4	2.61	0.48
38:U:61:THR:OG1	38:U:98:ASP:OD2	2.18	0.48
1:a:1332:U:OP1	13:m:99:GLY:N	2.47	0.48
3:c:55:GLU:OE1	3:c:55:GLU:N	2.46	0.48
23:A:1939:A:N7	23:A:1944:U:O4	2.47	0.48
30:M:59:ASN:N	30:M:128:GLY:O	2.45	0.47
1:a:461:C:H41	1:a:488:U:H3	1.61	0.47
1:a:605:G:O4'	17:q:30:TYR:OH	2.32	0.47
17:q:31:LYS:O	17:q:40:VAL:N	2.46	0.47
23:A:1155:A:O2'	23:A:1156:G:O4'	2.32	0.47
23:A:2868:G:C8	36:S:97:ALA:HB2	2.48	0.47
50:6:19:PHE:HD2	50:6:23:MET:HE2	1.78	0.47
1:a:1301:G:H21	9:i:42:PRO:HB3	1.79	0.47
3:c:69:THR:O	3:c:105:ILE:N	2.43	0.47
4:d:162:PRO:CG	4:d:165:LEU:HD12	2.44	0.47
6:f:31:ALA:HB2	6:f:37:VAL:HB	1.96	0.47
21:u:12:LEU:O	21:u:13:GLU:HG2	2.14	0.47
21:u:49:SER:C	21:u:51:ALA:H	2.20	0.47
22:v:20:TYR:CG	22:v:21:ILE:N	2.82	0.47
23:A:75:G:O2'	45:1:48:LYS:NZ	2.46	0.47
23:A:1396:A:OP2	23:A:1408:G:N1	2.42	0.47
25:D:52:HIS:ND1	25:D:52:HIS:O	2.47	0.47
29:H:8:ILE:C	29:H:9:ILE:HD12	2.39	0.47
1:a:1217:G:O4'	3:c:193:GLY:N	2.48	0.47
5:e:161:VAL:HG22	5:e:162:GLU:H	1.79	0.47
23:A:942:C:O2'	23:A:943:C:O5'	2.32	0.47
30:M:18:VAL:N	30:M:139:GLU:O	2.48	0.47
42:Y:27:VAL:O	42:Y:43:VAL:N	2.46	0.47
47:3:61:ARG:NH2	47:3:66:ALA:HB1	2.28	0.47
1:a:270:A:O2'	20:t:69:ASN:OD1	2.32	0.47
1:a:1147:U:O2'	1:a:1149:A:N7	2.40	0.47
22:v:7:HIS:NE2	22:v:41:HIS:CE1	2.82	0.47
1:a:128:U:OP2	17:q:4:ARG:NE	2.43	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:a:936:G:H22	22:v:91:LYS:HB3	1.76	0.47
9:i:43:PHE:N	9:i:44:GLU:OE1	2.43	0.47
20:t:4:ILE:CG2	20:t:8:ILE:HD11	2.44	0.47
21:u:25:LYS:HD3	21:u:25:LYS:HA	1.53	0.47
23:A:248:G:N7	51:7:8:ARG:NH2	2.62	0.47
37:T:115:ASP:OD1	37:T:116:ALA:N	2.48	0.47
38:U:7:THR:HG21	38:U:22:VAL:HG21	1.96	0.47
1:a:595:G:N2	1:a:762:C:OP2	2.47	0.47
1:a:1013:G:O2'	1:a:1015:C:OP1	2.33	0.47
1:a:1251:U:OP2	7:g:116:MET:HE2	2.14	0.47
1:a:1371:A:C8	14:n:18:VAL:HG11	2.50	0.47
4:d:46:GLU:OE1	4:d:46:GLU:N	2.44	0.47
10:j:24:LYS:CD	10:j:90:LEU:HD21	2.45	0.47
10:j:24:LYS:HD3	10:j:90:LEU:HD21	1.97	0.47
12:l:5:ASN:OD1	12:l:6:GLN:N	2.48	0.47
22:v:28:LEU:HD11	22:v:82:ASN:HD21	1.80	0.47
23:A:2380:G:N2	43:Z:42:GLY:O	2.41	0.47
23:A:2432:G:H21	23:A:2439:A:H62	1.63	0.47
23:A:2905:C:N3	48:4:39:LEU:HD22	2.30	0.47
36:S:48:VAL:HG12	36:S:49:VAL:O	2.15	0.47
7:g:58:ALA:O	7:g:62:PHE:N	2.40	0.47
12:l:68:VAL:HG22	12:l:69:ARG:O	2.15	0.47
22:v:55:GLU:HG3	22:v:68:GLU:HG2	1.96	0.47
22:v:58:ILE:CD1	22:v:85:LEU:HB2	2.44	0.47
22:v:87:ARG:HA	22:v:90:ARG:HG2	1.97	0.47
23:A:1892:U:C2'	23:A:1902:G:H22	2.27	0.47
1:a:1085:U:O2'	2:b:103:ASN:OD1	2.31	0.47
2:b:54:TYR:CD1	2:b:220:ALA:HB2	2.50	0.47
5:e:94:VAL:HG22	5:e:95:PHE:N	2.30	0.47
23:A:1631:G:OP1	23:A:1631:G:N2	2.48	0.47
23:A:1732:U:O2'	23:A:1744:A:N7	2.42	0.47
23:A:1836:A:O2'	23:A:1837:A:O4'	2.32	0.47
42:Y:14:THR:C	42:Y:18:LEU:CD2	2.85	0.47
1:a:1358:G:O2'	9:i:113:LYS:NZ	2.46	0.47
4:d:99:TYR:HD1	4:d:104:ALA:HB3	1.80	0.47
10:j:5:LYS:CB	10:j:77:VAL:CA	2.87	0.47
23:A:1826:G:N2	23:A:1846:A:OP2	2.40	0.47
47:3:9:TYR:OH	47:3:41:LYS:O	2.32	0.47
1:a:1447:C:H42	1:a:1477:U:H3	1.63	0.46
3:c:112:ALA:HB2	3:c:182:ASP:HB3	1.98	0.46
7:g:43:LEU:O	7:g:46:ALA:HB3	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:l:120:VAL:HG12	12:l:130:TYR:HB3	1.96	0.46
23:A:2276:U:N3	23:A:2280:G:OP2	2.48	0.46
51:7:34:ALA:HB3	51:7:37:SER:CB	2.45	0.46
1:a:910:A:O2'	1:a:911:A:O4'	2.22	0.46
21:u:46:LYS:CD	21:u:50:GLU:HG3	2.45	0.46
23:A:2085:A:N6	23:A:2086:A:N1	2.64	0.46
1:a:354:G:OP1	36:S:41:ARG:NH2	2.45	0.46
1:a:507:A:O4'	1:a:555:A:N6	2.49	0.46
1:a:726:A:C2	18:r:42:GLY:O	2.69	0.46
1:a:998:A:O4'	1:a:1024:A:N6	2.48	0.46
1:a:1129:A:N6	1:a:1167:G:H22	2.13	0.46
1:a:1538:G:N7	21:u:40:LYS:NZ	2.63	0.46
2:b:54:TYR:CE1	2:b:220:ALA:HB2	2.50	0.46
21:u:46:LYS:HD2	21:u:50:GLU:CG	2.45	0.46
23:A:1576:A:N6	23:A:1589:U:O4	2.49	0.46
23:A:1708:A:H61	23:A:2023:C:N4	2.14	0.46
23:A:2048:G:OP1	48:4:9:SER:OG	2.32	0.46
33:P:27:VAL:HG12	33:P:134:ARG:HD2	1.98	0.46
5:e:99:ALA:HB2	5:e:124:LEU:CD1	2.45	0.46
8:h:47:LYS:NZ	8:h:64:LEU:O	2.45	0.46
23:A:809:A:N3	25:D:211:ARG:NH1	2.63	0.46
23:A:1311:A:N6	23:A:1690:A:N3	2.63	0.46
23:A:1361:G:O2'	23:A:1363:U:OP2	2.22	0.46
23:A:2127:G:C6	23:A:2216:U:O2	2.69	0.46
23:A:2152:G:C2	23:A:2200:A:N6	2.84	0.46
33:P:110:SER:OG	33:P:111:GLU:N	2.49	0.46
43:Z:57:GLU:N	43:Z:57:GLU:OE1	2.48	0.46
49:5:39:GLU:OE1	49:5:39:GLU:N	2.48	0.46
1:a:472:G:H22	1:a:476:C:H5''	1.81	0.46
18:r:41:ARG:HG3	18:r:78:GLU:CB	2.46	0.46
23:A:318:A:N6	23:A:402:C:H42	2.14	0.46
23:A:1491:C:O2	23:A:1574:G:C2	2.67	0.46
29:H:35:ARG:HB3	29:H:37:LEU:HD21	1.98	0.46
1:a:106:G:H3'	1:a:107:G:H21	1.81	0.46
1:a:672:G:O2'	1:a:674:G:OP2	2.28	0.46
10:j:5:LYS:HD2	10:j:77:VAL:HG11	1.95	0.46
22:v:65:LEU:CD2	22:v:88:GLN:HE21	2.21	0.46
23:A:10:A:O2'	23:A:11:U:O4'	2.25	0.46
29:H:86:VAL:HG11	29:H:165:GLN:HE21	1.81	0.46
30:M:117:GLU:O	30:M:120:GLY:N	2.44	0.46
1:a:1517:G:N7	22:v:90:ARG:NH2	2.55	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:c:22:TRP:NE1	3:c:31:LEU:HD13	2.31	0.46
11:k:29:ASN:OD1	11:k:30:THR:N	2.48	0.46
22:v:31:TYR:CE2	22:v:89:VAL:C	2.93	0.46
23:A:1487:G:H22	23:A:1596:G:N2	2.14	0.46
23:A:1786:A:O2'	23:A:2741:G:O2'	2.31	0.46
23:A:2152:G:N2	23:A:2199:U:OP1	2.48	0.46
23:A:2172:C:O2'	23:A:2173:U:OP1	2.28	0.46
23:A:2860:U:C5'	34:Q:49:THR:HG21	2.46	0.46
25:D:215:ILE:HG22	25:D:216:ARG:N	2.31	0.46
38:U:59:THR:OG1	38:U:98:ASP:O	2.22	0.46
47:3:5:ILE:HD12	47:3:5:ILE:O	2.16	0.46
1:a:244:G:O3'	17:q:44:LYS:NZ	2.37	0.46
1:a:333:A:O2'	1:a:334:G:OP1	2.31	0.46
1:a:804:C:OP2	11:k:126:ARG:NH1	2.43	0.46
1:a:1236:A:O2'	19:s:82:GLY:O	2.34	0.46
15:o:32:LEU:HD13	15:o:62:ARG:HH21	1.80	0.46
17:q:68:PRO:C	17:q:69:LEU:HD22	2.41	0.46
23:A:1058:U:N3	23:A:1059:A:N7	2.64	0.46
35:R:74:THR:HB	35:R:111:ALA:HB2	1.98	0.46
40:W:52:SER:O	40:W:81:THR:HG22	2.15	0.46
2:b:96:TRP:CD1	2:b:172:ALA:HB2	2.51	0.46
8:h:23:GLU:OE1	8:h:23:GLU:N	2.48	0.46
23:A:1078:G:OP2	52:8:18:LYS:NZ	2.40	0.46
23:A:1576:A:H61	23:A:1587:C:H41	1.64	0.46
25:D:194:VAL:HG12	25:D:195:GLY:H	1.81	0.46
1:a:56:A:H61	1:a:365:G:H1'	1.81	0.46
7:g:105:VAL:O	7:g:108:ALA:HB3	2.16	0.46
13:m:107:ARG:N	13:m:110:LYS:O	2.49	0.46
23:A:1452:C:H42	23:A:1632:A:N6	2.11	0.46
23:A:1693:G:N2	34:Q:112:ASP:O	2.49	0.46
37:T:96:SER:O	37:T:99:ALA:HB3	2.15	0.46
1:a:1090:U:HO2'	1:a:1091:G:P	2.36	0.45
1:a:1321:U:OP1	13:m:79:ARG:NH2	2.50	0.45
3:c:90:LEU:O	3:c:94:THR:N	2.38	0.45
5:e:149:ASN:HD22	5:e:150:ALA:H	1.63	0.45
18:r:34:LEU:O	18:r:37:PHE:N	2.48	0.45
23:A:864:A:OP2	23:A:1226:G:N2	2.47	0.45
23:A:1099:G:H1	23:A:1148:C:H42	1.64	0.45
23:A:1539:A:N3	23:A:1624:C:O2'	2.46	0.45
23:A:2432:G:O2'	23:A:2433:C:OP2	2.15	0.45
23:A:2869:G:O2'	23:A:2886:G:N2	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:H:64:ASN:O	29:H:68:THR:OG1	2.23	0.45
39:V:23:LEU:HB2	39:V:24:ILE:HG23	1.97	0.45
1:a:386:G:N1	1:a:394:C:N3	2.63	0.45
20:t:57:VAL:O	20:t:61:ALA:N	2.44	0.45
46:2:11:SER:O	46:2:15:ARG:NH1	2.49	0.45
47:3:28:THR:HG22	47:3:30:THR:CG2	2.46	0.45
47:3:75:ASN:O	47:3:75:ASN:ND2	2.49	0.45
1:a:74:G:H22	1:a:94:G:H2'	1.82	0.45
1:a:467:U:O4	1:a:483:C:N4	2.48	0.45
14:n:33:VAL:HG23	14:n:40:CYS:HA	1.99	0.45
15:o:74:ASP:OD1	15:o:75:ILE:N	2.50	0.45
23:A:684:U:C2	23:A:694:G:O6	2.69	0.45
1:a:1318:U:O4	1:a:1342:G:N2	2.49	0.45
5:e:99:ALA:HB2	5:e:124:LEU:HD12	1.98	0.45
9:i:64:ASP:OD1	9:i:65:VAL:N	2.48	0.45
23:A:283:G:N7	23:A:284:C:O2'	2.44	0.45
41:X:70:LEU:HD23	41:X:76:ASN:ND2	2.31	0.45
51:7:32:LEU:HD11	51:7:33:PHE:CE1	2.52	0.45
6:f:49:ALA:HB1	18:r:74:PRO:HB3	1.97	0.45
20:t:50:VAL:O	20:t:54:VAL:HG23	2.17	0.45
21:u:12:LEU:HD23	21:u:12:LEU:HA	1.75	0.45
23:A:1042:C:OP2	37:T:58:ARG:NH2	2.49	0.45
23:A:1505:G:N7	23:A:1506:C:N4	2.65	0.45
23:A:1569:G:H21	23:A:1570:G:C4'	2.30	0.45
23:A:2161:A:C6	23:A:2184:G:N3	2.84	0.45
25:D:207:ALA:O	25:D:210:SER:N	2.48	0.45
26:E:195:ILE:N	26:E:195:ILE:HD12	2.32	0.45
29:H:11:ILE:HG23	29:H:15:VAL:HG11	1.98	0.45
40:W:56:MET:N	40:W:56:MET:SD	2.89	0.45
2:b:135:VAL:HG12	2:b:139:LYS:NZ	2.32	0.45
12:l:27:GLY:HA3	12:l:35:PHE:HB3	1.99	0.45
23:A:513:G:O2'	23:A:841:C:O2'	2.09	0.45
23:A:2778:G:N3	23:A:2778:G:O2'	2.44	0.45
24:B:82:C:HO2'	24:B:83:U:C4'	2.26	0.45
2:b:167:ARG:NH1	2:b:190:ASN:HD21	2.15	0.45
9:i:47:ILE:HA	9:i:50:LEU:HD13	1.99	0.45
12:l:91:SER:OG	12:l:92:VAL:N	2.50	0.45
20:t:68:SER:O	20:t:71:ALA:HB3	2.16	0.45
23:A:1001:A:N6	23:A:1003:A:N1	2.64	0.45
25:D:20:PHE:HB3	25:D:23:ILE:HD12	1.99	0.45
1:a:1250:A:C2'	1:a:1309:C:H42	2.30	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:A:160:G:O2'	23:A:167:U:O4	2.25	0.45
23:A:734:A:N3	23:A:824:A:O2'	2.48	0.45
23:A:903:G:OP2	43:Z:85:LYS:NZ	2.50	0.45
23:A:1767:G:HO2'	23:A:1768:C:P	2.40	0.45
26:E:138:ARG:HE	26:E:141:MET:HE3	1.82	0.45
5:e:124:LEU:HD12	5:e:124:LEU:N	2.32	0.45
9:i:41:LEU:HD22	9:i:74:PHE:HB2	1.99	0.45
15:o:3:ILE:HD12	15:o:7:ARG:CB	2.47	0.45
23:A:921:C:O2	23:A:945:A:N6	2.50	0.45
27:F:88:ILE:HG22	27:F:89:VAL:N	2.32	0.45
1:a:1518:U:N3	1:a:1534:U:OP1	2.50	0.45
4:d:191:GLU:HA	4:d:194:ILE:HG22	1.99	0.45
18:r:41:ARG:HA	18:r:78:GLU:CB	2.42	0.45
21:u:14:ASP:O	21:u:17:ARG:N	2.50	0.45
22:v:47:TYR:H	22:v:48:SER:HA	1.82	0.45
22:v:99:LYS:HD3	22:v:99:LYS:H	1.82	0.45
29:H:61:ASP:OD1	29:H:62:ARG:N	2.50	0.45
29:H:151:VAL:HG12	29:H:152:ARG:HG2	1.99	0.45
3:c:107:LYS:N	3:c:108:VAL:HA	2.31	0.44
5:e:44:GLY:N	5:e:118:ALA:O	2.45	0.44
11:k:31:ILE:HD12	11:k:32:VAL:N	2.32	0.44
23:A:1039:C:H42	30:M:4:THR:HG22	1.81	0.44
46:2:17:GLU:OE1	46:2:17:GLU:N	2.50	0.44
1:a:370:G:N1	1:a:373:U:OP2	2.49	0.44
1:a:827:A:N6	1:a:1541:G:O4'	2.49	0.44
1:a:1150:G:N2	1:a:1154:G:O6	2.49	0.44
1:a:1315:G:N2	1:a:1345:G:O6	2.50	0.44
3:c:88:ASN:O	3:c:92:ALA:N	2.44	0.44
9:i:132:ARG:O	22:v:37:ASN:ND2	2.47	0.44
11:k:80:LYS:O	11:k:106:GLU:N	2.43	0.44
22:v:92:TYR:O	22:v:92:TYR:CD1	2.70	0.44
23:A:2501:U:OP2	23:A:2502:C:N4	2.43	0.44
24:B:37:A:O2'	24:B:38:U:O4'	2.22	0.44
31:N:2:ILE:HG22	31:N:3:GLN:N	2.32	0.44
1:a:1146:U:O2	1:a:1152:U:N3	2.50	0.44
2:b:183:ILE:N	2:b:197:ASP:OD2	2.47	0.44
20:t:48:GLU:OE1	20:t:48:GLU:N	2.44	0.44
22:v:101:ARG:C	22:v:102:ASP:O	2.60	0.44
22:v:103:ARG:HG2	22:v:104:GLY:N	2.31	0.44
24:B:21:G:N1	24:B:59:U:C2	2.85	0.44
1:a:130:A:OP2	1:a:197:U:N3	2.49	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:c:24:ALA:HB3	10:j:97:ASP:CG	2.42	0.44
9:i:41:LEU:HD22	9:i:74:PHE:CB	2.47	0.44
23:A:1250:G:N2	23:A:1274:G:O2'	2.51	0.44
23:A:2710:C:O2	31:N:76:TYR:OH	2.33	0.44
34:Q:40:VAL:O	34:Q:44:VAL:HG22	2.17	0.44
1:a:590:U:H3	1:a:767:A:H62	1.65	0.44
2:b:59:GLN:NE2	2:b:63:ASP:OD2	2.50	0.44
11:k:17:GLU:O	11:k:81:THR:N	2.49	0.44
21:u:49:SER:C	21:u:51:ALA:N	2.75	0.44
23:A:572:C:HO2'	23:A:573:A:P	2.38	0.44
23:A:1124:A:O2'	23:A:1125:U:O4'	2.36	0.44
23:A:1726:A:P	23:A:1743:G:H22	2.38	0.44
26:E:5:ILE:O	26:E:211:ILE:N	2.42	0.44
27:F:144:SER:OG	27:F:186:ILE:HG21	2.17	0.44
37:T:94:MET:HE1	38:U:13:LYS:N	2.33	0.44
42:Y:14:THR:HB	42:Y:18:LEU:CD2	2.44	0.44
1:a:630:A:OP2	1:a:631:C:N4	2.42	0.44
23:A:6:A:HO2'	30:M:133:HIS:HD1	1.65	0.44
35:R:86:ASP:OD1	35:R:87:LYS:N	2.50	0.44
52:8:17:ILE:HD12	52:8:18:LYS:N	2.33	0.44
1:a:681:G:O3'	6:f:88:ARG:NH2	2.48	0.44
1:a:1360:A:H62	1:a:1384:G:N2	2.16	0.44
1:a:1547:C:H5'	21:u:54:LYS:CD	2.47	0.44
7:g:13:LEU:H	7:g:13:LEU:HD23	1.82	0.44
10:j:6:ILE:N	10:j:76:ILE:O	2.50	0.44
12:l:53:MET:HE3	12:l:65:TYR:OH	2.18	0.44
23:A:1290:G:O2'	23:A:1291:A:O4'	2.33	0.44
35:R:46:ASP:O	35:R:50:GLY:N	2.50	0.44
38:U:22:VAL:HG22	38:U:23:GLU:H	1.83	0.44
8:h:46:ILE:HD11	8:h:62:LEU:HB2	2.00	0.44
9:i:57:THR:HG23	9:i:96:TYR:CB	2.48	0.44
12:l:56:LYS:O	12:l:57:LYS:O	2.36	0.44
18:r:41:ARG:CZ	21:u:26:SER:HB3	2.48	0.44
23:A:32:C:N4	23:A:493:A:OP2	2.50	0.44
23:A:901:G:H2'	23:A:902:A:C8	2.53	0.44
23:A:2150:A:OP2	23:A:2197:G:O2'	2.35	0.44
26:E:9:LYS:NZ	26:E:201:VAL:HG23	2.32	0.44
39:V:108:SER:OG	39:V:110:GLY:N	2.51	0.44
1:a:455:G:H3'	1:a:456:A:C5'	2.47	0.44
1:a:961:G:N3	1:a:980:C:O2'	2.41	0.44
1:a:1203:C:P	3:c:4:LYS:HZ1	2.39	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:c:24:ALA:HB3	10:j:97:ASP:OD2	2.18	0.44
3:c:33:HIS:HE1	14:n:39:LEU:HD21	1.83	0.44
4:d:19:LEU:HD21	4:d:23:GLY:O	2.18	0.44
4:d:181:GLU:N	4:d:181:GLU:OE1	2.51	0.44
5:e:8:THR:O	5:e:8:THR:OG1	2.33	0.44
16:p:33:ILE:HG22	16:p:35:GLU:N	2.33	0.44
21:u:12:LEU:O	21:u:13:GLU:CG	2.65	0.44
23:A:744:A:N3	23:A:1677:G:O2'	2.45	0.44
30:M:74:VAL:HG11	30:M:76:TYR:CE1	2.53	0.44
35:R:95:ASP:OD1	35:R:96:ARG:N	2.47	0.44
40:W:14:GLU:O	40:W:17:SER:N	2.51	0.44
42:Y:24:SER:OG	42:Y:26:LYS:HG2	2.17	0.44
1:a:1235:U:HO2'	19:s:78:ARG:NH2	2.10	0.43
1:a:1370:C:O2'	1:a:1372:G:OP2	2.33	0.43
1:a:1371:A:N7	14:n:18:VAL:HG11	2.33	0.43
3:c:63:ILE:HD12	3:c:97:LYS:O	2.18	0.43
23:A:263:G:C2	23:A:264:G:C1'	2.96	0.43
23:A:660:A:C3'	23:A:661:U:H5'	2.48	0.43
23:A:1698:A:N6	23:A:2033:C:O4'	2.51	0.43
23:A:2261:G:O2'	23:A:2262:G:C5'	2.64	0.43
23:A:2757:U:O2'	26:E:181:GLN:O	2.34	0.43
31:N:65:THR:HG22	31:N:67:SER:N	2.32	0.43
47:3:9:TYR:HH	47:3:24:LEU:C	2.15	0.43
3:c:148:ILE:O	3:c:169:GLU:N	2.52	0.43
4:d:54:LYS:NZ	4:d:55:GLN:OE1	2.42	0.43
8:h:104:ALA:C	8:h:105:LEU:HD22	2.43	0.43
23:A:577:A:O2'	23:A:2048:G:N2	2.42	0.43
23:A:2302:C:C2	43:Z:18:THR:CG2	3.01	0.43
27:F:7:LEU:HD12	27:F:8:LYS:H	1.82	0.43
34:Q:24:LEU:O	34:Q:28:GLU:CA	2.64	0.43
39:V:32:ALA:HA	39:V:35:ILE:HD13	2.00	0.43
1:a:1538:G:OP2	21:u:41:PRO:HD2	2.19	0.43
11:k:101:GLN:HG2	21:u:12:LEU:HG	2.00	0.43
23:A:2733:A:O2'	34:Q:60:ARG:NH1	2.51	0.43
23:A:2854:A:N6	23:A:2899:A:O2'	2.50	0.43
27:F:39:LEU:HD23	27:F:39:LEU:C	2.44	0.43
45:1:10:THR:OG1	45:1:13:GLU:N	2.48	0.43
46:2:57:GLU:N	46:2:57:GLU:OE1	2.51	0.43
1:a:159:G:N2	1:a:162:A:OP2	2.44	0.43
1:a:735:G:N2	1:a:738:G:OP2	2.50	0.43
1:a:987:A:N6	1:a:1235:U:OP1	2.50	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:a:1384:G:OP2	9:i:75:THR:OG1	2.34	0.43
2:b:86:ARG:HH22	2:b:218:ALA:HB3	1.83	0.43
5:e:166:ASN:OD1	8:h:100:GLY:N	2.52	0.43
23:A:261:U:H3'	23:A:262:G:H8	1.82	0.43
47:3:12:VAL:HG12	47:3:45:VAL:HB	1.99	0.43
1:a:890:C:P	12:l:5:ASN:HD21	2.41	0.43
1:a:1001:U:O2	1:a:1224:A:N7	2.52	0.43
1:a:1267:C:H2'	1:a:1289:A:H62	1.83	0.43
1:a:1528:G:N2	1:a:1531:A:OP2	2.52	0.43
2:b:212:LEU:O	2:b:215:ALA:HB3	2.18	0.43
23:A:2467:C:HO2'	23:A:2468:C:C1'	2.31	0.43
25:D:138:THR:N	25:D:162:GLN:OE1	2.51	0.43
27:F:155:VAL:HG22	27:F:156:THR:C	2.44	0.43
31:N:24:VAL:HG11	31:N:33:ALA:HB2	2.01	0.43
50:6:20:ARG:O	50:6:24:SER:CB	2.66	0.43
7:g:30:ILE:O	7:g:32:LEU:N	2.51	0.43
13:m:78:LYS:HA	13:m:81:MET:HE3	2.01	0.43
23:A:720:A:N3	23:A:2470:C:O2'	2.39	0.43
23:A:774:G:OP2	25:D:206:LYS:NZ	2.49	0.43
23:A:2285:C:O2'	23:A:2453:A:O3'	2.35	0.43
1:a:967:U:O2'	1:a:969:A:N7	2.40	0.43
1:a:1085:U:HO2'	2:b:103:ASN:CG	2.26	0.43
5:e:22:ALA:HB1	5:e:30:ARG:O	2.19	0.43
23:A:260:A:N6	23:A:261:U:H3	2.15	0.43
23:A:628:G:H2'	23:A:1289:A:H62	1.84	0.43
23:A:1099:G:N2	23:A:1148:C:N3	2.67	0.43
29:H:9:ILE:HD11	29:H:69:ARG:HA	2.00	0.43
36:S:106:ARG:NE	36:S:106:ARG:HA	2.34	0.43
42:Y:17:ASP:C	42:Y:19:LYS:H	2.25	0.43
1:a:1265:G:H22	1:a:1270:C:HO2'	1.67	0.43
8:h:97:VAL:HG22	8:h:98:LEU:HD22	2.01	0.43
10:j:5:LYS:HB3	10:j:77:VAL:CA	2.48	0.43
10:j:8:ILE:HG22	10:j:99:GLU:O	2.19	0.43
15:o:14:GLU:OE1	15:o:14:GLU:N	2.46	0.43
22:v:31:TYR:CD2	22:v:89:VAL:CG1	2.98	0.43
22:v:65:LEU:HD23	22:v:66:ARG:C	2.44	0.43
23:A:1033:G:C8	46:2:13:ILE:HD11	2.54	0.43
25:D:159:ALA:HA	25:D:193:GLN:HE21	1.84	0.43
45:1:38:GLU:OE1	45:1:38:GLU:N	2.52	0.43
1:a:828:U:HO2'	1:a:829:G:P	2.37	0.43
3:c:69:THR:C	3:c:105:ILE:HG22	2.43	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:c:145:ALA:HB1	3:c:202:TYR:O	2.19	0.43
4:d:157:ILE:HD12	4:d:159:ASN:HD21	1.84	0.43
5:e:115:LEU:HD13	5:e:123:ILE:HD11	2.00	0.43
23:A:263:G:O2'	23:A:264:G:O5'	2.35	0.43
23:A:628:G:H2'	23:A:1289:A:N6	2.34	0.43
23:A:2869:G:N2	23:A:2886:G:O2'	2.50	0.43
24:B:22:G:O6	24:B:54:U:O2'	2.35	0.43
49:5:35:PHE:CE1	49:5:37:SER:CA	3.02	0.43
51:7:49:LEU:HD12	51:7:49:LEU:N	2.34	0.43
1:a:218:U:OP2	1:a:219:C:N4	2.51	0.43
16:p:57:ALA:O	16:p:61:LEU:HD23	2.19	0.43
22:v:47:TYR:N	22:v:48:SER:HA	2.33	0.43
23:A:9:U:O4	23:A:2656:A:N7	2.52	0.43
23:A:297:G:O2'	23:A:304:G:O2'	2.26	0.43
23:A:1305:U:O2	23:A:1305:U:H2'	2.18	0.43
25:D:107:LYS:N	25:D:193:GLN:O	2.43	0.43
41:X:34:VAL:HG22	41:X:62:ALA:HB2	2.01	0.43
1:a:629:A:H2'	1:a:630:A:O4'	2.19	0.42
4:d:94:LEU:HD13	4:d:131:TYR:HB3	2.01	0.42
11:k:94:GLU:N	11:k:94:GLU:OE1	2.52	0.42
22:v:51:ALA:O	22:v:52:THR:OG1	2.29	0.42
23:A:1885:G:C2'	23:A:1910:G:H22	2.32	0.42
29:H:128:ASN:OD1	29:H:129:THR:N	2.52	0.42
41:X:81:VAL:HG22	41:X:82:GLY:H	1.84	0.42
48:4:43:VAL:O	48:4:44:CYS:CB	2.67	0.42
51:7:32:LEU:HD11	51:7:33:PHE:CZ	2.54	0.42
1:a:452:A:N1	1:a:499:A:N6	2.67	0.42
1:a:530:C:OP2	12:l:63:ARG:NH2	2.53	0.42
1:a:590:U:O4	1:a:767:A:N7	2.52	0.42
1:a:1059:G:O3'	14:n:4:THR:HG21	2.18	0.42
2:b:206:ALA:O	2:b:209:ALA:N	2.52	0.42
8:h:27:LEU:O	8:h:60:LEU:N	2.44	0.42
12:l:117:THR:O	12:l:117:THR:HG23	2.20	0.42
14:n:33:VAL:HG23	14:n:39:LEU:C	2.44	0.42
23:A:1591:G:O2'	23:A:1592:A:O5'	2.37	0.42
24:B:74:G:H22	24:B:97:A:N6	2.16	0.42
34:Q:26:ILE:N	34:Q:26:ILE:HD12	2.34	0.42
39:V:28:ASN:OD1	39:V:29:ALA:N	2.49	0.42
41:X:8:ASN:OD1	41:X:9:VAL:N	2.51	0.42
50:6:35:ARG:HE	50:6:43:LEU:HA	1.85	0.42
23:A:13:A:O2'	23:A:15:G:N7	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:A:921:C:H1'	23:A:946:A:H61	1.84	0.42
23:A:1550:G:O2'	23:A:1551:U:O5'	2.37	0.42
23:A:2231:C:H2'	23:A:2232:A:C8	2.55	0.42
25:D:17:SER:OG	25:D:18:LEU:N	2.51	0.42
33:P:43:THR:OG1	33:P:44:SER:N	2.50	0.42
35:R:92:ILE:HD12	35:R:93:VAL:O	2.19	0.42
1:a:136:C:O2'	16:p:66:LYS:NZ	2.39	0.42
1:a:757:A:O2'	1:a:758:C:O5'	2.36	0.42
1:a:798:A:C4	22:v:30:ARG:HB3	2.54	0.42
4:d:32:ALA:HB1	4:d:33:PRO:HD2	2.01	0.42
11:k:17:GLU:OE1	11:k:80:LYS:N	2.52	0.42
22:v:58:ILE:CG1	22:v:65:LEU:HD22	2.50	0.42
23:A:99:U:O2	23:A:101:G:N1	2.51	0.42
31:N:65:THR:HG22	31:N:67:SER:H	1.84	0.42
34:Q:107:GLY:O	34:Q:116:SER:N	2.45	0.42
37:T:65:ILE:HD11	37:T:95:LEU:HB2	2.01	0.42
1:a:27:A:N6	1:a:566:G:O2'	2.50	0.42
1:a:984:A:OP2	14:n:41:ARG:NH2	2.53	0.42
2:b:57:LEU:HD21	2:b:221:ILE:HG13	2.01	0.42
6:f:31:ALA:HB1	6:f:35:ALA:O	2.19	0.42
23:A:1079:U:C4	23:A:1164:G:O6	2.71	0.42
23:A:1281:U:O4	23:A:1282:A:N6	2.53	0.42
23:A:1470:G:O2'	23:A:1619:A:N6	2.45	0.42
23:A:1822:C:H2'	23:A:1823:U:O4'	2.20	0.42
25:D:50:VAL:O	25:D:50:VAL:HG23	2.20	0.42
42:Y:21:LEU:CD1	42:Y:42:LYS:HG2	2.29	0.42
1:a:404:A:O2'	1:a:406:C:OP1	2.35	0.42
1:a:1287:G:O2'	1:a:1293:C:O4'	2.35	0.42
1:a:1316:G:HO2'	1:a:1342:G:H22	1.66	0.42
11:k:100:LEU:HD11	11:k:105:LEU:HD12	2.01	0.42
19:s:45:ILE:CG2	47:3:71:VAL:HG22	2.47	0.42
22:v:31:TYR:CE2	22:v:90:ARG:CA	3.02	0.42
23:A:1893:A:H2'	23:A:1894:G:O4'	2.20	0.42
25:D:223:VAL:HG23	25:D:224:MET:N	2.34	0.42
26:E:138:ARG:HE	26:E:141:MET:CE	2.33	0.42
42:Y:25:GLY:O	42:Y:27:VAL:HG23	2.20	0.42
1:a:725:C:H4'	11:k:119:ASN:HD22	1.84	0.42
1:a:960:U:H2'	1:a:961:G:C8	2.55	0.42
1:a:1003:G:H2'	1:a:1005:C:H41	1.85	0.42
1:a:1112:C:OP2	2:b:95:ARG:NE	2.53	0.42
2:b:87:ALA:HA	2:b:222:LEU:HD21	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:b:120:MET:HB2	2:b:125:LEU:HD22	2.01	0.42
10:j:44:THR:OG1	10:j:70:HIS:ND1	2.25	0.42
22:v:91:LYS:C	22:v:93:LYS:H	2.28	0.42
23:A:1449:A:N1	23:A:1633:A:O2'	2.45	0.42
23:A:2147:G:N2	23:A:2206:C:N3	2.68	0.42
26:E:118:VAL:HG12	26:E:211:ILE:HG12	2.01	0.42
35:R:16:ALA:O	35:R:20:THR:N	2.52	0.42
9:i:23:LEU:HD13	9:i:24:VAL:N	2.33	0.42
23:A:749:G:O2'	23:A:771:G:N2	2.47	0.42
23:A:1455:U:O4	23:A:1631:G:N1	2.53	0.42
1:a:466:G:N2	1:a:484:A:N1	2.62	0.42
1:a:958:C:OP2	13:m:107:ARG:NE	2.52	0.42
22:v:52:THR:OG1	22:v:72:ASP:O	2.36	0.42
23:A:1392:G:O6	23:A:1414:G:N2	2.53	0.42
23:A:1668:U:O4	23:A:1669:C:N4	2.52	0.42
23:A:2516:G:O6	23:A:2517:G:N2	2.53	0.42
23:A:2680:U:OP2	23:A:2681:A:O2'	2.30	0.42
46:2:8:LEU:HD23	46:2:31:THR:HA	2.01	0.42
50:6:27:ASN:O	50:6:31:VAL:HG23	2.20	0.42
20:t:34:ASN:O	20:t:38:ALA:N	2.51	0.42
23:A:341:G:O2'	23:A:383:A:N6	2.53	0.42
23:A:1495:C:N3	23:A:1504:U:N3	2.67	0.42
29:H:77:GLN:O	29:H:82:GLY:N	2.46	0.42
30:M:72:ASP:OD1	30:M:73:LYS:N	2.53	0.42
42:Y:22:ARG:HH21	42:Y:87:THR:HG23	1.68	0.42
1:a:8:G:C8	5:e:124:LEU:HD23	2.55	0.41
5:e:70:ASP:O	5:e:71:LEU:HD12	2.20	0.41
23:A:1094:A:H2	23:A:2778:G:H22	1.68	0.41
23:A:1099:G:H21	23:A:1128:A:H2	1.68	0.41
39:V:80:PRO:HD3	39:V:102:HIS:HE2	1.85	0.41
42:Y:70:ILE:HG22	42:Y:71:LYS:O	2.19	0.41
1:a:1260:C:O2'	9:i:72:GLY:O	2.31	0.41
8:h:37:ALA:HB1	8:h:49:VAL:HG11	2.02	0.41
13:m:80:LEU:HD11	13:m:87:ARG:HB2	2.03	0.41
23:A:672:A:N7	32:O:70:ASN:ND2	2.63	0.41
23:A:856:U:O2	32:O:21:ARG:HG2	2.20	0.41
23:A:1175:G:O6	30:M:80:ASN:ND2	2.53	0.41
23:A:1945:A:HO2'	23:A:1946:A:P	2.36	0.41
23:A:2342:U:H4'	35:R:2:ILE:HD11	2.01	0.41
30:M:46:THR:OG1	30:M:49:VAL:HG22	2.21	0.41
37:T:35:ALA:O	37:T:39:VAL:HG23	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:a:139:U:O4	1:a:140:A:N6	2.54	0.41
1:a:194:G:N1	1:a:197:U:OP2	2.50	0.41
9:i:18:VAL:O	9:i:69:VAL:HG23	2.19	0.41
9:i:24:VAL:HG13	9:i:64:ASP:HB3	2.02	0.41
10:j:62:ARG:HH12	10:j:64:GLN:HE21	1.68	0.41
23:A:1303:A:H1'	23:A:1305:U:C4	2.55	0.41
29:H:105:LEU:O	29:H:106:ASN:ND2	2.54	0.41
33:P:42:ILE:C	33:P:42:ILE:HD12	2.46	0.41
34:Q:26:ILE:HD12	34:Q:26:ILE:H	1.86	0.41
48:4:37:TYR:CE1	48:4:43:VAL:HG22	2.55	0.41
1:a:589:G:N1	1:a:767:A:OP2	2.42	0.41
1:a:916:G:O2'	1:a:917:A:O4'	2.38	0.41
1:a:1089:G:N2	1:a:1092:A:OP2	2.53	0.41
2:b:175:GLU:O	2:b:179:LEU:N	2.48	0.41
4:d:32:ALA:HB1	4:d:33:PRO:CD	2.50	0.41
9:i:17:SER:OG	9:i:71:GLY:O	2.28	0.41
19:s:4:SER:OG	19:s:5:ILE:N	2.51	0.41
22:v:32:PHE:CE2	22:v:34:ASP:HB2	2.51	0.41
23:A:1081:G:H22	23:A:1163:U:H1'	1.85	0.41
23:A:1382:C:N4	23:A:1383:G:O6	2.53	0.41
23:A:1798:C:H2'	23:A:1799:G:O4'	2.19	0.41
23:A:2657:G:N2	23:A:2911:A:N3	2.69	0.41
29:H:80:SER:OG	29:H:81:GLN:N	2.54	0.41
39:V:3:ALA:N	39:V:107:VAL:O	2.53	0.41
39:V:19:LEU:O	39:V:22:ASP:N	2.54	0.41
52:8:11:CYS:N	52:8:14:CYS:SG	2.88	0.41
2:b:163:VAL:HG22	2:b:164:VAL:H	1.85	0.41
8:h:73:VAL:HG23	8:h:74:ILE:HG13	2.01	0.41
15:o:2:ALA:HB3	15:o:3:ILE:HA	2.03	0.41
16:p:6:ARG:NH2	16:p:27:SER:OG	2.53	0.41
22:v:31:TYR:OH	22:v:90:ARG:HB3	2.20	0.41
22:v:58:ILE:HG12	22:v:65:LEU:HD22	2.02	0.41
23:A:2118:U:OP2	23:A:2119:U:O2'	2.33	0.41
25:D:126:GLY:O	25:D:128:ALA:N	2.54	0.41
33:P:56:ARG:O	33:P:59:LYS:NZ	2.53	0.41
36:S:72:VAL:HG22	36:S:73:GLU:H	1.85	0.41
49:5:35:PHE:CE1	49:5:37:SER:HA	2.54	0.41
1:a:701:G:C5'	22:v:100:SER:CB	2.96	0.41
8:h:40:LEU:HD12	8:h:45:PHE:CD2	2.55	0.41
17:q:7:ARG:NH1	17:q:65:GLU:OE2	2.50	0.41
20:t:76:SER:O	20:t:80:THR:OG1	2.28	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:b:78:GLU:O	2:b:82:SER:OG	2.30	0.41
3:c:52:SER:OG	3:c:53:HIS:N	2.54	0.41
13:m:84:SER:HB3	13:m:85:SER:HA	2.02	0.41
20:t:45:ASN:O	20:t:45:ASN:ND2	2.54	0.41
23:A:2161:A:C5	23:A:2184:G:N2	2.88	0.41
23:A:2679:U:H2'	23:A:2680:U:O4'	2.20	0.41
26:E:9:LYS:O	26:E:9:LYS:HG2	2.20	0.41
29:H:96:ALA:HA	29:H:105:LEU:HD23	2.03	0.41
35:R:68:THR:HG23	35:R:68:THR:O	2.20	0.41
1:a:473:U:N3	1:a:476:C:OP2	2.51	0.41
1:a:1266:G:N1	1:a:1294:C:N3	2.69	0.41
2:b:22:ARG:NE	2:b:22:ARG:HA	2.35	0.41
5:e:107:ALA:O	5:e:112:ARG:NH2	2.53	0.41
15:o:29:ILE:HD11	15:o:81:LEU:CD1	2.48	0.41
16:p:40:TYR:CD1	16:p:50:ILE:HG22	2.56	0.41
17:q:35:LEU:HD23	17:q:35:LEU:C	2.45	0.41
22:v:98:ARG:O	22:v:99:LYS:C	2.49	0.41
23:A:1206:G:H21	38:U:90:GLN:HE22	1.67	0.41
23:A:1390:A:OP2	23:A:1414:G:N1	2.41	0.41
27:F:136:THR:O	27:F:140:LYS:NZ	2.43	0.41
27:F:155:VAL:HG22	27:F:156:THR:O	2.20	0.41
1:a:24:C:OP2	1:a:569:U:N3	2.40	0.41
1:a:828:U:O2'	1:a:828:U:O2	2.39	0.41
5:e:134:ILE:HD12	5:e:134:ILE:H	1.86	0.41
18:r:31:THR:O	18:r:35:LYS:N	2.38	0.41
22:v:24:LYS:HA	22:v:27:LYS:HD3	2.02	0.41
22:v:82:ASN:O	22:v:84:LYS:N	2.54	0.41
22:v:101:ARG:O	22:v:102:ASP:C	2.62	0.41
22:v:102:ASP:CG	22:v:103:ARG:H	2.29	0.41
23:A:2162:A:H61	23:A:2183:G:C2'	2.34	0.41
23:A:2380:G:O2'	43:Z:41:GLY:O	2.39	0.41
24:B:46:A:O3'	35:R:102:HIS:NE2	2.50	0.41
25:D:190:THR:OG1	25:D:191:ILE:N	2.50	0.41
25:D:194:VAL:HG12	25:D:195:GLY:N	2.35	0.41
26:E:9:LYS:HZ3	26:E:201:VAL:HG23	1.85	0.41
26:E:169:MET:HB2	26:E:170:PRO:CD	2.51	0.41
30:M:53:ASP:N	30:M:53:ASP:OD1	2.53	0.41
32:O:30:THR:HG22	32:O:30:THR:O	2.21	0.41
33:P:38:THR:OG1	33:P:39:THR:N	2.54	0.41
34:Q:37:ALA:HA	34:Q:40:VAL:HG12	2.03	0.41
38:U:29:GLU:OE1	38:U:30:GLY:N	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
52:8:7:VAL:HG21	52:8:36:GLN:HB2	2.03	0.41
1:a:293:C:H2'	1:a:294:A:O4'	2.21	0.41
19:s:40:ILE:HG21	47:3:77:LYS:NZ	2.35	0.41
23:A:318:A:H61	23:A:402:C:H42	1.69	0.41
23:A:2152:G:N2	23:A:2200:A:N6	2.69	0.41
25:D:92:LEU:HD22	25:D:93:VAL:H	1.86	0.41
25:D:242:ARG:NH2	25:D:246:MET:HE3	2.35	0.41
31:N:102:VAL:CG2	31:N:121:VAL:HG22	2.51	0.41
37:T:108:GLN:O	37:T:111:THR:OG1	2.39	0.41
1:a:225:G:O2'	1:a:478:G:N2	2.49	0.40
1:a:1013:G:P	1:a:1036:C:H41	2.42	0.40
1:a:1332:U:OP1	13:m:90:ARG:NH1	2.55	0.40
4:d:64:THR:O	4:d:68:PHE:N	2.45	0.40
6:f:90:MET:HE1	18:r:69:HIS:HB3	2.02	0.40
22:v:95:ARG:CZ	22:v:96:ILE:CG2	2.87	0.40
23:A:1199:A:O3'	37:T:55:ARG:NH2	2.53	0.40
23:A:1584:A:H4'	23:A:1585:G:H5'	2.03	0.40
35:R:108:LEU:O	35:R:111:ALA:N	2.54	0.40
37:T:79:LEU:O	37:T:82:GLY:N	2.54	0.40
1:a:699:G:OP2	11:k:28:ASN:ND2	2.36	0.40
1:a:956:A:O2'	1:a:1344:A:N3	2.50	0.40
1:a:1261:A:H61	1:a:1365:U:H1'	1.86	0.40
2:b:169:GLU:O	2:b:172:ALA:HB3	2.22	0.40
16:p:12:SER:OG	16:p:13:LYS:N	2.55	0.40
23:A:85:G:OP1	41:X:26:THR:OG1	2.39	0.40
26:E:158:SER:O	26:E:161:SER:N	2.55	0.40
27:F:38:ASN:OD1	27:F:39:LEU:N	2.54	0.40
27:F:187:THR:OG1	27:F:188:ASN:N	2.54	0.40
1:a:271:A:H2'	1:a:272:C:H6	1.85	0.40
1:a:680:U:N3	1:a:681:G:N7	2.70	0.40
1:a:1076:G:N2	1:a:1202:A:OP2	2.48	0.40
1:a:1265:G:N1	1:a:1295:C:N3	2.69	0.40
9:i:6:VAL:HG13	9:i:6:VAL:O	2.21	0.40
23:A:198:A:H2'	23:A:201:C:H41	1.86	0.40
23:A:942:C:O2'	23:A:943:C:O4'	2.28	0.40
23:A:1241:A:O4'	27:F:41:ARG:NH2	2.53	0.40
23:A:2261:G:HO2'	23:A:2262:G:H5'	1.85	0.40
23:A:2599:A:OP2	26:E:157:ALA:HB3	2.21	0.40
25:D:247:SER:HB2	25:D:248:PRO:HD2	2.03	0.40
1:a:1267:C:H41	1:a:1288:C:H2'	1.86	0.40
4:d:151:ILE:O	4:d:155:VAL:HG23	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:h:40:LEU:O	8:h:43:GLU:N	2.54	0.40
12:l:53:MET:HE3	12:l:65:TYR:CZ	2.55	0.40
20:t:27:ALA:O	20:t:30:THR:OG1	2.33	0.40
23:A:1583:G:H3'	23:A:1584:A:C5'	2.50	0.40
34:Q:52:LYS:HG2	34:Q:90:ALA:HB1	2.03	0.40
40:W:18:GLU:O	40:W:21:ALA:HB3	2.21	0.40
51:7:31:HIS:O	51:7:33:PHE:N	2.54	0.40
1:a:1453:G:OP2	1:a:1454:A:N6	2.52	0.40
1:a:1542:G:O2'	1:a:1543:A:O4'	2.34	0.40
5:e:84:THR:OG1	5:e:96:MET:O	2.33	0.40
22:v:80:LEU:N	22:v:80:LEU:CD2	2.84	0.40
22:v:82:ASN:C	22:v:84:LYS:N	2.80	0.40
23:A:510:U:H2'	23:A:511:G:C8	2.57	0.40
23:A:2501:U:O2'	23:A:2502:C:OP1	2.36	0.40
27:F:39:LEU:HD13	27:F:101:MET:HE1	2.03	0.40
34:Q:33:THR:HB	34:Q:36:ARG:HE	1.86	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	b	220/255 (86%)	192 (87%)	27 (12%)	1 (0%)	24	56
3	c	201/217 (93%)	166 (83%)	34 (17%)	1 (0%)	24	56
4	d	193/200 (96%)	163 (84%)	30 (16%)	0	100	100
5	e	158/166 (95%)	124 (78%)	34 (22%)	0	100	100
6	f	92/98 (94%)	73 (79%)	18 (20%)	1 (1%)	11	42
7	g	139/156 (89%)	117 (84%)	20 (14%)	2 (1%)	9	37
8	h	129/132 (98%)	107 (83%)	21 (16%)	1 (1%)	16	48

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
9	i	8/132 (6%)	6 (75%)	2 (25%)	0	100	100
16	p	3/91 (3%)	2 (67%)	1 (33%)	0	100	100
19	s	16/92 (17%)	13 (81%)	3 (19%)	0	100	100
21	u	16/58 (28%)	13 (81%)	3 (19%)	0	100	100
25	D	273/277 (99%)	228 (84%)	44 (16%)	1 (0%)	30	60
26	E	216/220 (98%)	172 (80%)	41 (19%)	3 (1%)	9	37
27	F	197/207 (95%)	157 (80%)	40 (20%)	0	100	100
28	G	164/179 (92%)	123 (75%)	40 (24%)	1 (1%)	21	52
29	H	162/178 (91%)	140 (86%)	22 (14%)	0	100	100
30	M	143/145 (99%)	117 (82%)	25 (18%)	1 (1%)	18	50
31	N	120/122 (98%)	83 (69%)	37 (31%)	0	100	100
32	O	129/146 (88%)	90 (70%)	39 (30%)	0	100	100
33	P	131/144 (91%)	101 (77%)	30 (23%)	0	100	100
34	Q	115/122 (94%)	89 (77%)	26 (23%)	0	100	100
35	R	117/119 (98%)	95 (81%)	22 (19%)	0	100	100
36	S	105/116 (90%)	86 (82%)	17 (16%)	2 (2%)	6	33
37	T	114/118 (97%)	102 (90%)	12 (10%)	0	100	100
38	U	100/102 (98%)	79 (79%)	20 (20%)	1 (1%)	12	43
39	V	110/117 (94%)	98 (89%)	12 (11%)	0	100	100
40	W	87/91 (96%)	68 (78%)	19 (22%)	0	100	100
41	X	81/105 (77%)	50 (62%)	31 (38%)	0	100	100
42	Y	92/217 (42%)	68 (74%)	24 (26%)	0	100	100
43	Z	75/94 (80%)	65 (87%)	9 (12%)	1 (1%)	9	38
44	0	44/62 (71%)	33 (75%)	11 (25%)	0	100	100
45	1	63/69 (91%)	56 (89%)	7 (11%)	0	100	100
46	2	55/59 (93%)	48 (87%)	6 (11%)	1 (2%)	6	34
47	3	79/84 (94%)	47 (60%)	31 (39%)	1 (1%)	9	38
48	4	42/58 (72%)	36 (86%)	5 (12%)	1 (2%)	4	29
49	5	24/49 (49%)	19 (79%)	5 (21%)	0	100	100
50	6	42/45 (93%)	34 (81%)	6 (14%)	2 (5%)	2	17
51	7	58/66 (88%)	38 (66%)	20 (34%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
52	8	35/37 (95%)	27 (77%)	8 (23%)	0	100	100
All	All	4148/4945 (84%)	3325 (80%)	802 (19%)	21 (0%)	26	56

All (21) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	b	104	TYR
26	E	10	ILE
26	E	142	SER
36	S	105	LEU
43	Z	28	ARG
47	3	12	VAL
50	6	16	VAL
7	g	14	PRO
50	6	15	LYS
7	g	13	LEU
36	S	106	ARG
48	4	44	CYS
3	c	203	ARG
28	G	99	PHE
30	M	66	THR
38	U	23	GLU
8	h	100	GLY
46	2	30	LYS
6	f	12	PRO
25	D	252	PRO
26	E	154	VAL

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	b	192/221 (87%)	192 (100%)	0	100	100
3	c	164/175 (94%)	164 (100%)	0	100	100
4	d	172/175 (98%)	172 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	e	126/131 (96%)	124 (98%)	2 (2%)	55	68
6	f	82/86 (95%)	82 (100%)	0	100	100
7	g	122/132 (92%)	122 (100%)	0	100	100
8	h	112/113 (99%)	112 (100%)	0	100	100
9	i	106/109 (97%)	106 (100%)	0	100	100
10	j	89/91 (98%)	87 (98%)	2 (2%)	45	63
11	k	91/104 (88%)	90 (99%)	1 (1%)	65	73
12	l	117/119 (98%)	116 (99%)	1 (1%)	70	75
13	m	94/104 (90%)	94 (100%)	0	100	100
14	n	52/53 (98%)	52 (100%)	0	100	100
15	o	80/81 (99%)	79 (99%)	1 (1%)	61	71
16	p	76/77 (99%)	76 (100%)	0	100	100
17	q	80/82 (98%)	80 (100%)	0	100	100
18	r	51/68 (75%)	50 (98%)	1 (2%)	48	64
19	s	73/80 (91%)	73 (100%)	0	100	100
20	t	67/69 (97%)	67 (100%)	0	100	100
21	u	41/54 (76%)	33 (80%)	8 (20%)	1	9
22	v	91/173 (53%)	69 (76%)	22 (24%)	1	5
25	D	222/224 (99%)	220 (99%)	2 (1%)	70	75
26	E	175/177 (99%)	175 (100%)	0	100	100
27	F	163/169 (96%)	163 (100%)	0	100	100
28	G	147/158 (93%)	147 (100%)	0	100	100
29	H	144/155 (93%)	144 (100%)	0	100	100
30	M	123/123 (100%)	123 (100%)	0	100	100
31	N	100/100 (100%)	99 (99%)	1 (1%)	68	74
32	O	104/112 (93%)	103 (99%)	1 (1%)	68	74
33	P	110/119 (92%)	106 (96%)	4 (4%)	31	54
34	Q	98/102 (96%)	98 (100%)	0	100	100
35	R	95/95 (100%)	95 (100%)	0	100	100
36	S	93/102 (91%)	93 (100%)	0	100	100
37	T	96/98 (98%)	96 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
38	U	86/86 (100%)	86 (100%)	0	100	100
39	V	91/94 (97%)	91 (100%)	0	100	100
40	W	80/82 (98%)	80 (100%)	0	100	100
41	X	73/90 (81%)	73 (100%)	0	100	100
42	Y	83/190 (44%)	81 (98%)	2 (2%)	43	61
43	Z	60/75 (80%)	59 (98%)	1 (2%)	53	67
44	0	39/52 (75%)	39 (100%)	0	100	100
45	1	59/62 (95%)	59 (100%)	0	100	100
46	2	51/53 (96%)	51 (100%)	0	100	100
47	3	72/75 (96%)	71 (99%)	1 (1%)	59	70
48	4	41/51 (80%)	39 (95%)	2 (5%)	22	48
49	5	26/47 (55%)	26 (100%)	0	100	100
50	6	39/40 (98%)	39 (100%)	0	100	100
51	7	52/57 (91%)	52 (100%)	0	100	100
52	8	35/35 (100%)	35 (100%)	0	100	100
All	All	4635/5120 (90%)	4583 (99%)	52 (1%)	63	73

All (52) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
5	e	8	THR
5	e	9	LYS
10	j	4	GLN
10	j	5	LYS
11	k	14	LYS
12	l	101	LYS
15	o	47	LYS
18	r	40	GLU
21	u	11	SER
21	u	12	LEU
21	u	16	LEU
21	u	24	SER
21	u	25	LYS
21	u	44	LYS
21	u	53	ARG
21	u	54	LYS
22	v	20	TYR

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Mol	Chain	Res	Type
22	v	22	GLU
22	v	30	ARG
22	v	41	HIS
22	v	45	LYS
22	v	47	TYR
22	v	70	ARG
22	v	74	LEU
22	v	75	TYR
22	v	78	ILE
22	v	80	LEU
22	v	82	ASN
22	v	83	ASN
22	v	89	VAL
22	v	90	ARG
22	v	91	LYS
22	v	93	LYS
22	v	94	THR
22	v	96	ILE
22	v	99	LYS
22	v	101	ARG
22	v	103	ARG
25	D	197	LEU
25	D	254	LEU
31	N	63	VAL
32	O	23	VAL
33	P	51	ARG
33	P	133	LYS
33	P	135	GLU
33	P	136	GLU
42	Y	21	LEU
42	Y	22	ARG
43	Z	19	LYS
47	3	77	LYS
48	4	44	CYS
48	4	45	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (54) such sidechains are listed below:

Mol	Chain	Res	Type
2	b	19	GLN
2	b	36	ASN
3	c	88	ASN

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Mol	Chain	Res	Type
4	d	8	ASN
4	d	159	ASN
5	e	43	ASN
5	e	146	ASN
5	e	149	ASN
6	f	13	ASN
7	g	19	ASN
7	g	40	GLN
8	h	31	ASN
8	h	68	GLN
9	i	33	ASN
9	i	68	ASN
9	i	77	GLN
9	i	79	GLN
10	j	4	GLN
10	j	64	GLN
11	k	101	GLN
12	l	73	ASN
12	l	90	HIS
14	n	11	GLN
15	o	42	HIS
15	o	46	HIS
20	t	62	GLN
22	v	41	HIS
22	v	71	ASN
22	v	82	ASN
22	v	88	GLN
22	v	97	ASN
25	D	43	ASN
25	D	53	HIS
25	D	193	GLN
25	D	203	ASN
26	E	50	GLN
26	E	200	ASN
27	F	75	GLN
27	F	148	GLN
29	H	106	ASN
29	H	120	ASN
32	O	114	ASN
33	P	35	GLN
33	P	71	HIS
33	P	123	HIS

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Mol	Chain	Res	Type
36	S	4	HIS
37	T	44	GLN
39	V	90	GLN
39	V	97	ASN
41	X	76	ASN
42	Y	10	GLN
43	Z	20	ASN
44	0	32	ASN
45	1	17	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	a	1540/1556 (98%)	373 (24%)	0
23	A	2910/2923 (99%)	729 (25%)	13 (0%)
24	B	113/114 (99%)	23 (20%)	0
All	All	4563/4593 (99%)	1125 (24%)	13 (0%)

All (1125) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	a	8	G
1	a	9	A
1	a	10	G
1	a	11	A
1	a	15	U
1	a	28	G
1	a	31	U
1	a	32	G
1	a	33	A
1	a	40	G
1	a	44	C
1	a	48	C
1	a	49	C
1	a	51	A
1	a	52	A
1	a	53	U
1	a	58	G
1	a	61	A
1	a	62	G
1	a	67	G

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Mol	Chain	Res	Type
1	a	69	G
1	a	74	G
1	a	82	G
1	a	83	C
1	a	84	U
1	a	85	U
1	a	86	G
1	a	88	U
1	a	89	U
1	a	90	C
1	a	92	C
1	a	94	G
1	a	95	A
1	a	120	C
1	a	129	A
1	a	130	A
1	a	138	A
1	a	142	G
1	a	144	C
1	a	148	G
1	a	149	A
1	a	154	U
1	a	159	G
1	a	163	C
1	a	165	G
1	a	168	G
1	a	169	C
1	a	170	U
1	a	171	A
1	a	173	U
1	a	182	A
1	a	183	U
1	a	191	A
1	a	196	A
1	a	205	A
1	a	211	A
1	a	212	A
1	a	213	G
1	a	214	A
1	a	218	U
1	a	221	U
1	a	234	A

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Mol	Chain	Res	Type
1	a	247	C
1	a	248	U
1	a	252	U
1	a	255	G
1	a	259	G
1	a	260	U
1	a	269	U
1	a	274	G
1	a	275	C
1	a	287	A
1	a	297	G
1	a	301	A
1	a	307	G
1	a	314	A
1	a	315	U
1	a	333	A
1	a	334	G
1	a	336	C
1	a	354	G
1	a	355	G
1	a	356	G
1	a	360	C
1	a	361	A
1	a	362	G
1	a	364	A
1	a	373	U
1	a	375	U
1	a	380	C
1	a	402	G
1	a	405	A
1	a	406	C
1	a	414	G
1	a	419	A
1	a	420	U
1	a	421	G
1	a	422	A
1	a	429	U
1	a	431	G
1	a	432	G
1	a	436	G
1	a	437	U
1	a	438	A

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Mol	Chain	Res	Type
1	a	444	C
1	a	447	U
1	a	449	A
1	a	454	G
1	a	455	G
1	a	456	A
1	a	457	A
1	a	459	A
1	a	462	A
1	a	466	G
1	a	467	U
1	a	470	A
1	a	476	C
1	a	477	U
1	a	478	G
1	a	480	G
1	a	481	C
1	a	482	A
1	a	483	C
1	a	484	A
1	a	492	G
1	a	494	U
1	a	503	A
1	a	504	G
1	a	505	A
1	a	508	G
1	a	513	G
1	a	516	U
1	a	519	C
1	a	520	U
1	a	526	C
1	a	528	A
1	a	529	G
1	a	532	G
1	a	535	G
1	a	539	U
1	a	540	A
1	a	541	A
1	a	555	A
1	a	556	G
1	a	557	C
1	a	558	G

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Mol	Chain	Res	Type
1	a	567	A
1	a	569	U
1	a	570	U
1	a	572	U
1	a	575	G
1	a	576	G
1	a	580	A
1	a	581	A
1	a	583	G
1	a	584	C
1	a	585	G
1	a	587	G
1	a	588	C
1	a	604	A
1	a	613	U
1	a	615	A
1	a	634	U
1	a	635	G
1	a	640	G
1	a	641	U
1	a	647	G
1	a	650	A
1	a	661	U
1	a	669	G
1	a	673	A
1	a	693	G
1	a	695	A
1	a	701	G
1	a	710	A
1	a	711	G
1	a	725	C
1	a	726	A
1	a	731	U
1	a	736	A
1	a	741	G
1	a	742	A
1	a	756	A
1	a	757	A
1	a	758	C
1	a	763	G
1	a	774	A
1	a	781	G

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Mol	Chain	Res	Type
1	a	789	A
1	a	802	A
1	a	807	G
1	a	811	G
1	a	817	G
1	a	819	C
1	a	820	G
1	a	825	C
1	a	828	U
1	a	829	G
1	a	836	A
1	a	850	U
1	a	851	U
1	a	854	C
1	a	855	G
1	a	856	C
1	a	865	G
1	a	868	G
1	a	869	C
1	a	881	U
1	a	882	A
1	a	883	A
1	a	886	A
1	a	900	G
1	a	924	A
1	a	932	G
1	a	936	G
1	a	937	G
1	a	944	C
1	a	945	A
1	a	946	C
1	a	949	G
1	a	955	G
1	a	957	G
1	a	958	C
1	a	968	A
1	a	970	U
1	a	971	U
1	a	975	A
1	a	976	G
1	a	979	A
1	a	981	G

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Mol	Chain	Res	Type
1	a	985	A
1	a	986	G
1	a	992	U
1	a	993	A
1	a	994	C
1	a	999	U
1	a	1002	U
1	a	1003	G
1	a	1012	U
1	a	1014	A
1	a	1024	A
1	a	1027	U
1	a	1028	A
1	a	1030	A
1	a	1034	U
1	a	1036	C
1	a	1037	C
1	a	1038	C
1	a	1039	C
1	a	1040	U
1	a	1041	U
1	a	1042	C
1	a	1044	G
1	a	1049	C
1	a	1050	A
1	a	1057	C
1	a	1065	G
1	a	1067	A
1	a	1068	U
1	a	1076	G
1	a	1078	C
1	a	1083	C
1	a	1087	U
1	a	1091	G
1	a	1092	A
1	a	1097	U
1	a	1106	G
1	a	1107	U
1	a	1113	A
1	a	1117	A
1	a	1130	A
1	a	1139	G

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Mol	Chain	Res	Type
1	a	1141	C
1	a	1142	A
1	a	1144	C
1	a	1150	G
1	a	1151	U
1	a	1154	G
1	a	1157	A
1	a	1162	A
1	a	1163	A
1	a	1164	G
1	a	1165	U
1	a	1168	A
1	a	1169	C
1	a	1170	U
1	a	1171	G
1	a	1172	C
1	a	1179	C
1	a	1190	A
1	a	1195	G
1	a	1207	A
1	a	1208	A
1	a	1223	U
1	a	1225	U
1	a	1226	G
1	a	1232	G
1	a	1237	C
1	a	1239	C
1	a	1244	G
1	a	1249	A
1	a	1251	U
1	a	1261	A
1	a	1264	G
1	a	1271	G
1	a	1272	A
1	a	1273	A
1	a	1279	G
1	a	1281	G
1	a	1289	A
1	a	1291	A
1	a	1293	C
1	a	1296	A
1	a	1297	U

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Mol	Chain	Res	Type
1	a	1298	A
1	a	1304	G
1	a	1309	C
1	a	1310	A
1	a	1311	G
1	a	1313	U
1	a	1316	G
1	a	1323	G
1	a	1328	C
1	a	1330	A
1	a	1331	C
1	a	1333	C
1	a	1334	G
1	a	1335	A
1	a	1338	A
1	a	1346	C
1	a	1347	U
1	a	1356	U
1	a	1357	A
1	a	1358	G
1	a	1371	A
1	a	1375	U
1	a	1381	G
1	a	1386	A
1	a	1389	C
1	a	1390	G
1	a	1392	U
1	a	1406	C
1	a	1408	C
1	a	1410	C
1	a	1430	G
1	a	1437	A
1	a	1442	C
1	a	1443	G
1	a	1453	G
1	a	1454	A
1	a	1457	A
1	a	1459	C
1	a	1462	U
1	a	1463	U
1	a	1464	U
1	a	1465	A

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Mol	Chain	Res	Type
1	a	1478	C
1	a	1487	G
1	a	1492	A
1	a	1503	G
1	a	1505	A
1	a	1514	A
1	a	1515	A
1	a	1516	G
1	a	1517	G
1	a	1518	U
1	a	1519	A
1	a	1529	G
1	a	1532	G
1	a	1536	C
1	a	1541	G
1	a	1542	G
1	a	1546	A
23	A	15	G
23	A	23	G
23	A	28	A
23	A	34	U
23	A	39	C
23	A	46	C
23	A	52	A
23	A	61	A
23	A	63	U
23	A	64	A
23	A	71	A
23	A	75	G
23	A	76	C
23	A	80	G
23	A	82	G
23	A	85	G
23	A	90	A
23	A	100	U
23	A	102	A
23	A	104	C
23	A	108	A
23	A	117	A
23	A	118	A
23	A	119	U
23	A	121	G

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Mol	Chain	Res	Type
23	A	130	A
23	A	135	G
23	A	150	A
23	A	161	A
23	A	162	A
23	A	163	U
23	A	164	A
23	A	166	A
23	A	168	A
23	A	173	A
23	A	177	G
23	A	180	G
23	A	182	C
23	A	183	A
23	A	184	C
23	A	185	A
23	A	199	A
23	A	201	C
23	A	202	A
23	A	204	C
23	A	207	A
23	A	218	G
23	A	219	A
23	A	225	A
23	A	229	A
23	A	231	A
23	A	233	U
23	A	236	A
23	A	244	A
23	A	251	G
23	A	255	G
23	A	263	G
23	A	267	G
23	A	282	A
23	A	284	C
23	A	285	U
23	A	286	U
23	A	287	G
23	A	288	C
23	A	289	U
23	A	298	U
23	A	300	G

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Mol	Chain	Res	Type
23	A	301	U
23	A	305	A
23	A	312	A
23	A	314	A
23	A	316	G
23	A	317	G
23	A	318	A
23	A	319	G
23	A	320	U
23	A	321	U
23	A	329	A
23	A	330	C
23	A	331	G
23	A	337	A
23	A	338	G
23	A	342	A
23	A	345	C
23	A	353	A
23	A	354	A
23	A	355	G
23	A	364	A
23	A	365	A
23	A	373	A
23	A	374	U
23	A	389	A
23	A	393	G
23	A	398	C
23	A	401	U
23	A	404	U
23	A	411	A
23	A	418	G
23	A	432	G
23	A	438	U
23	A	451	U
23	A	457	G
23	A	464	U
23	A	468	A
23	A	482	U
23	A	489	A
23	A	490	C
23	A	502	C
23	A	503	A

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Mol	Chain	Res	Type
23	A	504	G
23	A	510	U
23	A	511	G
23	A	525	A
23	A	526	A
23	A	527	G
23	A	530	C
23	A	536	A
23	A	538	G
23	A	543	G
23	A	550	A
23	A	551	G
23	A	553	A
23	A	554	C
23	A	555	C
23	A	572	C
23	A	574	A
23	A	575	G
23	A	576	U
23	A	577	A
23	A	578	G
23	A	588	G
23	A	589	U
23	A	591	A
23	A	593	U
23	A	594	G
23	A	599	A
23	A	605	U
23	A	606	G
23	A	611	U
23	A	613	G
23	A	618	A
23	A	628	G
23	A	629	A
23	A	630	G
23	A	631	U
23	A	646	A
23	A	650	U
23	A	657	U
23	A	658	A
23	A	659	A
23	A	660	A

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Mol	Chain	Res	Type
23	A	661	U
23	A	663	U
23	A	665	G
23	A	682	A
23	A	683	G
23	A	690	U
23	A	693	G
23	A	698	U
23	A	713	A
23	A	715	A
23	A	716	C
23	A	727	G
23	A	731	U
23	A	732	C
23	A	733	U
23	A	760	A
23	A	762	C
23	A	763	A
23	A	771	G
23	A	774	G
23	A	775	A
23	A	777	C
23	A	785	C
23	A	792	U
23	A	793	G
23	A	795	A
23	A	797	A
23	A	806	A
23	A	807	U
23	A	809	A
23	A	820	G
23	A	827	A
23	A	828	A
23	A	829	U
23	A	834	A
23	A	835	U
23	A	837	G
23	A	838	A
23	A	845	A
23	A	847	A
23	A	848	U
23	A	850	G

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Mol	Chain	Res	Type
23	A	852	U
23	A	864	A
23	A	872	U
23	A	873	U
23	A	875	G
23	A	876	G
23	A	887	A
23	A	891	A
23	A	904	G
23	A	905	U
23	A	911	A
23	A	912	C
23	A	913	U
23	A	921	C
23	A	922	G
23	A	923	A
23	A	924	G
23	A	925	G
23	A	926	G
23	A	929	C
23	A	930	C
23	A	932	U
23	A	936	G
23	A	938	G
23	A	944	G
23	A	945	A
23	A	955	A
23	A	959	C
23	A	962	A
23	A	963	A
23	A	968	A
23	A	970	U
23	A	985	A
23	A	987	U
23	A	989	A
23	A	990	G
23	A	1001	A
23	A	1002	U
23	A	1003	A
23	A	1005	G
23	A	1006	G
23	A	1017	A

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Mol	Chain	Res	Type
23	A	1018	A
23	A	1033	G
23	A	1040	A
23	A	1041	G
23	A	1052	A
23	A	1053	A
23	A	1055	A
23	A	1056	U
23	A	1057	A
23	A	1066	G
23	A	1067	U
23	A	1069	G
23	A	1070	A
23	A	1073	A
23	A	1077	U
23	A	1079	U
23	A	1083	G
23	A	1085	U
23	A	1088	C
23	A	1091	G
23	A	1097	U
23	A	1098	A
23	A	1101	A
23	A	1104	U
23	A	1105	U
23	A	1106	G
23	A	1107	G
23	A	1108	C
23	A	1110	U
23	A	1112	G
23	A	1113	A
23	A	1114	A
23	A	1115	G
23	A	1116	C
23	A	1119	C
23	A	1120	C
23	A	1121	A
23	A	1122	U
23	A	1123	C
23	A	1124	A
23	A	1125	U
23	A	1126	U

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Mol	Chain	Res	Type
23	A	1128	A
23	A	1131	G
23	A	1132	A
23	A	1133	G
23	A	1134	U
23	A	1135	G
23	A	1138	U
23	A	1139	A
23	A	1140	A
23	A	1143	G
23	A	1145	U
23	A	1146	C
23	A	1149	U
23	A	1150	A
23	A	1154	G
23	A	1156	G
23	A	1158	G
23	A	1160	C
23	A	1163	U
23	A	1170	A
23	A	1172	A
23	A	1177	A
23	A	1178	C
23	A	1179	C
23	A	1185	U
23	A	1199	A
23	A	1213	C
23	A	1216	U
23	A	1217	U
23	A	1218	G
23	A	1225	G
23	A	1226	G
23	A	1234	G
23	A	1244	G
23	A	1245	G
23	A	1248	U
23	A	1250	G
23	A	1252	A
23	A	1258	A
23	A	1265	G
23	A	1267	A
23	A	1273	G

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Mol	Chain	Res	Type
23	A	1276	G
23	A	1278	G
23	A	1286	G
23	A	1287	U
23	A	1288	G
23	A	1289	A
23	A	1291	A
23	A	1293	U
23	A	1294	G
23	A	1300	G
23	A	1303	A
23	A	1305	U
23	A	1306	C
23	A	1308	C
23	A	1309	G
23	A	1310	A
23	A	1312	A
23	A	1323	A
23	A	1337	A
23	A	1338	U
23	A	1339	U
23	A	1345	A
23	A	1350	U
23	A	1358	A
23	A	1359	A
23	A	1361	G
23	A	1363	U
23	A	1369	G
23	A	1378	U
23	A	1379	A
23	A	1398	G
23	A	1404	A
23	A	1405	G
23	A	1416	U
23	A	1417	G
23	A	1421	A
23	A	1423	C
23	A	1429	G
23	A	1432	A
23	A	1435	C
23	A	1451	U
23	A	1452	C

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Mol	Chain	Res	Type
23	A	1454	U
23	A	1455	U
23	A	1458	A
23	A	1459	A
23	A	1463	A
23	A	1464	U
23	A	1471	A
23	A	1472	C
23	A	1473	G
23	A	1479	G
23	A	1480	G
23	A	1489	A
23	A	1490	G
23	A	1491	C
23	A	1494	G
23	A	1495	C
23	A	1496	G
23	A	1498	U
23	A	1499	U
23	A	1503	U
23	A	1504	U
23	A	1510	U
23	A	1511	C
23	A	1512	U
23	A	1519	U
23	A	1520	A
23	A	1522	G
23	A	1526	G
23	A	1533	A
23	A	1534	G
23	A	1536	C
23	A	1537	A
23	A	1550	G
23	A	1551	U
23	A	1552	U
23	A	1553	A
23	A	1555	G
23	A	1559	G
23	A	1561	G
23	A	1568	U
23	A	1570	G
23	A	1576	A

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Mol	Chain	Res	Type
23	A	1577	G
23	A	1578	A
23	A	1579	C
23	A	1580	A
23	A	1582	U
23	A	1583	G
23	A	1584	A
23	A	1586	U
23	A	1587	C
23	A	1590	C
23	A	1592	A
23	A	1593	G
23	A	1594	U
23	A	1605	A
23	A	1606	C
23	A	1614	A
23	A	1616	A
23	A	1625	U
23	A	1630	A
23	A	1631	G
23	A	1632	A
23	A	1633	A
23	A	1635	A
23	A	1636	U
23	A	1651	C
23	A	1652	A
23	A	1653	A
23	A	1655	C
23	A	1659	C
23	A	1660	A
23	A	1661	C
23	A	1662	A
23	A	1670	A
23	A	1678	A
23	A	1690	A
23	A	1691	G
23	A	1692	C
23	A	1697	G
23	A	1698	A
23	A	1704	C
23	A	1709	A
23	A	1717	G

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Mol	Chain	Res	Type
23	A	1718	G
23	A	1722	A
23	A	1738	C
23	A	1739	G
23	A	1742	A
23	A	1743	G
23	A	1751	G
23	A	1759	G
23	A	1768	C
23	A	1772	G
23	A	1784	U
23	A	1785	G
23	A	1790	G
23	A	1791	G
23	A	1800	A
23	A	1801	C
23	A	1808	U
23	A	1811	A
23	A	1827	C
23	A	1828	U
23	A	1829	A
23	A	1835	U
23	A	1836	A
23	A	1842	A
23	A	1843	U
23	A	1844	G
23	A	1846	A
23	A	1855	G
23	A	1856	A
23	A	1857	C
23	A	1885	G
23	A	1891	U
23	A	1893	A
23	A	1897	U
23	A	1898	C
23	A	1900	G
23	A	1902	G
23	A	1908	A
23	A	1930	G
23	A	1933	G
23	A	1939	A
23	A	1943	A

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Mol	Chain	Res	Type
23	A	1949	G
23	A	1952	C
23	A	1954	A
23	A	1956	G
23	A	1957	G
23	A	1958	U
23	A	1965	A
23	A	1967	U
23	A	1970	U
23	A	1979	A
23	A	1982	U
23	A	1989	C
23	A	1992	C
23	A	1993	A
23	A	1994	C
23	A	1997	A
23	A	1998	A
23	A	1999	G
23	A	2009	U
23	A	2018	U
23	A	2020	U
23	A	2023	C
23	A	2040	A
23	A	2047	A
23	A	2057	A
23	A	2058	A
23	A	2059	G
23	A	2060	A
23	A	2061	U
23	A	2063	C
23	A	2070	C
23	A	2073	G
23	A	2082	C
23	A	2083	G
23	A	2086	A
23	A	2087	A
23	A	2088	G
23	A	2089	A
23	A	2096	G
23	A	2103	U
23	A	2104	A
23	A	2107	G

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Mol	Chain	Res	Type
23	A	2120	G
23	A	2133	G
23	A	2135	U
23	A	2138	U
23	A	2139	A
23	A	2140	C
23	A	2141	A
23	A	2143	G
23	A	2144	A
23	A	2145	U
23	A	2146	A
23	A	2147	G
23	A	2148	G
23	A	2153	A
23	A	2155	C
23	A	2159	U
23	A	2160	G
23	A	2162	A
23	A	2163	A
23	A	2170	C
23	A	2172	C
23	A	2173	U
23	A	2175	G
23	A	2176	C
23	A	2178	U
23	A	2180	C
23	A	2184	G
23	A	2185	A
23	A	2188	C
23	A	2191	U
23	A	2193	G
23	A	2194	U
23	A	2195	G
23	A	2197	G
23	A	2200	A
23	A	2203	A
23	A	2206	C
23	A	2208	A
23	A	2209	G
23	A	2217	G
23	A	2221	U
23	A	2225	A

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Mol	Chain	Res	Type
23	A	2226	A
23	A	2230	G
23	A	2231	C
23	A	2240	U
23	A	2241	C
23	A	2252	A
23	A	2254	A
23	A	2265	G
23	A	2266	G
23	A	2270	U
23	A	2286	G
23	A	2290	C
23	A	2293	A
23	A	2294	A
23	A	2295	A
23	A	2305	A
23	A	2310	C
23	A	2314	A
23	A	2326	G
23	A	2331	G
23	A	2332	U
23	A	2335	G
23	A	2336	A
23	A	2337	A
23	A	2339	U
23	A	2347	A
23	A	2354	A
23	A	2360	A
23	A	2361	U
23	A	2362	A
23	A	2372	G
23	A	2374	C
23	A	2377	C
23	A	2380	G
23	A	2381	A
23	A	2402	G
23	A	2410	G
23	A	2412	C
23	A	2417	U
23	A	2418	G
23	A	2419	A
23	A	2429	U

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Mol	Chain	Res	Type
23	A	2430	C
23	A	2433	C
23	A	2447	C
23	A	2450	U
23	A	2451	C
23	A	2452	A
23	A	2454	C
23	A	2455	G
23	A	2456	G
23	A	2457	A
23	A	2458	U
23	A	2461	A
23	A	2462	A
23	A	2467	C
23	A	2468	C
23	A	2472	G
23	A	2475	A
23	A	2486	A
23	A	2492	C
23	A	2495	A
23	A	2496	A
23	A	2502	C
23	A	2505	A
23	A	2511	G
23	A	2516	G
23	A	2518	U
23	A	2525	C
23	A	2529	G
23	A	2530	A
23	A	2531	U
23	A	2532	G
23	A	2533	U
23	A	2545	A
23	A	2546	U
23	A	2547	C
23	A	2552	G
23	A	2561	C
23	A	2576	G
23	A	2579	U
23	A	2583	C
23	A	2589	U
23	A	2593	A

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Mol	Chain	Res	Type
23	A	2594	G
23	A	2599	A
23	A	2600	C
23	A	2601	G
23	A	2603	G
23	A	2604	A
23	A	2605	G
23	A	2612	U
23	A	2613	C
23	A	2623	U
23	A	2624	G
23	A	2629	A
23	A	2630	G
23	A	2636	U
23	A	2637	C
23	A	2638	C
23	A	2640	U
23	A	2641	A
23	A	2657	G
23	A	2667	G
23	A	2668	A
23	A	2681	A
23	A	2683	U
23	A	2688	G
23	A	2690	G
23	A	2704	A
23	A	2708	C
23	A	2716	U
23	A	2717	A
23	A	2739	U
23	A	2741	G
23	A	2753	U
23	A	2756	G
23	A	2760	A
23	A	2771	G
23	A	2775	A
23	A	2777	A
23	A	2778	G
23	A	2791	A
23	A	2792	A
23	A	2793	G
23	A	2794	C

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Mol	Chain	Res	Type
23	A	2798	C
23	A	2803	A
23	A	2805	A
23	A	2806	U
23	A	2807	G
23	A	2817	A
23	A	2820	U
23	A	2821	U
23	A	2822	C
23	A	2823	G
23	A	2824	G
23	A	2827	A
23	A	2828	U
23	A	2838	C
23	A	2840	A
23	A	2850	G
23	A	2853	U
23	A	2868	G
23	A	2869	G
23	A	2880	A
23	A	2881	C
23	A	2886	G
23	A	2887	G
23	A	2892	G
23	A	2896	A
23	A	2899	A
23	A	2900	C
23	A	2903	A
23	A	2906	G
23	A	2911	A
23	A	2913	G
23	A	2920	U
24	B	8	A
24	B	10	U
24	B	13	A
24	B	23	U
24	B	24	C
24	B	33	U
24	B	35	C
24	B	38	U
24	B	39	G
24	B	40	C

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Mol	Chain	Res	Type
24	B	42	G
24	B	49	G
24	B	51	A
24	B	55	A
24	B	60	C
24	B	67	G
24	B	84	U
24	B	87	G
24	B	88	U
24	B	92	G
24	B	93	C
24	B	106	U
24	B	113	G

All (13) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
23	A	162	A
23	A	179	A
23	A	311	U
23	A	437	A
23	A	593	U
23	A	863	G
23	A	961	G
23	A	2039	G
23	A	2360	A
23	A	2418	G
23	A	2432	G
23	A	2467	C
23	A	2501	U

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
23	A	1
42	Y	1
25	D	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	1569:G	O3'	1570:G	P	3.00
1	Y	25:GLY	C	26:LYS	N	1.74
1	D	5:TYR	C	6:LYS	N	1.17

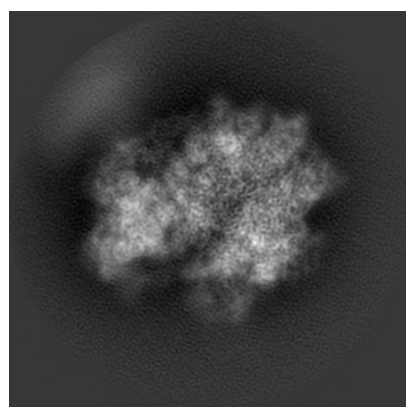
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-3625. These allow visual inspection of the internal detail of the map and identification of artifacts.

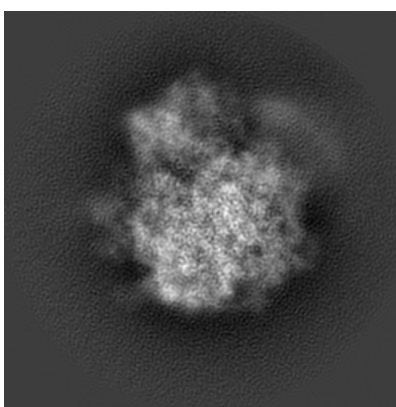
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

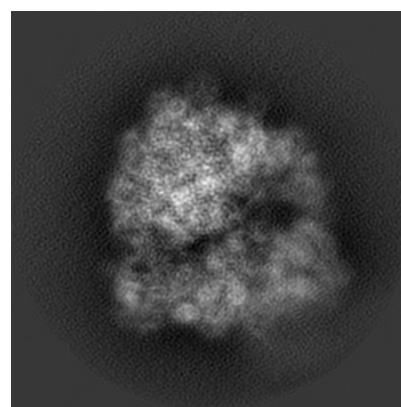
6.1.1 Primary map



X



Y

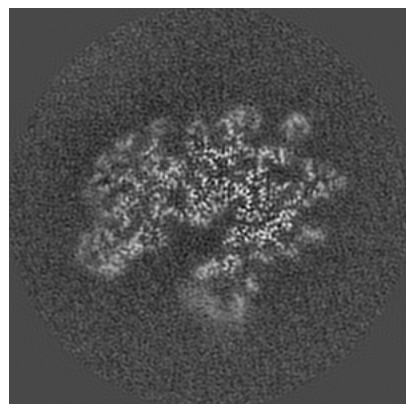


Z

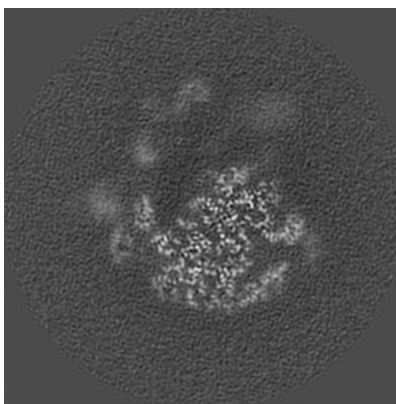
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

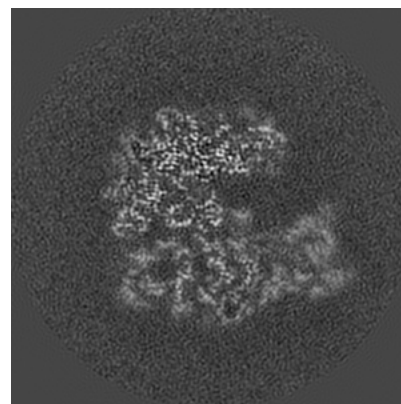
6.2.1 Primary map



X Index: 170



Y Index: 170

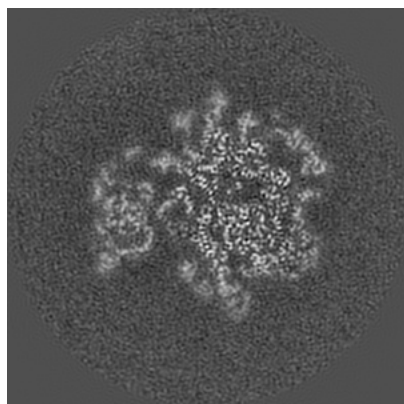


Z Index: 170

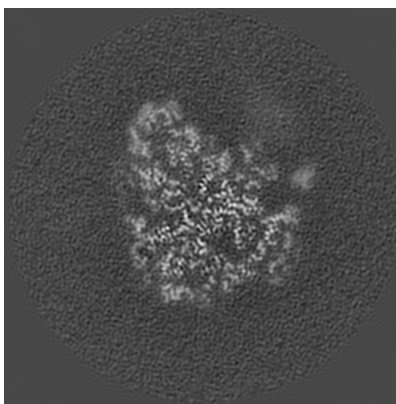
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

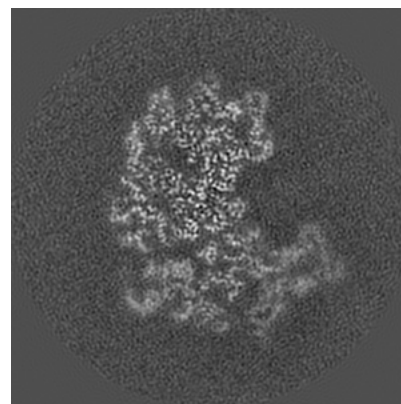
6.3.1 Primary map



X Index: 144



Y Index: 212

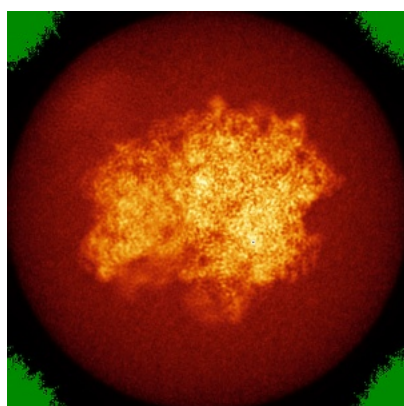


Z Index: 187

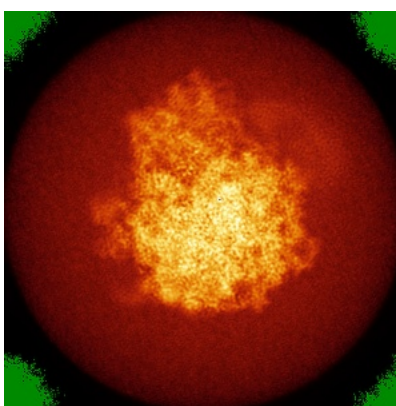
The images above show the largest variance slices of the map in three orthogonal directions.

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

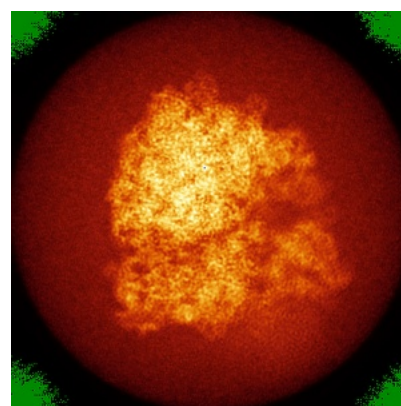
6.4.1 Primary map



X



Y

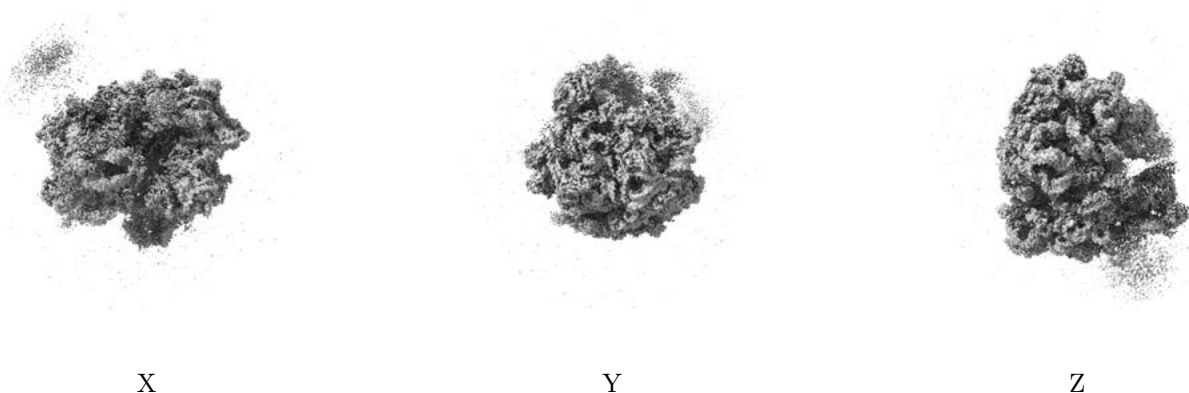


Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.05. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

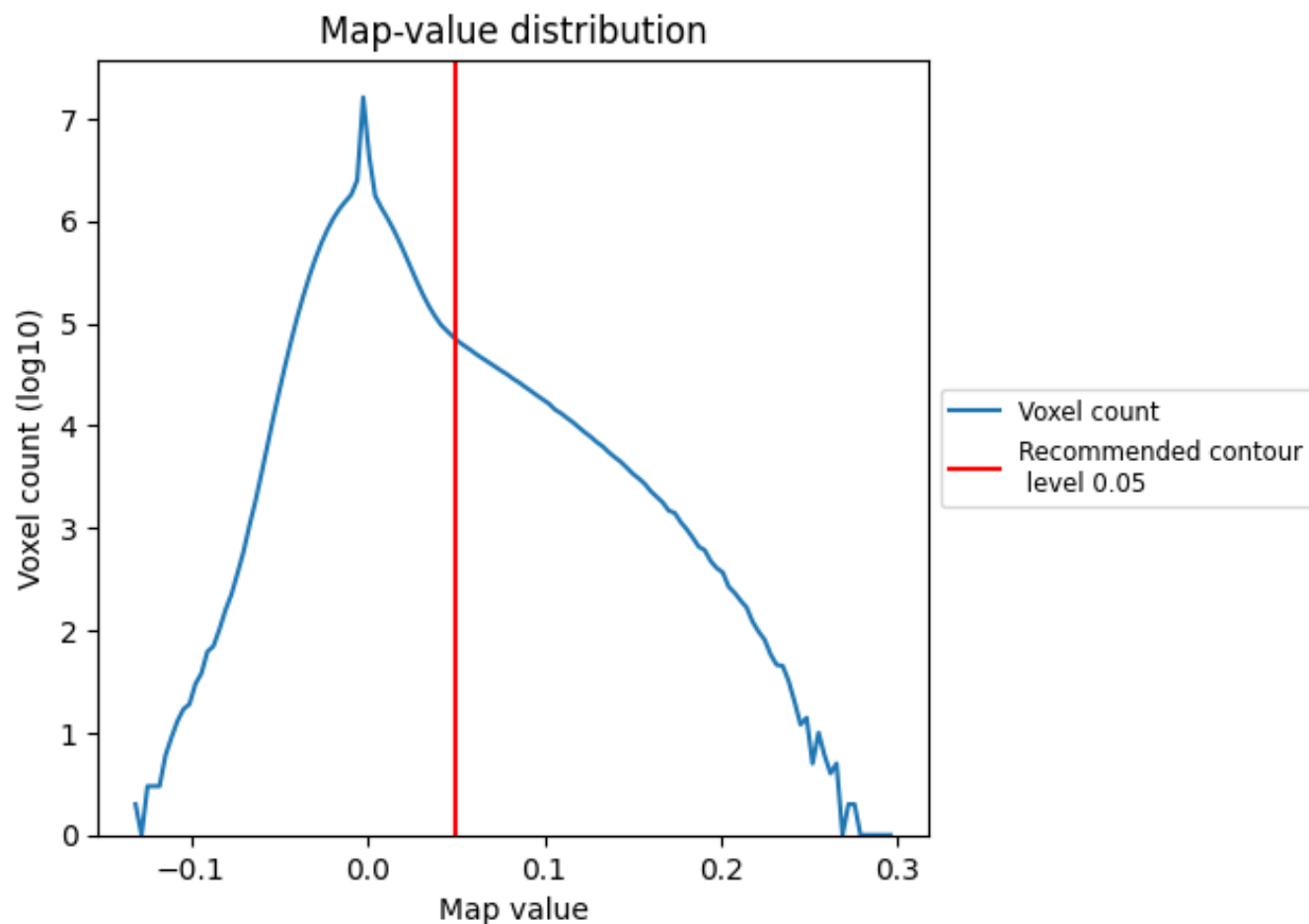
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

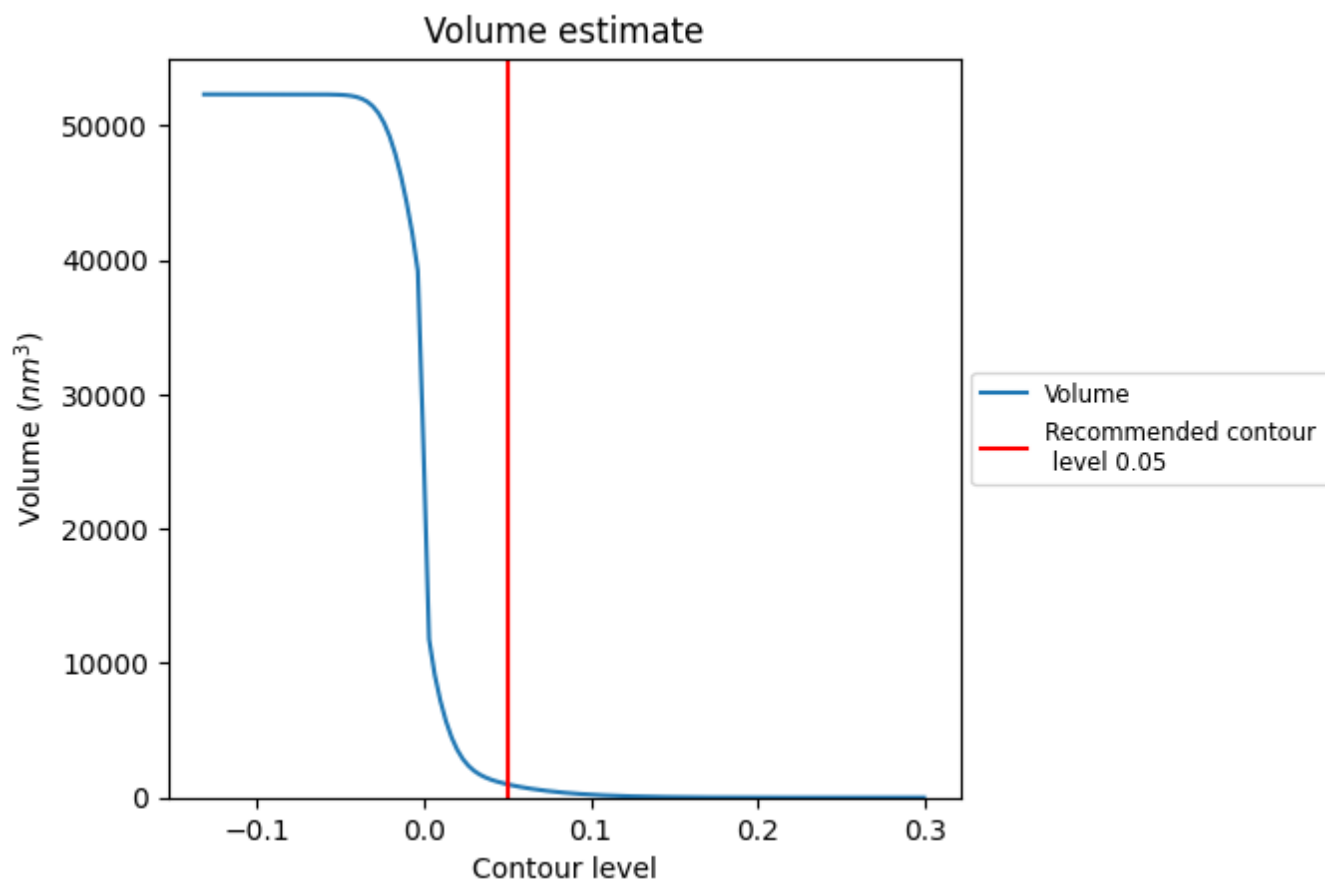
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

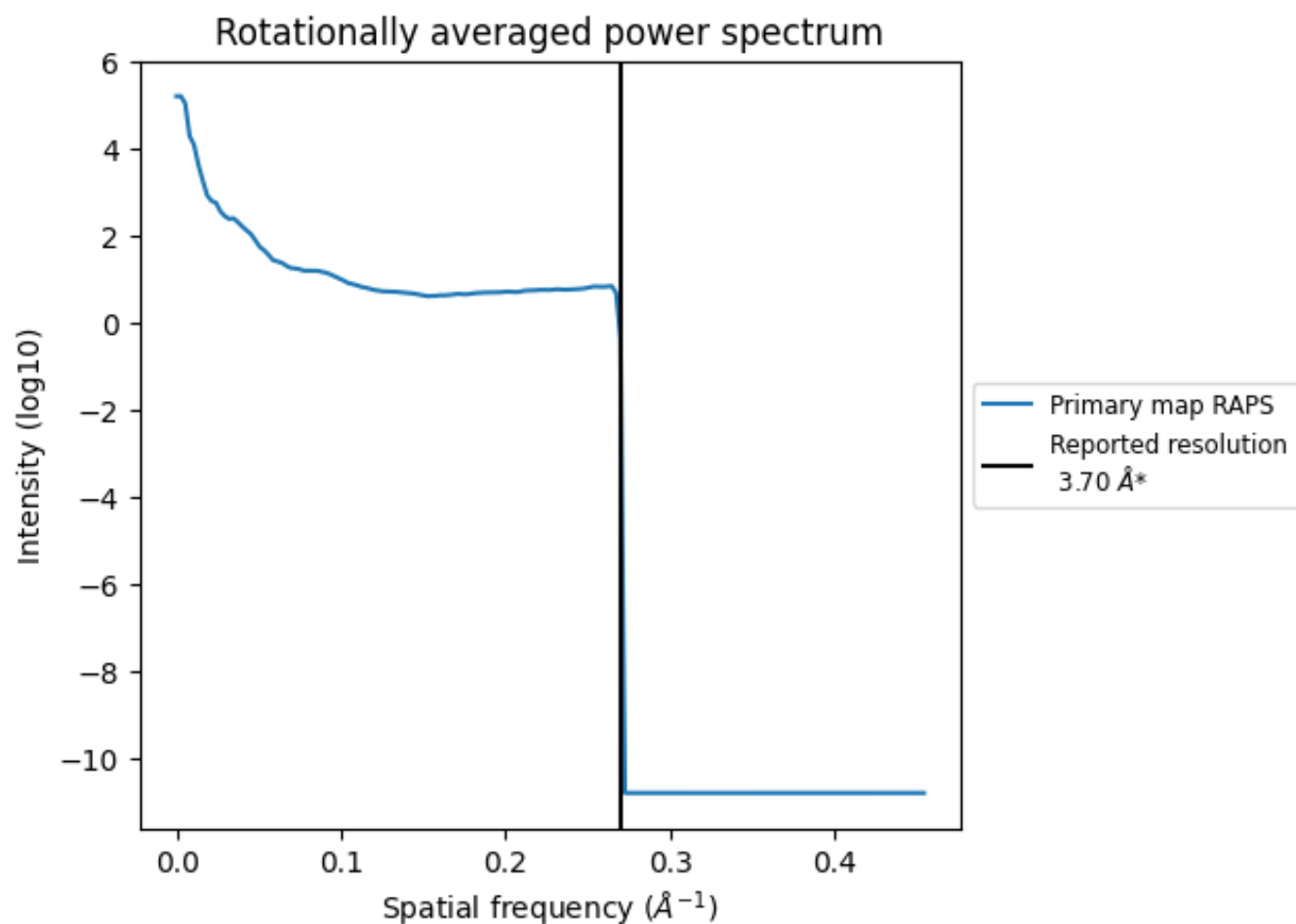
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 989 nm³; this corresponds to an approximate mass of 894 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 0.270 Å⁻¹

8 Fourier-Shell correlation

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

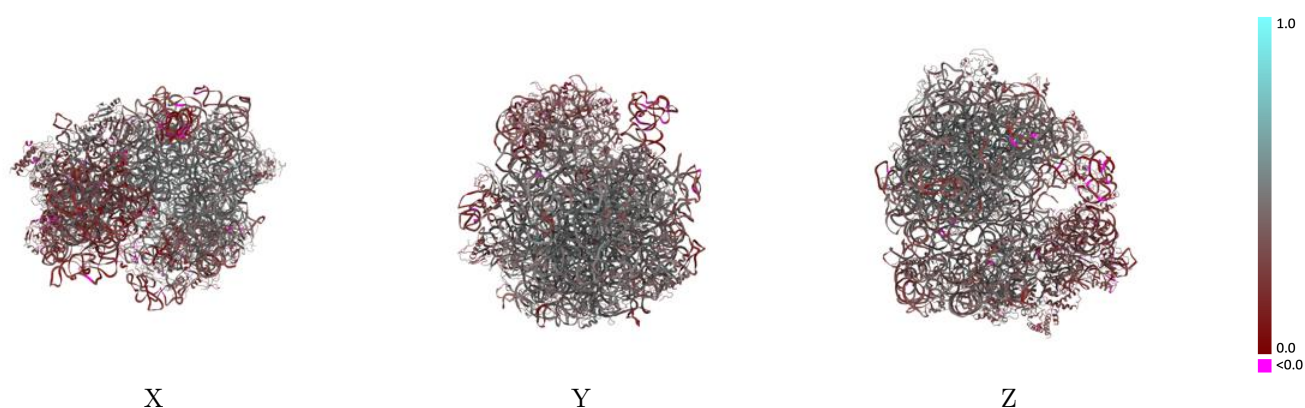
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-3625 and PDB model 5ND9. Per-residue inclusion information can be found in section 3 on page 13.

9.1 Map-model overlay [i](#)

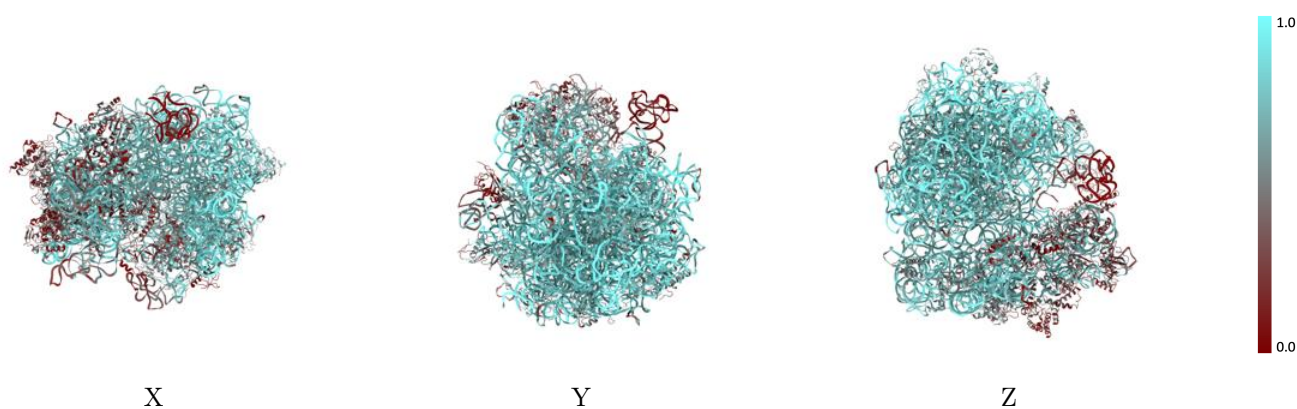
This section was not generated.

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



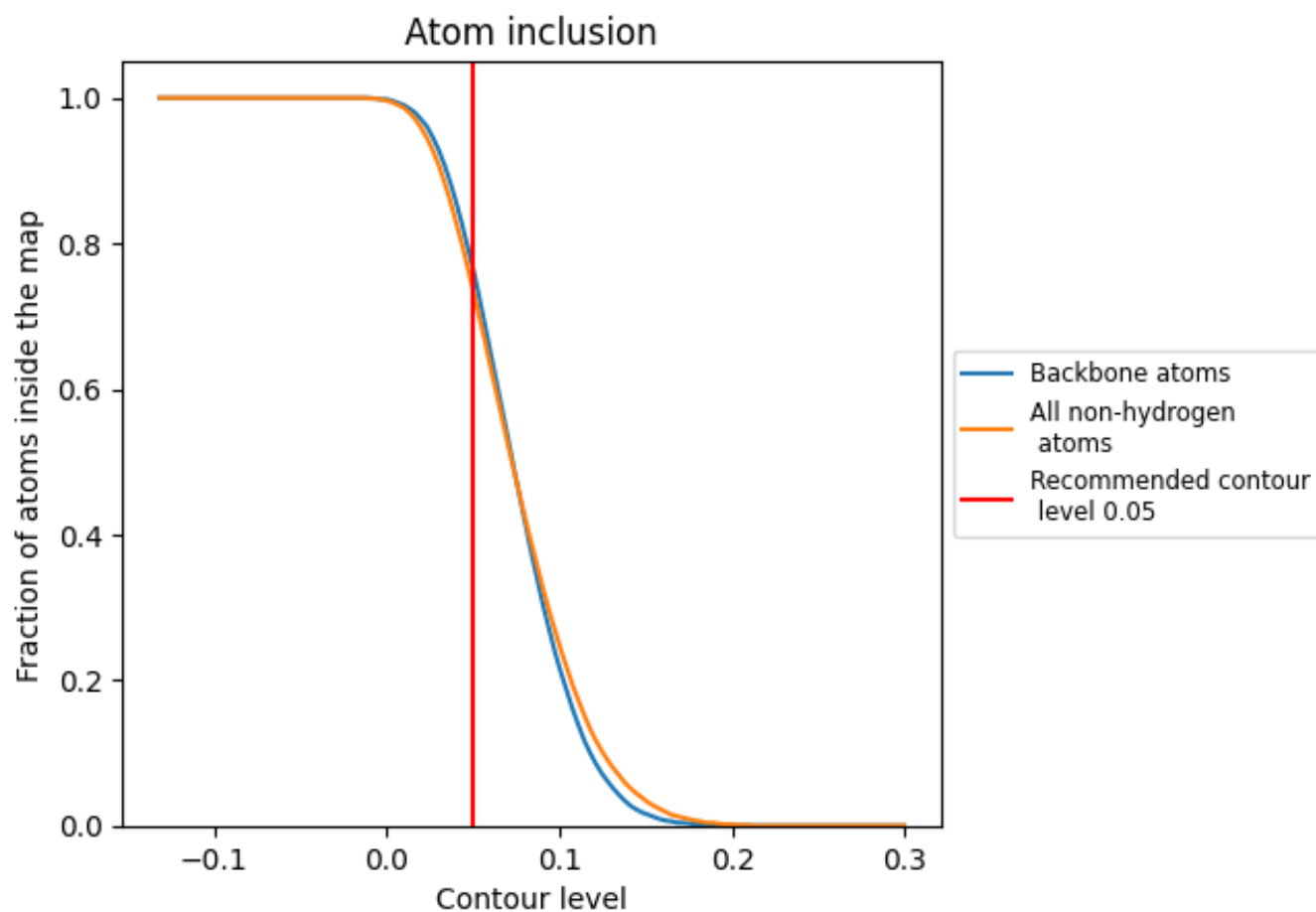
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.05).

9.4 Atom inclusion [i](#)



At the recommended contour level, 76% of all backbone atoms, 74% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.05) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7350	 0.3860
0	 0.5850	 0.4000
1	 0.5920	 0.3850
2	 0.6740	 0.4350
3	 0.1660	 0.2440
4	 0.5710	 0.4250
5	 0.1620	 0.3020
6	 0.7330	 0.4740
7	 0.6950	 0.4180
8	 0.6320	 0.4370
A	 0.8540	 0.4220
B	 0.8740	 0.3600
D	 0.7000	 0.4740
E	 0.6910	 0.4530
F	 0.6750	 0.4230
G	 0.3560	 0.2770
H	 0.5150	 0.3260
M	 0.7040	 0.4470
N	 0.5960	 0.4550
O	 0.6870	 0.4070
P	 0.6640	 0.4230
Q	 0.6610	 0.4210
R	 0.5610	 0.3230
S	 0.6390	 0.4320
T	 0.7330	 0.4450
U	 0.6520	 0.4290
V	 0.6830	 0.4580
W	 0.6150	 0.4130
X	 0.5830	 0.3730
Y	 0.1210	 0.3050
Z	 0.7200	 0.4400
a	 0.8050	 0.3510
b	 0.2800	 0.3130
c	 0.2190	 0.2750
d	 0.4100	 0.2760



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Chain	Atom inclusion	Q-score
e	 0.4340	 0.3600
f	 0.3650	 0.3660
g	 0.2340	 0.2470
h	 0.5300	 0.3770
i	 0.2430	 0.2360
j	 0.2080	 0.2290
k	 0.4840	 0.3560
l	 0.5710	 0.3890
m	 0.2000	 0.2280
n	 0.3220	 0.2550
o	 0.5420	 0.3410
p	 0.6010	 0.3850
q	 0.5240	 0.3650
r	 0.4320	 0.3540
s	 0.2570	 0.1900
t	 0.5400	 0.3160
u	 0.0800	 0.2820
v	 0.1950	 0.2990