



Full wwPDB EM Validation Report ⓘ

Mar 8, 2026 – 06:00 AM UTC

PDB ID : 5LI0 / pdb_00005li0
EMDB ID : EMD-4050
Title : 70S ribosome from Staphylococcus aureus
Authors : Khusainov, I.; Vicens, Q.; Bochler, A.; Grosse, F.; Myasnikov, A.; Menetret, J.F.; Chicher, J.; Marzi, S.; Romby, P.; Yusupova, G.; Yusupov, M.; Hashem, Y.
Deposited on : 2016-07-13
Resolution : 3.80 Å(reported)

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

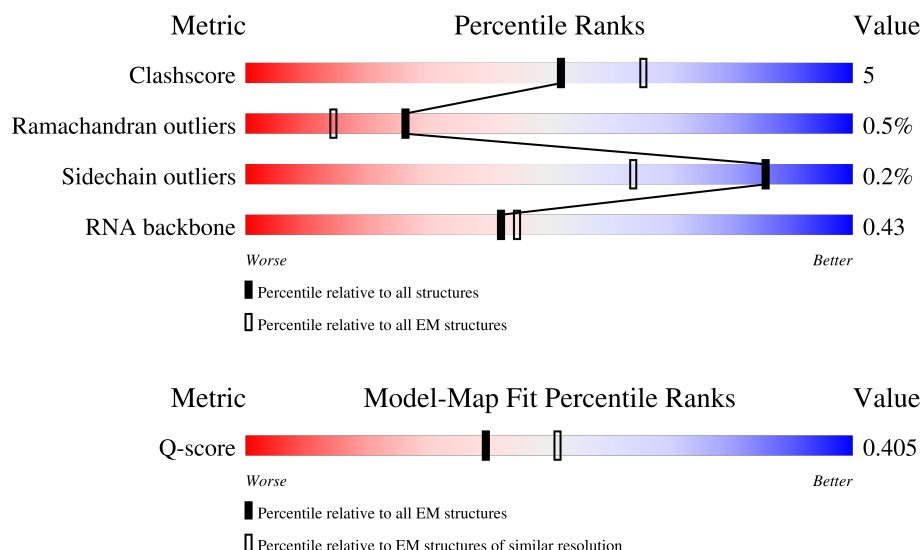
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDb archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh &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

1 Overall quality at a glance

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

The reported resolution of this entry is 3.80 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	10198 (3.30 - 4.30)

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	1547	
2	b	255	
3	c	217	

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Mol	Chain	Length	Quality of chain
4	d	199	
5	e	165	
6	f	96	
7	g	150	
8	h	131	
9	i	128	
10	j	102	
11	k	118	
12	l	135	
13	m	119	
14	n	60	
15	o	88	
16	p	90	
17	q	86	
18	r	71	
19	s	84	
20	t	80	
21	A	2918	
22	B	114	
23	D	275	
24	E	218	
25	F	199	
26	G	166	
27	H	164	
28	M	145	

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Mol	Chain	Length	Quality of chain
29	N	122	
30	O	131	
31	P	141	
32	Q	119	
33	R	119	
34	S	110	
35	T	116	
36	U	102	
37	V	112	
38	W	89	
39	X	100	
40	Y	94	
41	Z	82	
42	0	46	
43	1	65	
44	2	57	
45	3	84	
46	4	56	
47	5	39	
48	6	44	
49	7	60	
50	8	37	

2 Entry composition

There are 54 unique types of molecules in this entry. The entry contains 140825 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
1	a	1547	Total	C	N	O	P	0	0
			33126	14790	6036	10753	1547		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	b	224	Total	C	N	O	S	0	0
			1802	1147	315	333	7		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	c	208	Total	C	N	O	S	0	0
			1638	1032	306	298	2		

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
5	e	165	Total	C	N	O	S	0	0
			1239	775	229	233	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	f	96	Total	C	N	O	S	0	0
			799	503	139	154	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
7	g	147	Total	C	N	O	S	0	0
			1189	744	227	214	4		

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
10	j	102	Total	C	N	O	S	0	0
			813	512	148	150	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
11	k	118	Total	C	N	O	S	0	0
			881	543	169	166	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
12	l	135	Total	C	N	O	S	0	0
			1063	658	218	185	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
13	m	119	Total	C	N	O	S	0	0
			946	581	188	176	1		

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
17	q	86	Total	C	N	O	S	0	0
			707	447	126	133	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
18	r	71	Total	C	N	O	S	0	0
			590	372	115	100	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
19	s	84	Total	C	N	O	S	0	0
			678	434	120	122	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
20	t	80	Total	C	N	O	S	0	0
			607	367	119	119	2		

- Molecule 21 is a RNA chain called 23S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	A	2914	Total	C	N	O	P	0	0
			62475	27892	11424	20245	2914		

- Molecule 22 is a RNA chain called 5S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	B	114	Total	C	N	O	P	0	0
			2427	1086	436	792	113		

- Molecule 23 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	D	275	Total	C	N	O	S	0	0
			2104	1309	417	373	5		

- Molecule 24 is a protein called 50S ribosomal protein L3.

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

- Molecule 25 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	F	199	Total	C	N	O	S	0	0
			1525	955	281	287	2		

- Molecule 26 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	G	166	Total	C	N	O	S	0	0
			1312	832	223	251	6		

- Molecule 27 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	H	164	Total	C	N	O	S	0	0
			1285	799	232	251	3		

- Molecule 28 is a protein called 50S ribosomal protein L13.

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

- Molecule 29 is a protein called 50S ribosomal protein L14.

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

- Molecule 30 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	O	131	Total	C	N	O	S	0	0
			998	618	197	182	1		

- Molecule 31 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	P	141	Total	C	N	O	S	0	0
			1122	717	211	190	4		

- Molecule 32 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	Q	119	Total	C	N	O	S	0	0
			940	575	181	183	1		

- Molecule 33 is a protein called 50S ribosomal protein L18.

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

- Molecule 34 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	S	110	Total	C	N	O	S	0	0
			886	557	177	151	1		

- Molecule 35 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	T	116	Total	C	N	O	S	0	0
			944	593	189	158	4		

- Molecule 36 is a protein called 50S ribosomal protein L21.

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

- Molecule 37 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	V	112	Total	C	N	O	S	0	0
			863	537	164	159	3		

- Molecule 38 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	W	89	Total	C	N	O	S	0	0
			726	457	130	135	4		

- Molecule 39 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	X	87	Total	C	N	O	S	0	0
			669	423	122	123	1		

- Molecule 40 is a protein called 50S ribosomal protein L25.

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

- Molecule 41 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms				AltConf	Trace
41	Z	82	Total	C	N	O	0	0
			627	386	122	119		

- Molecule 42 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms				AltConf	Trace
42	0	46	Total	C	N	O	0	0
			374	231	83	60		

- Molecule 43 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms				AltConf	Trace
43	1	65	Total	C	N	O	0	0
			537	330	101	106		

- Molecule 44 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms				AltConf	Trace
44	2	57	Total	C	N	O	0	0
			442	274	83	85		

- Molecule 45 is a protein called 50S ribosomal protein L31 type B.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	3	83	Total	C	N	O	S	0	0
			677	430	116	128	3		

- Molecule 46 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	4	56	Total	C	N	O	S	0	0
			444	268	92	79	5		

- Molecule 47 is a protein called 50S ribosomal protein L33 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	5	28	Total	C	N	O	S	0	0
			229	137	45	43	4		

- Molecule 48 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	6	44	Total	C	N	O	S	0	0
			373	228	90	54	1		

- Molecule 49 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	7	60	Total	C	N	O	S	0	0
			488	300	108	78	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
50	8	37	Total	C	N	O	S	0	0
			297	186	60	46	5		

- Molecule 51 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
51	a	2	Total	Mg	0
			2	2	
51	A	29	Total	Mg	0
			29	29	

- Molecule 52 is OXYGEN ATOM (CCD ID: O) (formula: O).

Mol	Chain	Residues	Atoms		AltConf
52	A	9	Total	O	0
			9	9	

- Molecule 53 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
53	8	1	Total	Zn	0
			1	1	

- Molecule 54 is water.

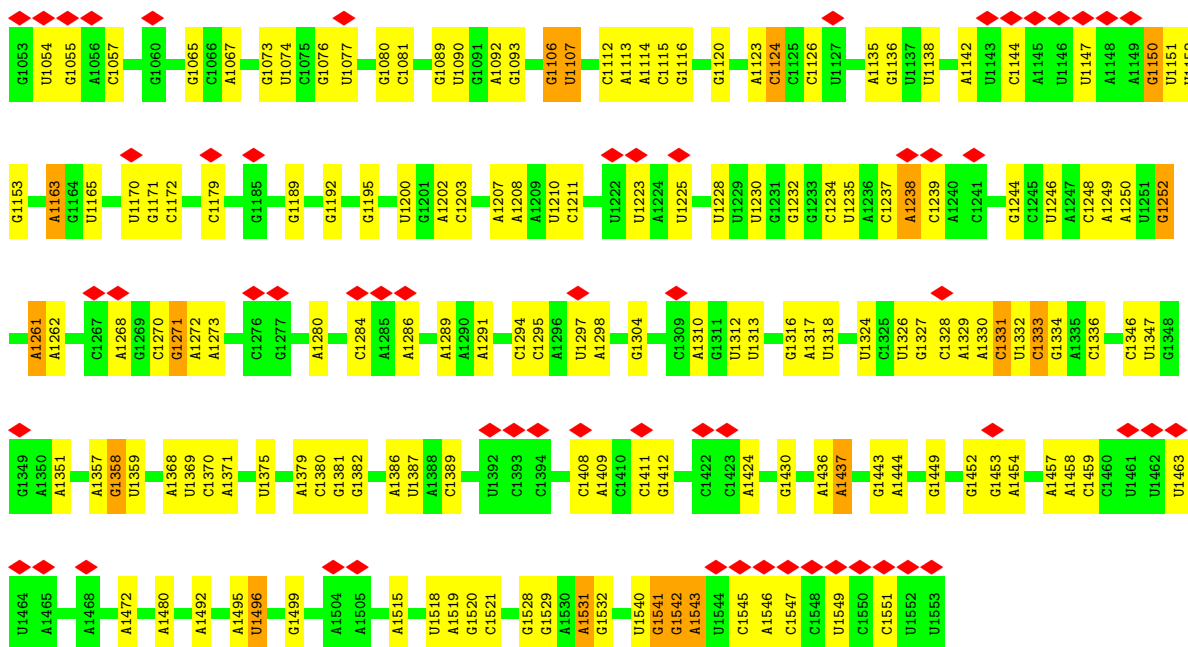
Mol	Chain	Residues	Atoms		AltConf
54	a	12	Total	O	0
			12	12	
54	A	143	Total	O	0
			143	143	
54	D	4	Total	O	0
			4	4	
54	T	2	Total	O	0
			2	2	
54	U	1	Total	O	0
			1	1	

3 Residue-property plots

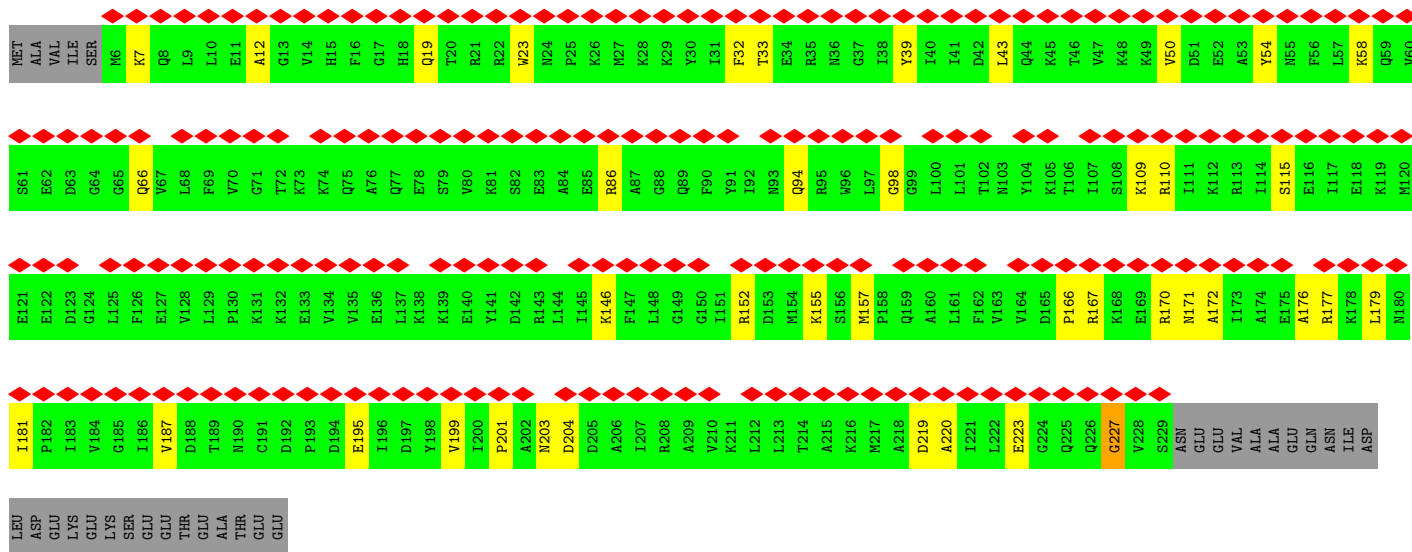
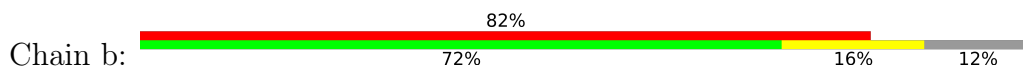
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

• Molecule 1: 16S ribosomal RNA

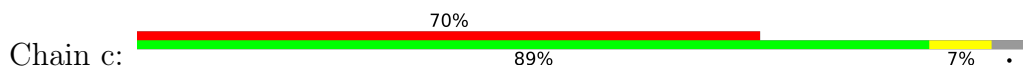


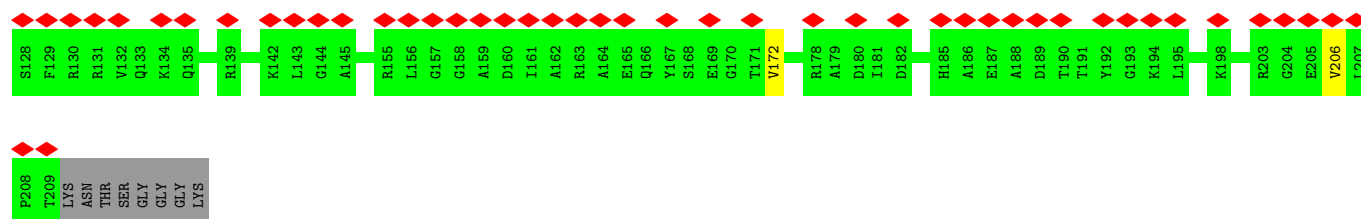


• Molecule 2: 30S ribosomal protein S2

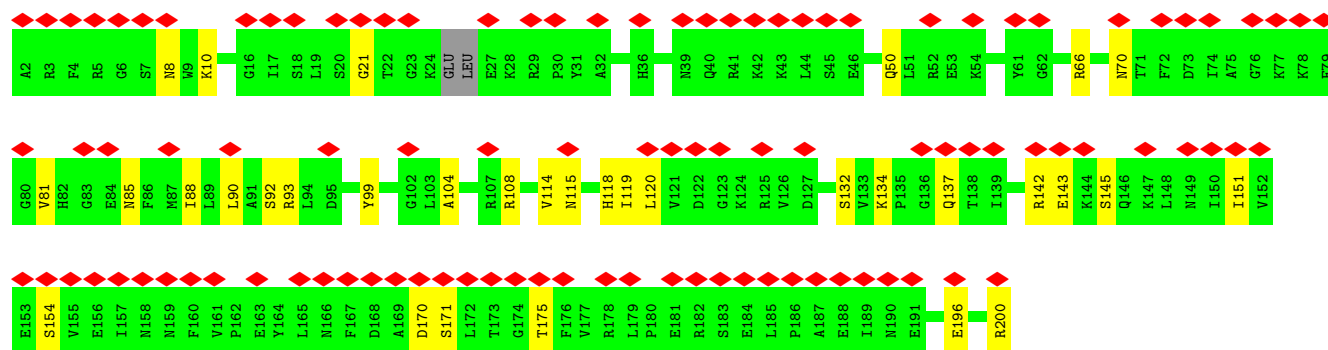
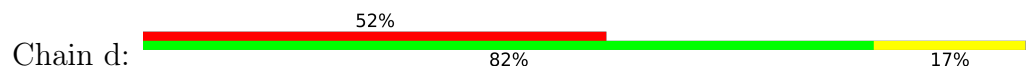


• Molecule 3: 30S ribosomal protein S3

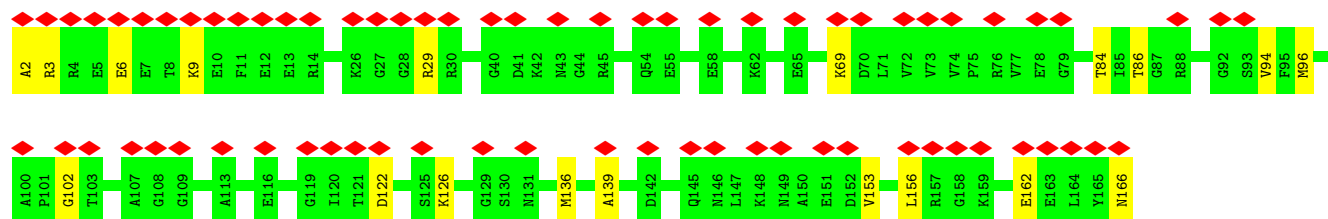
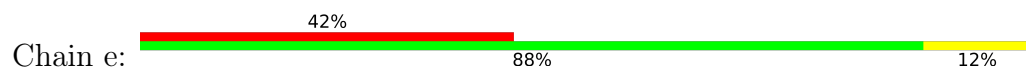




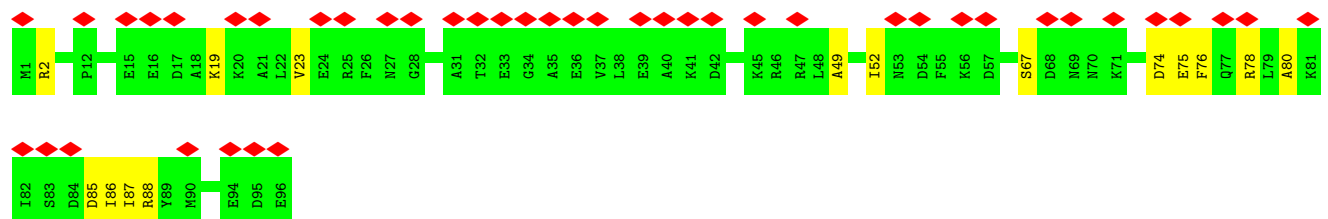
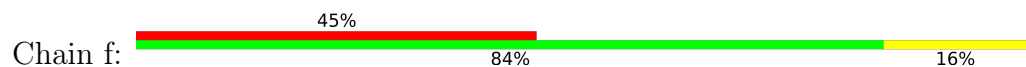
• Molecule 4: 30S ribosomal protein S4



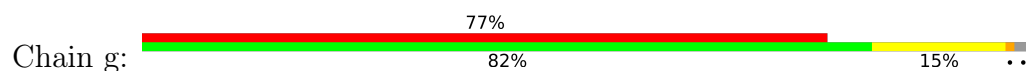
• Molecule 5: 30S ribosomal protein S5

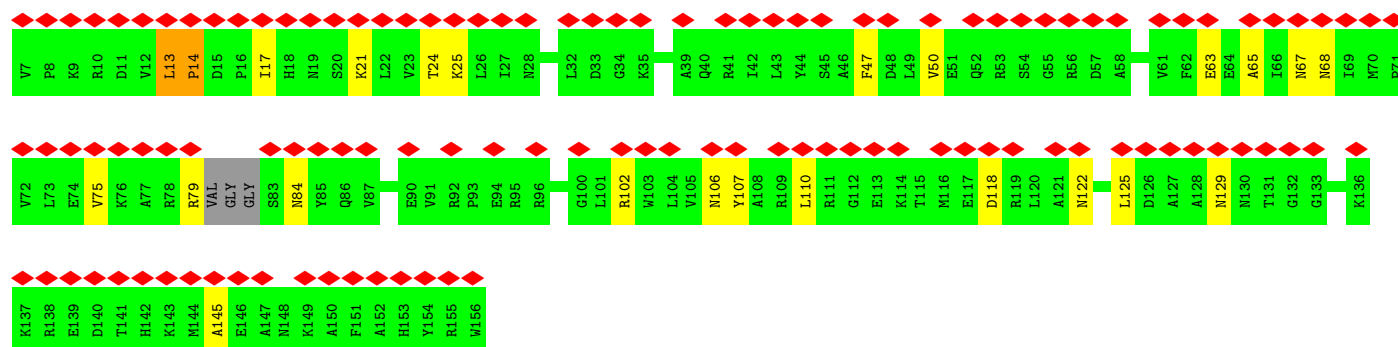


• Molecule 6: 30S ribosomal protein S6

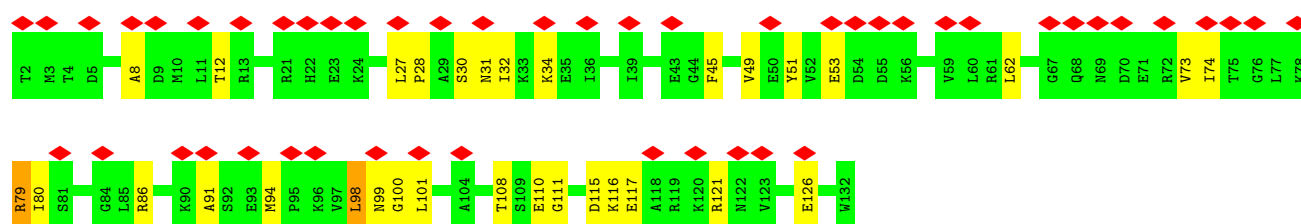
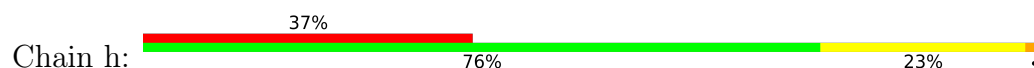


• Molecule 7: 30S ribosomal protein S7

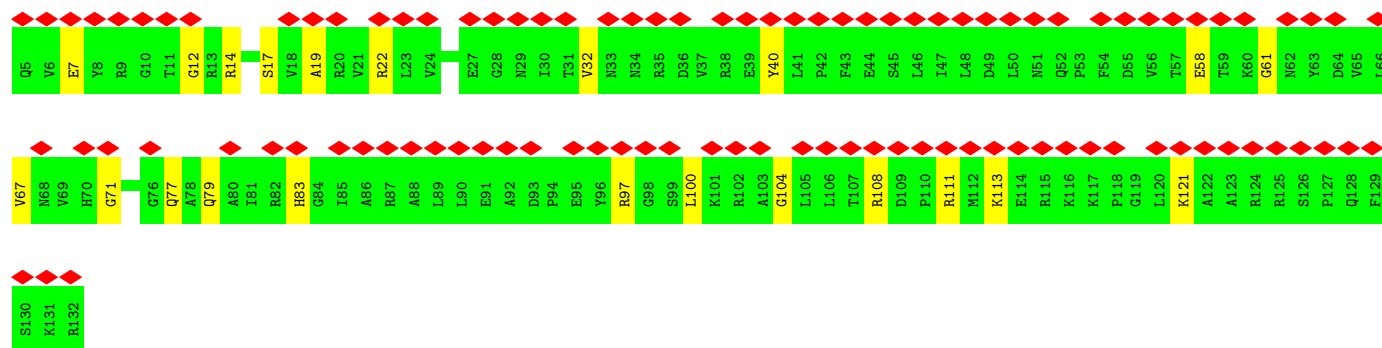
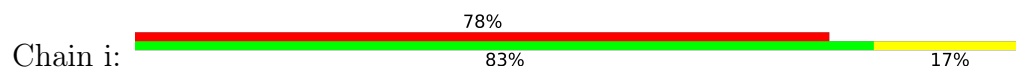




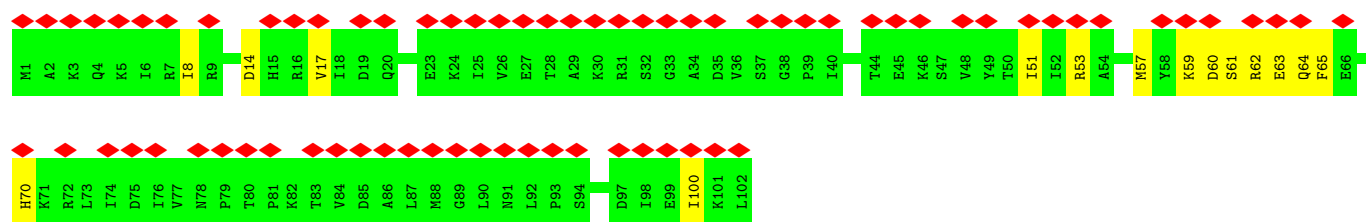
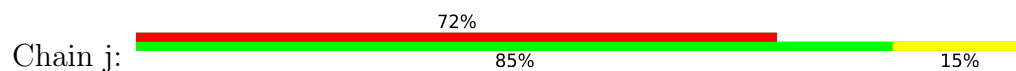
• Molecule 8: 30S ribosomal protein S8



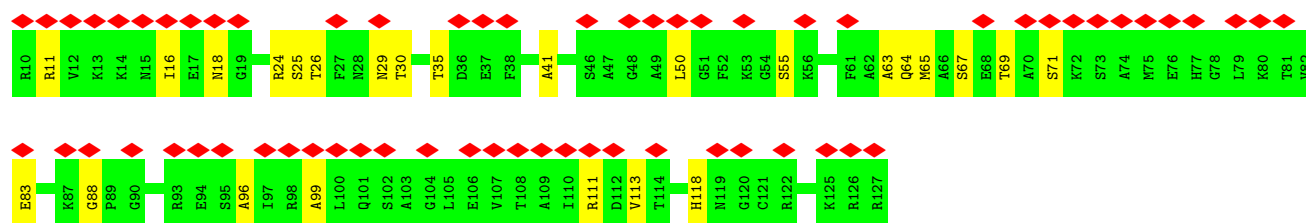
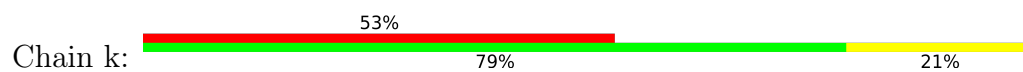
• Molecule 9: 30S ribosomal protein S9



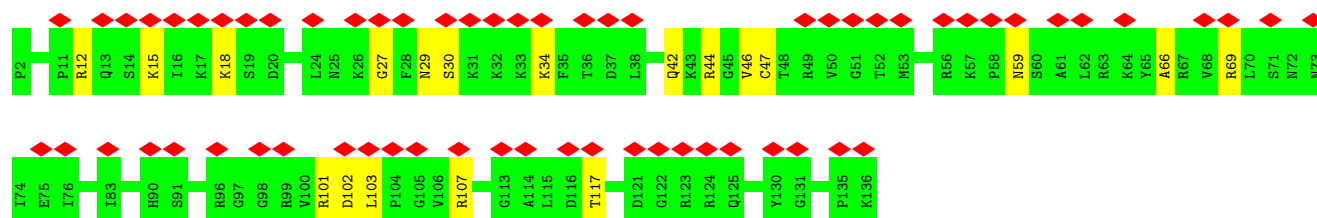
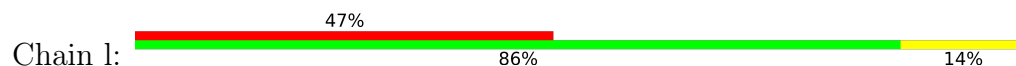
• Molecule 10: 30S ribosomal protein S10



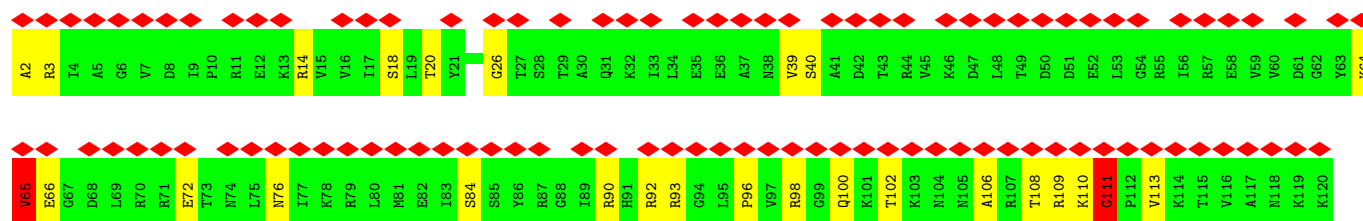
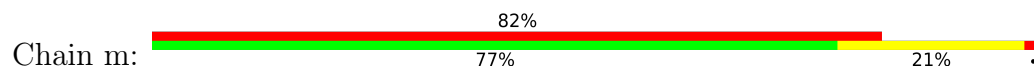
• Molecule 11: 30S ribosomal protein S11



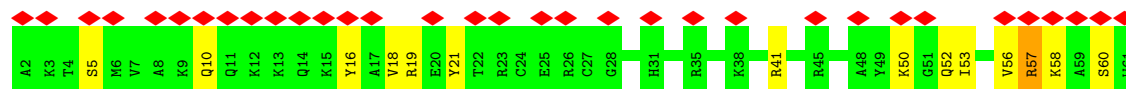
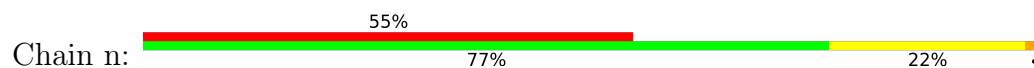
• Molecule 12: 30S ribosomal protein S12



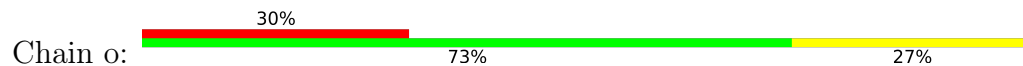
• Molecule 13: 30S ribosomal protein S13



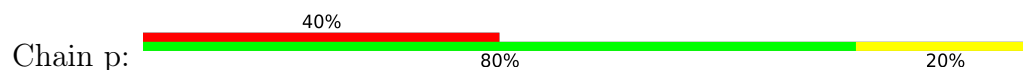
• Molecule 14: 30S ribosomal protein S14 type Z

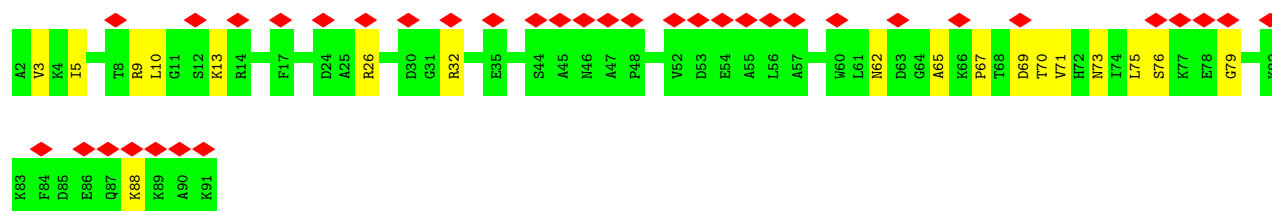


• Molecule 15: 30S ribosomal protein S15

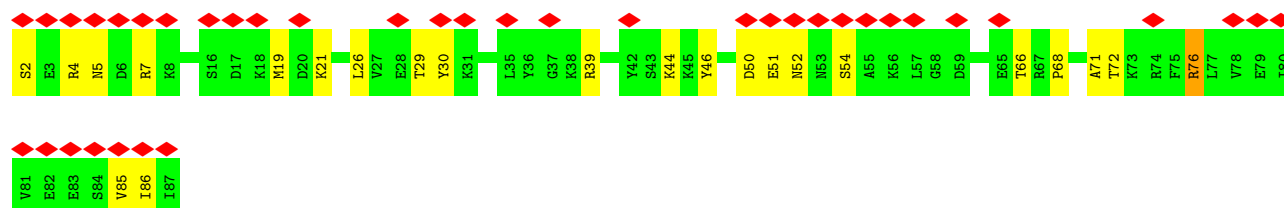
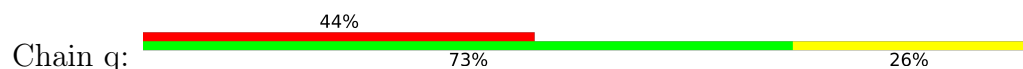


• Molecule 16: 30S ribosomal protein S16

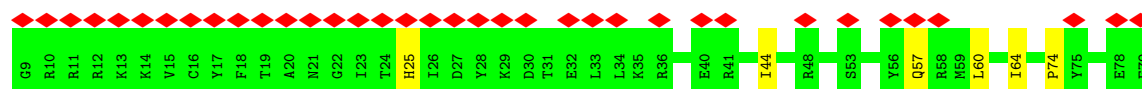
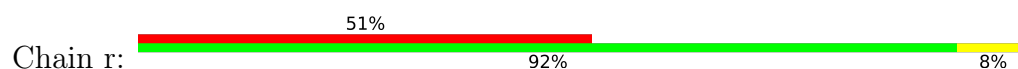




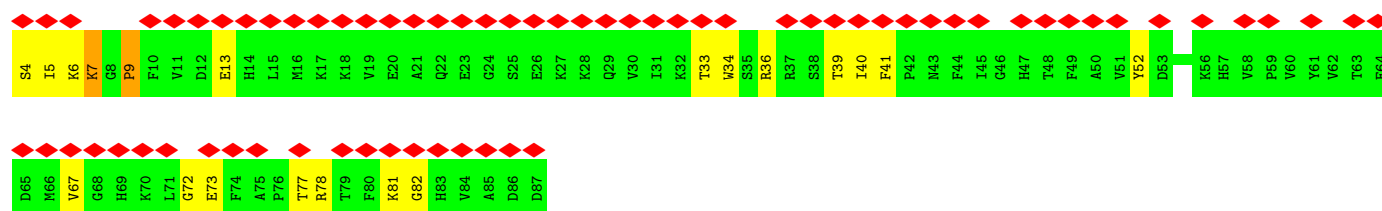
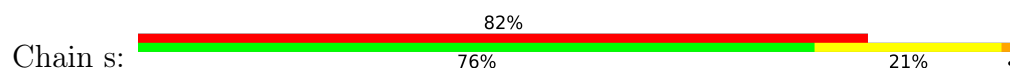
• Molecule 17: 30S ribosomal protein S17



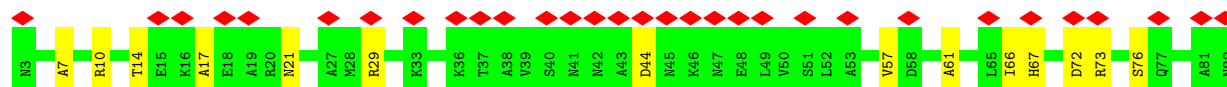
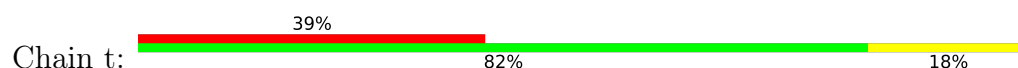
• Molecule 18: 30S ribosomal protein S18



• Molecule 19: 30S ribosomal protein S19

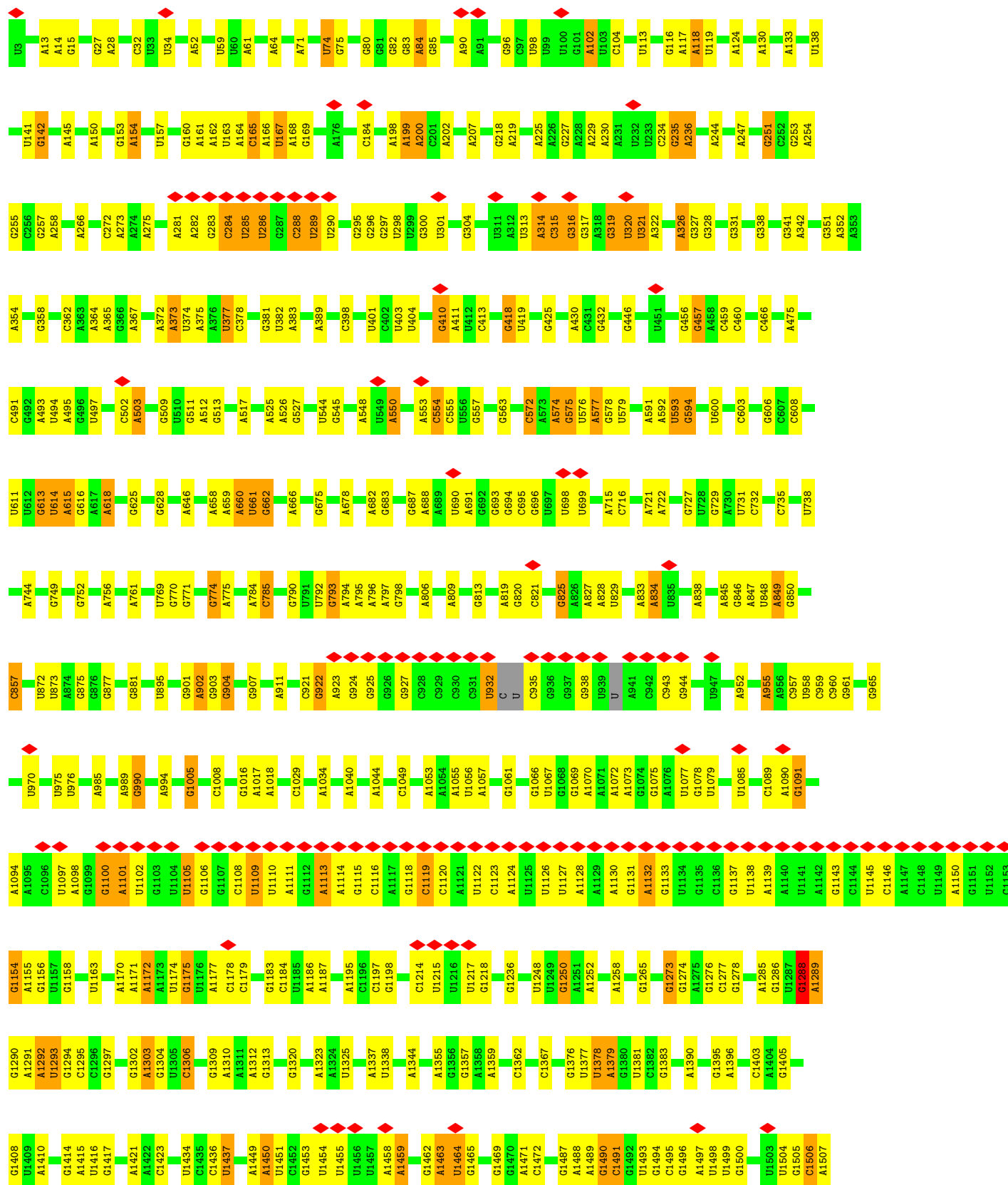


• Molecule 20: 30S ribosomal protein S20



• Molecule 21: 23S ribosomal RNA

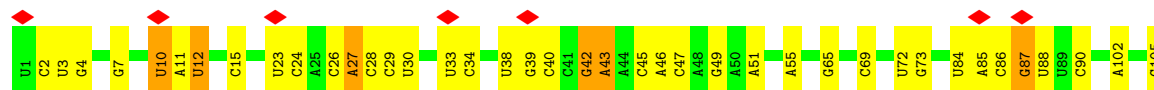




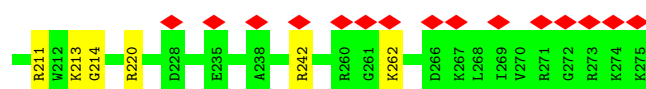
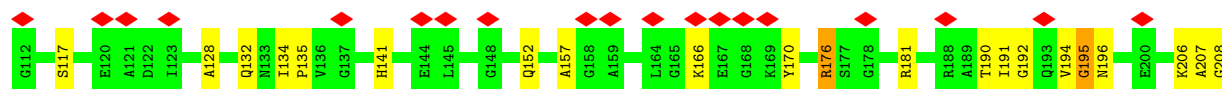
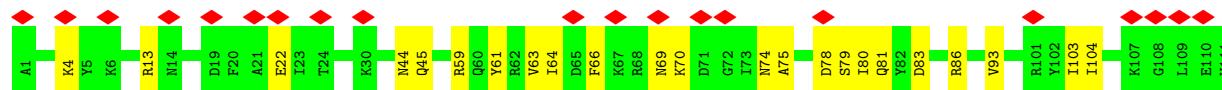
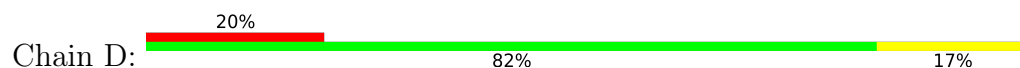




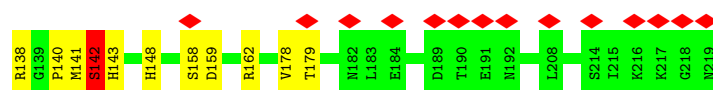
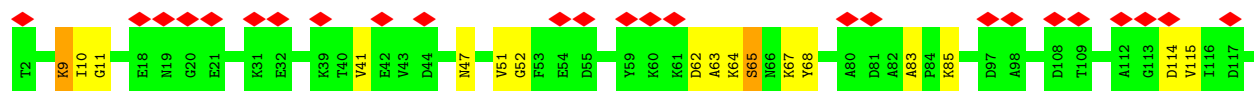
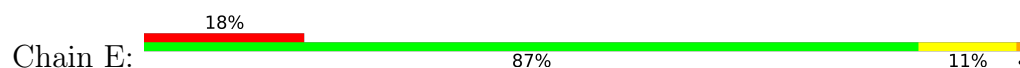
• Molecule 22: 5S ribosomal RNA



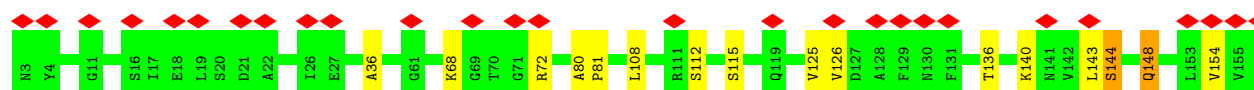
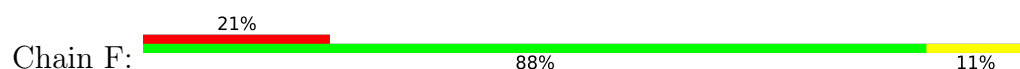
• Molecule 23: 50S ribosomal protein L2



• Molecule 24: 50S ribosomal protein L3

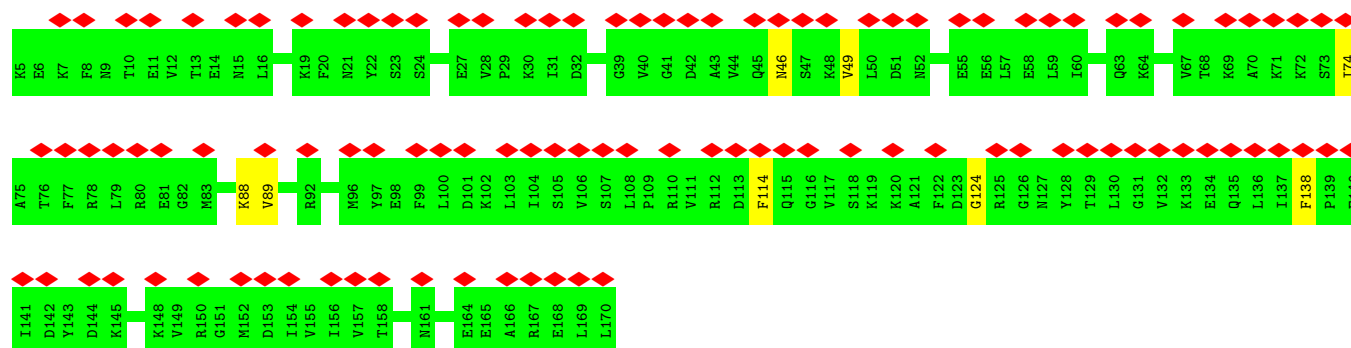


• Molecule 25: 50S ribosomal protein L4

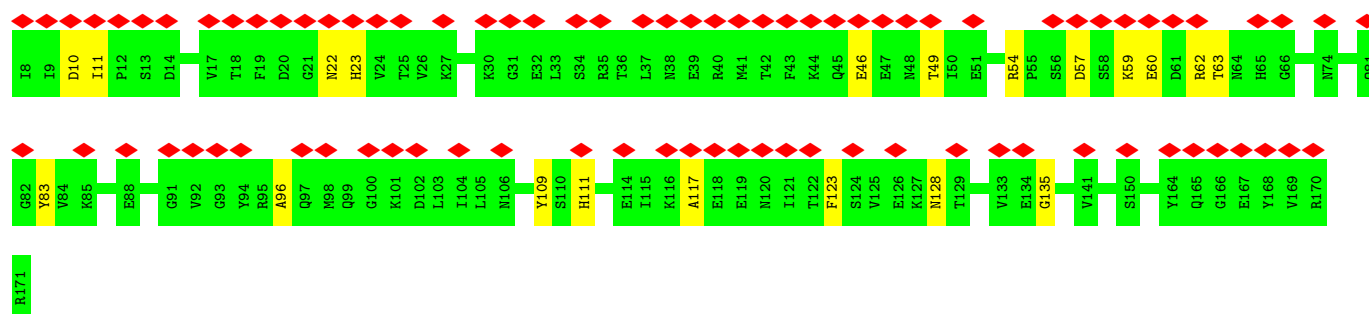
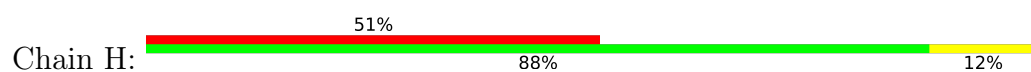




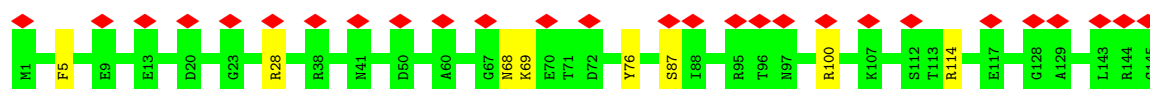
• Molecule 26: 50S ribosomal protein L5



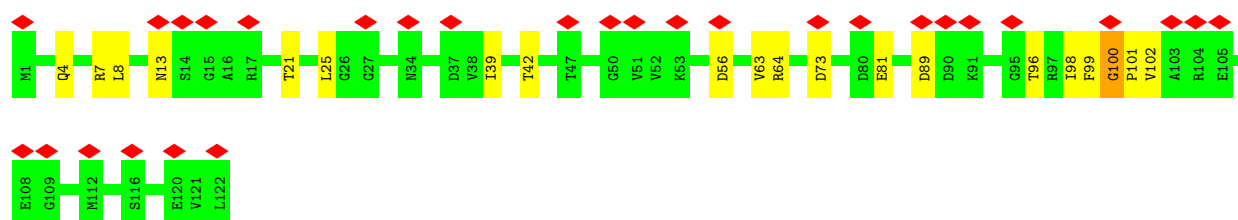
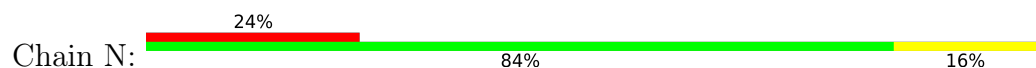
• Molecule 27: 50S ribosomal protein L6



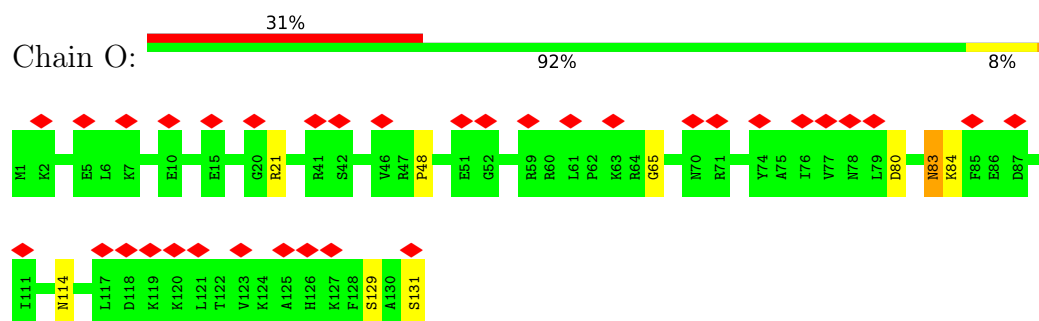
• Molecule 28: 50S ribosomal protein L13



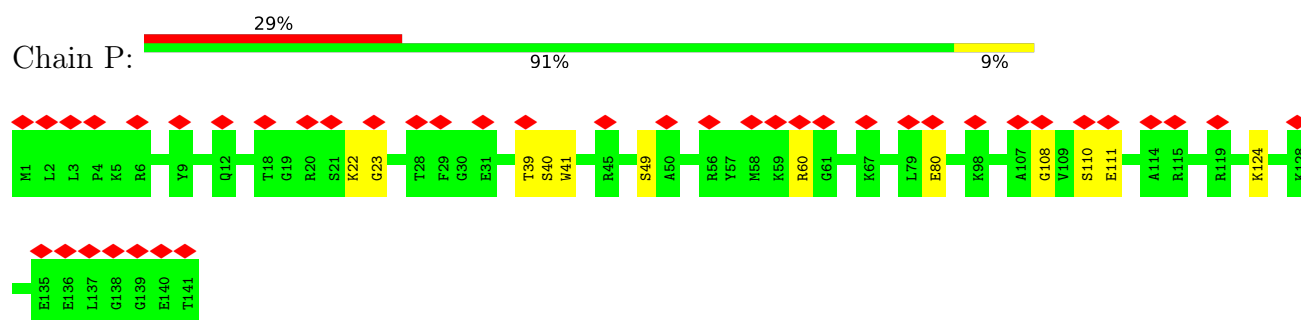
• Molecule 29: 50S ribosomal protein L14



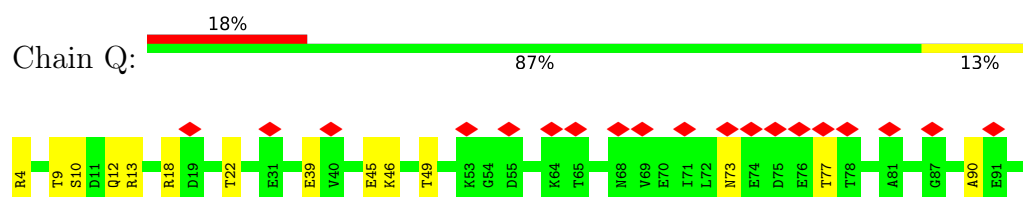
- Molecule 30: 50S ribosomal protein L15



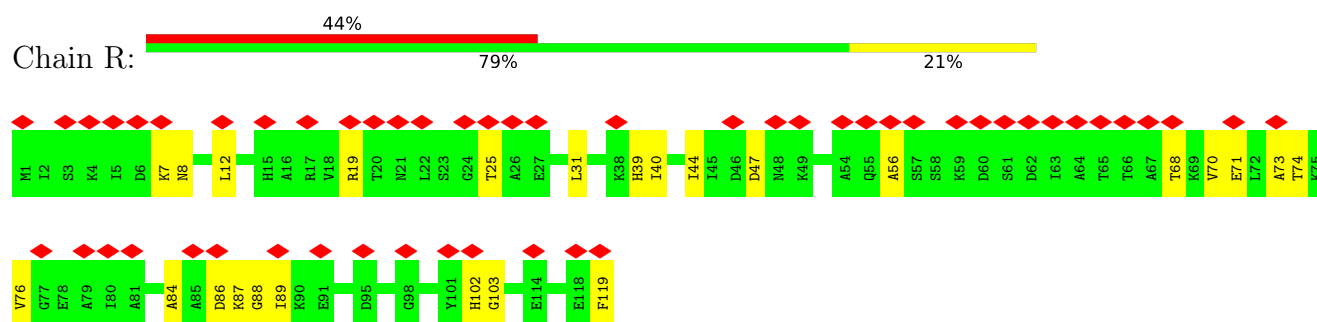
- Molecule 31: 50S ribosomal protein L16



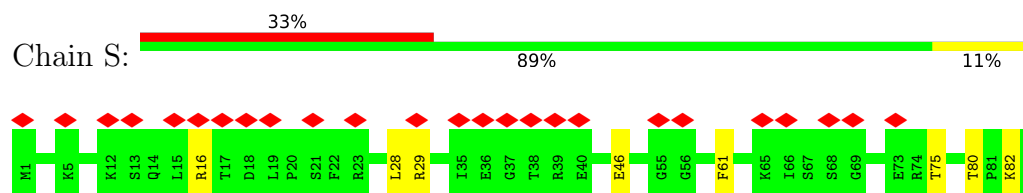
- Molecule 32: 50S ribosomal protein L17

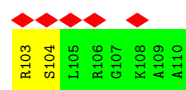


- Molecule 33: 50S ribosomal protein L18

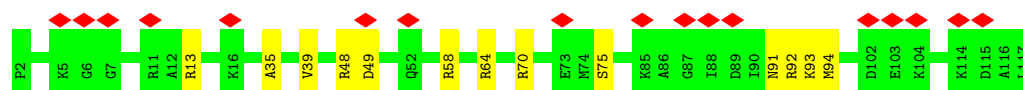
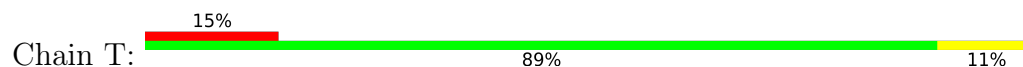


- Molecule 34: 50S ribosomal protein L19

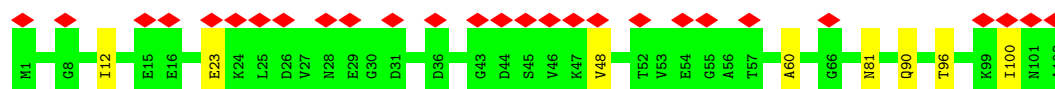




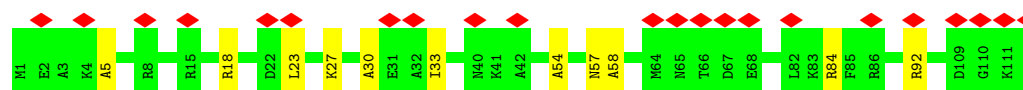
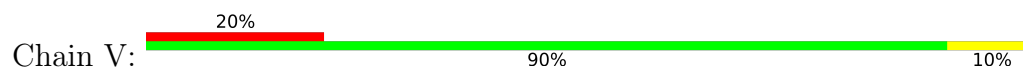
- Molecule 35: 50S ribosomal protein L20



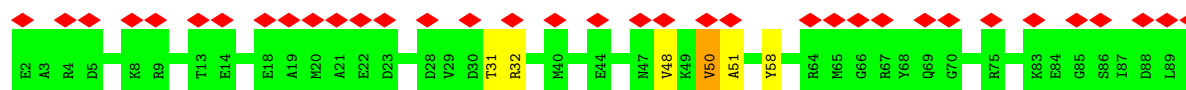
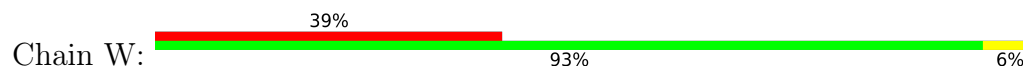
- Molecule 36: 50S ribosomal protein L21



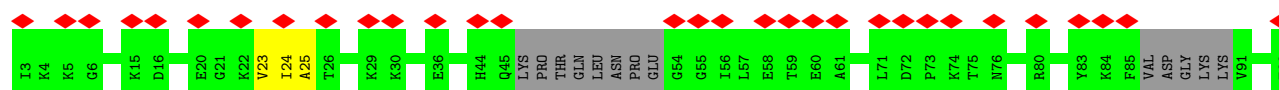
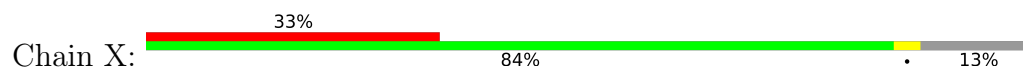
- Molecule 37: 50S ribosomal protein L22



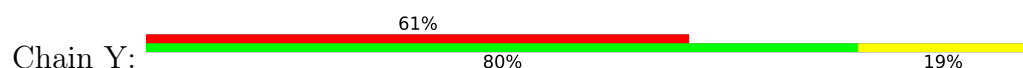
- Molecule 38: 50S ribosomal protein L23

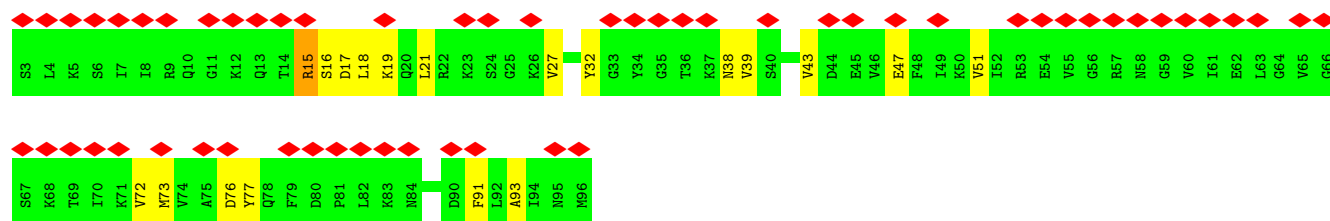


- Molecule 39: 50S ribosomal protein L24

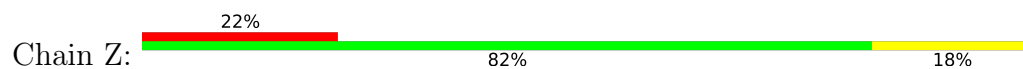


- Molecule 40: 50S ribosomal protein L25

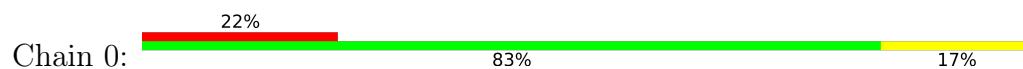




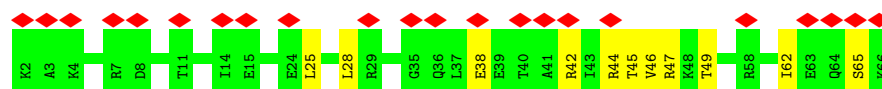
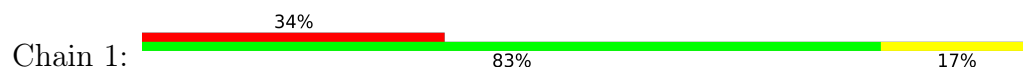
• Molecule 41: 50S ribosomal protein L27



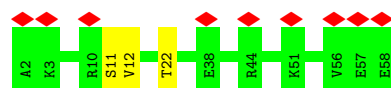
• Molecule 42: 50S ribosomal protein L28



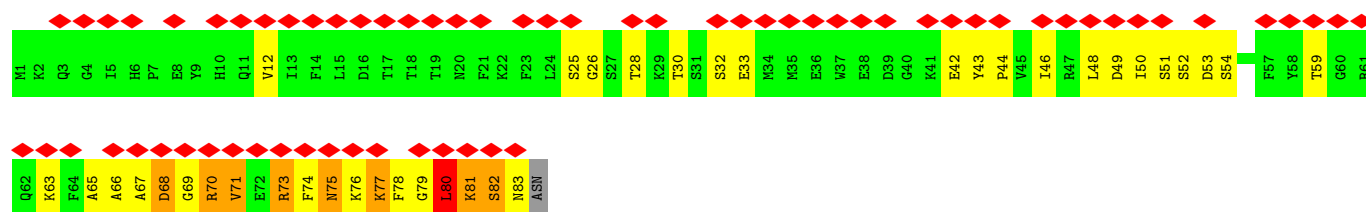
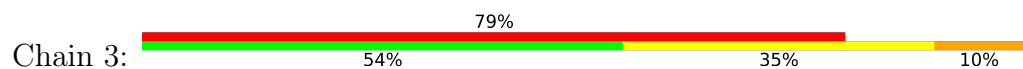
• Molecule 43: 50S ribosomal protein L29



• Molecule 44: 50S ribosomal protein L30

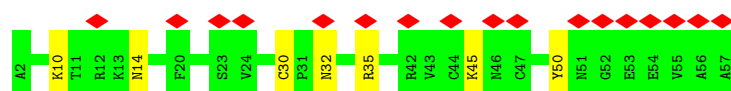
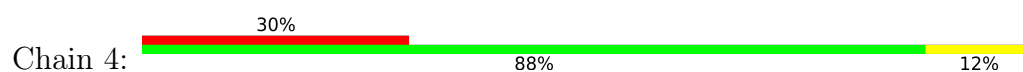


• Molecule 45: 50S ribosomal protein L31 type B



• Molecule 46: 50S ribosomal protein L32

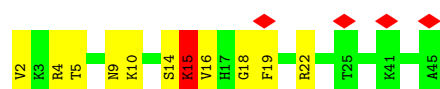
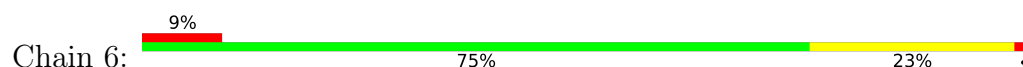




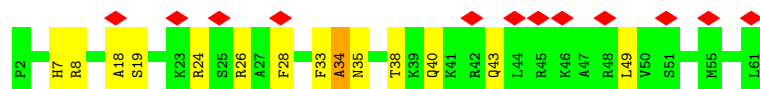
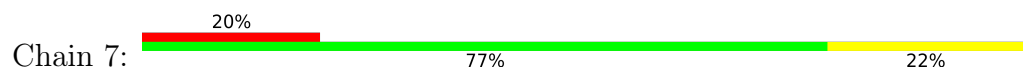
- Molecule 47: 50S ribosomal protein L33 2



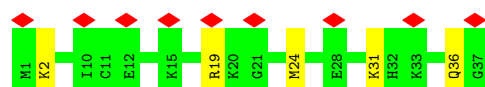
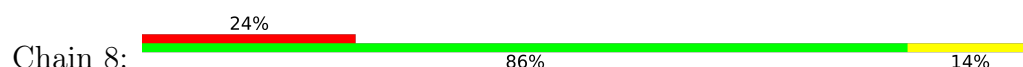
- Molecule 48: 50S ribosomal protein L34



- Molecule 49: 50S ribosomal protein L35



- Molecule 50: 50S ribosomal protein L36



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	110000	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	60	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	FEI FALCON II (4k x 4k)	Depositor
Maximum map value	0.447	Depositor
Minimum map value	-0.238	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.000	Depositor
Recommended contour level	0.095	Depositor
Map size ($\text{\AA}$)	365.2, 365.2, 365.2	wwPDB
Map dimensions	332, 332, 332	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.1, 1.1, 1.1	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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	0.41	0/37086	0.47	0/57833
2	b	0.35	0/1829	0.62	1/2454 (0.0%)
3	c	0.44	1/1661 (0.1%)	0.64	1/2233 (0.0%)
4	d	0.46	0/1629	0.67	0/2185
5	e	0.54	0/1253	0.66	0/1687
6	f	0.51	0/810	0.60	0/1085
7	g	0.41	0/1207	0.62	0/1625
8	h	0.56	0/1044	0.67	0/1401
9	i	0.39	0/1033	0.68	0/1386
10	j	0.41	0/825	0.62	0/1110
11	k	0.46	0/896	0.64	0/1207
12	l	0.51	0/1080	0.80	2/1445 (0.1%)
13	m	0.42	0/953	0.83	2/1275 (0.2%)
14	n	0.47	0/512	0.75	2/678 (0.3%)
15	o	0.52	0/747	0.73	0/996
16	p	0.51	0/723	0.67	0/971
17	q	0.52	0/715	0.76	0/955
18	r	0.46	0/599	0.70	0/797
19	s	0.38	0/696	0.83	1/934 (0.1%)
20	t	0.45	0/607	0.67	2/810 (0.2%)
21	A	0.88	23/69965 (0.0%)	0.57	29/109115 (0.0%)
22	B	0.39	0/2714	0.45	0/4228
23	D	0.74	0/2139	0.72	0/2869
24	E	0.65	0/1673	0.73	0/2243
25	F	0.62	0/1548	0.70	0/2088
26	G	0.39	0/1327	0.76	1/1780 (0.1%)
27	H	0.44	0/1303	0.60	0/1757
28	M	0.60	0/1173	0.64	0/1578
29	N	0.68	0/927	0.72	0/1243
30	O	0.62	0/1011	0.82	0/1344
31	P	0.64	0/1146	0.77	0/1536
32	Q	0.59	0/943	0.66	0/1259

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	R	0.50	0/931	0.70	0/1244
34	S	0.60	0/898	0.66	0/1199
35	T	0.69	0/956	0.71	0/1265
36	U	0.58	0/809	0.64	1/1080 (0.1%)
37	V	0.65	0/871	0.73	0/1171
38	W	0.58	0/734	0.70	0/978
39	X	0.46	0/673	0.72	0/893
40	Y	0.46	0/746	0.76	0/1000
41	Z	0.69	0/633	0.78	0/838
42	0	0.54	0/379	0.71	0/504
43	1	0.48	0/538	0.65	0/714
44	2	0.60	0/444	0.66	0/597
45	3	0.51	1/694 (0.1%)	0.97	2/930 (0.2%)
46	4	0.62	0/451	0.74	1/599 (0.2%)
47	5	0.53	0/230	0.91	0/303
48	6	0.72	0/377	0.76	0/491
49	7	0.67	0/492	0.98	1/643 (0.2%)
50	8	0.64	0/300	0.63	0/393
All	All	0.69	25/152930 (0.0%)	0.58	46/228949 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
3	c	0	2
5	e	0	1
7	g	0	3
8	h	0	2
13	m	0	5
14	n	0	2
17	q	0	3
19	s	0	3
23	D	0	1
24	E	0	6
25	F	0	5
26	G	0	4
28	M	0	2
29	N	0	1
30	O	0	4
31	P	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
33	R	0	2
34	S	0	1
35	T	0	1
36	U	0	1
38	W	0	2
40	Y	0	1
41	Z	0	4
45	3	0	3
46	4	0	2
47	5	0	1
48	6	0	2
49	7	0	2
All	All	0	67

All (25) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	A	2230	G	C1'-N9	64.12	2.44	1.48
21	A	1288	G	C6-N1	59.92	2.59	1.39
21	A	857	C	C5-C6	55.88	2.46	1.34
21	A	1288	G	N1-C2	55.43	2.48	1.37
21	A	1288	G	N3-C4	51.77	2.38	1.35
21	A	1288	G	C2-N3	49.67	2.32	1.32
21	A	1288	G	C5-C6	48.03	2.38	1.42
21	A	1828	U	N1-C2	44.18	2.27	1.38
21	A	1288	G	C5-C4	42.90	2.24	1.38
21	A	1828	U	C2-N3	41.95	2.21	1.37
21	A	857	C	C2-N3	41.84	2.19	1.35
21	A	1828	U	N3-C4	41.62	2.21	1.38
21	A	1828	U	N1-C6	40.59	2.19	1.38
21	A	1828	U	C4-C5	37.60	2.18	1.43
21	A	1828	U	C5-C6	36.68	2.07	1.34
21	A	2230	G	N9-C4	15.37	1.68	1.38
21	A	1510	U	O3'-P	-13.76	1.40	1.61
21	A	857	C	N3-C4	13.05	1.59	1.33
21	A	2230	G	N9-C8	11.65	1.61	1.37
45	3	80	LEU	C-N	7.79	1.43	1.33
21	A	857	C	C4-C5	-7.42	1.28	1.43
21	A	2230	G	N7-C5	-6.37	1.26	1.39
21	A	1511	C	O3'-P	6.33	1.70	1.61
3	c	206	VAL	C-N	6.21	1.42	1.32
21	A	857	C	C2-O2	5.51	1.35	1.24

All (46) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	A	857	C	N3-C4-C5	-31.76	26.62	121.90
21	A	857	C	C6-N1-C2	-30.28	29.37	120.20
21	A	2230	G	N9-C1'-C2'	16.34	136.51	112.00
21	A	857	C	C2-N3-C4	13.93	161.67	119.90
21	A	857	C	C5-C6-N1	13.68	162.03	121.00
21	A	2230	G	C8-N9-C4	-13.65	65.45	106.40
21	A	2230	G	N7-C8-N9	10.72	145.25	113.10
45	3	80	LEU	CA-C-N	-10.38	106.95	120.44
45	3	80	LEU	C-N-CA	-10.38	106.95	120.44
21	A	1510	U	P-O3'-C3'	-9.35	106.18	120.20
21	A	1511	C	OP2-P-O3'	9.07	135.22	108.00
19	s	67	VAL	N-CA-C	-8.88	104.70	111.90
21	A	1510	U	OP2-P-O3'	7.51	130.53	108.00
21	A	857	C	C4-C5-C6	7.46	139.78	117.40
21	A	2230	G	N9-C4-C5	7.26	127.19	105.40
21	A	2230	G	N3-C4-C5	-7.03	107.50	128.60
21	A	1288	G	C4-C5-N7	-6.98	89.86	110.80
21	A	2230	G	C8-N9-C1'	6.96	147.87	127.00
26	G	74	ILE	N-CA-C	-6.95	106.28	111.90
21	A	857	C	C6-N1-C1'	6.89	141.46	120.80
21	A	2002	G	N3-C2-N2	-6.86	99.32	119.90
21	A	1511	C	OP1-P-O3'	-6.84	87.47	108.00
21	A	2230	G	C4-N9-C1'	6.73	146.68	126.50
21	A	857	C	N3-C4-N4	6.42	137.24	118.00
21	A	1510	U	O3'-P-O5'	-6.22	94.66	104.00
21	A	785	C	N1-C1'-C2'	6.13	121.19	112.00
21	A	1938	U	C2'-C3'-O3'	5.57	117.86	109.50
13	m	65	VAL	N-CA-C	5.51	120.81	109.34
21	A	1288	G	N1-C6-O6	-5.36	103.82	119.90
13	m	106	ALA	N-CA-C	-5.31	107.35	113.88
21	A	1511	C	O3'-P-O5'	-5.29	96.07	104.00
20	t	44	ASP	CA-C-N	5.27	131.19	121.70
20	t	44	ASP	C-N-CA	5.27	131.19	121.70
3	c	25	GLU	N-CA-C	5.27	122.02	110.80
21	A	1288	G	C5-C6-O6	5.24	144.31	128.60
21	A	1857	C	C2-N1-C1'	5.20	134.39	118.80
21	A	1857	C	N1-C1'-C2'	5.15	119.72	112.00
2	b	227	GLY	N-CA-C	-5.14	106.02	111.93
46	4	50	TYR	N-CA-C	-5.11	107.11	113.55
14	n	56	VAL	CA-C-N	5.11	130.89	121.70
14	n	56	VAL	C-N-CA	5.11	130.89	121.70
12	l	34	LYS	CA-C-N	5.09	130.86	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	1	34	LYS	C-N-CA	5.09	130.86	121.70
49	7	34	ALA	N-CA-C	5.04	117.40	110.35
21	A	2816	C	O4'-C1'-N1	5.02	115.73	108.20
36	U	48	VAL	N-CA-C	-5.01	104.58	110.05

There are no chirality outliers.

All (67) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
45	3	43	TYR	Peptide
45	3	44	PRO	Peptide
45	3	63	LYS	Peptide
46	4	32	ASN	Peptide
46	4	45	LYS	Peptide
47	5	10	THR	Peptide
48	6	14	SER	Peptide
48	6	15	LYS	Peptide
49	7	28	PHE	Peptide
49	7	33	PHE	Peptide
23	D	176	ARG	Peptide
24	E	140	PRO	Peptide
24	E	142	SER	Peptide
24	E	62	ASP	Peptide
24	E	64	LYS	Peptide
24	E	65	SER	Peptide
24	E	9	LYS	Peptide
25	F	143	LEU	Peptide
25	F	148	GLN	Peptide
25	F	154	VAL	Peptide
25	F	171	PRO	Peptide
25	F	183	VAL	Peptide
26	G	114	PHE	Peptide
26	G	124	GLY	Peptide
26	G	138	PHE	Peptide
26	G	88	LYS	Peptide
28	M	68	ASN	Peptide
28	M	69	LYS	Peptide
29	N	89	ASP	Peptide
30	O	100	GLY	Peptide
30	O	65	GLY	Peptide
30	O	80	ASP	Peptide
30	O	83	ASN	Peptide

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Mol	Chain	Res	Type	Group
31	P	41	TRP	Peptide
33	R	103	GLY	Peptide
33	R	89	ILE	Peptide
34	S	104	SER	Peptide
35	T	91	ASN	Peptide
36	U	100	ILE	Peptide
38	W	48	VAL	Peptide
38	W	50	VAL	Peptide
40	Y	73	MET	Peptide
41	Z	16	SER	Peptide
41	Z	17	SER	Peptide
41	Z	19	LYS	Peptide
41	Z	22	ARG	Peptide
3	c	107	LYS	Peptide
3	c	24	ALA	Peptide
5	e	162	GLU	Peptide
7	g	13	LEU	Peptide
7	g	14	PRO	Peptide
7	g	17	ILE	Peptide
8	h	79	ARG	Peptide
8	h	98	LEU	Peptide
13	m	102	THR	Peptide
13	m	111	GLY	Peptide
13	m	64	LYS	Peptide
13	m	65	VAL	Peptide
13	m	84	SER	Peptide
14	n	18	VAL	Peptide
14	n	57	ARG	Peptide
17	q	5	ASN	Peptide
17	q	76	ARG	Peptide
17	q	85	VAL	Peptide
19	s	13	GLU	Peptide
19	s	7	LYS	Peptide
19	s	9	PRO	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	33126	0	16679	205	0
2	b	1802	0	1861	28	0
3	c	1638	0	1702	10	0
4	d	1600	0	1628	20	0
5	e	1239	0	1298	13	0
6	f	799	0	794	10	0
7	g	1189	0	1218	12	0
8	h	1032	0	1082	23	0
9	i	1017	0	1039	15	0
10	j	813	0	859	14	0
11	k	881	0	899	21	0
12	l	1063	0	1130	14	0
13	m	946	0	1001	14	0
14	n	502	0	527	10	0
15	o	738	0	769	15	0
16	p	712	0	744	12	0
17	q	707	0	749	16	0
18	r	590	0	628	5	0
19	s	678	0	672	25	0
20	t	607	0	650	8	0
21	A	62475	0	31402	485	0
22	B	2427	0	1230	23	0
23	D	2104	0	2221	36	0
24	E	1649	0	1689	15	0
25	F	1525	0	1570	13	0
26	G	1312	0	1366	1	0
27	H	1285	0	1301	12	0
28	M	1151	0	1145	5	0
29	N	920	0	981	10	0
30	O	998	0	1044	5	0
31	P	1122	0	1185	8	0
32	Q	940	0	990	12	0
33	R	922	0	968	14	0
34	S	886	0	957	6	0
35	T	944	0	1014	9	0
36	U	799	0	836	4	0
37	V	863	0	920	7	0
38	W	726	0	761	3	0
39	X	669	0	725	2	0
40	Y	738	0	787	11	0
41	Z	627	0	645	11	0
42	0	374	0	407	5	0
43	1	537	0	567	8	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
44	2	442	0	478	3	0
45	3	677	0	655	67	0
46	4	444	0	453	2	0
47	5	229	0	224	15	0
48	6	373	0	420	6	0
49	7	488	0	548	9	0
50	8	297	0	339	5	0
51	A	29	0	0	0	0
51	a	2	0	0	0	0
52	A	9	0	0	1	0
53	8	1	0	0	0	0
54	A	143	0	0	13	0
54	D	4	0	0	0	0
54	T	2	0	0	0	0
54	U	1	0	0	1	0
54	a	12	0	0	0	0
All	All	140825	0	93757	1131	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 5.

All (1131) 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)
21:A:1828:U:C6	21:A:1828:U:C5	2.07	1.42
21:A:2230:G:N9	21:A:2230:G:C4	1.68	1.39
21:A:857:C:N3	21:A:857:C:C6	1.94	1.34
21:A:1828:U:C5	21:A:1828:U:C4	2.18	1.31
21:A:1288:G:C4	21:A:1288:G:C5	2.24	1.23
21:A:857:C:N3	21:A:1288:G:N1	1.96	1.14
21:A:1828:U:N1	21:A:2230:G:H1'	1.65	1.12
21:A:1794:C:C2	21:A:2013:G:N2	2.18	1.11
21:A:1288:G:C5	21:A:1288:G:C6	2.38	1.11
19:s:9:PRO:CG	45:3:81:LYS:HD2	1.82	1.10
21:A:1828:U:C6	21:A:1828:U:N1	2.19	1.08
21:A:857:C:N3	21:A:857:C:C2	2.19	1.08
21:A:1828:U:N3	21:A:1828:U:C2	2.21	1.07
21:A:1828:U:C4	21:A:1828:U:N3	2.21	1.07
21:A:857:C:C6	21:A:857:C:C5	2.46	1.04
47:5:35:PHE:HD1	47:5:36:CYS:N	1.54	1.03
21:A:1828:U:N1	21:A:1828:U:C2	2.26	1.02

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:A:1793:C:C2	21:A:2014:G:N2	2.28	1.01
21:A:903:G:N1	21:A:2295:A:C2	2.28	1.01
1:a:972:C:H42	1:a:984:A:H61	0.99	0.99
45:3:71:VAL:HA	45:3:74:PHE:CE1	1.97	0.99
21:A:1288:G:N3	21:A:1288:G:C2	2.32	0.98
1:a:1271:G:H21	1:a:1286:A:N6	1.63	0.96
1:a:1271:G:N2	1:a:1286:A:H62	1.64	0.95
1:a:972:C:H42	1:a:984:A:N6	1.65	0.94
21:A:1828:U:N3	21:A:2230:G:O4'	2.01	0.94
45:3:75:ASN:HA	45:3:78:PHE:CE2	2.02	0.93
45:3:70:ARG:HD2	45:3:71:VAL:H	1.33	0.91
21:A:1288:G:C4	21:A:1288:G:N3	2.39	0.91
19:s:9:PRO:HG2	45:3:81:LYS:HB3	1.53	0.90
21:A:790:G:HO2'	21:A:793:G:HO2'	1.06	0.89
1:a:972:C:N4	1:a:984:A:H61	1.69	0.89
1:a:1271:G:H21	1:a:1286:A:H62	0.90	0.88
45:3:70:ARG:NE	45:3:71:VAL:HG23	1.89	0.88
21:A:857:C:C2	21:A:1288:G:N1	2.42	0.87
21:A:628:G:C2	21:A:1289:A:N1	2.42	0.87
21:A:857:C:N3	21:A:1288:G:C6	2.42	0.87
45:3:77:LYS:HE2	45:3:77:LYS:HA	1.56	0.87
21:A:857:C:C5	21:A:1288:G:C4	2.62	0.87
47:5:35:PHE:CD1	47:5:36:CYS:N	2.42	0.87
1:a:420:U:O2'	1:a:421:G:O4'	1.92	0.87
31:P:80:GLU:O	41:Z:12:LYS:NZ	2.08	0.86
45:3:70:ARG:CD	45:3:71:VAL:HG23	2.05	0.85
21:A:1828:U:C2	21:A:2230:G:C1'	2.58	0.85
21:A:857:C:N3	21:A:1288:G:C2	2.44	0.85
21:A:1828:U:C6	21:A:2230:G:N9	2.44	0.85
21:A:1306:C:C2	21:A:2040:A:C6	2.64	0.84
21:A:1971:U:O4'	21:A:1982:U:O2'	1.93	0.84
1:a:319:C:OP1	16:p:32:ARG:NH1	2.10	0.84
1:a:1333:C:OP1	19:s:78:ARG:NH2	2.11	0.84
45:3:70:ARG:HD2	45:3:71:VAL:N	1.92	0.84
21:A:2397:G:N2	47:5:35:PHE:CE2	2.46	0.84
22:B:15:C:H42	22:B:105:G:H21	1.25	0.84
21:A:2397:G:H21	47:5:35:PHE:HE2	1.21	0.83
45:3:70:ARG:O	45:3:73:ARG:HG3	1.78	0.83
21:A:903:G:C6	21:A:2295:A:C2	2.66	0.83
21:A:857:C:C6	21:A:1288:G:C4	2.67	0.83
21:A:1828:U:C2	21:A:2230:G:N9	2.46	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:A:1987:A:H5''	21:A:1987:A:H8	1.43	0.83
21:A:1288:G:N1	21:A:1288:G:C2	2.48	0.81
21:A:1828:U:N3	21:A:2230:G:N9	2.29	0.81
1:a:1081:C:O2'	1:a:1203:C:O2	1.98	0.81
21:A:857:C:C5	21:A:1288:G:N3	2.49	0.81
21:A:1312:A:O4'	32:Q:12:GLN:NE2	2.14	0.81
21:A:1828:U:C4	21:A:2230:G:C1'	2.64	0.81
21:A:2230:G:N9	21:A:2230:G:C1'	2.44	0.81
21:A:2250:A:OP1	23:D:170:TYR:OH	1.99	0.81
21:A:1828:U:N3	21:A:2230:G:C1'	2.44	0.80
21:A:2471:G:OP2	25:F:68:LYS:NZ	2.15	0.80
21:A:321:U:OP1	21:A:326:A:N6	2.15	0.80
21:A:2649:U:O2'	21:A:2845:G:N2	2.15	0.80
19:s:9:PRO:HG3	45:3:81:LYS:HD2	1.61	0.79
21:A:1094:A:N3	21:A:2778:G:N2	2.29	0.79
21:A:2060:A:O2'	21:A:2062:G:OP2	1.99	0.79
45:3:75:ASN:HA	45:3:78:PHE:CD2	2.18	0.79
21:A:1987:A:O2'	21:A:1988:C:H5'	1.81	0.79
4:d:66:ARG:O	4:d:70:ASN:ND2	2.16	0.79
21:A:628:G:N2	21:A:1289:A:C2	2.51	0.79
21:A:1520:A:N6	21:A:1562:C:O2	2.16	0.79
21:A:1806:U:OP2	21:A:1811:A:N6	2.15	0.79
21:A:1569:G:H21	21:A:1570:G:H5'	1.46	0.78
11:k:65:MET:O	11:k:69:THR:OG1	2.01	0.78
21:A:83:G:N2	21:A:102:A:OP2	2.17	0.78
21:A:1828:U:N1	21:A:2230:G:N9	2.30	0.78
21:A:857:C:C5	21:A:1288:G:C2	2.70	0.78
21:A:275:A:H62	21:A:296:G:H21	1.29	0.78
15:o:44:ARG:NH2	21:A:761:A:O2'	2.16	0.78
21:A:932:U:C2	21:A:935:C:N4	2.51	0.78
21:A:1101:A:N6	21:A:1131:G:OP2	2.16	0.78
1:a:587:G:O2'	15:o:54:ARG:NH1	2.17	0.78
21:A:575:G:O2'	21:A:577:A:N7	2.17	0.78
47:5:35:PHE:HE1	47:5:37:SER:N	1.81	0.78
21:A:289:U:O2'	21:A:290:U:O4'	2.01	0.78
21:A:1415:A:O2'	21:A:1417:G:N7	2.17	0.78
21:A:857:C:C5	21:A:1288:G:C5	2.72	0.77
1:a:919:A:OP1	12:l:18:LYS:NZ	2.16	0.77
21:A:61:A:OP1	43:1:44:ARG:NE	2.17	0.77
17:q:52:ASN:OD1	17:q:54:SER:OG	2.03	0.77
7:g:79:ARG:NH2	7:g:84:ASN:OD1	2.17	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:B:29:C:O2	22:B:51:A:N6	2.17	0.77
21:A:2717:A:OP1	32:Q:4:ARG:NH2	2.17	0.77
23:D:4:LYS:NZ	23:D:13:ARG:O	2.17	0.77
1:a:388:G:N2	1:a:391:A:OP2	2.17	0.77
9:i:14:ARG:NH1	9:i:79:GLN:OE1	2.17	0.77
25:F:112:SER:O	25:F:115:SER:OG	2.02	0.77
21:A:2102:U:OP1	23:D:242:ARG:NH2	2.17	0.77
21:A:2285:C:O2'	21:A:2454:C:OP2	2.02	0.77
13:m:90:ARG:NH1	13:m:96:PRO:O	2.18	0.77
47:5:35:PHE:CE1	47:5:37:SER:N	2.52	0.77
21:A:2017:C:OP2	54:A:3101:HOH:O	2.03	0.76
21:A:1794:C:O2	21:A:2013:G:N2	2.18	0.76
29:N:64:ARG:NH1	29:N:100:GLY:O	2.18	0.76
1:a:1200:U:OP1	10:j:53:ARG:NH2	2.18	0.76
21:A:661:U:O2'	21:A:662:G:OP2	2.02	0.76
21:A:857:C:C6	21:A:1288:G:N3	2.54	0.76
21:A:1819:G:N7	54:A:3110:HOH:O	2.18	0.76
1:a:415:A:OP1	4:d:108:ARG:NH2	2.17	0.76
21:A:304:G:O6	21:A:410:G:N2	2.17	0.76
21:A:1828:U:C4	21:A:2230:G:N9	2.53	0.76
45:3:70:ARG:HD2	45:3:71:VAL:HG23	1.67	0.76
21:A:797:A:C5	21:A:1808:U:O2	2.39	0.76
1:a:987:A:O2'	1:a:989:C:OP2	2.01	0.76
6:f:75:GLU:OE1	6:f:78:ARG:NH2	2.19	0.76
21:A:1828:U:C6	21:A:2230:G:C1'	2.69	0.76
21:A:2747:U:OP1	54:A:3103:HOH:O	2.04	0.76
25:F:144:SER:OG	25:F:148:GLN:NE2	2.19	0.76
21:A:834:A:N1	48:6:4:ARG:NH1	2.33	0.76
21:A:1828:U:C5	21:A:2230:G:N9	2.54	0.76
29:N:73:ASP:OD2	34:S:82:LYS:NZ	2.19	0.76
21:A:321:U:C2	21:A:326:A:N6	2.54	0.76
21:A:628:G:N3	21:A:1289:A:C6	2.54	0.75
21:A:1323:A:O2'	21:A:1325:U:OP2	2.03	0.75
21:A:1828:U:N1	21:A:2230:G:C1'	2.47	0.75
22:B:72:U:O2'	40:Y:38:ASN:ND2	2.18	0.75
19:s:9:PRO:CD	45:3:81:LYS:HD2	2.15	0.75
21:A:628:G:C2	21:A:1289:A:C2	2.74	0.75
21:A:313:U:O2'	21:A:314:A:N3	2.19	0.75
21:A:857:C:C6	21:A:1288:G:C2	2.75	0.75
21:A:907:G:OP2	54:A:3104:HOH:O	2.05	0.75
33:R:71:GLU:O	33:R:74:THR:OG1	2.03	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:a:1273:A:N6	1:a:1284:C:O2	2.19	0.75
16:p:62:ASN:OD1	16:p:88:LYS:NZ	2.19	0.75
21:A:955:A:OP1	54:A:3102:HOH:O	2.04	0.75
25:F:178:ALA:O	25:F:182:ASN:ND2	2.20	0.75
8:h:86:ARG:NH2	8:h:126:GLU:OE2	2.19	0.75
21:A:903:G:OP1	41:Z:52:LYS:NZ	2.18	0.75
1:a:666:G:C4	1:a:757:A:N6	2.55	0.75
14:n:53:ILE:O	14:n:57:ARG:NH2	2.20	0.75
21:A:2328:A:OP2	21:A:2336:A:N6	2.20	0.75
21:A:419:U:OP2	42:0:52:ARG:NH1	2.20	0.74
21:A:628:G:C2	21:A:1289:A:C6	2.75	0.74
32:Q:73:ASN:ND2	32:Q:77:THR:O	2.19	0.74
3:c:50:SER:OG	3:c:71:LYS:NZ	2.20	0.74
21:A:857:C:C2	21:A:1288:G:C6	2.75	0.74
20:t:72:ASP:O	20:t:76:SER:OG	2.04	0.74
21:A:1493:U:O4	21:A:1506:C:N3	2.20	0.74
21:A:2153:A:O2'	21:A:2189:G:N2	2.20	0.74
23:D:132:GLN:O	23:D:166:LYS:NZ	2.21	0.74
45:3:70:ARG:CD	45:3:71:VAL:H	2.01	0.74
21:A:1854:U:OP2	23:D:220:ARG:NH1	2.21	0.74
21:A:2126:C:O2'	21:A:2127:G:O4'	2.06	0.74
21:A:2667:G:OP1	28:M:100:ARG:NH1	2.20	0.73
45:3:71:VAL:HA	45:3:74:PHE:CD1	2.22	0.73
1:a:1189:G:OP1	9:i:97:ARG:NH1	2.21	0.73
21:A:2272:U:O2'	21:A:2463:G:OP2	2.03	0.73
27:H:57:ASP:O	27:H:62:ARG:NH1	2.20	0.73
47:5:35:PHE:HE1	47:5:37:SER:CA	2.01	0.73
2:b:187:VAL:HG21	2:b:199:VAL:HG13	1.71	0.73
21:A:59:U:O2'	21:A:74:U:OP2	2.07	0.73
21:A:2157:U:O2'	21:A:2185:A:N1	2.19	0.73
1:a:1379:A:OP1	10:j:62:ARG:NH2	2.21	0.73
27:H:60:GLU:O	27:H:63:THR:OG1	2.04	0.73
1:a:731:U:O2	1:a:865:G:O2'	2.06	0.73
1:a:81:A:O2'	1:a:82:G:N7	2.21	0.73
21:A:142:G:N2	21:A:1640:U:O3'	2.22	0.73
21:A:315:C:O2'	21:A:316:G:N7	2.17	0.73
21:A:375:A:O2'	21:A:377:U:OP2	2.04	0.73
16:p:73:ASN:O	16:p:76:SER:OG	2.03	0.73
21:A:2397:G:N2	47:5:35:PHE:CD2	2.57	0.72
21:A:2622:G:N2	21:A:2625:A:OP2	2.22	0.72
50:8:2:LYS:NZ	50:8:31:LYS:O	2.22	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:A:625:G:C6	21:A:1297:G:N1	2.57	0.72
32:Q:18:ARG:O	32:Q:22:THR:OG1	2.03	0.72
1:a:1126:C:O2'	14:n:60:SER:OG	2.05	0.72
21:A:774:G:C2	21:A:1802:U:C2	2.77	0.72
21:A:2530:A:O2'	21:A:2532:G:OP2	2.08	0.72
22:B:65:G:O6	22:B:105:G:N2	2.19	0.72
21:A:613:G:C6	21:A:2057:A:N6	2.57	0.72
23:D:93:VAL:HG21	23:D:103:ILE:HD13	1.72	0.72
43:1:46:VAL:O	43:1:49:THR:OG1	2.07	0.72
21:A:364:A:O2'	21:A:383:A:N3	2.23	0.72
21:A:2804:G:OP2	21:A:2808:A:O2'	2.07	0.72
22:B:29:C:O2'	22:B:51:A:N1	2.17	0.72
37:V:23:LEU:O	37:V:27:LYS:NZ	2.22	0.72
21:A:857:C:C6	21:A:1288:G:C5	2.78	0.71
1:a:413:U:OP1	1:a:414:G:O2'	2.02	0.71
21:A:425:G:O6	54:A:3105:HOH:O	2.05	0.71
21:A:1828:U:C5	21:A:2230:G:C1'	2.73	0.71
1:a:370:G:N2	1:a:373:U:OP2	2.23	0.71
2:b:94:GLN:NE2	2:b:146:LYS:O	2.23	0.71
45:3:71:VAL:HA	45:3:74:PHE:HE1	1.52	0.71
1:a:986:G:OP2	1:a:1369:U:O2'	2.08	0.71
21:A:1771:A:O2'	21:A:1772:G:O5'	2.06	0.71
21:A:2599:A:N7	24:E:158:SER:OG	2.23	0.71
5:e:3:ARG:N	5:e:69:LYS:O	2.23	0.71
21:A:1288:G:N1	21:A:1288:G:C6	2.59	0.71
1:a:1047:G:OP2	1:a:1048:A:N6	2.23	0.70
1:a:1443:G:N2	1:a:1480:A:OP2	2.23	0.70
1:a:370:G:OP2	12:l:44:ARG:NH2	2.25	0.70
1:a:1238:A:OP2	13:m:110:LYS:NZ	2.24	0.70
5:e:6:GLU:OE2	5:e:9:LYS:NZ	2.23	0.70
1:a:692:U:OP1	11:k:11:ARG:NH1	2.24	0.70
21:A:614:U:O2'	21:A:616:G:OP2	2.09	0.70
5:e:84:THR:OG1	5:e:96:MET:O	2.09	0.70
8:h:8:ALA:O	8:h:12:THR:OG1	2.04	0.70
21:A:283:G:N7	21:A:284:C:O2'	2.23	0.70
1:a:283:G:O2'	17:q:19:MET:SD	2.49	0.70
17:q:30:TYR:O	17:q:39:ARG:NH2	2.25	0.70
21:A:1488:A:N1	21:A:1490:G:C6	2.59	0.70
22:B:34:C:N4	22:B:47:C:O2	2.25	0.70
4:d:137:GLN:O	4:d:175:THR:OG1	2.05	0.70
21:A:922:G:O6	21:A:943:C:N4	2.24	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:A:1978:U:O2'	21:A:1980:A:N7	2.22	0.70
45:3:75:ASN:ND2	45:3:78:PHE:HE2	1.90	0.70
1:a:908:G:N2	1:a:911:A:OP2	2.23	0.69
21:A:2815:C:O2'	21:A:2829:A:N3	2.23	0.69
42:0:29:TRP:CZ3	42:0:31:ALA:HB2	2.26	0.69
21:A:425:G:N7	54:A:3113:HOH:O	2.25	0.69
1:a:930:U:O2'	1:a:1093:G:O2'	2.11	0.69
3:c:121:ARG:NH1	3:c:124:GLU:OE1	2.25	0.69
4:d:81:VAL:O	4:d:85:ASN:ND2	2.26	0.69
21:A:1987:A:C2'	21:A:1988:C:H5'	2.22	0.69
21:A:1377:U:OP2	38:W:58:TYR:OH	2.11	0.69
21:A:2015:C:OP2	54:A:3106:HOH:O	2.08	0.69
45:3:30:THR:OG1	45:3:33:GLU:O	2.06	0.69
21:A:688:A:N1	21:A:2396:A:O2'	2.21	0.69
43:1:62:ILE:O	43:1:65:SER:OG	2.10	0.69
1:a:534:C:OP2	12:l:101:ARG:NH1	2.26	0.69
21:A:628:G:C4	21:A:1289:A:C6	2.81	0.69
21:A:1569:G:H3'	21:A:1569:G:N3	2.08	0.69
8:h:30:SER:O	8:h:34:LYS:NZ	2.26	0.69
21:A:2229:C:O2'	21:A:2231:C:OP1	2.10	0.69
1:a:65:G:O6	1:a:100:A:N6	2.26	0.68
1:a:353:C:O2	1:a:354:G:N2	2.26	0.68
21:A:321:U:N3	21:A:326:A:C6	2.61	0.68
11:k:63:ALA:HB1	11:k:96:ALA:HB2	1.75	0.68
21:A:1320:G:N2	21:A:1323:A:OP2	2.26	0.68
21:A:1658:A:N6	37:V:92:ARG:O	2.26	0.68
21:A:2019:G:N2	21:A:2023:C:O2	2.24	0.68
1:a:996:A:N3	19:s:52:TYR:OH	2.23	0.68
1:a:1408:C:OP2	5:e:29:ARG:NH2	2.25	0.68
9:i:58:GLU:O	9:i:61:GLY:N	2.27	0.68
21:A:616:G:O2'	21:A:618:A:OP1	2.11	0.68
21:A:2089:A:OP1	54:A:3107:HOH:O	2.10	0.68
1:a:269:U:O4	20:t:73:ARG:NH1	2.26	0.68
1:a:476:C:O2'	1:a:478:G:OP2	2.08	0.68
1:a:1237:C:OP1	13:m:93:ARG:NH1	2.25	0.68
1:a:1043:G:OP2	1:a:1043:G:N2	2.24	0.68
42:0:12:ALA:O	42:0:14:THR:OG1	2.11	0.68
1:a:456:A:O2'	1:a:492:G:N2	2.26	0.68
21:A:903:G:N1	21:A:2295:A:H2	1.91	0.68
21:A:257:G:O2'	21:A:258:A:O4'	2.11	0.67
21:A:1816:A:OP1	23:D:220:ARG:NE	2.27	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:A:2695:G:O2'	27:H:111:HIS:NE2	2.25	0.67
21:A:1379:A:O2'	21:A:1381:U:OP2	2.11	0.67
22:B:38:U:O2'	22:B:43:A:N6	2.22	0.67
8:h:51:TYR:OH	8:h:53:GLU:OE1	2.10	0.67
21:A:234:C:O2'	21:A:235:G:O4'	2.12	0.67
21:A:1897:U:O2'	21:A:1898:C:O4'	2.13	0.67
1:a:1228:U:OP1	14:n:5:SER:OG	2.07	0.67
21:A:1465:G:O2'	21:A:1537:A:N6	2.27	0.67
1:a:1047:G:O2'	1:a:1048:A:O4'	2.12	0.67
1:a:784:G:N2	1:a:810:A:OP2	2.27	0.67
1:a:1387:U:OP1	7:g:25:LYS:NZ	2.29	0.66
21:A:613:G:N1	21:A:2057:A:N7	2.42	0.66
21:A:857:C:C4	21:A:1288:G:N1	2.63	0.66
45:3:70:ARG:CZ	45:3:71:VAL:HG23	2.24	0.66
2:b:54:TYR:CE1	2:b:220:ALA:HB2	2.30	0.66
21:A:2457:A:O2'	21:A:2458:U:O5'	2.12	0.66
21:A:32:C:N4	21:A:493:A:OP2	2.28	0.66
21:A:2127:G:N2	21:A:2216:U:O2	2.29	0.66
21:A:2477:A:OP1	21:A:2524:A:O2'	2.08	0.66
22:B:45:C:OP2	33:R:7:LYS:NZ	2.28	0.66
21:A:2717:A:N6	32:Q:39:GLU:OE1	2.27	0.66
45:3:73:ARG:HG3	45:3:74:PHE:H	1.61	0.66
23:D:208:GLY:O	23:D:211:ARG:N	2.29	0.66
13:m:92:ARG:O	13:m:109:ARG:NH1	2.28	0.66
1:a:666:G:N2	1:a:757:A:N7	2.43	0.66
49:7:26:ARG:O	49:7:40:GLN:NE2	2.28	0.66
21:A:1172:A:C6	21:A:2545:A:C6	2.84	0.65
1:a:1332:U:OP1	13:m:98:ARG:HA	1.96	0.65
21:A:592:A:O2'	21:A:593:U:O5'	2.13	0.65
21:A:675:G:N2	21:A:678:A:OP2	2.25	0.65
21:A:1987:A:H2'	21:A:1988:C:C5'	2.25	0.65
21:A:199:A:O2'	21:A:200:A:OP1	2.12	0.65
21:A:1053:A:N3	21:A:1197:C:O2'	2.27	0.65
21:A:2599:A:OP1	21:A:2601:G:O2'	2.12	0.65
1:a:823:A:N6	1:a:1521:C:O2'	2.30	0.65
21:A:857:C:O2	21:A:1288:G:N1	2.29	0.65
1:a:9:A:N6	4:d:200:ARG:O	2.29	0.65
21:A:266:A:O2'	21:A:475:A:N3	2.23	0.65
21:A:1518:G:HO2'	21:A:1519:U:P	2.19	0.65
27:H:54:ARG:NH2	27:H:57:ASP:OD1	2.29	0.65
1:a:989:C:N3	14:n:16:TYR:OH	2.29	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:A:275:A:H62	21:A:296:G:N2	1.95	0.65
21:A:2505:A:OP1	50:8:31:LYS:NZ	2.29	0.65
22:B:84:U:O2'	22:B:86:C:O2	2.11	0.65
2:b:177:ARG:NH2	2:b:195:GLU:O	2.30	0.65
21:A:2747:U:OP2	54:A:3108:HOH:O	2.14	0.65
34:S:16:ARG:NH2	34:S:80:THR:O	2.30	0.65
23:D:83:ASP:OD2	23:D:86:ARG:NH2	2.30	0.64
1:a:702:A:OP1	11:k:55:SER:OG	2.14	0.64
1:a:1037:C:OP2	1:a:1039:C:N4	2.30	0.64
1:a:1262:A:N3	1:a:1380:C:O2'	2.26	0.64
1:a:1280:A:O2'	1:a:1336:C:O2'	2.15	0.64
11:k:63:ALA:O	11:k:67:SER:OG	2.12	0.64
1:a:195:C:N4	17:q:2:SER:O	2.29	0.64
1:a:377:C:OP2	1:a:396:G:N2	2.28	0.64
21:A:138:U:N3	21:A:141:U:OP2	2.29	0.64
21:A:2752:A:O2'	21:A:2753:U:O5'	2.15	0.64
1:a:128:U:OP2	17:q:4:ARG:NE	2.30	0.64
1:a:988:A:N6	1:a:1327:G:O2'	2.29	0.64
3:c:20:ALA:HB1	3:c:22:TRP:HZ3	1.62	0.64
46:4:10:LYS:O	46:4:14:ASN:ND2	2.30	0.64
1:a:1318:U:OP1	13:m:100:GLN:NE2	2.30	0.64
21:A:572:C:N4	21:A:2806:U:OP2	2.30	0.64
21:A:1359:A:O2'	37:V:84:ARG:NH2	2.31	0.64
21:A:2024:A:OP2	24:E:138:ARG:NH1	2.31	0.64
1:a:541:A:O2'	1:a:543:A:OP2	2.10	0.64
19:s:9:PRO:HG2	45:3:81:LYS:HD2	1.74	0.64
21:A:1570:G:O5'	21:A:1570:G:H8	1.80	0.64
21:A:2070:C:OP1	21:A:2804:G:O2'	2.15	0.64
1:a:1135:A:N6	1:a:1136:G:O6	2.31	0.64
1:a:1270:C:O2'	1:a:1294:C:O2	2.16	0.64
21:A:1987:A:H2'	21:A:1988:C:H5'	1.80	0.64
21:A:1215:U:O2'	21:A:1217:U:OP2	2.14	0.63
21:A:1172:A:N6	21:A:2545:A:C6	2.66	0.63
9:i:100:LEU:O	9:i:104:GLY:N	2.31	0.63
15:o:61:GLY:O	15:o:65:HIS:ND1	2.31	0.63
21:A:230:A:H61	21:A:456:G:H21	1.46	0.63
47:5:35:PHE:HE1	47:5:37:SER:HA	1.63	0.63
20:t:10:ARG:O	20:t:14:THR:OG1	2.13	0.63
21:A:1295:C:OP1	25:F:72:ARG:NH2	2.32	0.63
21:A:2717:A:OP2	32:Q:13:ARG:NH2	2.32	0.63
25:F:144:SER:O	25:F:148:GLN:NE2	2.32	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:A:457:G:OP2	21:A:2433:C:O2'	2.14	0.63
21:A:1302:G:O6	21:A:1303:A:N6	2.31	0.63
21:A:1306:C:N3	21:A:2040:A:C6	2.67	0.63
21:A:2877:G:N2	21:A:2880:A:OP2	2.31	0.63
42:O:19:SER:N	42:O:27:ARG:O	2.30	0.63
1:a:728:C:O3'	18:r:57:GLN:NE2	2.31	0.63
3:c:20:ALA:HB3	14:n:52:GLN:O	1.99	0.63
15:o:56:LEU:O	15:o:59:MET:N	2.31	0.63
21:A:1828:U:C6	21:A:2230:G:H1'	2.33	0.63
21:A:1845:U:O2'	23:D:152:GLN:O	2.11	0.63
21:A:2404:A:O2'	33:R:119:PHE:OXT	2.16	0.63
21:A:251:G:O2'	21:A:2459:A:OP1	2.09	0.63
22:B:7:G:OP1	33:R:19:ARG:NH1	2.32	0.62
1:a:921:U:OP2	12:l:107:ARG:NH2	2.32	0.62
5:e:166:ASN:OD1	8:h:100:GLY:N	2.32	0.62
21:A:1578:A:N6	21:A:1591:G:N7	2.45	0.62
21:A:661:U:HO2'	21:A:662:G:P	2.22	0.62
1:a:1107:U:OP1	1:a:1120:G:N2	2.22	0.62
11:k:24:ARG:O	11:k:30:THR:OG1	2.10	0.62
21:A:1395:G:O2'	21:A:1410:A:N6	2.31	0.62
1:a:1436:A:O2'	1:a:1437:A:O4'	2.17	0.62
21:A:735:C:O2'	21:A:825:G:OP1	2.18	0.62
21:A:1250:G:O2'	21:A:1274:G:N2	2.33	0.62
1:a:195:C:O2	17:q:7:ARG:NE	2.31	0.62
7:g:118:ASP:OD1	7:g:122:ASN:ND2	2.33	0.62
21:A:1612:C:O2'	21:A:1614:A:N7	2.30	0.62
21:A:1987:A:H5''	21:A:1987:A:C8	2.32	0.62
21:A:628:G:N2	21:A:1289:A:N1	2.46	0.62
1:a:583:G:O2'	1:a:829:G:OP2	2.12	0.62
21:A:774:G:OP2	23:D:206:LYS:NZ	2.31	0.62
21:A:1306:C:C2	21:A:2040:A:N6	2.67	0.62
2:b:12:ALA:HB1	2:b:43:LEU:HD22	1.80	0.62
21:A:460:C:O2	21:A:1891:U:O2'	2.18	0.62
1:a:1382:G:OP2	9:i:113:LYS:NZ	2.29	0.61
21:A:1097:U:O4	21:A:1098:A:N6	2.33	0.61
1:a:1436:A:O2'	1:a:1437:A:O5'	2.18	0.61
9:i:12:GLY:N	9:i:19:ALA:O	2.34	0.61
21:A:74:U:OP1	43:l:47:ARG:NH2	2.34	0.61
21:A:2510:C:O2	31:P:49:SER:OG	2.15	0.61
1:a:1123:A:O2'	1:a:1124:C:O4'	2.19	0.61
8:h:117:GLU:OE2	8:h:121:ARG:NE	2.33	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:A:790:G:H21	21:A:795:A:H61	1.46	0.61
21:A:1518:G:O2'	21:A:1519:U:O5'	2.12	0.61
21:A:321:U:C2	21:A:326:A:C6	2.89	0.61
21:A:857:C:N3	21:A:1288:G:C5	2.68	0.61
21:A:2418:G:OP1	49:7:26:ARG:NH2	2.34	0.61
32:Q:46:LYS:O	32:Q:49:THR:OG1	2.17	0.61
21:A:1313:G:OP2	21:A:1689:G:O2'	2.09	0.61
43:1:42:ARG:O	43:1:45:THR:OG1	2.16	0.61
39:X:24:ILE:HG22	39:X:25:ALA:H	1.65	0.61
31:P:39:THR:O	31:P:40:SER:OG	2.14	0.61
1:a:34:A:O2'	12:l:42:GLN:NE2	2.34	0.60
1:a:194:G:N2	1:a:197:U:OP2	2.25	0.60
21:A:284:C:N4	21:A:286:U:O4'	2.34	0.60
22:B:87:G:C2	31:P:39:THR:HA	2.34	0.60
1:a:756:A:O2'	1:a:757:A:O4'	2.16	0.60
1:a:63:U:O2'	1:a:387:C:O2	2.19	0.60
1:a:827:A:N6	1:a:1541:G:N3	2.49	0.60
7:g:102:ARG:O	7:g:106:ASN:ND2	2.35	0.60
21:A:1793:C:C2	21:A:2014:G:C2	2.89	0.60
21:A:1828:U:C4	21:A:2230:G:C8	2.88	0.60
23:D:117:SER:HA	23:D:128:ALA:HB3	1.82	0.60
19:s:39:THR:OG1	19:s:40:ILE:N	2.33	0.60
21:A:857:C:C5	21:A:1288:G:C6	2.86	0.60
21:A:1453:G:N2	21:A:1631:G:N7	2.49	0.60
21:A:321:U:N3	21:A:326:A:N6	2.50	0.60
9:i:83:HIS:HB3	9:i:108:ARG:HE	1.67	0.60
21:A:965:G:N2	21:A:2296:A:OP2	2.35	0.60
1:a:272:C:O2'	17:q:68:PRO:O	2.20	0.60
19:s:41:PHE:CG	45:3:82:SER:OG	2.54	0.60
21:A:1581:U:C5	21:A:1584:A:H8	2.19	0.60
21:A:2239:A:N7	21:A:2241:C:N4	2.50	0.60
1:a:827:A:N6	1:a:1541:G:C2	2.70	0.60
2:b:152:ARG:O	2:b:155:LYS:NZ	2.35	0.60
21:A:1306:C:O2	21:A:2040:A:N1	2.34	0.59
21:A:2161:A:N6	21:A:2184:G:O2'	2.29	0.59
1:a:1324:U:OP1	19:s:7:LYS:NZ	2.35	0.59
21:A:1172:A:C6	21:A:2545:A:N1	2.70	0.59
21:A:1938:U:O2'	21:A:1939:A:O5'	2.20	0.59
1:a:404:A:O2'	1:a:406:C:OP1	2.21	0.59
21:A:2575:G:O2'	29:N:4:GLN:OE1	2.20	0.59
21:A:2650:G:O5'	21:A:2845:G:N2	2.35	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:A:236:A:H61	21:A:475:A:H61	1.50	0.59
27:H:22:ASN:OD1	27:H:23:HIS:N	2.36	0.59
1:a:800:A:O2'	1:a:802:A:N7	2.31	0.59
2:b:7:LYS:HE3	2:b:12:ALA:HB2	1.84	0.59
15:o:80:GLU:O	15:o:84:SER:OG	2.11	0.59
21:A:628:G:C4	21:A:1289:A:N6	2.71	0.59
21:A:1462:G:O2'	21:A:1463:A:O4'	2.18	0.59
21:A:2361:U:O2'	21:A:2362:A:OP1	2.17	0.59
1:a:409:C:O2'	1:a:629:A:N3	2.36	0.58
29:N:42:THR:OG1	29:N:56:ASP:O	2.13	0.58
45:3:67:ALA:O	45:3:68:ASP:HB2	2.01	0.58
1:a:10:G:OP2	5:e:126:LYS:NZ	2.36	0.58
21:A:153:G:O2'	21:A:154:A:O5'	2.21	0.58
21:A:1794:C:C2	21:A:2013:G:C2	2.90	0.58
21:A:774:G:N1	21:A:1802:U:N3	2.50	0.58
1:a:127:A:O2'	17:q:7:ARG:NH1	2.36	0.58
12:l:47:CYS:SG	12:l:66:ALA:HB1	2.43	0.58
21:A:932:U:N3	21:A:935:C:N4	2.51	0.58
21:A:1290:G:OP2	35:T:13:ARG:NH2	2.34	0.58
48:6:9:ASN:OD1	48:6:10:LYS:N	2.36	0.58
21:A:1005:G:O6	21:A:2482:G:O2'	2.21	0.58
21:A:1079:U:OP1	27:H:59:LYS:NZ	2.33	0.58
44:2:11:SER:OG	44:2:12:VAL:N	2.33	0.58
47:5:35:PHE:HD1	47:5:36:CYS:H	1.40	0.58
21:A:2195:G:N1	21:A:2197:G:N7	2.52	0.58
1:a:535:G:O6	12:l:59:ASN:ND2	2.37	0.58
1:a:694:U:O4	1:a:711:G:O2'	2.20	0.58
1:a:1542:G:O2'	1:a:1543:A:O5'	2.20	0.58
21:A:1304:G:O2'	21:A:2039:G:O6	2.13	0.58
21:A:1828:U:C2	21:A:2230:G:H1'	2.37	0.58
1:a:1142:A:O3'	9:i:22:ARG:NH1	2.37	0.58
8:h:110:GLU:OE2	8:h:121:ARG:NH1	2.36	0.58
2:b:7:LYS:CE	2:b:12:ALA:HB2	2.34	0.57
21:A:1708:A:C6	21:A:2753:U:N3	2.72	0.57
8:h:98:LEU:O	8:h:100:GLY:N	2.37	0.57
19:s:33:THR:OG1	19:s:34:TRP:N	2.36	0.57
21:A:857:C:C2	21:A:1288:G:C2	2.89	0.57
21:A:990:G:O6	21:A:1016:G:N2	2.37	0.57
40:Y:47:GLU:O	40:Y:51:VAL:HG23	2.05	0.57
1:a:1230:U:OP1	14:n:19:ARG:NH1	2.37	0.57
21:A:593:U:O2'	21:A:594:G:OP1	2.19	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
45:3:73:ARG:HD3	45:3:74:PHE:N	2.18	0.57
1:a:1368:A:OP2	1:a:1370:C:N4	2.37	0.57
2:b:223:GLU:O	2:b:227:GLY:N	2.37	0.57
21:A:2402:G:N2	21:A:2405:A:OP2	2.26	0.57
8:h:108:THR:OG1	8:h:111:GLY:N	2.38	0.57
21:A:895:U:HO2'	44:2:22:THR:HG1	1.53	0.57
1:a:550:U:OP1	4:d:10:LYS:NZ	2.34	0.57
19:s:9:PRO:HD3	45:3:81:LYS:HD2	1.86	0.57
21:A:1568:U:H5'	21:A:1570:G:H1'	1.87	0.57
1:a:109:C:O2'	16:p:26:ARG:O	2.20	0.57
12:l:102:ASP:OD1	12:l:103:LEU:N	2.35	0.57
21:A:833:A:N3	48:6:5:THR:OG1	2.37	0.57
21:A:1934:G:O6	21:A:1951:C:N4	2.38	0.57
41:Z:64:ASP:OD1	41:Z:66:THR:HG23	2.04	0.57
18:r:44:ILE:HD11	18:r:64:ILE:HD11	1.86	0.57
21:A:795:A:OP1	21:A:1659:C:N4	2.37	0.57
17:q:66:THR:HG23	17:q:76:ARG:HE	1.70	0.56
19:s:9:PRO:HD3	45:3:81:LYS:CD	2.34	0.56
21:A:1091:G:N2	21:A:1154:G:HO2'	2.03	0.56
2:b:171:ASN:OD1	2:b:172:ALA:N	2.38	0.56
15:o:52:SER:O	15:o:55:GLY:N	2.38	0.56
21:A:1458:A:N1	21:A:1459:A:N6	2.53	0.56
25:F:80:ALA:HB1	25:F:81:PRO:HD2	1.87	0.56
21:A:857:C:C4	21:A:1288:G:C6	2.94	0.56
21:A:1962:G:C4	21:A:1991:G:N2	2.74	0.56
21:A:2860:U:H5''	32:Q:49:THR:HG21	1.87	0.56
24:E:114:ASP:OD1	24:E:115:VAL:N	2.38	0.56
21:A:2372:G:O6	21:A:2398:G:N2	2.37	0.56
45:3:69:GLY:O	45:3:73:ARG:HB3	2.05	0.56
1:a:125:G:OP1	1:a:613:U:O2'	2.20	0.56
2:b:199:VAL:HG12	2:b:201:PRO:HD3	1.86	0.56
25:F:136:THR:O	25:F:140:LYS:NZ	2.21	0.55
1:a:1271:G:OP1	1:a:1295:C:O2'	2.23	0.55
1:a:1331:C:N4	19:s:36:ARG:O	2.38	0.55
1:a:410:G:OP2	4:d:66:ARG:NH1	2.39	0.55
21:A:574:A:N6	21:A:2069:A:N3	2.54	0.55
21:A:613:G:N1	21:A:2057:A:C5	2.74	0.55
21:A:1110:U:O2'	21:A:1113:A:N6	2.38	0.55
21:A:1828:U:C5	21:A:2230:G:C8	2.94	0.55
46:4:30:CYS:N	46:4:35:ARG:O	2.40	0.55
21:A:796:A:N7	21:A:834:A:N6	2.54	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:A:1659:C:OP2	21:A:1661:C:N4	2.37	0.55
40:Y:76:ASP:OD1	40:Y:77:TYR:N	2.39	0.55
45:3:77:LYS:HA	45:3:77:LYS:CE	2.34	0.55
21:A:1491:C:H42	21:A:1508:C:H42	1.54	0.55
21:A:1788:U:O4	21:A:1789:A:N6	2.39	0.55
30:O:110:LYS:NZ	30:O:131:SER:OG	2.35	0.55
37:V:57:ASN:OD1	37:V:58:ALA:N	2.40	0.55
21:A:2680:U:OP2	21:A:2681:A:O2'	2.17	0.55
34:S:61:PHE:O	34:S:75:THR:OG1	2.19	0.55
1:a:692:U:O2	11:k:41:ALA:HB3	2.05	0.55
21:A:904:G:O2'	21:A:961:G:O6	2.24	0.55
21:A:903:G:O2'	21:A:904:G:O4'	2.25	0.55
21:A:1569:G:H21	21:A:1570:G:C5'	2.19	0.55
21:A:1828:U:C2	21:A:2230:G:C4	2.94	0.55
8:h:27:LEU:HD12	8:h:28:PRO:HD2	1.89	0.55
18:r:25:HIS:CE1	18:r:60:LEU:HD21	2.42	0.55
21:A:1506:C:O2'	21:A:1507:A:O4'	2.21	0.54
1:a:988:A:C6	1:a:1371:A:N1	2.75	0.54
1:a:1248:C:O2'	1:a:1346:C:O4'	2.25	0.54
1:a:1261:A:OP1	9:i:71:GLY:N	2.41	0.54
15:o:16:ARG:NH1	15:o:19:GLU:O	2.41	0.54
21:A:254:A:OP1	49:7:7:HIS:NE2	2.41	0.54
23:D:44:ASN:OD1	23:D:45:GLN:N	2.40	0.54
45:3:74:PHE:C	45:3:74:PHE:CD2	2.85	0.54
21:A:806:A:N6	52:A:3004:O:O	2.41	0.54
34:S:102:LEU:O	34:S:103:ARG:NH1	2.36	0.54
1:a:788:A:N6	1:a:809:U:OP2	2.39	0.54
21:A:857:C:H5	21:A:1288:G:C4	2.23	0.54
21:A:2089:A:N6	21:A:2530:A:N7	2.56	0.54
23:D:74:ASN:OD1	23:D:75:ALA:N	2.40	0.54
45:3:78:PHE:CD1	45:3:78:PHE:C	2.85	0.54
1:a:789:A:OP2	1:a:808:G:N1	2.38	0.54
21:A:545:G:N1	21:A:548:A:OP2	2.40	0.54
21:A:1569:G:N2	21:A:1570:G:H5'	2.20	0.54
1:a:525:G:N1	1:a:541:A:OP2	2.36	0.54
21:A:2276:U:N3	21:A:2280:G:OP2	2.41	0.54
10:j:60:ASP:OD1	10:j:61:SER:N	2.41	0.54
21:A:283:G:N2	21:A:289:U:O2	2.40	0.54
45:3:75:ASN:CA	45:3:78:PHE:CE2	2.86	0.54
1:a:332:G:N2	1:a:335:A:OP2	2.41	0.54
1:a:1073:G:OP1	3:c:2:GLY:N	2.41	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:A:342:A:N3	21:A:362:C:O2'	2.40	0.54
45:3:46:ILE:HD12	45:3:48:LEU:HD11	1.90	0.54
16:p:75:LEU:O	16:p:79:GLY:N	2.41	0.53
21:A:2869:G:O3'	21:A:2886:G:N2	2.34	0.53
36:U:81:ASN:ND2	54:U:201:HOH:O	2.41	0.53
45:3:51:SER:O	45:3:52:SER:OG	2.20	0.53
21:A:2549:U:O2'	21:A:2674:U:OP1	2.23	0.53
21:A:903:G:C2	21:A:2295:A:C2	2.96	0.53
29:N:64:ARG:NE	29:N:81:GLU:OE2	2.40	0.53
4:d:99:TYR:HD1	4:d:104:ALA:HB3	1.74	0.53
17:q:21:LYS:O	17:q:50:ASP:N	2.38	0.53
21:A:1581:U:C6	21:A:1584:A:H8	2.27	0.53
21:A:2465:U:O2'	21:A:2467:C:OP1	2.26	0.53
19:s:41:PHE:CB	45:3:82:SER:OG	2.57	0.53
21:A:994:A:O3'	22:B:85:A:N6	2.42	0.53
48:6:19:PHE:O	48:6:22:ARG:N	2.42	0.53
1:a:983:G:O3'	14:n:41:ARG:NH1	2.40	0.53
21:A:2282:G:N2	41:Z:14:GLY:O	2.42	0.53
40:Y:15:ARG:O	40:Y:17:ASP:N	2.41	0.53
45:3:75:ASN:HA	45:3:78:PHE:HE2	1.64	0.53
31:P:22:LYS:NZ	31:P:23:GLY:O	2.42	0.53
45:3:74:PHE:CD2	45:3:75:ASN:N	2.77	0.53
1:a:1089:G:N2	1:a:1092:A:OP2	2.39	0.53
6:f:52:ILE:CD1	6:f:87:ILE:HG21	2.39	0.53
21:A:418:G:O2'	21:A:446:G:O6	2.10	0.53
21:A:625:G:C4	21:A:1297:G:N2	2.77	0.53
21:A:2693:C:H42	27:H:109:TYR:HA	1.74	0.53
25:F:108:LEU:O	25:F:112:SER:OG	2.22	0.53
8:h:108:THR:OG1	8:h:111:GLY:O	2.17	0.53
15:o:47:LYS:O	15:o:53:ARG:NH2	2.42	0.53
21:A:1712:A:N3	21:A:1714:C:N4	2.57	0.53
5:e:86:THR:OG1	5:e:94:VAL:O	2.16	0.52
21:A:550:A:HO2'	21:A:554:C:HO2'	1.54	0.52
21:A:615:A:H61	21:A:2056:G:H21	1.58	0.52
21:A:2281:C:H42	41:Z:14:GLY:HA3	1.73	0.52
21:A:857:C:C6	21:A:1288:G:C6	2.94	0.52
27:H:10:ASP:OD1	27:H:11:ILE:N	2.42	0.52
45:3:75:ASN:CG	45:3:78:PHE:HE2	2.17	0.52
47:5:35:PHE:CD1	47:5:35:PHE:C	2.86	0.52
2:b:32:PHE:O	2:b:33:THR:OG1	2.18	0.52
21:A:1794:C:N3	21:A:2013:G:C2	2.77	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:a:675:G:OP1	1:a:740:C:O2'	2.25	0.52
8:h:31:ASN:OD1	8:h:32:ILE:N	2.42	0.52
10:j:51:ILE:HD13	10:j:65:PHE:CD2	2.45	0.52
23:D:61:TYR:CE2	23:D:63:VAL:HG22	2.45	0.52
37:V:30:ALA:HA	37:V:33:ILE:HD12	1.92	0.52
29:N:63:VAL:HG21	29:N:102:VAL:HG23	1.91	0.52
11:k:29:ASN:OD1	11:k:30:THR:N	2.43	0.52
16:p:69:ASP:OD1	16:p:70:THR:N	2.43	0.52
19:s:36:ARG:NH1	19:s:73:GLU:OE1	2.37	0.52
50:8:19:ARG:NE	50:8:24:MET:SD	2.82	0.52
1:a:1327:G:N1	1:a:1330:A:OP2	2.42	0.52
8:h:45:PHE:CD1	8:h:74:ILE:HG23	2.45	0.52
21:A:608:C:O3'	54:A:3111:HOH:O	2.19	0.52
21:A:628:G:N3	21:A:1289:A:N6	2.57	0.52
21:A:1575:A:O2'	21:A:1577:G:O6	2.23	0.52
21:A:1828:U:N1	21:A:2230:G:C4	2.78	0.52
21:A:2059:G:N2	24:E:159:ASP:OD2	2.42	0.52
2:b:203:ASN:OD1	2:b:204:ASP:N	2.42	0.52
25:F:190:ASP:OD1	25:F:191:SER:N	2.42	0.52
45:3:73:ARG:CG	45:3:74:PHE:N	2.73	0.52
21:A:903:G:C6	21:A:2295:A:N1	2.78	0.52
21:A:932:U:N3	21:A:935:C:C4	2.78	0.52
21:A:1288:G:OP2	30:O:21:ARG:NH2	2.43	0.52
21:A:2260:A:O2'	21:A:2261:G:H5'	2.10	0.52
21:A:1569:G:N3	21:A:1569:G:C2'	2.73	0.51
21:A:1710:G:N1	21:A:2022:U:O4	2.43	0.51
21:A:1987:A:C2'	21:A:1988:C:C5'	2.85	0.51
21:A:2110:G:O6	21:A:2264:G:N2	2.43	0.51
1:a:1458:A:OP1	1:a:1459:C:N4	2.37	0.51
11:k:26:THR:OG1	11:k:29:ASN:N	2.43	0.51
13:m:111:GLY:O	13:m:113:VAL:N	2.43	0.51
21:A:13:A:O2'	21:A:15:G:N7	2.43	0.51
21:A:352:A:N7	21:A:373:A:N6	2.58	0.51
45:3:78:PHE:CD1	45:3:79:GLY:N	2.78	0.51
13:m:72:GLU:O	13:m:76:ASN:ND2	2.44	0.51
21:A:1075:G:H21	50:8:36:GLN:HE22	1.58	0.51
21:A:1568:U:O4'	21:A:1570:G:C4	2.64	0.51
21:A:1569:G:N3	21:A:1569:G:C3'	2.73	0.51
21:A:1570:G:H2'	21:A:1571:G:C8	2.45	0.51
34:S:29:ARG:NH1	34:S:46:GLU:OE2	2.44	0.51
41:Z:48:GLN:OE1	41:Z:53:ILE:N	2.44	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:k:113:VAL:O	11:k:113:VAL:HG13	2.11	0.51
20:t:17:ALA:O	20:t:21:ASN:ND2	2.44	0.51
21:A:752:G:O6	21:A:770:G:N2	2.44	0.51
21:A:1581:U:C5	21:A:1584:A:C8	2.98	0.51
22:B:38:U:N3	22:B:42:G:OP2	2.44	0.51
23:D:69:ASN:OD1	23:D:70:LYS:N	2.43	0.51
1:a:874:A:O2'	1:a:1090:U:O4	2.27	0.51
2:b:115:SER:OG	2:b:152:ARG:NH2	2.42	0.51
21:A:550:A:O2'	21:A:554:C:O2'	2.26	0.51
21:A:1172:A:C5	21:A:2545:A:N1	2.79	0.51
21:A:1519:U:O2'	21:A:1560:A:N1	2.43	0.51
21:A:1570:G:H8	21:A:1570:G:P	2.33	0.51
21:A:1708:A:N6	21:A:2753:U:C4	2.78	0.51
1:a:666:G:C2	1:a:757:A:C5	2.99	0.51
1:a:672:G:H22	1:a:749:G:H1	1.58	0.51
21:A:1175:G:N7	24:E:162:ARG:NH2	2.59	0.51
21:A:1568:U:C5'	21:A:1570:G:H1'	2.39	0.51
21:A:1962:G:O2'	21:A:1963:A:O5'	2.26	0.51
21:A:2002:G:O6	21:A:2003:U:N3	2.43	0.51
22:B:90:C:OP1	40:Y:19:LYS:NZ	2.40	0.51
45:3:32:SER:OG	45:3:54:SER:OG	2.19	0.51
9:i:7:GLU:N	9:i:7:GLU:OE1	2.43	0.51
31:P:110:SER:OG	31:P:111:GLU:N	2.44	0.51
4:d:151:ILE:O	4:d:154:SER:N	2.44	0.51
21:A:166:A:O2'	21:A:167:U:O4'	2.28	0.51
45:3:33:GLU:O	45:3:51:SER:OG	2.26	0.51
1:a:1114:A:O2'	2:b:98:GLY:N	2.40	0.51
21:A:563:G:O5'	37:V:18:ARG:NH1	2.44	0.51
21:A:1306:C:C2	21:A:2040:A:N1	2.78	0.51
21:A:749:G:O2'	21:A:771:G:N2	2.44	0.50
21:A:1711:G:O2'	21:A:2018:U:O4	2.24	0.50
40:Y:27:VAL:N	40:Y:43:VAL:O	2.44	0.50
1:a:1358:G:OP2	9:i:111:ARG:NE	2.44	0.50
21:A:1123:C:N4	21:A:1132:A:O4'	2.43	0.50
21:A:1836:A:O2'	21:A:1837:A:O4'	2.20	0.50
42:0:18:ARG:O	42:0:29:TRP:NE1	2.44	0.50
1:a:1002:U:HO2'	1:a:1054:U:H3	1.59	0.50
11:k:67:SER:O	11:k:71:SER:OG	2.21	0.50
21:A:2860:U:C5'	32:Q:49:THR:HG21	2.42	0.50
33:R:84:ALA:O	33:R:88:GLY:N	2.39	0.50
1:a:827:A:C6	1:a:1541:G:C2	3.00	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:a:1449:G:OP2	20:t:29:ARG:NH1	2.44	0.50
21:A:83:G:O2'	21:A:84:A:OP2	2.24	0.50
23:D:190:THR:OG1	23:D:191:ILE:N	2.45	0.50
17:q:50:ASP:OD1	17:q:51:GLU:N	2.44	0.50
21:A:1855:G:N2	54:A:3126:HOH:O	2.45	0.50
21:A:2140:C:N4	21:A:2195:G:O2'	2.44	0.50
45:3:66:ALA:HA	45:3:67:ALA:HB3	1.94	0.50
11:k:50:LEU:HD23	11:k:65:MET:HE2	1.94	0.50
21:A:319:G:N2	21:A:320:U:O3'	2.44	0.50
1:a:988:A:N6	1:a:1371:A:C2	2.79	0.50
21:A:902:A:N1	21:A:903:G:N2	2.59	0.50
21:A:1236:G:H1'	21:A:1288:G:H21	1.77	0.50
1:a:760:G:OP1	15:o:73:LYS:NZ	2.41	0.50
6:f:52:ILE:HD12	6:f:87:ILE:HG21	1.93	0.50
21:A:687:G:H21	21:A:691:A:H62	1.59	0.50
24:E:41:VAL:N	24:E:47:ASN:OD1	2.43	0.50
10:j:51:ILE:O	10:j:63:GLU:N	2.43	0.49
15:o:12:ILE:HG22	15:o:27:VAL:HG13	1.94	0.49
21:A:198:A:OP2	21:A:199:A:O2'	2.29	0.49
21:A:1463:A:HO2'	21:A:1464:U:P	2.36	0.49
21:A:2362:A:N6	21:A:2364:G:N3	2.59	0.49
45:3:75:ASN:ND2	45:3:78:PHE:CE2	2.78	0.49
10:j:51:ILE:HD13	10:j:65:PHE:CE2	2.47	0.49
15:o:74:ASP:OD1	15:o:75:ILE:N	2.41	0.49
21:A:1292:A:O2'	21:A:1293:U:OP1	2.30	0.49
1:a:1443:G:O2'	1:a:1444:A:OP2	2.30	0.49
2:b:54:TYR:CD1	2:b:220:ALA:HB2	2.47	0.49
9:i:17:SER:OG	9:i:71:GLY:O	2.18	0.49
15:o:29:ILE:O	15:o:33:THR:OG1	2.19	0.49
21:A:285:U:OP1	21:A:288:C:N4	2.42	0.49
21:A:2603:G:O2'	21:A:2606:C:OP2	2.31	0.49
48:6:15:LYS:O	48:6:18:GLY:N	2.44	0.49
21:A:613:G:C5	21:A:2057:A:N6	2.80	0.49
49:7:34:ALA:O	49:7:38:THR:OG1	2.18	0.49
21:A:1510:U:C2'	21:A:1511:C:H5'	2.43	0.49
45:3:70:ARG:CZ	45:3:71:VAL:CG2	2.90	0.49
1:a:1116:G:O2'	2:b:109:LYS:NZ	2.41	0.49
21:A:738:U:O2'	21:A:1390:A:N3	2.42	0.49
21:A:790:G:N2	21:A:795:A:H61	2.10	0.49
5:e:136:MET:O	5:e:139:ALA:HB3	2.13	0.49
21:A:1436:C:O2'	21:A:1437:U:O5'	2.31	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:U:23:GLU:OE1	36:U:90:GLN:NE2	2.45	0.49
41:Z:64:ASP:CG	41:Z:66:THR:HG23	2.38	0.49
21:A:230:A:H61	21:A:456:G:N2	2.11	0.49
21:A:281:A:N1	21:A:282:A:N6	2.60	0.49
21:A:613:G:C6	21:A:2057:A:C6	3.00	0.49
21:A:1828:U:C5	21:A:2230:G:C2'	2.96	0.49
27:H:96:ALA:N	27:H:128:ASN:O	2.38	0.49
1:a:666:G:C5	1:a:757:A:N6	2.81	0.48
1:a:989:C:OP1	1:a:1234:C:N4	2.46	0.48
21:A:1752:C:H42	21:A:1777:G:H1	1.61	0.48
21:A:1809:C:O2	21:A:2635:G:O2'	2.23	0.48
41:Z:35:ASP:OD1	41:Z:36:GLY:N	2.46	0.48
1:a:958:C:OP1	13:m:108:THR:OG1	2.27	0.48
1:a:419:A:N6	1:a:437:U:O4'	2.45	0.48
17:q:71:ALA:O	17:q:72:THR:OG1	2.20	0.48
21:A:1708:A:N6	21:A:2753:U:N3	2.62	0.48
21:A:2268:A:N7	54:A:3121:HOH:O	2.35	0.48
2:b:58:LYS:NZ	2:b:223:GLU:OE1	2.45	0.48
21:A:2616:A:N1	21:A:2633:C:N4	2.61	0.48
23:D:64:ILE:HD11	23:D:86:ARG:HH22	1.77	0.48
43:1:38:GLU:N	43:1:38:GLU:OE1	2.46	0.48
45:3:28:THR:HG23	45:3:48:LEU:HD12	1.94	0.48
2:b:7:LYS:HB2	2:b:50:VAL:HG11	1.96	0.48
11:k:25:SER:OG	11:k:88:GLY:O	2.30	0.48
21:A:1828:U:C6	21:A:2230:G:C2'	2.96	0.48
40:Y:32:TYR:O	40:Y:93:ALA:N	2.41	0.48
45:3:71:VAL:CA	45:3:74:PHE:CE1	2.86	0.48
1:a:971:U:O2	1:a:993:A:O2'	2.26	0.48
7:g:75:VAL:HG13	7:g:145:ALA:HB2	1.94	0.48
21:A:796:A:H62	21:A:834:A:H62	1.59	0.48
47:5:35:PHE:HE1	47:5:37:SER:H	1.38	0.48
1:a:1147:U:N3	1:a:1150:G:OP2	2.44	0.48
21:A:1187:A:N7	28:M:28:ARG:NH1	2.62	0.48
45:3:42:GLU:N	45:3:42:GLU:OE1	2.46	0.48
21:A:749:G:O2'	21:A:771:G:N1	2.46	0.48
29:N:98:ILE:HG22	29:N:99:PHE:O	2.13	0.48
47:5:32:MET:SD	47:5:32:MET:N	2.87	0.48
7:g:63:GLU:OE2	7:g:67:ASN:ND2	2.41	0.48
20:t:57:VAL:O	20:t:61:ALA:HB2	2.13	0.48
21:A:1793:C:N1	21:A:2014:G:N2	2.60	0.48
22:B:15:C:N4	22:B:105:G:H21	2.03	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:c:49:ALA:O	3:c:50:SER:OG	2.29	0.48
21:A:1828:U:C6	21:A:2230:G:H2'	2.49	0.48
24:E:83:ALA:O	24:E:85:LYS:NZ	2.42	0.48
11:k:16:ILE:HD12	11:k:18:ASN:O	2.13	0.47
21:A:1072:A:N3	21:A:2513:G:O2'	2.41	0.47
21:A:1306:C:N3	21:A:2040:A:C5	2.81	0.47
38:W:31:THR:HG22	38:W:32:ARG:H	1.78	0.47
45:3:75:ASN:CG	45:3:78:PHE:CE2	2.92	0.47
1:a:374:C:O2'	1:a:375:U:O5'	2.31	0.47
9:i:32:VAL:HG23	9:i:67:VAL:HG13	1.96	0.47
35:T:94:MET:HE1	36:U:12:ILE:C	2.39	0.47
45:3:77:LYS:HE2	45:3:77:LYS:CA	2.37	0.47
8:h:45:PHE:CD1	8:h:73:VAL:HG23	2.49	0.47
23:D:141:HIS:ND1	23:D:192:GLY:O	2.44	0.47
2:b:86:ARG:NH1	2:b:219:ASP:OD1	2.45	0.47
21:A:895:U:O2'	44:2:22:THR:OG1	2.24	0.47
21:A:2355:A:H2'	21:A:2356:A:C8	2.49	0.47
21:A:2510:C:H42	31:P:124:LYS:HE2	1.79	0.47
32:Q:9:THR:OG1	32:Q:10:SER:N	2.45	0.47
1:a:419:A:N6	1:a:437:U:O5'	2.46	0.47
8:h:45:PHE:HD1	8:h:73:VAL:HG23	1.79	0.47
21:A:1709:A:N1	21:A:2023:C:N4	2.58	0.47
4:d:114:VAL:CG2	4:d:119:ILE:HD11	2.44	0.47
21:A:1252:A:N6	21:A:1273:G:O2'	2.39	0.47
21:A:1450:A:H3'	21:A:1634:A:H61	1.79	0.47
21:A:1982:U:H3	21:A:2579:U:C4'	2.28	0.47
35:T:70:ARG:NH1	35:T:75:SER:OG	2.48	0.47
1:a:446:G:O2'	1:a:502:C:N4	2.48	0.47
1:a:572:U:OP1	12:l:12:ARG:NH2	2.48	0.47
1:a:1112:C:N4	1:a:1115:C:OP1	2.48	0.47
4:d:8:ASN:O	4:d:21:GLY:N	2.47	0.47
7:g:65:ALA:O	7:g:68:ASN:N	2.48	0.47
7:g:125:LEU:O	7:g:129:ASN:ND2	2.48	0.47
21:A:1469:G:N2	21:A:1621:C:N3	2.63	0.47
21:A:2870:A:P	21:A:2886:G:H22	2.37	0.47
33:R:70:VAL:O	33:R:73:ALA:HB3	2.15	0.47
36:U:60:ALA:HB1	36:U:96:THR:O	2.15	0.47
38:W:31:THR:HG22	38:W:32:ARG:N	2.30	0.47
40:Y:27:VAL:HB	40:Y:43:VAL:HG13	1.97	0.47
21:A:164:A:O2'	21:A:165:C:O5'	2.32	0.47
21:A:1817:C:O2'	23:D:207:ALA:HB2	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:A:2822:C:O2'	21:A:2823:G:O4'	2.33	0.47
45:3:65:ALA:O	45:3:67:ALA:HB3	2.15	0.47
1:a:130:A:H61	1:a:241:U:H1'	1.79	0.47
4:d:132:SER:OG	4:d:134:LYS:NZ	2.48	0.47
8:h:45:PHE:CE1	8:h:74:ILE:HG23	2.50	0.47
8:h:49:VAL:HG12	8:h:62:LEU:HG	1.97	0.47
22:B:69:C:H42	22:B:102:A:H61	1.61	0.47
45:3:80:LEU:HD23	45:3:80:LEU:HA	1.77	0.47
1:a:1271:G:O2'	1:a:1272:A:OP2	2.29	0.46
21:A:82:G:N1	21:A:102:A:OP2	2.44	0.46
33:R:31:LEU:HD13	33:R:44:ILE:HG13	1.98	0.46
1:a:1002:U:O2'	1:a:1054:U:N3	2.45	0.46
3:c:20:ALA:HB1	3:c:22:TRP:CZ3	2.45	0.46
5:e:153:VAL:O	5:e:156:LEU:N	2.45	0.46
10:j:14:ASP:HB2	10:j:17:VAL:HG12	1.98	0.46
21:A:83:G:HO2'	21:A:84:A:P	2.38	0.46
21:A:1172:A:N6	21:A:2545:A:N6	2.63	0.46
22:B:4:G:H1	22:B:111:A:H62	1.62	0.46
45:3:73:ARG:HG3	45:3:74:PHE:N	2.25	0.46
1:a:681:G:O3'	6:f:88:ARG:NH2	2.48	0.46
21:A:319:G:H21	21:A:320:U:C4'	2.29	0.46
22:B:10:U:O2'	22:B:12:U:OP1	2.32	0.46
32:Q:90:ALA:O	32:Q:94:THR:HG23	2.15	0.46
15:o:24:SER:O	15:o:26:GLU:N	2.48	0.46
21:A:1091:G:N2	21:A:1154:G:O2'	2.47	0.46
21:A:1858:G:H22	21:A:2002:G:N2	2.13	0.46
1:a:1232:G:O3'	19:s:77:THR:HG21	2.15	0.46
1:a:184:A:N6	1:a:208:U:O4	2.48	0.46
21:A:695:C:N4	21:A:696:G:O6	2.48	0.46
21:A:1390:A:OP2	21:A:1414:G:N1	2.42	0.46
21:A:2255:G:P	23:D:262:LYS:HZ1	2.39	0.46
22:B:11:A:OP1	41:Z:82:ARG:NE	2.44	0.46
1:a:1074:U:O4	3:c:3:GLN:NE2	2.48	0.46
1:a:1495:A:H5''	1:a:1496:U:OP2	2.16	0.46
4:d:170:ASP:OD1	4:d:171:SER:N	2.49	0.46
10:j:64:GLN:N	10:j:64:GLN:OE1	2.49	0.46
14:n:10:GLN:OE1	14:n:21:TYR:N	2.44	0.46
21:A:1704:C:H42	21:A:2027:G:H1	1.64	0.46
21:A:2093:C:N4	21:A:2094:G:O6	2.49	0.46
1:a:633:G:H5''	16:p:10:LEU:HD23	1.98	0.46
11:k:63:ALA:HB1	11:k:96:ALA:CB	2.43	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:A:1044:A:OP2	21:A:1198:G:N1	2.40	0.46
1:a:640:G:O2'	1:a:641:U:O2	2.34	0.46
8:h:91:ALA:O	8:h:94:MET:HE3	2.16	0.46
23:D:64:ILE:HG21	23:D:66:PHE:CE1	2.51	0.46
45:3:53:ASP:OD1	45:3:59:THR:OG1	2.34	0.46
1:a:1065:G:O2'	1:a:1210:U:OP2	2.24	0.46
11:k:35:THR:HG22	11:k:41:ALA:HA	1.98	0.46
21:A:1008:C:O2'	21:A:2300:A:N3	2.38	0.46
21:A:2039:G:O2'	21:A:2040:A:O5'	2.29	0.46
21:A:2375:U:OP2	49:7:35:ASN:ND2	2.43	0.46
21:A:2485:U:HO2'	21:A:2517:G:H1	1.63	0.46
24:E:63:ALA:HB1	24:E:68:TYR:HD2	1.81	0.46
40:Y:18:LEU:O	40:Y:21:LEU:N	2.47	0.46
1:a:1458:A:P	1:a:1459:C:H41	2.39	0.45
21:A:1488:A:N7	21:A:1596:G:N1	2.63	0.45
1:a:412:G:OP1	4:d:115:ASN:ND2	2.46	0.45
1:a:1067:A:H62	1:a:1211:C:H42	1.64	0.45
21:A:600:U:OP1	28:M:114:ARG:NH1	2.47	0.45
21:A:1897:U:HO2'	21:A:1898:C:C1'	2.29	0.45
33:R:8:ASN:O	33:R:12:LEU:N	2.49	0.45
21:A:625:G:C6	21:A:1297:G:C6	3.04	0.45
21:A:1927:A:O2'	21:A:1928:A:OP1	2.32	0.45
21:A:2127:G:C2	21:A:2216:U:O2	2.69	0.45
45:3:77:LYS:HD3	45:3:77:LYS:C	2.40	0.45
19:s:81:LYS:H	19:s:82:GLY:HA2	1.81	0.45
20:t:7:ALA:O	20:t:10:ARG:N	2.50	0.45
29:N:7:ARG:C	29:N:8:LEU:HD12	2.42	0.45
45:3:67:ALA:O	45:3:68:ASP:CB	2.65	0.45
49:7:18:ALA:O	49:7:19:SER:OG	2.29	0.45
5:e:153:VAL:HG21	8:h:101:LEU:HD21	1.98	0.45
21:A:790:G:O2'	21:A:793:G:O2'	1.96	0.45
21:A:1718:G:H21	21:A:1721:A:H61	1.64	0.45
24:E:142:SER:O	24:E:143:HIS:ND1	2.48	0.45
1:a:364:A:N3	1:a:376:U:O2'	2.35	0.45
21:A:903:G:O6	21:A:2295:A:N1	2.50	0.45
21:A:1989:C:H6	21:A:1989:C:O5'	2.00	0.45
1:a:420:U:O4	1:a:439:A:N6	2.50	0.45
15:o:51:HIS:NE2	15:o:52:SER:OG	2.50	0.45
21:A:116:G:OP2	21:A:118:A:O2'	2.35	0.45
43:1:45:THR:O	43:1:49:THR:HG23	2.16	0.45
1:a:225:G:H1'	1:a:478:G:H21	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:a:1246:U:O2'	1:a:1316:G:OP1	2.30	0.45
1:a:1528:G:N2	1:a:1531:A:OP2	2.48	0.45
1:a:1123:A:O2'	1:a:1124:C:O5'	2.33	0.45
6:f:19:LYS:O	6:f:23:VAL:HG23	2.17	0.45
10:j:63:GLU:OE2	14:n:58:LYS:NZ	2.32	0.45
12:l:29:ASN:OD1	12:l:30:SER:N	2.48	0.45
21:A:1100:G:O2'	21:A:1130:A:N7	2.47	0.45
21:A:2354:A:N7	21:A:2415:A:N6	2.65	0.45
30:O:114:ASN:ND2	30:O:129:SER:O	2.50	0.45
45:3:75:ASN:O	45:3:78:PHE:CD2	2.70	0.45
1:a:245:C:P	17:q:44:LYS:HZ3	2.39	0.44
1:a:261:U:C1'	1:a:283:G:H21	2.31	0.44
1:a:1163:A:OP1	10:j:70:HIS:ND1	2.45	0.44
21:A:729:G:N2	21:A:819:A:N1	2.65	0.44
21:A:1105:U:O2'	21:A:1109:U:O4	2.32	0.44
31:P:60:ARG:NH1	31:P:108:GLY:O	2.45	0.44
37:V:5:ALA:HB3	37:V:54:ALA:HB2	1.98	0.44
1:a:1054:U:H2'	1:a:1055:G:N7	2.32	0.44
1:a:1316:G:O2'	1:a:1317:A:OP2	2.34	0.44
1:a:1331:C:H42	19:s:36:ARG:HB3	1.83	0.44
5:e:102:GLY:N	5:e:122:ASP:OD2	2.47	0.44
11:k:63:ALA:HB1	11:k:96:ALA:CA	2.48	0.44
21:A:721:A:H2	21:A:847:A:H61	1.64	0.44
21:A:1865:C:H41	21:A:1926:A:H5'	1.82	0.44
21:A:2370:U:HO2'	21:A:2400:U:HO2'	1.58	0.44
32:Q:45:GLU:O	32:Q:49:THR:HG23	2.18	0.44
1:a:1424:A:H2	1:a:1499:G:H22	1.66	0.44
3:c:8:ILE:HD12	14:n:50:LYS:HA	2.00	0.44
45:3:71:VAL:O	45:3:74:PHE:CD1	2.70	0.44
2:b:166:PRO:O	2:b:170:ARG:N	2.50	0.44
21:A:1793:C:N3	21:A:2014:G:C2	2.85	0.44
21:A:1847:U:O2'	23:D:157:ALA:HB3	2.18	0.44
23:D:59:ARG:NH2	23:D:213:LYS:O	2.50	0.44
10:j:8:ILE:HG22	10:j:100:ILE:HA	1.99	0.44
21:A:1357:G:N1	21:A:1367:C:OP2	2.48	0.44
21:A:1828:U:H3'	21:A:1829:A:C5'	2.48	0.44
21:A:2195:G:N2	21:A:2197:G:O6	2.50	0.44
21:A:2458:U:N3	21:A:2461:A:OP2	2.45	0.44
47:5:35:PHE:CD1	47:5:37:SER:N	2.81	0.44
2:b:66:GLN:NE2	2:b:157:MET:O	2.50	0.44
12:l:46:VAL:N	12:l:69:ARG:O	2.50	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:A:877:G:N2	30:O:48:PRO:O	2.47	0.44
24:E:9:LYS:O	24:E:11:GLY:N	2.51	0.44
27:H:83:TYR:N	27:H:135:GLY:O	2.47	0.44
1:a:949:G:OP1	7:g:102:ARG:NH1	2.51	0.44
2:b:23:TRP:NE1	2:b:39:TYR:OH	2.50	0.44
21:A:660:A:C2	25:F:36:ALA:HB1	2.53	0.44
21:A:628:G:H2'	21:A:1289:A:H62	1.82	0.43
21:A:2033:C:O2'	21:A:2843:A:N3	2.51	0.43
21:A:2126:C:HO2'	21:A:2127:G:H8	1.66	0.43
23:D:22:GLU:O	23:D:80:ILE:HG21	2.18	0.43
33:R:68:THR:O	33:R:68:THR:HG23	2.18	0.43
40:Y:38:ASN:OD1	40:Y:39:VAL:N	2.51	0.43
45:3:46:ILE:HD12	45:3:48:LEU:CD1	2.48	0.43
45:3:80:LEU:O	45:3:81:LYS:C	2.60	0.43
49:7:49:LEU:N	49:7:49:LEU:HD12	2.32	0.43
1:a:982:C:OP2	10:j:59:LYS:NZ	2.46	0.43
1:a:1542:G:O2'	1:a:1543:A:O4'	2.35	0.43
21:A:1198:G:OP2	35:T:58:ARG:NE	2.35	0.43
21:A:1828:U:C4	21:A:2230:G:O4'	2.71	0.43
45:3:25:SER:OG	45:3:26:GLY:N	2.52	0.43
1:a:728:C:O2'	18:r:57:GLN:NE2	2.46	0.43
1:a:1080:G:N7	1:a:1106:G:O2'	2.50	0.43
2:b:176:ALA:HB1	2:b:181:ILE:HD11	1.99	0.43
21:A:1569:G:N3	21:A:1569:G:H2'	2.33	0.43
21:A:1570:G:H2'	21:A:1571:G:H8	1.82	0.43
23:D:80:ILE:HG22	23:D:81:GLN:N	2.33	0.43
30:O:83:ASN:OD1	30:O:84:LYS:N	2.51	0.43
33:R:39:HIS:HA	33:R:40:ILE:HD12	2.00	0.43
33:R:86:ASP:OD1	33:R:87:LYS:N	2.51	0.43
49:7:24:ARG:NH2	49:7:43:GLN:O	2.49	0.43
17:q:44:LYS:NZ	17:q:46:TYR:OH	2.27	0.43
19:s:9:PRO:CD	45:3:81:LYS:CD	2.89	0.43
21:A:932:U:C2	21:A:935:C:C4	3.07	0.43
21:A:1118:G:O2'	21:A:1119:C:O5'	2.33	0.43
21:A:2292:U:O2	21:A:2301:A:N6	2.44	0.43
21:A:2673:C:OP2	21:A:2759:G:O2'	2.35	0.43
28:M:76:TYR:HE1	28:M:87:SER:HG	1.66	0.43
17:q:29:THR:OG1	17:q:30:TYR:N	2.51	0.43
21:A:27:G:O2'	21:A:557:G:N2	2.51	0.43
21:A:1816:A:H2'	21:A:1817:C:O4'	2.19	0.43
21:A:1827:C:OP2	23:D:181:ARG:NH1	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
45:3:49:ASP:OD1	45:3:50:ILE:N	2.51	0.43
10:j:53:ARG:NH2	10:j:63:GLU:OE1	2.51	0.43
11:k:83:GLU:OE2	11:k:111:ARG:NE	2.42	0.43
12:l:117:THR:O	12:l:117:THR:HG23	2.18	0.43
22:B:26:C:H2'	22:B:27:A:O4'	2.18	0.43
24:E:65:SER:O	24:E:67:LYS:N	2.52	0.43
2:b:19:GLN:OE1	2:b:167:ARG:NH2	2.41	0.43
6:f:85:ASP:OD1	6:f:86:ILE:N	2.51	0.43
17:q:26:LEU:HD23	17:q:26:LEU:O	2.18	0.43
21:A:273:A:OP2	21:A:297:G:N1	2.45	0.43
21:A:503:A:N6	21:A:517:A:OP2	2.49	0.43
1:a:666:G:C2	1:a:757:A:C6	3.07	0.43
1:a:969:A:N6	19:s:77:THR:O	2.52	0.43
1:a:1452:G:O2'	1:a:1472:A:N6	2.46	0.43
9:i:40:TYR:OH	9:i:77:GLN:NE2	2.51	0.43
21:A:790:G:H21	21:A:795:A:N6	2.15	0.43
24:E:9:LYS:O	24:E:9:LYS:HG2	2.19	0.43
40:Y:72:VAL:HG21	40:Y:91:PHE:CD1	2.54	0.43
1:a:944:C:H42	1:a:948:A:H61	1.67	0.43
11:k:63:ALA:HB1	11:k:96:ALA:N	2.34	0.43
21:A:903:G:H22	21:A:965:G:H1	1.67	0.43
21:A:903:G:H1	21:A:2295:A:H2	1.60	0.43
21:A:975:U:O2'	21:A:976:U:O4'	2.35	0.43
1:a:528:A:H61	1:a:541:A:H61	1.67	0.43
4:d:88:ILE:O	4:d:92:SER:N	2.52	0.43
22:B:3:U:H3	22:B:112:G:H22	1.67	0.43
21:A:1510:U:O2'	21:A:1511:C:H5'	2.19	0.42
1:a:886:A:H1'	8:h:12:THR:HG21	2.00	0.42
1:a:974:A:O2'	10:j:57:MET:HE1	2.19	0.42
5:e:2:ALA:HB1	5:e:69:LYS:HD3	2.00	0.42
21:A:1987:A:H2'	21:A:1988:C:O5'	2.18	0.42
1:a:225:G:C1'	1:a:478:G:H21	2.31	0.42
1:a:1115:C:O2'	2:b:110:ARG:NH2	2.51	0.42
23:D:157:ALA:O	23:D:176:ARG:NH2	2.51	0.42
27:H:117:ALA:HB2	27:H:123:PHE:CE2	2.54	0.42
1:a:504:G:H21	1:a:505:A:H5''	1.85	0.42
1:a:1326:U:OP2	19:s:6:LYS:NZ	2.50	0.42
1:a:1495:A:O5'	1:a:1495:A:H8	2.03	0.42
13:m:2:ALA:HB1	13:m:3:ARG:HB2	2.00	0.42
21:A:628:G:N3	21:A:1289:A:N1	2.62	0.42
21:A:1828:U:C5	21:A:2230:G:H2'	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:A:1989:C:O2'	21:A:1991:G:OP2	2.32	0.42
25:F:125:VAL:HG22	25:F:126:VAL:N	2.34	0.42
28:M:5:PHE:O	35:T:64:ARG:NH2	2.46	0.42
1:a:401:A:OP2	16:p:13:LYS:NZ	2.45	0.42
21:A:848:U:O4	21:A:849:A:N6	2.52	0.42
29:N:13:ASN:OD1	29:N:96:THR:OG1	2.28	0.42
20:t:66:ILE:HB	20:t:67:HIS:HA	2.01	0.42
21:A:247:A:OP2	49:7:8:ARG:NH1	2.50	0.42
23:D:78:ASP:O	23:D:79:SER:OG	2.36	0.42
23:D:194:VAL:HG12	23:D:195:GLY:N	2.35	0.42
24:E:141:MET:SD	24:E:148:HIS:ND1	2.92	0.42
34:S:28:LEU:HD11	34:S:86:ILE:CG2	2.49	0.42
48:6:2:VAL:HG21	48:6:4:ARG:HE	1.84	0.42
1:a:399:G:OP1	16:p:9:ARG:NH2	2.52	0.42
1:a:681:G:H2'	1:a:682:G:C8	2.55	0.42
1:a:726:A:C1'	11:k:118:HIS:HD1	2.31	0.42
1:a:899:A:N6	1:a:918:A:OP2	2.47	0.42
4:d:120:LEU:HD11	4:d:142:ARG:HA	2.02	0.42
23:D:213:LYS:N	23:D:214:GLY:HA2	2.35	0.42
45:3:28:THR:OG1	45:3:46:ILE:HD11	2.20	0.42
45:3:73:ARG:HE	45:3:73:ARG:HB2	1.64	0.42
2:b:176:ALA:O	2:b:179:LEU:N	2.52	0.42
21:A:319:G:H21	21:A:320:U:H4'	1.84	0.42
21:A:579:U:O2'	35:T:49:ASP:OD2	2.12	0.42
21:A:1344:A:OP2	21:A:1650:G:N1	2.49	0.42
21:A:1396:A:OP2	21:A:1408:G:N2	2.51	0.42
21:A:1515:G:HO2'	21:A:1516:C:H6	1.63	0.42
27:H:46:GLU:HB2	27:H:49:THR:HG23	2.01	0.42
33:R:25:THR:OG1	33:R:47:ASP:N	2.52	0.42
1:a:184:A:N1	1:a:208:U:C4	2.88	0.42
1:a:569:U:O3'	12:l:15:LYS:NZ	2.53	0.42
4:d:50:GLN:NE2	4:d:196:GLU:OE1	2.53	0.42
7:g:107:TYR:O	7:g:110:LEU:N	2.53	0.42
21:A:1378:U:OP1	21:A:1434:U:N3	2.53	0.42
1:a:666:G:C2	1:a:757:A:N7	2.88	0.42
1:a:774:A:N7	1:a:821:U:O4	2.53	0.42
1:a:988:A:N6	1:a:1371:A:C6	2.88	0.42
6:f:49:ALA:HB1	18:r:74:PRO:HB3	2.02	0.42
6:f:76:PHE:O	6:f:80:ALA:HB2	2.19	0.42
7:g:47:PHE:HA	7:g:50:VAL:HG12	2.00	0.42
21:A:491:C:O2'	21:A:495:A:N3	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:A:2774:G:H21	21:A:2784:A:H62	1.67	0.42
23:D:103:ILE:HG22	23:D:104:ILE:O	2.20	0.42
13:m:20:THR:OG1	13:m:26:GLY:O	2.30	0.41
41:Z:64:ASP:OD1	41:Z:64:ASP:N	2.52	0.41
1:a:111:G:H21	1:a:362:G:C4'	2.32	0.41
1:a:839:U:O2'	1:a:1551:C:OP1	2.34	0.41
1:a:1249:A:H2	1:a:1252:G:H21	1.68	0.41
21:A:1693:G:H1	21:A:2035:C:H42	1.67	0.41
21:A:1949:G:H2'	21:A:1950:U:O4'	2.20	0.41
1:a:24:C:OP2	1:a:569:U:N3	2.47	0.41
1:a:693:G:N1	1:a:712:A:OP2	2.49	0.41
6:f:2:ARG:N	6:f:67:SER:O	2.47	0.41
6:f:74:ASP:O	6:f:78:ARG:NE	2.53	0.41
1:a:456:A:N7	1:a:493:G:O2'	2.39	0.41
3:c:172:VAL:HG13	3:c:172:VAL:O	2.20	0.41
11:k:64:GLN:HG2	11:k:99:ALA:HB2	2.02	0.41
21:A:922:G:N2	21:A:944:G:O6	2.47	0.41
33:R:56:ALA:HB1	33:R:76:VAL:HG13	2.02	0.41
35:T:35:ALA:O	35:T:39:VAL:HG23	2.20	0.41
1:a:1106:G:O2'	1:a:1107:U:OP1	2.37	0.41
21:A:2023:C:O2	21:A:2023:C:O2'	2.36	0.41
23:D:80:ILE:HG22	23:D:81:GLN:H	1.84	0.41
29:N:21:THR:HG22	29:N:39:ILE:HD12	2.01	0.41
4:d:114:VAL:HG23	4:d:119:ILE:HD11	2.02	0.41
16:p:3:VAL:HG23	16:p:65:ALA:HA	2.02	0.41
16:p:71:VAL:HG12	16:p:75:LEU:HD13	2.02	0.41
21:A:688:A:H61	21:A:2396:A:H1'	1.85	0.41
21:A:1105:U:O2	21:A:1108:C:N4	2.49	0.41
21:A:1122:U:O2'	21:A:1132:A:N3	2.47	0.41
21:A:1858:G:H1	21:A:2002:G:N2	2.19	0.41
1:a:111:G:H21	1:a:362:G:H4'	1.85	0.41
12:l:27:GLY:O	12:l:29:ASN:N	2.53	0.41
15:o:51:HIS:CE1	15:o:52:SER:HG	2.39	0.41
21:A:2207:U:O4	21:A:2208:A:N6	2.52	0.41
21:A:2770:U:OP2	21:A:2782:C:N4	2.54	0.41
22:B:28:C:H1'	22:B:55:A:H61	1.86	0.41
23:D:194:VAL:HG12	23:D:195:GLY:H	1.86	0.41
24:E:51:VAL:HG12	24:E:52:GLY:N	2.35	0.41
45:3:73:ARG:CD	45:3:74:PHE:N	2.84	0.41
1:a:560:U:O4	1:a:561:A:N6	2.54	0.41
1:a:1495:A:H3'	1:a:1496:U:O4'	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:b:179:LEU:O	2:b:181:ILE:HG23	2.21	0.41
13:m:14:ARG:O	13:m:18:SER:OG	2.22	0.41
1:a:784:G:H22	1:a:810:A:P	2.44	0.41
1:a:1067:A:H62	1:a:1211:C:N4	2.19	0.41
4:d:118:HIS:NE2	4:d:145:SER:O	2.47	0.41
5:e:153:VAL:HG11	8:h:101:LEU:HD11	2.02	0.41
8:h:79:ARG:O	8:h:80:ILE:HD13	2.21	0.41
16:p:5:ILE:HD11	16:p:67:PRO:HB3	2.03	0.41
21:A:341:G:N1	21:A:382:U:OP2	2.54	0.41
21:A:509:G:N2	21:A:512:A:OP2	2.53	0.41
21:A:901:G:H2'	21:A:902:A:C8	2.56	0.41
21:A:1487:G:N2	21:A:1597:U:O2	2.54	0.41
21:A:1733:A:OP2	21:A:1742:A:N6	2.51	0.41
21:A:1865:C:N4	21:A:1926:A:O4'	2.54	0.41
21:A:2397:G:N2	47:5:35:PHE:HE2	2.00	0.41
23:D:134:ILE:HG22	23:D:135:PRO:O	2.21	0.41
23:D:157:ALA:HB1	23:D:196:ASN:O	2.21	0.41
1:a:181:A:N1	1:a:208:U:N3	2.69	0.41
19:s:4:SER:OG	19:s:5:ILE:N	2.53	0.41
19:s:36:ARG:NH1	19:s:72:GLY:O	2.54	0.41
21:A:236:A:H61	21:A:475:A:N6	2.16	0.41
21:A:1828:U:C2	21:A:2230:G:N3	2.89	0.41
21:A:1979:A:N3	21:A:2587:C:O2'	2.43	0.41
21:A:2146:A:H61	21:A:2195:G:H1	1.69	0.41
21:A:2261:G:C6	21:A:2262:G:C6	3.08	0.41
22:B:46:A:O3'	33:R:102:HIS:NE2	2.46	0.41
19:s:9:PRO:HD3	45:3:81:LYS:HD3	2.03	0.40
35:T:92:ARG:O	35:T:93:LYS:HG2	2.21	0.40
7:g:21:LYS:O	7:g:24:THR:N	2.53	0.40
21:A:603:C:O2'	35:T:48:ARG:NH2	2.54	0.40
21:A:1500:G:N2	21:A:2731:C:C2	2.90	0.40
25:F:173:VAL:O	25:F:173:VAL:HG22	2.20	0.40
26:G:46:ASN:O	26:G:49:VAL:N	2.54	0.40
4:d:90:LEU:HD12	4:d:93:ARG:HE	1.87	0.40
8:h:115:ASP:OD1	8:h:116:LYS:N	2.54	0.40
13:m:65:VAL:O	13:m:66:GLU:HG2	2.22	0.40
21:A:327:G:N1	21:A:328:G:N7	2.70	0.40
21:A:955:A:N3	21:A:2291:C:O2'	2.50	0.40
21:A:1712:A:O2'	21:A:1718:G:N7	2.52	0.40
21:A:1770:C:H42	21:A:1771:A:N6	2.19	0.40
21:A:2357:G:H21	41:Z:50:GLY:N	2.20	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:a:374:C:HO2'	1:a:375:U:P	2.45	0.40
1:a:1244:G:H4'	9:i:121:LYS:HE3	2.04	0.40
13:m:39:VAL:O	13:m:40:SER:OG	2.34	0.40
21:A:1075:G:N2	50:8:36:GLN:HE22	2.18	0.40
24:E:178:VAL:HG12	24:E:179:THR:N	2.36	0.40
39:X:23:VAL:O	39:X:24:ILE:HD13	2.20	0.40
43:1:25:LEU:O	43:1:28:LEU:N	2.55	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	b	222/255 (87%)	199 (90%)	23 (10%)	0	100	100
3	c	206/217 (95%)	172 (84%)	34 (16%)	0	100	100
4	d	193/199 (97%)	171 (89%)	21 (11%)	1 (0%)	24	57
5	e	163/165 (99%)	140 (86%)	23 (14%)	0	100	100
6	f	94/96 (98%)	85 (90%)	9 (10%)	0	100	100
7	g	143/150 (95%)	124 (87%)	17 (12%)	2 (1%)	9	37
8	h	129/131 (98%)	109 (84%)	19 (15%)	1 (1%)	16	48
9	i	126/128 (98%)	114 (90%)	12 (10%)	0	100	100
10	j	100/102 (98%)	89 (89%)	11 (11%)	0	100	100
11	k	116/118 (98%)	99 (85%)	17 (15%)	0	100	100
12	l	133/135 (98%)	103 (77%)	30 (23%)	0	100	100
13	m	117/119 (98%)	92 (79%)	23 (20%)	2 (2%)	7	34
14	n	58/60 (97%)	49 (84%)	9 (16%)	0	100	100
15	o	86/88 (98%)	75 (87%)	11 (13%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
16	p	88/90 (98%)	74 (84%)	14 (16%)	0	100	100
17	q	84/86 (98%)	66 (79%)	17 (20%)	1 (1%)	10	40
18	r	69/71 (97%)	58 (84%)	11 (16%)	0	100	100
19	s	82/84 (98%)	66 (80%)	16 (20%)	0	100	100
20	t	78/80 (98%)	71 (91%)	7 (9%)	0	100	100
23	D	273/275 (99%)	236 (86%)	36 (13%)	1 (0%)	30	62
24	E	216/218 (99%)	181 (84%)	33 (15%)	2 (1%)	14	45
25	F	197/199 (99%)	166 (84%)	30 (15%)	1 (0%)	24	57
26	G	164/166 (99%)	132 (80%)	31 (19%)	1 (1%)	21	54
27	H	162/164 (99%)	148 (91%)	14 (9%)	0	100	100
28	M	143/145 (99%)	126 (88%)	17 (12%)	0	100	100
29	N	120/122 (98%)	98 (82%)	19 (16%)	3 (2%)	4	28
30	O	129/131 (98%)	90 (70%)	39 (30%)	0	100	100
31	P	139/141 (99%)	106 (76%)	33 (24%)	0	100	100
32	Q	117/119 (98%)	104 (89%)	13 (11%)	0	100	100
33	R	117/119 (98%)	104 (89%)	13 (11%)	0	100	100
34	S	108/110 (98%)	97 (90%)	11 (10%)	0	100	100
35	T	114/116 (98%)	106 (93%)	8 (7%)	0	100	100
36	U	100/102 (98%)	82 (82%)	18 (18%)	0	100	100
37	V	110/112 (98%)	102 (93%)	8 (7%)	0	100	100
38	W	87/89 (98%)	75 (86%)	10 (12%)	2 (2%)	5	30
39	X	81/100 (81%)	66 (82%)	15 (18%)	0	100	100
40	Y	92/94 (98%)	73 (79%)	17 (18%)	2 (2%)	5	30
41	Z	80/82 (98%)	67 (84%)	13 (16%)	0	100	100
42	0	44/46 (96%)	30 (68%)	14 (32%)	0	100	100
43	1	63/65 (97%)	62 (98%)	1 (2%)	0	100	100
44	2	55/57 (96%)	48 (87%)	7 (13%)	0	100	100
45	3	81/84 (96%)	54 (67%)	24 (30%)	3 (4%)	2	21
46	4	54/56 (96%)	46 (85%)	8 (15%)	0	100	100
47	5	24/39 (62%)	15 (62%)	9 (38%)	0	100	100
48	6	42/44 (96%)	35 (83%)	5 (12%)	2 (5%)	2	17

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
49	7	58/60 (97%)	47 (81%)	11 (19%)	0	100	100
50	8	35/37 (95%)	29 (83%)	6 (17%)	0	100	100
All	All	5292/5466 (97%)	4481 (85%)	787 (15%)	24 (0%)	26	57

All (24) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
7	g	13	LEU
8	h	99	ASN
38	W	50	VAL
45	3	12	VAL
45	3	68	ASP
24	E	10	ILE
29	N	100	GLY
48	6	15	LYS
48	6	16	VAL
13	m	111	GLY
24	E	142	SER
4	d	143	GLU
25	F	144	SER
29	N	25	LEU
40	Y	15	ARG
7	g	14	PRO
38	W	51	ALA
40	Y	16	SER
23	D	195	GLY
45	3	71	VAL
29	N	101	PRO
13	m	65	VAL
26	G	89	VAL
17	q	86	ILE

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	b	194/221 (88%)	194 (100%)	0	100	100
3	c	169/175 (97%)	169 (100%)	0	100	100
4	d	172/174 (99%)	172 (100%)	0	100	100
5	e	130/130 (100%)	130 (100%)	0	100	100
6	f	84/84 (100%)	84 (100%)	0	100	100
7	g	126/127 (99%)	126 (100%)	0	100	100
8	h	112/112 (100%)	112 (100%)	0	100	100
9	i	106/106 (100%)	106 (100%)	0	100	100
10	j	91/91 (100%)	91 (100%)	0	100	100
11	k	94/94 (100%)	94 (100%)	0	100	100
12	l	117/117 (100%)	117 (100%)	0	100	100
13	m	102/102 (100%)	102 (100%)	0	100	100
14	n	52/52 (100%)	52 (100%)	0	100	100
15	o	80/80 (100%)	80 (100%)	0	100	100
16	p	76/76 (100%)	76 (100%)	0	100	100
17	q	81/81 (100%)	81 (100%)	0	100	100
18	r	63/63 (100%)	63 (100%)	0	100	100
19	s	73/73 (100%)	73 (100%)	0	100	100
20	t	67/67 (100%)	67 (100%)	0	100	100
23	D	222/222 (100%)	222 (100%)	0	100	100
24	E	175/175 (100%)	175 (100%)	0	100	100
25	F	163/163 (100%)	163 (100%)	0	100	100
26	G	147/147 (100%)	147 (100%)	0	100	100
27	H	144/144 (100%)	144 (100%)	0	100	100
28	M	123/123 (100%)	123 (100%)	0	100	100
29	N	100/100 (100%)	100 (100%)	0	100	100
30	O	104/104 (100%)	104 (100%)	0	100	100
31	P	116/116 (100%)	116 (100%)	0	100	100
32	Q	100/100 (100%)	100 (100%)	0	100	100
33	R	95/95 (100%)	95 (100%)	0	100	100
34	S	96/96 (100%)	96 (100%)	0	100	100
35	T	96/96 (100%)	96 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
36	U	86/86 (100%)	86 (100%)	0	100	100
37	V	91/91 (100%)	91 (100%)	0	100	100
38	W	80/80 (100%)	80 (100%)	0	100	100
39	X	73/85 (86%)	73 (100%)	0	100	100
40	Y	83/83 (100%)	83 (100%)	0	100	100
41	Z	64/64 (100%)	64 (100%)	0	100	100
42	0	39/39 (100%)	39 (100%)	0	100	100
43	1	59/59 (100%)	59 (100%)	0	100	100
44	2	51/51 (100%)	51 (100%)	0	100	100
45	3	74/75 (99%)	65 (88%)	9 (12%)	5	21
46	4	49/49 (100%)	49 (100%)	0	100	100
47	5	26/37 (70%)	26 (100%)	0	100	100
48	6	39/39 (100%)	39 (100%)	0	100	100
49	7	52/52 (100%)	52 (100%)	0	100	100
50	8	35/35 (100%)	35 (100%)	0	100	100
All	All	4571/4631 (99%)	4562 (100%)	9 (0%)	85	87

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
45	3	70	ARG
45	3	73	ARG
45	3	75	ASN
45	3	76	LYS
45	3	77	LYS
45	3	80	LEU
45	3	81	LYS
45	3	82	SER
45	3	83	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
2	b	15	HIS
3	c	3	GLN
4	d	50	GLN

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Mol	Chain	Res	Type
4	d	85	ASN
7	g	129	ASN
9	i	16	ASN
9	i	77	GLN
12	l	42	GLN
20	t	47	ASN
23	D	133	ASN
24	E	182	ASN
25	F	148	GLN
27	H	45	GLN
28	M	41	ASN
35	T	52	GLN
36	U	81	ASN
37	V	97	ASN
39	X	39	ASN
40	Y	38	ASN
44	2	32	ASN
44	2	40	ASN
45	3	10	HIS
45	3	75	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	a	1546/1547 (99%)	268 (17%)	0
21	A	2910/2918 (99%)	631 (21%)	8 (0%)
22	B	113/114 (99%)	18 (15%)	0
All	All	4569/4579 (99%)	917 (20%)	8 (0%)

All (917) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	a	10	G
1	a	11	A
1	a	16	G
1	a	23	G
1	a	31	U
1	a	32	G
1	a	33	A
1	a	34	A
1	a	40	G

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Mol	Chain	Res	Type
1	a	42	G
1	a	48	C
1	a	49	C
1	a	51	A
1	a	52	A
1	a	62	G
1	a	74	G
1	a	82	G
1	a	85	U
1	a	87	C
1	a	88	U
1	a	89	U
1	a	92	C
1	a	107	G
1	a	108	A
1	a	115	A
1	a	120	C
1	a	129	A
1	a	130	A
1	a	131	C
1	a	144	C
1	a	151	A
1	a	156	C
1	a	159	G
1	a	163	C
1	a	182	A
1	a	183	U
1	a	185	U
1	a	196	A
1	a	198	G
1	a	206	A
1	a	211	A
1	a	212	A
1	a	213	G
1	a	219	C
1	a	221	U
1	a	234	A
1	a	248	U
1	a	249	G
1	a	252	U
1	a	255	G
1	a	259	G

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Mol	Chain	Res	Type
1	a	260	U
1	a	274	G
1	a	275	C
1	a	286	A
1	a	287	A
1	a	294	A
1	a	297	G
1	a	307	G
1	a	315	U
1	a	324	C
1	a	336	C
1	a	337	A
1	a	355	G
1	a	360	C
1	a	362	G
1	a	374	C
1	a	375	U
1	a	376	U
1	a	380	C
1	a	385	G
1	a	390	A
1	a	396	G
1	a	401	A
1	a	405	A
1	a	414	G
1	a	418	G
1	a	419	A
1	a	420	U
1	a	421	G
1	a	422	A
1	a	429	U
1	a	432	G
1	a	437	U
1	a	449	A
1	a	456	A
1	a	457	A
1	a	462	A
1	a	466	G
1	a	471	A
1	a	477	U
1	a	481	C
1	a	482	A

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Mol	Chain	Res	Type
1	a	483	C
1	a	492	G
1	a	493	G
1	a	499	A
1	a	505	A
1	a	517	A
1	a	519	C
1	a	528	A
1	a	529	G
1	a	532	G
1	a	535	G
1	a	538	G
1	a	539	U
1	a	540	A
1	a	554	A
1	a	555	A
1	a	557	C
1	a	570	U
1	a	571	A
1	a	580	A
1	a	584	C
1	a	585	G
1	a	587	G
1	a	589	G
1	a	595	G
1	a	604	A
1	a	641	U
1	a	650	A
1	a	661	U
1	a	666	G
1	a	673	A
1	a	674	G
1	a	695	A
1	a	703	A
1	a	710	A
1	a	729	A
1	a	741	G
1	a	742	A
1	a	757	A
1	a	759	U
1	a	763	G
1	a	769	G

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Mol	Chain	Res	Type
1	a	782	G
1	a	785	A
1	a	802	A
1	a	803	C
1	a	807	G
1	a	821	U
1	a	825	C
1	a	826	G
1	a	829	G
1	a	836	A
1	a	840	G
1	a	854	C
1	a	855	G
1	a	861	U
1	a	863	G
1	a	865	G
1	a	879	A
1	a	882	A
1	a	886	A
1	a	899	A
1	a	924	A
1	a	936	G
1	a	944	C
1	a	945	A
1	a	947	A
1	a	970	U
1	a	979	A
1	a	981	G
1	a	984	A
1	a	985	A
1	a	986	G
1	a	992	U
1	a	993	A
1	a	999	U
1	a	1002	U
1	a	1003	G
1	a	1012	U
1	a	1014	A
1	a	1016	A
1	a	1025	G
1	a	1027	U
1	a	1028	A

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Mol	Chain	Res	Type
1	a	1034	U
1	a	1035	U
1	a	1036	C
1	a	1037	C
1	a	1038	C
1	a	1039	C
1	a	1041	U
1	a	1044	G
1	a	1051	A
1	a	1057	C
1	a	1076	G
1	a	1077	U
1	a	1106	G
1	a	1107	U
1	a	1113	A
1	a	1124	C
1	a	1138	U
1	a	1144	C
1	a	1150	G
1	a	1151	U
1	a	1152	U
1	a	1153	G
1	a	1163	A
1	a	1165	U
1	a	1170	U
1	a	1171	G
1	a	1172	C
1	a	1179	C
1	a	1192	G
1	a	1195	G
1	a	1202	A
1	a	1207	A
1	a	1208	A
1	a	1223	U
1	a	1225	U
1	a	1235	U
1	a	1238	A
1	a	1239	C
1	a	1250	A
1	a	1252	G
1	a	1261	A
1	a	1268	A

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Mol	Chain	Res	Type
1	a	1271	G
1	a	1289	A
1	a	1291	A
1	a	1297	U
1	a	1298	A
1	a	1304	G
1	a	1310	A
1	a	1312	U
1	a	1313	U
1	a	1328	C
1	a	1329	A
1	a	1331	C
1	a	1333	C
1	a	1334	G
1	a	1347	U
1	a	1351	A
1	a	1357	A
1	a	1358	G
1	a	1359	U
1	a	1375	U
1	a	1381	G
1	a	1386	A
1	a	1389	C
1	a	1409	A
1	a	1411	C
1	a	1412	G
1	a	1430	G
1	a	1437	A
1	a	1453	G
1	a	1454	A
1	a	1457	A
1	a	1463	U
1	a	1492	A
1	a	1496	U
1	a	1515	A
1	a	1518	U
1	a	1519	A
1	a	1520	G
1	a	1529	G
1	a	1531	A
1	a	1532	G
1	a	1540	U

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Mol	Chain	Res	Type
1	a	1541	G
1	a	1542	G
1	a	1543	A
1	a	1545	C
1	a	1546	A
1	a	1547	C
1	a	1549	U
21	A	14	A
21	A	28	A
21	A	34	U
21	A	52	A
21	A	64	A
21	A	71	A
21	A	74	U
21	A	75	G
21	A	80	G
21	A	84	A
21	A	85	G
21	A	90	A
21	A	96	G
21	A	98	U
21	A	102	A
21	A	104	C
21	A	113	U
21	A	117	A
21	A	118	A
21	A	119	U
21	A	124	A
21	A	130	A
21	A	133	A
21	A	142	G
21	A	145	A
21	A	150	A
21	A	154	A
21	A	157	U
21	A	160	G
21	A	161	A
21	A	162	A
21	A	163	U
21	A	165	C
21	A	167	U
21	A	168	A

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Mol	Chain	Res	Type
21	A	169	G
21	A	184	C
21	A	199	A
21	A	200	A
21	A	202	A
21	A	207	A
21	A	218	G
21	A	219	A
21	A	225	A
21	A	227	G
21	A	229	A
21	A	235	G
21	A	236	A
21	A	244	A
21	A	251	G
21	A	253	G
21	A	255	G
21	A	272	C
21	A	284	C
21	A	285	U
21	A	286	U
21	A	288	C
21	A	289	U
21	A	295	G
21	A	298	U
21	A	300	G
21	A	301	U
21	A	314	A
21	A	315	C
21	A	316	G
21	A	317	G
21	A	319	G
21	A	320	U
21	A	321	U
21	A	322	A
21	A	326	A
21	A	331	G
21	A	338	G
21	A	351	G
21	A	354	A
21	A	358	G
21	A	365	A

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Mol	Chain	Res	Type
21	A	367	A
21	A	372	A
21	A	373	A
21	A	374	U
21	A	378	C
21	A	381	G
21	A	389	A
21	A	398	C
21	A	401	U
21	A	403	U
21	A	404	U
21	A	410	G
21	A	411	A
21	A	413	C
21	A	418	G
21	A	430	A
21	A	432	G
21	A	457	G
21	A	459	C
21	A	466	C
21	A	494	U
21	A	497	U
21	A	502	C
21	A	503	A
21	A	511	G
21	A	513	G
21	A	525	A
21	A	526	A
21	A	527	G
21	A	544	U
21	A	550	A
21	A	553	A
21	A	554	C
21	A	555	C
21	A	572	C
21	A	574	A
21	A	575	G
21	A	576	U
21	A	577	A
21	A	578	G
21	A	591	A
21	A	593	U

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Mol	Chain	Res	Type
21	A	594	G
21	A	606	G
21	A	611	U
21	A	613	G
21	A	614	U
21	A	615	A
21	A	618	A
21	A	646	A
21	A	658	A
21	A	659	A
21	A	660	A
21	A	661	U
21	A	662	G
21	A	666	A
21	A	682	A
21	A	683	G
21	A	690	U
21	A	693	G
21	A	694	G
21	A	698	U
21	A	699	U
21	A	715	A
21	A	716	C
21	A	722	A
21	A	727	G
21	A	731	U
21	A	732	C
21	A	744	A
21	A	756	A
21	A	769	U
21	A	774	G
21	A	775	A
21	A	784	A
21	A	785	C
21	A	792	U
21	A	793	G
21	A	794	A
21	A	798	G
21	A	809	A
21	A	813	G
21	A	820	G
21	A	821	C

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Mol	Chain	Res	Type
21	A	825	G
21	A	827	A
21	A	828	A
21	A	829	U
21	A	834	A
21	A	838	A
21	A	845	A
21	A	846	G
21	A	849	A
21	A	850	G
21	A	872	U
21	A	873	U
21	A	875	G
21	A	881	G
21	A	902	A
21	A	904	G
21	A	911	A
21	A	921	C
21	A	922	G
21	A	923	A
21	A	924	G
21	A	925	G
21	A	927	G
21	A	932	U
21	A	938	G
21	A	952	A
21	A	955	A
21	A	957	C
21	A	958	U
21	A	959	C
21	A	960	C
21	A	970	U
21	A	985	A
21	A	989	A
21	A	990	G
21	A	1005	G
21	A	1017	A
21	A	1018	A
21	A	1029	C
21	A	1034	A
21	A	1040	A
21	A	1049	C

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Mol	Chain	Res	Type
21	A	1055	A
21	A	1056	U
21	A	1057	A
21	A	1061	G
21	A	1066	G
21	A	1067	U
21	A	1069	G
21	A	1070	A
21	A	1073	A
21	A	1077	U
21	A	1078	G
21	A	1085	U
21	A	1089	C
21	A	1090	A
21	A	1091	G
21	A	1100	G
21	A	1101	A
21	A	1102	U
21	A	1105	U
21	A	1106	G
21	A	1109	U
21	A	1111	A
21	A	1113	A
21	A	1114	A
21	A	1115	G
21	A	1116	C
21	A	1119	C
21	A	1120	C
21	A	1124	A
21	A	1126	U
21	A	1127	U
21	A	1128	A
21	A	1132	A
21	A	1133	G
21	A	1137	G
21	A	1138	U
21	A	1139	A
21	A	1143	G
21	A	1145	U
21	A	1146	C
21	A	1150	A
21	A	1154	G

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Mol	Chain	Res	Type
21	A	1155	A
21	A	1156	G
21	A	1158	G
21	A	1163	U
21	A	1170	A
21	A	1171	A
21	A	1172	A
21	A	1174	U
21	A	1175	G
21	A	1177	A
21	A	1178	C
21	A	1179	C
21	A	1183	G
21	A	1184	C
21	A	1186	A
21	A	1195	A
21	A	1214	C
21	A	1218	G
21	A	1248	U
21	A	1250	G
21	A	1258	A
21	A	1265	G
21	A	1273	G
21	A	1276	G
21	A	1277	C
21	A	1278	G
21	A	1285	A
21	A	1286	G
21	A	1288	G
21	A	1289	A
21	A	1291	A
21	A	1292	A
21	A	1293	U
21	A	1294	G
21	A	1303	A
21	A	1306	C
21	A	1309	G
21	A	1310	A
21	A	1337	A
21	A	1338	U
21	A	1355	A
21	A	1362	C

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Mol	Chain	Res	Type
21	A	1376	G
21	A	1378	U
21	A	1379	A
21	A	1383	G
21	A	1403	C
21	A	1405	G
21	A	1416	U
21	A	1421	A
21	A	1423	C
21	A	1437	U
21	A	1449	A
21	A	1450	A
21	A	1451	U
21	A	1454	U
21	A	1455	U
21	A	1459	A
21	A	1463	A
21	A	1464	U
21	A	1471	A
21	A	1472	C
21	A	1489	A
21	A	1490	G
21	A	1491	C
21	A	1494	G
21	A	1495	C
21	A	1496	G
21	A	1497	A
21	A	1498	U
21	A	1499	U
21	A	1504	U
21	A	1505	G
21	A	1506	C
21	A	1510	U
21	A	1512	U
21	A	1516	C
21	A	1519	U
21	A	1520	A
21	A	1521	A
21	A	1525	U
21	A	1527	A
21	A	1534	G
21	A	1536	C

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Mol	Chain	Res	Type
21	A	1537	A
21	A	1540	U
21	A	1551	U
21	A	1552	U
21	A	1553	A
21	A	1555	G
21	A	1561	G
21	A	1567	A
21	A	1568	U
21	A	1569	G
21	A	1570	G
21	A	1571	G
21	A	1576	A
21	A	1577	G
21	A	1579	C
21	A	1580	A
21	A	1582	U
21	A	1583	G
21	A	1584	A
21	A	1585	G
21	A	1586	U
21	A	1587	C
21	A	1605	A
21	A	1606	C
21	A	1613	G
21	A	1614	A
21	A	1616	A
21	A	1621	C
21	A	1625	U
21	A	1629	U
21	A	1631	G
21	A	1632	A
21	A	1633	A
21	A	1636	U
21	A	1651	C
21	A	1652	A
21	A	1655	C
21	A	1659	C
21	A	1660	A
21	A	1662	A
21	A	1678	A
21	A	1684	A

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Mol	Chain	Res	Type
21	A	1690	A
21	A	1691	G
21	A	1692	C
21	A	1704	C
21	A	1709	A
21	A	1716	C
21	A	1717	G
21	A	1718	G
21	A	1737	U
21	A	1738	C
21	A	1739	G
21	A	1740	G
21	A	1742	A
21	A	1746	G
21	A	1759	G
21	A	1768	C
21	A	1772	G
21	A	1775	G
21	A	1777	G
21	A	1782	A
21	A	1783	G
21	A	1785	G
21	A	1790	G
21	A	1791	G
21	A	1800	A
21	A	1801	C
21	A	1808	U
21	A	1811	A
21	A	1818	A
21	A	1826	G
21	A	1827	C
21	A	1828	U
21	A	1829	A
21	A	1833	C
21	A	1835	U
21	A	1843	U
21	A	1844	G
21	A	1846	A
21	A	1855	G
21	A	1856	A
21	A	1861	U
21	A	1862	G

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Mol	Chain	Res	Type
21	A	1865	C
21	A	1893	A
21	A	1895	C
21	A	1897	U
21	A	1899	U
21	A	1926	A
21	A	1928	A
21	A	1933	G
21	A	1939	A
21	A	1950	U
21	A	1956	G
21	A	1957	G
21	A	1958	U
21	A	1963	A
21	A	1964	A
21	A	1965	A
21	A	1968	C
21	A	1969	C
21	A	1970	U
21	A	1972	G
21	A	1982	U
21	A	1983	U
21	A	1989	C
21	A	1994	C
21	A	1997	A
21	A	1998	A
21	A	1999	G
21	A	2002	G
21	A	2008	A
21	A	2018	U
21	A	2020	U
21	A	2048	G
21	A	2050	A
21	A	2057	A
21	A	2058	A
21	A	2059	G
21	A	2060	A
21	A	2061	U
21	A	2070	C
21	A	2079	G
21	A	2082	C
21	A	2083	G

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Mol	Chain	Res	Type
21	A	2087	A
21	A	2088	G
21	A	2096	G
21	A	2119	U
21	A	2120	G
21	A	2127	G
21	A	2139	A
21	A	2140	C
21	A	2143	G
21	A	2145	U
21	A	2147	G
21	A	2155	C
21	A	2160	G
21	A	2161	A
21	A	2162	A
21	A	2165	G
21	A	2172	C
21	A	2173	U
21	A	2174	A
21	A	2175	G
21	A	2185	A
21	A	2186	G
21	A	2188	C
21	A	2194	U
21	A	2195	G
21	A	2198	A
21	A	2208	A
21	A	2212	G
21	A	2217	G
21	A	2226	A
21	A	2230	G
21	A	2231	C
21	A	2238	U
21	A	2240	U
21	A	2241	C
21	A	2252	A
21	A	2265	G
21	A	2266	G
21	A	2275	C
21	A	2278	G
21	A	2290	C
21	A	2293	A

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Mol	Chain	Res	Type
21	A	2294	A
21	A	2295	A
21	A	2305	A
21	A	2306	G
21	A	2310	C
21	A	2314	A
21	A	2333	U
21	A	2334	G
21	A	2335	G
21	A	2337	A
21	A	2339	U
21	A	2342	U
21	A	2346	U
21	A	2347	A
21	A	2348	G
21	A	2349	A
21	A	2352	G
21	A	2353	U
21	A	2354	A
21	A	2358	G
21	A	2361	U
21	A	2362	A
21	A	2363	A
21	A	2372	G
21	A	2374	C
21	A	2377	C
21	A	2410	G
21	A	2412	C
21	A	2415	A
21	A	2419	A
21	A	2429	U
21	A	2430	C
21	A	2433	C
21	A	2449	C
21	A	2450	U
21	A	2452	A
21	A	2456	G
21	A	2457	A
21	A	2458	U
21	A	2462	A
21	A	2467	C
21	A	2468	C

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Mol	Chain	Res	Type
21	A	2472	G
21	A	2475	A
21	A	2492	C
21	A	2497	G
21	A	2505	A
21	A	2518	U
21	A	2521	G
21	A	2525	C
21	A	2526	C
21	A	2529	G
21	A	2530	A
21	A	2532	G
21	A	2533	U
21	A	2540	A
21	A	2545	A
21	A	2549	U
21	A	2552	G
21	A	2560	U
21	A	2561	C
21	A	2562	G
21	A	2576	G
21	A	2579	U
21	A	2582	U
21	A	2583	C
21	A	2589	U
21	A	2593	A
21	A	2594	G
21	A	2599	A
21	A	2600	C
21	A	2601	G
21	A	2605	G
21	A	2609	G
21	A	2612	U
21	A	2613	C
21	A	2624	G
21	A	2629	A
21	A	2630	G
21	A	2636	U
21	A	2638	C
21	A	2640	U
21	A	2648	G
21	A	2657	G

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Mol	Chain	Res	Type
21	A	2661	A
21	A	2666	A
21	A	2683	U
21	A	2690	G
21	A	2708	C
21	A	2709	U
21	A	2716	U
21	A	2717	A
21	A	2741	G
21	A	2753	U
21	A	2756	G
21	A	2760	A
21	A	2766	U
21	A	2767	A
21	A	2771	G
21	A	2783	U
21	A	2784	A
21	A	2785	A
21	A	2788	A
21	A	2791	A
21	A	2792	A
21	A	2793	G
21	A	2803	A
21	A	2804	G
21	A	2805	A
21	A	2806	U
21	A	2807	G
21	A	2817	A
21	A	2820	U
21	A	2821	U
21	A	2824	G
21	A	2827	A
21	A	2838	C
21	A	2845	G
21	A	2846	A
21	A	2850	G
21	A	2853	U
21	A	2855	A
21	A	2856	U
21	A	2869	G
21	A	2882	A
21	A	2887	G

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Mol	Chain	Res	Type
21	A	2892	G
21	A	2899	A
21	A	2900	C
21	A	2903	A
21	A	2905	C
21	A	2906	G
21	A	2913	G
21	A	2917	U
22	B	2	C
22	B	10	U
22	B	12	U
22	B	23	U
22	B	24	C
22	B	27	A
22	B	30	U
22	B	33	U
22	B	39	G
22	B	40	C
22	B	42	G
22	B	43	A
22	B	49	G
22	B	73	G
22	B	87	G
22	B	88	U
22	B	106	U
22	B	108	G

All (8) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
21	A	160	G
21	A	199	A
21	A	377	U
21	A	661	U
21	A	1127	U
21	A	1938	U
21	A	1962	G
21	A	2230	G

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 41 ligands modelled in this entry, 41 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

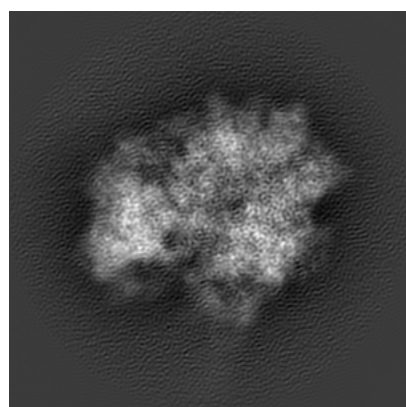
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-4050. These allow visual inspection of the internal detail of the map and identification of artifacts.

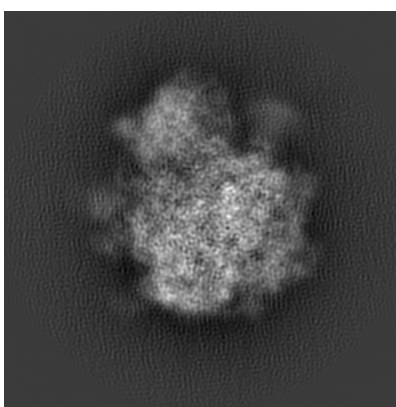
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

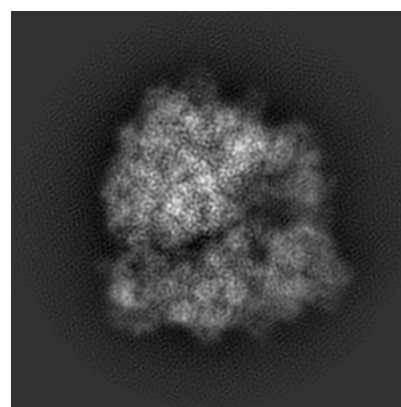
6.1.1 Primary map



X



Y

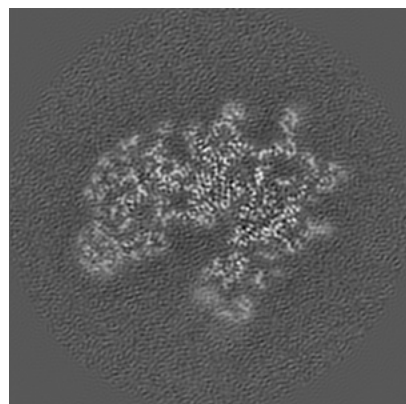


Z

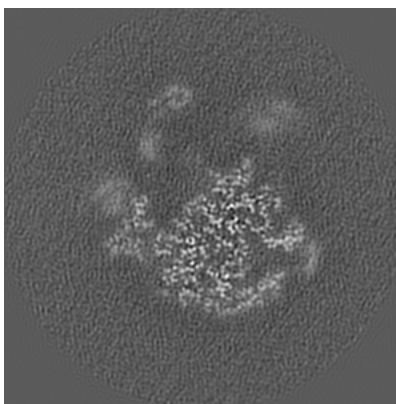
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

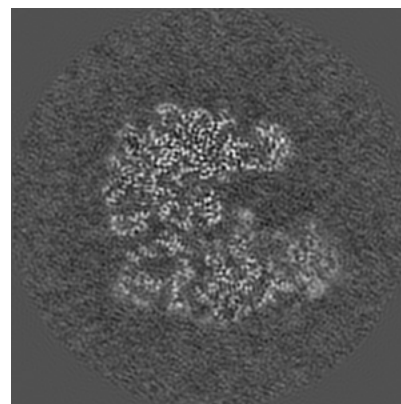
6.2.1 Primary map



X Index: 166



Y Index: 166

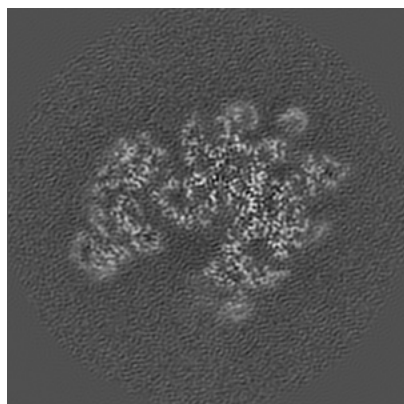


Z Index: 166

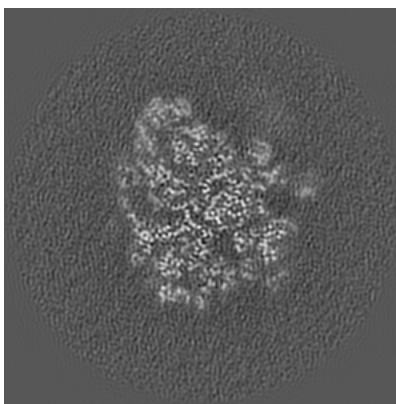
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

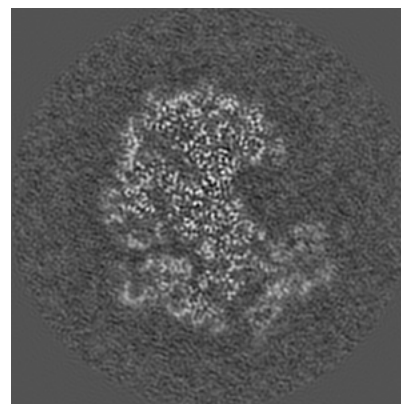
6.3.1 Primary map



X Index: 160



Y Index: 211

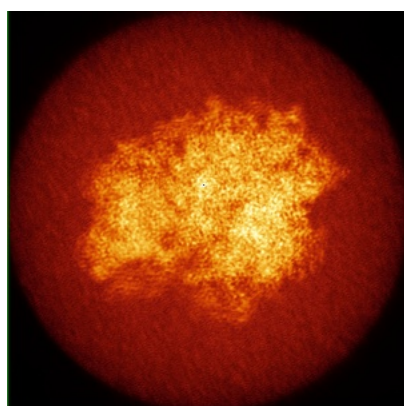


Z Index: 182

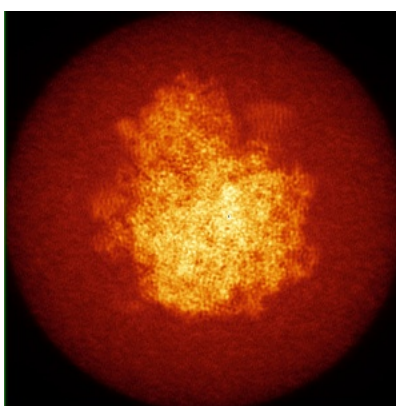
The images above show the largest variance slices of the map in three orthogonal directions.

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

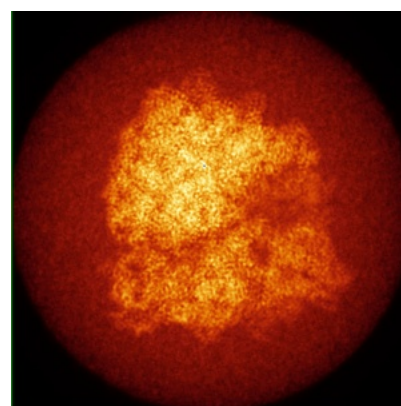
6.4.1 Primary map



X



Y

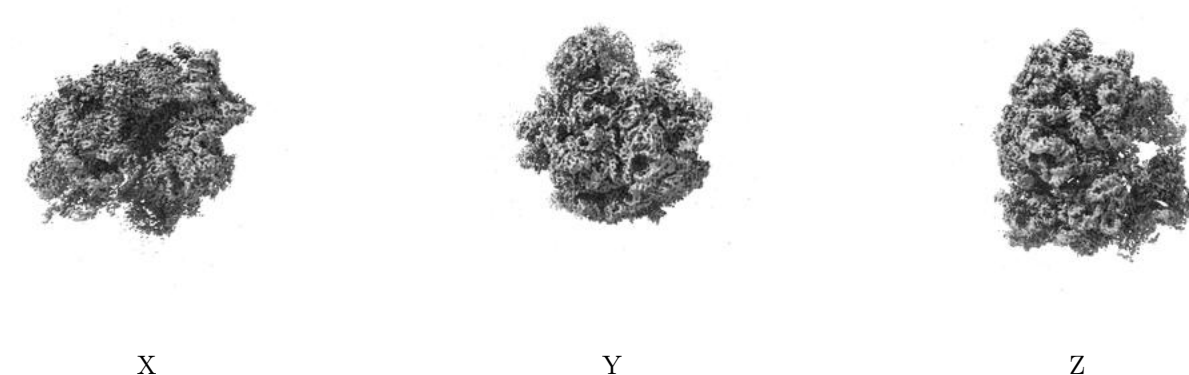


Z

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

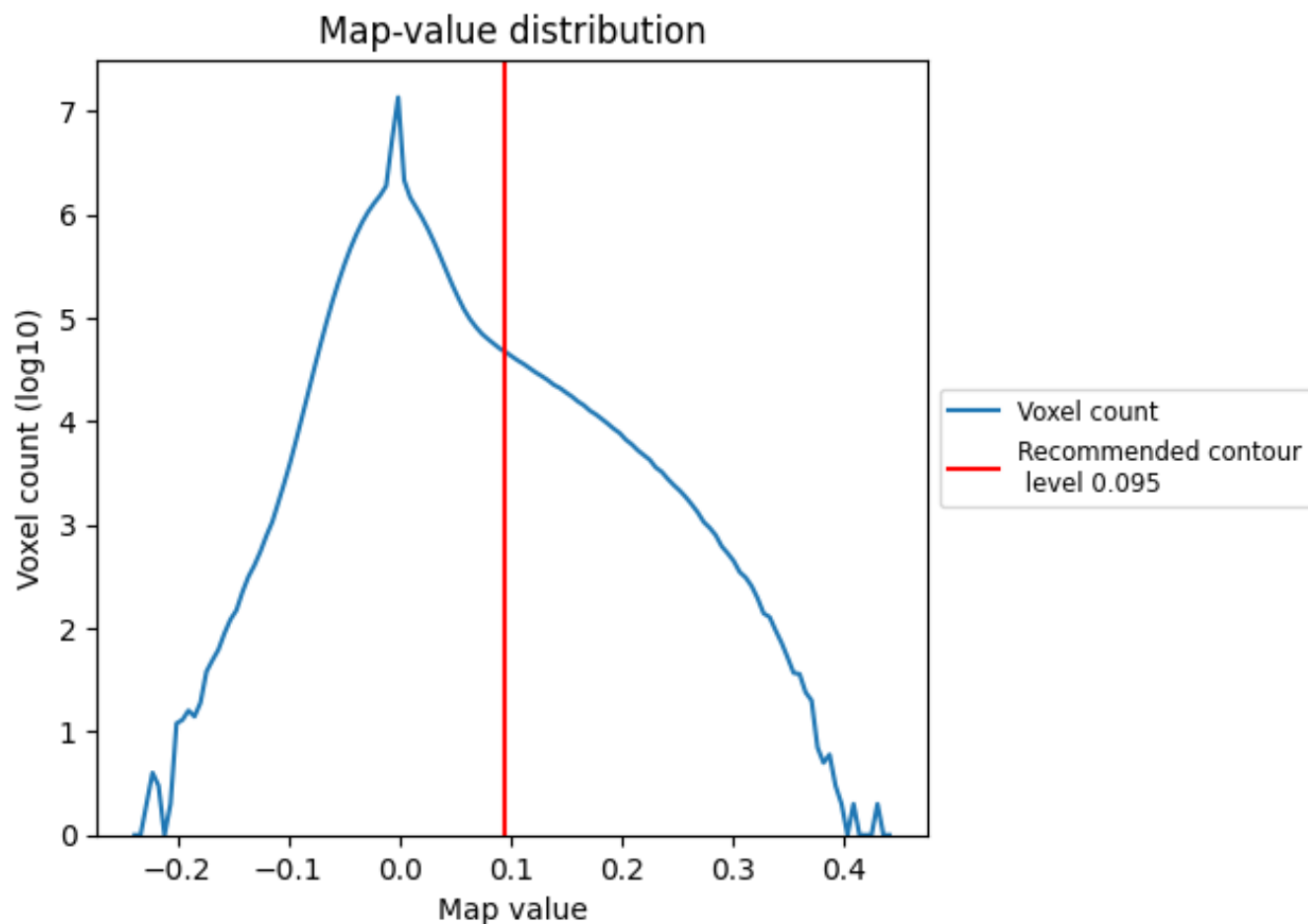
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

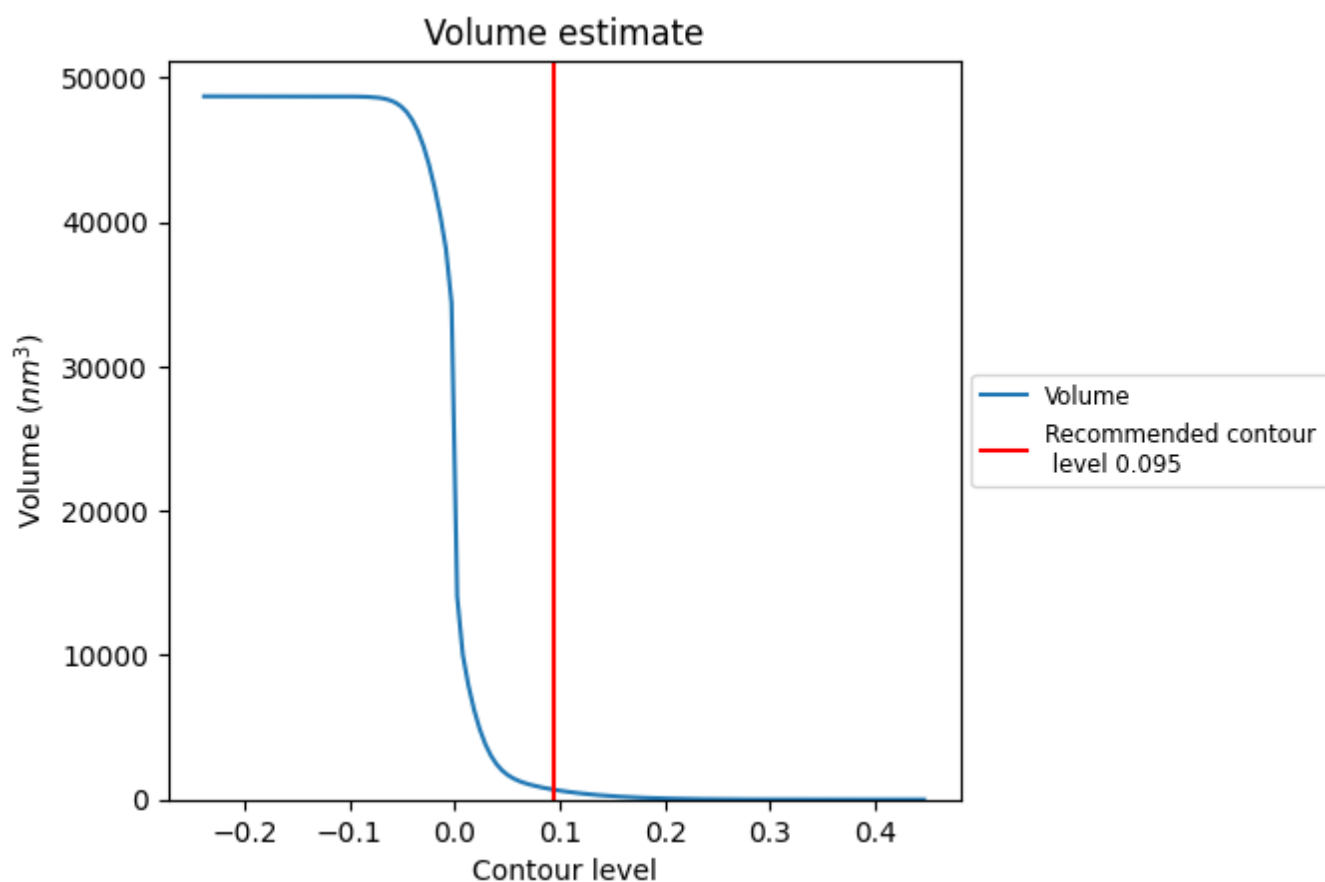
This section contains the results of statistical analysis of the map.

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.

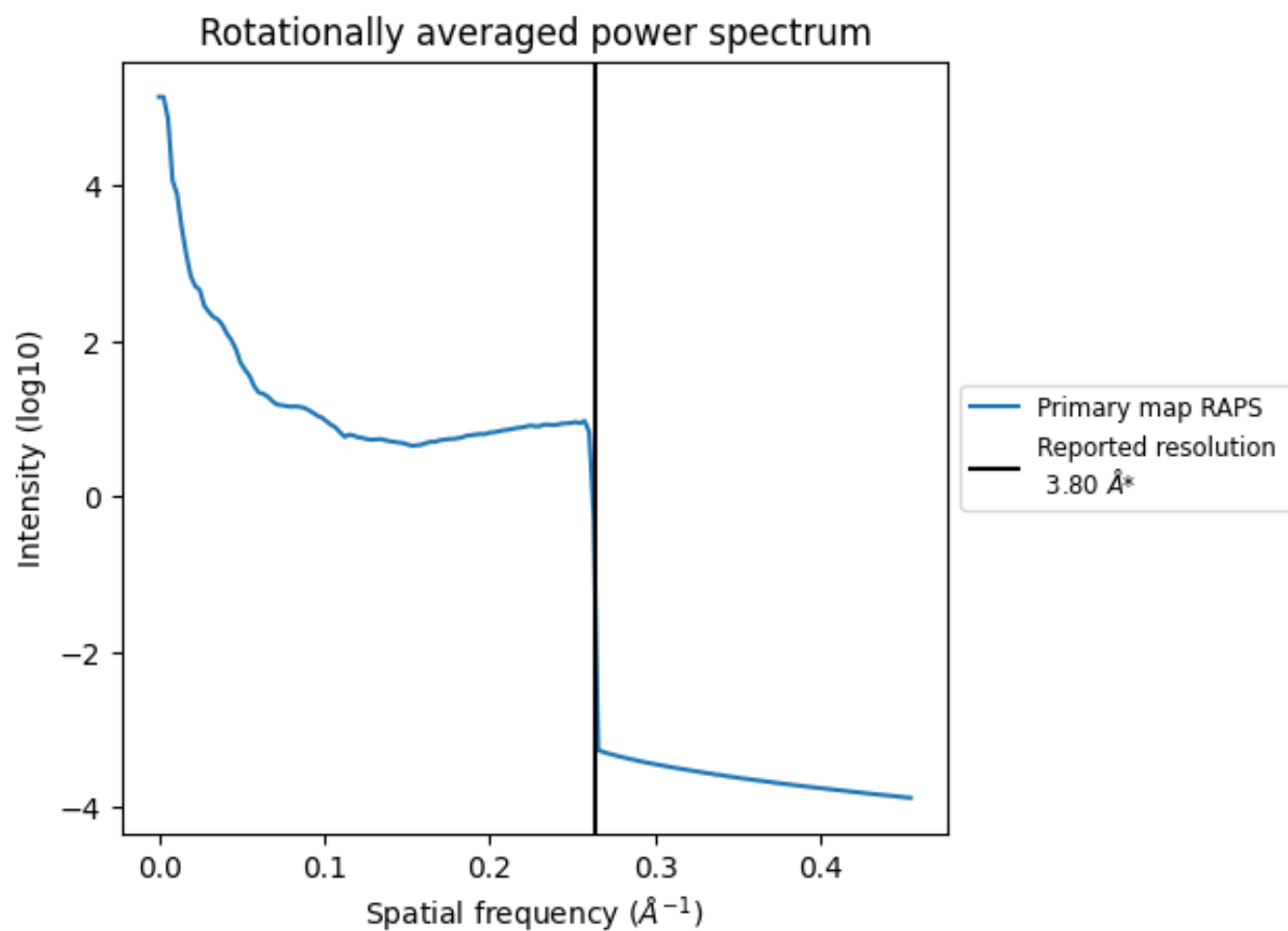
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 679 nm³; this corresponds to an approximate mass of 613 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 0.263 Å⁻¹

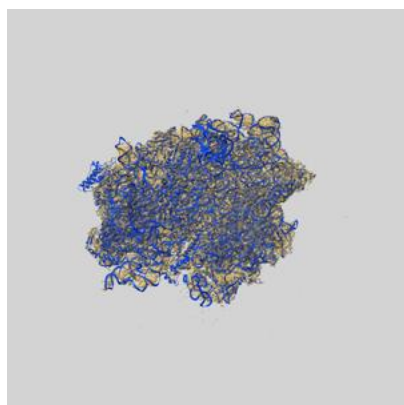
8 Fourier-Shell correlation

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

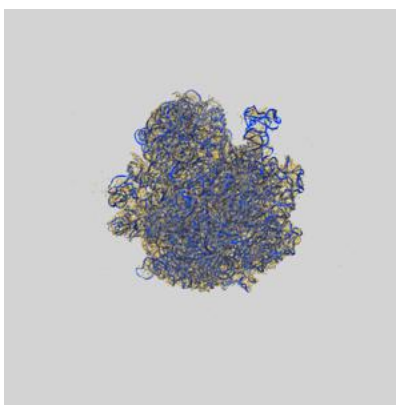
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-4050 and PDB model 5LI0. Per-residue inclusion information can be found in [section 3](#) on [page 13](#).

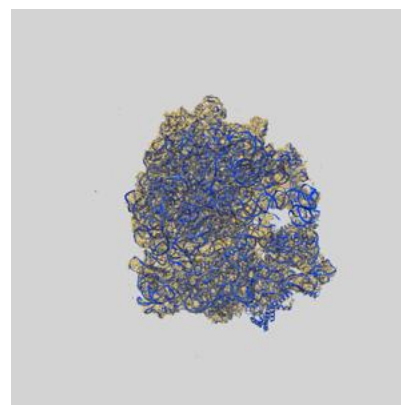
9.1 Map-model overlay [i](#)



X



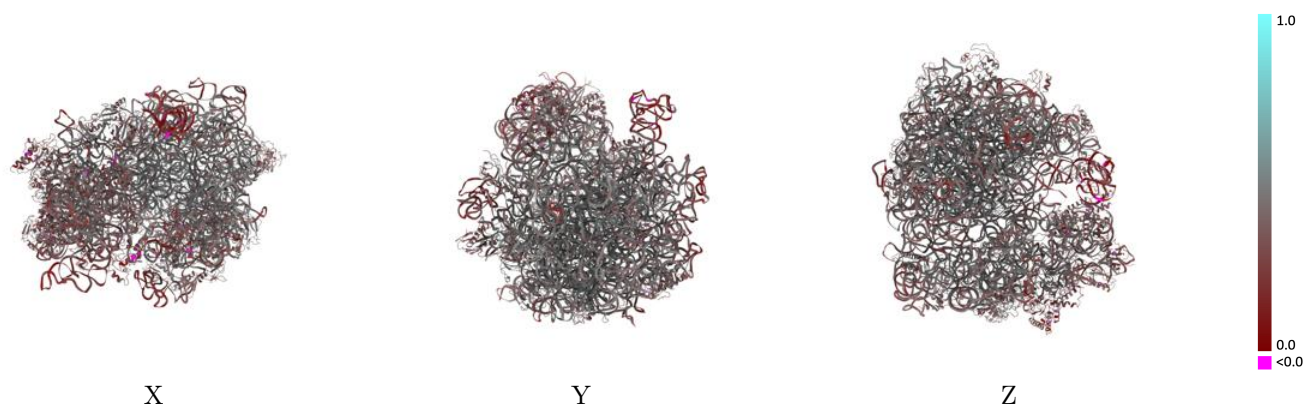
Y



Z

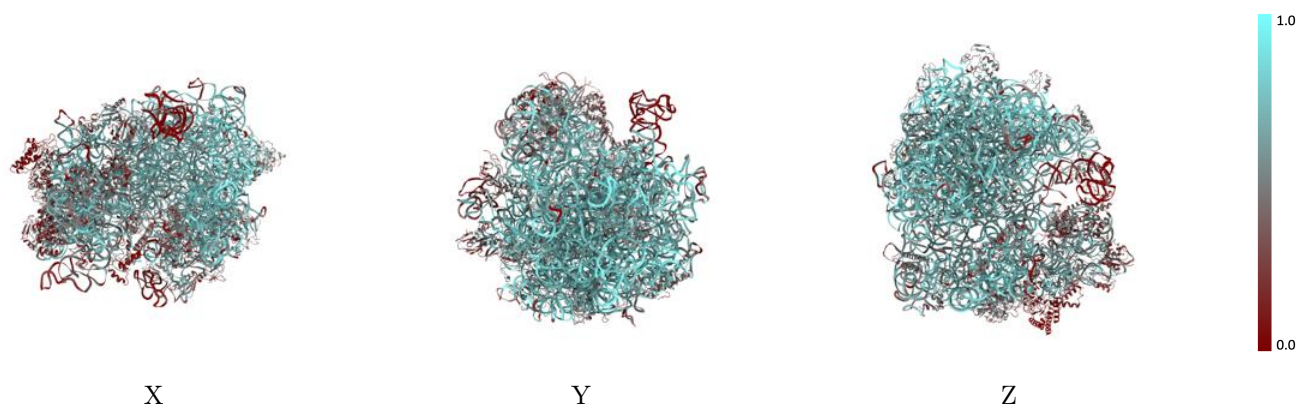
The images above show the 3D surface view of the map at the recommended contour level 0.095 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



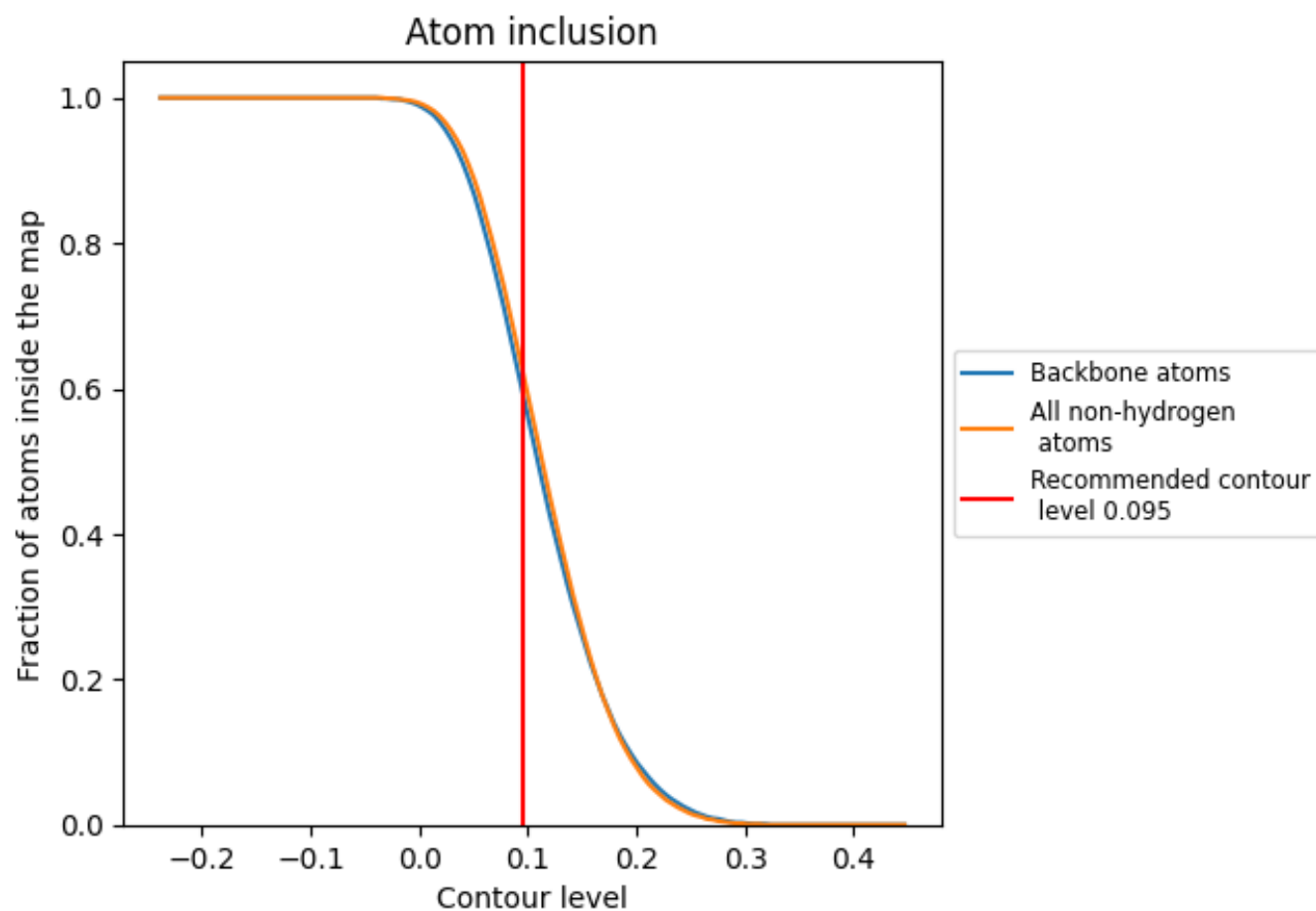
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.095).

9.4 Atom inclusion [i](#)



At the recommended contour level, 60% of all backbone atoms, 62% 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 (0.095) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6250	 0.4050
0	 0.5530	 0.4180
1	 0.4760	 0.3730
2	 0.5620	 0.4520
3	 0.1620	 0.2260
4	 0.5120	 0.4080
5	 0.5400	 0.3790
6	 0.6360	 0.4550
7	 0.5960	 0.4100
8	 0.5410	 0.4420
A	 0.7330	 0.4210
B	 0.7020	 0.3920
D	 0.5940	 0.4630
E	 0.5800	 0.4540
F	 0.5460	 0.4160
G	 0.3280	 0.2920
H	 0.3770	 0.3630
M	 0.5770	 0.4480
N	 0.5320	 0.4600
O	 0.5480	 0.3990
P	 0.5060	 0.4150
Q	 0.5530	 0.4200
R	 0.4380	 0.3590
S	 0.5140	 0.4400
T	 0.6200	 0.4490
U	 0.5310	 0.4440
V	 0.5530	 0.4480
W	 0.4940	 0.4010
X	 0.4470	 0.3890
Y	 0.3560	 0.3870
Z	 0.5620	 0.4420
a	 0.6680	 0.3980
b	 0.1340	 0.3060
c	 0.3010	 0.3470
d	 0.3810	 0.3530



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Chain	Atom inclusion	Q-score
e	 0.4330	 0.4010
f	 0.4370	 0.3970
g	 0.2690	 0.3330
h	 0.4750	 0.4040
i	 0.2770	 0.3380
j	 0.2590	 0.3530
k	 0.3670	 0.3690
l	 0.4060	 0.3860
m	 0.2050	 0.2880
n	 0.3530	 0.3370
o	 0.5110	 0.3950
p	 0.4600	 0.3860
q	 0.4350	 0.4070
r	 0.3660	 0.3720
s	 0.1890	 0.2760
t	 0.4370	 0.3600