



Full wwPDB EM Validation Report ⓘ

May 14, 2025 – 06:11 AM EDT

PDB ID : 5TCU / pdb_00005tcu
EMDB ID : EMD-8402
Title : Methicillin sensitive Staphylococcus aureus 70S ribosome
Authors : Eyal, Z.; Ahmed, T.; Belousoff, N.; Mishra, S.; Matzov, D.; Bashan, A.; Zimmermann, E.; Lithgow, T.; Bhushan, S.; Yonath, A.
Deposited on : 2016-09-15
Resolution : 3.90 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.dev118
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0rc1
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.43.1

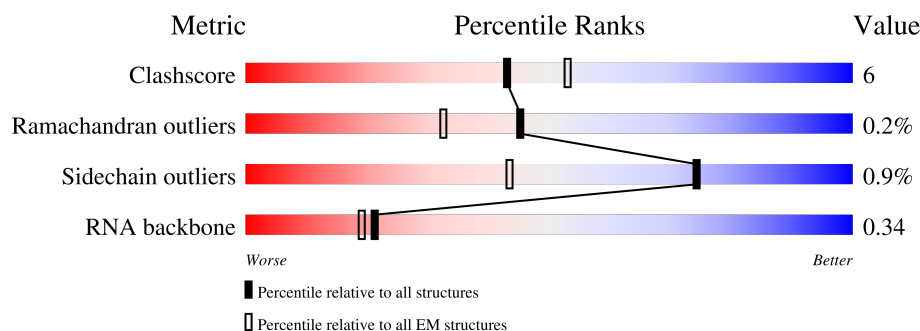
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.90 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)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415
RNA backbone	6643	2191

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	1555	<div> <div>5%</div> <div>43%</div> <div>41%</div> <div>11%</div> <div>6%</div> </div>
2	SB	202	<div> <div>44%</div> <div>77%</div> <div>23%</div> </div>
3	SC	198	<div> <div>40%</div> <div>92%</div> <div>8%</div> </div>
4	SD	156	<div> <div>9%</div> <div>81%</div> <div>19%</div> </div>
5	SE	95	<div> <div>22%</div> <div>75%</div> <div>25%</div> </div>
6	SG	155	<div> <div>50%</div> <div>83%</div> <div>17%</div> </div>
7	SF	130	<div> <div>13%</div> <div>72%</div> <div>28%</div> </div>



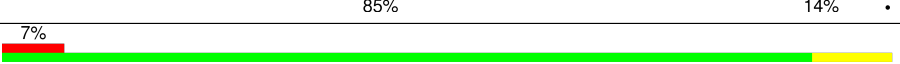
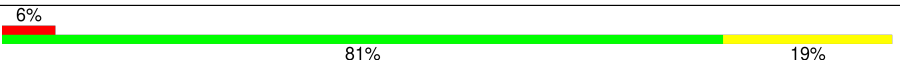


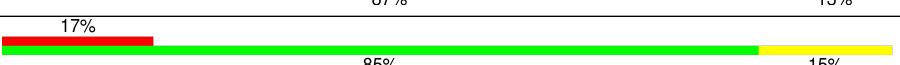
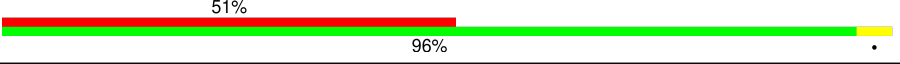
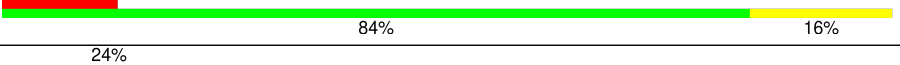

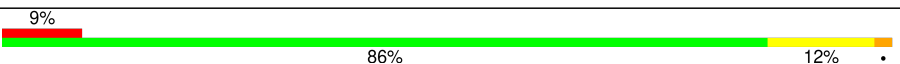
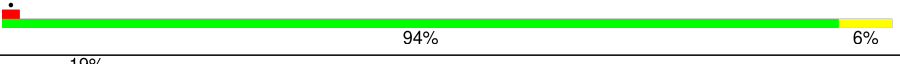

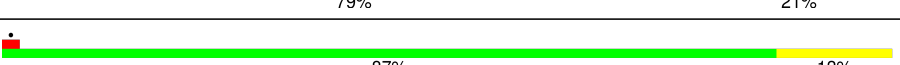

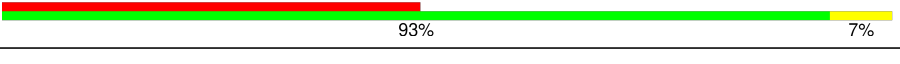




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Mol	Chain	Length	Quality of chain
8	SH	127	
9	S1	80	
10	S2	114	
11	S3	136	
12	S4	113	
13	S5	60	
14	S6	88	
15	S7	83	
16	S8	80	
17	S9	56	
18	SI	78	
19	SA	79	
20	X	13	
21	E	75	
22	D	76	
23	B	2923	
24	C	114	
25	L2	274	
26	LC	215	
27	LJ	205	
28	LK	166	
29	LL	174	
30	LM	145	
31	LN	122	
32	LO	145	

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Mol	Chain	Length	Quality of chain
33	LP	136	
34	LQ	119	
35	LR	113	
36	L1	109	
37	L3	116	
38	L4	102	
39	L5	112	
40	L6	89	
41	L7	103	
42	L8	93	
43	L9	82	
44	LA	58	
45	LB	62	
46	LD	57	
47	LE	47	
48	LS	47	
49	LG	43	
50	LH	60	
51	LI	37	
52	LF	74	

2 Entry composition

There are 54 unique types of molecules in this entry. The entry contains 133876 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 rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1464	Total	C	N	O	P	0	0
			31369	14007	5741	10159	1462		

- Molecule 2 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	SB	202	Total	C	N	O	S	0	0
			1551	979	293	278	1		

- Molecule 3 is a protein called 30S ribosomal protein S4.

Mol	Chain	Residues	Atoms				AltConf	Trace
3	SC	198	Total	C	N	O	0	0
			1058	634	211	213		

- Molecule 4 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	SD	156	Total	C	N	O	S	0	0
			1153	727	211	213	2		

- Molecule 5 is a protein called 30S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	SE	95	Total	C	N	O	S	0	0
			785	496	138	149	2		

- Molecule 6 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	SG	155	Total	C	N	O	S	0	0
			1164	724	220	217	3		

- Molecule 7 is a protein called 30S ribosomal protein S8.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	SF	130	Total	C	N	O	S	0	0
			1007	639	180	184	4		

- Molecule 8 is a protein called 30S ribosomal protein S9.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	SH	127	Total	C	N	O	S	0	0
			975	605	194	175	1		

- Molecule 9 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms				AltConf	Trace
9	S1	80	Total	C	N	O	0	0
			626	394	116	116		

- Molecule 10 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	S2	114	Total	C	N	O	S	0	0
			826	507	158	159	2		

- Molecule 11 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	S3	136	Total	C	N	O	S	0	0
			976	611	190	173	2		

- Molecule 12 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	S4	113	Total	C	N	O	S	0	0
			828	510	168	149	1		

- Molecule 13 is a protein called 30S ribosomal protein S14 type Z.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	S5	60	Total	C	N	O	S	0	0
			497	314	99	79	5		

- Molecule 14 is a protein called 30S ribosomal protein S15.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	S6	88	Total	C	N	O	S	0	0
			713	441	148	123	1		

- Molecule 15 is a protein called 30S ribosomal protein S16.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	S7	83	Total	C	N	O	S	0	0
			537	335	105	96	1		

- Molecule 16 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms				AltConf	Trace
16	S8	80	Total	C	N	O	0	0
			520	327	97	96		

- Molecule 17 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	S9	56	Total	C	N	O	S	0	0
			458	292	88	76	2		

- Molecule 18 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	SI	78	Total	C	N	O	S	0	0
			541	340	104	96	1		

- Molecule 19 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	SA	78	Total	C	N	O	S	0	0
			503	303	100	99	1		

- Molecule 20 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	X	10	Total	C	N	O	P	0	0
			213	96	39	68	10		

- Molecule 21 is a RNA chain called P-site tRNA CHAIN.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	E	75	Total	C	N	O	P	0	0
			1600	713	285	527	75		

- Molecule 22 is a RNA chain called E-site tRNA CHAIN.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	D	76	Total	C	N	O	P	0	0
			1619	723	290	531	75		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
23	B	2755	Total	C	N	O	P	0	0
			59059	26368	10814	19122	2755		

- Molecule 24 is a RNA chain called 5S rRNA CHAIN.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	C	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	L2	274	Total	C	N	O	S	0	0
			2066	1288	414	359	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
26	LC	215	Total	C	N	O	S	0	0
			1570	987	295	283	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
27	LJ	205	Total	C	N	O	S	0	0
			1514	953	282	277	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
28	LK	166	Total	C	N	O	S	0	0
			1026	635	185	204	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
29	LL	174	Total	C	N	O	S	0	0
			1062	660	205	195	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
30	LM	145	Total	C	N	O	S	0	0
			1124	703	205	213	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
31	LN	122	Total	C	N	O	S	0	0
			918	572	174	168	4		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
32	LO	145	Total	C	N	O	0	0
			1020	631	207	182		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
33	LP	136	Total	C	N	O	S	0	0
			1043	672	202	165	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
34	LQ	119	Total	C	N	O	S	0	0
			898	551	176	170	1		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
35	LR	113	Total	C	N	O	0	0
			765	474	145	146		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
36	L1	109	Total	C	N	O	0	0
			832	529	169	134		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
37	L3	116	Total	C	N	O	S	0	0
			942	593	189	156	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
38	L4	102	Total	C	N	O	S	0	0
			749	474	140	134	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
39	L5	112	Total	C	N	O	S	0	0
			837	526	163	146	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
40	L6	89	Total	C	N	O	S	0	0
			694	436	126	128	4		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
41	L7	103	Total	C	N	O	0	0
			734	462	137	135		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
42	L8	93	Total	C	N	O	0	0
			648	411	115	122		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
43	L9	82	Total	C	N	O	0	0
			615	382	122	111		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
44	LA	58	Total	C	N	O	0	0
			443	276	96	71		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
45	LB	62	Total	C	N	O	0	0
			493	304	93	96		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
46	LD	57	Total	C	N	O	0	0
			436	272	83	81		

- Molecule 47 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	LE	47	Total	C	N	O	S	0	0
			356	218	77	59	2		

- Molecule 48 is a protein called 50S ribosomal protein L33 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	LS	47	Total	C	N	O	S	0	0
			380	233	75	68	4		

- Molecule 49 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	LG	43	Total	C	N	O	S	0	0
			367	225	89	52	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
50	LH	60	Total	C	N	O	S	0	0
			446	277	92	75	2		

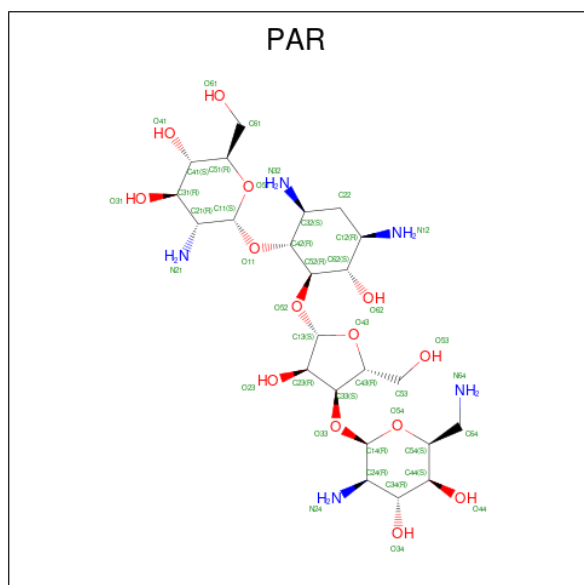
- Molecule 51 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	LI	37	Total	C	N	O	S	0	0
			272	170	57	40	5		

- Molecule 52 is a protein called 50S ribosomal protein L31 type B.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	LF	74	Total	C	N	O	S	0	0
			447	269	86	91	1		

- Molecule 53 is PAROMOMYCIN (CCD ID: PAR) (formula: $C_{23}H_{45}N_5O_{14}$).



Mol	Chain	Residues	Atoms				AltConf
53	A	1	Total	C	N	O	0
			42	23	5	14	

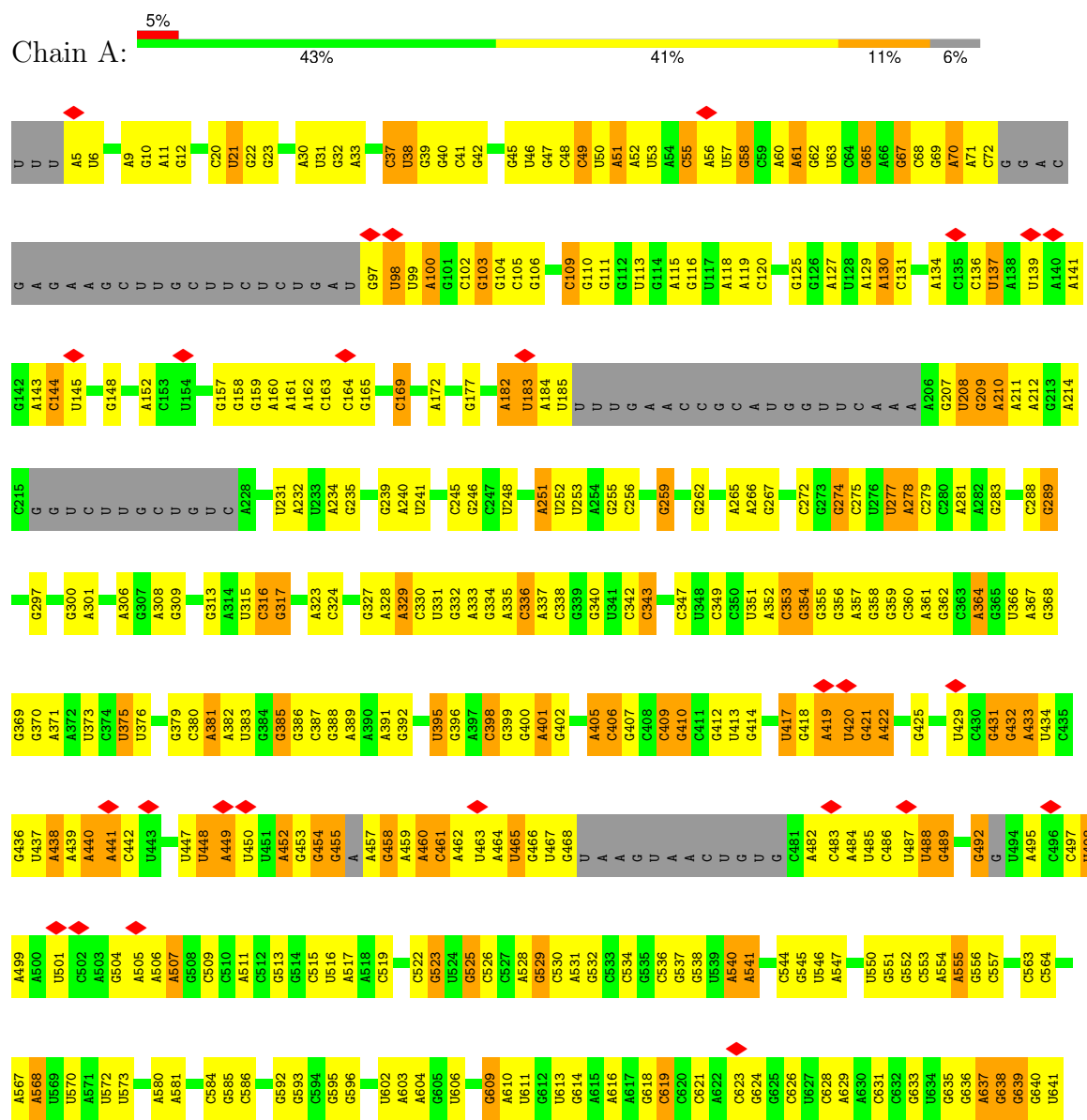
- Molecule 54 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
54	A	27	Total 27	Mg 27	0
54	SG	1	Total 1	Mg 1	0
54	B	99	Total 99	Mg 99	0
54	C	2	Total 2	Mg 2	0

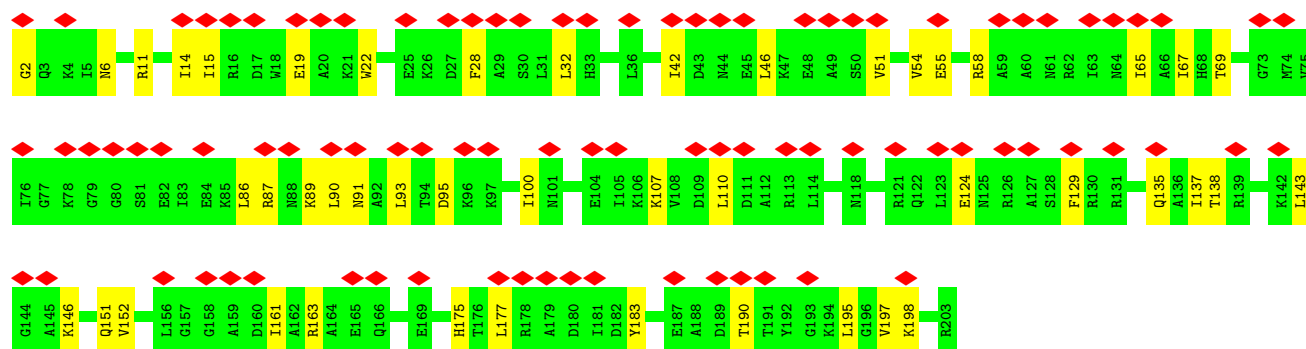
3 Residue-property plots [i](#)

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

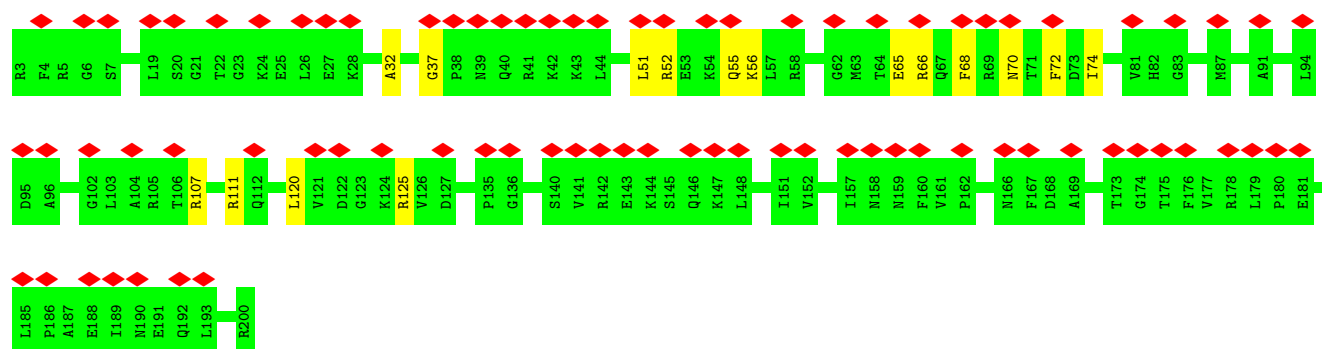
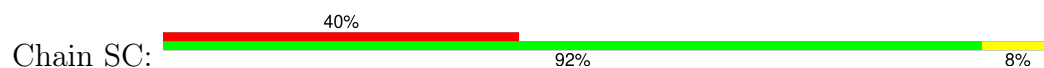
• Molecule 1: 16S rRNA



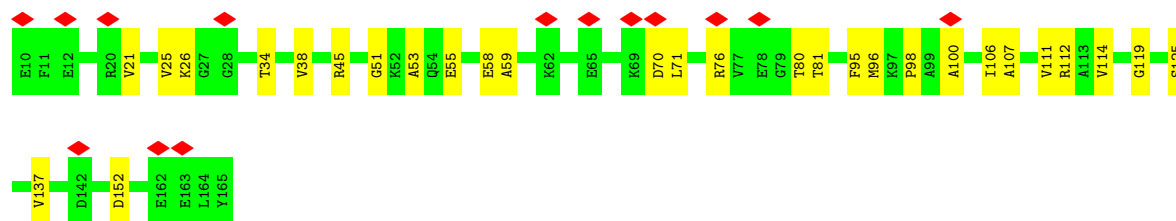
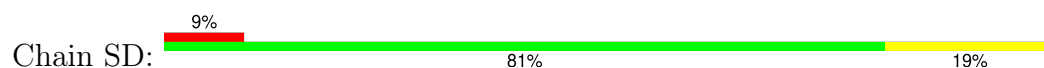




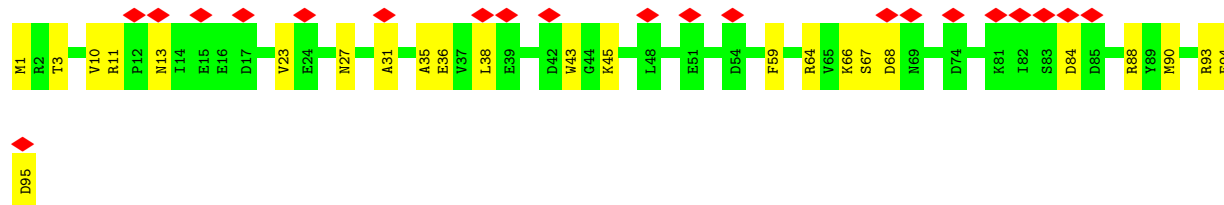
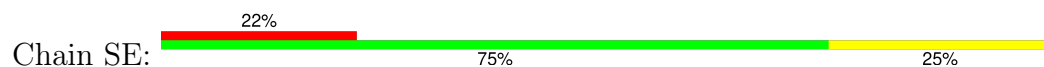
• Molecule 3: 30S ribosomal protein S4



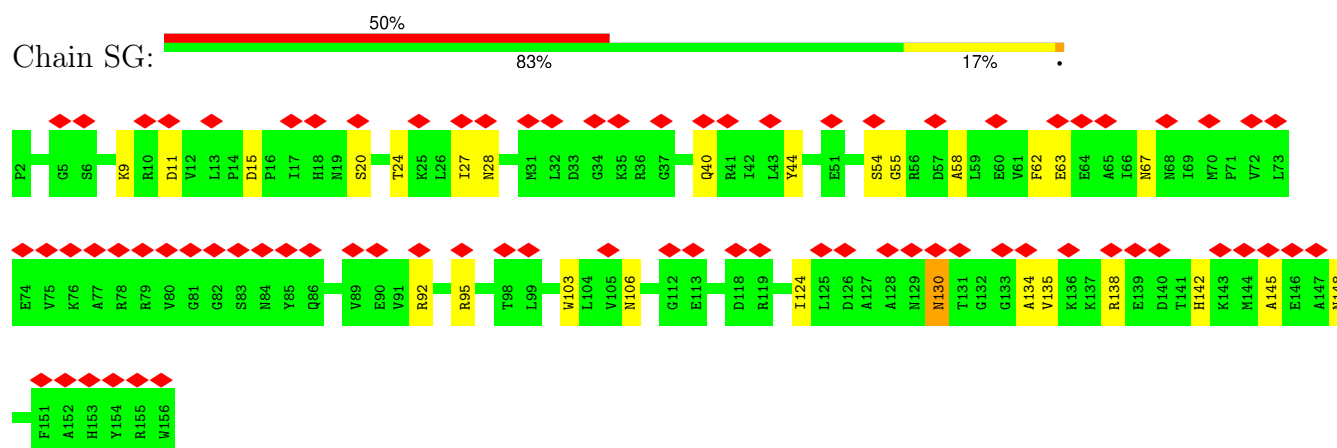
• Molecule 4: 30S ribosomal protein S5



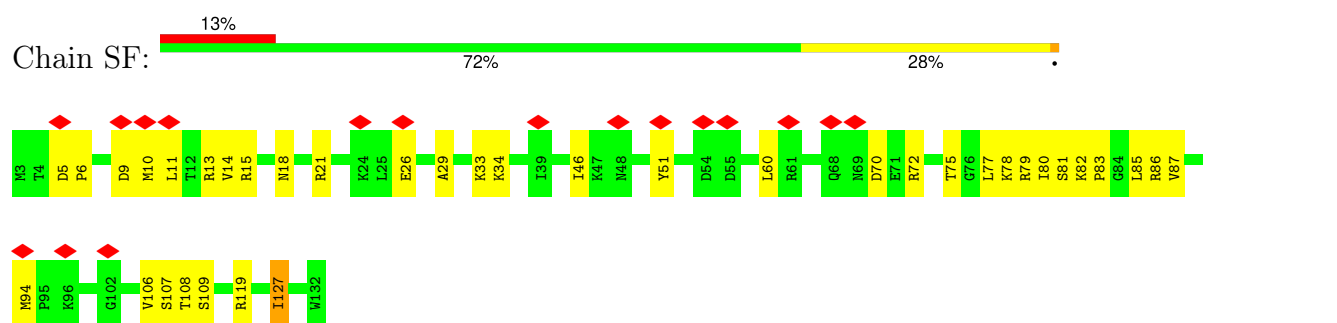
• Molecule 5: 30S ribosomal protein S6



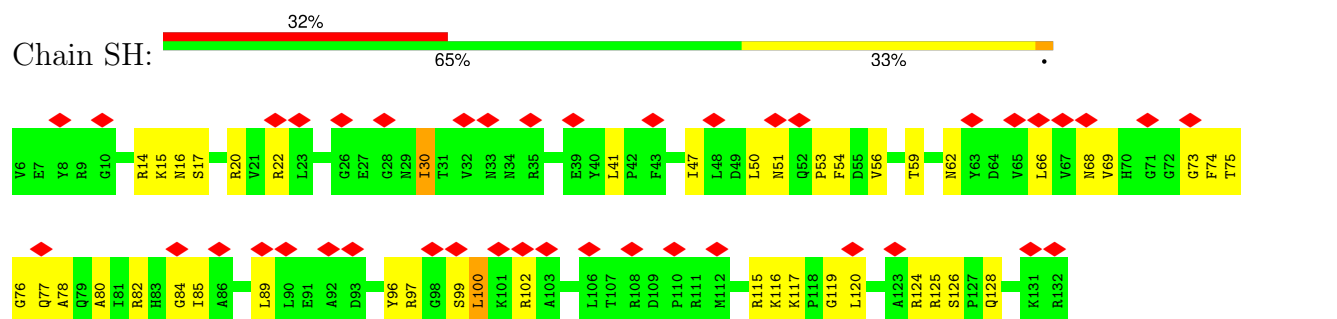
• Molecule 6: 30S ribosomal protein S7



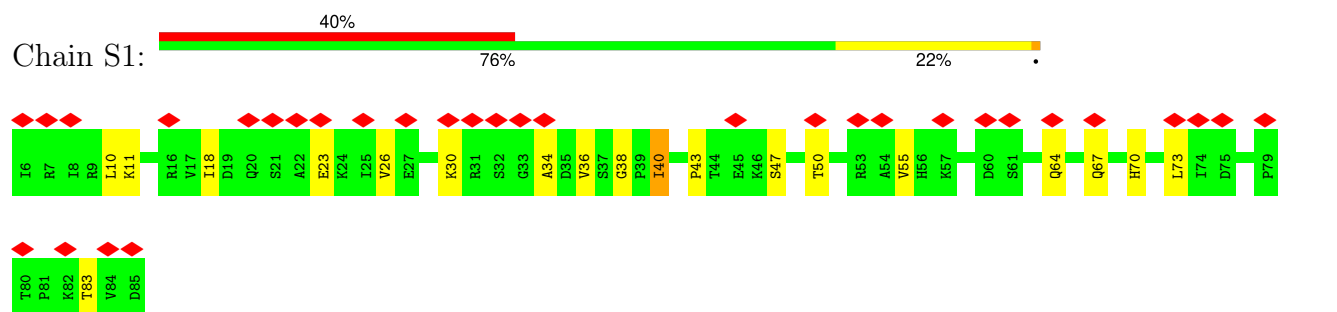
• Molecule 7: 30S ribosomal protein S8



• Molecule 8: 30S ribosomal protein S9

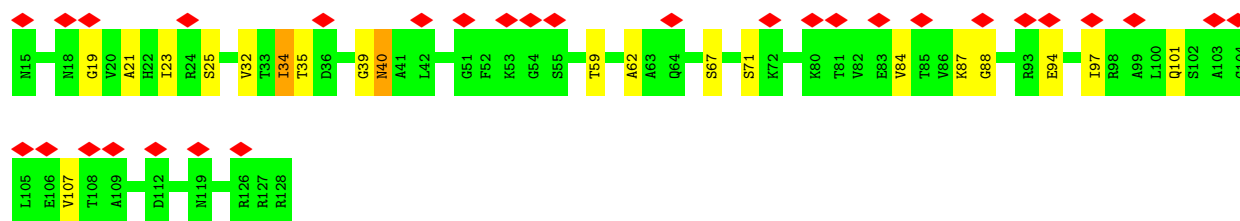


• Molecule 9: 30S ribosomal protein S10

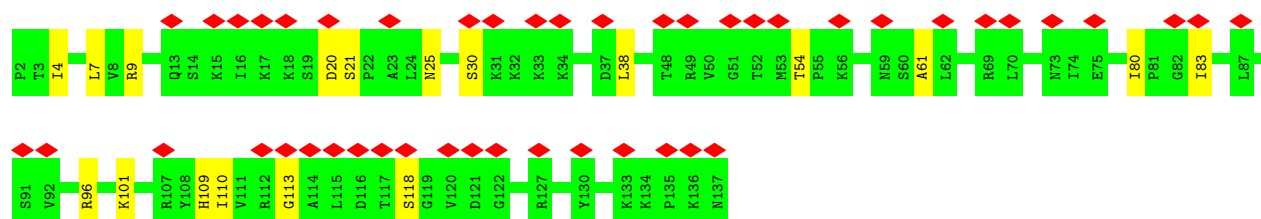
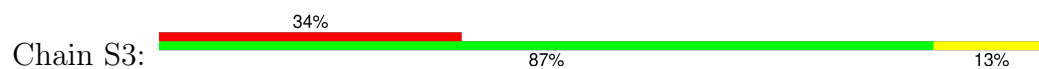


• Molecule 10: 30S ribosomal protein S11

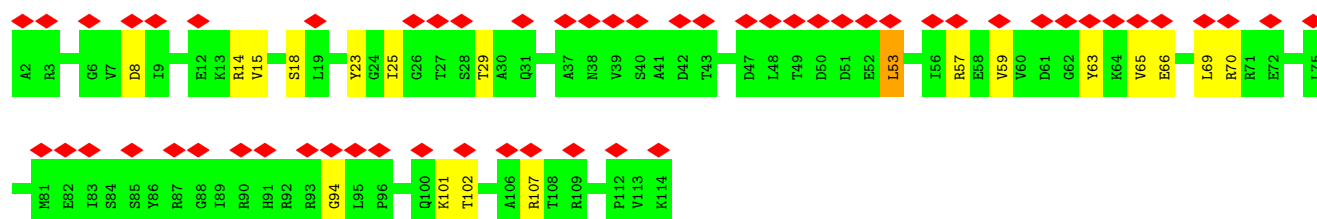
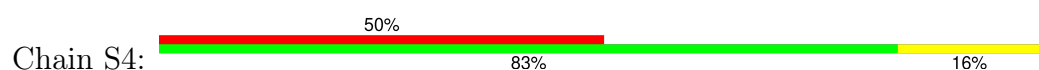




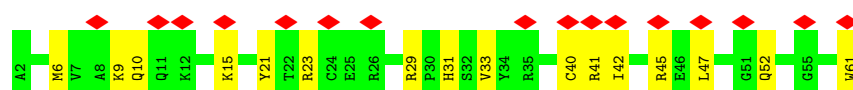
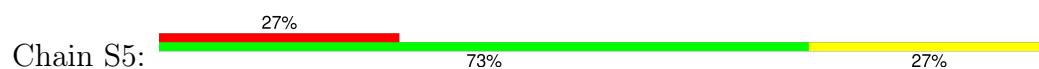
• Molecule 11: 30S ribosomal protein S12



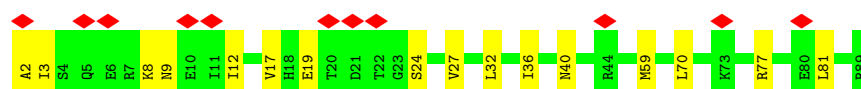
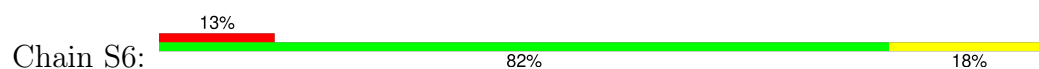
• Molecule 12: 30S ribosomal protein S13



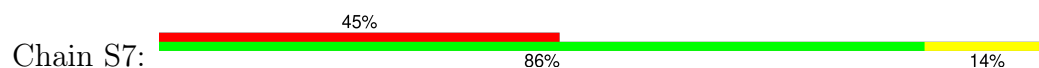
• Molecule 13: 30S ribosomal protein S14 type Z

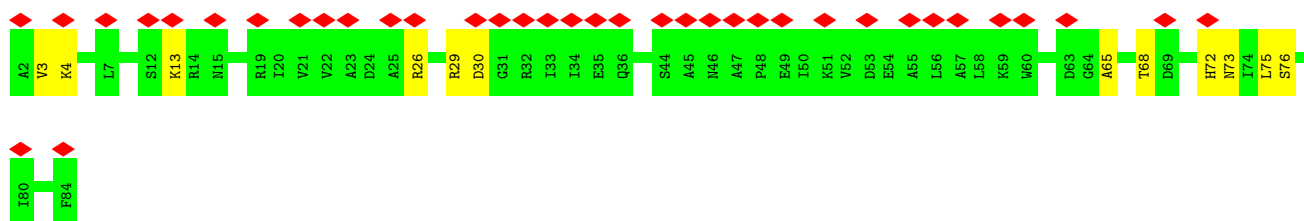


• Molecule 14: 30S ribosomal protein S15

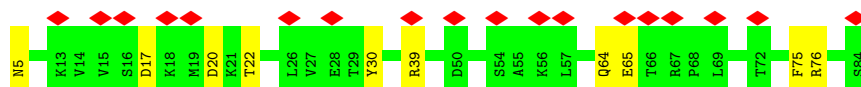
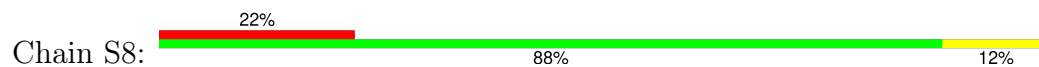


• Molecule 15: 30S ribosomal protein S16

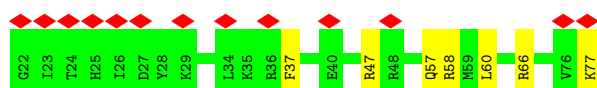
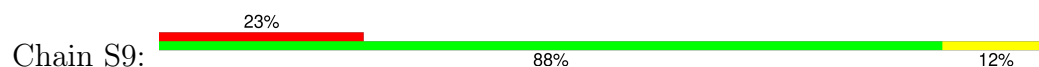




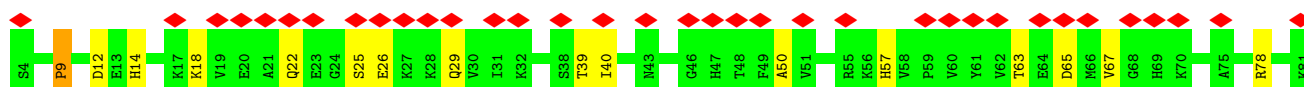
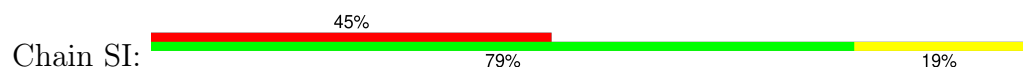
- Molecule 16: 30S ribosomal protein S17



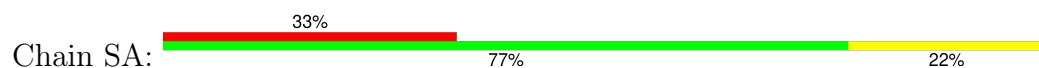
- Molecule 17: 30S ribosomal protein S18



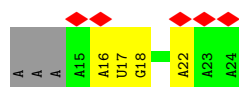
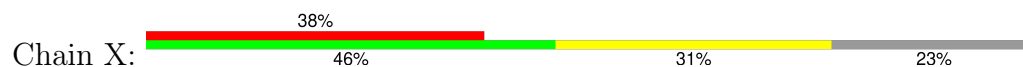
- Molecule 18: 30S ribosomal protein S19



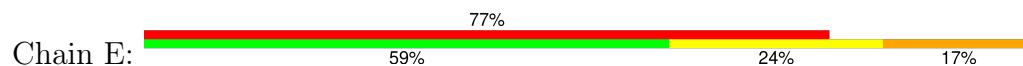
- Molecule 19: 30S ribosomal protein S20

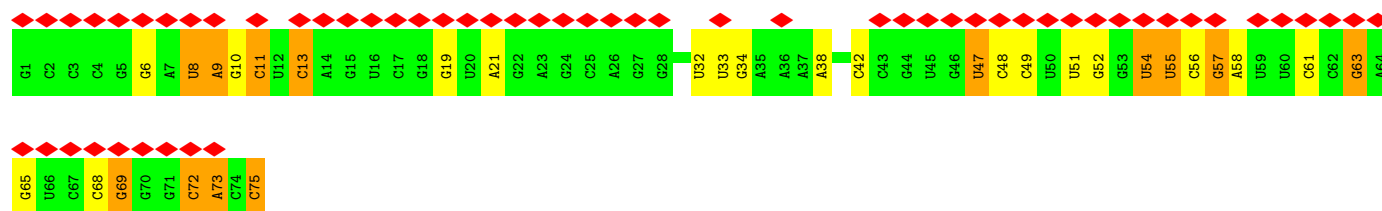


- Molecule 20: mRNA

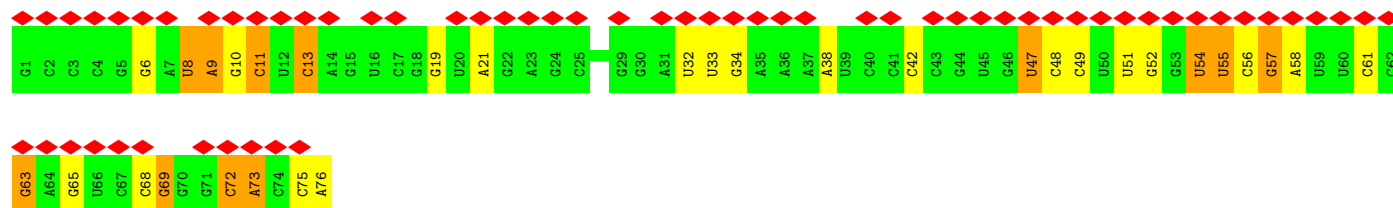
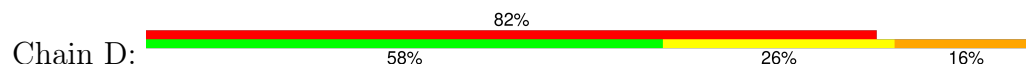


- Molecule 21: P-site tRNA CHAIN

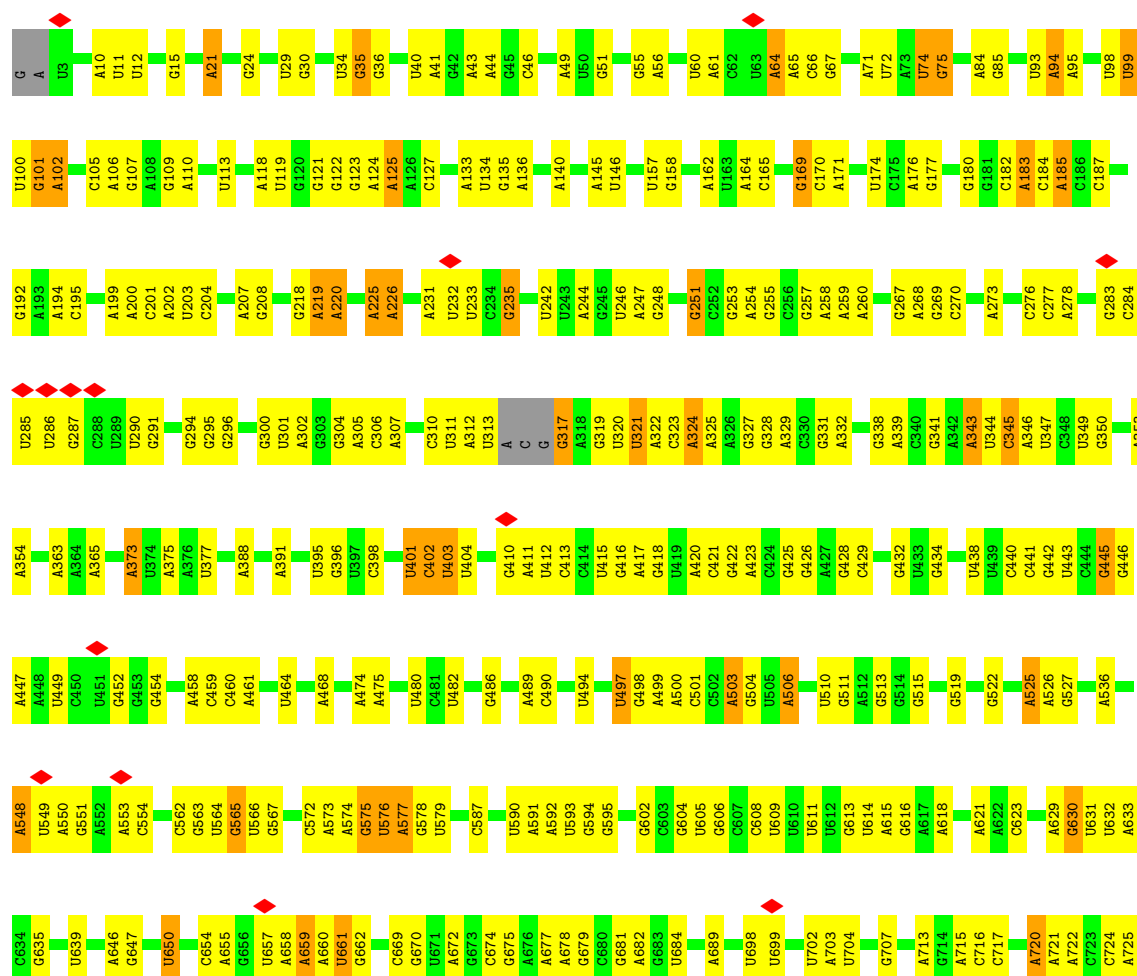


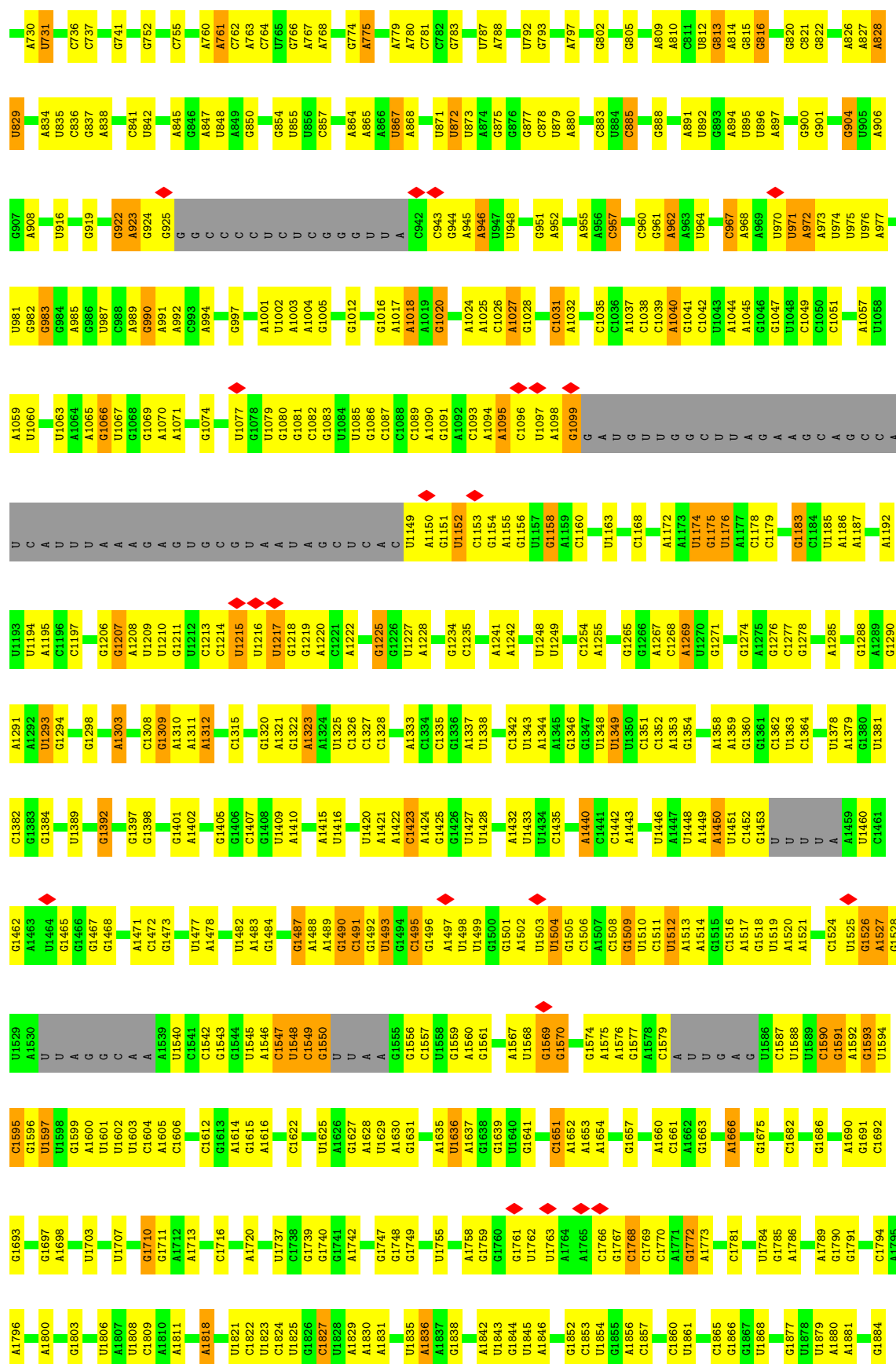


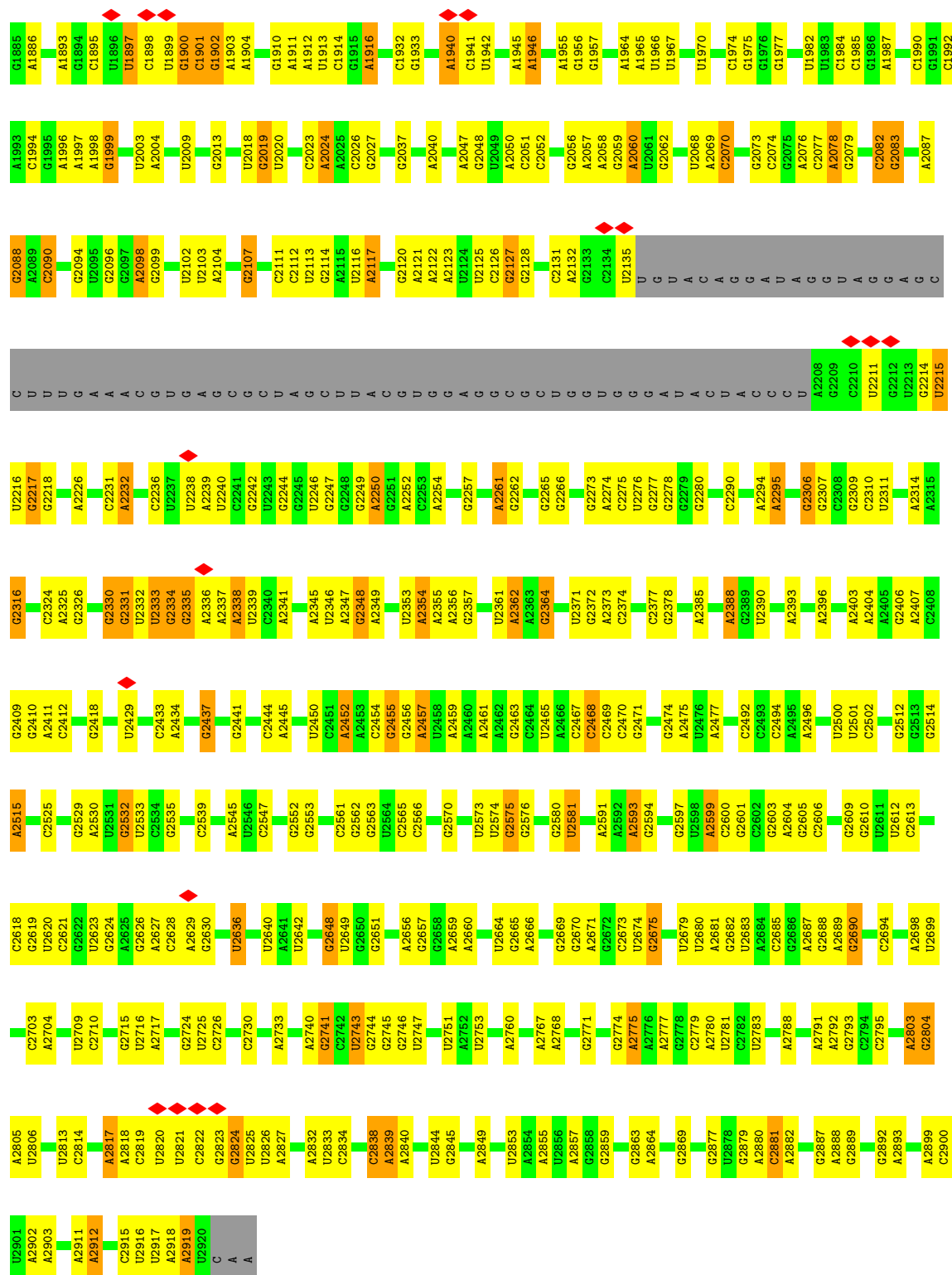
• Molecule 22: E-site tRNA CHAIN



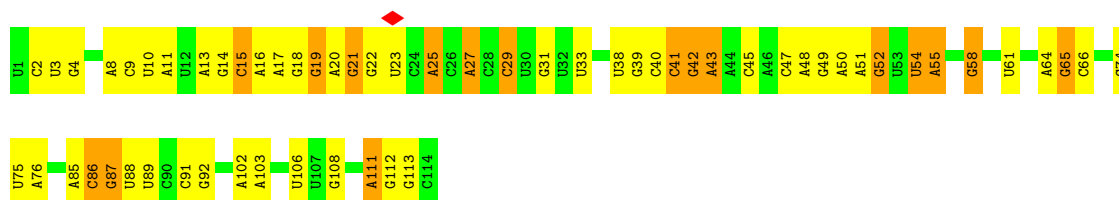
• Molecule 23: 23S RRNA



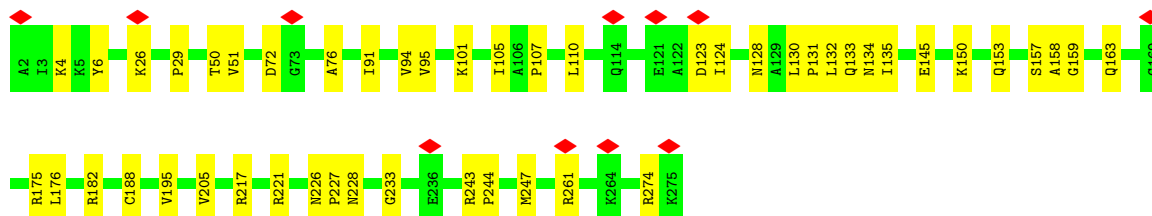
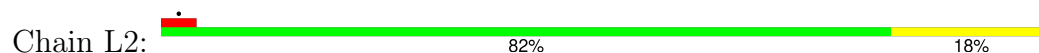




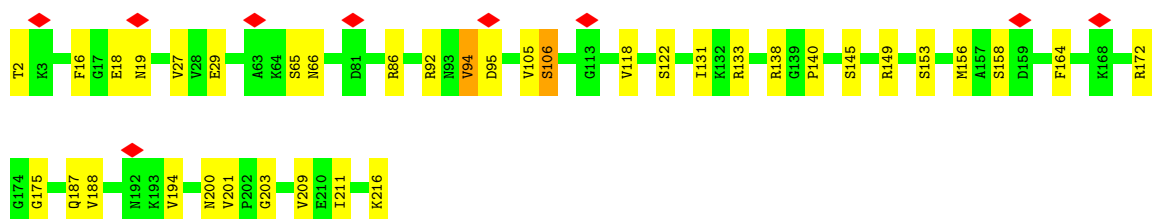
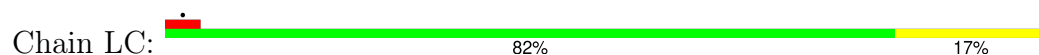
• Molecule 24: 5S rRNA CHAIN



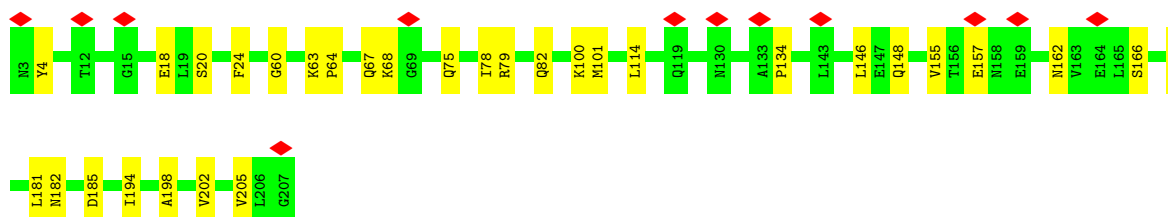
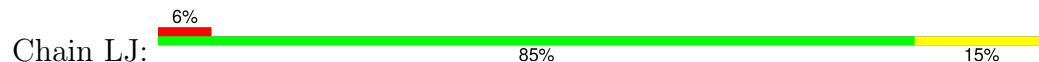
• Molecule 25: 50S ribosomal protein L2



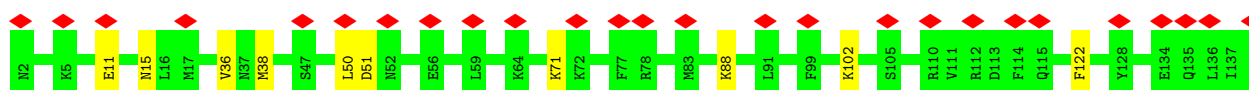
• Molecule 26: 50S ribosomal protein L3

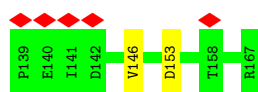


• Molecule 27: 50S ribosomal protein L4

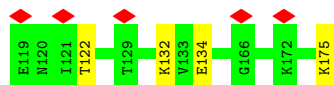
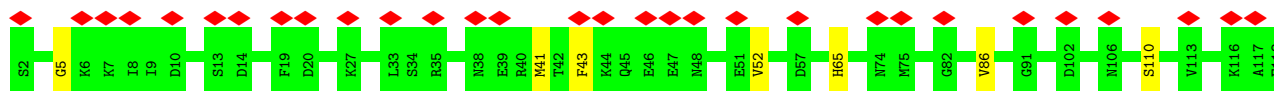


• Molecule 28: 50S ribosomal protein L5

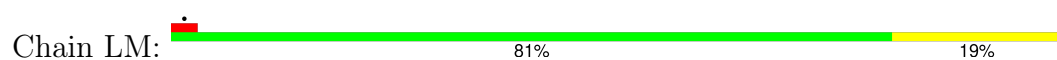




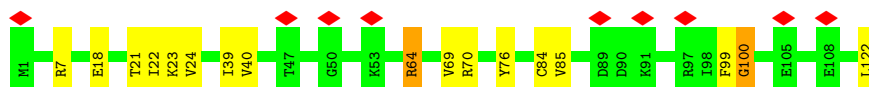
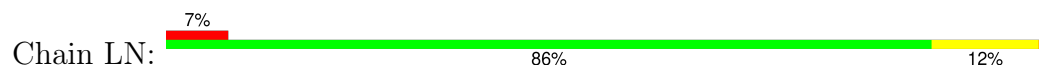
- Molecule 29: 50S ribosomal protein L6



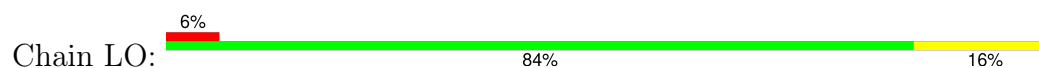
- Molecule 30: 50S ribosomal protein L13



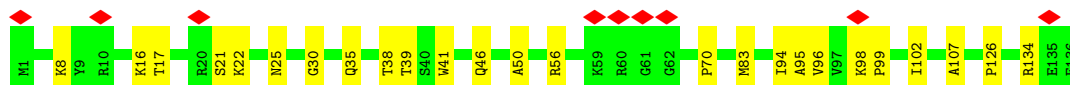
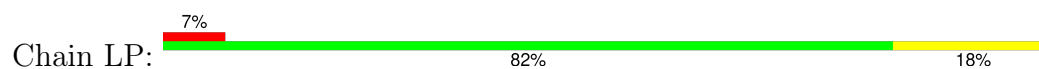
- Molecule 31: 50S ribosomal protein L14



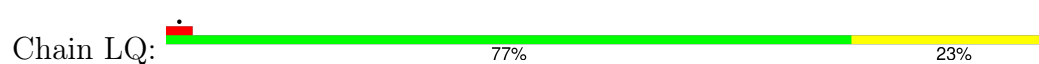
- Molecule 32: 50S ribosomal protein L15

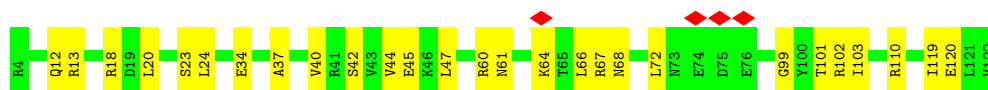


- Molecule 33: 50S ribosomal protein L16

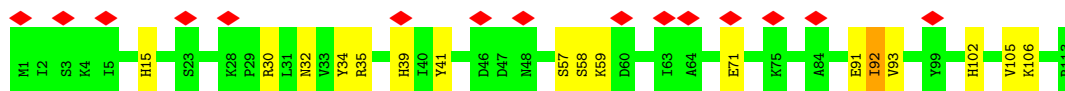
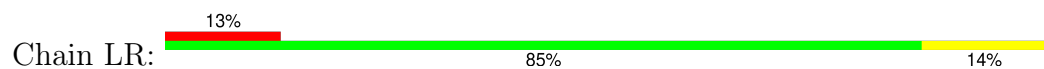


- Molecule 34: 50S ribosomal protein L17

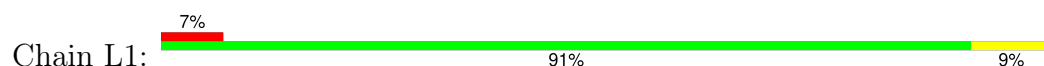




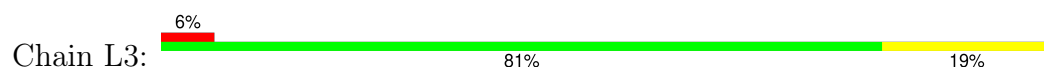
- Molecule 35: 50S ribosomal protein L18



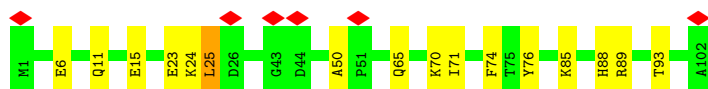
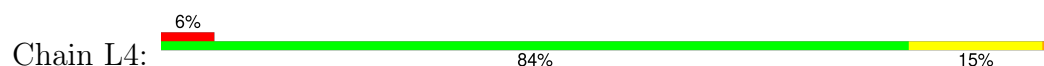
- Molecule 36: 50S ribosomal protein L19



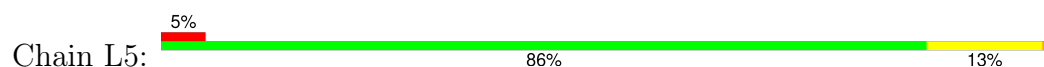
- Molecule 37: 50S ribosomal protein L20



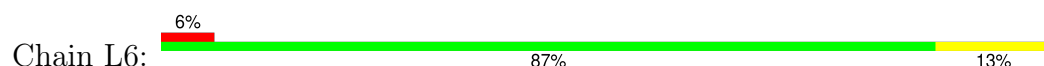
- Molecule 38: 50S ribosomal protein L21



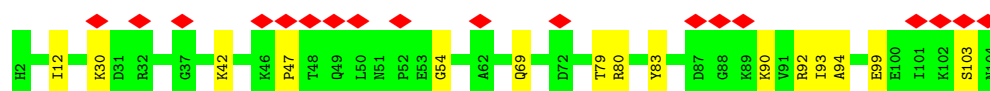
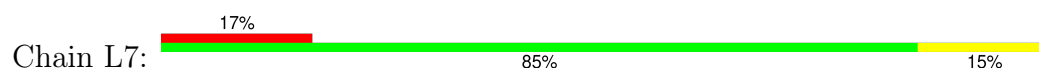
- Molecule 39: 50S ribosomal protein L22



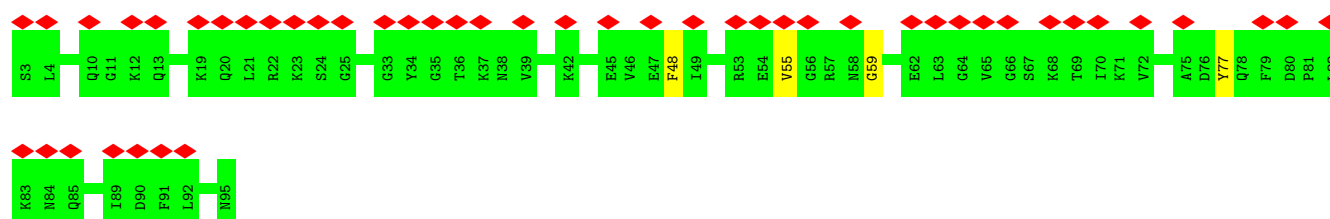
- Molecule 40: 50S ribosomal protein L23



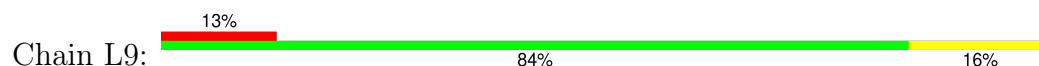
- Molecule 41: 50S ribosomal protein L24



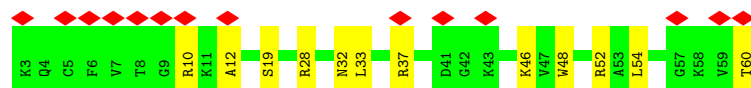
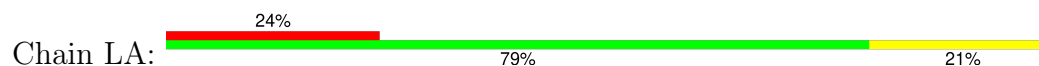
- Molecule 42: 50S ribosomal protein L25



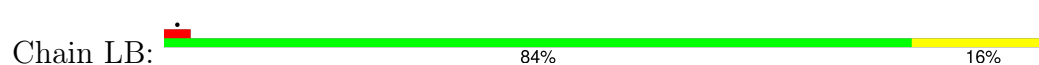
- Molecule 43: 50S ribosomal protein L27



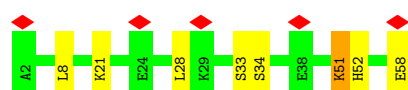
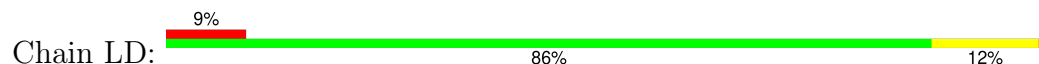
- Molecule 44: 50S ribosomal protein L28



- Molecule 45: 50S ribosomal protein L29

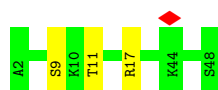


- Molecule 46: 50S ribosomal protein L30

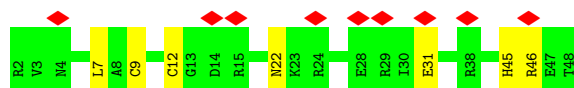
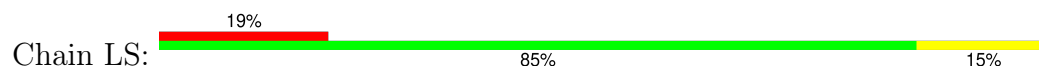


- Molecule 47: 50S ribosomal protein L32

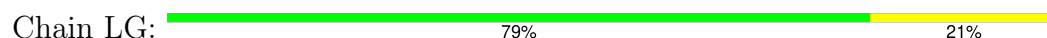




- Molecule 48: 50S ribosomal protein L33 1



- Molecule 49: 50S ribosomal protein L34



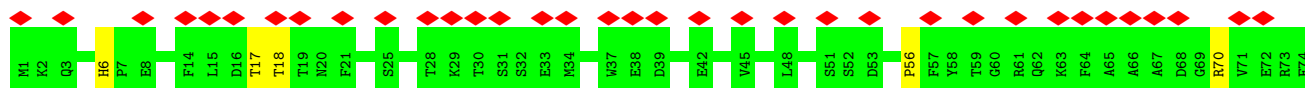
- Molecule 50: 50S ribosomal protein L35



- Molecule 51: 50S ribosomal protein L36



- Molecule 52: 50S ribosomal protein L31 type B



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	126000	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TECNAI ARCTICA	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	40	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	0.370	Depositor
Minimum map value	-0.205	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.021	Depositor
Recommended contour level	0.065	Depositor
Map size (Å)	393.6, 393.6, 393.6	wwPDB
Map dimensions	410, 410, 410	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.96000004, 0.96000004, 0.96000004	Depositor

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.45	0/35118	0.55	6/54749 (0.0%)
2	SB	0.38	0/1573	0.72	0/2121
3	SC	0.29	0/1062	0.67	2/1465 (0.1%)
4	SD	0.46	0/1167	0.71	0/1576
5	SE	0.39	0/796	0.65	0/1069
6	SG	0.34	0/1180	0.69	0/1595
7	SF	0.47	0/1019	0.79	0/1371
8	SH	0.35	0/990	0.84	1/1332 (0.1%)
9	S1	0.40	0/637	0.69	1/865 (0.1%)
10	S2	0.39	0/840	0.68	0/1137
11	S3	0.41	0/991	0.80	0/1337
12	S4	0.36	0/835	0.89	4/1123 (0.4%)
13	S5	0.40	0/507	0.78	0/674
14	S6	0.44	0/721	0.70	0/964
15	S7	0.32	0/541	0.69	0/733
16	S8	0.31	0/527	0.61	0/721
17	S9	0.37	0/465	0.68	0/620
18	SI	0.31	0/551	0.76	0/747
19	SA	0.29	0/502	0.52	0/679
20	X	0.39	0/238	0.54	0/368
21	E	0.27	0/1787	0.51	0/2784
22	D	0.28	0/1809	0.51	0/2819
23	B	0.62	0/66138	0.56	7/103134 (0.0%)
24	C	0.46	0/2717	0.54	1/4232 (0.0%)
25	L2	0.63	0/2101	0.71	0/2823
26	LC	0.56	0/1593	0.79	0/2143
27	LJ	0.56	0/1536	0.75	0/2078
28	LK	0.35	0/1033	0.69	0/1412
29	LL	0.29	0/1074	0.54	0/1467
30	LM	0.51	0/1146	0.73	0/1546
31	LN	0.58	0/925	0.85	1/1242 (0.1%)
32	LO	0.56	0/1034	0.79	0/1388

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	LP	0.52	0/1067	0.70	0/1436
34	LQ	0.54	0/900	0.76	0/1205
35	LR	0.41	0/770	0.70	0/1044
36	L1	0.50	0/844	0.66	0/1134
37	L3	0.61	0/954	0.74	0/1264
38	L4	0.51	0/758	0.70	0/1014
39	L5	0.60	0/845	0.74	0/1140
40	L6	0.56	0/701	0.72	0/939
41	L7	0.38	0/742	0.71	2/1001 (0.2%)
42	L8	0.31	0/655	0.65	0/888
43	L9	0.54	0/621	0.75	0/824
44	LA	0.48	0/449	0.71	0/600
45	LB	0.44	0/494	0.70	0/660
46	LD	0.50	0/438	0.74	0/591
47	LE	0.56	0/361	0.71	0/481
48	LS	0.43	0/385	0.72	0/518
49	LG	0.67	0/371	0.79	0/484
50	LH	0.51	0/450	0.84	2/597 (0.3%)
51	LI	0.49	0/275	0.70	0/366
52	LF	0.25	0/454	0.58	0/624
All	All	0.53	0/145687	0.60	27/219124 (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
5	SE	0	1
6	SG	0	1
10	S2	0	1
11	S3	0	1
13	S5	0	1
15	S7	0	1
18	SI	0	1
25	L2	0	1
26	LC	0	3
28	LK	0	1
30	LM	0	1
31	LN	0	1
33	LP	0	1
34	LQ	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
38	L4	0	2
42	L8	0	2
43	L9	0	1
48	LS	0	1
50	LH	0	1
All	All	0	23

There are no bond length outliers.

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	B	317	G	OP1-P-O3'	-9.59	79.22	108.00
12	S4	8	ASP	CA-C-N	6.40	126.58	120.43
12	S4	8	ASP	C-N-CA	6.40	126.58	120.43
23	B	317	G	OP2-P-O3'	-5.89	90.33	108.00
12	S4	94	GLY	CA-C-N	5.74	129.03	122.83
12	S4	94	GLY	C-N-CA	5.74	129.03	122.83
8	SH	100	LEU	N-CA-C	-5.57	107.49	114.56
50	LH	28	PHE	CA-C-N	5.49	132.03	121.54
50	LH	28	PHE	C-N-CA	5.49	132.03	121.54
1	A	1076	G	P-O3'-C3'	5.45	128.38	120.20
23	B	1897	U	P-O3'-C3'	5.41	128.32	120.20
23	B	1900	G	C2'-C3'-O3'	5.31	117.46	109.50
31	LN	64	ARG	CA-CB-CG	5.30	124.71	114.10
1	A	465	U	P-O3'-C3'	5.30	128.15	120.20
23	B	1276	G	O4'-C1'-N9	5.25	116.07	108.20
3	SC	65	GLU	CA-C-N	5.23	131.54	121.54
3	SC	65	GLU	C-N-CA	5.23	131.54	121.54
9	S1	40	ILE	CA-C-O	5.14	122.53	119.19
23	B	577	A	P-O3'-C3'	5.12	127.89	120.20
1	A	1002	U	P-O3'-C3'	5.12	127.89	120.20
1	A	1510	U	P-O3'-C3'	5.07	127.81	120.20
1	A	609	G	P-O3'-C3'	5.07	127.80	120.20
23	B	1636	U	P-O3'-C3'	5.04	127.76	120.20
24	C	86	C	C2-N1-C1'	5.03	133.89	118.80
41	L7	30	LYS	CA-C-N	5.03	131.15	121.54
41	L7	30	LYS	C-N-CA	5.03	131.15	121.54
1	A	70	A	P-O3'-C3'	5.00	127.70	120.20

There are no chirality outliers.

All (23) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
25	L2	131	PRO	Peptide
38	L4	15	GLU	Peptide
38	L4	25	LEU	Peptide
42	L8	48	PHE	Peptide
42	L8	77	TYR	Peptide
43	L9	21	GLY	Peptide
26	LC	158	SER	Peptide
26	LC	18	GLU	Peptide
26	LC	94	VAL	Peptide
50	LH	10	ALA	Peptide
28	LK	71	LYS	Peptide
30	LM	141	TYR	Peptide
31	LN	99	PHE	Peptide
33	LP	38	THR	Peptide
34	LQ	68	ASN	Peptide
48	LS	22	ASN	Peptide
10	S2	40	ASN	Peptide
11	S3	54	THR	Peptide
13	S5	15	LYS	Peptide
15	S7	68	THR	Peptide
5	SE	43	TRP	Peptide
6	SG	124	ILE	Peptide
18	SI	29	GLN	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	31369	0	15803	351	0
2	SB	1551	0	1570	31	0
3	SC	1058	0	568	8	0
4	SD	1153	0	1210	19	0
5	SE	785	0	781	16	0
6	SG	1164	0	1146	20	0
7	SF	1007	0	1050	22	0
8	SH	975	0	970	37	0
9	S1	626	0	628	12	0
10	S2	826	0	817	13	0
11	S3	976	0	966	11	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
12	S4	828	0	809	10	0
13	S5	497	0	512	13	0
14	S6	713	0	733	12	0
15	S7	537	0	462	9	0
16	S8	520	0	415	6	0
17	S9	458	0	496	7	0
18	SI	541	0	482	10	0
19	SA	503	0	451	13	0
20	X	213	0	108	0	0
21	E	1600	0	810	15	0
22	D	1619	0	822	14	0
23	B	59059	0	29695	460	0
24	C	2430	0	1229	28	0
25	L2	2066	0	2161	32	0
26	LC	1570	0	1593	22	0
27	LJ	1514	0	1540	21	0
28	LK	1026	0	797	8	0
29	LL	1062	0	808	6	0
30	LM	1124	0	1101	17	0
31	LN	918	0	981	8	0
32	LO	1020	0	998	18	0
33	LP	1043	0	1084	16	0
34	LQ	898	0	932	19	0
35	LR	765	0	720	11	0
36	L1	832	0	875	10	0
37	L3	942	0	1014	20	0
38	L4	749	0	730	10	0
39	L5	837	0	893	13	0
40	L6	694	0	705	7	0
41	L7	734	0	731	11	0
42	L8	648	0	598	1	0
43	L9	615	0	637	9	0
44	LA	443	0	461	8	0
45	LB	493	0	503	6	0
46	LD	436	0	474	5	0
47	LE	356	0	354	4	0
48	LS	380	0	379	3	0
49	LG	367	0	415	8	0
50	LH	446	0	465	4	0
51	LI	272	0	290	9	0
52	LF	447	0	289	4	0
53	A	42	0	44	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
54	A	27	0	0	0	0
54	B	99	0	0	0	0
54	C	2	0	0	0	0
54	SG	1	0	0	0	0
All	All	133876	0	85105	1269	0

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

All (1269) 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)
23:B:1037:A:N7	23:B:1206:G:N1	2.02	1.08
23:B:1037:A:C5	23:B:1206:G:N1	2.22	1.07
1:A:251:A:C5	1:A:289:G:N2	2.26	1.03
23:B:497:U:C2	23:B:499:A:N7	2.27	1.02
23:B:420:A:H62	23:B:446:G:N2	1.62	0.98
23:B:615:A:N6	23:B:2056:G:H21	1.61	0.98
1:A:1145:A:C2	1:A:1153:G:N1	2.32	0.97
23:B:615:A:H61	23:B:2056:G:N2	1.63	0.97
23:B:1493:U:H3	23:B:1506:C:N4	1.62	0.97
23:B:1884:G:H21	23:B:1912:A:H62	0.98	0.97
1:A:300:G:H21	1:A:616:A:H61	1.05	0.96
1:A:1201:G:HO2'	2:SB:2:GLY:N	1.62	0.96
23:B:420:A:H62	23:B:446:G:H21	0.97	0.95
23:B:1884:G:N2	23:B:1912:A:H62	1.65	0.95
23:B:1493:U:H3	23:B:1506:C:H42	1.06	0.95
21:E:54:U:H3	21:E:58:A:H62	1.14	0.94
22:D:54:U:H3	22:D:58:A:H62	1.14	0.94
23:B:1037:A:N7	23:B:1206:G:C6	2.36	0.93
1:A:300:G:H21	1:A:616:A:N6	1.67	0.91
23:B:1884:G:H21	23:B:1912:A:N6	1.70	0.90
1:A:145:U:H3	1:A:177:G:H1	1.13	0.90
1:A:1145:A:N1	1:A:1153:G:C6	2.41	0.89
23:B:420:A:N6	23:B:446:G:H21	1.71	0.88
1:A:300:G:N2	1:A:616:A:H61	1.71	0.87
18:SI:18:LYS:O	18:SI:22:GLN:HB2	1.75	0.86
23:B:1037:A:N7	23:B:1206:G:C2	2.43	0.86
23:B:2863:G:HO2'	36:L1:2:THR:N	1.72	0.86
23:B:317:G:H1	23:B:403:U:H3	1.16	0.85
23:B:497:U:N3	23:B:499:A:N7	2.26	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:B:1037:A:N6	23:B:1206:G:O6	2.11	0.83
23:B:615:A:H61	23:B:2056:G:H21	0.86	0.82
23:B:1794:C:O2	23:B:2013:G:N2	2.13	0.81
1:A:251:A:C6	1:A:289:G:N2	2.49	0.80
10:S2:19:GLY:HA2	10:S2:35:THR:O	1.81	0.79
1:A:22:G:H21	1:A:924:A:H62	1.30	0.79
22:D:54:U:H3	22:D:58:A:N6	1.83	0.77
21:E:54:U:H3	21:E:58:A:N6	1.83	0.76
23:B:497:U:N3	23:B:499:A:C8	2.53	0.76
8:SH:85:ILE:O	8:SH:89:LEU:HB2	1.84	0.76
1:A:425:G:H1	1:A:434:U:H3	1.29	0.76
23:B:24:G:N2	23:B:562:C:O2	2.19	0.75
1:A:251:A:N7	1:A:289:G:C2	2.55	0.74
1:A:385:G:C2	1:A:395:U:O2	2.42	0.72
1:A:182:A:N1	1:A:208:U:N3	2.36	0.72
1:A:385:G:C6	1:A:395:U:N3	2.58	0.72
23:B:1526:G:H21	23:B:1527:A:H61	1.35	0.72
1:A:507:A:N6	1:A:554:A:N3	2.37	0.72
23:B:1037:A:C8	23:B:1206:G:C2	2.78	0.71
1:A:385:G:N1	1:A:395:U:N3	2.39	0.71
23:B:1528:G:H1	23:B:1549:C:H42	1.39	0.70
6:SG:138:ARG:O	6:SG:142:HIS:HB2	1.91	0.70
2:SB:51:VAL:HA	2:SB:69:THR:HA	1.74	0.69
32:LO:92:THR:HG22	32:LO:94:ALA:H	1.57	0.69
1:A:385:G:N1	1:A:395:U:C2	2.60	0.69
23:B:2685:C:H42	23:B:2690:G:H1	1.41	0.69
8:SH:51:ASN:O	8:SH:54:PHE:HB2	1.92	0.69
6:SG:58:ALA:O	6:SG:62:PHE:HB2	1.93	0.69
23:B:1526:G:H22	23:B:1550:G:H1	1.39	0.68
1:A:251:A:C5	1:A:289:G:C2	2.81	0.68
1:A:957:G:N1	1:A:1246:U:C2	2.61	0.68
1:A:995:C:H2'	1:A:996:A:H8	1.58	0.68
1:A:1001:U:O2	1:A:1224:A:N7	2.27	0.67
23:B:2649:U:H4'	26:LC:172:ARG:HH21	1.59	0.67
23:B:497:U:C4	23:B:499:A:C8	2.82	0.67
23:B:1004:A:H61	33:LP:83:MET:HE1	1.59	0.67
33:LP:70:PRO:HA	33:LP:95:ALA:HB2	1.77	0.67
1:A:1145:A:N1	1:A:1153:G:O6	2.27	0.67
5:SE:3:THR:HB	5:SE:94:GLU:O	1.95	0.67
23:B:1528:G:N2	23:B:1549:C:N3	2.43	0.67
23:B:574:A:N3	23:B:575:G:N2	2.43	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:507:A:H61	1:A:554:A:H1'	1.59	0.66
24:C:29:C:O2'	24:C:52:G:N2	2.28	0.66
23:B:1977:G:N2	23:B:1984:C:N3	2.44	0.66
1:A:1189:G:H4'	8:SH:97:ARG:HH22	1.61	0.65
1:A:1228:U:OP1	13:S5:9:LYS:NZ	2.29	0.65
23:B:1037:A:C6	23:B:1206:G:N1	2.57	0.65
23:B:1352:C:H2'	23:B:1353:A:H8	1.61	0.65
23:B:659:A:N6	23:B:661:U:O2	2.30	0.65
1:A:1171:G:H1	1:A:1193:G:H1	1.45	0.65
1:A:1358:G:O6	8:SH:14:ARG:NH2	2.29	0.65
6:SG:63:GLU:O	6:SG:67:ASN:HB2	1.96	0.65
23:B:1492:G:N3	23:B:1574:G:N2	2.41	0.65
1:A:152:A:N6	1:A:169:C:O2	2.28	0.65
1:A:1064:U:O2	1:A:1211:C:C4	2.49	0.65
1:A:5:A:H62	4:SD:100:ALA:HA	1.62	0.65
7:SF:15:ARG:HE	7:SF:77:LEU:HD12	1.60	0.65
1:A:912:G:H2'	1:A:913:G:H8	1.61	0.64
23:B:1168:C:O2	51:LI:36:GLN:NE2	2.31	0.64
23:B:325:A:N1	23:B:402:C:O2'	2.31	0.64
23:B:2378:G:OP2	50:LH:42:ARG:NH2	2.30	0.64
33:LP:39:THR:HG22	33:LP:99:PRO:HD3	1.78	0.64
23:B:426:G:N2	23:B:441:C:N3	2.45	0.64
23:B:1854:U:OP2	25:L2:221:ARG:NH1	2.30	0.64
1:A:421:G:O2'	1:A:438:A:N6	2.31	0.64
1:A:183:U:H3	1:A:232:A:H4'	1.63	0.64
23:B:1657:G:O2'	49:LG:4:ARG:NH1	2.31	0.64
4:SD:107:ALA:HB1	4:SD:111:VAL:HG23	1.79	0.63
23:B:609:U:OP1	32:LO:29:LYS:NZ	2.31	0.63
1:A:67:G:N2	1:A:172:A:O2'	2.26	0.63
23:B:1290:G:H1	37:L3:37:GLN:HE21	1.46	0.63
3:SC:66:ARG:O	3:SC:70:ASN:ND2	2.31	0.63
23:B:363:A:N3	27:LJ:169:ASN:ND2	2.47	0.63
23:B:2917:U:H2'	23:B:2918:A:H8	1.62	0.63
1:A:366:U:H2'	1:A:367:A:H8	1.64	0.63
23:B:1349:U:O4	40:L6:59:LYS:NZ	2.31	0.63
23:B:2566:C:H5'	51:LI:3:VAL:HG21	1.81	0.63
43:L9:48:GLN:HE21	43:L9:51:THR:HA	1.63	0.63
23:B:1037:A:C5	23:B:1206:G:C2	2.87	0.63
23:B:1290:G:OP2	37:L3:14:ARG:NH2	2.31	0.63
22:D:9:A:OP2	22:D:13:C:N4	2.32	0.62
23:B:2294:A:H5''	23:B:2295:A:H5''	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:E:9:A:OP2	21:E:13:C:N4	2.32	0.62
23:B:632:U:H2'	23:B:633:A:H8	1.65	0.62
13:S5:29:ARG:NH2	13:S5:31:HIS:O	2.33	0.62
23:B:1288:G:OP2	32:LO:21:ARG:NH2	2.32	0.62
4:SD:38:VAL:HG21	4:SD:114:VAL:HG12	1.82	0.62
23:B:1825:U:OP2	25:L2:274:ARG:NH2	2.32	0.62
24:C:4:G:H1	24:C:111:A:H62	1.48	0.62
25:L2:107:PRO:HD2	25:L2:110:LEU:HD21	1.82	0.62
23:B:1861:U:O2	23:B:1999:G:N2	2.33	0.62
2:SB:11:ARG:HB3	2:SB:15:ILE:HD11	1.82	0.61
23:B:1320:G:N2	23:B:1323:A:OP2	2.32	0.61
1:A:400:G:OP2	15:S7:13:LYS:NZ	2.33	0.61
1:A:691:G:N2	10:S2:39:GLY:O	2.34	0.61
50:LH:58:VAL:HG23	50:LH:59:LYS:HG2	1.81	0.61
5:SE:90:MET:HE1	17:S9:66:ARG:HB2	1.81	0.61
1:A:1145:A:C2	1:A:1153:G:C2	2.87	0.61
46:LD:8:LEU:HB2	46:LD:28:LEU:HD13	1.82	0.61
2:SB:87:ARG:O	2:SB:91:ASN:HB2	2.00	0.61
23:B:1809:C:H1'	23:B:2636:U:H5'	1.83	0.61
2:SB:151:GLN:HE21	2:SB:198:LYS:HD2	1.66	0.61
38:L4:74:PHE:HD1	38:L4:85:LYS:HB3	1.66	0.61
9:S1:10:LEU:HB3	9:S1:18:ILE:HD11	1.83	0.61
25:L2:227:PRO:HB3	25:L2:233:GLY:HA3	1.83	0.60
1:A:773:G:H1	1:A:820:G:HO2'	1.49	0.60
1:A:1361:A:OP1	8:SH:125:ARG:NH2	2.33	0.60
23:B:1379:A:O2'	23:B:1381:U:OP2	2.19	0.60
23:B:124:A:OP2	49:LG:20:ARG:NH2	2.33	0.60
37:L3:60:LEU:HD21	37:L3:64:ARG:HH21	1.66	0.60
13:S5:10:GLN:NE2	13:S5:21:TYR:O	2.35	0.60
31:LN:22:ILE:HG13	31:LN:23:LYS:HG3	1.83	0.60
1:A:452:A:N6	1:A:498:U:O2	2.34	0.60
1:A:681:G:H4'	5:SE:88:ARG:HE	1.67	0.60
5:SE:1:MET:N	5:SE:67:SER:O	2.33	0.60
23:B:967:C:H2'	23:B:968:A:H8	1.67	0.60
1:A:540:A:H2	1:A:1217:G:H21	1.50	0.60
23:B:901:G:N2	23:B:967:C:N3	2.50	0.60
23:B:2512:G:OP1	33:LP:46:GLN:NE2	2.34	0.60
1:A:1378:U:H5''	8:SH:119:GLY:H	1.66	0.60
5:SE:1:MET:N	5:SE:68:ASP:OD1	2.35	0.60
23:B:2309:G:C2	23:B:2452:A:C6	2.90	0.60
23:B:2649:U:O2'	23:B:2845:G:N2	2.35	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:B:787:U:H2'	23:B:788:A:H8	1.66	0.59
23:B:2128:G:H1	23:B:2215:U:H3	1.49	0.59
16:S8:65:GLU:HA	16:S8:75:PHE:HA	1.84	0.59
23:B:515:G:O6	49:LG:40:ARG:NH1	2.33	0.59
8:SH:99:SER:O	8:SH:102:ARG:NH1	2.35	0.59
23:B:247:A:OP2	50:LH:8:ARG:NH2	2.31	0.59
23:B:1335:C:H42	23:B:1686:G:H1	1.51	0.59
39:L5:11:ARG:NH2	39:L5:11:ARG:O	2.36	0.59
1:A:274:G:N2	1:A:274:G:OP1	2.34	0.59
26:LC:16:PHE:O	36:L1:14:GLN:NE2	2.35	0.59
39:L5:22:ASP:OD1	39:L5:25:ARG:NH2	2.35	0.59
1:A:51:A:N6	11:S3:30:SER:OG	2.36	0.59
1:A:1140:C:O2	1:A:1158:C:N4	2.36	0.59
21:E:9:A:H2'	21:E:11:C:H41	1.67	0.59
42:L8:55:VAL:HG11	42:L8:59:GLY:HA3	1.84	0.59
1:A:63:U:O2	1:A:387:C:O2'	2.21	0.59
1:A:1050:A:H2'	1:A:1051:A:H8	1.67	0.59
1:A:957:G:N1	1:A:1246:U:N3	2.50	0.59
23:B:72:U:OP2	45:LB:54:LYS:NZ	2.35	0.59
23:B:2470:C:H2'	23:B:2471:G:H8	1.67	0.59
11:S3:80:ILE:HG13	11:S3:110:ILE:HD13	1.84	0.59
23:B:1234:G:N2	23:B:1235:C:N3	2.50	0.59
1:A:1367:G:H2'	1:A:1368:A:C8	2.38	0.58
23:B:522:G:N1	23:B:525:A:OP2	2.36	0.58
23:B:838:A:H61	25:L2:228:ASN:HD22	1.50	0.58
23:B:1217:U:OP2	23:B:1218:G:N2	2.36	0.58
28:LK:102:LYS:HZ3	52:LF:56:PRO:HD3	1.67	0.58
1:A:159:G:N1	1:A:162:A:OP2	2.36	0.58
1:A:681:G:O3'	5:SE:88:ARG:NH1	2.33	0.58
23:B:2743:U:H2'	23:B:2744:G:H8	1.67	0.58
35:LR:57:SER:OG	35:LR:58:SER:N	2.36	0.58
1:A:1123:A:N6	2:SB:175:HIS:O	2.35	0.58
1:A:1438:C:H2'	1:A:1439:A:H8	1.68	0.58
2:SB:110:LEU:HD21	2:SB:143:LEU:HB3	1.84	0.58
5:SE:11:ARG:NH2	5:SE:84:ASP:O	2.35	0.58
23:B:669:C:H2'	23:B:670:G:H8	1.68	0.58
1:A:967:U:O2'	1:A:969:A:OP2	2.20	0.58
1:A:1089:G:N2	1:A:1091:G:O2'	2.37	0.58
7:SF:15:ARG:HD3	7:SF:77:LEU:HB3	1.86	0.58
23:B:1513:A:N6	23:B:1567:A:O2'	2.37	0.58
23:B:2362:A:N6	23:B:2364:G:N3	2.51	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:LJ:146:LEU:O	27:LJ:148:GLN:NE2	2.36	0.58
1:A:127:A:OP1	16:S8:5:ASN:ND2	2.36	0.58
7:SF:106:VAL:HB	7:SF:127:ILE:HG22	1.86	0.58
13:S5:33:VAL:HG12	13:S5:40:CYS:HB3	1.86	0.58
35:LR:30:ARG:NH1	35:LR:91:GLU:OE1	2.37	0.58
23:B:276:C:N3	23:B:296:G:N2	2.51	0.58
23:B:317:G:O6	23:B:403:U:O4	2.22	0.58
23:B:2532:G:N2	23:B:2533:U:O4	2.36	0.58
26:LC:156:MET:SD	26:LC:156:MET:N	2.77	0.58
1:A:888:U:OP1	7:SF:82:LYS:NZ	2.37	0.58
22:D:9:A:H2'	22:D:11:C:H41	1.67	0.58
1:A:1064:U:N3	1:A:1211:C:N3	2.52	0.57
22:D:54:U:O4	22:D:58:A:N7	2.37	0.57
1:A:1236:A:H5''	12:S4:102:THR:HG22	1.86	0.57
8:SH:80:ALA:O	8:SH:84:GLY:N	2.37	0.57
23:B:349:U:H3	23:B:353:A:H62	1.50	0.57
23:B:350:G:H8	23:B:373:A:H61	1.51	0.57
1:A:385:G:N2	1:A:395:U:O2	2.38	0.57
23:B:923:A:N6	23:B:946:A:OP2	2.38	0.57
23:B:2127:G:O6	23:B:2216:U:O2	2.22	0.57
1:A:425:G:N2	1:A:434:U:O2	2.34	0.57
26:LC:65:SER:OG	26:LC:66:ASN:N	2.37	0.57
37:L3:50:ARG:HG2	37:L3:53:ARG:HH21	1.69	0.57
1:A:957:G:N2	1:A:1246:U:O2	2.37	0.57
43:L9:45:LEU:HD11	43:L9:75:VAL:HG11	1.86	0.57
45:LB:6:ILE:HG12	45:LB:52:ARG:HH22	1.68	0.57
1:A:1102:U:HO2'	1:A:1182:A:HO2'	1.52	0.57
1:A:1145:A:C2	1:A:1153:G:C6	2.88	0.57
23:B:2733:A:O2'	34:LQ:60:ARG:NH1	2.37	0.57
1:A:937:G:OP1	1:A:1517:G:N2	2.38	0.57
36:L1:16:ARG:NH2	36:L1:80:THR:O	2.37	0.57
21:E:54:U:O4	21:E:58:A:N7	2.37	0.57
23:B:277:C:O2	23:B:295:G:N2	2.38	0.57
1:A:1402:U:H2'	1:A:1403:G:H8	1.70	0.57
9:S1:23:GLU:HA	9:S1:26:VAL:HG12	1.86	0.57
23:B:1364:C:O2'	34:LQ:110:ARG:NH2	2.38	0.57
36:L1:33:ARG:NE	36:L1:84:GLU:OE2	2.36	0.57
1:A:431:G:H21	1:A:432:G:H1'	1.70	0.56
23:B:1037:A:N6	23:B:1206:G:C6	2.69	0.56
25:L2:145:GLU:HB2	25:L2:188:CYS:HB3	1.87	0.56
1:A:1271:G:OP1	1:A:1295:C:O2'	2.23	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:SH:50:LEU:HB2	8:SH:82:ARG:HB2	1.87	0.56
23:B:106:A:H2'	23:B:107:G:H8	1.70	0.56
23:B:446:G:O6	44:LA:52:ARG:NH2	2.38	0.56
23:B:1063:U:OP1	23:B:1079:U:O2'	2.21	0.56
23:B:1308:C:H42	23:B:2037:G:H1	1.53	0.56
23:B:2273:G:H2'	23:B:2274:A:H8	1.70	0.56
45:LB:9:LEU:O	45:LB:60:ARG:NH1	2.38	0.56
1:A:381:A:H61	1:A:399:G:H1'	1.70	0.56
2:SB:28:PHE:O	2:SB:32:LEU:HB2	2.05	0.56
23:B:226:A:N6	23:B:468:A:N1	2.54	0.56
24:C:54:U:H4'	24:C:55:A:H5'	1.86	0.56
1:A:626:C:N4	1:A:629:A:OP2	2.38	0.56
5:SE:93:ARG:NH1	5:SE:95:ASP:OD2	2.38	0.56
26:LC:122:SER:HB2	26:LC:175:GLY:HA2	1.88	0.56
1:A:63:U:O2'	1:A:387:C:O2	2.24	0.56
1:A:106:G:N7	19:SA:10:ARG:NH1	2.53	0.56
1:A:983:G:O6	1:A:984:A:N6	2.38	0.56
1:A:1264:G:H1	1:A:1295:C:H42	1.51	0.56
23:B:29:U:H2'	23:B:30:G:H8	1.70	0.56
23:B:957:C:OP1	33:LP:8:LYS:NZ	2.36	0.56
23:B:2355:A:H2'	23:B:2356:A:C8	2.41	0.56
1:A:953:U:H2'	1:A:954:G:H8	1.71	0.56
1:A:843:A:OP1	17:S9:58:ARG:NH2	2.38	0.56
2:SB:107:LYS:HB3	2:SB:110:LEU:HD23	1.86	0.56
11:S3:25:ASN:O	11:S3:38:LEU:N	2.35	0.56
23:B:1423:C:O2'	23:B:1512:U:O2	2.19	0.56
25:L2:123:ASP:O	25:L2:128:ASN:ND2	2.38	0.56
1:A:962:U:H2'	1:A:963:G:H8	1.70	0.56
23:B:1081:G:N2	23:B:1163:U:O2	2.38	0.56
23:B:1901:C:H1'	23:B:1902:G:H5'	1.88	0.56
28:LK:36:VAL:HG22	28:LK:146:VAL:HG12	1.88	0.56
10:S2:101:GLN:HE22	10:S2:107:VAL:H	1.54	0.56
23:B:576:U:OP1	23:B:604:G:N2	2.39	0.56
1:A:209:G:H2'	1:A:210:A:C4	2.41	0.56
1:A:316:C:H2'	1:A:317:G:H8	1.71	0.56
1:A:1383:U:OP1	8:SH:76:GLY:N	2.37	0.56
23:B:816:G:O2'	23:B:1392:G:O2'	2.24	0.56
33:LP:16:LYS:O	33:LP:98:LYS:NZ	2.38	0.56
1:A:592:G:O6	1:A:766:G:N2	2.39	0.55
23:B:1215:U:O2'	23:B:1218:G:N2	2.33	0.55
1:A:336:C:H4'	1:A:337:A:H5'	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:537:G:H22	11:S3:61:ALA:HB2	1.71	0.55
11:S3:96:ARG:HB3	11:S3:109:HIS:HB2	1.88	0.55
1:A:381:A:HO2'	1:A:489:G:H21	1.54	0.55
1:A:525:G:N1	1:A:541:A:OP2	2.36	0.55
23:B:85:G:O2'	23:B:102:A:N6	2.39	0.55
23:B:1440:A:O2'	23:B:1514:A:O2'	2.23	0.55
26:LC:29:GLU:HA	26:LC:194:VAL:HG12	1.88	0.55
1:A:596:G:H5''	7:SF:6:PRO:HG3	1.88	0.55
1:A:1418:C:H2'	1:A:1419:A:H8	1.72	0.55
7:SF:13:ARG:NH1	7:SF:26:GLU:O	2.40	0.55
8:SH:120:LEU:HD12	8:SH:126:SER:HA	1.89	0.55
23:B:162:A:H8	23:B:2244:G:H21	1.55	0.55
23:B:2357:G:H21	43:L9:50:GLY:HA2	1.70	0.55
1:A:42:G:O6	1:A:409:C:N4	2.39	0.55
23:B:2471:G:OP2	27:LJ:68:LYS:NZ	2.36	0.55
23:B:1303:A:H61	23:B:2040:A:H5''	1.71	0.55
23:B:2902:A:OP1	34:LQ:102:ARG:NH1	2.40	0.55
25:L2:159:GLY:H	25:L2:195:VAL:HG13	1.72	0.55
27:LJ:182:ASN:OD1	27:LJ:182:ASN:N	2.39	0.55
4:SD:107:ALA:O	4:SD:112:ARG:NH2	2.40	0.55
23:B:201:C:N4	23:B:251:G:O6	2.39	0.55
23:B:319:G:H1	23:B:401:U:H3	1.55	0.55
28:LK:11:GLU:O	28:LK:15:ASN:ND2	2.40	0.55
30:LM:53:ASP:N	30:LM:53:ASP:OD1	2.39	0.55
1:A:381:A:H2'	1:A:382:A:H8	1.72	0.55
1:A:419:A:H62	1:A:439:A:H61	1.55	0.55
1:A:955:G:N2	1:A:1345:G:O3'	2.40	0.55
23:B:2659:A:H2'	23:B:2660:A:H8	1.71	0.55
31:LN:21:THR:HG22	31:LN:39:ILE:HD13	1.89	0.55
3:SC:107:ARG:O	3:SC:111:ARG:CB	2.55	0.55
23:B:675:G:H21	23:B:677:A:H8	1.55	0.55
23:B:1363:U:HO2'	23:B:2037:G:HO2'	1.53	0.55
23:B:2128:G:O6	23:B:2215:U:O4	2.25	0.55
44:LA:12:ALA:O	44:LA:28:ARG:NH2	2.34	0.55
12:S4:66:GLU:HG2	12:S4:69:LEU:HD22	1.88	0.54
23:B:2102:U:OP1	25:L2:243:ARG:NH2	2.37	0.54
23:B:2863:G:O2'	36:L1:2:THR:N	2.38	0.54
44:LA:33:LEU:HD12	44:LA:48:TRP:HB3	1.89	0.54
1:A:688:C:H42	1:A:718:G:H1	1.56	0.54
1:A:1132:C:H2'	1:A:1133:U:H6	1.71	0.54
29:LL:43:PHE:HA	29:LL:52:VAL:HA	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:E:9:A:O2'	21:E:10:G:N7	2.39	0.54
23:B:826:A:OP1	25:L2:217:ARG:NH2	2.40	0.54
23:B:2665:G:H22	23:B:2803:A:H5'	1.71	0.54
24:C:75:U:H2'	24:C:76:A:H8	1.71	0.54
1:A:432:G:H2'	1:A:433:A:H8	1.72	0.54
1:A:695:A:H62	1:A:711:G:H21	1.56	0.54
1:A:986:G:H22	1:A:1373:C:H2'	1.72	0.54
21:E:68:C:H2'	21:E:69:G:C8	2.42	0.54
39:L5:36:LEU:O	39:L5:44:SER:OG	2.26	0.54
1:A:626:C:H42	1:A:631:C:H42	1.56	0.54
1:A:1243:U:H5'	8:SH:128:GLN:HE21	1.72	0.54
9:S1:11:LYS:HA	9:S1:70:HIS:O	2.08	0.54
23:B:421:C:N4	23:B:445:G:O6	2.41	0.54
1:A:277:U:H2'	1:A:278:A:H8	1.72	0.54
7:SF:5:ASP:OD2	7:SF:79:ARG:NH1	2.40	0.54
23:B:1450:A:OP1	23:B:1635:A:N6	2.40	0.54
23:B:339:A:O3'	41:L7:90:LYS:NZ	2.41	0.54
23:B:1308:C:H5'	23:B:1309:G:H5'	1.90	0.54
23:B:2048:G:OP1	47:LE:11:THR:OG1	2.26	0.54
33:LP:46:GLN:HG2	33:LP:126:PRO:HD3	1.90	0.54
39:L5:43:SER:HB3	39:L5:46:VAL:HB	1.90	0.54
1:A:1064:U:N3	1:A:1211:C:C2	2.74	0.54
7:SF:34:LYS:HD2	7:SF:51:TYR:HB2	1.89	0.54
19:SA:18:GLU:HA	19:SA:21:ASN:HB2	1.90	0.54
1:A:1456:U:O2	1:A:1469:G:C6	2.60	0.54
23:B:630:G:OP2	32:LO:21:ARG:NH1	2.40	0.54
23:B:2496:A:H4'	33:LP:56:ARG:HH22	1.73	0.54
32:LO:123:VAL:HG23	32:LO:143:HIS:HB3	1.90	0.54
1:A:109:C:O2'	15:S7:26:ARG:O	2.26	0.53
22:D:68:C:H2'	22:D:69:G:C8	2.42	0.53
23:B:1040:A:O2'	37:L3:91:ASN:ND2	2.38	0.53
23:B:1495:C:N4	23:B:1504:U:O4	2.41	0.53
1:A:20:C:O2	1:A:927:G:N2	2.41	0.53
1:A:259:G:N2	1:A:274:G:O4'	2.41	0.53
1:A:329:A:H2'	1:A:330:C:H6	1.73	0.53
14:S6:36:ILE:HD13	14:S6:59:MET:HE3	1.90	0.53
23:B:344:U:OP2	41:L7:80:ARG:NH2	2.41	0.53
23:B:1210:U:H2'	23:B:1211:G:H8	1.73	0.53
23:B:422:G:H2'	23:B:423:A:H8	1.73	0.53
35:LR:102:HIS:HA	35:LR:105:VAL:HG12	1.91	0.53
1:A:681:G:H2'	1:A:682:G:C8	2.43	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:S6:40:ASN:ND2	23:B:761:A:N7	2.39	0.53
23:B:1214:C:O2	23:B:1219:G:N2	2.42	0.53
23:B:2468:C:H2'	23:B:2469:C:H6	1.74	0.53
23:B:64:A:H2'	23:B:65:A:H8	1.73	0.53
23:B:1020:G:O6	23:B:1031:C:N4	2.37	0.53
31:LN:64:ARG:NH1	31:LN:100:GLY:O	2.42	0.53
1:A:1235:U:O2	12:S4:101:LYS:NZ	2.33	0.53
23:B:169:G:O2'	23:B:2236:C:O2'	2.26	0.53
23:B:2535:G:O2'	23:B:2581:U:O2'	2.26	0.53
38:L4:71:ILE:HD11	38:L4:88:HIS:HD2	1.72	0.53
23:B:901:G:H1	23:B:967:C:H42	1.55	0.53
24:C:22:G:N2	24:C:25:A:H61	2.06	0.53
40:L6:50:VAL:HG12	40:L6:82:LEU:HB3	1.89	0.53
1:A:534:C:OP2	11:S3:101:LYS:NZ	2.42	0.53
7:SF:10:MET:HG3	7:SF:33:LYS:HD3	1.91	0.53
23:B:2316:G:N2	23:B:2371:U:O2	2.42	0.53
34:LQ:37:ALA:HA	34:LQ:40:VAL:HG12	1.90	0.53
1:A:672:G:H22	1:A:749:G:H1	1.57	0.53
7:SF:72:ARG:HG3	7:SF:75:THR:HG22	1.91	0.53
23:B:1041:G:OP1	37:L3:92:ARG:NH1	2.42	0.53
27:LJ:78:ILE:HG23	27:LJ:79:ARG:HG2	1.90	0.53
45:LB:31:GLN:HE21	45:LB:36:GLN:HG2	1.74	0.53
1:A:137:U:O2	1:A:235:G:N2	2.42	0.53
23:B:1039:C:H5	30:LM:1:MET:HE2	1.73	0.52
1:A:152:A:N6	1:A:169:C:C2	2.76	0.52
1:A:672:G:OP1	17:S9:58:ARG:NH1	2.42	0.52
1:A:1141:C:OP1	8:SH:20:ARG:NH1	2.42	0.52
23:B:611:U:OP2	32:LO:36:LYS:NZ	2.42	0.52
23:B:971:U:O4	23:B:972:A:N6	2.41	0.52
23:B:2514:G:H2'	23:B:2515:A:H8	1.74	0.52
1:A:1064:U:C2	1:A:1211:C:C4	2.97	0.52
23:B:497:U:O2	23:B:499:A:N7	2.38	0.52
23:B:788:A:O2'	23:B:1703:U:OP1	2.27	0.52
1:A:381:A:O2'	1:A:489:G:N2	2.40	0.52
1:A:528:A:H61	1:A:544:C:H1'	1.73	0.52
1:A:891:G:OP2	11:S3:9:ARG:NH1	2.42	0.52
1:A:1339:C:H2'	1:A:1340:A:C8	2.44	0.52
22:D:9:A:O2'	22:D:10:G:N7	2.39	0.52
25:L2:226:ASN:N	25:L2:226:ASN:OD1	2.41	0.52
31:LN:24:VAL:HA	31:LN:39:ILE:HG22	1.90	0.52
38:L4:65:GLN:HG2	38:L4:93:THR:HG22	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:B:548:A:O2'	23:B:551:G:OP2	2.26	0.52
23:B:632:U:H2'	23:B:633:A:C8	2.44	0.52
23:B:906:A:H62	23:B:961:G:H21	1.56	0.52
23:B:1651:C:N4	23:B:1666:A:OP2	2.41	0.52
39:L5:15:ARG:HH21	47:LE:17:ARG:HH12	1.56	0.52
43:L9:75:VAL:HG12	43:L9:89:VAL:HG22	1.92	0.52
1:A:984:A:OP1	13:S5:29:ARG:NH1	2.42	0.52
23:B:1174:U:OP2	23:B:2597:G:N2	2.41	0.52
23:B:1781:C:H41	36:L1:96:ARG:HH21	1.56	0.52
26:LC:156:MET:HE1	26:LC:164:PHE:HE2	1.74	0.52
32:LO:88:GLY:HA2	32:LO:121:LEU:HD22	1.91	0.52
1:A:343:C:O2'	1:A:1444:A:N3	2.38	0.52
25:L2:4:LYS:HE3	25:L2:6:TYR:HE1	1.73	0.52
32:LO:67:THR:OG1	32:LO:68:ASN:N	2.42	0.52
1:A:103:G:N7	19:SA:9:LYS:NZ	2.57	0.52
1:A:454:G:N2	1:A:497:C:N3	2.47	0.52
1:A:1379:A:H5''	8:SH:116:LYS:HB3	1.92	0.52
2:SB:152:VAL:HG22	2:SB:197:VAL:HG22	1.91	0.52
23:B:678:A:OP1	32:LO:68:ASN:ND2	2.43	0.52
23:B:2881:C:H2'	23:B:2882:A:H8	1.74	0.52
26:LC:94:VAL:HG22	26:LC:95:ASP:HB2	1.90	0.52
27:LJ:185:ASP:OD1	27:LJ:185:ASP:N	2.42	0.52
49:LG:24:SER:OG	49:LG:25:THR:N	2.43	0.52
14:S6:9:ASN:HA	14:S6:12:ILE:HG12	1.91	0.52
23:B:1359:A:O2'	39:L5:84:ARG:NH2	2.43	0.52
1:A:331:U:H5'	19:SA:18:GLU:HB3	1.90	0.52
23:B:1482:U:H2'	23:B:1483:A:H8	1.73	0.52
23:B:1492:G:N2	23:B:1508:C:N3	2.57	0.52
1:A:670:A:O2'	1:A:844:G:OP1	2.26	0.51
23:B:105:C:H2'	23:B:106:A:H8	1.74	0.51
23:B:922:G:N3	23:B:946:A:N6	2.58	0.51
23:B:2273:G:H2'	23:B:2274:A:C8	2.44	0.51
1:A:161:A:N6	1:A:162:A:N7	2.57	0.51
1:A:1162:A:H4'	9:S1:43:PRO:HB3	1.91	0.51
8:SH:59:THR:OG1	8:SH:62:ASN:ND2	2.38	0.51
23:B:2311:U:H3	23:B:2411:A:H62	1.57	0.51
6:SG:145:ALA:HA	6:SG:148:ASN:HB3	1.91	0.51
12:S4:25:ILE:HG23	12:S4:29:THR:HG23	1.91	0.51
23:B:306:C:H2'	23:B:307:A:H8	1.75	0.51
23:B:474:A:N6	23:B:475:A:N1	2.58	0.51
23:B:2099:G:N2	23:B:2465:U:O2	2.43	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:145:U:O2	1:A:177:G:N2	2.35	0.51
4:SD:53:ALA:HB3	4:SD:59:ALA:HB2	1.92	0.51
23:B:40:U:H2'	23:B:41:A:H8	1.74	0.51
23:B:813:G:H2'	23:B:814:A:H8	1.75	0.51
40:L6:13:THR:OG1	40:L6:16:SER:N	2.40	0.51
1:A:39:G:O2'	1:A:555:A:N6	2.43	0.51
23:B:1759:G:N2	23:B:1772:G:OP1	2.44	0.51
24:C:42:G:N3	24:C:45:C:N4	2.58	0.51
27:LJ:20:SER:HB2	27:LJ:24:PHE:HB2	1.92	0.51
4:SD:114:VAL:HG11	4:SD:137:VAL:HG13	1.93	0.51
8:SH:96:TYR:O	8:SH:100:LEU:N	2.44	0.51
23:B:1786:A:HO2'	23:B:2741:G:HO2'	1.57	0.51
23:B:2574:U:O2	23:B:2593:A:N6	2.44	0.51
30:LM:30:SER:OG	30:LM:105:SER:O	2.26	0.51
40:L6:33:VAL:O	40:L6:76:ARG:NH1	2.44	0.51
1:A:46:U:H2'	1:A:47:G:H8	1.76	0.51
1:A:61:A:N1	1:A:106:G:O2'	2.39	0.51
23:B:2306:G:N7	43:L9:22:ARG:NH1	2.43	0.51
29:LL:86:VAL:HA	29:LL:132:LYS:HA	1.92	0.51
3:SC:32:ALA:HB3	3:SC:37:GLY:HA2	1.93	0.51
7:SF:29:ALA:HB2	7:SF:60:LEU:HB2	1.92	0.51
23:B:2019:G:N2	23:B:2023:C:O2	2.43	0.51
27:LJ:146:LEU:HD12	27:LJ:148:GLN:HE22	1.76	0.51
1:A:1201:G:H5'	2:SB:175:HIS:HE1	1.75	0.51
1:A:1522:C:H42	1:A:1537:G:H1	1.59	0.51
24:C:91:C:H2'	24:C:92:G:C8	2.45	0.51
30:LM:117:GLU:O	30:LM:121:LYS:NZ	2.42	0.51
1:A:681:G:H2'	1:A:682:G:H8	1.76	0.50
3:SC:52:ARG:O	3:SC:56:LYS:CB	2.59	0.50
23:B:1360:G:OP1	39:L5:84:ARG:NH1	2.36	0.50
24:C:47:C:H2'	24:C:48:A:H8	1.75	0.50
44:LA:10:ARG:HH22	44:LA:52:ARG:HB2	1.76	0.50
1:A:461:C:N3	1:A:488:U:O4	2.44	0.50
1:A:1452:G:H2'	1:A:1453:G:H21	1.76	0.50
2:SB:54:VAL:HG12	2:SB:67:ILE:HG12	1.92	0.50
23:B:75:G:O2'	45:LB:48:LYS:NZ	2.39	0.50
23:B:1493:U:N3	23:B:1506:C:N4	2.42	0.50
23:B:2335:G:OP1	23:B:2338:A:N6	2.36	0.50
23:B:2403:A:H61	35:LR:92:ILE:HG12	1.76	0.50
30:LM:66:THR:O	30:LM:69:LYS:NZ	2.44	0.50
1:A:332:G:N1	1:A:335:A:OP2	2.39	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:SD:76:ARG:NH1	4:SD:119:GLY:O	2.44	0.50
13:S5:47:LEU:HA	13:S5:52:GLN:HE21	1.77	0.50
23:B:506:A:H2	23:B:515:G:H21	1.58	0.50
1:A:902:A:O2'	1:A:1426:G:O2'	2.29	0.50
1:A:1296:A:H5'	1:A:1297:U:H5	1.76	0.50
14:S6:77:ARG:O	14:S6:81:LEU:HB2	2.11	0.50
23:B:1427:U:H3	23:B:1432:A:H62	1.59	0.50
23:B:2694:C:N3	29:LL:110:SER:OG	2.40	0.50
24:C:108:G:N2	24:C:108:G:OP2	2.45	0.50
1:A:1064:U:C2	1:A:1211:C:N3	2.79	0.50
6:SG:130:ASN:HD21	6:SG:135:VAL:HG11	1.77	0.50
8:SH:100:LEU:HA	8:SH:102:ARG:HH11	1.77	0.50
23:B:774:G:H5'	23:B:775:A:H5''	1.92	0.50
23:B:1595:C:H2'	23:B:1596:G:C8	2.47	0.50
23:B:1911:A:H2'	23:B:1912:A:H8	1.76	0.50
23:B:2127:G:C6	23:B:2216:U:O2	2.64	0.50
24:C:22:G:H21	24:C:25:A:H61	1.59	0.50
27:LJ:134:PRO:HA	27:LJ:162:ASN:HD21	1.76	0.50
27:LJ:162:ASN:ND2	27:LJ:166:SER:OG	2.45	0.50
48:LS:7:LEU:HB3	48:LS:45:HIS:HB3	1.93	0.50
1:A:861:U:H2'	1:A:862:A:H8	1.76	0.50
1:A:987:A:O2'	1:A:989:C:OP2	2.28	0.50
15:S7:73:ASN:O	15:S7:76:SER:OG	2.29	0.50
23:B:55:G:H2'	23:B:56:A:H8	1.76	0.50
23:B:2047:A:H5'	47:LE:9:SER:HB3	1.94	0.50
35:LR:102:HIS:O	35:LR:106:LYS:N	2.40	0.50
23:B:1268:C:H2'	23:B:1269:A:C8	2.47	0.50
23:B:2574:U:H2'	23:B:2575:G:H8	1.76	0.50
36:L1:19:LEU:HD12	36:L1:86:ILE:HD12	1.93	0.50
7:SF:81:SER:HB2	7:SF:87:VAL:HG22	1.93	0.50
10:S2:25:SER:H	10:S2:88:GLY:HA3	1.76	0.50
23:B:170:C:H2'	23:B:171:A:H8	1.75	0.50
23:B:422:G:H2'	23:B:423:A:C8	2.47	0.50
23:B:2774:G:N2	23:B:2775:A:N7	2.59	0.50
34:LQ:101:THR:OG1	34:LQ:120:GLU:O	2.27	0.50
1:A:385:G:OP2	15:S7:4:LYS:NZ	2.45	0.50
1:A:1456:U:O2	1:A:1469:G:O6	2.30	0.50
6:SG:138:ARG:O	6:SG:142:HIS:CB	2.60	0.50
23:B:681:G:H1	32:LO:76:ILE:HD13	1.77	0.50
27:LJ:155:VAL:HB	27:LJ:194:ILE:HG22	1.93	0.50
23:B:225:A:N6	23:B:235:G:N3	2.60	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:B:674:C:N4	23:B:675:G:O6	2.45	0.49
23:B:1241:A:H2'	23:B:1242:A:C8	2.47	0.49
23:B:1710:G:O6	23:B:1711:G:N2	2.44	0.49
23:B:2849:A:OP1	26:LC:86:ARG:NH2	2.45	0.49
24:C:21:G:H1	24:C:58:G:H22	1.60	0.49
33:LP:17:THR:HG22	33:LP:96:VAL:HG21	1.94	0.49
1:A:129:A:H5''	1:A:130:A:H5'	1.95	0.49
1:A:690:U:H2'	1:A:691:G:H8	1.76	0.49
11:S3:113:GLY:HA2	11:S3:118:SER:HA	1.93	0.49
23:B:1254:C:H2'	23:B:1255:A:H8	1.77	0.49
23:B:2325:A:H2	23:B:2348:G:H2'	1.75	0.49
23:B:2565:C:H2'	23:B:2566:C:H6	1.77	0.49
25:L2:95:VAL:HG22	25:L2:101:LYS:HG2	1.93	0.49
1:A:682:G:H2'	1:A:683:A:H8	1.76	0.49
5:SE:45:LYS:HD3	5:SE:59:PHE:HE1	1.78	0.49
12:S4:59:VAL:O	12:S4:63:TYR:N	2.45	0.49
22:D:51:U:H3	22:D:63:G:H22	1.60	0.49
23:B:904:G:O2'	23:B:961:G:O6	2.30	0.49
23:B:1085:U:O2	23:B:1158:G:O6	2.30	0.49
23:B:2309:G:C2	23:B:2452:A:C5	3.00	0.49
1:A:410:G:OP1	1:A:629:A:O2'	2.30	0.49
23:B:1207:G:H21	38:L4:88:HIS:HE1	1.59	0.49
23:B:2599:A:H5''	23:B:2601:G:H4'	1.94	0.49
23:B:2715:G:N1	23:B:2747:U:OP2	2.40	0.49
1:A:448:U:N3	1:A:449:A:N7	2.61	0.49
23:B:1041:G:H5'	37:L3:91:ASN:HD22	1.77	0.49
23:B:2354:A:H2'	23:B:2355:A:C8	2.47	0.49
40:L6:9:ARG:NH2	40:L6:28:ASP:OD2	2.45	0.49
1:A:551:G:H2'	1:A:552:G:H8	1.77	0.49
23:B:1065:A:H2'	23:B:1066:G:H4'	1.95	0.49
23:B:2603:G:O2'	23:B:2606:C:OP2	2.31	0.49
27:LJ:4:TYR:HA	27:LJ:18:GLU:HA	1.94	0.49
1:A:251:A:N6	1:A:289:G:O2'	2.45	0.49
23:B:2330:G:O2'	23:B:2331:G:O4'	2.27	0.49
23:B:2492:C:H4'	51:LI:5:PRO:HG2	1.95	0.49
26:LC:200:ASN:OD1	26:LC:200:ASN:N	2.46	0.49
1:A:65:G:C2	1:A:100:A:N6	2.81	0.49
1:A:245:C:H2'	1:A:246:G:H8	1.78	0.49
6:SG:27:ILE:HD11	6:SG:40:GLN:HB3	1.95	0.49
7:SF:14:VAL:O	7:SF:18:ASN:HB2	2.12	0.49
21:E:51:U:H3	21:E:63:G:H22	1.60	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:B:579:U:O2'	37:L3:49:ASP:OD2	2.23	0.49
26:LC:118:VAL:HG11	26:LC:201:VAL:HB	1.94	0.49
26:LC:140:PRO:O	26:LC:145:SER:OG	2.31	0.49
41:L7:93:ILE:HG22	41:L7:99:GLU:HB3	1.95	0.49
1:A:1262:A:H4'	8:SH:16:ASN:HD21	1.78	0.49
1:A:1384:G:H1	8:SH:15:LYS:HE3	1.78	0.49
2:SB:28:PHE:O	2:SB:32:LEU:CB	2.61	0.49
23:B:1713:A:O2'	23:B:2576:G:OP1	2.30	0.49
23:B:2088:G:H2'	23:B:2090:C:H41	1.77	0.49
23:B:2824:G:O2'	23:B:2825:U:O4'	2.31	0.49
34:LQ:18:ARG:NE	34:LQ:67:ARG:HH21	2.11	0.49
2:SB:183:TYR:OH	2:SB:198:LYS:NZ	2.35	0.48
4:SD:95:PHE:O	4:SD:125:SER:HA	2.13	0.48
23:B:1490:G:O2'	23:B:1491:C:O4'	2.31	0.48
23:B:623:C:H42	23:B:1298:G:H1	1.61	0.48
23:B:720:A:OP1	27:LJ:63:LYS:NZ	2.46	0.48
30:LM:7:ALA:H	30:LM:46:THR:HG21	1.78	0.48
1:A:1025:G:H2'	1:A:1026:A:C8	2.48	0.48
5:SE:31:ALA:HA	5:SE:35:ALA:HB2	1.96	0.48
8:SH:74:PHE:O	8:SH:78:ALA:N	2.42	0.48
23:B:105:C:H2'	23:B:106:A:C8	2.48	0.48
23:B:1398:G:O2'	23:B:2242:G:O2'	2.27	0.48
23:B:2116:U:H2'	23:B:2117:A:H8	1.77	0.48
1:A:736:A:H2'	1:A:737:A:H8	1.78	0.48
3:SC:51:LEU:O	3:SC:55:GLN:CB	2.62	0.48
23:B:829:U:H3	25:L2:228:ASN:HD21	1.61	0.48
23:B:867:U:H2'	23:B:868:A:H8	1.79	0.48
23:B:1018:A:C5	23:B:1225:G:C2	3.01	0.48
23:B:1047:G:N2	23:B:1197:C:N3	2.61	0.48
23:B:1409:U:O4	23:B:1410:A:N6	2.46	0.48
23:B:1442:C:H2'	23:B:1443:A:C8	2.49	0.48
24:C:9:C:H2'	24:C:13:A:H61	1.78	0.48
1:A:567:A:H4'	1:A:568:A:H3'	1.96	0.48
1:A:602:U:C2	1:A:654:G:N1	2.82	0.48
1:A:1107:U:OP2	1:A:1120:G:N1	2.41	0.48
23:B:375:A:O2'	23:B:377:U:OP2	2.26	0.48
23:B:1175:G:N2	23:B:1176:U:O4	2.40	0.48
23:B:1315:C:O2'	34:LQ:23:SER:OG	2.29	0.48
23:B:1490:G:N2	23:B:1491:C:N3	2.62	0.48
23:B:2060:A:O2'	23:B:2062:G:OP2	2.31	0.48
23:B:908:A:OP2	33:LP:22:LYS:NZ	2.32	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:B:1227:U:H2'	23:B:1228:A:H8	1.79	0.48
34:LQ:103:ILE:HG22	34:LQ:119:ILE:HG22	1.94	0.48
41:L7:92:ARG:NH2	41:L7:103:SER:OG	2.44	0.48
1:A:422:A:H8	1:A:438:A:H61	1.60	0.48
1:A:449:A:H61	1:A:501:U:H1'	1.78	0.48
1:A:619:C:H42	1:A:638:G:H1	1.62	0.48
1:A:1306:U:O3'	12:S4:14:ARG:NH1	2.47	0.48
2:SB:14:ILE:HG13	2:SB:15:ILE:HG13	1.96	0.48
10:S2:21:ALA:HB3	10:S2:84:VAL:HA	1.95	0.48
39:L5:11:ARG:HH12	39:L5:98:LYS:HE2	1.79	0.48
4:SD:34:THR:HA	4:SD:51:GLY:O	2.14	0.48
23:B:813:G:H2'	23:B:814:A:C8	2.48	0.48
23:B:896:U:H2'	23:B:897:A:H8	1.79	0.48
23:B:1255:A:OP1	37:L3:15:LYS:NZ	2.37	0.48
23:B:1821:U:H2'	23:B:1822:C:C6	2.48	0.48
24:C:16:A:N3	24:C:65:G:N2	2.62	0.48
1:A:37:C:O2'	1:A:38:U:O5'	2.29	0.48
1:A:353:C:H5'	1:A:354:G:H5'	1.96	0.48
1:A:1388:A:OP2	6:SG:95:ARG:NH1	2.46	0.48
1:A:1448:C:H2'	1:A:1449:G:H8	1.79	0.48
1:A:1454:A:H2'	1:A:1455:G:H8	1.78	0.48
9:S1:40:ILE:HB	9:S1:73:LEU:HB3	1.95	0.48
23:B:1423:C:H2'	23:B:1424:A:C8	2.49	0.48
36:L1:16:ARG:H	36:L1:79:HIS:HD2	1.60	0.48
1:A:509:C:O2'	1:A:557:C:O2	2.32	0.48
23:B:66:C:H2'	23:B:67:G:H8	1.79	0.48
23:B:702:U:H2'	23:B:703:A:C8	2.48	0.48
23:B:896:U:H2'	23:B:897:A:C8	2.49	0.48
23:B:2465:U:O2'	23:B:2467:C:OP1	2.31	0.48
23:B:2703:C:H2'	23:B:2704:A:H8	1.79	0.48
1:A:432:G:H2'	1:A:433:A:C8	2.49	0.47
1:A:1148:A:H3'	1:A:1149:A:H4'	1.95	0.47
1:A:1367:G:H2'	1:A:1368:A:H8	1.78	0.47
23:B:1037:A:C5	23:B:1206:G:C6	2.92	0.47
23:B:2717:A:OP2	34:LQ:13:ARG:NH2	2.34	0.47
8:SH:14:ARG:O	8:SH:17:SER:OG	2.32	0.47
21:E:55:U:O2'	21:E:57:G:N7	2.47	0.47
23:B:829:U:O4	25:L2:228:ASN:ND2	2.48	0.47
23:B:1575:A:O2'	23:B:1576:A:O4'	2.31	0.47
23:B:2333:U:OP2	23:B:2334:G:N2	2.47	0.47
27:LJ:202:VAL:HA	27:LJ:205:VAL:HG12	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1380:C:H2'	1:A:1381:G:C8	2.49	0.47
1:A:1505:A:H3'	23:B:1940:A:H62	1.79	0.47
1:A:1524:U:H2'	1:A:1525:A:H8	1.80	0.47
9:S1:55:VAL:HG12	13:S5:42:ILE:HG12	1.97	0.47
22:D:72:C:H5'	22:D:73:A:C8	2.50	0.47
23:B:343:A:H3'	41:L7:80:ARG:HH22	1.80	0.47
23:B:441:C:H2'	23:B:442:G:H8	1.79	0.47
23:B:1652:A:O2'	23:B:1654:A:OP2	2.33	0.47
23:B:1880:A:N6	23:B:1916:A:N7	2.63	0.47
34:LQ:20:LEU:HD22	34:LQ:40:VAL:HG21	1.96	0.47
49:LG:25:THR:HG23	49:LG:28:GLY:H	1.79	0.47
1:A:209:G:H21	1:A:231:U:H1'	1.79	0.47
1:A:405:A:N6	1:A:555:A:O3'	2.46	0.47
1:A:722:G:H2'	1:A:723:A:H8	1.80	0.47
4:SD:45:ARG:HB3	4:SD:71:LEU:HD23	1.96	0.47
16:S8:64:GLN:O	16:S8:76:ARG:N	2.37	0.47
23:B:724:C:H2'	23:B:725:A:H8	1.79	0.47
23:B:797:A:OP1	49:LG:4:ARG:NH2	2.46	0.47
23:B:982:G:H2'	23:B:983:G:H8	1.79	0.47
1:A:157:G:H2'	1:A:158:G:H8	1.80	0.47
1:A:718:G:H2'	1:A:719:G:H8	1.79	0.47
23:B:1945:A:O2'	23:B:1946:A:N7	2.46	0.47
23:B:2455:G:H21	32:LO:60:ARG:NH2	2.13	0.47
23:B:2774:G:H1	23:B:2781:U:H2'	1.79	0.47
1:A:1410:C:N3	1:A:1514:A:N6	2.62	0.47
21:E:72:C:H5'	21:E:73:A:C8	2.50	0.47
23:B:904:G:N2	23:B:962:A:OP2	2.35	0.47
23:B:1460:U:H3	23:B:1628:A:H62	1.63	0.47
2:SB:22:TRP:HB3	2:SB:58:ARG:H	1.80	0.47
8:SH:75:THR:HA	8:SH:78:ALA:HB3	1.97	0.47
19:SA:32:VAL:HG12	19:SA:53:ALA:HB1	1.96	0.47
23:B:194:A:H2'	23:B:195:C:H6	1.80	0.47
23:B:900:G:O2'	43:L9:35:ASP:OD2	2.27	0.47
23:B:2068:U:H2'	23:B:2069:A:H8	1.78	0.47
23:B:2232:A:N1	23:B:2247:G:C2	2.83	0.47
23:B:2246:U:H2'	23:B:2247:G:C8	2.50	0.47
34:LQ:45:GLU:OE2	34:LQ:99:GLY:N	2.41	0.47
34:LQ:47:LEU:HD21	34:LQ:66:LEU:HD11	1.96	0.47
46:LD:33:SER:OG	46:LD:34:SER:N	2.47	0.47
1:A:550:U:H2'	1:A:551:G:H8	1.80	0.47
1:A:745:U:H2'	1:A:746:U:H6	1.80	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:832:U:H2'	1:A:833:G:H8	1.78	0.47
3:SC:68:PHE:O	3:SC:72:PHE:HB2	2.15	0.47
3:SC:120:LEU:HA	3:SC:125:ARG:HA	1.97	0.47
8:SH:53:PRO:HA	8:SH:56:VAL:HG22	1.95	0.47
19:SA:7:ALA:O	19:SA:10:ARG:N	2.48	0.47
23:B:1254:C:H2'	23:B:1255:A:C8	2.50	0.47
24:C:43:A:C8	28:LK:88:LYS:HE2	2.50	0.47
1:A:1402:U:H2'	1:A:1403:G:C8	2.49	0.47
23:B:21:A:N1	23:B:565:G:N1	2.60	0.47
4:SD:106:ILE:O	4:SD:125:SER:OG	2.32	0.47
4:SD:152:ASP:N	4:SD:152:ASP:OD1	2.47	0.47
14:S6:24:SER:H	14:S6:27:VAL:HG12	1.79	0.47
21:E:75:C:H42	23:B:2280:G:H1	1.63	0.47
23:B:246:U:H2'	23:B:247:A:H8	1.80	0.47
23:B:341:G:OP1	41:L7:83:TYR:N	2.43	0.47
23:B:1442:C:H2'	23:B:1443:A:H8	1.80	0.47
23:B:1794:C:C2	23:B:2013:G:N2	2.83	0.47
23:B:2082:C:H5'	23:B:2083:G:H5''	1.97	0.47
25:L2:50:THR:OG1	25:L2:51:VAL:N	2.47	0.47
1:A:650:A:N3	7:SF:107:SER:OG	2.43	0.46
1:A:1013:G:N1	1:A:1014:A:O2'	2.42	0.46
23:B:1520:A:C2	23:B:1521:A:H1'	2.50	0.46
23:B:2074:C:N4	23:B:2648:G:O6	2.47	0.46
1:A:118:A:N3	1:A:119:A:N6	2.64	0.46
23:B:459:C:N4	23:B:2437:G:O6	2.49	0.46
23:B:594:G:H2'	23:B:595:G:H8	1.80	0.46
23:B:1467:G:H2'	23:B:1468:G:C8	2.50	0.46
1:A:143:A:H5''	1:A:144:C:H5'	1.97	0.46
1:A:417:U:H3'	1:A:418:G:H8	1.79	0.46
1:A:637:A:H2'	1:A:638:G:H2'	1.97	0.46
1:A:1250:A:O2'	1:A:1309:C:N4	2.43	0.46
5:SE:36:GLU:HB2	5:SE:66:LYS:H	1.81	0.46
23:B:1218:G:O2'	23:B:1219:G:O4'	2.33	0.46
23:B:2388:A:OP1	50:LH:25:SER:OG	2.29	0.46
25:L2:26:LYS:HZ1	25:L2:29:PRO:HD3	1.79	0.46
30:LM:1:MET:SD	30:LM:1:MET:N	2.87	0.46
1:A:125:G:OP1	1:A:613:U:O2'	2.30	0.46
1:A:592:G:H2'	1:A:593:G:H8	1.81	0.46
1:A:1049:C:H2'	1:A:1050:A:O4'	2.15	0.46
9:S1:47:SER:OG	9:S1:67:GLN:NE2	2.49	0.46
23:B:345:C:H2'	23:B:346:A:C8	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:B:838:A:OP2	23:B:2098:A:O2'	2.26	0.46
23:B:872:U:N3	23:B:2457:A:C6	2.84	0.46
23:B:1569:G:H3'	23:B:1570:G:C8	2.50	0.46
24:C:87:G:N2	24:C:87:G:OP2	2.46	0.46
49:LG:5:THR:OG1	49:LG:6:TYR:N	2.49	0.46
1:A:765:U:OP1	1:A:830:A:O2'	2.31	0.46
1:A:1135:A:H4'	9:S1:38:GLY:HA3	1.98	0.46
7:SF:21:ARG:HH12	7:SF:70:ASP:HB3	1.81	0.46
12:S4:53:LEU:HD13	12:S4:57:ARG:HH12	1.79	0.46
23:B:1974:C:H2'	23:B:1975:G:H8	1.80	0.46
33:LP:21:SER:OG	33:LP:99:PRO:O	2.33	0.46
25:L2:157:SER:OG	25:L2:158:ALA:N	2.46	0.46
1:A:544:C:N4	1:A:545:G:O6	2.49	0.46
1:A:988:A:N6	1:A:1329:A:N7	2.64	0.46
1:A:1238:A:OP1	12:S4:107:ARG:NH2	2.44	0.46
1:A:1360:A:H5'	8:SH:125:ARG:HB2	1.97	0.46
2:SB:55:GLU:O	2:SB:65:ILE:HA	2.15	0.46
6:SG:24:THR:O	6:SG:28:ASN:ND2	2.48	0.46
13:S5:21:TYR:OH	13:S5:23:ARG:NH2	2.46	0.46
18:SI:12:ASP:OD2	18:SI:14:HIS:NE2	2.49	0.46
21:E:8:U:O2'	21:E:47:U:O2	2.28	0.46
22:D:8:U:O2'	22:D:47:U:O2	2.28	0.46
23:B:64:A:H2'	23:B:65:A:C8	2.50	0.46
23:B:1353:A:H2'	23:B:1354:G:H8	1.80	0.46
24:C:23:U:O2'	24:C:27:A:N6	2.49	0.46
31:LN:84:CYS:SG	31:LN:85:VAL:N	2.88	0.46
1:A:130:A:N6	1:A:241:U:O2'	2.49	0.46
1:A:1287:G:N2	1:A:1294:C:O4'	2.49	0.46
23:B:1099:G:N2	23:B:1149:U:OP2	2.49	0.46
23:B:2331:G:O2'	28:LK:122:PHE:O	2.33	0.46
29:LL:41:MET:HE1	29:LL:65:HIS:CD2	2.51	0.46
2:SB:90:LEU:HA	2:SB:93:LEU:HD23	1.98	0.46
7:SF:94:MET:HB3	7:SF:119:ARG:HH12	1.80	0.46
23:B:304:G:H2'	23:B:305:A:H8	1.81	0.46
23:B:2070:C:N3	23:B:2804:G:N2	2.64	0.46
23:B:2725:U:H2'	23:B:2726:C:C6	2.51	0.46
37:L3:52:GLN:HG2	37:L3:55:ARG:HH21	1.81	0.46
46:LD:51:LYS:O	46:LD:52:HIS:ND1	2.49	0.46
1:A:440:A:H5''	1:A:441:A:N7	2.31	0.46
1:A:703:A:H2'	1:A:704:A:C8	2.51	0.46
1:A:1108:C:O2'	1:A:1181:A:O2'	2.31	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:S6:17:VAL:HG23	14:S6:19:GLU:HG2	1.98	0.46
23:B:614:U:N3	23:B:2057:A:N1	2.63	0.46
23:B:2783:U:OP2	51:LI:19:ARG:NH2	2.49	0.46
1:A:143:A:H1'	1:A:210:A:H2'	1.98	0.45
1:A:425:G:O6	1:A:434:U:O4	2.34	0.45
1:A:894:U:H4'	1:A:895:G:H5''	1.98	0.45
6:SG:103:TRP:CD1	6:SG:106:ASN:HD21	2.34	0.45
23:B:123:G:N2	23:B:125:A:O2'	2.48	0.45
23:B:259:A:H2'	23:B:260:A:C8	2.51	0.45
23:B:828:A:H2'	23:B:829:U:H4'	1.98	0.45
23:B:1548:U:O4	23:B:1549:C:N4	2.48	0.45
23:B:2539:C:O2	26:LC:153:SER:OG	2.34	0.45
1:A:385:G:H2'	1:A:386:G:C8	2.51	0.45
8:SH:115:ARG:HH22	13:S5:61:TRP:CD1	2.34	0.45
23:B:35:G:H2'	23:B:36:G:H8	1.81	0.45
23:B:306:C:H2'	23:B:307:A:C8	2.52	0.45
23:B:443:U:H5''	44:LA:32:ASN:HB2	1.98	0.45
23:B:608:C:H2'	23:B:609:U:C6	2.52	0.45
31:LN:22:ILE:HG23	31:LN:40:VAL:HG13	1.97	0.45
1:A:22:G:N2	1:A:924:A:H62	2.05	0.45
10:S2:67:SER:O	10:S2:71:SER:OG	2.29	0.45
16:S8:17:ASP:OD1	16:S8:22:THR:OG1	2.30	0.45
23:B:192:G:H2'	23:B:208:G:H22	1.79	0.45
23:B:1037:A:N6	23:B:1206:G:H1	2.14	0.45
23:B:1039:C:O2'	37:L3:93:LYS:NZ	2.48	0.45
23:B:1407:C:O2'	23:B:1838:G:O2'	2.35	0.45
33:LP:30:GLY:HA2	33:LP:107:ALA:HB2	1.99	0.45
51:LI:19:ARG:HD2	51:LI:24:MET:HG3	1.98	0.45
2:SB:86:LEU:HA	2:SB:89:LYS:HB3	1.98	0.45
4:SD:81:THR:HG23	4:SD:98:PRO:HG3	1.98	0.45
23:B:2051:C:H2'	23:B:2052:C:H6	1.82	0.45
25:L2:133:GLN:NE2	25:L2:134:ASN:OD1	2.49	0.45
37:L3:108:GLN:O	37:L3:111:THR:OG1	2.26	0.45
1:A:522:C:H2'	1:A:523:G:C8	2.52	0.45
1:A:1337:U:H2'	1:A:1338:A:C8	2.51	0.45
6:SG:103:TRP:HB3	6:SG:134:ALA:HB1	1.99	0.45
9:S1:50:THR:HA	9:S1:64:GLN:HA	1.98	0.45
10:S2:94:GLU:HA	10:S2:97:ILE:HG22	1.99	0.45
23:B:1835:U:O2'	23:B:1836:A:O4'	2.34	0.45
23:B:2077:C:N4	23:B:2078:A:N1	2.64	0.45
23:B:2514:G:H2'	23:B:2515:A:C8	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:B:2767:A:H2'	23:B:2768:A:H8	1.81	0.45
23:B:2877:G:N2	23:B:2880:A:OP2	2.40	0.45
1:A:722:G:H2'	1:A:723:A:C8	2.51	0.45
1:A:916:G:O2'	1:A:917:A:O4'	2.31	0.45
1:A:1221:C:N4	1:A:1222:U:O4	2.50	0.45
17:S9:47:ARG:HA	17:S9:57:GLN:HE22	1.82	0.45
23:B:968:A:H4'	43:L9:37:GLN:HB3	1.99	0.45
23:B:1590:C:H2'	23:B:1591:G:C4	2.52	0.45
23:B:1823:U:H2'	23:B:1824:C:H6	1.82	0.45
23:B:2406:G:H2'	23:B:2407:A:H8	1.81	0.45
1:A:251:A:N7	1:A:289:G:N2	2.61	0.45
1:A:1260:C:O2'	8:SH:77:GLN:OE1	2.31	0.45
10:S2:23:ILE:HG22	10:S2:32:VAL:HA	1.98	0.45
23:B:84:A:N1	23:B:98:U:O2'	2.49	0.45
23:B:2618:C:H2'	23:B:2619:G:C8	2.51	0.45
32:LO:91:VAL:HG22	32:LO:123:VAL:HA	1.98	0.45
35:LR:15:HIS:NE2	35:LR:91:GLU:OE2	2.49	0.45
1:A:383:U:O2	15:S7:29:ARG:NH2	2.50	0.45
3:SC:70:ASN:O	3:SC:74:ILE:CB	2.64	0.45
19:SA:15:GLU:O	19:SA:19:ALA:CB	2.64	0.45
19:SA:15:GLU:O	19:SA:19:ALA:HB2	2.17	0.45
1:A:65:G:C2	1:A:100:A:C6	3.05	0.45
1:A:431:G:O2'	1:A:432:G:O4'	2.35	0.45
1:A:1245:C:O2'	1:A:1375:U:O2	2.30	0.45
1:A:1248:C:O2'	1:A:1345:G:N2	2.49	0.45
1:A:1266:G:H3'	1:A:1290:A:H61	1.82	0.45
1:A:1359:U:H4'	8:SH:124:ARG:HG3	1.99	0.45
23:B:460:C:H2'	23:B:461:A:H8	1.81	0.45
23:B:741:G:H1	23:B:812:U:H3	1.64	0.45
36:L1:16:ARG:H	36:L1:79:HIS:CD2	2.35	0.45
37:L3:50:ARG:O	37:L3:54:LYS:NZ	2.48	0.45
41:L7:12:ILE:HD11	41:L7:69:GLN:HB2	1.99	0.45
48:LS:9:CYS:HB3	48:LS:12:CYS:HB2	1.49	0.45
1:A:370:G:N2	1:A:373:U:OP2	2.50	0.45
1:A:1374:A:O2'	1:A:1376:G:N7	2.37	0.45
6:SG:9:LYS:HD3	6:SG:11:ASP:H	1.81	0.45
7:SF:78:LYS:NZ	7:SF:79:ARG:O	2.48	0.45
19:SA:69:ASN:HD22	19:SA:72:ASP:HB3	1.82	0.45
23:B:1768:C:H2'	23:B:1769:C:C6	2.51	0.45
23:B:2026:C:H2'	23:B:2027:G:H8	1.81	0.45
26:LC:2:THR:HA	26:LC:94:VAL:HG11	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:800:A:O2'	1:A:802:A:N7	2.44	0.44
2:SB:6:ASN:OD1	2:SB:6:ASN:N	2.51	0.44
17:S9:57:GLN:HA	17:S9:60:LEU:HB2	1.98	0.44
23:B:94:A:H2'	23:B:95:A:C8	2.52	0.44
23:B:1493:U:O2	23:B:1506:C:N3	2.50	0.44
23:B:2833:U:H2'	23:B:2834:C:H6	1.82	0.44
41:L7:47:PRO:HA	41:L7:54:GLY:H	1.81	0.44
1:A:379:G:H21	1:A:381:A:H62	1.66	0.44
1:A:461:C:C4	1:A:488:U:O4	2.70	0.44
1:A:529:G:H4'	11:S3:83:ILE:HG13	1.99	0.44
1:A:1271:G:N2	1:A:1286:A:H62	2.16	0.44
4:SD:55:GLU:OE1	4:SD:58:GLU:N	2.47	0.44
18:SI:25:SER:OG	18:SI:26:GLU:N	2.50	0.44
19:SA:72:ASP:O	19:SA:76:SER:CB	2.65	0.44
24:C:47:C:OP2	35:LR:35:ARG:NH1	2.29	0.44
39:L5:12:ILE:H	39:L5:12:ILE:HG13	1.42	0.44
1:A:405:A:N6	1:A:555:A:O2'	2.51	0.44
1:A:1133:U:H3	1:A:1164:G:H22	1.66	0.44
1:A:1246:U:O2'	1:A:1316:G:OP1	2.31	0.44
5:SE:23:VAL:O	5:SE:27:ASN:ND2	2.50	0.44
23:B:885:C:H42	23:B:982:G:H1	1.64	0.44
23:B:990:G:O6	23:B:1016:G:N2	2.50	0.44
23:B:2494:C:OP1	51:LI:8:LYS:NZ	2.48	0.44
25:L2:132:LEU:HD22	25:L2:135:ILE:HD12	1.98	0.44
32:LO:19:VAL:HG22	32:LO:31:SER:HB2	2.00	0.44
35:LR:32:ASN:HA	35:LR:91:GLU:HB3	1.99	0.44
40:L6:51:ALA:N	40:L6:81:THR:O	2.46	0.44
52:LF:17:THR:HG23	52:LF:18:THR:HG23	1.98	0.44
1:A:277:U:H2'	1:A:278:A:C8	2.51	0.44
1:A:1167:G:H21	1:A:1191:A:H61	1.65	0.44
1:A:1198:G:O5'	8:SH:117:LYS:NZ	2.47	0.44
23:B:1600:A:O2'	23:B:1601:U:O4'	2.34	0.44
23:B:1767:G:H5''	23:B:1768:C:H5	1.82	0.44
23:B:2813:U:H2'	23:B:2814:C:H6	1.82	0.44
2:SB:95:ASP:OD1	2:SB:95:ASP:N	2.51	0.44
21:E:72:C:H3'	21:E:73:A:H8	1.83	0.44
22:D:72:C:H3'	22:D:73:A:H8	1.83	0.44
23:B:106:A:H2'	23:B:107:G:C8	2.52	0.44
23:B:1210:U:H2'	23:B:1211:G:C8	2.52	0.44
23:B:1763:U:O2	23:B:1767:G:N1	2.49	0.44
23:B:2553:G:O2'	51:LI:1:MET:N	2.36	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:B:2574:U:H2'	23:B:2575:G:C8	2.53	0.44
1:A:614:G:H2'	1:A:639:G:H2'	1.99	0.44
1:A:1120:G:H5'	2:SB:175:HIS:HD2	1.83	0.44
1:A:1464:U:C4	1:A:1465:A:H1'	2.53	0.44
13:S5:6:MET:HA	13:S5:9:LYS:HE2	1.99	0.44
23:B:1183:G:OP1	30:LM:105:SER:OG	2.24	0.44
29:LL:5:GLY:HA2	29:LL:65:HIS:CE1	2.52	0.44
37:L3:103:GLU:O	37:L3:107:ALA:N	2.51	0.44
1:A:623:C:H2'	1:A:624:G:C8	2.52	0.44
5:SE:10:VAL:HB	5:SE:59:PHE:HB2	2.00	0.44
6:SG:135:VAL:HG13	6:SG:138:ARG:HD2	1.99	0.44
23:B:991:A:H2'	23:B:992:A:C8	2.53	0.44
23:B:2216:U:H2'	23:B:2217:G:C8	2.53	0.44
23:B:2659:A:H2'	23:B:2660:A:C8	2.52	0.44
23:B:2670:G:H2'	23:B:2671:A:H8	1.82	0.44
1:A:103:G:H2'	1:A:104:G:C8	2.53	0.44
1:A:158:G:H2'	1:A:159:G:C8	2.53	0.44
1:A:1489:C:H2'	1:A:1490:A:C8	2.53	0.44
5:SE:11:ARG:HG2	5:SE:13:ASN:H	1.83	0.44
14:S6:3:ILE:HD12	14:S6:8:LYS:HB2	1.99	0.44
23:B:526:A:O2'	41:L7:42:LYS:O	2.33	0.44
23:B:631:U:H2'	23:B:632:U:C6	2.52	0.44
23:B:1477:U:H2'	23:B:1478:A:C8	2.53	0.44
24:C:41:C:OP1	52:LF:6:HIS:NE2	2.48	0.44
27:LJ:60:GLY:HA2	27:LJ:78:ILE:HG22	2.00	0.44
30:LM:126:TYR:CE2	30:LM:132:PRO:HD2	2.53	0.44
1:A:387:C:H2'	1:A:388:G:H8	1.83	0.44
1:A:420:U:H4'	1:A:421:G:C5	2.53	0.44
1:A:420:U:H4'	1:A:421:G:N7	2.32	0.44
1:A:924:A:H2'	1:A:925:A:C8	2.52	0.44
10:S2:35:THR:OG1	10:S2:40:ASN:N	2.51	0.44
23:B:323:C:N4	23:B:324:A:N1	2.65	0.44
23:B:345:C:H2'	23:B:346:A:H8	1.82	0.44
23:B:1051:C:H4'	30:LM:111:PRO:HD3	1.99	0.44
23:B:2767:A:H2'	23:B:2768:A:C8	2.53	0.44
6:SG:54:SER:OG	6:SG:55:GLY:N	2.51	0.43
8:SH:30:ILE:H	8:SH:30:ILE:HG13	1.55	0.43
18:SI:9:PRO:HB2	18:SI:39:THR:HG21	2.00	0.43
23:B:145:A:H2'	23:B:146:U:C6	2.53	0.43
23:B:498:G:H21	23:B:503:A:H8	1.66	0.43
23:B:2048:G:OP1	47:LE:9:SER:OG	2.35	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:C:15:C:H42	24:C:66:C:H42	1.66	0.43
38:L4:23:GLU:OE1	38:L4:24:LYS:N	2.50	0.43
1:A:1454:A:H2'	1:A:1455:G:C8	2.53	0.43
12:S4:23:TYR:HE2	12:S4:70:ARG:HH22	1.66	0.43
16:S8:30:TYR:HB3	16:S8:39:ARG:HD2	2.00	0.43
23:B:277:C:H2'	23:B:278:A:C8	2.53	0.43
23:B:1423:C:H2'	23:B:1424:A:H8	1.83	0.43
25:L2:76:ALA:HB1	25:L2:94:VAL:HB	1.99	0.43
27:LJ:101:MET:HE2	27:LJ:101:MET:HB2	1.86	0.43
27:LJ:157:GLU:HA	27:LJ:198:ALA:HB2	2.00	0.43
5:SE:38:LEU:HB3	5:SE:64:ARG:HH21	1.83	0.43
8:SH:22:ARG:HH11	8:SH:66:LEU:HD12	1.83	0.43
19:SA:57:VAL:O	19:SA:61:ALA:HB2	2.19	0.43
23:B:681:G:N7	32:LO:110:LYS:NZ	2.52	0.43
23:B:1865:C:H4'	23:B:1866:G:H5'	1.99	0.43
23:B:2113:U:H2'	23:B:2114:G:H8	1.82	0.43
23:B:2274:A:H2'	23:B:2275:C:H6	1.84	0.43
23:B:2591:A:OP1	23:B:2675:G:O2'	2.34	0.43
28:LK:38:MET:HE1	28:LK:50:LEU:HB3	1.99	0.43
30:LM:38:ARG:HA	30:LM:119:GLN:NE2	2.32	0.43
4:SD:25:VAL:HG12	4:SD:26:LYS:H	1.82	0.43
7:SF:108:THR:OG1	7:SF:109:SER:N	2.52	0.43
22:D:55:U:O2'	22:D:57:G:N7	2.47	0.43
23:B:994:A:OP1	24:C:85:A:N6	2.51	0.43
23:B:1044:A:H2'	23:B:1045:A:C8	2.52	0.43
23:B:1818:A:H4'	25:L2:205:VAL:HG23	2.01	0.43
23:B:1827:C:OP2	25:L2:182:ARG:NH2	2.48	0.43
44:LA:37:ARG:HA	44:LA:46:LYS:HA	2.01	0.43
1:A:385:G:O6	1:A:395:U:C4	2.72	0.43
1:A:400:G:H2'	1:A:401:A:C8	2.53	0.43
1:A:1137:U:H5	9:S1:73:LEU:HD11	1.83	0.43
8:SH:69:VAL:HG13	8:SH:77:GLN:HE21	1.82	0.43
12:S4:15:VAL:HA	12:S4:18:SER:HB3	1.99	0.43
23:B:320:U:O2'	23:B:321:U:O4'	2.32	0.43
30:LM:89:THR:HB	30:LM:93:LEU:HD12	1.99	0.43
33:LP:35:GLN:HB3	33:LP:102:ILE:HD13	1.99	0.43
34:LQ:24:LEU:HD12	34:LQ:44:VAL:HG21	2.01	0.43
39:L5:4:LYS:HB3	39:L5:106:VAL:HG12	2.00	0.43
1:A:974:A:C8	1:A:979:A:H1'	2.53	0.43
2:SB:19:GLU:HB3	13:S5:52:GLN:HA	2.01	0.43
7:SF:85:LEU:HD12	11:S3:4:ILE:HG13	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:SH:56:VAL:O	8:SH:102:ARG:NH2	2.50	0.43
23:B:1095:A:H61	23:B:1152:U:H3	1.65	0.43
1:A:385:G:H2'	1:A:386:G:H8	1.83	0.43
1:A:842:U:H2'	1:A:843:A:H8	1.84	0.43
1:A:1138:U:H2'	1:A:1292:U:H1'	2.01	0.43
23:B:273:A:N1	23:B:415:U:O2'	2.51	0.43
23:B:1323:A:H5''	34:LQ:110:ARG:HD2	2.01	0.43
23:B:2122:A:H2'	23:B:2123:A:H8	1.84	0.43
1:A:406:C:H2'	1:A:407:G:C8	2.53	0.43
1:A:973:G:O2'	1:A:974:A:O4'	2.35	0.43
1:A:984:A:OP2	13:S5:41:ARG:NE	2.52	0.43
1:A:1457:A:N7	1:A:1458:A:N6	2.66	0.43
6:SG:130:ASN:ND2	6:SG:135:VAL:HG11	2.34	0.43
9:S1:34:ALA:HB2	9:S1:83:THR:HG21	2.00	0.43
15:S7:3:VAL:HG23	15:S7:65:ALA:HA	2.00	0.43
17:S9:37:PHE:CD2	17:S9:60:LEU:HD21	2.54	0.43
23:B:497:U:C2	23:B:499:A:C8	2.96	0.43
23:B:1241:A:H2'	23:B:1242:A:H8	1.82	0.43
28:LK:51:ASP:OD1	28:LK:51:ASP:N	2.51	0.43
1:A:419:A:C8	1:A:421:G:H5'	2.54	0.43
1:A:1526:U:H2'	1:A:1527:C:H6	1.83	0.43
7:SF:83:PRO:HA	7:SF:86:ARG:HH12	1.83	0.43
23:B:767:A:H2'	23:B:768:A:H8	1.84	0.43
23:B:1039:C:OP1	37:L3:53:ARG:NH1	2.51	0.43
34:LQ:61:ASN:HA	34:LQ:64:LYS:HG2	2.01	0.43
39:L5:11:ARG:NH1	39:L5:98:LYS:HB3	2.33	0.43
41:L7:83:TYR:CE1	41:L7:92:ARG:HG2	2.54	0.43
1:A:798:A:H2'	1:A:799:G:C8	2.54	0.43
1:A:1252:G:H2'	1:A:1253:G:H8	1.82	0.43
2:SB:152:VAL:HG13	2:SB:195:LEU:HD21	2.00	0.43
23:B:994:A:H5''	24:C:85:A:H61	1.84	0.43
23:B:1831:A:OP2	25:L2:261:ARG:NH2	2.52	0.43
23:B:2070:C:OP1	23:B:2804:G:O2'	2.32	0.43
43:L9:26:SER:OG	43:L9:28:ARG:NH2	2.52	0.43
6:SG:15:ASP:CG	6:SG:20:SER:H	2.27	0.42
23:B:736:C:H2'	23:B:737:C:H6	1.83	0.42
23:B:894:A:O3'	46:LD:21:LYS:NZ	2.52	0.42
23:B:2107:G:H5'	44:LA:19:SER:HB2	2.02	0.42
23:B:2915:C:H2'	23:B:2916:U:C6	2.54	0.42
25:L2:163:GLN:HE21	25:L2:175:ARG:HD2	1.84	0.42
51:LI:2:LYS:HE3	51:LI:4:ARG:HH12	1.83	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:775:A:H2'	1:A:776:A:H8	1.83	0.42
2:SB:124:GLU:HB2	2:SB:190:THR:HG23	2.01	0.42
2:SB:135:GLN:HA	2:SB:138:THR:HG22	2.00	0.42
6:SG:15:ASP:OD2	6:SG:20:SER:N	2.51	0.42
23:B:1085:U:H2'	23:B:1086:G:H8	1.84	0.42
23:B:2094:G:N2	23:B:2471:G:N3	2.66	0.42
1:A:32:G:N2	1:A:49:C:OP1	2.44	0.42
1:A:57:U:H2'	1:A:58:G:C8	2.54	0.42
1:A:551:G:H2'	1:A:552:G:C8	2.52	0.42
23:B:257:G:O2'	23:B:258:A:O4'	2.35	0.42
23:B:923:A:N6	23:B:946:A:N7	2.66	0.42
23:B:1823:U:H2'	23:B:1824:C:C6	2.54	0.42
23:B:2838:C:O2'	23:B:2839:A:H8	2.02	0.42
31:LN:7:ARG:NE	31:LN:18:GLU:OE2	2.52	0.42
38:L4:70:LYS:HB2	38:L4:89:ARG:HH11	1.84	0.42
1:A:461:C:N3	1:A:488:U:C4	2.88	0.42
1:A:773:G:N1	1:A:820:G:O2'	2.49	0.42
1:A:861:U:H2'	1:A:862:A:C8	2.55	0.42
1:A:1024:A:H2'	1:A:1025:G:C8	2.55	0.42
2:SB:161:ILE:HG13	2:SB:163:ARG:HH11	1.84	0.42
8:SH:41:LEU:HD12	8:SH:47:ILE:HG23	2.01	0.42
8:SH:85:ILE:O	8:SH:89:LEU:CB	2.62	0.42
9:S1:30:LYS:HE3	9:S1:36:VAL:HB	2.02	0.42
11:S3:20:ASP:OD1	11:S3:21:SER:N	2.51	0.42
18:SI:67:VAL:HG23	52:LF:70:ARG:HH12	1.84	0.42
23:B:865:A:N3	23:B:987:U:O2'	2.43	0.42
29:LL:122:THR:N	29:LL:134:GLU:O	2.53	0.42
32:LO:123:VAL:HG21	32:LO:136:ILE:HD13	2.02	0.42
7:SF:11:LEU:HD13	7:SF:77:LEU:HD11	2.02	0.42
15:S7:30:ASP:OD1	15:S7:30:ASP:N	2.49	0.42
23:B:1911:A:H2'	23:B:1912:A:C8	2.53	0.42
23:B:2111:C:H2'	23:B:2112:C:C6	2.55	0.42
23:B:2355:A:H2'	23:B:2356:A:H8	1.83	0.42
23:B:2918:A:H2'	23:B:2919:A:C8	2.55	0.42
25:L2:91:ILE:HD12	25:L2:105:ILE:HA	2.02	0.42
1:A:455:G:OP1	1:A:495:A:N6	2.52	0.42
1:A:748:U:OP1	14:S6:2:ALA:N	2.52	0.42
6:SG:92:ARG:HH12	6:SG:95:ARG:HE	1.66	0.42
1:A:387:C:H2'	1:A:388:G:C8	2.54	0.42
1:A:988:A:O2'	1:A:1333:C:N3	2.47	0.42
1:A:1133:U:H3	1:A:1164:G:N2	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1134:U:H2'	1:A:1135:A:C8	2.55	0.42
1:A:1136:G:H22	1:A:1161:U:H3	1.67	0.42
1:A:1423:C:H2'	1:A:1424:A:C8	2.55	0.42
2:SB:14:ILE:HD11	2:SB:177:LEU:HD12	2.01	0.42
10:S2:34:ILE:H	10:S2:34:ILE:HG13	1.61	0.42
23:B:650:U:O3'	27:LJ:100:LYS:NZ	2.53	0.42
23:B:654:C:H2'	23:B:655:A:H8	1.85	0.42
23:B:780:A:H3'	23:B:781:C:H6	1.84	0.42
23:B:1587:C:H2'	23:B:1588:U:C2	2.55	0.42
30:LM:21:ALA:HB1	30:LM:63:ILE:HD11	2.01	0.42
1:A:157:G:H2'	1:A:158:G:C8	2.55	0.42
1:A:719:G:H2'	1:A:720:A:H8	1.85	0.42
1:A:745:U:H2'	1:A:746:U:C6	2.55	0.42
1:A:904:G:H2'	1:A:905:A:H8	1.84	0.42
1:A:960:U:H2'	1:A:961:G:H8	1.84	0.42
23:B:109:G:H2'	23:B:110:A:C8	2.55	0.42
23:B:219:A:H2'	23:B:220:A:C8	2.54	0.42
23:B:1027:A:N6	23:B:1028:G:O6	2.52	0.42
23:B:2649:U:H5'	26:LC:172:ARG:HE	1.84	0.42
24:C:20:A:H2'	24:C:21:G:C8	2.55	0.42
25:L2:72:ASP:OD1	25:L2:72:ASP:N	2.52	0.42
26:LC:105:VAL:HG23	26:LC:106:SER:H	1.85	0.42
1:A:240:A:H2'	1:A:241:U:C6	2.54	0.42
1:A:364:A:N3	1:A:376:U:O2'	2.51	0.42
1:A:1048:A:H2'	1:A:1049:C:C4	2.54	0.42
1:A:1201:G:O2'	2:SB:2:GLY:N	2.39	0.42
23:B:675:G:N2	23:B:677:A:H3'	2.35	0.42
23:B:1037:A:N6	23:B:1206:G:N1	2.67	0.42
23:B:1487:G:H1	23:B:1597:U:H3	1.68	0.42
23:B:2444:C:H2'	23:B:2445:A:H8	1.85	0.42
24:C:2:C:H2'	24:C:3:U:H6	1.85	0.42
1:A:328:A:H2'	1:A:329:A:C8	2.55	0.42
1:A:398:C:H4'	15:S7:29:ARG:HH12	1.85	0.42
1:A:1092:A:H5''	4:SD:21:VAL:HG11	2.01	0.42
14:S6:36:ILE:O	14:S6:40:ASN:N	2.44	0.42
23:B:60:U:O2	23:B:74:U:O2'	2.32	0.42
23:B:872:U:C2	23:B:2457:A:C6	3.08	0.42
23:B:2864:A:O4'	36:L1:2:THR:N	2.53	0.42
24:C:18:G:H1	24:C:61:U:H3	1.67	0.42
30:LM:30:SER:OG	30:LM:30:SER:O	2.38	0.42
40:L6:20:MET:HE3	40:L6:20:MET:HB3	1.92	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:904:G:H2'	1:A:905:A:C8	2.55	0.41
4:SD:70:ASP:OD1	4:SD:70:ASP:N	2.53	0.41
15:S7:72:HIS:HA	15:S7:75:LEU:HB2	2.02	0.41
18:SI:50:ALA:HB1	18:SI:57:HIS:CG	2.54	0.41
23:B:1577:G:H21	23:B:1590:C:H41	1.68	0.41
23:B:2024:A:O5'	26:LC:138:ARG:NH1	2.52	0.41
23:B:2562:G:H2'	23:B:2563:G:H8	1.85	0.41
24:C:47:C:H2'	24:C:48:A:C8	2.55	0.41
32:LO:68:ASN:ND2	32:LO:70:ASN:O	2.52	0.41
37:L3:53:ARG:HH11	37:L3:53:ARG:HD2	1.69	0.41
1:A:509:C:H42	1:A:553:C:H42	1.67	0.41
1:A:699:G:N2	1:A:704:A:OP2	2.47	0.41
1:A:721:G:H2'	1:A:722:G:C8	2.55	0.41
1:A:1261:A:H2'	1:A:1262:A:C8	2.54	0.41
1:A:1498:G:H2'	1:A:1499:G:C8	2.56	0.41
21:E:51:U:H2'	21:E:52:G:C8	2.55	0.41
21:E:51:U:H2'	21:E:52:G:H8	1.84	0.41
23:B:879:U:H2'	23:B:880:A:H8	1.85	0.41
33:LP:25:ASN:HA	33:LP:102:ILE:HG12	2.02	0.41
1:A:329:A:H2'	1:A:330:C:C6	2.53	0.41
1:A:614:G:C8	1:A:639:G:H3'	2.55	0.41
1:A:1071:U:O3'	13:S5:45:ARG:NH2	2.51	0.41
14:S6:70:LEU:HD21	14:S6:77:ARG:HB2	2.02	0.41
22:D:51:U:H2'	22:D:52:G:H8	1.84	0.41
23:B:317:G:O6	23:B:403:U:C4	2.73	0.41
23:B:877:G:H2'	23:B:878:C:C6	2.55	0.41
23:B:2406:G:H2'	23:B:2407:A:C8	2.55	0.41
23:B:2623:U:O4	23:B:2624:G:N2	2.54	0.41
38:L4:6:GLU:HB3	38:L4:11:GLN:HG2	2.02	0.41
1:A:1095:U:O2'	1:A:1114:A:OP2	2.24	0.41
1:A:1182:A:H2'	1:A:1183:C:C6	2.55	0.41
1:A:1209:A:H2'	1:A:1210:U:C6	2.55	0.41
1:A:1485:G:H2'	1:A:1486:G:C8	2.55	0.41
10:S2:59:THR:OG1	10:S2:62:ALA:N	2.47	0.41
23:B:187:C:O2'	23:B:220:A:N3	2.52	0.41
23:B:290:U:H2'	23:B:291:G:C8	2.55	0.41
23:B:1059:A:H2'	23:B:1060:U:H6	1.86	0.41
23:B:1312:A:N7	34:LQ:12:GLN:NE2	2.60	0.41
23:B:1326:C:H2'	23:B:1327:C:H6	1.83	0.41
25:L2:124:ILE:HG22	25:L2:130:LEU:HD21	2.03	0.41
25:L2:150:LYS:HD2	25:L2:153:GLN:HE22	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:LO:55:LEU:HA	32:LO:56:PRO:HD3	1.91	0.41
34:LQ:34:GLU:O	34:LQ:37:ALA:N	2.53	0.41
35:LR:34:TYR:HB3	35:LR:41:TYR:HB2	2.02	0.41
48:LS:31:GLU:HG2	48:LS:46:ARG:HA	2.02	0.41
1:A:11:A:H2'	1:A:12:G:H8	1.83	0.41
1:A:460:A:O2'	1:A:461:C:O4'	2.39	0.41
1:A:718:G:H2'	1:A:719:G:C8	2.54	0.41
1:A:994:C:H2'	1:A:995:C:C6	2.55	0.41
10:S2:101:GLN:NE2	10:S2:107:VAL:H	2.18	0.41
23:B:731:U:O4'	49:LG:12:LYS:NZ	2.52	0.41
24:C:19:G:H2'	24:C:20:A:C8	2.56	0.41
25:L2:243:ARG:HA	25:L2:244:PRO:HD3	1.88	0.41
38:L4:25:LEU:HD13	38:L4:25:LEU:HA	1.85	0.41
39:L5:8:ARG:HD3	39:L5:102:HIS:HE1	1.85	0.41
45:LB:7:ARG:HD2	45:LB:9:LEU:HD13	2.02	0.41
1:A:55:C:OP1	1:A:359:G:N2	2.53	0.41
1:A:97:G:H1'	1:A:98:U:H5	1.86	0.41
1:A:148:G:H21	1:A:1458:A:H2	1.67	0.41
1:A:618:G:N2	1:A:619:C:O2	2.53	0.41
1:A:636:G:H2'	1:A:637:A:N3	2.35	0.41
1:A:842:U:H2'	1:A:843:A:C8	2.55	0.41
1:A:962:U:H2'	1:A:963:G:C8	2.52	0.41
1:A:1260:C:O2'	8:SH:73:GLY:O	2.38	0.41
1:A:1271:G:H21	1:A:1286:A:N6	2.19	0.41
1:A:1496:U:HO2'	23:B:1987:A:HO2'	1.69	0.41
7:SF:9:ASP:OD1	7:SF:9:ASP:N	2.54	0.41
23:B:346:A:H2'	23:B:347:U:C6	2.56	0.41
23:B:621:A:OP1	23:B:1293:U:O2'	2.34	0.41
23:B:2703:C:H2'	23:B:2704:A:C8	2.55	0.41
1:A:375:U:O5'	1:A:402:G:N2	2.54	0.41
1:A:1292:U:OP2	1:A:1293:C:N4	2.45	0.41
22:D:51:U:H2'	22:D:52:G:C8	2.55	0.41
23:B:2122:A:H2'	23:B:2123:A:C8	2.56	0.41
27:LJ:18:GLU:O	27:LJ:20:SER:N	2.51	0.41
28:LK:153:ASP:OD1	28:LK:153:ASP:N	2.51	0.41
34:LQ:72:LEU:HD13	34:LQ:72:LEU:HA	1.90	0.41
37:L3:44:GLN:HE22	38:L4:76:TYR:H	1.69	0.41
1:A:251:A:N7	1:A:289:G:N1	2.69	0.41
1:A:830:A:N6	1:A:889:C:H42	2.18	0.41
1:A:1029:G:H2'	1:A:1030:A:C8	2.56	0.41
18:SI:39:THR:OG1	18:SI:40:ILE:N	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:B:290:U:H2'	23:B:291:G:H8	1.85	0.41
23:B:1508:C:N3	23:B:1509:G:N1	2.68	0.41
24:C:112:G:H2'	24:C:113:G:C8	2.56	0.41
35:LR:39:HIS:CG	35:LR:59:LYS:HB3	2.55	0.41
37:L3:50:ARG:HG2	37:L3:53:ARG:NH2	2.36	0.41
41:L7:79:THR:HG21	41:L7:94:ALA:HB1	2.02	0.41
44:LA:54:LEU:HD13	44:LA:54:LEU:HA	1.92	0.41
1:A:262:G:O2'	16:S8:20:ASP:O	2.39	0.41
1:A:331:U:H2'	1:A:332:G:O4'	2.21	0.41
1:A:368:G:H2'	1:A:369:G:C8	2.56	0.41
1:A:715:U:OP1	10:S2:87:LYS:NZ	2.47	0.41
1:A:801:U:H3'	1:A:802:A:H5''	2.01	0.41
1:A:1080:G:N7	1:A:1106:G:O2'	2.48	0.41
2:SB:65:ILE:HG13	2:SB:100:ILE:HD13	2.03	0.41
6:SG:135:VAL:HA	6:SG:138:ARG:HG3	2.03	0.41
17:S9:77:LYS:HE2	17:S9:77:LYS:HB2	1.94	0.41
19:SA:36:LYS:HA	19:SA:39:VAL:HG22	2.02	0.41
23:B:183:A:O2'	23:B:185:A:OP2	2.31	0.41
23:B:981:U:H2'	23:B:982:G:C8	2.55	0.41
23:B:1363:U:O2'	23:B:2037:G:O2'	2.28	0.41
23:B:1517:A:H2'	23:B:1518:G:C8	2.56	0.41
23:B:1528:G:O6	23:B:1547:C:N4	2.38	0.41
23:B:1796:A:O2'	23:B:1985:C:OP1	2.36	0.41
23:B:1880:A:H2'	23:B:1881:A:C8	2.56	0.41
23:B:2664:U:H5''	26:LC:92:ARG:HH11	1.85	0.41
23:B:2859:G:OP1	34:LQ:42:SER:OG	2.38	0.41
23:B:2863:G:H2'	23:B:2864:A:H8	1.84	0.41
25:L2:176:LEU:HD13	25:L2:176:LEU:HA	1.83	0.41
25:L2:243:ARG:HE	25:L2:247:MET:HE1	1.85	0.41
26:LC:118:VAL:HG22	26:LC:211:ILE:HG22	2.02	0.41
26:LC:133:ARG:HA	26:LC:173:MET:HE1	2.03	0.41
26:LC:187:GLN:NE2	26:LC:188:VAL:O	2.54	0.41
27:LJ:75:GLN:HE22	27:LJ:82:GLN:NE2	2.19	0.41
30:LM:59:ASN:HA	30:LM:128:GLY:HA2	2.03	0.41
37:L3:91:ASN:HB3	37:L3:92:ARG:H	1.73	0.41
38:L4:24:LYS:HA	38:L4:93:THR:HG23	2.02	0.41
46:LD:51:LYS:HG2	46:LD:52:HIS:H	1.84	0.41
51:LI:14:CYS:SG	51:LI:32:HIS:ND1	2.85	0.41
1:A:385:G:O6	1:A:395:U:O4	2.39	0.41
1:A:458:G:N2	1:A:492:G:O6	2.49	0.41
1:A:1428:G:O2'	1:A:1495:A:N6	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:SH:17:SER:OG	8:SH:76:GLY:O	2.38	0.41
14:S6:32:LEU:O	14:S6:36:ILE:HG12	2.21	0.41
30:LM:22:GLU:HG3	30:LM:23:GLY:H	1.86	0.41
32:LO:83:ASN:ND2	32:LO:116:SER:O	2.45	0.41
43:L9:34:ALA:H	43:L9:37:GLN:HE21	1.67	0.41
1:A:736:A:H2'	1:A:737:A:C8	2.55	0.40
14:S6:9:ASN:HD22	14:S6:12:ILE:HD11	1.86	0.40
23:B:2249:G:H2'	23:B:2250:A:C8	2.56	0.40
31:LN:70:ARG:NH1	31:LN:76:TYR:OH	2.50	0.40
35:LR:15:HIS:CD2	35:LR:93:VAL:HG21	2.56	0.40
1:A:185:U:H4'	19:SA:80:THR:HG22	2.03	0.40
1:A:546:U:H2'	1:A:547:A:H8	1.86	0.40
1:A:563:C:H2'	1:A:564:C:C6	2.57	0.40
1:A:623:C:H2'	1:A:624:G:H8	1.84	0.40
1:A:745:U:H5''	5:SE:93:ARG:HB2	2.04	0.40
4:SD:96:MET:HE2	4:SD:96:MET:HB2	1.95	0.40
18:SI:63:THR:O	18:SI:65:ASP:N	2.53	0.40
23:B:787:U:H2'	23:B:788:A:C8	2.52	0.40
23:B:1593:G:N7	23:B:1594:U:N3	2.69	0.40
23:B:2112:C:H42	23:B:2261:A:H61	1.69	0.40
23:B:2500:U:H6	23:B:2500:U:H2'	1.74	0.40
33:LP:46:GLN:O	33:LP:50:ALA:N	2.51	0.40
39:L5:49:LYS:HD3	39:L5:49:LYS:HA	1.90	0.40
1:A:932:G:N1	1:A:933:A:N1	2.70	0.40
4:SD:80:THR:OG1	4:SD:81:THR:N	2.53	0.40
23:B:703:A:H2'	23:B:704:U:C6	2.57	0.40
23:B:1042:C:P	37:L3:92:ARG:HH22	2.44	0.40
23:B:2620:U:H2'	23:B:2621:C:C6	2.56	0.40
27:LJ:181:LEU:HD23	27:LJ:181:LEU:HA	1.83	0.40
30:LM:21:ALA:HB3	30:LM:60:ALA:H	1.86	0.40
1:A:22:G:H21	1:A:924:A:N6	2.06	0.40
1:A:682:G:H2'	1:A:683:A:C8	2.55	0.40
1:A:1233:G:H5''	18:SI:78:ARG:HH21	1.85	0.40
2:SB:42:ILE:HG23	2:SB:46:LEU:HD12	2.01	0.40
8:SH:68:ASN:OD1	8:SH:69:VAL:N	2.54	0.40
18:SI:50:ALA:HB1	18:SI:57:HIS:CD2	2.57	0.40
23:B:2817:A:N6	23:B:2912:A:N7	2.70	0.40
24:C:75:U:H2'	24:C:76:A:C8	2.55	0.40
26:LC:131:ILE:HD11	26:LC:149:ARG:NH1	2.36	0.40
1:A:20:C:H2'	1:A:21:U:C6	2.57	0.40
1:A:660:U:O4	1:A:760:G:O2'	2.28	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:957:G:O2'	1:A:958:C:O5'	2.37	0.40
6:SG:40:GLN:HB2	6:SG:44:TYR:CD2	2.57	0.40
23:B:99:U:O2	23:B:101:G:N1	2.55	0.40
23:B:841:C:H2'	23:B:842:U:C6	2.56	0.40
23:B:878:C:H2'	23:B:879:U:H6	1.86	0.40
23:B:1352:C:H2'	23:B:1353:A:C8	2.48	0.40
23:B:1913:U:H2'	23:B:1914:C:C6	2.57	0.40
23:B:2278:G:C2	23:B:2477:A:H1'	2.57	0.40
23:B:2745:G:H2'	23:B:2746:G:H8	1.87	0.40
33:LP:41:TRP:CD2	33:LP:94:ILE:HD11	2.57	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	SB	200/202 (99%)	165 (82%)	34 (17%)	1 (0%)	25	60
3	SC	196/198 (99%)	151 (77%)	45 (23%)	0	100	100
4	SD	154/156 (99%)	135 (88%)	19 (12%)	0	100	100
5	SE	93/95 (98%)	87 (94%)	6 (6%)	0	100	100
6	SG	153/155 (99%)	134 (88%)	19 (12%)	0	100	100
7	SF	128/130 (98%)	110 (86%)	18 (14%)	0	100	100
8	SH	125/127 (98%)	101 (81%)	24 (19%)	0	100	100
9	S1	78/80 (98%)	72 (92%)	6 (8%)	0	100	100
10	S2	112/114 (98%)	85 (76%)	27 (24%)	0	100	100
11	S3	134/136 (98%)	98 (73%)	36 (27%)	0	100	100
12	S4	111/113 (98%)	87 (78%)	24 (22%)	0	100	100
13	S5	58/60 (97%)	49 (84%)	9 (16%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
14	S6	86/88 (98%)	77 (90%)	9 (10%)	0	100	100
15	S7	81/83 (98%)	60 (74%)	21 (26%)	0	100	100
16	S8	78/80 (98%)	58 (74%)	20 (26%)	0	100	100
17	S9	54/56 (96%)	50 (93%)	4 (7%)	0	100	100
18	SI	76/78 (97%)	54 (71%)	21 (28%)	1 (1%)	10	41
19	SA	76/79 (96%)	74 (97%)	2 (3%)	0	100	100
25	L2	272/274 (99%)	230 (85%)	42 (15%)	0	100	100
26	LC	213/215 (99%)	164 (77%)	46 (22%)	3 (1%)	9	39
27	LJ	203/205 (99%)	174 (86%)	27 (13%)	2 (1%)	13	46
28	LK	164/166 (99%)	120 (73%)	44 (27%)	0	100	100
29	LL	172/174 (99%)	136 (79%)	36 (21%)	0	100	100
30	LM	143/145 (99%)	118 (82%)	24 (17%)	1 (1%)	19	54
31	LN	120/122 (98%)	97 (81%)	22 (18%)	1 (1%)	16	51
32	LO	143/145 (99%)	107 (75%)	36 (25%)	0	100	100
33	LP	134/136 (98%)	114 (85%)	19 (14%)	1 (1%)	19	54
34	LQ	117/119 (98%)	98 (84%)	19 (16%)	0	100	100
35	LR	111/113 (98%)	85 (77%)	25 (22%)	1 (1%)	14	48
36	L1	107/109 (98%)	95 (89%)	12 (11%)	0	100	100
37	L3	114/116 (98%)	107 (94%)	7 (6%)	0	100	100
38	L4	100/102 (98%)	83 (83%)	16 (16%)	1 (1%)	13	46
39	L5	110/112 (98%)	97 (88%)	13 (12%)	0	100	100
40	L6	87/89 (98%)	75 (86%)	12 (14%)	0	100	100
41	L7	101/103 (98%)	80 (79%)	21 (21%)	0	100	100
42	L8	91/93 (98%)	78 (86%)	13 (14%)	0	100	100
43	L9	80/82 (98%)	67 (84%)	13 (16%)	0	100	100
44	LA	56/58 (97%)	47 (84%)	9 (16%)	0	100	100
45	LB	60/62 (97%)	53 (88%)	7 (12%)	0	100	100
46	LD	55/57 (96%)	48 (87%)	7 (13%)	0	100	100
47	LE	45/47 (96%)	37 (82%)	8 (18%)	0	100	100
48	LS	45/47 (96%)	39 (87%)	6 (13%)	0	100	100
49	LG	41/43 (95%)	38 (93%)	3 (7%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
50	LH	58/60 (97%)	46 (79%)	12 (21%)	0	100	100
51	LI	35/37 (95%)	27 (77%)	8 (23%)	0	100	100
52	LF	72/74 (97%)	46 (64%)	26 (36%)	0	100	100
All	All	5042/5135 (98%)	4153 (82%)	877 (17%)	12 (0%)	45	75

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
35	LR	71	GLU
2	SB	129	PHE
18	SI	9	PRO
27	LJ	67	GLN
26	LC	19	ASN
26	LC	106	SER
30	LM	23	GLY
33	LP	134	ARG
38	L4	50	ALA
27	LJ	64	PRO
26	LC	203	GLY
31	LN	100	GLY

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	SB	151/164 (92%)	149 (99%)	2 (1%)	65	76
3	SC	23/174 (13%)	23 (100%)	0	100	100
4	SD	120/122 (98%)	120 (100%)	0	100	100
5	SE	82/83 (99%)	82 (100%)	0	100	100
6	SG	115/131 (88%)	114 (99%)	1 (1%)	75	83
7	SF	107/111 (96%)	104 (97%)	3 (3%)	38	59
8	SH	96/105 (91%)	95 (99%)	1 (1%)	73	81

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
9	S1	67/73 (92%)	67 (100%)	0	100	100
10	S2	85/90 (94%)	84 (99%)	1 (1%)	67	78
11	S3	95/118 (80%)	94 (99%)	1 (1%)	70	79
12	S4	75/97 (77%)	73 (97%)	2 (3%)	40	60
13	S5	51/52 (98%)	51 (100%)	0	100	100
14	S6	74/80 (92%)	74 (100%)	0	100	100
15	S7	36/70 (51%)	36 (100%)	0	100	100
16	S8	35/75 (47%)	35 (100%)	0	100	100
17	S9	49/50 (98%)	49 (100%)	0	100	100
18	SI	45/69 (65%)	45 (100%)	0	100	100
19	SA	37/66 (56%)	37 (100%)	0	100	100
25	L2	212/221 (96%)	212 (100%)	0	100	100
26	LC	158/173 (91%)	155 (98%)	3 (2%)	52	70
27	LJ	154/168 (92%)	153 (99%)	1 (1%)	84	88
28	LK	67/147 (46%)	67 (100%)	0	100	100
29	LL	61/152 (40%)	60 (98%)	1 (2%)	58	73
30	LM	117/123 (95%)	114 (97%)	3 (3%)	41	61
31	LN	100/100 (100%)	98 (98%)	2 (2%)	50	68
32	LO	91/111 (82%)	91 (100%)	0	100	100
33	LP	101/113 (89%)	101 (100%)	0	100	100
34	LQ	90/100 (90%)	90 (100%)	0	100	100
35	LR	63/90 (70%)	62 (98%)	1 (2%)	58	73
36	L1	83/95 (87%)	83 (100%)	0	100	100
37	L3	96/96 (100%)	93 (97%)	3 (3%)	35	56
38	L4	68/86 (79%)	68 (100%)	0	100	100
39	L5	84/91 (92%)	83 (99%)	1 (1%)	67	78
40	L6	72/80 (90%)	72 (100%)	0	100	100
41	L7	71/88 (81%)	71 (100%)	0	100	100
42	L8	58/82 (71%)	58 (100%)	0	100	100
43	L9	61/64 (95%)	61 (100%)	0	100	100
44	LA	43/49 (88%)	42 (98%)	1 (2%)	45	64

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
45	LB	52/57 (91%)	51 (98%)	1 (2%)	52	70
46	LD	50/51 (98%)	48 (96%)	2 (4%)	27	51
47	LE	35/43 (81%)	35 (100%)	0	100	100
48	LS	42/45 (93%)	42 (100%)	0	100	100
49	LG	39/39 (100%)	39 (100%)	0	100	100
50	LH	44/52 (85%)	43 (98%)	1 (2%)	45	64
51	LI	29/35 (83%)	29 (100%)	0	100	100
52	LF	23/66 (35%)	23 (100%)	0	100	100
All	All	3507/4347 (81%)	3476 (99%)	31 (1%)	74	83

All (31) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	SB	137	ILE
2	SB	146	LYS
6	SG	130	ASN
7	SF	46	ILE
7	SF	80	ILE
7	SF	127	ILE
8	SH	30	ILE
10	S2	34	ILE
11	S3	7	LEU
12	S4	53	LEU
12	S4	65	VAL
26	LC	27	VAL
26	LC	209	VAL
26	LC	216	LYS
27	LJ	114	LEU
29	LL	175	LYS
30	LM	8	ASN
30	LM	58	ILE
30	LM	106	ILE
31	LN	69	VAL
31	LN	122	LEU
35	LR	92	ILE
37	L3	4	VAL
37	L3	109	LEU
37	L3	117	LEU
39	L5	12	ILE

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Mol	Chain	Res	Type
44	LA	60	THR
45	LB	66	LYS
46	LD	51	LYS
46	LD	58	GLU
50	LH	61	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (70) such sidechains are listed below:

Mol	Chain	Res	Type
2	SB	53	HIS
2	SB	61	ASN
2	SB	64	ASN
2	SB	68	HIS
2	SB	151	GLN
3	SC	85	ASN
4	SD	43	ASN
4	SD	146	ASN
5	SE	27	ASN
5	SE	70	ASN
6	SG	28	ASN
6	SG	40	GLN
6	SG	68	ASN
6	SG	84	ASN
6	SG	130	ASN
7	SF	22	HIS
8	SH	33	ASN
8	SH	51	ASN
8	SH	62	ASN
9	S1	67	GLN
10	S2	40	ASN
10	S2	64	GLN
10	S2	101	GLN
11	S3	13	GLN
11	S3	42	GLN
11	S3	73	ASN
11	S3	77	ASN
14	S6	28	GLN
14	S6	51	HIS
17	S9	57	GLN
19	SA	69	ASN
25	L2	11	ASN
25	L2	15	ASN

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Mol	Chain	Res	Type
25	L2	133	GLN
25	L2	143	ASN
25	L2	163	GLN
25	L2	228	ASN
26	LC	47	ASN
26	LC	143	HIS
27	LJ	29	ASN
27	LJ	40	GLN
27	LJ	75	GLN
27	LJ	130	ASN
27	LJ	148	GLN
27	LJ	162	ASN
28	LK	21	ASN
29	LL	77	GLN
29	LL	106	ASN
30	LM	8	ASN
32	LO	38	GLN
35	LR	8	ASN
36	L1	79	HIS
37	L3	37	GLN
37	L3	44	GLN
37	L3	91	ASN
38	L4	88	HIS
39	L5	77	ASN
40	L6	73	ASN
41	L7	67	ASN
42	L8	84	ASN
44	LA	16	ASN
44	LA	32	ASN
45	LB	17	GLN
45	LB	27	ASN
45	LB	31	GLN
47	LE	40	HIS
48	LS	40	ASN
49	LG	17	HIS
50	LH	7	HIS
50	LH	35	ASN

5.3.3 RNA ⓘ

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	1455/1555 (93%)	523 (35%)	24 (1%)
20	X	9/13 (69%)	4 (44%)	1 (11%)
21	E	74/75 (98%)	25 (33%)	1 (1%)
22	D	75/76 (98%)	26 (34%)	1 (1%)
23	B	2746/2923 (93%)	817 (29%)	28 (1%)
24	C	113/114 (99%)	37 (32%)	1 (0%)
All	All	4472/4756 (94%)	1432 (32%)	56 (1%)

All (1432) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	6	U
1	A	9	A
1	A	10	G
1	A	21	U
1	A	23	G
1	A	30	A
1	A	31	U
1	A	33	A
1	A	37	C
1	A	38	U
1	A	40	G
1	A	41	C
1	A	45	G
1	A	48	C
1	A	49	C
1	A	50	U
1	A	51	A
1	A	52	A
1	A	53	U
1	A	55	C
1	A	56	A
1	A	58	G
1	A	60	A
1	A	61	A
1	A	62	G
1	A	65	G
1	A	67	G
1	A	68	C
1	A	69	G
1	A	70	A

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Mol	Chain	Res	Type
1	A	71	A
1	A	72	C
1	A	98	U
1	A	99	U
1	A	100	A
1	A	102	C
1	A	103	G
1	A	105	C
1	A	109	C
1	A	110	G
1	A	111	G
1	A	113	U
1	A	115	A
1	A	116	G
1	A	120	C
1	A	130	A
1	A	131	C
1	A	134	A
1	A	136	C
1	A	137	U
1	A	139	U
1	A	141	A
1	A	144	C
1	A	160	A
1	A	163	C
1	A	164	C
1	A	165	G
1	A	169	C
1	A	182	A
1	A	183	U
1	A	184	A
1	A	207	G
1	A	208	U
1	A	209	G
1	A	210	A
1	A	211	A
1	A	212	A
1	A	214	A
1	A	234	A
1	A	239	G
1	A	248	U
1	A	251	A

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Mol	Chain	Res	Type
1	A	253	U
1	A	255	G
1	A	256	C
1	A	259	G
1	A	265	A
1	A	266	A
1	A	267	G
1	A	272	C
1	A	274	G
1	A	275	C
1	A	277	U
1	A	278	A
1	A	279	C
1	A	281	A
1	A	283	G
1	A	288	C
1	A	289	G
1	A	297	G
1	A	301	A
1	A	306	A
1	A	308	A
1	A	309	G
1	A	313	G
1	A	315	U
1	A	316	C
1	A	317	G
1	A	323	A
1	A	324	C
1	A	327	G
1	A	329	A
1	A	333	A
1	A	334	G
1	A	336	C
1	A	338	C
1	A	340	G
1	A	343	C
1	A	347	C
1	A	349	C
1	A	351	U
1	A	352	A
1	A	353	C
1	A	354	G

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Mol	Chain	Res	Type
1	A	355	G
1	A	356	G
1	A	358	G
1	A	360	C
1	A	361	A
1	A	362	G
1	A	364	A
1	A	371	A
1	A	375	U
1	A	380	C
1	A	381	A
1	A	385	G
1	A	389	A
1	A	391	A
1	A	392	G
1	A	395	U
1	A	396	G
1	A	398	C
1	A	401	A
1	A	405	A
1	A	406	C
1	A	409	C
1	A	410	G
1	A	412	G
1	A	413	U
1	A	414	G
1	A	417	U
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	433	A
1	A	436	G
1	A	437	U
1	A	438	A
1	A	440	A
1	A	441	A
1	A	442	C
1	A	447	U

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Mol	Chain	Res	Type
1	A	448	U
1	A	449	A
1	A	450	U
1	A	452	A
1	A	453	G
1	A	454	G
1	A	455	G
1	A	458	G
1	A	459	A
1	A	460	A
1	A	461	C
1	A	462	A
1	A	463	U
1	A	464	A
1	A	465	U
1	A	466	G
1	A	467	U
1	A	468	G
1	A	482	A
1	A	483	C
1	A	484	A
1	A	485	U
1	A	486	C
1	A	487	U
1	A	488	U
1	A	489	G
1	A	492	G
1	A	498	U
1	A	499	A
1	A	504	G
1	A	505	A
1	A	506	A
1	A	507	A
1	A	511	A
1	A	513	G
1	A	515	C
1	A	516	U
1	A	517	A
1	A	519	C
1	A	523	G
1	A	525	G
1	A	526	C

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Mol	Chain	Res	Type
1	A	529	G
1	A	530	C
1	A	531	A
1	A	532	G
1	A	536	C
1	A	538	G
1	A	540	A
1	A	541	A
1	A	555	A
1	A	556	G
1	A	568	A
1	A	570	U
1	A	572	U
1	A	573	U
1	A	580	A
1	A	581	A
1	A	584	C
1	A	585	G
1	A	586	C
1	A	595	G
1	A	603	A
1	A	604	A
1	A	606	U
1	A	610	A
1	A	611	U
1	A	619	C
1	A	621	C
1	A	628	C
1	A	633	G
1	A	635	G
1	A	638	G
1	A	639	G
1	A	640	G
1	A	641	U
1	A	642	C
1	A	647	G
1	A	650	A
1	A	652	U
1	A	656	A
1	A	661	U
1	A	669	G
1	A	671	A

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Mol	Chain	Res	Type
1	A	673	A
1	A	675	G
1	A	694	U
1	A	695	A
1	A	696	G
1	A	700	U
1	A	710	A
1	A	711	G
1	A	712	A
1	A	713	G
1	A	715	U
1	A	716	A
1	A	725	C
1	A	726	A
1	A	731	U
1	A	732	G
1	A	756	A
1	A	758	C
1	A	763	G
1	A	768	U
1	A	769	G
1	A	774	A
1	A	781	G
1	A	782	G
1	A	787	C
1	A	796	U
1	A	799	G
1	A	800	A
1	A	801	U
1	A	802	A
1	A	807	G
1	A	821	U
1	A	822	A
1	A	825	C
1	A	826	G
1	A	827	A
1	A	828	U
1	A	829	G
1	A	835	U
1	A	836	A
1	A	837	A
1	A	840	G

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Mol	Chain	Res	Type
1	A	846	G
1	A	848	G
1	A	849	U
1	A	856	C
1	A	859	C
1	A	863	G
1	A	869	C
1	A	874	A
1	A	882	A
1	A	888	U
1	A	890	C
1	A	899	A
1	A	912	G
1	A	924	A
1	A	929	A
1	A	932	G
1	A	941	C
1	A	944	C
1	A	947	A
1	A	952	G
1	A	956	A
1	A	957	G
1	A	958	C
1	A	964	G
1	A	970	U
1	A	971	U
1	A	973	G
1	A	974	A
1	A	975	A
1	A	978	A
1	A	979	A
1	A	981	G
1	A	983	G
1	A	986	G
1	A	987	A
1	A	992	U
1	A	997	A
1	A	998	A
1	A	1002	U
1	A	1003	G
1	A	1004	A
1	A	1008	C

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Mol	Chain	Res	Type
1	A	1011	U
1	A	1012	U
1	A	1013	G
1	A	1014	A
1	A	1015	C
1	A	1016	A
1	A	1017	A
1	A	1019	U
1	A	1032	C
1	A	1033	C
1	A	1034	U
1	A	1035	U
1	A	1036	C
1	A	1038	C
1	A	1039	C
1	A	1040	U
1	A	1041	U
1	A	1042	C
1	A	1043	G
1	A	1044	G
1	A	1045	G
1	A	1046	G
1	A	1047	G
1	A	1048	A
1	A	1049	C
1	A	1053	G
1	A	1054	U
1	A	1057	C
1	A	1063	G
1	A	1064	U
1	A	1065	G
1	A	1066	C
1	A	1067	A
1	A	1068	U
1	A	1077	U
1	A	1082	U
1	A	1084	G
1	A	1086	G
1	A	1090	U
1	A	1092	A
1	A	1093	G
1	A	1096	G

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Mol	Chain	Res	Type
1	A	1097	U
1	A	1098	U
1	A	1106	G
1	A	1107	U
1	A	1113	A
1	A	1114	A
1	A	1120	G
1	A	1124	C
1	A	1133	U
1	A	1135	A
1	A	1136	G
1	A	1137	U
1	A	1138	U
1	A	1139	G
1	A	1140	C
1	A	1141	C
1	A	1142	A
1	A	1143	U
1	A	1144	C
1	A	1146	U
1	A	1148	A
1	A	1149	A
1	A	1150	G
1	A	1151	U
1	A	1152	U
1	A	1153	G
1	A	1155	G
1	A	1157	A
1	A	1159	U
1	A	1160	C
1	A	1161	U
1	A	1163	A
1	A	1164	G
1	A	1165	U
1	A	1166	U
1	A	1167	G
1	A	1168	A
1	A	1169	C
1	A	1171	G
1	A	1172	C
1	A	1173	C
1	A	1174	G

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Mol	Chain	Res	Type
1	A	1176	U
1	A	1177	G
1	A	1179	C
1	A	1182	A
1	A	1184	C
1	A	1188	G
1	A	1189	G
1	A	1190	A
1	A	1191	A
1	A	1192	G
1	A	1193	G
1	A	1194	U
1	A	1195	G
1	A	1203	C
1	A	1204	G
1	A	1207	A
1	A	1208	A
1	A	1209	A
1	A	1223	U
1	A	1224	A
1	A	1225	U
1	A	1226	G
1	A	1228	U
1	A	1235	U
1	A	1237	C
1	A	1238	A
1	A	1239	C
1	A	1243	U
1	A	1244	G
1	A	1249	A
1	A	1251	U
1	A	1256	A
1	A	1259	A
1	A	1268	A
1	A	1269	G
1	A	1271	G
1	A	1281	G
1	A	1284	C
1	A	1286	A
1	A	1287	G
1	A	1291	A
1	A	1292	U

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Mol	Chain	Res	Type
1	A	1293	C
1	A	1297	U
1	A	1298	A
1	A	1311	G
1	A	1312	U
1	A	1314	C
1	A	1316	G
1	A	1317	A
1	A	1320	G
1	A	1327	G
1	A	1329	A
1	A	1331	C
1	A	1333	C
1	A	1334	G
1	A	1339	C
1	A	1340	A
1	A	1342	G
1	A	1343	A
1	A	1348	G
1	A	1353	C
1	A	1354	G
1	A	1357	A
1	A	1358	G
1	A	1360	A
1	A	1361	A
1	A	1362	U
1	A	1364	G
1	A	1370	C
1	A	1374	A
1	A	1379	A
1	A	1389	C
1	A	1392	U
1	A	1398	G
1	A	1405	A
1	A	1407	A
1	A	1408	C
1	A	1409	A
1	A	1411	C
1	A	1412	G
1	A	1413	C
1	A	1417	U
1	A	1422	C

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Mol	Chain	Res	Type
1	A	1426	G
1	A	1429	A
1	A	1430	G
1	A	1434	G
1	A	1440	C
1	A	1443	G
1	A	1451	U
1	A	1452	G
1	A	1454	A
1	A	1456	U
1	A	1457	A
1	A	1458	A
1	A	1459	C
1	A	1463	U
1	A	1465	A
1	A	1468	A
1	A	1480	A
1	A	1484	U
1	A	1503	G
1	A	1504	A
1	A	1509	G
1	A	1511	A
1	A	1514	A
1	A	1515	A
1	A	1516	G
1	A	1519	A
1	A	1520	G
1	A	1529	G
1	A	1541	G
1	A	1542	G
1	A	1544	U
20	X	16	A
20	X	17	U
20	X	18	G
20	X	22	A
21	E	6	G
21	E	8	U
21	E	9	A
21	E	11	C
21	E	13	C
21	E	19	G
21	E	21	A

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Mol	Chain	Res	Type
21	E	33	U
21	E	34	G
21	E	38	A
21	E	42	C
21	E	47	U
21	E	48	C
21	E	49	C
21	E	54	U
21	E	55	U
21	E	56	C
21	E	57	G
21	E	61	C
21	E	63	G
21	E	65	G
21	E	69	G
21	E	72	C
21	E	73	A
21	E	75	C
22	D	6	G
22	D	8	U
22	D	9	A
22	D	11	C
22	D	13	C
22	D	19	G
22	D	21	A
22	D	33	U
22	D	34	G
22	D	38	A
22	D	42	C
22	D	47	U
22	D	48	C
22	D	49	C
22	D	54	U
22	D	55	U
22	D	56	C
22	D	57	G
22	D	61	C
22	D	63	G
22	D	65	G
22	D	69	G
22	D	72	C
22	D	73	A

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Mol	Chain	Res	Type
22	D	75	C
22	D	76	A
23	B	10	A
23	B	11	U
23	B	12	U
23	B	15	G
23	B	21	A
23	B	34	U
23	B	35	G
23	B	43	A
23	B	44	A
23	B	46	C
23	B	49	A
23	B	51	G
23	B	61	A
23	B	64	A
23	B	71	A
23	B	74	U
23	B	75	G
23	B	93	U
23	B	94	A
23	B	99	U
23	B	100	U
23	B	101	G
23	B	102	A
23	B	113	U
23	B	118	A
23	B	119	U
23	B	121	G
23	B	122	G
23	B	125	A
23	B	127	C
23	B	133	A
23	B	134	U
23	B	135	G
23	B	136	A
23	B	140	A
23	B	157	U
23	B	158	G
23	B	164	A
23	B	165	C
23	B	169	G

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Mol	Chain	Res	Type
23	B	174	U
23	B	176	A
23	B	177	G
23	B	180	G
23	B	182	C
23	B	183	A
23	B	184	C
23	B	185	A
23	B	199	A
23	B	200	A
23	B	202	A
23	B	203	U
23	B	204	C
23	B	207	A
23	B	218	G
23	B	219	A
23	B	220	A
23	B	225	A
23	B	226	A
23	B	231	A
23	B	232	U
23	B	233	U
23	B	235	G
23	B	242	U
23	B	244	A
23	B	248	G
23	B	251	G
23	B	253	G
23	B	254	A
23	B	255	G
23	B	267	G
23	B	268	A
23	B	269	G
23	B	270	C
23	B	283	G
23	B	284	C
23	B	285	U
23	B	286	U
23	B	287	G
23	B	294	G
23	B	300	G
23	B	301	U

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Mol	Chain	Res	Type
23	B	302	A
23	B	310	C
23	B	311	U
23	B	312	A
23	B	313	U
23	B	321	U
23	B	322	A
23	B	324	A
23	B	327	G
23	B	328	G
23	B	329	A
23	B	331	G
23	B	332	A
23	B	338	G
23	B	343	A
23	B	345	C
23	B	354	A
23	B	365	A
23	B	373	A
23	B	388	A
23	B	391	A
23	B	395	U
23	B	396	G
23	B	398	C
23	B	401	U
23	B	402	C
23	B	403	U
23	B	404	U
23	B	410	G
23	B	411	A
23	B	412	U
23	B	413	C
23	B	416	G
23	B	417	A
23	B	418	G
23	B	425	G
23	B	428	G
23	B	429	C
23	B	432	G
23	B	434	G
23	B	438	U
23	B	440	C

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Mol	Chain	Res	Type
23	B	445	G
23	B	447	A
23	B	449	U
23	B	452	G
23	B	454	G
23	B	458	A
23	B	464	U
23	B	480	U
23	B	482	U
23	B	486	G
23	B	489	A
23	B	490	C
23	B	494	U
23	B	497	U
23	B	500	A
23	B	501	C
23	B	503	A
23	B	504	G
23	B	506	A
23	B	510	U
23	B	511	G
23	B	513	G
23	B	519	G
23	B	525	A
23	B	527	G
23	B	536	A
23	B	549	U
23	B	550	A
23	B	553	A
23	B	554	C
23	B	563	G
23	B	564	U
23	B	565	G
23	B	566	U
23	B	567	G
23	B	572	C
23	B	573	A
23	B	575	G
23	B	576	U
23	B	577	A
23	B	578	G
23	B	587	C

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Mol	Chain	Res	Type
23	B	590	U
23	B	591	A
23	B	592	A
23	B	593	U
23	B	602	G
23	B	605	U
23	B	606	G
23	B	613	G
23	B	616	G
23	B	618	A
23	B	629	A
23	B	630	G
23	B	635	G
23	B	639	U
23	B	646	A
23	B	647	G
23	B	650	U
23	B	657	U
23	B	658	A
23	B	659	A
23	B	660	A
23	B	661	U
23	B	662	G
23	B	672	A
23	B	679	G
23	B	682	A
23	B	684	U
23	B	689	A
23	B	698	U
23	B	699	U
23	B	707	G
23	B	713	A
23	B	715	A
23	B	716	C
23	B	717	C
23	B	720	A
23	B	721	A
23	B	722	A
23	B	730	A
23	B	731	U
23	B	752	G
23	B	755	C

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Mol	Chain	Res	Type
23	B	760	A
23	B	761	A
23	B	762	C
23	B	763	A
23	B	764	C
23	B	766	G
23	B	775	A
23	B	779	A
23	B	783	G
23	B	792	U
23	B	793	G
23	B	802	G
23	B	805	G
23	B	809	A
23	B	810	A
23	B	813	G
23	B	815	G
23	B	816	G
23	B	820	G
23	B	821	C
23	B	822	G
23	B	827	A
23	B	828	A
23	B	829	U
23	B	834	A
23	B	836	C
23	B	837	G
23	B	845	A
23	B	847	A
23	B	848	U
23	B	850	G
23	B	855	U
23	B	857	C
23	B	864	A
23	B	867	U
23	B	871	U
23	B	872	U
23	B	873	U
23	B	875	G
23	B	883	C
23	B	885	C
23	B	888	G

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Mol	Chain	Res	Type
23	B	891	A
23	B	892	U
23	B	895	U
23	B	904	G
23	B	916	U
23	B	919	G
23	B	922	G
23	B	923	A
23	B	924	G
23	B	925	G
23	B	943	C
23	B	944	G
23	B	945	A
23	B	946	A
23	B	948	U
23	B	951	G
23	B	952	A
23	B	955	A
23	B	957	C
23	B	960	C
23	B	962	A
23	B	964	U
23	B	967	C
23	B	970	U
23	B	971	U
23	B	972	A
23	B	973	A
23	B	974	U
23	B	975	U
23	B	976	U
23	B	977	A
23	B	983	G
23	B	985	A
23	B	989	A
23	B	990	G
23	B	997	G
23	B	1001	A
23	B	1002	U
23	B	1003	A
23	B	1005	G
23	B	1012	G
23	B	1017	A

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Mol	Chain	Res	Type
23	B	1018	A
23	B	1020	G
23	B	1024	A
23	B	1025	A
23	B	1026	C
23	B	1027	A
23	B	1031	C
23	B	1032	A
23	B	1035	C
23	B	1038	C
23	B	1040	A
23	B	1049	C
23	B	1057	A
23	B	1066	G
23	B	1067	U
23	B	1069	G
23	B	1070	A
23	B	1071	A
23	B	1074	G
23	B	1077	U
23	B	1080	G
23	B	1082	C
23	B	1083	G
23	B	1087	C
23	B	1089	C
23	B	1090	A
23	B	1091	G
23	B	1093	C
23	B	1094	A
23	B	1095	A
23	B	1096	C
23	B	1097	U
23	B	1098	A
23	B	1099	G
23	B	1150	A
23	B	1151	G
23	B	1152	U
23	B	1153	C
23	B	1154	G
23	B	1155	A
23	B	1156	G
23	B	1158	G

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Mol	Chain	Res	Type
23	B	1160	C
23	B	1172	A
23	B	1174	U
23	B	1175	G
23	B	1176	U
23	B	1178	C
23	B	1179	C
23	B	1183	G
23	B	1186	A
23	B	1187	A
23	B	1192	A
23	B	1194	U
23	B	1195	A
23	B	1207	G
23	B	1208	A
23	B	1209	U
23	B	1213	C
23	B	1215	U
23	B	1216	U
23	B	1217	U
23	B	1220	A
23	B	1222	A
23	B	1225	G
23	B	1248	U
23	B	1249	U
23	B	1265	G
23	B	1267	A
23	B	1269	A
23	B	1271	G
23	B	1274	G
23	B	1277	C
23	B	1278	G
23	B	1285	A
23	B	1291	A
23	B	1293	U
23	B	1294	G
23	B	1303	A
23	B	1309	G
23	B	1310	A
23	B	1311	A
23	B	1312	A
23	B	1321	A

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Mol	Chain	Res	Type
23	B	1322	G
23	B	1323	A
23	B	1325	U
23	B	1328	C
23	B	1333	A
23	B	1337	A
23	B	1338	U
23	B	1342	C
23	B	1343	U
23	B	1344	A
23	B	1346	G
23	B	1348	U
23	B	1349	U
23	B	1351	C
23	B	1358	A
23	B	1362	C
23	B	1378	U
23	B	1382	C
23	B	1384	G
23	B	1389	U
23	B	1392	G
23	B	1397	G
23	B	1401	G
23	B	1402	A
23	B	1405	G
23	B	1415	A
23	B	1416	U
23	B	1420	U
23	B	1421	A
23	B	1422	A
23	B	1423	C
23	B	1425	G
23	B	1428	U
23	B	1433	U
23	B	1435	C
23	B	1440	A
23	B	1446	U
23	B	1448	U
23	B	1449	A
23	B	1450	A
23	B	1451	U
23	B	1452	C

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Mol	Chain	Res	Type
23	B	1453	G
23	B	1462	G
23	B	1465	G
23	B	1471	A
23	B	1472	C
23	B	1473	G
23	B	1484	G
23	B	1487	G
23	B	1488	A
23	B	1489	A
23	B	1490	G
23	B	1491	C
23	B	1493	U
23	B	1495	C
23	B	1496	G
23	B	1497	A
23	B	1498	U
23	B	1499	U
23	B	1501	G
23	B	1502	A
23	B	1503	U
23	B	1504	U
23	B	1505	G
23	B	1509	G
23	B	1510	U
23	B	1511	C
23	B	1512	U
23	B	1516	C
23	B	1519	U
23	B	1524	C
23	B	1525	U
23	B	1526	G
23	B	1527	A
23	B	1540	U
23	B	1542	C
23	B	1543	G
23	B	1545	U
23	B	1546	A
23	B	1547	C
23	B	1548	U
23	B	1549	C
23	B	1550	G

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Mol	Chain	Res	Type
23	B	1556	G
23	B	1557	C
23	B	1560	A
23	B	1561	G
23	B	1568	U
23	B	1569	G
23	B	1570	G
23	B	1579	C
23	B	1590	C
23	B	1591	G
23	B	1592	A
23	B	1593	G
23	B	1595	C
23	B	1597	U
23	B	1599	G
23	B	1602	U
23	B	1603	U
23	B	1604	C
23	B	1605	A
23	B	1606	C
23	B	1612	C
23	B	1614	A
23	B	1615	G
23	B	1616	A
23	B	1622	C
23	B	1625	U
23	B	1627	G
23	B	1629	U
23	B	1630	A
23	B	1631	G
23	B	1636	U
23	B	1637	A
23	B	1639	G
23	B	1641	G
23	B	1651	C
23	B	1653	A
23	B	1660	A
23	B	1661	C
23	B	1663	G
23	B	1666	A
23	B	1675	G
23	B	1682	C

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Mol	Chain	Res	Type
23	B	1690	A
23	B	1691	G
23	B	1692	C
23	B	1693	G
23	B	1697	G
23	B	1698	A
23	B	1707	U
23	B	1710	G
23	B	1716	C
23	B	1720	A
23	B	1737	U
23	B	1739	G
23	B	1740	G
23	B	1742	A
23	B	1747	G
23	B	1748	G
23	B	1749	G
23	B	1755	U
23	B	1758	A
23	B	1761	G
23	B	1762	U
23	B	1766	C
23	B	1768	C
23	B	1770	C
23	B	1772	G
23	B	1773	A
23	B	1784	U
23	B	1785	G
23	B	1789	A
23	B	1790	G
23	B	1791	G
23	B	1800	A
23	B	1803	G
23	B	1806	U
23	B	1808	U
23	B	1811	A
23	B	1818	A
23	B	1827	C
23	B	1829	A
23	B	1830	A
23	B	1836	A
23	B	1842	A

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Mol	Chain	Res	Type
23	B	1843	U
23	B	1844	G
23	B	1846	A
23	B	1852	G
23	B	1853	C
23	B	1856	A
23	B	1857	C
23	B	1860	C
23	B	1868	U
23	B	1877	G
23	B	1879	U
23	B	1886	A
23	B	1893	A
23	B	1895	C
23	B	1898	C
23	B	1899	U
23	B	1900	G
23	B	1901	C
23	B	1902	G
23	B	1903	A
23	B	1904	A
23	B	1910	G
23	B	1916	A
23	B	1932	C
23	B	1933	G
23	B	1940	A
23	B	1941	C
23	B	1942	U
23	B	1946	A
23	B	1955	A
23	B	1956	G
23	B	1957	G
23	B	1964	A
23	B	1965	A
23	B	1966	U
23	B	1967	U
23	B	1970	U
23	B	1982	U
23	B	1990	C
23	B	1992	C
23	B	1994	C
23	B	1996	A

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Mol	Chain	Res	Type
23	B	1997	A
23	B	1998	A
23	B	1999	G
23	B	2003	U
23	B	2004	A
23	B	2009	U
23	B	2018	U
23	B	2019	G
23	B	2020	U
23	B	2024	A
23	B	2050	A
23	B	2058	A
23	B	2059	G
23	B	2060	A
23	B	2070	C
23	B	2073	G
23	B	2076	A
23	B	2078	A
23	B	2079	G
23	B	2082	C
23	B	2083	G
23	B	2087	A
23	B	2088	G
23	B	2090	C
23	B	2096	G
23	B	2098	A
23	B	2103	U
23	B	2104	A
23	B	2107	G
23	B	2117	A
23	B	2120	G
23	B	2121	A
23	B	2125	U
23	B	2126	C
23	B	2127	G
23	B	2131	C
23	B	2132	A
23	B	2135	U
23	B	2211	U
23	B	2214	G
23	B	2215	U
23	B	2217	G

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Mol	Chain	Res	Type
23	B	2218	G
23	B	2226	A
23	B	2231	C
23	B	2232	A
23	B	2238	U
23	B	2239	A
23	B	2240	U
23	B	2250	A
23	B	2252	A
23	B	2254	A
23	B	2257	G
23	B	2261	A
23	B	2262	G
23	B	2265	G
23	B	2266	G
23	B	2276	U
23	B	2277	G
23	B	2290	C
23	B	2295	A
23	B	2306	G
23	B	2307	G
23	B	2310	C
23	B	2314	A
23	B	2316	G
23	B	2324	C
23	B	2326	G
23	B	2330	G
23	B	2331	G
23	B	2332	U
23	B	2333	U
23	B	2334	G
23	B	2335	G
23	B	2336	A
23	B	2337	A
23	B	2338	A
23	B	2339	U
23	B	2341	A
23	B	2345	A
23	B	2346	U
23	B	2347	A
23	B	2348	G
23	B	2349	A

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Mol	Chain	Res	Type
23	B	2353	U
23	B	2354	A
23	B	2361	U
23	B	2362	A
23	B	2364	G
23	B	2372	G
23	B	2373	A
23	B	2374	C
23	B	2377	C
23	B	2385	A
23	B	2388	A
23	B	2390	U
23	B	2393	A
23	B	2396	A
23	B	2404	A
23	B	2409	G
23	B	2410	G
23	B	2412	C
23	B	2418	G
23	B	2429	U
23	B	2433	C
23	B	2434	A
23	B	2437	G
23	B	2441	G
23	B	2450	U
23	B	2452	A
23	B	2454	C
23	B	2455	G
23	B	2456	G
23	B	2457	A
23	B	2459	A
23	B	2461	A
23	B	2463	G
23	B	2468	C
23	B	2474	G
23	B	2475	A
23	B	2501	U
23	B	2502	C
23	B	2515	A
23	B	2525	C
23	B	2529	G
23	B	2530	A

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Mol	Chain	Res	Type
23	B	2532	G
23	B	2545	A
23	B	2547	C
23	B	2552	G
23	B	2561	C
23	B	2570	G
23	B	2573	U
23	B	2575	G
23	B	2580	G
23	B	2581	U
23	B	2593	A
23	B	2594	G
23	B	2599	A
23	B	2600	C
23	B	2604	A
23	B	2605	G
23	B	2609	G
23	B	2610	G
23	B	2612	U
23	B	2613	C
23	B	2626	G
23	B	2627	A
23	B	2628	C
23	B	2629	A
23	B	2630	G
23	B	2636	U
23	B	2640	U
23	B	2642	U
23	B	2648	G
23	B	2651	G
23	B	2656	A
23	B	2657	G
23	B	2666	A
23	B	2669	G
23	B	2673	C
23	B	2674	U
23	B	2675	G
23	B	2679	U
23	B	2680	U
23	B	2681	A
23	B	2682	G
23	B	2683	U

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Mol	Chain	Res	Type
23	B	2687	A
23	B	2688	G
23	B	2689	A
23	B	2690	G
23	B	2698	A
23	B	2699	U
23	B	2709	U
23	B	2710	C
23	B	2716	U
23	B	2724	G
23	B	2730	C
23	B	2740	A
23	B	2741	G
23	B	2743	U
23	B	2751	U
23	B	2753	U
23	B	2760	A
23	B	2771	G
23	B	2775	A
23	B	2777	A
23	B	2779	C
23	B	2780	A
23	B	2788	A
23	B	2791	A
23	B	2792	A
23	B	2793	G
23	B	2795	C
23	B	2803	A
23	B	2804	G
23	B	2805	A
23	B	2806	U
23	B	2817	A
23	B	2818	A
23	B	2819	C
23	B	2820	U
23	B	2821	U
23	B	2822	C
23	B	2823	G
23	B	2824	G
23	B	2826	U
23	B	2827	A
23	B	2832	A

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Mol	Chain	Res	Type
23	B	2838	C
23	B	2839	A
23	B	2840	A
23	B	2844	U
23	B	2853	U
23	B	2855	A
23	B	2857	A
23	B	2869	G
23	B	2879	G
23	B	2881	C
23	B	2887	G
23	B	2888	A
23	B	2889	G
23	B	2892	G
23	B	2893	A
23	B	2899	A
23	B	2900	C
23	B	2903	A
23	B	2911	A
23	B	2912	A
23	B	2919	A
24	C	8	A
24	C	10	U
24	C	11	A
24	C	14	G
24	C	15	C
24	C	17	A
24	C	19	G
24	C	21	G
24	C	25	A
24	C	27	A
24	C	29	C
24	C	31	G
24	C	33	U
24	C	38	U
24	C	39	G
24	C	40	C
24	C	41	C
24	C	42	G
24	C	43	A
24	C	49	G
24	C	50	A

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Mol	Chain	Res	Type
24	C	51	A
24	C	52	G
24	C	54	U
24	C	55	A
24	C	58	G
24	C	64	A
24	C	65	G
24	C	74	G
24	C	86	C
24	C	87	G
24	C	88	U
24	C	89	U
24	C	102	A
24	C	103	A
24	C	106	U
24	C	111	A

All (56) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	60	A
1	A	70	A
1	A	252	U
1	A	342	C
1	A	357	A
1	A	409	C
1	A	457	A
1	A	460	A
1	A	465	U
1	A	531	A
1	A	585	G
1	A	609	G
1	A	637	A
1	A	695	A
1	A	711	G
1	A	1002	U
1	A	1038	C
1	A	1076	G
1	A	1176	U
1	A	1202	A
1	A	1268	A
1	A	1296	A

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Mol	Chain	Res	Type
1	A	1311	G
1	A	1510	U
20	X	16	A
21	E	32	U
22	D	32	U
23	B	184	C
23	B	267	G
23	B	548	A
23	B	577	A
23	B	660	A
23	B	716	C
23	B	763	A
23	B	835	U
23	B	850	G
23	B	854	G
23	B	922	G
23	B	1024	A
23	B	1185	U
23	B	1293	U
23	B	1489	A
23	B	1559	G
23	B	1636	U
23	B	1761	G
23	B	1845	U
23	B	1852	G
23	B	1897	U
23	B	1900	G
23	B	1940	A
23	B	1967	U
23	B	2238	U
23	B	2338	A
23	B	2529	G
23	B	2709	U
24	C	40	C

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 130 ligands modelled in this entry, 129 are monoatomic - leaving 1 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
53	PAR	A	1601	-	44,45,45	0.28	0	63,67,67	1.09	6 (9%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
53	PAR	A	1601	-	-	3/18/94/94	0/4/4/4

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
53	A	1601	PAR	O52-C13-O43	-3.60	107.69	111.37
53	A	1601	PAR	C13-C23-C33	-3.23	98.21	102.10
53	A	1601	PAR	O33-C14-C24	-2.96	103.24	108.08
53	A	1601	PAR	C32-C22-C12	-2.57	106.61	111.02
53	A	1601	PAR	O11-C42-C32	-2.21	103.90	109.18
53	A	1601	PAR	O54-C14-C24	2.11	114.75	110.08

There are no chirality outliers.

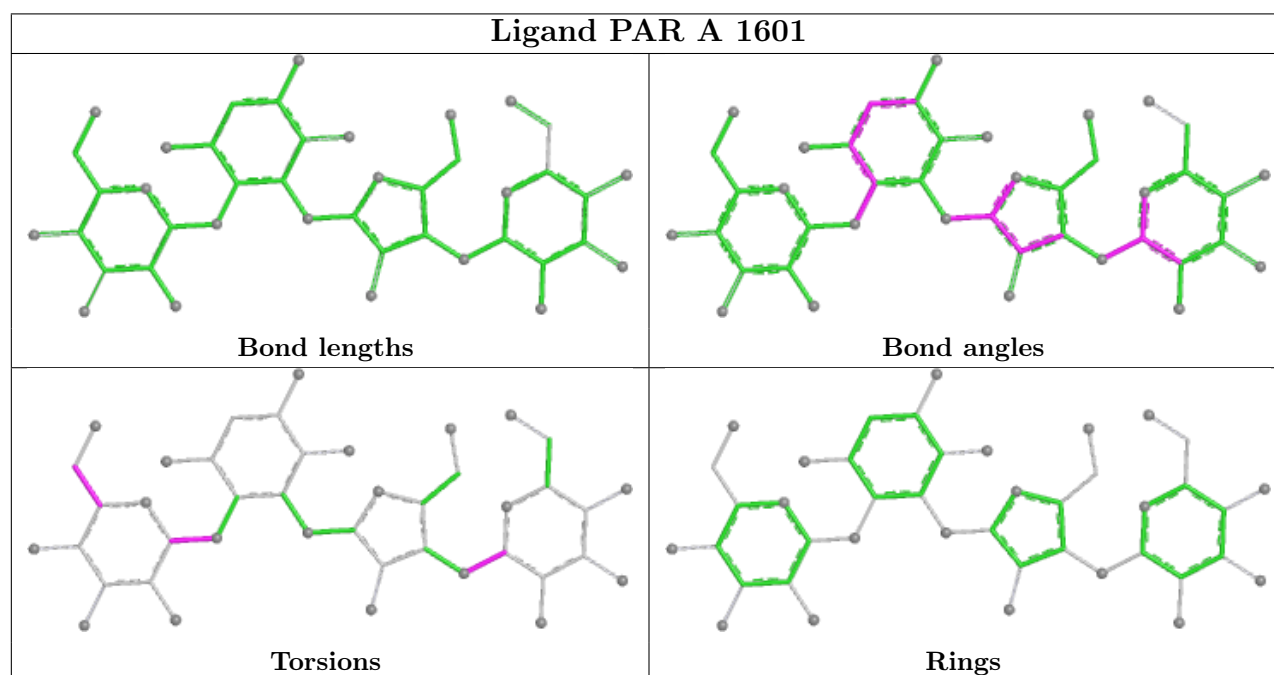
All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
53	A	1601	PAR	O54-C14-O33-C33
53	A	1601	PAR	O51-C11-O11-C42
53	A	1601	PAR	O51-C51-C61-O61

There are no ring outliers.

No monomer is involved in short contacts.

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



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	1460:C	O3'	1461:U	P	4.77

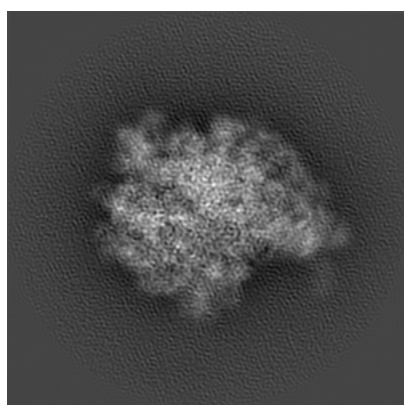
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-8402. These allow visual inspection of the internal detail of the map and identification of artifacts.

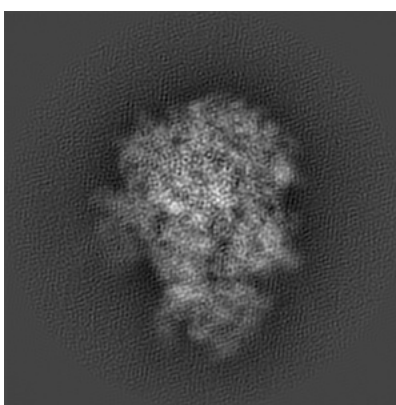
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

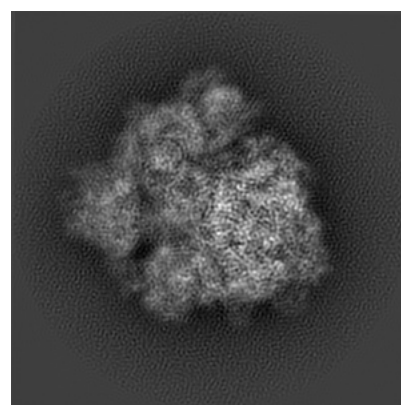
6.1.1 Primary map



X



Y

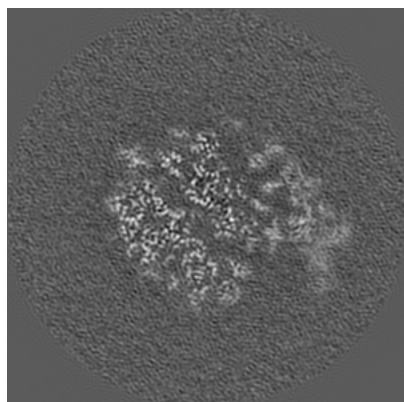


Z

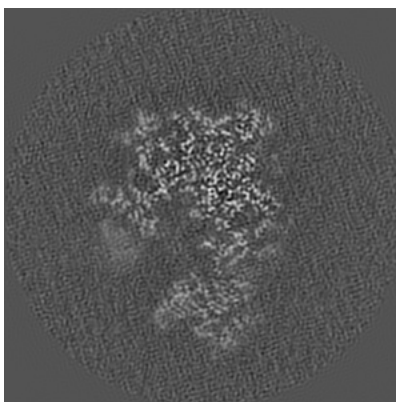
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

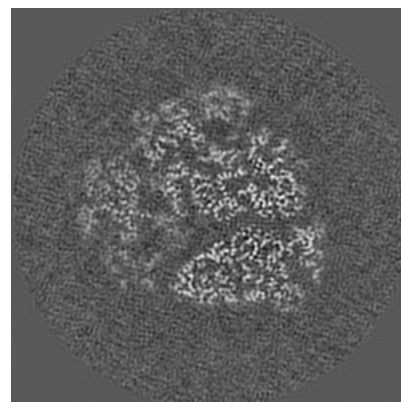
6.2.1 Primary map



X Index: 205



Y Index: 205

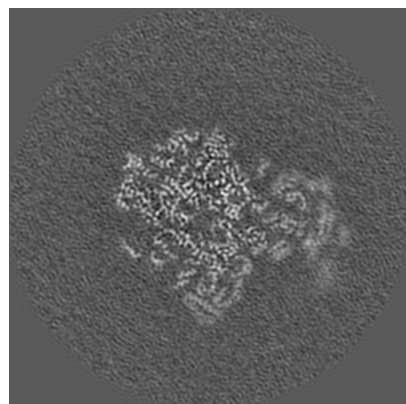


Z Index: 205

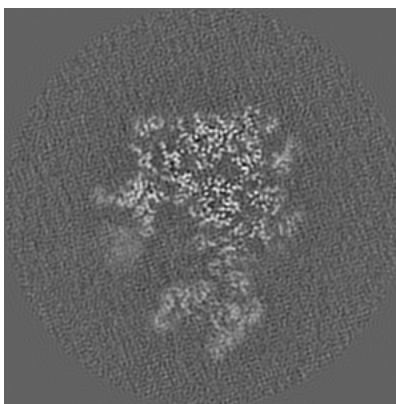
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

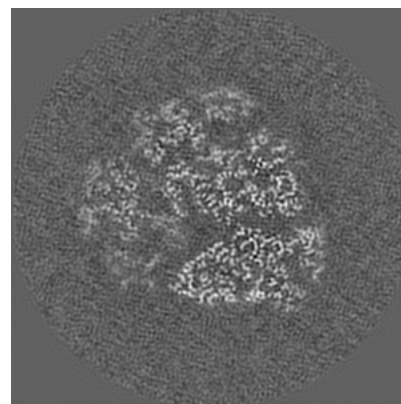
6.3.1 Primary map



X Index: 215



Y Index: 211

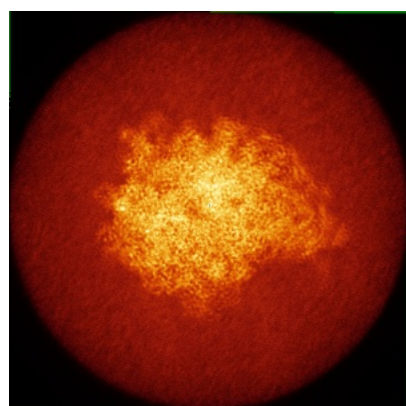


Z Index: 206

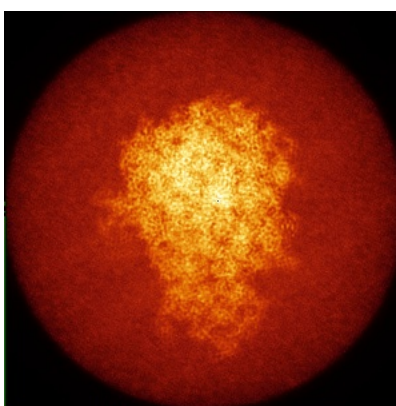
The images above show the largest variance slices of the map in three orthogonal directions.

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

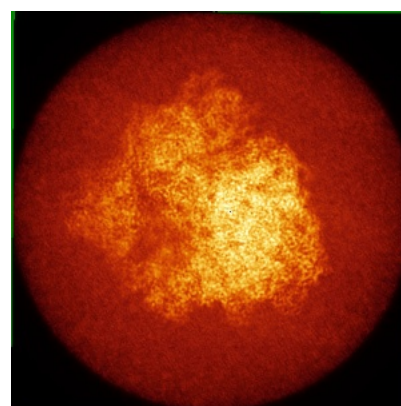
6.4.1 Primary map



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 0.065. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

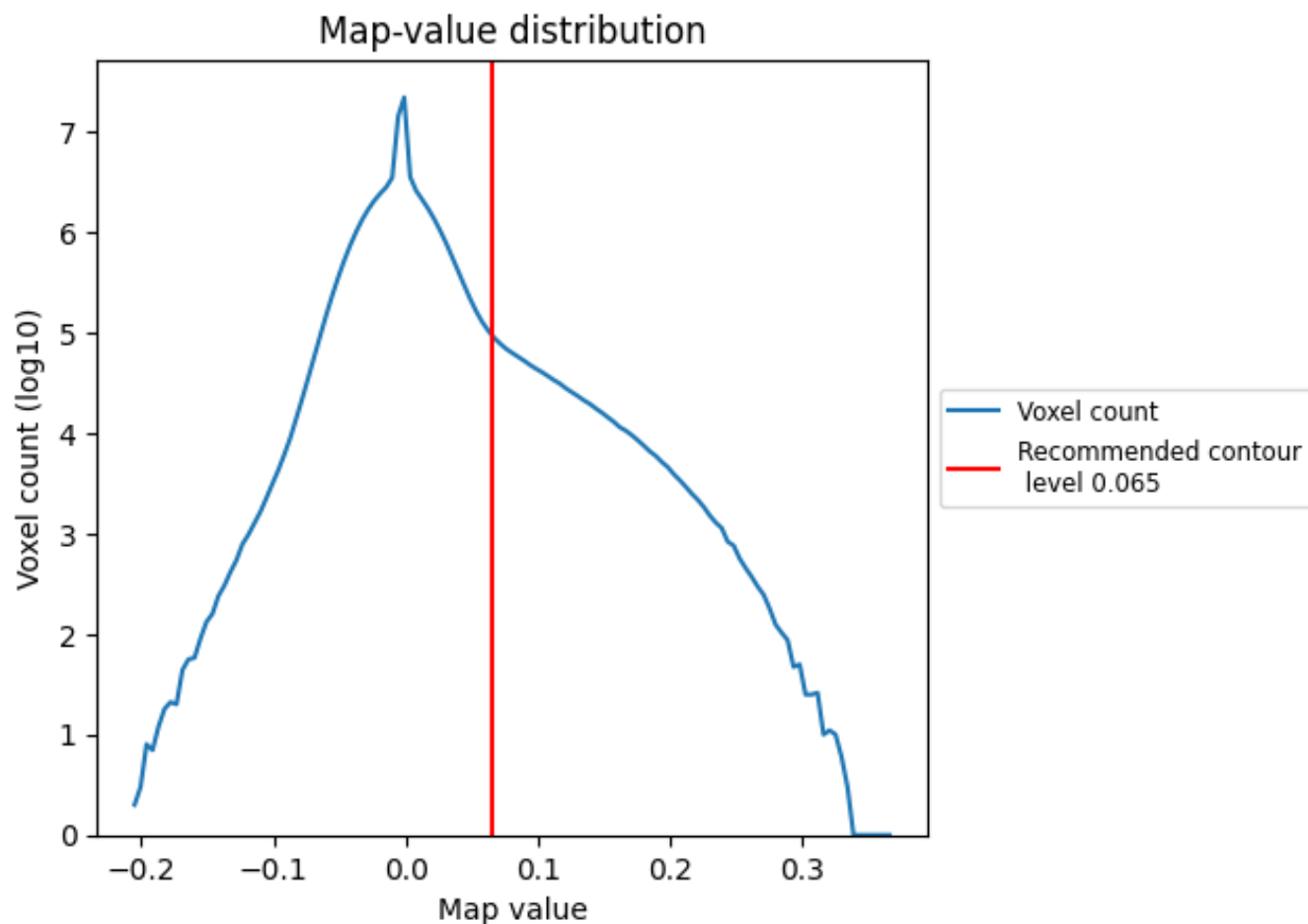
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

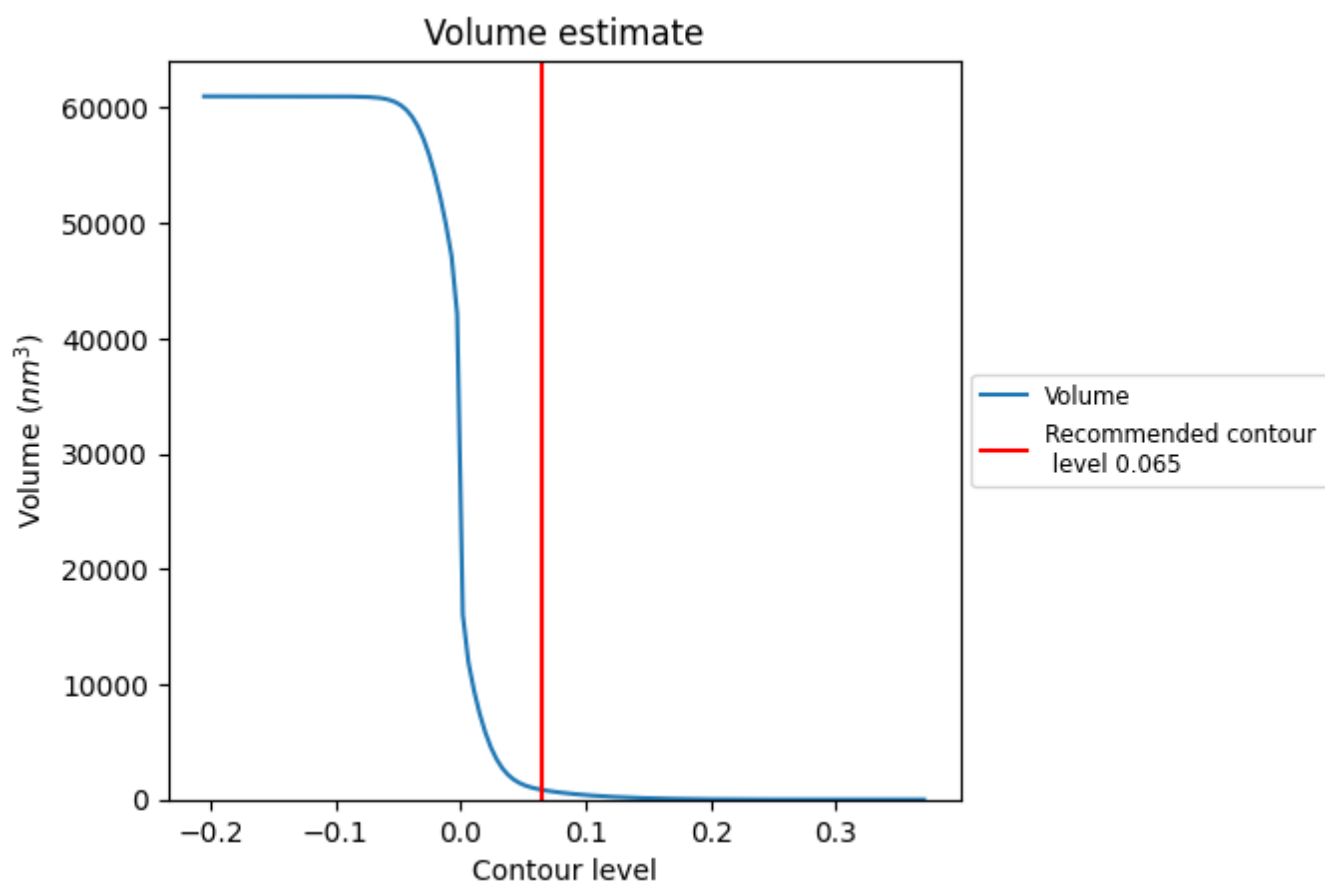
This section contains the results of statistical analysis of the map.

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.

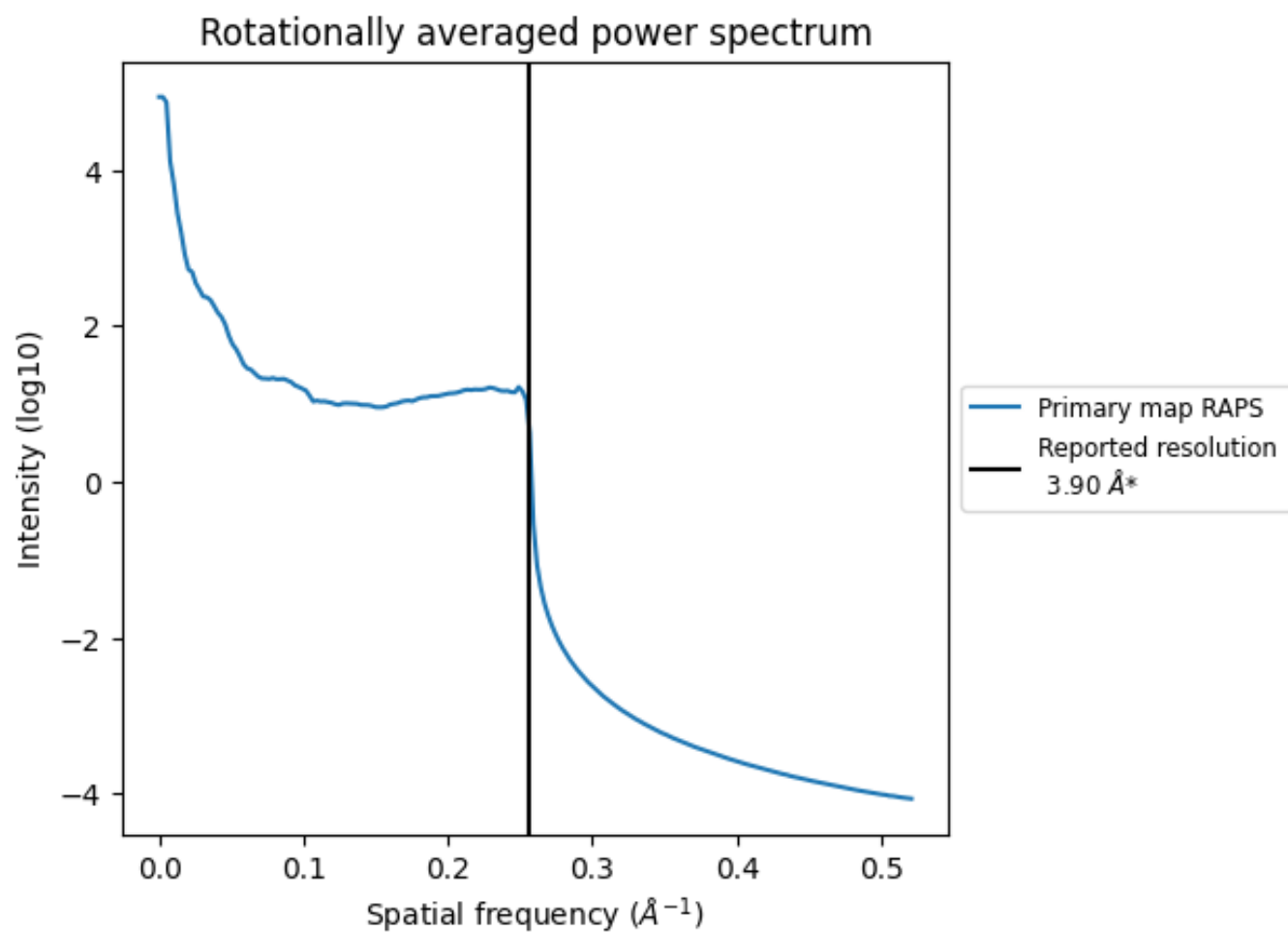
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 844 nm³; this corresponds to an approximate mass of 762 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 0.256 Å⁻¹

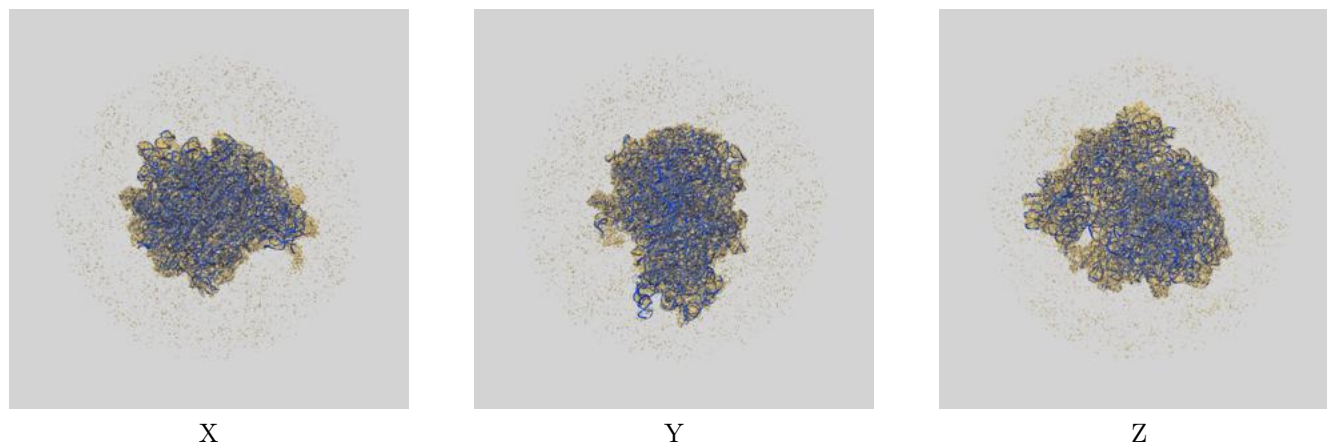
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

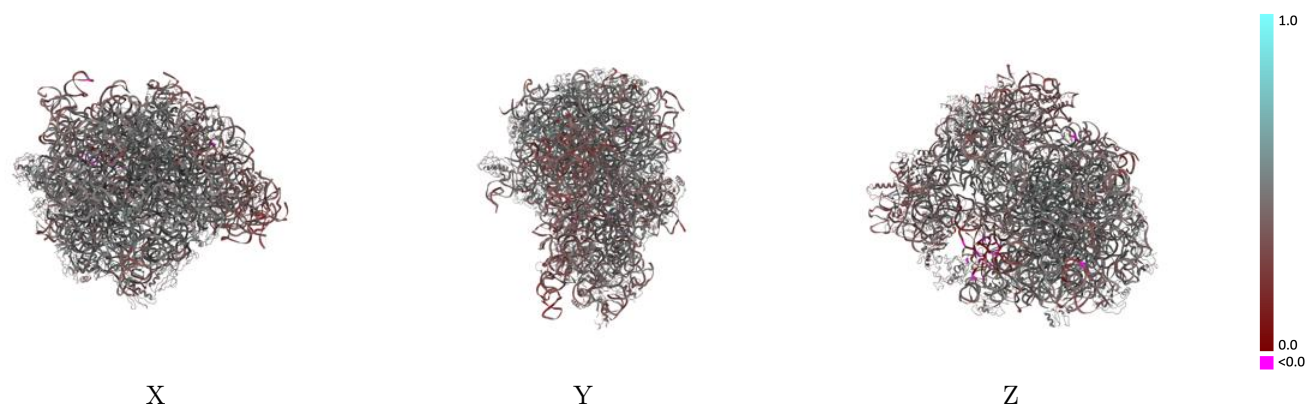
This section contains information regarding the fit between EMDB map EMD-8402 and PDB model 5TCU. Per-residue inclusion information can be found in section [3](#) on page [14](#).

9.1 Map-model overlay [i](#)



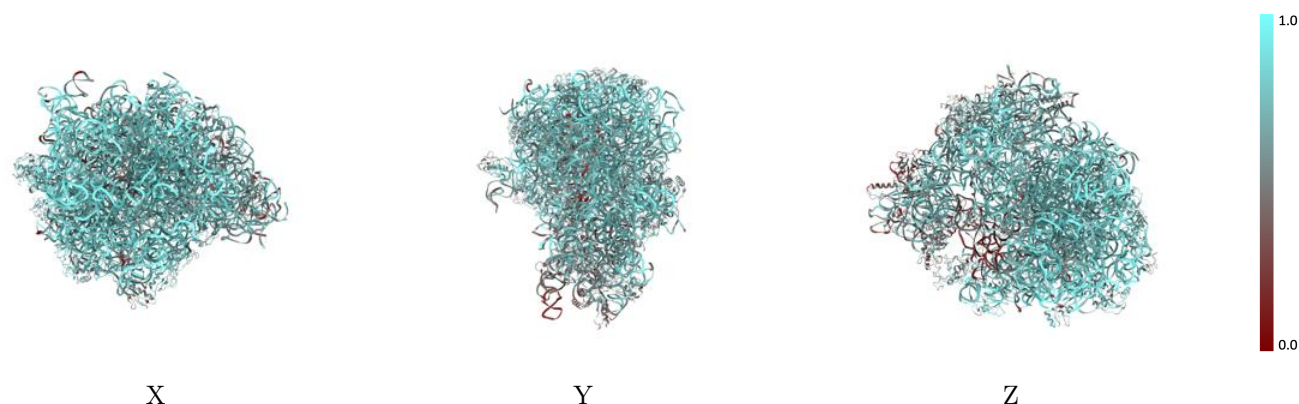
The images above show the 3D surface view of the map at the recommended contour level 0.065 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



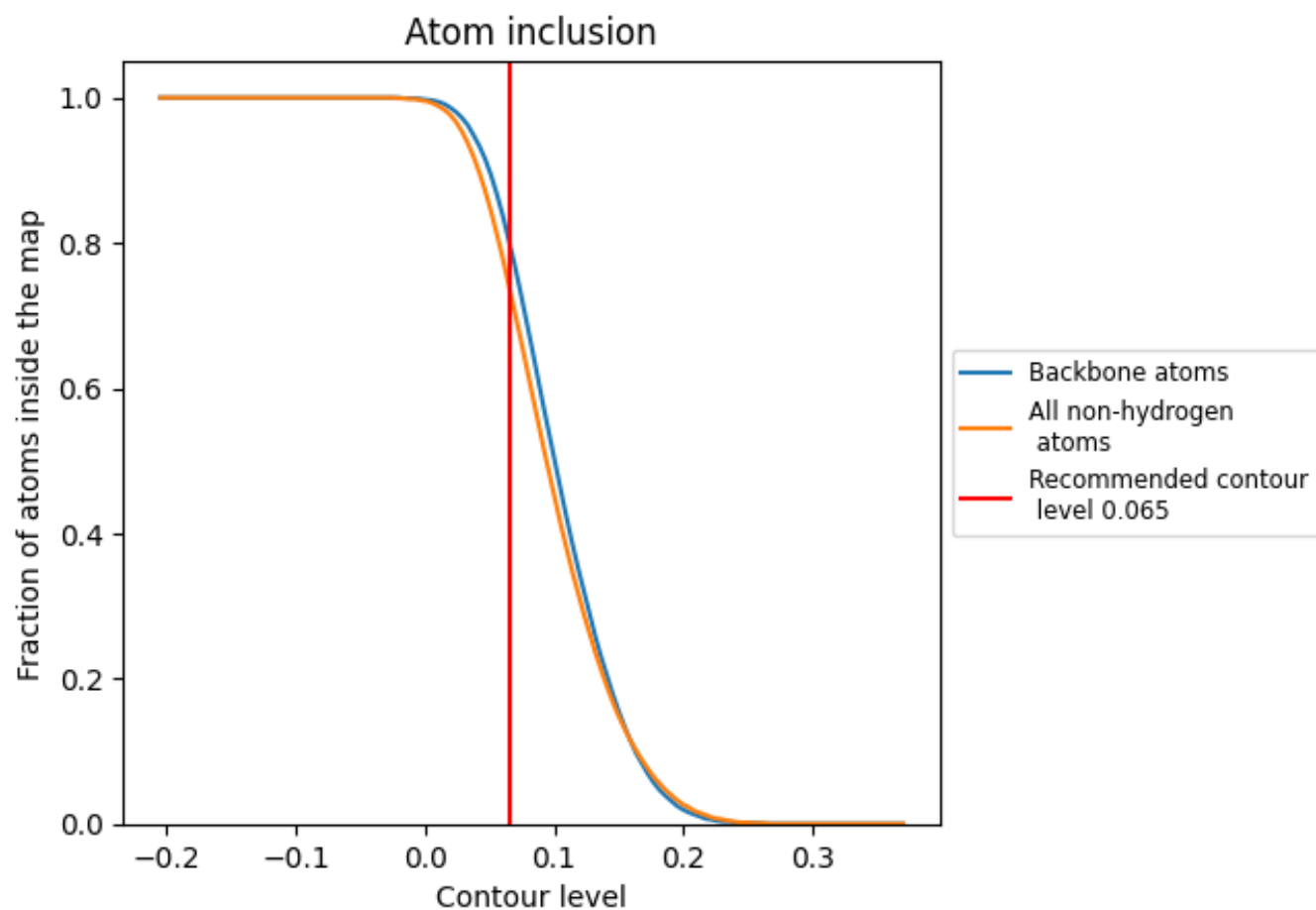
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.065).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 80% 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 (0.065) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7410	 0.4310
A	 0.7350	 0.3970
B	 0.8450	 0.4480
C	 0.8290	 0.4150
D	 0.2460	 0.1320
E	 0.2540	 0.2870
L1	 0.7020	 0.4910
L2	 0.7320	 0.5000
L3	 0.7290	 0.4710
L4	 0.7310	 0.4780
L5	 0.6950	 0.4870
L6	 0.6930	 0.4630
L7	 0.5790	 0.4400
L8	 0.4020	 0.4390
L9	 0.6830	 0.4890
LA	 0.5790	 0.4600
LB	 0.7060	 0.4520
LC	 0.7330	 0.4820
LD	 0.6780	 0.4860
LE	 0.7230	 0.4860
LF	 0.4920	 0.4100
LG	 0.7430	 0.4970
LH	 0.7980	 0.5100
LI	 0.6960	 0.4930
LJ	 0.7140	 0.4740
LK	 0.6300	 0.4380
LL	 0.6320	 0.4390
LM	 0.6810	 0.4750
LN	 0.6460	 0.4900
LO	 0.7360	 0.4800
LP	 0.6850	 0.4890
LQ	 0.7160	 0.4820
LR	 0.6780	 0.4310
LS	 0.6100	 0.4690
S1	 0.4910	 0.4130



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Chain	Atom inclusion	Q-score
S2	 0.5280	 0.4240
S3	 0.5180	 0.4320
S4	 0.4080	 0.3840
S5	 0.5190	 0.4440
S6	 0.6410	 0.4290
S7	 0.5020	 0.3830
S8	 0.5750	 0.4260
S9	 0.5600	 0.4390
SA	 0.5170	 0.3590
SB	 0.4450	 0.4140
SC	 0.5110	 0.3810
SD	 0.6060	 0.4600
SE	 0.5760	 0.4280
SF	 0.6220	 0.4430
SG	 0.4270	 0.4130
SH	 0.5130	 0.4010
SI	 0.4160	 0.3940
X	 0.4550	 0.4080