



Full wwPDB EM Validation Report ⓘ

Jul 3, 2025 – 08:43 AM EDT

PDB ID : 8UXB / pdb_00008uxb
EMDB ID : EMD-42721
Title : E. coli 70S ribosome with unmodified P/E-tRNA^{Pro}(GGG) bound to slippery
P-site CCC-C codon
Authors : Kimbrough, E.M.; Dunham, C.M.; Nguyen, H.A.
Deposited on : 2023-11-09
Resolution : 2.90 Å(reported)

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev118
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0rc1
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.44

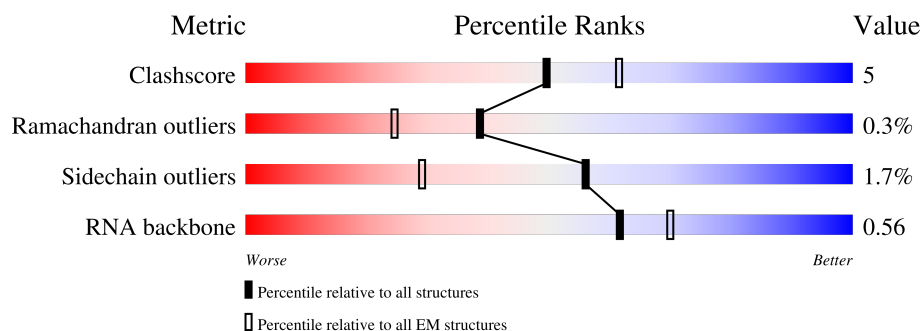
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.90 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415
RNA backbone	6643	2191

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

Mol	Chain	Length	Quality of chain
1	1	2904	<div> <div>9%</div> <div>68%</div> <div>25%</div> <div>6%</div> </div>
2	2	1540	<div> <div>13%</div> <div>69%</div> <div>26%</div> <div>5%</div> </div>
3	3	120	<div> <div>7%</div> <div>74%</div> <div>21%</div> <div>5%</div> </div>
4	4	18	<div> <div>22%</div> <div>17%</div> <div>33%</div> <div>50%</div> </div>
5	5	77	<div> <div>6%</div> <div>60%</div> <div>35%</div> <div>5%</div> </div>
6	B	273	<div> <div>83%</div> <div>15%</div> </div>
7	C	209	<div> <div>11%</div> <div>88%</div> <div>12%</div> </div>



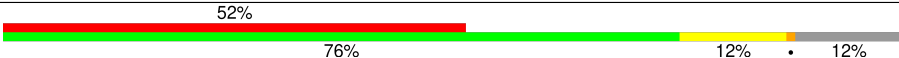

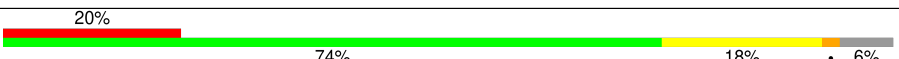
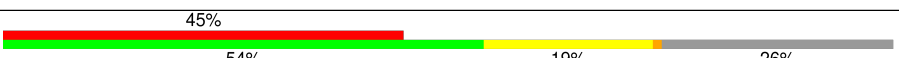

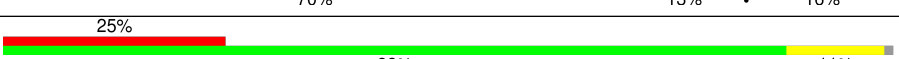










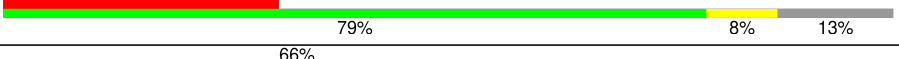


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Mol	Chain	Length	Quality of chain
8	D	201	
9	E	179	
10	F	177	
11	G	149	
12	J	142	
13	K	123	
14	L	144	
15	M	136	
16	N	127	
17	O	117	
18	P	115	
19	Q	118	
20	R	103	
21	S	110	
22	T	100	
23	U	104	
24	V	94	
25	W	84	
26	X	78	
27	Y	63	
28	Z	59	
29	b	57	
30	c	55	
31	d	46	
32	e	65	

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Mol	Chain	Length	Quality of chain
33	f	38	
34	g	241	
35	h	233	
36	i	206	
37	j	167	
38	k	135	
39	l	179	
40	m	130	
41	n	130	
42	o	103	
43	p	129	
44	q	124	
45	r	118	
46	s	102	
47	t	89	
48	u	82	
49	v	84	
50	w	75	
51	x	92	
52	y	87	
53	z	71	

2 Entry composition

There are 55 unique types of molecules in this entry. The entry contains 145220 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 23S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	1	2900	Total	C	N	O	P	0	0
			62262	27774	11460	20128	2900		

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
1	747	C	U	conflict	GB 1109114233
1	887	A	U	conflict	GB 1109114233
1	1847	G	A	conflict	GB 1109114233

- Molecule 2 is a RNA chain called 16S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	2	1539	Total	C	N	O	P	0	0
			33015	14725	6052	10699	1539		

- Molecule 3 is a RNA chain called 5S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	3	120	Total	C	N	O	P	0	0
			2572	1145	471	836	120		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
3	120	A	U	conflict	GB 1370526515

- Molecule 4 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	4	9	Total	C	N	O	P	0	0
			188	84	31	64	9		

- Molecule 5 is a RNA chain called tRNA^{Pro}L (GGG).

Mol	Chain	Residues	Atoms					AltConf	Trace
5	5	77	Total	C	N	O	P	0	0
			1648	733	297	541	77		

- Molecule 6 is a protein called 50S ribosomal protein L2.

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

- Molecule 7 is a protein called 50S ribosomal protein L3.

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

- Molecule 8 is a protein called 50S ribosomal protein L4.

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

- Molecule 9 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	E	177	Total	C	N	O	S	0	0
			1410	899	249	256	6		

- Molecule 10 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	F	176	Total	C	N	O	S	0	0
			1323	832	243	246	2		

- Molecule 11 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	G	149	Total	C	N	O	S	0	0
			1111	699	197	214	1		

- Molecule 12 is a protein called 50S ribosomal protein L13.

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

- Molecule 13 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	K	122	Total	C	N	O	S	0	0
			938	587	180	165	6		

- Molecule 14 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	L	143	Total	C	N	O	S	0	0
			1045	649	206	189	1		

- Molecule 15 is a protein called 50S ribosomal protein L16.

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

- Molecule 16 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	N	120	Total	C	N	O	S	0	0
			960	593	196	166	5		

- Molecule 17 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms				AltConf	Trace
17	O	116	Total	C	N	O	0	0
			892	552	178	162		

- Molecule 18 is a protein called 50S ribosomal protein L19.

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

- Molecule 19 is a protein called 50S ribosomal protein L20.

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

- Molecule 20 is a protein called 50S ribosomal protein L21.

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

- Molecule 21 is a protein called 50S ribosomal protein L22.

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

- Molecule 22 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	T	93	Total	C	N	O	S	0	0
			738	466	139	131	2		

- Molecule 23 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms				AltConf	Trace
23	U	102	Total	C	N	O	0	0
			779	492	146	141		

- Molecule 24 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	V	94	Total	C	N	O	S	0	0
			753	479	137	134	3		

- Molecule 25 is a protein called 50S ribosomal protein L27.

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

- Molecule 26 is a protein called 50S ribosomal protein L28.

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

- Molecule 27 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	Y	63	Total	C	N	O	S	0	0
			509	313	99	95	2		

- Molecule 28 is a protein called 50S ribosomal protein L30.

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

- Molecule 29 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	b	56	Total	C	N	O	S	0	0
			444	269	94	80	1		

- Molecule 30 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms				AltConf	Trace
30	c	50	Total	C	N	O	0	0
			409	263	75	71		

- Molecule 31 is a protein called 50S ribosomal protein L34.

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

- Molecule 32 is a protein called 50S ribosomal protein L35.

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

- Molecule 33 is a protein called 50S ribosomal protein L36.

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

- Molecule 34 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	g	218	Total	C	N	O	S	0	0
			1704	1081	305	311	7		

- Molecule 35 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	h	206	Total	C	N	O	S	0	0
			1624	1028	305	288	3		

- Molecule 36 is a protein called 30S ribosomal protein S4.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	i	205	Total	C	N	O	S	0	0
			1643	1026	315	298	4		

- Molecule 37 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	j	157	Total	C	N	O	S	0	0
			1141	709	218	208	6		

- Molecule 38 is a protein called 30S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	k	100	Total	C	N	O	S	0	0
			817	515	148	148	6		

- Molecule 39 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	l	151	Total	C	N	O	S	0	0
			1181	735	227	215	4		

- Molecule 40 is a protein called 30S ribosomal protein S8.

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

- Molecule 41 is a protein called 30S ribosomal protein S9.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	n	127	Total	C	N	O	S	0	0
			1022	634	206	179	3		

- Molecule 42 is a protein called 30S ribosomal protein S10.

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

- Molecule 43 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	p	116	Total	C	N	O	S	0	0
			869	535	173	158	3		

- Molecule 44 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	q	123	Total	C	N	O	S	0	0
			957	591	196	165	5		

- Molecule 45 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	r	114	Total	C	N	O	S	0	0
			883	546	178	156	3		

- Molecule 46 is a protein called 30S ribosomal protein S14.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	s	101	Total	C	N	O	S	0	0
			799	498	165	133	3		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
s	36	ALA	-	insertion	UNP C3SR07

- Molecule 47 is a protein called 30S ribosomal protein S15.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	t	88	Total	C	N	O	S	0	0
			714	439	144	130	1		

- Molecule 48 is a protein called 30S ribosomal protein S16.

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

- Molecule 49 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	v	80	Total	C	N	O	S	0	0
			648	411	121	113	3		

- Molecule 50 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms				AltConf	Trace
50	w	65	Total	C	N	O	0	0
			504	317	96	91		

- Molecule 51 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	x	79	Total	C	N	O	S	0	0
			637	408	120	107	2		

- Molecule 52 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	y	85	Total	C	N	O	S	0	0
			665	411	137	114	3		

- Molecule 53 is a protein called 30S ribosomal protein S21.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	z	65	Total	C	N	O	S	0	0
			495	307	100	87	1		

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

Mol	Chain	Residues	Atoms		AltConf
54	1	203	Total	Mg	0
			203	203	
54	2	76	Total	Mg	0
			76	76	
54	3	1	Total	Mg	0
			1	1	
54	5	1	Total	Mg	0
			1	1	
54	B	2	Total	Mg	0
			2	2	
54	D	1	Total	Mg	0
			1	1	
54	Q	1	Total	Mg	0
			1	1	
54	b	1	Total	Mg	0
			1	1	
54	e	1	Total	Mg	0
			1	1	

- Molecule 55 is water.

Mol	Chain	Residues	Atoms		AltConf
55	1	935	Total	O	0
			935	935	
55	2	356	Total	O	0
			356	356	
55	3	14	Total	O	0
			14	14	
55	4	1	Total	O	0
			1	1	
55	5	10	Total	O	0
			10	10	
55	B	7	Total	O	0
			7	7	
55	C	5	Total	O	0
			5	5	
55	D	5	Total	O	0
			5	5	

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Mol	Chain	Residues	Atoms		AltConf
55	E	3	Total 3	O 3	0
55	F	4	Total 4	O 4	0
55	G	1	Total 1	O 1	0
55	J	3	Total 3	O 3	0
55	K	2	Total 2	O 2	0
55	L	4	Total 4	O 4	0
55	M	4	Total 4	O 4	0
55	O	3	Total 3	O 3	0
55	P	5	Total 5	O 5	0
55	Q	3	Total 3	O 3	0
55	R	3	Total 3	O 3	0
55	S	2	Total 2	O 2	0
55	V	2	Total 2	O 2	0
55	W	2	Total 2	O 2	0
55	X	1	Total 1	O 1	0
55	Y	2	Total 2	O 2	0
55	b	1	Total 1	O 1	0
55	c	1	Total 1	O 1	0
55	d	3	Total 3	O 3	0
55	f	1	Total 1	O 1	0
55	g	9	Total 9	O 9	0

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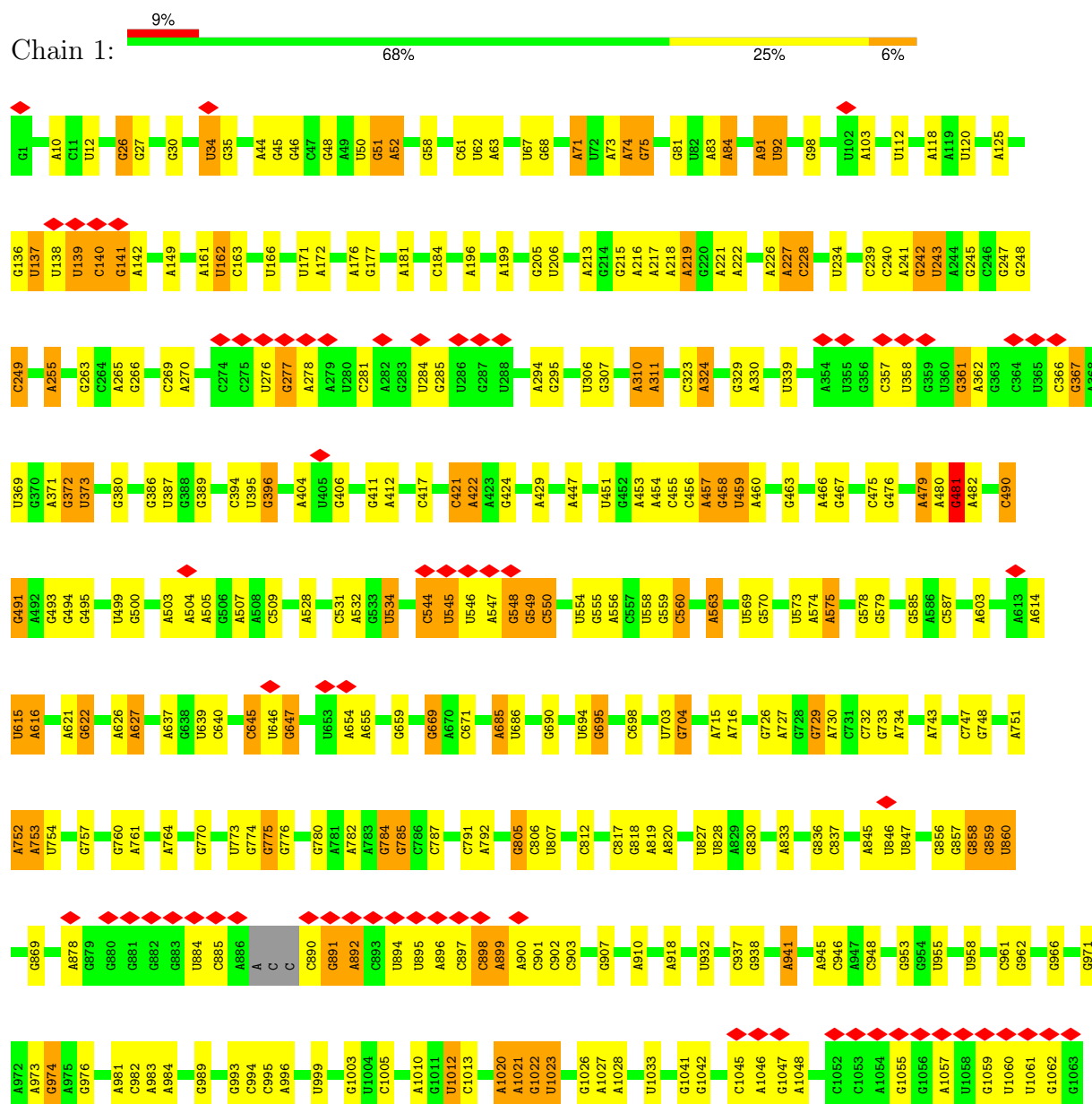
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Mol	Chain	Residues	Atoms		AltConf
55	h	7	Total 7	O 7	0
55	i	8	Total 8	O 8	0
55	j	1	Total 1	O 1	0
55	k	2	Total 2	O 2	0
55	l	10	Total 10	O 10	0
55	m	1	Total 1	O 1	0
55	o	1	Total 1	O 1	0
55	p	1	Total 1	O 1	0
55	q	2	Total 2	O 2	0
55	r	7	Total 7	O 7	0
55	s	2	Total 2	O 2	0
55	t	1	Total 1	O 1	0
55	u	3	Total 3	O 3	0
55	v	4	Total 4	O 4	0
55	x	4	Total 4	O 4	0
55	z	3	Total 3	O 3	0

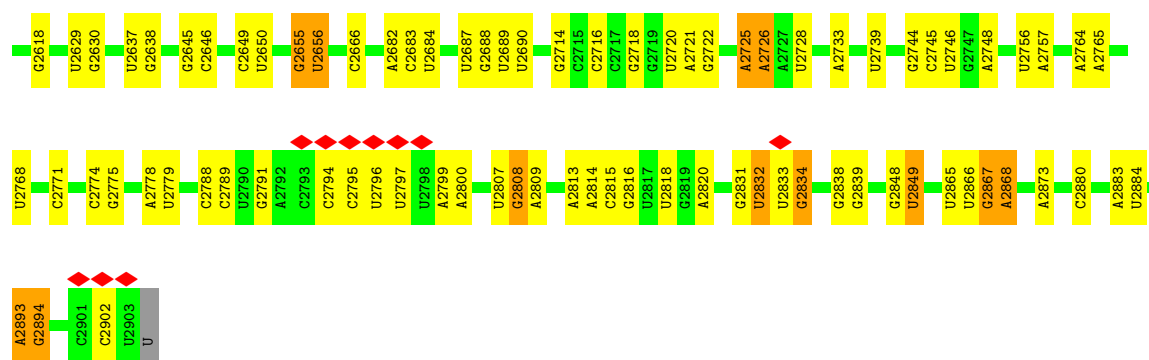
3 Residue-property plots

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.

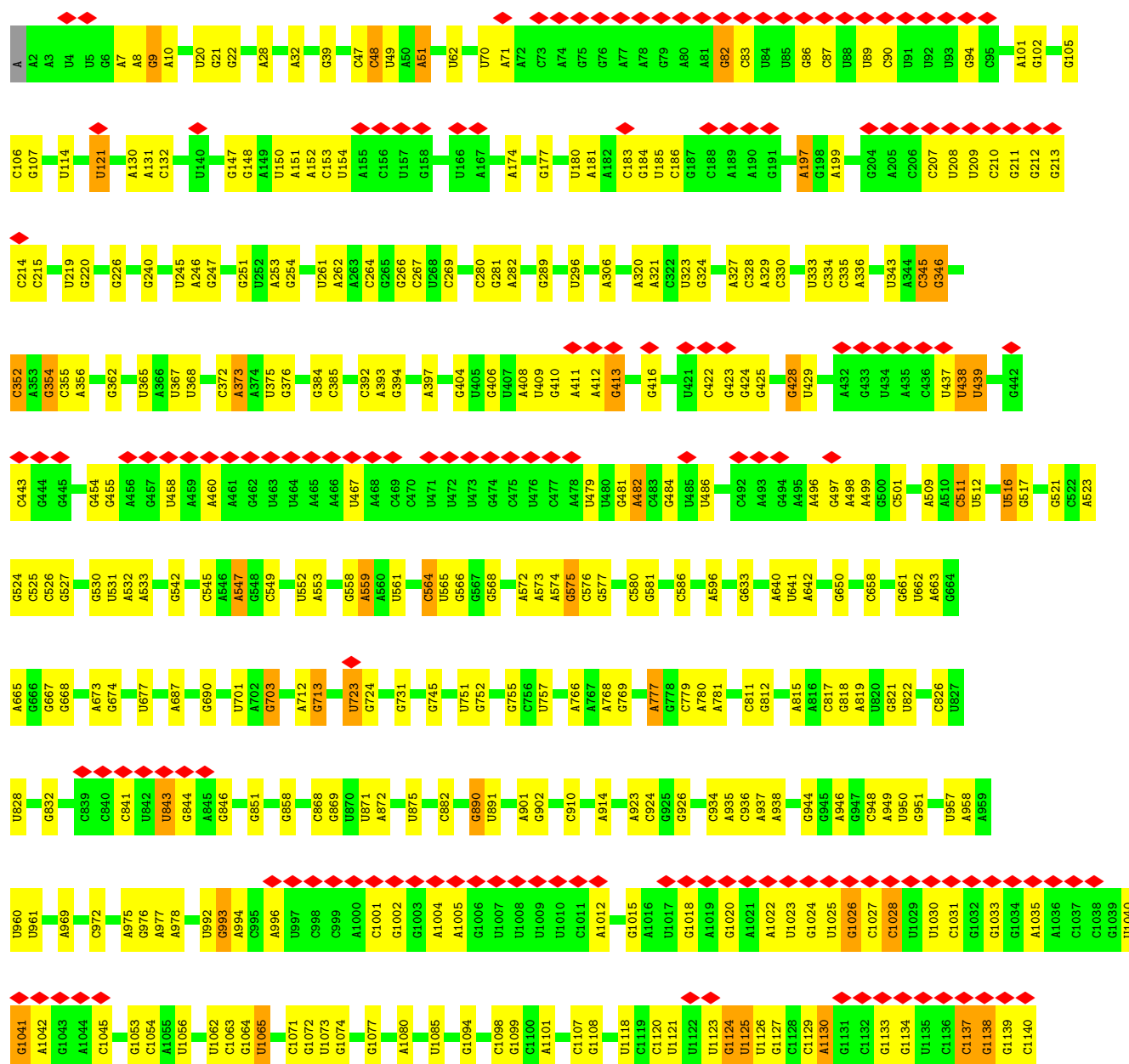
• Molecule 1: 23S ribosomal RNA

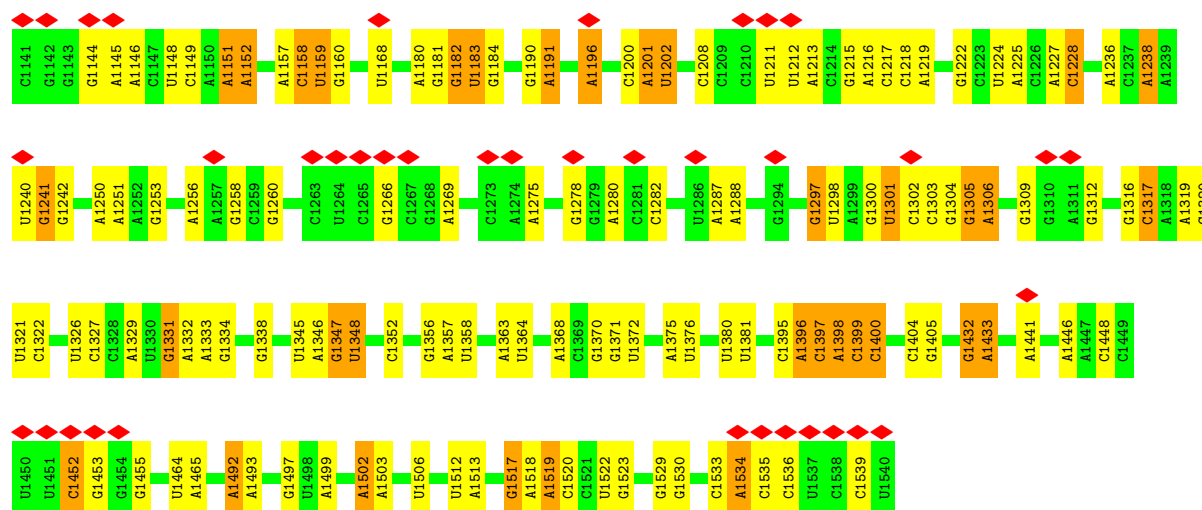


A2503	U2504	G2505	U2506	C2512	A2513	A2516	C2517	A2518	U2519	C2520	G2526	G2529	G2535	A2547	C2551	U2552	G2553	U2554	C2559	A2566	G2567	A2572	C2573	G2574	C2575	G2576	C2579	U2580	G2581	C2582	U2585	U2586	A2587	C2588	A2589	A2590	A2602	G2603	U2604	U2605	C2606	U2609	C2610	U2613												
G2383	U2384	C2385	G2391	A2392	U2393	C2394	C2395	A2396	U2402	C2403	U2404	G2405	A2406	A2407	G2410	U2423	C2424	A2425	G2428	G2429	A2430	A2435	U2441	G2446	G2447	A2448	U2449	C2452	U2453	C2467	A2468	C2475	A2476	U2477	A2478	C2486	U2489	G2490	C2496	A2497	C2498	C2499	G2502													
G2258	A2266	A2267	G2279	G2280	A2281	C2282	C2283	G2286	A2287	A2288	U2291	U2292	G2293	G2294	C2295	U2296	G2304	U2305	C2306	G2307	G2308	A2309	U2312	C2313	A2314	U2320	G2325	C2326	A2327	A2328	U2329	A2333	U2334	G2345	A2346	C2347	U2348	G2349	C2350	C2354	G2361	C2364	G2365	A2369												
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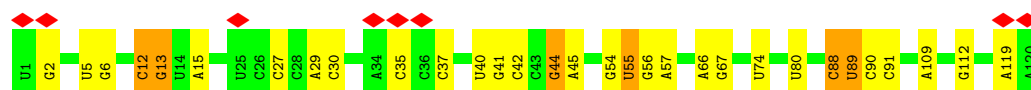
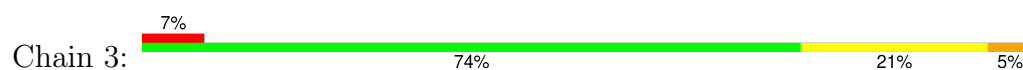


• Molecule 2: 16S ribosomal RNA





• Molecule 3: 5S ribosomal RNA



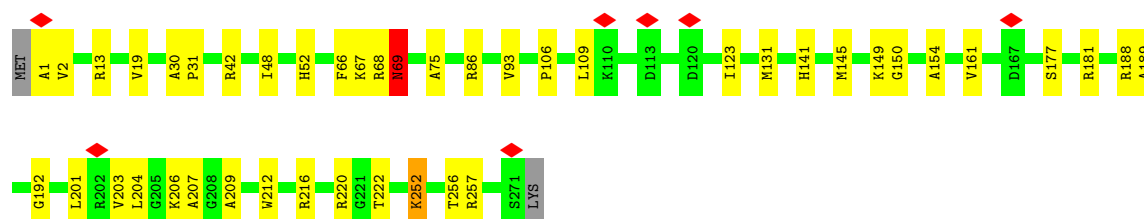
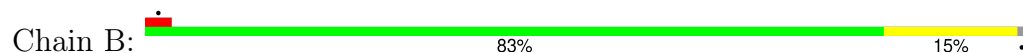
• Molecule 4: mRNA



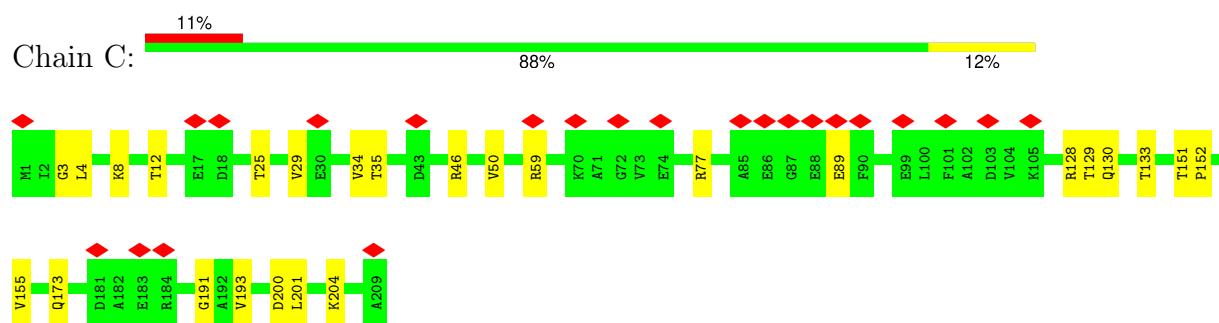
• Molecule 5: tRNA^{ProL} (GGG)



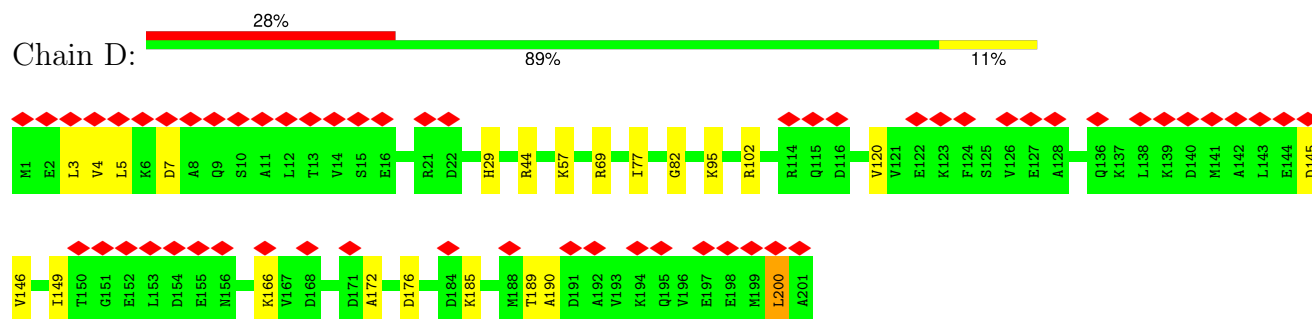
• Molecule 6: 50S ribosomal protein L2



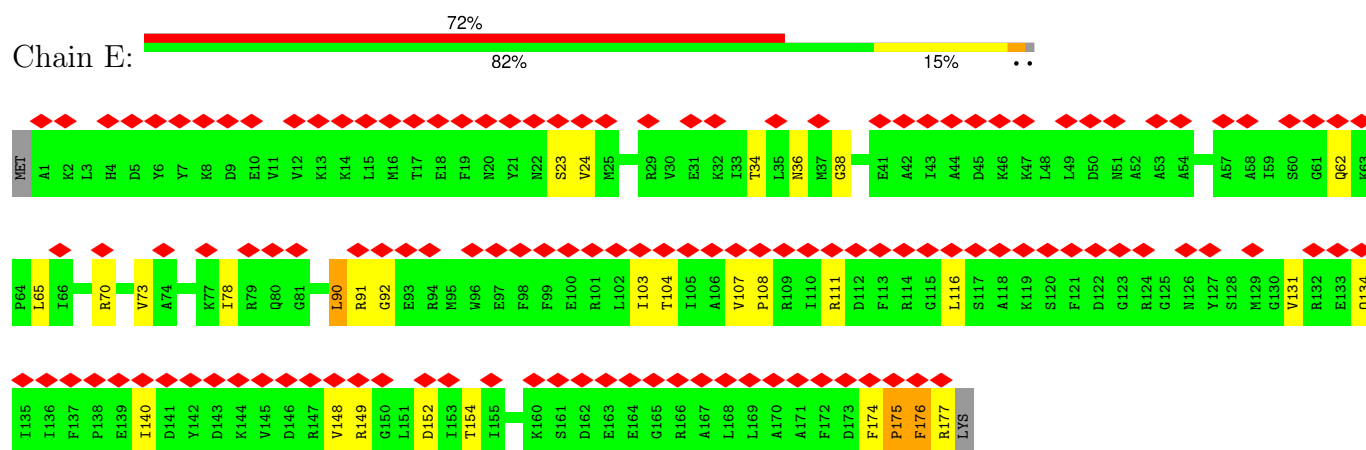
• Molecule 7: 50S ribosomal protein L3



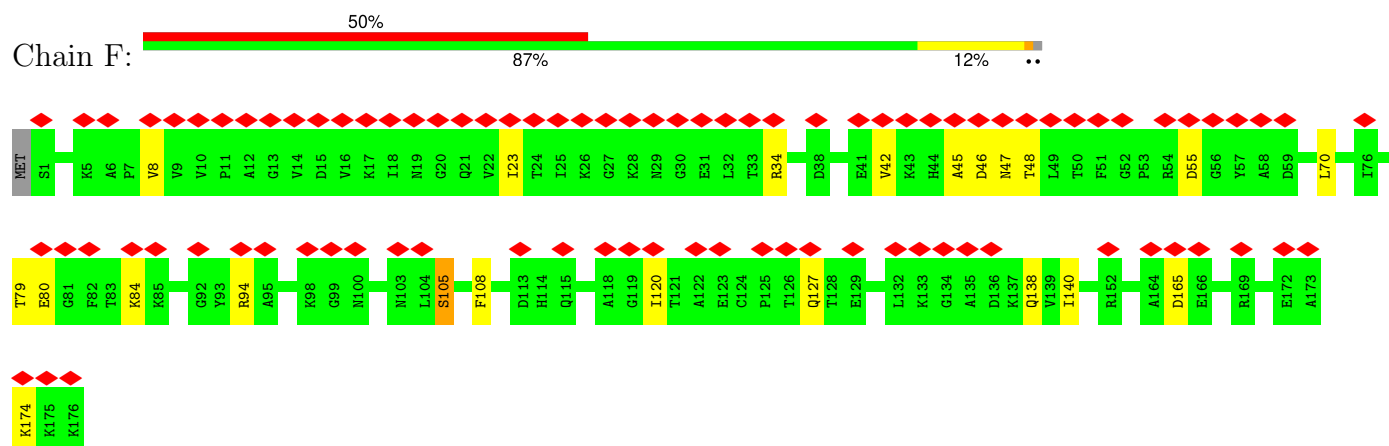
• Molecule 8: 50S ribosomal protein L4

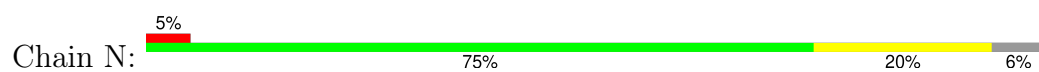


• Molecule 9: 50S ribosomal protein L5

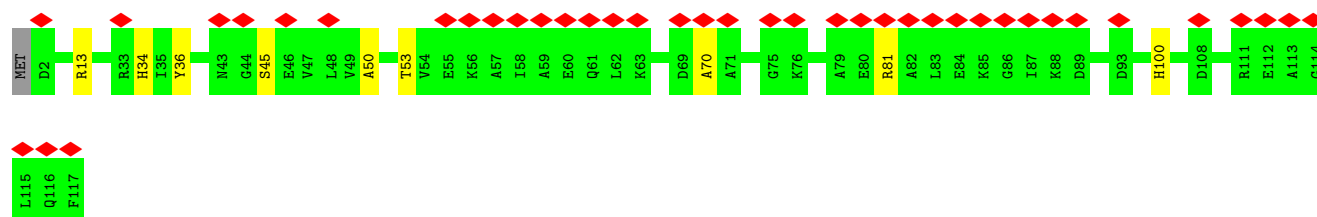


• Molecule 10: 50S ribosomal protein L6

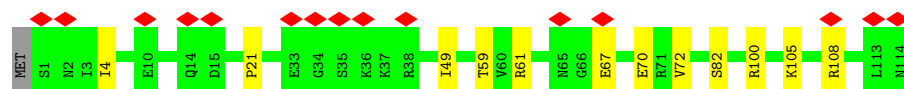
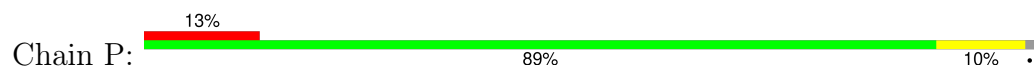




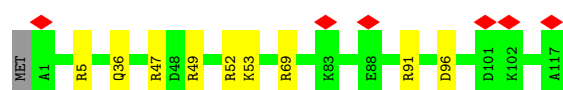
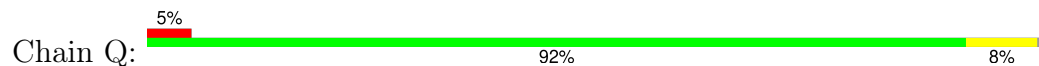
- Molecule 17: 50S ribosomal protein L18



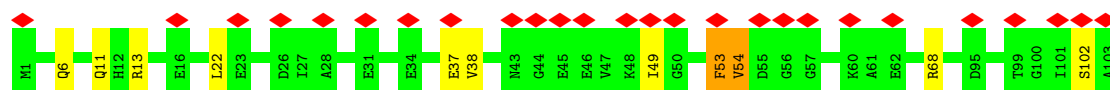
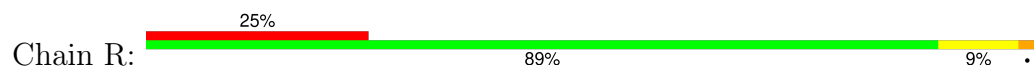
- Molecule 18: 50S ribosomal protein L19



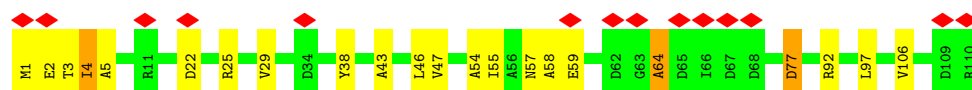
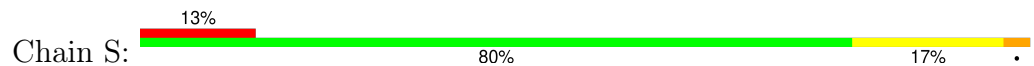
- Molecule 19: 50S ribosomal protein L20



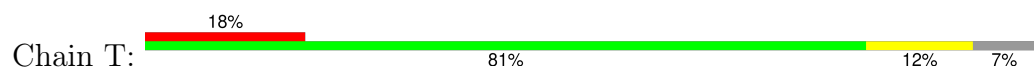
- Molecule 20: 50S ribosomal protein L21



- Molecule 21: 50S ribosomal protein L22

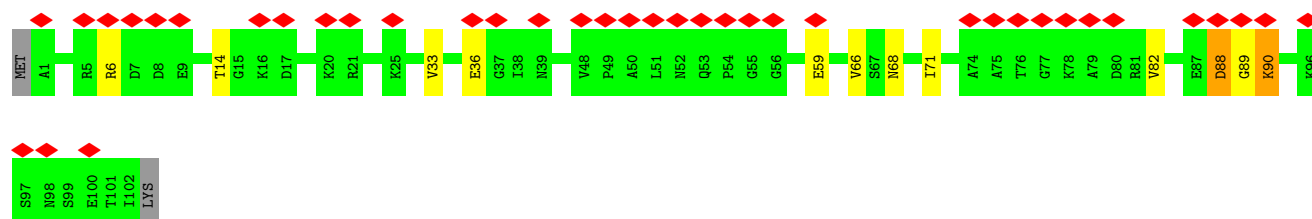
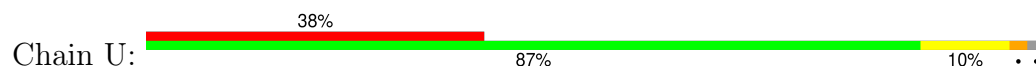


- Molecule 22: 50S ribosomal protein L23

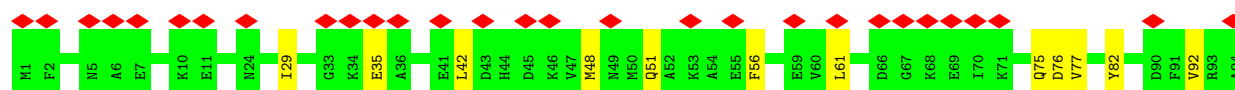
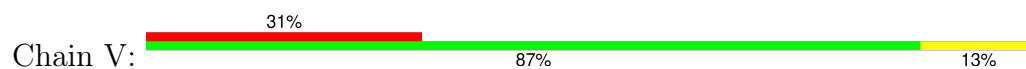




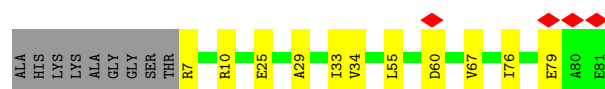
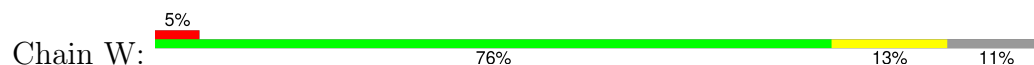
- Molecule 23: 50S ribosomal protein L24



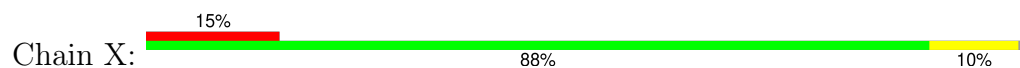
- Molecule 24: 50S ribosomal protein L25



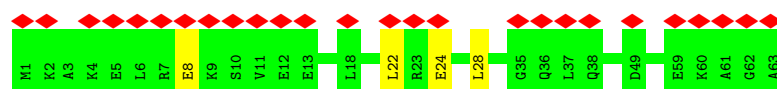
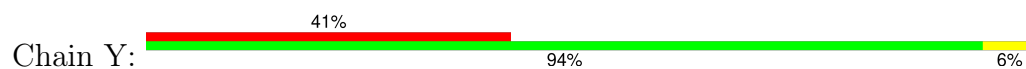
- Molecule 25: 50S ribosomal protein L27



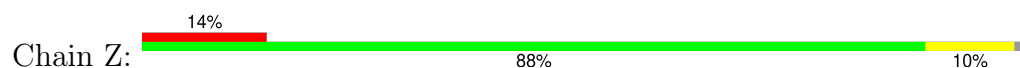
- Molecule 26: 50S ribosomal protein L28

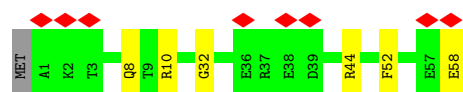


- Molecule 27: 50S ribosomal protein L29

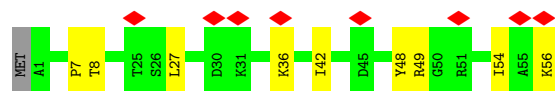
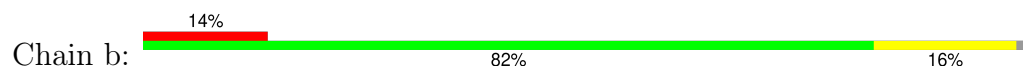


- Molecule 28: 50S ribosomal protein L30

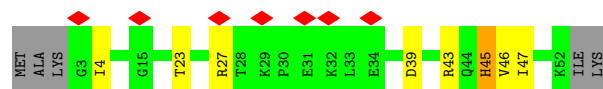
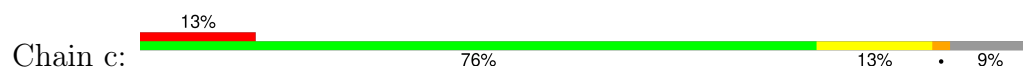




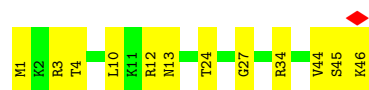
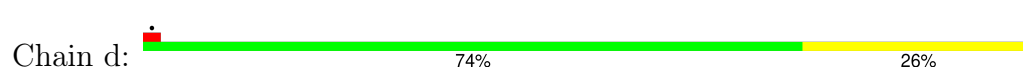
- Molecule 29: 50S ribosomal protein L32



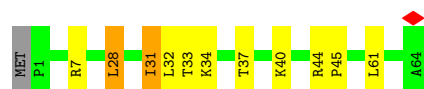
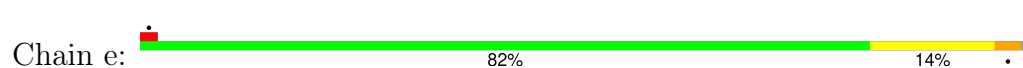
- Molecule 30: 50S ribosomal protein L33



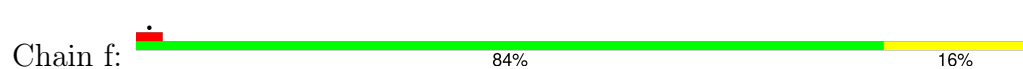
- Molecule 31: 50S ribosomal protein L34



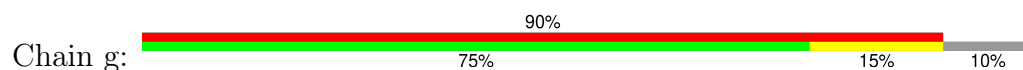
- Molecule 32: 50S ribosomal protein L35



- Molecule 33: 50S ribosomal protein L36

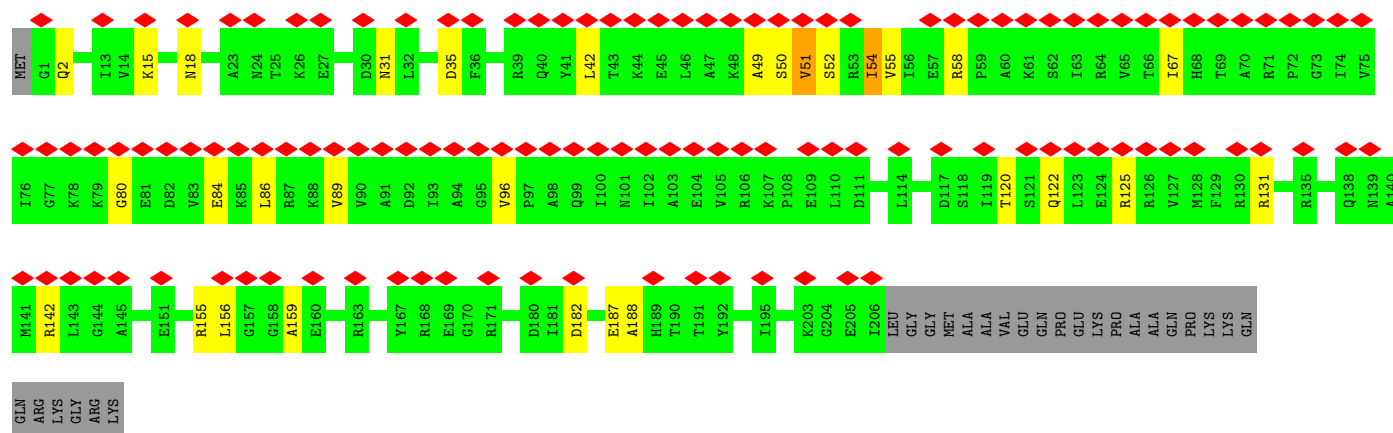
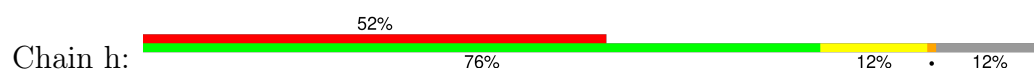


- Molecule 34: 30S ribosomal protein S2

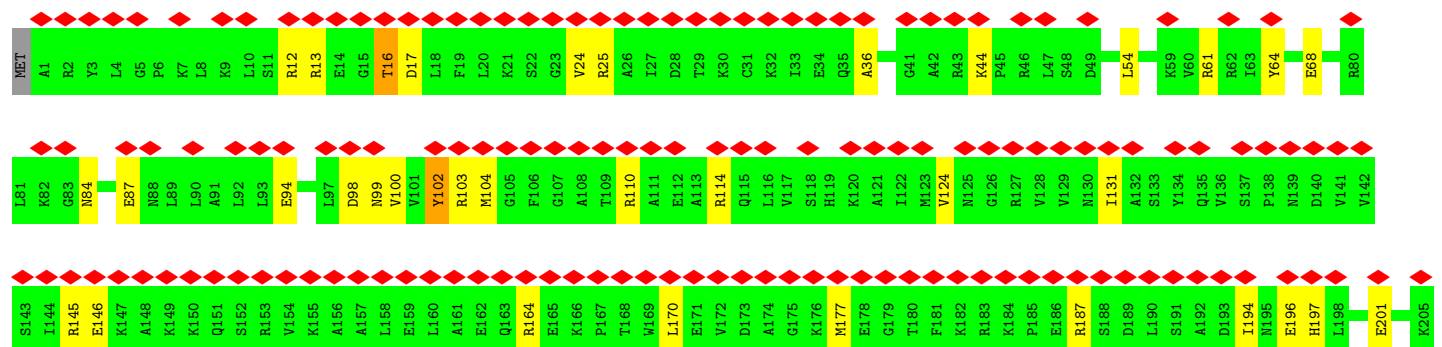
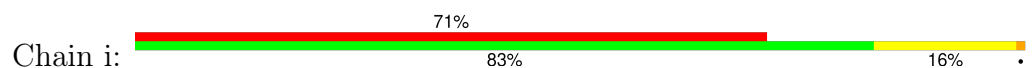




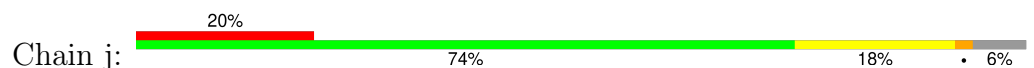
• Molecule 35: 30S ribosomal protein S3

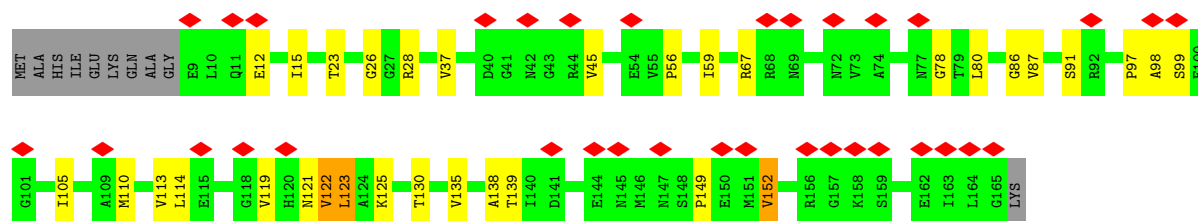


• Molecule 36: 30S ribosomal protein S4

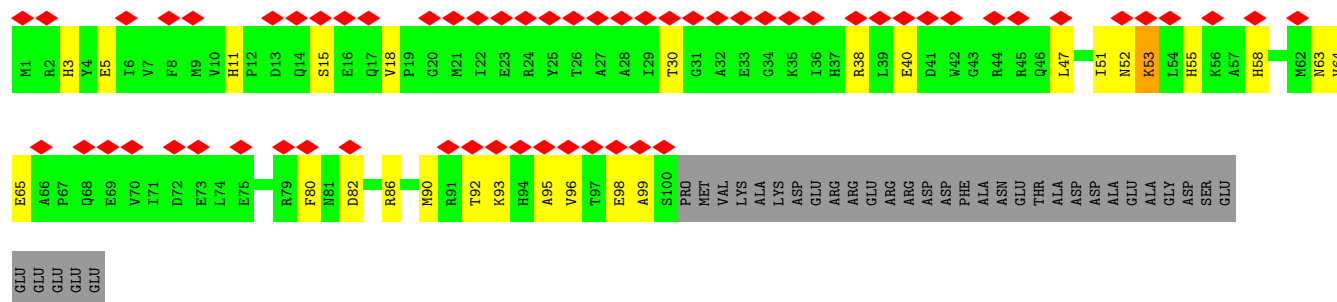


• Molecule 37: 30S ribosomal protein S5

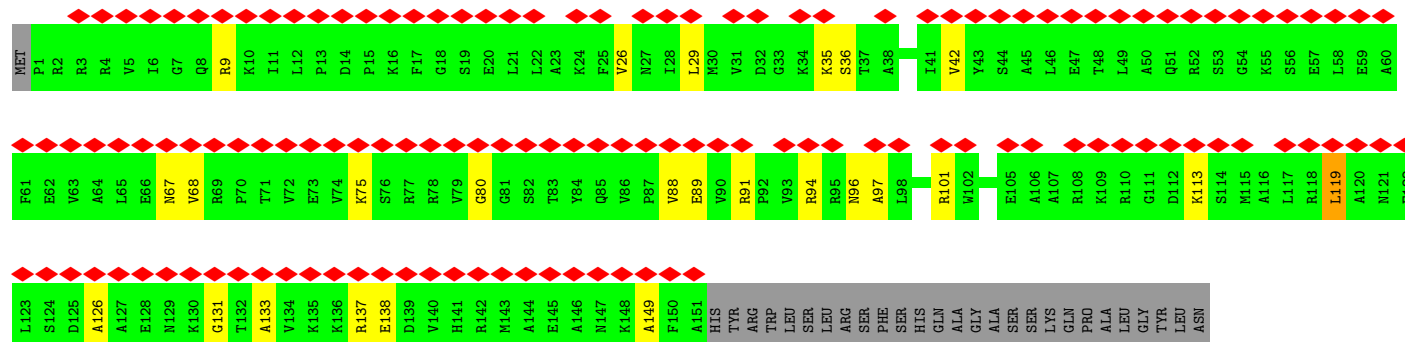
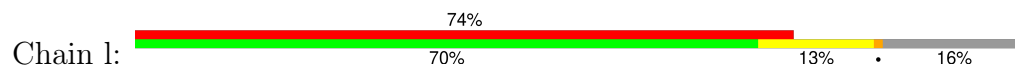




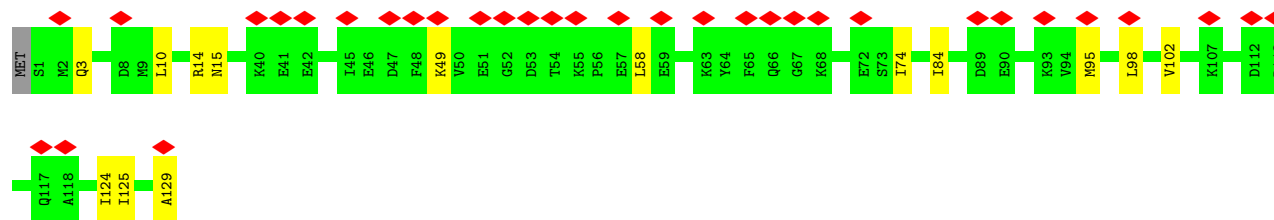
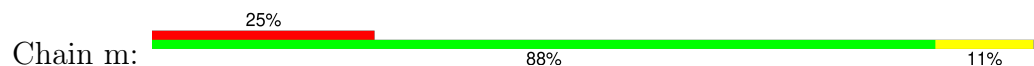
• Molecule 38: 30S ribosomal protein S6



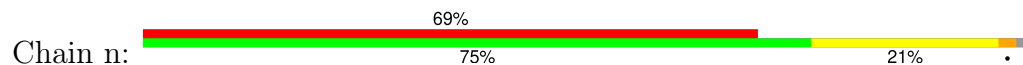
• Molecule 39: 30S ribosomal protein S7

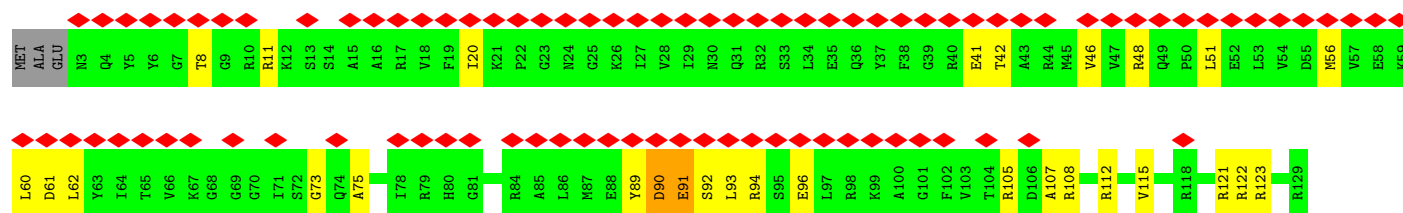


• Molecule 40: 30S ribosomal protein S8

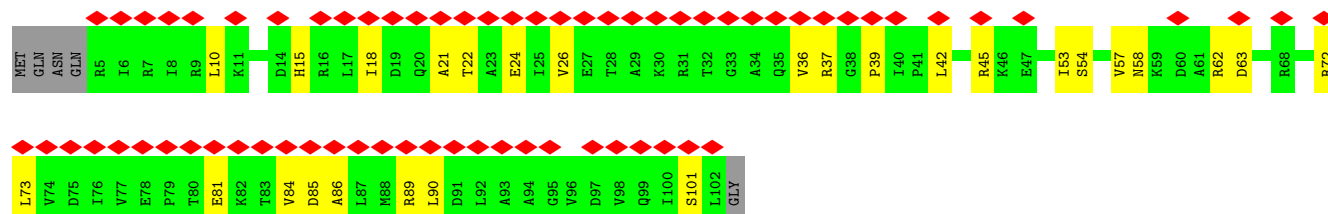


• Molecule 41: 30S ribosomal protein S9

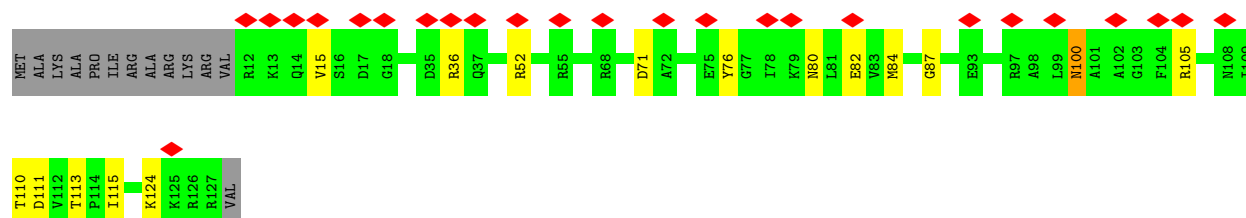
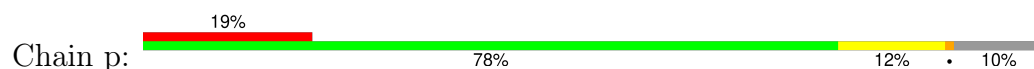




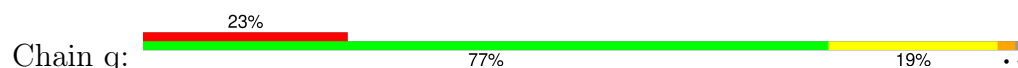
• Molecule 42: 30S ribosomal protein S10



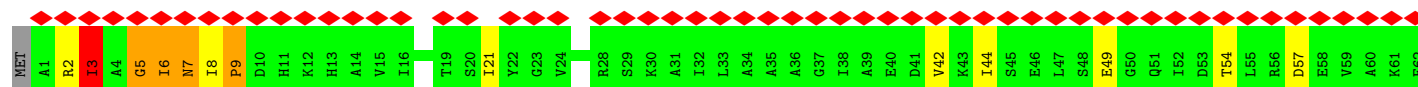
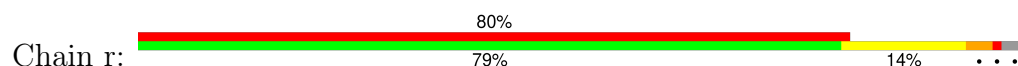
• Molecule 43: 30S ribosomal protein S11

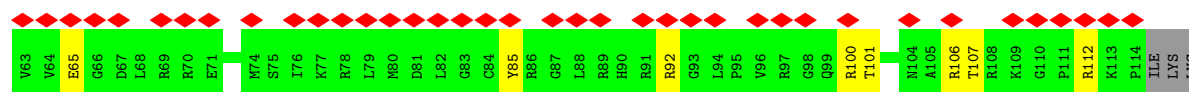


• Molecule 44: 30S ribosomal protein S12

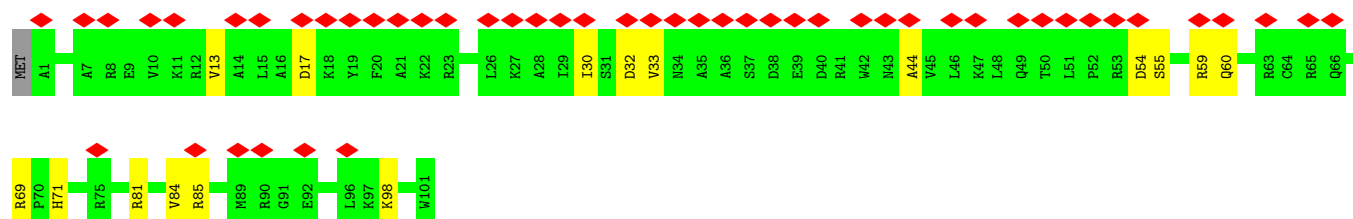
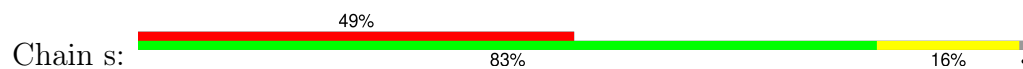


• Molecule 45: 30S ribosomal protein S13

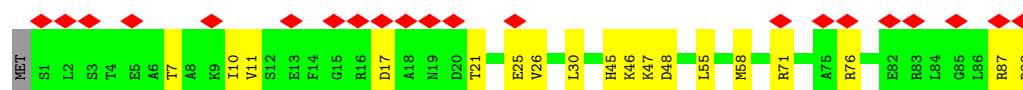
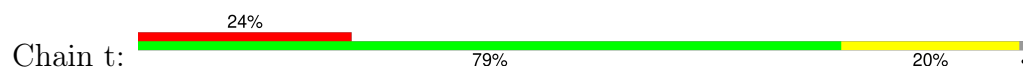




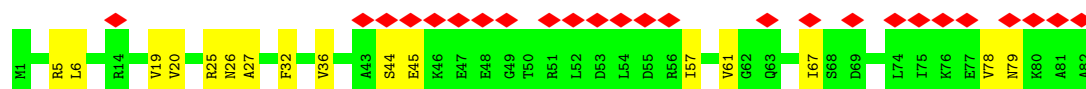
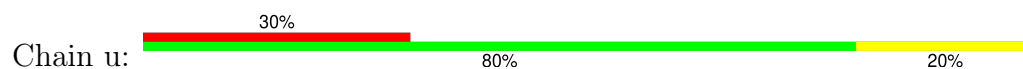
- Molecule 46: 30S ribosomal protein S14



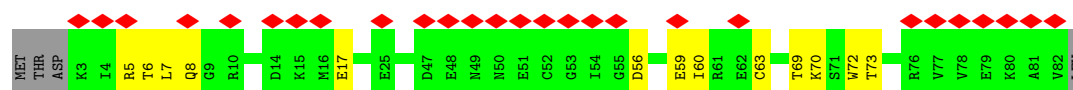
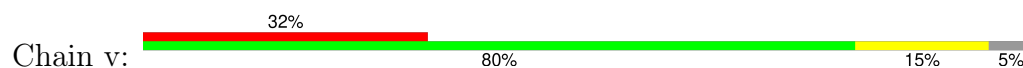
- Molecule 47: 30S ribosomal protein S15



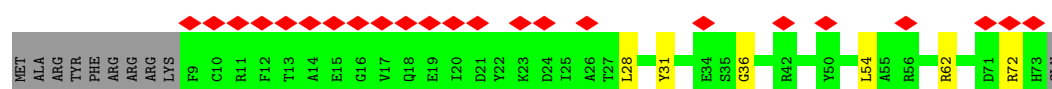
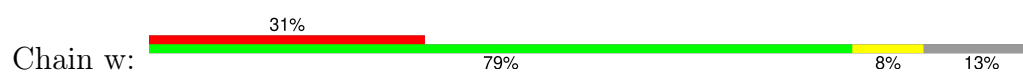
- Molecule 48: 30S ribosomal protein S16



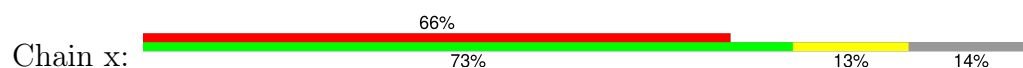
- Molecule 49: 30S ribosomal protein S17

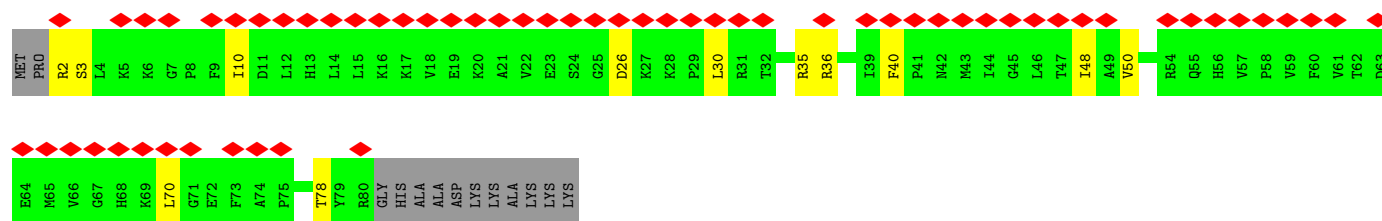


- Molecule 50: 30S ribosomal protein S18

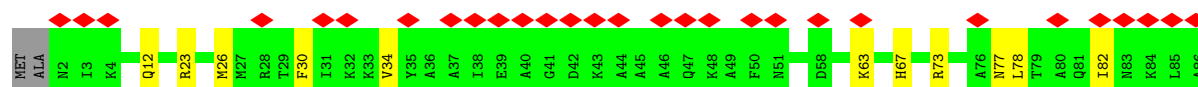
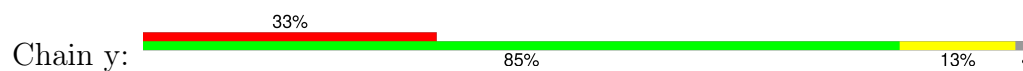


- Molecule 51: 30S ribosomal protein S19

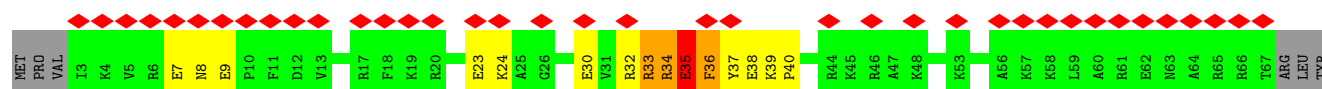




- Molecule 52: 30S ribosomal protein S20



- Molecule 53: 30S ribosomal protein S21



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	361087	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TALOS ARCTICA	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	61.23	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2700	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.053	Depositor
Minimum map value	-0.004	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.004	Depositor
Recommended contour level	0.0198	Depositor
Map size (Å)	427.64, 427.64, 427.64	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.0691, 1.0691, 1.0691	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: 0TD, MG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	1	0.17	0/69734	0.30	7/108788 (0.0%)
2	2	0.15	0/36966	0.28	2/57666 (0.0%)
3	3	0.15	0/2876	0.29	0/4483
4	4	0.39	0/208	0.69	0/321
5	5	0.16	0/1841	0.35	0/2870
6	B	0.29	0/2121	0.46	1/2852 (0.0%)
7	C	0.20	0/1586	0.39	0/2134
8	D	0.35	0/1571	0.44	1/2113 (0.0%)
9	E	0.30	0/1434	0.47	0/1926
10	F	0.29	0/1343	0.50	1/1816 (0.1%)
11	G	0.22	0/1122	0.48	0/1515
12	J	0.20	0/1152	0.34	0/1551
13	K	0.20	0/947	0.43	0/1268
14	L	0.21	0/1054	0.45	0/1403
15	M	0.37	1/1093 (0.1%)	0.49	1/1460 (0.1%)
16	N	0.21	0/973	0.45	0/1301
17	O	0.17	0/902	0.39	0/1209
18	P	0.20	0/929	0.34	0/1242
19	Q	0.21	0/960	0.39	0/1278
20	R	0.29	0/829	0.44	0/1107
21	S	0.21	0/864	0.40	0/1156
22	T	0.18	0/744	0.34	0/994
23	U	0.48	0/787	0.73	5/1051 (0.5%)
24	V	0.29	0/766	0.36	0/1025
25	W	0.19	0/582	0.37	0/769
26	X	0.20	0/635	0.31	0/848
27	Y	0.17	0/510	0.39	0/677
28	Z	0.20	0/453	0.35	0/605
29	b	0.19	0/450	0.38	0/599
30	c	0.16	0/416	0.32	0/554
31	d	0.23	0/380	0.45	0/498
32	e	0.47	0/513	0.50	0/676

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	f	0.20	0/303	0.40	0/397
34	g	0.19	0/1735	0.44	0/2338
35	h	0.20	0/1651	0.49	4/2225 (0.2%)
36	i	0.28	0/1665	0.44	1/2227 (0.0%)
37	j	0.18	0/1154	0.45	0/1554
38	k	0.22	0/835	0.45	0/1128
39	l	0.22	0/1195	0.41	0/1602
40	m	0.17	0/989	0.35	0/1326
41	n	0.17	0/1034	0.45	0/1375
42	o	0.18	0/796	0.45	0/1077
43	p	0.33	0/885	0.48	1/1195 (0.1%)
44	q	0.24	0/960	0.53	0/1286
45	r	0.23	0/892	0.52	1/1193 (0.1%)
46	s	0.17	0/811	0.41	0/1081
47	t	0.17	0/722	0.35	0/964
48	u	0.17	0/659	0.38	0/884
49	v	0.28	0/657	0.47	0/881
50	w	0.16	0/511	0.37	0/689
51	x	0.13	0/652	0.29	0/877
52	y	0.14	0/671	0.36	0/888
53	z	0.44	1/500 (0.2%)	0.80	2/668 (0.3%)
All	All	0.19	2/156018 (0.0%)	0.34	27/233610 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
53	z	33	ARG	CA-C	-6.84	1.43	1.52
15	M	58	LYS	CA-C	-5.24	1.46	1.52

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	U	88	ASP	N-CA-C	-8.62	98.35	110.50
35	h	50	SER	N-CA-C	8.56	123.51	111.52
23	U	6	ARG	N-CA-C	8.23	119.88	111.07
8	D	82	GLY	N-CA-C	8.04	122.83	112.54
15	M	57	VAL	N-CA-C	-6.88	96.57	106.55
6	B	69	ASN	N-CA-C	6.75	121.22	112.92
10	F	45	ALA	N-CA-C	6.70	120.49	111.24
53	z	35	GLU	CA-C-N	6.70	134.34	121.54
53	z	35	GLU	C-N-CA	6.70	134.34	121.54
45	r	8	ILE	N-CA-C	-6.51	101.11	107.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	h	52	SER	N-CA-C	6.38	118.04	111.14
1	1	1826	G	C1'-C2'-O2'	-6.17	99.15	108.40
43	p	100	ASN	N-CA-C	-5.95	105.11	112.90
1	1	560	C	C3'-C2'-O2'	-5.92	101.82	110.70
36	i	102	TYR	N-CA-C	-5.87	104.79	111.07
1	1	481	G	C2'-C3'-O3'	-5.83	104.95	113.70
1	1	534	U	C3'-C2'-O2'	-5.71	102.13	110.70
35	h	49	ALA	N-CA-C	5.65	119.48	112.59
2	2	1301	U	C3'-C2'-O2'	5.64	119.17	110.70
2	2	1301	U	C2'-C3'-O3'	5.56	122.04	113.70
1	1	479	A	C2'-C3'-O3'	-5.54	101.19	109.50
1	1	1961	C	C4'-C3'-O3'	-5.35	104.97	113.00
35	h	51	VAL	N-CA-C	5.31	116.02	107.73
1	1	2287	A	C1'-C2'-O2'	-5.23	100.56	108.40
23	U	90	LYS	N-CA-C	5.13	117.67	110.23
23	U	6	ARG	CA-C-N	-5.03	115.97	123.11
23	U	6	ARG	C-N-CA	-5.03	115.97	123.11

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	1	62262	0	31314	453	0
2	2	33015	0	16617	254	0
3	3	2572	0	1302	20	0
4	4	188	0	98	4	0
5	5	1648	0	834	9	0
6	B	2082	0	2157	34	0
7	C	1565	0	1616	18	0
8	D	1552	0	1619	17	0
9	E	1410	0	1447	31	0
10	F	1323	0	1374	16	0
11	G	1111	0	1148	20	0
12	J	1129	0	1162	8	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
13	K	938	0	1012	21	0
14	L	1045	0	1117	19	0
15	M	1074	0	1157	24	0
16	N	960	0	1000	17	0
17	O	892	0	923	8	0
18	P	917	0	965	8	0
19	Q	947	0	1022	8	0
20	R	816	0	839	9	0
21	S	857	0	922	15	0
22	T	738	0	807	8	0
23	U	779	0	834	6	0
24	V	753	0	780	7	0
25	W	575	0	592	6	0
26	X	625	0	655	6	0
27	Y	509	0	543	4	0
28	Z	449	0	491	3	0
29	b	444	0	461	9	0
30	c	409	0	440	5	0
31	d	377	0	418	10	0
32	e	504	0	574	10	0
33	f	302	0	343	6	0
34	g	1704	0	1732	23	0
35	h	1624	0	1699	17	0
36	i	1643	0	1710	27	0
37	j	1141	0	1170	24	0
38	k	817	0	808	19	0
39	l	1181	0	1240	22	0
40	m	979	0	1034	12	0
41	n	1022	0	1070	24	0
42	o	786	0	828	23	0
43	p	869	0	878	12	0
44	q	957	0	1017	19	0
45	r	883	0	944	17	0
46	s	799	0	841	8	0
47	t	714	0	737	14	0
48	u	649	0	666	10	0
49	v	648	0	691	13	0
50	w	504	0	502	3	0
51	x	637	0	665	11	0
52	y	665	0	714	8	0
53	z	495	0	486	17	0
54	1	203	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
54	2	76	0	0	0	0
54	3	1	0	0	0	0
54	5	1	0	0	0	0
54	B	2	0	0	0	0
54	D	1	0	0	0	0
54	Q	1	0	0	0	0
54	b	1	0	0	0	0
54	e	1	0	0	0	0
55	1	935	0	0	69	0
55	2	356	0	0	29	0
55	3	14	0	0	5	0
55	4	1	0	0	0	0
55	5	10	0	0	0	0
55	B	7	0	0	2	0
55	C	5	0	0	2	0
55	D	5	0	0	2	0
55	E	3	0	0	2	0
55	F	4	0	0	0	0
55	G	1	0	0	3	0
55	J	3	0	0	0	0
55	K	2	0	0	3	0
55	L	4	0	0	0	0
55	M	4	0	0	4	0
55	O	3	0	0	1	0
55	P	5	0	0	1	0
55	Q	3	0	0	0	0
55	R	3	0	0	0	0
55	S	2	0	0	2	0
55	V	2	0	0	0	0
55	W	2	0	0	1	0
55	X	1	0	0	1	0
55	Y	2	0	0	0	0
55	b	1	0	0	0	0
55	c	1	0	0	2	0
55	d	3	0	0	1	0
55	f	1	0	0	0	0
55	g	9	0	0	3	0
55	h	7	0	0	6	0
55	i	8	0	0	3	0
55	j	1	0	0	0	0
55	k	2	0	0	2	0
55	l	10	0	0	8	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
55	m	1	0	0	0	0
55	o	1	0	0	1	0
55	p	1	0	0	0	0
55	q	2	0	0	0	0
55	r	7	0	0	7	0
55	s	2	0	0	4	0
55	t	1	0	0	1	0
55	u	3	0	0	2	0
55	v	4	0	0	3	0
55	x	4	0	0	2	0
55	z	3	0	0	4	0
All	All	145220	0	96015	1260	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 (1260) 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)
1:1:2142:A:H3'	55:1:3339:HOH:O	1.28	1.24
1:1:2168:G:H5'	55:1:3875:HOH:O	1.36	1.24
1:1:2136:G:H1'	55:1:3846:HOH:O	1.45	1.15
2:2:723:U:H1'	55:2:1751:HOH:O	1.46	1.15
46:s:85:ARG:HD2	55:s:201:HOH:O	1.50	1.12
2:2:416:G:H5''	55:2:2009:HOH:O	1.50	1.10
7:C:204:LYS:HE3	55:C:302:HOH:O	1.51	1.08
2:2:1211:U:H2'	55:2:1736:HOH:O	1.52	1.07
39:l:80:GLY:HA3	55:l:202:HOH:O	1.55	1.05
42:o:53:ILE:HG13	55:s:201:HOH:O	1.58	1.03
2:2:443:C:H4'	55:2:1978:HOH:O	1.59	1.02
55:c:101:HOH:O	32:e:33:THR:HG22	1.61	1.01
53:z:30:GLU:HB3	55:z:101:HOH:O	1.58	1.01
1:1:1493:C:H1'	55:1:3559:HOH:O	1.60	1.01
1:1:891:G:H2'	1:1:892:A:C8	1.95	1.00
36:i:145:ARG:HD3	55:i:305:HOH:O	1.65	0.96
39:l:119:LEU:HB2	55:l:210:HOH:O	1.67	0.94
42:o:45:ARG:HB3	55:o:201:HOH:O	1.67	0.94
39:l:149:ALA:HB3	55:l:208:HOH:O	1.66	0.94
1:1:890:C:H2'	55:1:4113:HOH:O	1.69	0.92
1:1:2808:G:H5'	55:1:3580:HOH:O	1.70	0.92
45:r:42:VAL:HA	55:r:206:HOH:O	1.69	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:B:69:ASN:HA	6:B:188:ARG:HH12	1.36	0.90
1:1:2326:C:O2'	1:1:2327:A:OP1	1.89	0.89
53:z:35:GLU:HG3	53:z:36:PHE:H	1.38	0.89
2:2:1492:A:H8	4:4:19:U:HO2'	0.89	0.87
1:1:1130:U:O2'	1:1:1131:G:OP1	1.93	0.86
22:T:8:LEU:HD11	27:Y:22:LEU:HD12	1.57	0.86
1:1:1084:A:C4	55:1:3317:HOH:O	2.27	0.86
1:1:2137:U:H3'	55:1:3746:HOH:O	1.73	0.86
1:1:2126:A:C4	55:1:3444:HOH:O	2.27	0.86
2:2:1026:G:O2'	2:2:1027:C:O4'	1.92	0.85
1:1:2116:G:H4'	55:1:3435:HOH:O	1.77	0.85
2:2:1025:U:C3'	55:2:1730:HOH:O	2.24	0.85
1:1:2184:A:O2'	1:1:2185:U:O4'	1.94	0.85
1:1:1070:A:H2	55:1:3737:HOH:O	1.56	0.84
41:n:122:ARG:NH1	41:n:123:ARG:O	2.11	0.84
2:2:1025:U:H2'	55:2:1730:HOH:O	1.78	0.84
8:D:57:LYS:HE2	55:D:403:HOH:O	1.78	0.84
1:1:548:G:O2'	1:1:549:G:O4'	1.96	0.84
39:l:149:ALA:CB	55:l:208:HOH:O	2.24	0.83
2:2:1492:A:H8	4:4:19:U:O2'	1.62	0.83
14:L:29:LYS:O	14:L:30:THR:OG1	1.97	0.83
55:1:3553:HOH:O	30:c:45:HIS:CD2	2.30	0.83
1:1:1900:A:O2'	1:1:1901:A:OP2	1.97	0.82
1:1:1920:C:H4'	55:1:3546:HOH:O	1.79	0.82
16:N:69:ARG:O	16:N:70:THR:OG1	1.98	0.82
35:h:142:ARG:HD3	55:h:304:HOH:O	1.77	0.82
2:2:1025:U:H3'	55:2:1730:HOH:O	1.78	0.82
1:1:858:G:O2'	1:1:859:G:OP1	1.98	0.81
45:r:85:TYR:HE1	55:r:204:HOH:O	1.63	0.80
34:g:38:HIS:CD2	55:g:301:HOH:O	2.33	0.80
43:p:84:MET:SD	43:p:110:THR:OG1	2.38	0.80
55:1:3393:HOH:O	15:M:18:ARG:CD	2.31	0.79
49:v:63:CYS:SG	49:v:73:THR:OG1	2.28	0.79
55:2:1887:HOH:O	39:l:91:ARG:HD3	1.81	0.79
1:1:227:A:O2'	1:1:228:C:O5'	1.99	0.79
1:1:1209:U:H5	55:1:3721:HOH:O	1.64	0.78
2:2:1320:C:N3	51:x:35:ARG:NH1	2.32	0.78
55:c:101:HOH:O	32:e:33:THR:CG2	2.24	0.78
45:r:85:TYR:CE1	55:r:204:HOH:O	2.35	0.78
1:1:310:A:O2'	1:1:311:A:O5'	2.00	0.78
42:o:53:ILE:CG1	55:s:201:HOH:O	2.23	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:2618:G:H21	7:C:155:VAL:HG21	1.50	0.77
53:z:8:ASN:HA	55:z:102:HOH:O	1.84	0.77
1:1:1125:G:OP2	1:1:1126:A:O2'	2.02	0.76
6:B:145:MET:SD	6:B:181:ARG:NH2	2.59	0.76
38:k:80:PHE:HD1	55:k:202:HOH:O	1.70	0.75
1:1:2832:U:O4	29:b:49:ARG:NH2	2.20	0.75
1:1:1936:A:C8	55:1:4098:HOH:O	2.38	0.75
38:k:38:ARG:NH2	38:k:40:GLU:OE1	2.20	0.75
2:2:422:C:O2'	2:2:423:G:N2	2.20	0.75
5:5:15:G:N2	5:5:48:C:O2	2.20	0.75
40:m:95:MET:SD	40:m:129:ALA:HB1	2.27	0.74
1:1:2768:U:O2'	12:J:95:ARG:NH2	2.20	0.74
1:1:2745:C:O2	10:F:138:GLN:NE2	2.21	0.74
49:v:5:ARG:NE	55:v:101:HOH:O	2.20	0.74
49:v:8:GLN:NE2	49:v:59:GLU:OE2	2.21	0.74
37:j:97:PRO:HA	37:j:122:VAL:HG12	1.68	0.74
1:1:1087:G:C2	55:1:3374:HOH:O	2.41	0.73
1:1:2725:A:O2'	1:1:2726:A:O5'	2.03	0.73
28:Z:44:ARG:NH2	28:Z:58:GLU:OE2	2.22	0.73
31:d:12:ARG:HE	31:d:44:VAL:HG21	1.51	0.73
3:3:37:C:O2	17:O:100:HIS:NE2	2.22	0.73
10:F:34:ARG:HE	10:F:70:LEU:HD13	1.53	0.73
37:j:78:GLY:O	37:j:121:ASN:ND2	2.22	0.73
35:h:31:ASN:OD1	35:h:58:ARG:NH2	2.22	0.73
2:2:404:G:O2'	2:2:498:A:N1	2.21	0.73
1:1:2305:U:C2	55:1:3305:HOH:O	2.40	0.72
42:o:85:ASP:OD1	42:o:89:ARG:NH2	2.22	0.72
2:2:1151:A:O2'	42:o:72:ARG:NH2	2.23	0.72
23:U:14:THR:OG1	23:U:68:ASN:ND2	2.21	0.72
43:p:111:ASP:O	50:w:72:ARG:NH2	2.22	0.72
2:2:1309:G:O6	2:2:1329:A:N6	2.22	0.72
2:2:455:G:H4'	55:2:1925:HOH:O	1.89	0.72
45:r:9:PRO:HG2	45:r:44:ILE:HG13	1.72	0.72
1:1:587:C:O2	14:L:33:ARG:NH1	2.22	0.72
1:1:1754:A:N1	1:1:2716:C:O2'	2.22	0.72
39:l:131:GLY:HA3	55:l:201:HOH:O	1.90	0.72
1:1:2865:U:OP2	1:1:2866:U:O2'	2.04	0.72
25:W:25:GLU:HG3	55:W:102:HOH:O	1.90	0.72
1:1:704:G:O2'	1:1:727:A:N6	2.21	0.72
11:G:38:PRO:O	11:G:43:ASN:ND2	2.23	0.71
1:1:2305:U:N3	55:1:3305:HOH:O	2.22	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:2505:G:O2'	1:1:2506:U:O5'	2.08	0.71
1:1:976:G:HO2'	1:1:1155:A:HO2'	1.37	0.71
2:2:207:C:N4	55:2:1705:HOH:O	2.24	0.71
2:2:1228:C:OP1	45:r:106:ARG:NH1	2.23	0.70
36:i:87:GLU:N	36:i:87:GLU:OE1	2.25	0.70
41:n:90:ASP:O	41:n:92:SER:N	2.24	0.70
1:1:548:G:O2'	1:1:549:G:O5'	2.08	0.70
1:1:1095:A:H5'	55:1:3334:HOH:O	1.90	0.70
1:1:2110:G:H3'	55:1:3459:HOH:O	1.91	0.70
55:1:3393:HOH:O	15:M:18:ARG:HD3	1.88	0.70
55:1:3393:HOH:O	15:M:18:ARG:HD2	1.91	0.70
2:2:1397:C:OP2	37:j:28:ARG:NH2	2.24	0.70
1:1:1328:A:O2'	1:1:1329:U:O5'	2.10	0.70
1:1:1365:A:OP1	26:X:2:ARG:NH1	2.25	0.70
2:2:121:U:C2	55:2:1799:HOH:O	2.45	0.70
6:B:66:PHE:HZ	6:B:86:ARG:HH12	1.38	0.70
2:2:1124:G:H1	2:2:1149:C:H42	1.38	0.69
8:D:57:LYS:CE	55:D:403:HOH:O	2.37	0.69
11:G:148:ALA:N	55:G:201:HOH:O	2.24	0.69
41:n:48:ARG:HA	41:n:51:LEU:HD12	1.74	0.69
48:u:26:ASN:ND2	55:u:101:HOH:O	2.25	0.69
1:1:227:A:HO2'	1:1:228:C:P	2.15	0.69
2:2:1144:G:O2'	2:2:1145:A:O4'	2.10	0.69
2:2:1023:U:H4'	55:2:1857:HOH:O	1.91	0.68
2:2:1028:C:C4	55:2:1744:HOH:O	2.45	0.68
2:2:501:C:OP1	44:q:114:ARG:NH2	2.26	0.68
45:r:65:GLU:HB2	55:r:202:HOH:O	1.91	0.68
9:E:70:ARG:HD3	55:E:203:HOH:O	1.94	0.68
2:2:1201:A:O2'	2:2:1202:U:OP2	2.07	0.68
5:5:15:G:N2	5:5:48:C:C2	2.62	0.68
11:G:148:ALA:CA	55:G:201:HOH:O	2.42	0.68
35:h:131:ARG:NE	55:h:301:HOH:O	2.27	0.68
1:1:1244:A:HO2'	8:D:29:HIS:HE2	1.42	0.68
1:1:219:A:N3	1:1:234:U:O2'	2.26	0.68
1:1:456:C:H5'	55:1:3427:HOH:O	1.94	0.68
1:1:1315:C:O2'	1:1:1392:A:N3	2.24	0.68
1:1:2312:U:O2	9:E:36:ASN:ND2	2.26	0.68
9:E:62:GLN:N	9:E:62:GLN:OE1	2.27	0.68
2:2:1025:U:C2'	55:2:1730:HOH:O	2.31	0.67
42:o:42:LEU:HD11	42:o:73:LEU:HG	1.77	0.67
1:1:2121:G:OP1	5:5:56:C:N4	2.27	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:690:G:O6	43:p:52:ARG:NH2	2.27	0.67
1:1:1070:A:C2	55:1:3737:HOH:O	2.35	0.67
1:1:51:G:O2'	1:1:52:A:OP1	2.08	0.67
1:1:2391:G:O2'	1:1:2429:G:N2	2.27	0.67
53:z:34:ARG:HD2	53:z:36:PHE:CZ	2.30	0.67
15:M:66:ARG:NH1	15:M:104:GLU:OE2	2.28	0.67
1:1:1418:G:N2	1:1:1579:A:N7	2.43	0.67
2:2:1312:G:N1	2:2:1326:U:O4	2.28	0.67
2:2:523:A:H61	44:q:89:0TD:H6	1.59	0.67
1:1:1084:A:N9	55:1:3317:HOH:O	2.25	0.66
2:2:1266:G:N2	2:2:1269:A:OP2	2.26	0.66
2:2:1224:U:H4'	55:2:1836:HOH:O	1.96	0.66
43:p:87:GLY:H	43:p:113:THR:HG22	1.59	0.66
2:2:1137:C:O2'	2:2:1138:G:N2	2.28	0.66
3:3:88:C:O2'	3:3:89:U:O5'	2.12	0.66
2:2:197:A:N1	2:2:220:G:O2'	2.29	0.66
8:D:149:ILE:HD11	8:D:172:ALA:HA	1.78	0.66
2:2:1306:A:N6	2:2:1331:G:O2'	2.28	0.66
32:e:31:ILE:HG22	32:e:34:LYS:HE3	1.78	0.66
1:1:918:A:N3	3:3:80:U:O2'	2.28	0.66
15:M:10:ARG:HD3	55:M:204:HOH:O	1.95	0.66
1:1:91:A:O2'	1:1:92:U:O4'	2.14	0.66
11:G:1:MET:N	11:G:20:ASN:OD1	2.29	0.66
1:1:807:U:OP2	14:L:41:ARG:NH1	2.29	0.65
1:1:1490:A:O2'	1:1:1491:G:OP1	2.14	0.65
1:1:1069:A:H5''	55:1:4007:HOH:O	1.95	0.65
25:W:29:ALA:N	25:W:60:ASP:OD1	2.30	0.65
7:C:46:ARG:NH2	7:C:89:GLU:OE1	2.28	0.65
1:1:2602:A:C2	55:1:3618:HOH:O	2.49	0.65
55:1:3614:HOH:O	8:D:69:ARG:HG3	1.97	0.65
1:1:1454:C:O2'	16:N:60:VAL:HG13	1.96	0.65
1:1:690:G:H21	6:B:42:ARG:HH12	1.44	0.65
2:2:1305:G:O2'	2:2:1306:A:O5'	2.14	0.65
1:1:1089:A:H1'	55:1:3374:HOH:O	1.97	0.65
1:1:2683:C:O2	13:K:70:ARG:NH2	2.30	0.65
16:N:114:GLU:N	16:N:114:GLU:OE1	2.30	0.65
23:U:36:GLU:N	23:U:36:GLU:OE1	2.29	0.65
1:1:139:U:O2'	1:1:140:C:O2	2.15	0.65
1:1:563:A:N3	19:Q:36:GLN:NE2	2.45	0.65
2:2:826:C:O2	40:m:15:ASN:ND2	2.29	0.65
43:p:80:ASN:HB3	43:p:105:ARG:HD3	1.77	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:k:11:HIS:O	38:k:15:SER:N	2.30	0.65
35:h:142:ARG:CD	55:h:304:HOH:O	2.42	0.64
13:K:35:VAL:HG22	13:K:69:VAL:HG12	1.79	0.64
1:1:213:A:H5''	55:1:3901:HOH:O	1.96	0.64
2:2:1441:A:N6	55:2:1712:HOH:O	2.30	0.64
5:5:56:C:O2'	5:5:57:A:OP1	2.09	0.64
13:K:113:MET:SD	55:K:202:HOH:O	2.54	0.64
6:B:1:ALA:N	6:B:19:VAL:O	2.30	0.64
9:E:111:ARG:NH1	55:E:202:HOH:O	2.30	0.64
12:J:56:VAL:HB	12:J:124:VAL:HG12	1.80	0.64
21:S:92:ARG:HD3	55:S:202:HOH:O	1.98	0.64
51:x:30:LEU:HB2	51:x:48:ILE:HG22	1.79	0.64
2:2:1151:A:HO2'	2:2:1152:A:P	2.21	0.64
2:2:1297:G:N2	39:l:113:LYS:O	2.31	0.64
1:1:1363:C:O2'	1:1:1809:A:N3	2.30	0.63
6:B:203:VAL:HG12	55:B:404:HOH:O	1.98	0.63
40:m:10:LEU:HD22	40:m:74:ILE:HD11	1.79	0.63
42:o:57:VAL:HG22	42:o:58:ASN:H	1.64	0.63
1:1:1244:A:O2'	8:D:29:HIS:NE2	2.23	0.63
34:g:30:ILE:HD12	34:g:30:ILE:O	1.99	0.63
35:h:15:LYS:NZ	35:h:182:ASP:OD1	2.29	0.63
1:1:1069:A:N7	1:1:1073:A:N6	2.47	0.63
1:1:2512:C:OP2	7:C:128:ARG:NH2	2.32	0.63
13:K:116:ILE:HD11	55:K:202:HOH:O	1.99	0.63
1:1:770:G:H5''	31:d:10:LEU:HD23	1.81	0.62
1:1:898:C:O2'	1:1:899:A:OP1	2.16	0.62
1:1:1322:A:N1	1:1:1333:G:O2'	2.26	0.62
2:2:875:U:O2'	40:m:14:ARG:NH1	2.32	0.62
27:Y:24:GLU:O	27:Y:28:LEU:HD12	1.98	0.62
1:1:2831:G:N2	1:1:2884:U:OP2	2.33	0.62
2:2:1064:G:N2	2:2:1191:A:OP1	2.31	0.62
12:J:17:VAL:HG23	12:J:137:PRO:HB2	1.80	0.62
2:2:105:G:OP2	52:y:12:GLN:NE2	2.33	0.62
1:1:2123:G:N2	1:1:2124:G:O6	2.34	0.61
2:2:1317:C:O2	51:x:36:ARG:NH2	2.32	0.61
46:s:32:ASP:OD1	46:s:33:VAL:N	2.32	0.61
2:2:1316:G:N1	2:2:1319:A:OP2	2.33	0.61
38:k:15:SER:HA	38:k:18:VAL:HG23	1.81	0.61
2:2:948:C:H2'	2:2:949:A:H8	1.64	0.61
2:2:1151:A:O2'	2:2:1152:A:OP1	2.14	0.61
47:t:45:HIS:O	47:t:47:LYS:N	2.33	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
39:l:80:GLY:CA	55:l:202:HOH:O	2.29	0.61
1:1:1668:A:O2'	1:1:1674:G:N7	2.25	0.61
2:2:437:U:H4'	55:2:1748:HOH:O	2.00	0.61
36:i:12:ARG:NH1	36:i:36:ALA:O	2.33	0.61
53:z:32:ARG:HG3	53:z:33:ARG:HG2	1.82	0.61
36:i:146:GLU:OE2	36:i:146:GLU:N	2.34	0.60
2:2:9:G:OP2	37:j:125:LYS:NZ	2.33	0.60
1:1:585:G:N7	19:Q:5:ARG:NH1	2.49	0.60
2:2:658:C:H1'	47:t:21:THR:HG21	1.83	0.60
2:2:1534:A:N6	55:2:1725:HOH:O	2.35	0.60
1:1:621:A:OP2	14:L:99:ASN:ND2	2.34	0.60
6:B:69:ASN:HA	6:B:188:ARG:NH1	2.13	0.60
36:i:102:TYR:O	36:i:164:ARG:NH1	2.34	0.60
41:n:89:TYR:HB3	41:n:93:LEU:HD12	1.83	0.60
1:1:1712:U:OP2	1:1:1713:A:O2'	2.12	0.60
2:2:1222:G:OP2	2:2:1322:C:N4	2.34	0.60
37:j:105:ILE:HD11	37:j:123:LEU:HD23	1.82	0.60
1:1:1837:C:O2'	1:1:1927:A:N3	2.32	0.60
9:E:116:LEU:O	9:E:177:ARG:N	2.35	0.60
2:2:413:G:H2'	2:2:428:G:N2	2.16	0.60
1:1:898:C:HO2'	1:1:899:A:P	2.25	0.60
1:1:2106:U:H2'	1:1:2107:G:C8	2.37	0.60
1:1:549:G:O2'	1:1:550:C:OP1	2.19	0.59
1:1:743:A:H5''	55:C:304:HOH:O	2.00	0.59
16:N:20:MET:HE1	16:N:40:LYS:HE3	1.84	0.59
23:U:33:VAL:HG13	23:U:66:VAL:HG22	1.84	0.59
11:G:103:VAL:HG12	11:G:108:VAL:O	2.02	0.59
12:J:109:LEU:HD22	12:J:118:MET:SD	2.43	0.59
1:1:30:G:O2'	1:1:1214:A:N3	2.34	0.59
2:2:261:U:N3	2:2:264:C:OP2	2.35	0.59
1:1:495:G:O2'	21:S:57:ASN:ND2	2.35	0.59
1:1:2295:C:H5	55:1:4063:HOH:O	1.84	0.59
2:2:362:G:N2	2:2:365:U:OP2	2.35	0.59
21:S:43:ALA:O	21:S:47:VAL:HG12	2.03	0.59
28:Z:10:ARG:NH2	28:Z:52:PHE:O	2.35	0.59
1:1:1930:G:O2'	1:1:1931:U:O5'	2.20	0.59
10:F:79:THR:OG1	10:F:80:GLU:OE1	2.15	0.59
22:T:4:GLU:OE2	27:Y:22:LEU:HD11	2.03	0.59
41:n:20:ILE:CG1	41:n:60:LEU:HD13	2.33	0.59
55:1:3553:HOH:O	30:c:45:HIS:HD2	1.77	0.59
38:k:80:PHE:CD1	55:k:202:HOH:O	2.51	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:499:A:O4'	2:2:547:A:N6	2.36	0.59
1:1:626:A:N3	14:L:78:ARG:NH2	2.50	0.58
2:2:1001:C:N4	2:2:1002:G:O6	2.35	0.58
55:3:301:HOH:O	9:E:91:ARG:C	2.46	0.58
13:K:69:VAL:HG21	13:K:104:THR:HG21	1.85	0.58
25:W:7:ARG:O	25:W:10:ARG:NH1	2.35	0.58
1:1:1730:C:O2	1:1:1731:G:N1	2.36	0.58
1:1:245:G:N7	32:e:7:ARG:NH2	2.49	0.58
41:n:115:VAL:HG21	42:o:62:ARG:HB2	1.85	0.58
47:t:71:ARG:NH1	55:t:101:HOH:O	2.36	0.58
21:S:92:ARG:CD	55:S:202:HOH:O	2.51	0.58
52:y:77:ASN:OD1	52:y:78:LEU:N	2.37	0.58
1:1:2306:C:N4	9:E:38:GLY:O	2.35	0.58
1:1:2156:G:O6	1:1:2157:G:N2	2.36	0.58
11:G:14:SER:O	11:G:14:SER:OG	2.20	0.58
1:1:380:G:N2	55:1:3369:HOH:O	2.37	0.58
8:D:102:ARG:NH1	8:D:200:LEU:O	2.37	0.58
1:1:372:G:O2'	1:1:373:U:O5'	2.21	0.58
1:1:578:G:OP1	1:1:1255:U:O2'	2.22	0.58
2:2:1347:G:O6	41:n:11:ARG:NH2	2.37	0.58
8:D:3:LEU:HD13	8:D:120:VAL:HG21	1.86	0.57
37:j:80:LEU:HD13	37:j:122:VAL:HG11	1.85	0.57
37:j:149:PRO:HA	37:j:152:VAL:HG22	1.86	0.57
1:1:2162:G:C1'	55:1:3370:HOH:O	2.51	0.57
36:i:197:HIS:NE2	36:i:201:GLU:OE2	2.37	0.57
5:5:1:C:H5	5:5:72:G:H1	1.49	0.57
1:1:372:G:O6	26:X:56:ARG:NH2	2.37	0.57
1:1:2140:G:N2	1:1:2152:G:N7	2.51	0.57
1:1:2572:A:O2'	1:1:2573:C:OP1	2.20	0.57
1:1:2137:U:C3'	55:1:3746:HOH:O	2.41	0.57
1:1:1111:A:O2'	1:1:1112:G:OP1	2.21	0.57
2:2:811:C:O2'	2:2:901:A:N1	2.38	0.57
2:2:1399:C:O2	2:2:1502:A:N6	2.36	0.57
12:J:122:LEU:HG	12:J:124:VAL:HG13	1.87	0.57
1:1:554:U:H2'	1:1:555:G:O4'	2.05	0.57
2:2:1118:U:OP1	41:n:105:ARG:NE	2.33	0.57
2:2:1376:U:O4	39:l:9:ARG:NH1	2.34	0.57
38:k:63:ASN:ND2	38:k:96:VAL:HG22	2.19	0.57
1:1:1992:G:N2	1:1:1996:C:O2'	2.38	0.57
2:2:1452:C:O3'	2:2:1453:G:N2	2.38	0.57
40:m:74:ILE:HG23	40:m:74:ILE:O	2.05	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
55:1:3333:HOH:O	22:T:82:LYS:NZ	2.38	0.57
22:T:6:ARG:O	22:T:10:VAL:HG23	2.04	0.57
1:1:1248:G:OP1	8:D:44:ARG:NH2	2.33	0.56
2:2:1398:A:N6	37:j:26:GLY:O	2.38	0.56
2:2:1518:A:C8	2:2:1519:A:C2	2.93	0.56
1:1:2184:A:H2'	1:1:2185:U:C6	2.41	0.56
2:2:687:A:N6	2:2:703:G:O2'	2.37	0.56
2:2:1159:U:OP1	34:g:131:LYS:NZ	2.33	0.56
20:R:11:GLN:N	20:R:11:GLN:OE1	2.38	0.56
1:1:1068:G:N2	1:1:1095:A:O2'	2.32	0.56
2:2:356:A:N3	2:2:368:U:O2'	2.35	0.56
11:G:77:THR:HA	11:G:143:ILE:O	2.06	0.56
1:1:2684:U:O4'	13:K:70:ARG:NH1	2.39	0.56
34:g:33:ALA:HB2	34:g:39:ILE:HD11	1.88	0.56
39:l:26:VAL:HG22	39:l:42:VAL:HG21	1.88	0.56
1:1:1914:C:H1'	55:1:3568:HOH:O	2.04	0.56
1:1:2110:G:H2'	55:1:3354:HOH:O	2.04	0.56
36:i:61:ARG:NH1	36:i:68:GLU:OE1	2.39	0.56
41:n:41:GLU:N	41:n:41:GLU:OE1	2.39	0.56
2:2:324:G:N1	2:2:327:A:OP2	2.38	0.56
11:G:78:VAL:HG12	11:G:79:THR:H	1.70	0.56
25:W:33:ILE:HG22	25:W:34:VAL:HG23	1.87	0.56
1:1:310:A:HO2'	1:1:311:A:P	2.26	0.55
1:1:1936:A:H8	55:1:4098:HOH:O	1.80	0.55
6:B:204:LEU:O	6:B:206:LYS:N	2.36	0.55
15:M:58:LYS:O	15:M:60:GLN:N	2.39	0.55
37:j:86:GLY:O	37:j:138:ALA:HB1	2.06	0.55
49:v:5:ARG:HD2	55:v:101:HOH:O	2.05	0.55
1:1:805:G:OP2	1:1:806:C:N4	2.38	0.55
34:g:212:TYR:O	34:g:216:VAL:HG23	2.07	0.55
43:p:111:ASP:OD1	43:p:113:THR:HG23	2.05	0.55
1:1:1416:G:H1	1:1:1582:C:H42	1.53	0.55
10:F:79:THR:HG1	10:F:80:GLU:CD	2.11	0.55
42:o:54:SER:O	46:s:81:ARG:NH1	2.38	0.55
45:r:7:ASN:O	45:r:9:PRO:HD3	2.05	0.55
2:2:545:C:OP1	36:i:61:ARG:NH1	2.31	0.55
1:1:2144:G:O2'	1:1:2147:A:N1	2.34	0.55
2:2:410:G:OP1	36:i:25:ARG:NH1	2.40	0.55
44:q:57:LEU:HD21	44:q:82:ILE:HD12	1.88	0.55
1:1:1275:A:N1	1:1:1295:C:O2'	2.36	0.55
9:E:176:PHE:O	9:E:177:ARG:C	2.49	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:L:95:LEU:HD22	14:L:100:ILE:HD11	1.89	0.55
35:h:187:GLU:OE1	35:h:187:GLU:N	2.34	0.55
2:2:1045:C:N4	55:2:1736:HOH:O	2.40	0.55
1:1:2579:C:H2'	1:1:2580:U:O2	2.06	0.55
55:3:301:HOH:O	9:E:92:GLY:CA	2.55	0.55
1:1:500:G:N1	1:1:503:A:OP2	2.34	0.55
1:1:1066:U:H2'	1:1:1068:G:OP2	2.07	0.54
1:1:1084:A:C8	55:1:3317:HOH:O	2.61	0.54
23:U:88:ASP:O	23:U:90:LYS:N	2.41	0.54
52:y:30:PHE:O	52:y:34:VAL:HG23	2.07	0.54
1:1:2306:C:OP2	1:1:2307:G:O2'	2.24	0.54
1:1:2529:G:H4'	10:F:174:LYS:HD3	1.89	0.54
2:2:1157:A:N7	2:2:1180:A:N6	2.55	0.54
7:C:3:GLY:C	7:C:4:LEU:HD12	2.32	0.54
15:M:80:VAL:HG12	55:M:202:HOH:O	2.08	0.54
25:W:79:GLU:OE1	25:W:79:GLU:N	2.40	0.54
49:v:5:ARG:CD	55:v:101:HOH:O	2.54	0.54
1:1:966:G:O4'	1:1:2267:A:N6	2.41	0.54
1:1:307:G:N1	1:1:310:A:OP2	2.41	0.54
3:3:74:U:O2	24:V:29:ILE:HD13	2.07	0.54
16:N:56:LYS:NZ	16:N:87:PHE:O	2.41	0.54
49:v:56:ASP:OD1	49:v:56:ASP:N	2.40	0.54
1:1:1223:G:OP1	20:R:68:ARG:NH2	2.41	0.54
2:2:1347:G:O2'	2:2:1348:U:P	2.65	0.54
6:B:220:ARG:NH1	6:B:222:THR:OG1	2.41	0.54
9:E:116:LEU:HD13	9:E:175:PRO:HD2	1.89	0.54
1:1:560:C:O2'	19:Q:47:ARG:NH2	2.41	0.54
2:2:523:A:N1	44:q:89:OTD:H6	2.23	0.54
2:2:662:U:H2'	2:2:663:A:C8	2.43	0.54
2:2:1028:C:N3	55:2:1744:HOH:O	2.41	0.54
14:L:85:VAL:HG13	14:L:94:THR:O	2.07	0.54
45:r:112:ARG:NH1	55:r:203:HOH:O	2.41	0.54
1:1:1153:C:OP1	19:Q:91:ARG:NH2	2.41	0.54
13:K:78:ARG:NH2	18:P:70:GLU:OE2	2.41	0.54
36:i:103:ARG:HB2	36:i:170:LEU:HD21	1.89	0.54
1:1:2162:G:H2'	1:1:2163:A:C8	2.43	0.53
15:M:110:GLU:OE2	15:M:114:ARG:NH1	2.38	0.53
19:Q:49:ARG:O	19:Q:53:LYS:NZ	2.38	0.53
53:z:35:GLU:HG3	53:z:36:PHE:N	2.16	0.53
1:1:2114:A:N6	1:1:2119:A:N1	2.56	0.53
15:M:57:VAL:O	15:M:58:LYS:C	2.50	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:S:77:ASP:OD1	21:S:77:ASP:N	2.40	0.53
44:q:66:TYR:O	44:q:97:THR:HG22	2.08	0.53
1:1:729:G:C8	6:B:206:LYS:HE3	2.43	0.53
2:2:177:G:OP2	52:y:63:LYS:NZ	2.42	0.53
2:2:523:A:N1	44:q:89:OTD:SB	2.81	0.53
2:2:1125:U:H2'	2:2:1127:G:N7	2.23	0.53
39:l:75:LYS:HE3	39:l:88:VAL:HG11	1.89	0.53
2:2:1123:U:H2'	2:2:1124:G:O4'	2.08	0.53
2:2:1518:A:N7	2:2:1519:A:C2	2.77	0.53
2:2:424:G:H2'	2:2:425:G:C8	2.43	0.53
39:l:35:LYS:HD3	55:l:205:HOH:O	2.08	0.53
1:1:1022:G:H1'	1:1:1023:U:OP2	2.08	0.53
1:1:1203:U:OP2	1:1:1204:A:O2'	2.14	0.53
1:1:716:A:OP2	47:t:88:ARG:NH2	2.42	0.53
1:1:948:C:O2	1:1:984:A:O2'	2.20	0.53
1:1:1328:A:HO2'	1:1:1329:U:P	2.31	0.53
1:1:2505:G:HO2'	1:1:2506:U:P	2.31	0.53
23:U:71:ILE:HD11	23:U:82:VAL:HG22	1.91	0.53
1:1:372:G:O2'	1:1:373:U:P	2.67	0.53
1:1:615:U:H4'	1:1:616:A:OP2	2.09	0.53
26:X:26:ARG:NH1	55:X:101:HOH:O	2.42	0.53
1:1:463:G:N2	1:1:466:A:OP2	2.32	0.53
8:D:176:ASP:OD1	8:D:176:ASP:N	2.41	0.53
50:w:36:GLY:O	50:w:62:ARG:NH2	2.40	0.53
1:1:140:C:O2'	1:1:141:G:O5'	2.20	0.53
1:1:780:G:OP1	6:B:216:ARG:NH2	2.41	0.53
1:1:971:G:OP2	1:1:974:G:N2	2.42	0.53
41:n:46:VAL:CG2	41:n:75:ALA:HB1	2.39	0.53
41:n:91:GLU:HA	41:n:94:ARG:HB2	1.91	0.53
39:l:67:ASN:ND2	39:l:126:ALA:O	2.42	0.52
1:1:859:G:O2'	1:1:860:U:P	2.66	0.52
16:N:69:ARG:C	16:N:70:THR:HG1	2.06	0.52
2:2:745:G:OP1	2:2:851:G:O2'	2.25	0.52
53:z:8:ASN:CA	55:z:102:HOH:O	2.49	0.52
1:1:242:G:O2'	1:1:243:U:P	2.67	0.52
1:1:1953:A:O2'	1:1:2559:C:O2	2.27	0.52
2:2:677:U:O2	2:2:777:A:O2'	2.25	0.52
13:K:116:ILE:CD1	55:K:202:HOH:O	2.56	0.52
36:i:103:ARG:CB	36:i:170:LEU:HD21	2.39	0.52
2:2:454:G:H5''	55:2:1931:HOH:O	2.09	0.52
21:S:38:TYR:CE2	29:b:27:LEU:HD21	2.45	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:673:A:H2'	2:2:674:G:C8	2.44	0.52
44:q:101:ALA:O	44:q:102:LEU:HG	2.10	0.52
2:2:948:C:H2'	2:2:949:A:C8	2.44	0.52
38:k:18:VAL:HG21	38:k:58:HIS:CD2	2.45	0.52
1:1:1095:A:C5'	55:1:3334:HOH:O	2.54	0.52
2:2:333:U:H2'	2:2:334:C:C6	2.45	0.52
36:i:177:MET:N	36:i:177:MET:SD	2.82	0.52
47:t:10:ILE:HG21	47:t:30:LEU:HD12	1.92	0.52
1:1:458:G:O2'	1:1:459:U:P	2.68	0.52
16:N:79:LEU:HD23	16:N:83:LEU:HD12	1.91	0.52
34:g:116:LEU:HD22	34:g:140:LEU:HD12	1.90	0.52
1:1:2467:C:H2'	1:1:2468:A:O4'	2.10	0.52
1:1:1542:U:H2'	1:1:1543:G:O4'	2.10	0.51
1:1:2029:G:N1	1:1:2033:A:OP2	2.40	0.51
1:1:2137:U:C2'	55:1:3746:HOH:O	2.57	0.51
1:1:2314:A:H1'	9:E:154:THR:HG21	1.92	0.51
1:1:2478:A:OP2	33:f:2:LYS:NZ	2.42	0.51
8:D:4:VAL:C	8:D:5:LEU:HD12	2.35	0.51
1:1:91:A:O2'	1:1:92:U:P	2.68	0.51
1:1:1028:A:OP2	1:1:1126:A:N6	2.39	0.51
1:1:2167:U:H3	1:1:2170:A:H62	1.59	0.51
2:2:8:A:N6	36:i:201:GLU:O	2.43	0.51
15:M:35:ALA:HB2	15:M:102:LEU:HD11	1.93	0.51
1:1:2134:A:O2'	1:1:2159:G:N3	2.43	0.51
3:3:42:C:C5	9:E:65:LEU:HD22	2.46	0.51
32:e:31:ILE:CG2	32:e:34:LYS:HE3	2.41	0.51
45:r:92:ARG:NH1	55:r:201:HOH:O	2.25	0.51
1:1:84:A:N1	1:1:98:G:O2'	2.41	0.51
2:2:768:A:N3	2:2:1512:U:O2'	2.43	0.51
2:2:1005:A:N6	2:2:1024:G:O2'	2.44	0.51
10:F:34:ARG:NE	10:F:70:LEU:HD13	2.22	0.51
22:T:57:VAL:HG12	22:T:86:THR:OG1	2.11	0.51
45:r:85:TYR:HA	55:r:205:HOH:O	2.11	0.51
1:1:490:C:O2'	1:1:491:G:OP2	2.26	0.51
2:2:1134:G:N7	55:2:1723:HOH:O	2.34	0.51
42:o:84:VAL:HG13	42:o:85:ASP:N	2.25	0.51
48:u:61:VAL:HG22	48:u:67:ILE:HD11	1.93	0.51
1:1:447:A:N1	1:1:454:A:O2'	2.35	0.51
2:2:1432:G:HO2'	2:2:1433:A:P	2.33	0.51
21:S:22:ASP:OD1	21:S:25:ARG:NH2	2.43	0.51
1:1:2655:G:O2'	1:1:2656:U:P	2.69	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:523:A:N6	44:q:89:0TD:H6	2.26	0.51
5:5:48:C:N4	5:5:59:A:N7	2.59	0.51
48:u:25:ARG:NH1	55:u:102:HOH:O	2.43	0.51
2:2:766:A:OP2	2:2:812:G:N2	2.44	0.51
37:j:105:ILE:HD11	37:j:123:LEU:CD2	2.41	0.51
42:o:10:LEU:HD12	42:o:18:ILE:HD11	1.93	0.51
48:u:6:LEU:CD2	48:u:19:VAL:HG22	2.41	0.51
1:1:1416:G:O2'	1:1:1417:C:O5'	2.26	0.51
14:L:76:GLU:HB2	14:L:111:ILE:HD13	1.92	0.51
39:l:96:ASN:OD1	39:l:97:ALA:N	2.44	0.51
1:1:1869:G:H3'	1:1:1870:C:C5'	2.42	0.50
51:x:50:VAL:HG21	51:x:70:LEU:HB3	1.94	0.50
1:1:858:G:HO2'	1:1:859:G:P	2.33	0.50
1:1:1020:A:H1'	1:1:1021:A:OP2	2.11	0.50
2:2:1320:C:O5'	51:x:2:ARG:NH2	2.44	0.50
43:p:36:ARG:NH2	43:p:82:GLU:OE2	2.41	0.50
2:2:957:U:H4'	51:x:78:THR:O	2.11	0.50
35:h:155:ARG:NE	35:h:159:ALA:O	2.35	0.50
51:x:10:ILE:HG21	51:x:40:PHE:CE2	2.46	0.50
1:1:549:G:HO2'	1:1:550:C:P	2.35	0.50
1:1:2134:A:N6	1:1:2157:G:O4'	2.45	0.50
1:1:2771:C:O2'	7:C:173:GLN:NE2	2.43	0.50
2:2:944:G:N1	2:2:1338:G:OP2	2.41	0.50
1:1:2326:C:HO2'	1:1:2327:A:P	2.27	0.50
13:K:90:ASN:OD1	13:K:91:SER:N	2.44	0.50
15:M:58:LYS:O	15:M:60:GLN:HG3	2.12	0.50
34:g:95:TRP:NE1	34:g:99:MET:SD	2.85	0.50
1:1:1111:A:HO2'	1:1:1112:G:P	2.35	0.50
1:1:1625:C:H2'	1:1:1626:A:O4'	2.12	0.50
55:1:3332:HOH:O	6:B:52:HIS:HD2	1.94	0.50
10:F:105:SER:O	10:F:105:SER:OG	2.30	0.50
49:v:6:THR:C	49:v:7:LEU:HD12	2.36	0.50
34:g:93:HIS:ND1	34:g:145:ASN:O	2.44	0.50
41:n:96:GLU:OE2	41:n:96:GLU:N	2.44	0.50
1:1:247:G:OP2	1:1:249:C:N4	2.40	0.50
1:1:962:G:H21	1:1:2250:G:H1	1.59	0.50
2:2:1211:U:C2'	55:2:1736:HOH:O	2.30	0.50
6:B:106:PRO:HD2	6:B:109:LEU:HD22	1.93	0.50
1:1:242:G:N2	1:1:255:A:OP2	2.40	0.50
1:1:1236:G:O2'	1:1:1237:A:O5'	2.27	0.50
13:K:99:ILE:HD13	13:K:115:ILE:HG23	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:M:22:GLN:NE2	55:M:203:HOH:O	2.45	0.50
1:1:1282:U:H2'	1:1:1283:G:O4'	2.12	0.49
2:2:254:G:H5''	49:v:70:LYS:HD3	1.93	0.49
2:2:424:G:H2'	2:2:425:G:H8	1.77	0.49
13:K:35:VAL:HG11	13:K:106:GLU:HB2	1.94	0.49
13:K:86:LEU:O	13:K:87:LEU:HD23	2.11	0.49
19:Q:96:ASP:OD2	20:R:13:ARG:NH2	2.43	0.49
2:2:408:A:O2'	36:i:24:VAL:HG23	2.11	0.49
2:2:545:C:O2'	2:2:549:C:OP1	2.30	0.49
2:2:1306:A:C2	45:r:107:THR:HG21	2.46	0.49
6:B:66:PHE:HZ	6:B:86:ARG:NH1	2.07	0.49
40:m:10:LEU:HD22	40:m:74:ILE:CD1	2.41	0.49
44:q:33:VAL:HG22	44:q:79:VAL:HG12	1.95	0.49
1:1:1942:C:OP2	1:1:1943:U:O2'	2.21	0.49
1:1:2020:A:H5'	29:b:8:THR:HG21	1.94	0.49
1:1:2725:A:H3'	55:1:3944:HOH:O	2.12	0.49
9:E:148:VAL:HG12	9:E:148:VAL:O	2.11	0.49
24:V:35:GLU:N	24:V:35:GLU:OE1	2.45	0.49
1:1:205:G:HO2'	1:1:206:U:P	2.35	0.49
1:1:958:U:OP2	15:M:14:LYS:NZ	2.45	0.49
2:2:781:A:O2'	2:2:1522:U:O2	2.28	0.49
35:h:42:LEU:HD23	35:h:54:ILE:HG21	1.94	0.49
38:k:92:THR:OG1	38:k:93:LYS:N	2.44	0.49
40:m:95:MET:HE2	40:m:98:LEU:HD11	1.94	0.49
1:1:558:U:H2'	1:1:559:G:C8	2.48	0.49
1:1:1099:G:N7	55:1:3356:HOH:O	2.35	0.49
6:B:67:LYS:HG2	6:B:150:GLY:HA2	1.93	0.49
1:1:856:G:H2'	1:1:857:G:C8	2.48	0.49
1:1:1319:C:H2'	1:1:1320:C:O4'	2.13	0.49
1:1:1328:A:O2'	1:1:1329:U:P	2.70	0.49
1:1:2848:G:O2'	1:1:2849:U:O5'	2.28	0.49
13:K:35:VAL:HG13	13:K:69:VAL:HG11	1.94	0.49
13:K:80:ASP:OD2	18:P:61:ARG:NH1	2.43	0.49
16:N:2:ARG:O	16:N:2:ARG:HD3	2.12	0.49
52:y:67:HIS:O	52:y:67:HIS:ND1	2.46	0.49
1:1:2250:G:H21	1:1:2496:C:H4'	1.75	0.49
1:1:1003:G:O2'	1:1:1010:A:N1	2.42	0.49
1:1:2137:U:H2'	55:1:3746:HOH:O	2.13	0.49
24:V:75:GLN:HB2	24:V:92:VAL:HG23	1.94	0.49
34:g:119:GLN:HG2	55:g:308:HOH:O	2.12	0.49
1:1:499:U:H2'	1:1:500:G:O4'	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:1204:A:O4'	1:1:1206:G:C8	2.66	0.49
2:2:1158:C:N4	2:2:1160:G:C8	2.81	0.49
2:2:1492:A:C8	4:4:19:U:O2'	2.50	0.49
10:F:8:VAL:O	10:F:48:THR:HA	2.13	0.49
27:Y:8:GLU:N	27:Y:8:GLU:OE1	2.45	0.49
34:g:25:LYS:NZ	55:g:302:HOH:O	2.46	0.49
1:1:645:C:H2'	1:1:647:G:N7	2.28	0.49
1:1:1176:U:H2'	1:1:1177:G:C8	2.48	0.49
1:1:1847:G:O2'	1:1:1848:A:O5'	2.25	0.49
1:1:1869:G:O2'	1:1:1872:A:N6	2.46	0.49
1:1:2489:U:H2'	1:1:2490:G:O4'	2.13	0.49
34:g:75:ALA:HB2	34:g:209:VAL:HG21	1.95	0.49
38:k:47:LEU:HD13	38:k:51:ILE:HD12	1.94	0.49
46:s:30:ILE:HG21	46:s:44:ALA:HB2	1.95	0.49
48:u:36:VAL:HG11	48:u:57:ILE:HG13	1.95	0.49
1:1:74:A:H4'	1:1:75:G:O5'	2.13	0.48
1:1:555:G:HO2'	1:1:556:A:H8	1.59	0.48
1:1:1357:C:H2'	1:1:1358:G:O4'	2.13	0.48
1:1:1799:G:OP1	6:B:257:ARG:NE	2.46	0.48
1:1:2452:C:H2'	1:1:2453:A:O4'	2.12	0.48
1:1:2477:U:O2	33:f:4:ARG:NH2	2.45	0.48
2:2:28:A:O2'	2:2:296:U:OP1	2.30	0.48
2:2:151:A:C2	2:2:152:A:H1'	2.48	0.48
2:2:261:U:OP2	52:y:73:ARG:NH2	2.46	0.48
16:N:49:GLU:OE2	16:N:95:THR:HG22	2.13	0.48
53:z:33:ARG:O	53:z:34:ARG:C	2.53	0.48
1:1:140:C:O2'	1:1:141:G:P	2.71	0.48
18:P:105:LYS:O	18:P:108:ARG:NH2	2.46	0.48
30:c:4:ILE:HG21	30:c:27:ARG:NH2	2.29	0.48
24:V:76:ASP:OD1	24:V:77:VAL:N	2.45	0.48
2:2:993:G:H21	2:2:996:A:H61	1.62	0.48
44:q:74:LEU:HD21	44:q:80:ILE:HG21	1.96	0.48
1:1:1930:G:O2'	1:1:1931:U:P	2.71	0.48
1:1:2266:A:H4'	1:1:2267:A:O5'	2.13	0.48
14:L:128:THR:OG1	14:L:129:LYS:N	2.45	0.48
1:1:2348:U:OP1	32:e:37:THR:HG21	2.13	0.48
7:C:151:THR:HB	7:C:152:PRO:HD3	1.95	0.48
10:F:94:ARG:NE	10:F:127:GLN:OE1	2.47	0.48
53:z:34:ARG:HD2	53:z:36:PHE:HZ	1.76	0.48
2:2:530:G:O6	4:4:20:U:O2'	2.32	0.48
26:X:64:ASP:OD2	26:X:64:ASP:N	2.46	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:k:5:GLU:HB2	38:k:90:MET:HE3	1.95	0.48
41:n:46:VAL:HG23	41:n:75:ALA:HB1	1.95	0.48
1:1:1055:G:O2'	1:1:1085:A:N1	2.38	0.48
1:1:2655:G:O2'	1:1:2656:U:O5'	2.32	0.48
2:2:335:C:H2'	2:2:336:A:C8	2.49	0.48
42:o:63:ASP:OD2	46:s:98:LYS:NZ	2.44	0.48
1:1:1853:A:N3	1:1:2233:U:O2'	2.42	0.48
1:1:2166:U:H4'	55:1:3481:HOH:O	2.13	0.48
1:1:1499:C:C2	1:1:1500:G:C8	3.02	0.47
41:n:20:ILE:HG13	41:n:60:LEU:HD13	1.94	0.47
1:1:2032:G:N2	7:C:151:THR:OG1	2.47	0.47
1:1:2139:U:O2	1:1:2152:G:O6	2.32	0.47
1:1:240:C:OP2	1:1:241:A:O2'	2.22	0.47
2:2:246:A:C2	2:2:282:A:C5	3.02	0.47
2:2:413:G:H2'	2:2:428:G:H22	1.79	0.47
2:2:1041:G:H2'	2:2:1042:A:C8	2.49	0.47
2:2:1157:A:H4'	2:2:1158:C:O4'	2.15	0.47
31:d:1:MET:HE1	31:d:3:ARG:NH1	2.29	0.47
1:1:44:A:H2'	1:1:45:G:O4'	2.13	0.47
1:1:549:G:O2'	1:1:550:C:P	2.71	0.47
1:1:2013:A:OP1	21:S:97:LEU:N	2.42	0.47
2:2:938:A:O2'	39:l:94:ARG:NH2	2.45	0.47
2:2:1023:U:C4'	55:2:1857:HOH:O	2.57	0.47
2:2:1064:G:H4'	2:2:1065:U:OP1	2.14	0.47
6:B:2:VAL:HG21	6:B:201:LEU:HD12	1.97	0.47
24:V:48:MET:O	24:V:51:GLN:HG3	2.15	0.47
32:e:28:LEU:HA	32:e:32:LEU:HD21	1.96	0.47
1:1:26:G:O2'	1:1:27:G:O4'	2.31	0.47
1:1:2867:G:C2'	1:1:2868:A:OP2	2.62	0.47
2:2:20:U:H2'	2:2:21:G:O4'	2.14	0.47
2:2:1304:G:N2	2:2:1334:G:C6	2.83	0.47
9:E:152:ASP:OD1	9:E:152:ASP:N	2.46	0.47
20:R:38:VAL:HG13	20:R:38:VAL:O	2.14	0.47
1:1:2394:C:H42	5:5:76:A:H1'	1.80	0.47
2:2:1040:U:O2'	2:2:1041:G:O5'	2.33	0.47
2:2:1182:G:H5'	2:2:1183:U:OP1	2.14	0.47
1:1:1251:C:O2'	1:1:1253:A:OP2	2.33	0.47
1:1:2194:U:O2'	1:1:2195:U:P	2.72	0.47
1:1:2832:U:O2	1:1:2834:G:N2	2.48	0.47
2:2:526:C:P	44:q:88:LYS:HZ3	2.38	0.47
2:2:951:G:OP2	45:r:100:ARG:NH2	2.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:1054:C:N4	2:2:1196:A:N7	2.63	0.47
2:2:1182:G:H4'	2:2:1183:U:O5'	2.15	0.47
9:E:90:LEU:HD12	9:E:90:LEU:O	2.15	0.47
9:E:116:LEU:H	9:E:175:PRO:HB2	1.79	0.47
14:L:77:ILE:HD11	14:L:101:ILE:HG21	1.96	0.47
15:M:76:LYS:NZ	15:M:83:GLY:O	2.44	0.47
37:j:12:GLU:OE1	37:j:67:ARG:NH2	2.48	0.47
46:s:54:ASP:OD1	46:s:59:ARG:NE	2.45	0.47
51:x:26:ASP:HA	55:x:101:HOH:O	2.13	0.47
1:1:242:G:HO2'	1:1:243:U:P	2.36	0.47
1:1:837:C:N3	1:1:941:A:N6	2.62	0.47
1:1:1358:G:N7	55:1:3363:HOH:O	2.35	0.47
1:1:1913:A:N6	55:1:3446:HOH:O	2.48	0.47
2:2:580:C:H2'	2:2:581:G:O4'	2.15	0.47
11:G:72:ILE:HG23	11:G:73:ASN:N	2.29	0.47
11:G:76:GLU:HG2	11:G:142:VAL:HG22	1.97	0.47
1:1:645:C:H2'	1:1:647:G:C8	2.50	0.47
1:1:1107:G:C2	1:1:1108:U:C5	3.03	0.47
1:1:2123:G:H3'	55:1:3487:HOH:O	2.13	0.47
1:1:2831:G:OP2	7:C:59:ARG:NH1	2.48	0.47
13:K:92:GLU:O	13:K:93:GLN:C	2.58	0.47
21:S:1:MET:HG3	21:S:2:GLU:N	2.30	0.47
34:g:14:HIS:O	34:g:15:PHE:C	2.57	0.47
42:o:86:ALA:O	42:o:90:LEU:HD12	2.14	0.47
1:1:1980:G:O2'	1:1:1982:U:OP2	2.28	0.47
2:2:524:G:H2'	2:2:525:C:C6	2.50	0.47
15:M:80:VAL:CG1	55:M:202:HOH:O	2.63	0.47
17:O:53:THR:HG21	17:O:70:ALA:HB1	1.96	0.47
34:g:33:ALA:HB3	34:g:37:VAL:CG1	2.45	0.47
1:1:1856:U:H2'	1:1:1857:G:O4'	2.15	0.46
1:1:2333:A:H4'	1:1:2334:U:O5'	2.15	0.46
2:2:511:C:O2'	2:2:512:U:O5'	2.30	0.46
5:5:12:G:C6	5:5:24:G:C6	3.04	0.46
8:D:7:ASP:OD1	8:D:7:ASP:N	2.44	0.46
11:G:58:LEU:HD23	11:G:62:LEU:HD12	1.97	0.46
42:o:15:HIS:HA	42:o:18:ILE:HG22	1.97	0.46
49:v:60:ILE:HG22	49:v:72:TRP:HE3	1.80	0.46
53:z:33:ARG:HH21	53:z:34:ARG:HE	1.63	0.46
2:2:1063:C:OP2	2:2:1064:G:O2'	2.31	0.46
3:3:112:G:N2	17:O:45:SER:O	2.33	0.46
14:L:111:ILE:HD12	14:L:111:ILE:H	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:528:A:C2	1:1:2043:C:H4'	2.50	0.46
1:1:818:G:N1	1:1:1188:U:OP2	2.37	0.46
1:1:859:G:HO2'	1:1:860:U:P	2.37	0.46
55:1:3332:HOH:O	6:B:52:HIS:CD2	2.67	0.46
1:1:695:G:OP1	1:1:1380:G:O2'	2.33	0.46
2:2:254:G:N2	49:v:17:GLU:OE1	2.49	0.46
2:2:950:U:H2'	2:2:951:G:C8	2.51	0.46
39:l:80:GLY:C	55:l:202:HOH:O	2.55	0.46
53:z:36:PHE:C	53:z:38:GLU:H	2.23	0.46
1:1:981:A:OP2	1:1:982:C:N4	2.39	0.46
2:2:180:U:H2'	2:2:181:A:O4'	2.15	0.46
2:2:438:U:HO2'	2:2:439:U:P	2.38	0.46
26:X:11:PRO:HB3	26:X:29:LEU:HD23	1.98	0.46
53:z:23:GLU:O	53:z:24:LYS:C	2.59	0.46
1:1:372:G:HO2'	1:1:373:U:P	2.38	0.46
1:1:627:A:OP2	55:1:3301:HOH:O	2.20	0.46
11:G:78:VAL:HG12	11:G:79:THR:N	2.31	0.46
11:G:103:VAL:HG12	11:G:108:VAL:N	2.30	0.46
12:J:7:LYS:O	12:J:11:VAL:HG23	2.16	0.46
37:j:105:ILE:HG13	37:j:105:ILE:O	2.16	0.46
1:1:753:A:H8	1:1:753:A:OP2	1.99	0.46
2:2:1144:G:H21	2:2:1146:A:H62	1.62	0.46
6:B:75:ALA:HB1	6:B:93:VAL:CG1	2.46	0.46
18:P:70:GLU:OE2	18:P:100:ARG:NH1	2.42	0.46
46:s:69:ARG:NH1	46:s:71:HIS:O	2.48	0.46
1:1:394:C:H2'	1:1:395:U:O4'	2.16	0.46
1:1:1378:A:C4'	1:1:1379:U:OP1	2.64	0.46
2:2:542:G:O2'	36:i:13:ARG:NH2	2.48	0.46
3:3:5:U:H2'	3:3:6:G:C8	2.50	0.46
1:1:1528:A:OP2	1:1:1543:G:N2	2.49	0.46
55:1:4154:HOH:O	15:M:6:ARG:HD3	2.16	0.46
2:2:48:C:H5'	2:2:49:U:OP2	2.15	0.46
2:2:868:C:H2'	2:2:869:G:O4'	2.16	0.46
2:2:936:C:C4	2:2:937:A:N7	2.84	0.46
2:2:1309:G:O6	2:2:1329:A:C6	2.69	0.46
31:d:13:ASN:O	55:d:101:HOH:O	2.21	0.46
44:q:48:ALA:C	44:q:49:LEU:HD22	2.40	0.46
47:t:25:GLU:OE2	47:t:76:ARG:NH1	2.49	0.46
47:t:87:ARG:O	47:t:88:ARG:C	2.59	0.46
1:1:34:U:N3	55:1:3361:HOH:O	2.35	0.45
1:1:1906:G:H2'	1:1:1907:G:O4'	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:2446:G:N2	1:1:2449:U:O2	2.49	0.45
7:C:25:THR:OG1	7:C:191:GLY:O	2.25	0.45
2:2:393:A:C2	2:2:394:G:C8	3.04	0.45
2:2:1040:U:H2'	2:2:1041:G:C8	2.51	0.45
2:2:1200:C:H5''	2:2:1201:A:H3'	1.98	0.45
2:2:1224:U:C4'	55:2:1836:HOH:O	2.61	0.45
2:2:1345:U:OP1	41:n:121:ARG:NH1	2.49	0.45
3:3:12:C:O2	3:3:12:C:O4'	2.34	0.45
11:G:69:ALA:O	11:G:72:ILE:HG22	2.16	0.45
35:h:18:ASN:O	35:h:55:VAL:HG13	2.16	0.45
1:1:1131:G:O2'	1:1:2025:C:O2'	2.32	0.45
2:2:373:A:N3	2:2:482:A:N6	2.64	0.45
21:S:38:TYR:CD2	29:b:27:LEU:HD21	2.51	0.45
1:1:754:U:O2'	1:1:1272:A:N1	2.47	0.45
1:1:974:G:O2'	1:1:989:G:N2	2.50	0.45
1:1:2098:U:H2'	1:1:2099:U:O4'	2.17	0.45
1:1:2305:U:C4	55:1:3305:HOH:O	2.56	0.45
2:2:343:U:O2'	2:2:346:G:O6	2.25	0.45
40:m:102:VAL:O	40:m:125:ILE:N	2.43	0.45
1:1:226:A:H2'	1:1:227:A:O4'	2.15	0.45
1:1:575:A:OP2	1:1:2499:C:O2'	2.34	0.45
1:1:671:C:OP1	14:L:43:GLY:N	2.41	0.45
1:1:1693:U:O2'	6:B:13:ARG:NH2	2.49	0.45
1:1:2333:A:O2'	1:1:2334:U:O5'	2.31	0.45
1:1:2687:U:H2'	1:1:2688:G:O4'	2.16	0.45
2:2:1107:C:C4	2:2:1108:G:C8	3.05	0.45
39:l:36:SER:HA	41:n:42:THR:HG21	1.98	0.45
45:r:7:ASN:HB2	45:r:21:ILE:HD11	1.99	0.45
48:u:78:VAL:HG13	48:u:78:VAL:O	2.16	0.45
1:1:48:G:N2	1:1:177:G:OP2	2.50	0.45
1:1:748:G:O6	1:1:751:A:H4'	2.17	0.45
1:1:2194:U:O2'	1:1:2195:U:OP1	2.32	0.45
2:2:875:U:HO2'	40:m:14:ARG:NH1	2.15	0.45
2:2:1148:U:H5''	41:n:8:THR:HG23	1.98	0.45
2:2:1216:A:C2	2:2:1217:C:C5	3.05	0.45
2:2:1347:G:O2'	2:2:1348:U:OP2	2.35	0.45
55:3:301:HOH:O	9:E:92:GLY:HA3	2.16	0.45
7:C:129:THR:HG22	7:C:130:GLN:O	2.16	0.45
14:L:77:ILE:CD1	14:L:108:ALA:HB1	2.46	0.45
16:N:36:THR:OG1	16:N:37:THR:N	2.50	0.45
21:S:4:ILE:HG22	21:S:106:VAL:HG22	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:h:125:ARG:NH1	55:h:302:HOH:O	2.28	0.45
1:1:161:A:H3'	1:1:162:U:H5''	1.99	0.45
1:1:1737:G:O3'	1:1:1738:G:O4'	2.35	0.45
2:2:751:U:H2'	2:2:752:G:O4'	2.16	0.45
2:2:757:U:OP1	2:2:822:U:O2'	2.32	0.45
3:3:54:G:O2'	9:E:24:VAL:HG11	2.17	0.45
1:1:357:C:C2	1:1:358:U:C5	3.04	0.45
1:1:579:G:O2'	1:1:2019:A:OP1	2.35	0.45
1:1:2313:C:O2'	9:E:34:THR:HG21	2.17	0.45
2:2:564:C:OP2	44:q:12:ARG:NH2	2.45	0.45
2:2:779:C:H2'	2:2:780:A:O4'	2.16	0.45
2:2:1396:A:H2	37:j:23:THR:HG21	1.82	0.45
20:R:6:GLN:OE1	20:R:11:GLN:NE2	2.50	0.45
34:g:27:LYS:N	34:g:28:PRO:CD	2.80	0.45
37:j:114:LEU:O	37:j:119:VAL:HG22	2.16	0.45
38:k:3:HIS:HB2	38:k:92:THR:HA	1.99	0.45
39:l:89:GLU:OE1	39:l:89:GLU:N	2.44	0.45
53:z:36:PHE:O	53:z:38:GLU:N	2.50	0.45
1:1:891:G:O2'	1:1:892:A:O4'	2.33	0.45
55:1:3346:HOH:O	31:d:45:SER:HB3	2.16	0.45
2:2:923:A:O2'	2:2:1399:C:OP2	2.32	0.45
34:g:33:ALA:HB3	34:g:37:VAL:HG13	1.99	0.45
37:j:110:MET:HA	37:j:113:VAL:HG12	1.98	0.45
1:1:1521:G:OP2	1:1:1522:A:O2'	2.27	0.44
1:1:1558:C:O4'	1:1:1560:G:C8	2.69	0.44
9:E:73:VAL:HG22	9:E:78:ILE:HD11	1.99	0.44
36:i:44:LYS:HE2	55:i:306:HOH:O	2.17	0.44
1:1:61:C:H2'	1:1:62:U:O4'	2.18	0.44
1:1:493:G:H2'	1:1:494:G:O4'	2.17	0.44
1:1:1028:A:N3	1:1:2486:C:O2'	2.41	0.44
1:1:2194:U:HO2'	1:1:2195:U:P	2.40	0.44
1:1:2266:A:H4'	1:1:2267:A:N3	2.31	0.44
2:2:978:A:C4	2:2:1319:A:C2	3.05	0.44
2:2:1380:U:H5''	55:2:1952:HOH:O	2.17	0.44
40:m:84:ILE:HG21	40:m:124:ILE:HD11	1.98	0.44
45:r:3:ILE:H	45:r:3:ILE:HG12	1.30	0.44
47:t:17:ASP:OD1	47:t:17:ASP:N	2.50	0.44
1:1:306:U:H3	1:1:310:A:H62	1.64	0.44
1:1:937:C:C2	1:1:938:G:C8	3.05	0.44
1:1:1048:A:OP2	1:1:1110:G:N2	2.50	0.44
1:1:1716:U:OP2	1:1:1743:G:N1	2.45	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:1901:A:H4'	6:B:252:LYS:HD3	1.98	0.44
2:2:558:G:OP2	2:2:559:A:O2'	2.28	0.44
3:3:27:C:OP1	17:O:34:HIS:NE2	2.50	0.44
55:3:301:HOH:O	9:E:91:ARG:HG3	2.17	0.44
7:C:8:LYS:HB2	7:C:201:LEU:HD11	2.00	0.44
14:L:85:VAL:HG12	14:L:86:GLU:N	2.32	0.44
18:P:67:GLU:OE1	55:P:201:HOH:O	2.21	0.44
21:S:5:ALA:HB3	21:S:54:ALA:HB2	1.99	0.44
22:T:56:GLU:N	22:T:86:THR:O	2.48	0.44
40:m:49:LYS:O	40:m:58:LEU:HD12	2.16	0.44
48:u:78:VAL:O	48:u:79:ASN:C	2.61	0.44
1:1:75:G:N3	1:1:75:G:H2'	2.31	0.44
1:1:2168:G:N3	1:1:2168:G:H2'	2.32	0.44
2:2:1201:A:H1'	2:2:1202:U:OP2	2.17	0.44
21:S:3:THR:HG21	21:S:58:ALA:CA	2.47	0.44
26:X:39:VAL:O	26:X:43:LYS:N	2.50	0.44
37:j:15:ILE:HD13	37:j:37:VAL:HG23	2.00	0.44
6:B:141:HIS:ND1	6:B:192:GLY:O	2.44	0.44
7:C:4:LEU:HD23	7:C:29:VAL:HG11	1.99	0.44
11:G:148:ALA:HA	55:G:201:HOH:O	2.09	0.44
29:b:54:ILE:HG23	29:b:56:LYS:N	2.32	0.44
45:r:54:THR:O	45:r:57:ASP:OD1	2.36	0.44
1:1:698:C:O2'	1:1:734:A:N6	2.50	0.44
1:1:2011:U:H2'	1:1:2012:G:O4'	2.18	0.44
1:1:2327:A:H2'	1:1:2328:A:C8	2.53	0.44
1:1:2505:G:H2'	1:1:2576:G:H1	1.83	0.44
2:2:132:C:O3'	52:y:67:HIS:NE2	2.51	0.44
8:D:77:ILE:O	8:D:77:ILE:HG22	2.17	0.44
42:o:10:LEU:HD12	42:o:10:LEU:O	2.18	0.44
1:1:263:G:O2'	1:1:429:A:N3	2.48	0.44
1:1:558:U:H2'	1:1:559:G:H8	1.83	0.44
1:1:1041:G:C2	1:1:1042:G:N7	2.85	0.44
1:1:1370:C:H2'	1:1:1371:G:O4'	2.18	0.44
1:1:1379:U:OP1	1:1:1379:U:C6	2.70	0.44
1:1:1695:G:N7	6:B:13:ARG:NH2	2.66	0.44
1:1:1730:C:O2'	1:1:1731:G:O4'	2.35	0.44
1:1:2526:G:N3	33:f:1:MET:N	2.66	0.44
2:2:524:G:N2	55:2:1768:HOH:O	2.48	0.44
2:2:1218:C:H2'	2:2:1219:A:C8	2.52	0.44
3:3:30:C:H1'	3:3:57:A:H61	1.83	0.44
13:K:88:ASN:O	13:K:90:ASN:N	2.49	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:1288:G:OP2	1:1:1288:G:N2	2.33	0.44
1:1:1619:G:O2'	31:d:1:MET:N	2.51	0.44
1:1:2138:G:H8	55:1:3746:HOH:O	1.97	0.44
1:1:2345:G:C8	1:1:2347:C:C5	3.06	0.44
1:1:2604:U:O2	1:1:2604:U:O4'	2.36	0.44
1:1:2605:U:C5	1:1:2606:C:C5	3.06	0.44
7:C:25:THR:HG21	7:C:193:VAL:HG22	1.99	0.44
10:F:84:LYS:HG2	10:F:140:ILE:HD13	1.99	0.44
15:M:57:VAL:HG12	15:M:112:LEU:HG	2.00	0.44
34:g:20:ARG:O	34:g:22:TRP:N	2.51	0.44
38:k:51:ILE:HD13	38:k:86:ARG:NH1	2.33	0.44
42:o:53:ILE:CD1	55:s:201:HOH:O	2.62	0.44
1:1:833:A:O2'	55:1:3302:HOH:O	2.21	0.44
2:2:345:C:O2'	2:2:346:G:N2	2.51	0.44
2:2:411:A:O2'	2:2:413:G:OP2	2.31	0.44
2:2:458:U:OP2	55:2:1701:HOH:O	2.21	0.44
2:2:924:C:O2'	2:2:1502:A:N1	2.48	0.44
2:2:1396:A:C2	37:j:23:THR:HG21	2.53	0.44
6:B:123:ILE:HG22	6:B:123:ILE:O	2.16	0.44
13:K:7:MET:HE1	13:K:44:LYS:HG3	1.99	0.44
35:h:2:GLN:N	35:h:2:GLN:OE1	2.50	0.44
36:i:94:GLU:OE1	36:i:99:ASN:ND2	2.51	0.44
45:r:49:GLU:OE2	45:r:49:GLU:N	2.51	0.44
46:s:13:VAL:HG22	46:s:60:GLN:OE1	2.18	0.44
1:1:270:A:N1	1:1:369:U:O2'	2.43	0.43
1:1:2893:A:H4'	1:1:2894:G:O5'	2.18	0.43
2:2:62:U:O3'	2:2:384:G:N2	2.51	0.43
2:2:668:G:O2'	47:t:45:HIS:HB3	2.16	0.43
3:3:29:A:H2'	3:3:30:C:O4'	2.17	0.43
14:L:79:LEU:HD12	14:L:112:LEU:HD12	1.98	0.43
15:M:53:MET:O	15:M:57:VAL:HG22	2.18	0.43
37:j:87:VAL:HG23	37:j:91:SER:O	2.18	0.43
39:l:137:ARG:NH2	39:l:138:GLU:OE2	2.51	0.43
1:1:83:A:O2'	1:1:103:A:N6	2.51	0.43
1:1:902:C:C2	1:1:903:C:C5	3.06	0.43
1:1:1295:C:C2	1:1:1296:G:C8	3.06	0.43
1:1:2395:C:H2'	1:1:2396:G:O4'	2.18	0.43
1:1:2795:C:H2'	1:1:2796:U:O4'	2.18	0.43
2:2:993:G:H2'	2:2:993:G:N3	2.33	0.43
2:2:1347:G:HO2'	2:2:1348:U:P	2.39	0.43
11:G:72:ILE:CG2	11:G:108:VAL:HG22	2.47	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
44:q:70:GLU:H	44:q:107:VAL:HG21	1.82	0.43
1:1:490:C:O2'	1:1:491:G:P	2.76	0.43
1:1:752:A:C1'	1:1:753:A:OP2	2.66	0.43
1:1:2033:A:O2'	1:1:2035:G:OP1	2.33	0.43
1:1:2050:C:O2'	1:1:2051:A:O5'	2.36	0.43
2:2:1372:U:OP1	41:n:73:GLY:N	2.51	0.43
20:R:49:ILE:CG2	20:R:54:VAL:HG22	2.49	0.43
25:W:55:LEU:HD12	25:W:76:ILE:HD12	2.00	0.43
31:d:3:ARG:HD3	31:d:4:THR:H	1.82	0.43
42:o:22:THR:O	42:o:26:VAL:HG23	2.17	0.43
1:1:81:G:O2'	1:1:295:G:O2'	2.35	0.43
1:1:395:U:H2'	1:1:396:G:C8	2.53	0.43
1:1:2467:C:O2	15:M:123:LYS:NZ	2.44	0.43
2:2:1321:U:OP2	2:2:1322:C:O2'	2.28	0.43
9:E:134:GLN:NE2	9:E:149:ARG:O	2.51	0.43
28:Z:8:GLN:O	28:Z:32:GLY:N	2.41	0.43
37:j:98:ALA:O	37:j:99:SER:C	2.61	0.43
38:k:52:ASN:O	38:k:53:LYS:O	2.36	0.43
38:k:98:GLU:CD	38:k:98:GLU:H	2.26	0.43
44:q:114:ARG:CG	44:q:119:VAL:HG13	2.48	0.43
1:1:140:C:H4'	1:1:141:G:OP1	2.19	0.43
1:1:732:C:H2'	1:1:733:G:O4'	2.19	0.43
14:L:29:LYS:O	14:L:30:THR:CB	2.67	0.43
2:2:516:U:O4	2:2:533:A:N7	2.52	0.43
2:2:1181:G:H1'	2:2:1182:G:C4	2.53	0.43
2:2:1238:A:H2'	2:2:1238:A:N3	2.34	0.43
15:M:2:LEU:N	15:M:2:LEU:HD12	2.34	0.43
22:T:80:TRP:H	22:T:80:TRP:CD1	2.37	0.43
29:b:54:ILE:HG23	29:b:56:LYS:H	1.83	0.43
41:n:62:LEU:N	41:n:62:LEU:HD12	2.33	0.43
43:p:80:ASN:OD1	43:p:80:ASN:N	2.52	0.43
1:1:752:A:H1'	1:1:753:A:OP2	2.18	0.43
2:2:404:G:OP2	36:i:114:ARG:NH2	2.47	0.43
3:3:5:U:H2'	3:3:6:G:H8	1.82	0.43
17:O:34:HIS:HA	17:O:53:THR:OG1	2.18	0.43
18:P:21:PRO:HD3	18:P:49:ILE:HD12	2.00	0.43
51:x:10:ILE:C	51:x:10:ILE:HD12	2.43	0.43
1:1:58:G:O2'	1:1:73:A:N1	2.40	0.43
1:1:715:A:C2	47:t:55:LEU:HD21	2.54	0.43
1:1:1790:C:O2'	6:B:207:ALA:HB2	2.19	0.43
2:2:375:U:C2	2:2:376:G:C8	3.06	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:1218:C:O2	2:2:1219:A:N7	2.51	0.43
8:D:146:VAL:HG12	8:D:185:LYS:HB2	2.00	0.43
11:G:3:VAL:CG1	11:G:36:ALA:HB1	2.49	0.43
1:1:458:G:C2'	1:1:459:U:OP2	2.67	0.43
1:1:1386:C:H2'	1:1:1387:A:H8	1.84	0.43
1:1:2328:A:H2'	1:1:2329:U:C6	2.53	0.43
1:1:2637:U:H2'	1:1:2638:G:O4'	2.19	0.43
2:2:552:U:H2'	2:2:553:A:C8	2.54	0.43
2:2:769:G:H4'	2:2:1513:A:H4'	2.01	0.43
2:2:1071:C:H2'	2:2:1072:G:H8	1.83	0.43
2:2:1347:G:C2'	2:2:1348:U:OP2	2.66	0.43
2:2:1399:C:H1'	2:2:1400:C:OP2	2.19	0.43
36:i:196:GLU:OE1	36:i:196:GLU:N	2.51	0.43
1:1:1177:G:H2'	1:1:1178:C:O4'	2.19	0.43
1:1:2404:U:H2'	1:1:2405:G:O4'	2.18	0.43
1:1:2604:U:C4	1:1:2605:U:C2	3.06	0.43
2:2:51:A:N7	2:2:114:U:O2'	2.47	0.43
2:2:1026:G:H2'	2:2:1027:C:C6	2.53	0.43
7:C:12:THR:CG2	18:P:4:ILE:HG23	2.49	0.43
16:N:73:ASN:HA	16:N:76:VAL:HG12	2.00	0.43
35:h:86:LEU:HA	35:h:89:VAL:HG22	2.01	0.43
41:n:61:ASP:C	41:n:62:LEU:HD12	2.43	0.43
43:p:115:ILE:HD11	53:z:23:GLU:HG3	2.00	0.43
1:1:569:U:H2'	1:1:570:G:O4'	2.18	0.42
1:1:773:U:H1'	55:B:401:HOH:O	2.18	0.42
1:1:966:G:C1'	1:1:2267:A:H62	2.32	0.42
1:1:1681:G:OP2	1:1:1757:A:N6	2.51	0.42
1:1:2250:G:OP1	15:M:84:LYS:HE3	2.19	0.42
1:1:2590:A:N1	1:1:2604:U:O4	2.51	0.42
2:2:575:G:O2'	2:2:821:G:OP2	2.37	0.42
2:2:910:C:OP2	44:q:18:LYS:NZ	2.45	0.42
2:2:1062:U:H2'	2:2:1063:C:C6	2.53	0.42
2:2:1370:G:C2	2:2:1371:G:C8	3.07	0.42
16:N:70:THR:O	16:N:71:ARG:C	2.61	0.42
1:1:239:C:HO2'	1:1:622:G:HO2'	1.63	0.42
1:1:1378:A:O2'	1:1:1380:G:OP2	2.36	0.42
2:2:1304:G:O3'	2:2:1305:G:O4'	2.36	0.42
3:3:55:U:H2'	3:3:56:G:C8	2.54	0.42
35:h:142:ARG:NE	55:h:304:HOH:O	2.49	0.42
41:n:90:ASP:O	41:n:91:GLU:C	2.62	0.42
48:u:5:ARG:NH2	48:u:27:ALA:O	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:269:C:H2'	1:1:270:A:C8	2.54	0.42
1:1:994:C:OP1	19:Q:52:ARG:NH2	2.52	0.42
1:1:1321:A:H2'	1:1:1321:A:N3	2.35	0.42
1:1:1564:C:H2'	1:1:1565:C:C6	2.55	0.42
1:1:1846:G:H2'	1:1:1847:G:C1'	2.50	0.42
1:1:1872:A:H2'	1:1:1873:G:O4'	2.19	0.42
1:1:2477:U:O4	33:f:10:LEU:HD22	2.20	0.42
1:1:2609:U:H5'	1:1:2610:C:OP2	2.20	0.42
1:1:2774:C:H2'	1:1:2775:G:O4'	2.18	0.42
2:2:523:A:N1	44:q:89:0TD:CB	2.82	0.42
2:2:1305:G:O2'	2:2:1306:A:H8	2.02	0.42
2:2:1326:U:O2'	2:2:1327:C:H5'	2.19	0.42
13:K:109:SER:O	13:K:111:LYS:N	2.52	0.42
47:t:26:VAL:O	47:t:30:LEU:HD13	2.19	0.42
51:x:30:LEU:CD1	55:x:104:HOH:O	2.66	0.42
1:1:456:C:C5'	55:1:3427:HOH:O	2.59	0.42
1:1:544:C:O3'	1:1:545:U:O4'	2.37	0.42
1:1:784:G:H5'	1:1:785:G:OP1	2.20	0.42
1:1:1087:G:N3	55:1:3374:HOH:O	2.49	0.42
1:1:1263:U:O2'	29:b:7:PRO:HD2	2.19	0.42
2:2:323:U:H2'	2:2:324:G:O4'	2.19	0.42
2:2:409:U:H2'	2:2:410:G:O4'	2.20	0.42
2:2:1288:A:N3	2:2:1352:C:O2'	2.40	0.42
11:G:51:ARG:O	11:G:55:GLU:N	2.52	0.42
29:b:27:LEU:HD23	29:b:36:LYS:HB3	2.00	0.42
31:d:24:THR:HG23	31:d:27:GLY:H	1.84	0.42
35:h:42:LEU:HD21	35:h:67:ILE:HD11	1.99	0.42
41:n:90:ASP:C	41:n:92:SER:N	2.78	0.42
1:1:703:U:H2'	1:1:704:G:O4'	2.19	0.42
1:1:1323:C:O2'	1:1:1324:G:H5'	2.19	0.42
1:1:2364:C:H2'	1:1:2365:G:O4'	2.19	0.42
1:1:2603:G:OP1	55:1:3304:HOH:O	2.21	0.42
1:1:2649:C:H2'	1:1:2650:U:C6	2.54	0.42
2:2:106:C:H2'	2:2:107:G:O4'	2.19	0.42
2:2:972:C:H1'	42:o:57:VAL:HG23	2.02	0.42
2:2:1241:G:H2'	2:2:1242:G:H8	1.84	0.42
11:G:90:LEU:HD21	11:G:94:ILE:HD12	2.02	0.42
43:p:15:VAL:HG12	43:p:76:TYR:HB3	2.00	0.42
44:q:82:ILE:CG2	44:q:83:ARG:N	2.82	0.42
47:t:55:LEU:O	47:t:58:MET:HG2	2.19	0.42
1:1:1298:C:H2'	1:1:1299:G:O4'	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:2127:G:N1	1:1:2162:G:N7	2.67	0.42
1:1:2185:U:C5	1:1:2186:G:N7	2.88	0.42
1:1:2551:C:H2'	1:1:2552:U:O4'	2.20	0.42
2:2:254:G:OP1	49:v:69:THR:HG22	2.19	0.42
2:2:352:C:N3	2:2:356:A:N6	2.66	0.42
16:N:66:ALA:O	16:N:69:ARG:O	2.36	0.42
30:c:46:VAL:HG12	30:c:47:ILE:N	2.35	0.42
38:k:3:HIS:HB2	38:k:92:THR:HB	2.02	0.42
39:l:68:VAL:HG11	39:l:133:ALA:HB3	2.01	0.42
48:u:20:VAL:HG21	48:u:32:PHE:CG	2.55	0.42
49:v:6:THR:OG1	49:v:59:GLU:OE1	2.32	0.42
1:1:820:A:H4'	1:1:836:G:H22	1.84	0.42
1:1:1398:C:C2	1:1:1399:C:C5	3.08	0.42
1:1:1864:U:OP1	1:1:2410:G:O2'	2.35	0.42
1:1:2588:G:OP1	55:1:3303:HOH:O	2.21	0.42
1:1:2605:U:O2	1:1:2605:U:O4'	2.36	0.42
2:2:185:U:C2	2:2:186:C:C5	3.08	0.42
3:3:40:U:N3	3:3:44:G:OP2	2.39	0.42
23:U:71:ILE:CD1	23:U:82:VAL:HG22	2.50	0.42
32:e:61:LEU:HD12	32:e:61:LEU:O	2.19	0.42
1:1:467:G:OP2	31:d:34:ARG:HD3	2.20	0.42
1:1:1020:A:H4'	1:1:1021:A:O5'	2.20	0.42
1:1:1341:G:OP1	1:1:1397:U:N3	2.44	0.42
1:1:1733:G:C2	1:1:1734:G:N7	2.88	0.42
1:1:2281:A:O2'	1:1:2282:G:H5'	2.20	0.42
1:1:2813:A:C4	1:1:2814:A:C8	3.08	0.42
2:2:890:G:C2'	2:2:891:U:OP2	2.68	0.42
2:2:1040:U:O2	2:2:1041:G:N7	2.53	0.42
2:2:1077:G:N2	2:2:1080:A:OP2	2.39	0.42
2:2:1250:A:H2'	2:2:1251:A:C8	2.55	0.42
2:2:1357:A:H2'	2:2:1358:U:O4'	2.19	0.42
2:2:1404:C:H2'	2:2:1405:G:C8	2.54	0.42
35:h:122:GLN:HG2	55:h:302:HOH:O	2.19	0.42
36:i:99:ASN:CG	36:i:110:ARG:HH12	2.28	0.42
43:p:80:ASN:HB3	43:p:105:ARG:HH11	1.84	0.42
1:1:242:G:C2'	1:1:243:U:OP2	2.68	0.42
1:1:791:C:H2'	55:1:3631:HOH:O	2.19	0.42
1:1:859:G:O2'	1:1:860:U:O5'	2.34	0.42
1:1:1084:A:C5	55:1:3317:HOH:O	2.64	0.42
1:1:2349:G:O6	1:1:2369:A:N6	2.53	0.42
6:B:67:LYS:HA	6:B:150:GLY:HA2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:c:39:ASP:O	30:c:43:ARG:N	2.53	0.42
38:k:5:GLU:HA	38:k:63:ASN:HA	2.02	0.42
38:k:64:VAL:HG22	38:k:65:GLU:N	2.35	0.42
42:o:36:VAL:HG22	42:o:37:ARG:H	1.85	0.42
1:1:1720:U:H2'	1:1:1721:G:O4'	2.19	0.42
1:1:1799:G:N7	6:B:177:SER:OG	2.51	0.42
1:1:2756:U:H4'	1:1:2757:A:OP1	2.20	0.42
2:2:89:U:H2'	2:2:90:C:O4'	2.20	0.42
3:3:42:C:H5	9:E:65:LEU:HD22	1.85	0.42
6:B:154:ALA:HB2	6:B:161:VAL:HG23	2.01	0.42
6:B:209:ALA:HA	6:B:212:TRP:CE2	2.55	0.42
9:E:103:ILE:HG13	9:E:104:THR:HG23	2.02	0.42
15:M:20:LEU:N	15:M:20:LEU:HD12	2.35	0.42
36:i:100:VAL:O	36:i:104:MET:HG2	2.19	0.42
38:k:82:ASP:OD1	38:k:82:ASP:N	2.49	0.42
38:k:98:GLU:O	38:k:99:ALA:HB3	2.19	0.42
53:z:33:ARG:HB2	53:z:34:ARG:H	1.54	0.42
1:1:2121:G:H2'	1:1:2122:U:O4'	2.19	0.41
2:2:841:C:HO2'	2:2:843:U:C1'	2.33	0.41
2:2:1129:C:H5''	2:2:1130:A:OP1	2.20	0.41
55:3:301:HOH:O	9:E:92:GLY:N	2.51	0.41
9:E:140:ILE:HD12	9:E:140:ILE:N	2.35	0.41
10:F:120:ILE:HD12	10:F:140:ILE:HG22	2.02	0.41
10:F:165:ASP:OD1	10:F:165:ASP:N	2.52	0.41
31:d:12:ARG:NE	31:d:44:VAL:HG21	2.25	0.41
47:t:7:THR:O	47:t:11:VAL:HG23	2.20	0.41
1:1:1797:G:O2'	6:B:256:THR:OG1	2.37	0.41
1:1:2304:G:H22	1:1:2312:U:H3	1.69	0.41
1:1:2728:U:H5	55:1:3362:HOH:O	2.01	0.41
55:1:3373:HOH:O	14:L:53:GLY:HA3	2.19	0.41
2:2:568:G:O2'	2:2:574:A:N1	2.52	0.41
6:B:131:MET:HE3	6:B:189:ALA:HB2	2.02	0.41
12:J:32:LEU:HD22	12:J:54:ILE:HG21	2.02	0.41
13:K:1:MET:HE3	13:K:1:MET:HB2	1.97	0.41
16:N:82:GLU:O	16:N:86:ARG:HB2	2.20	0.41
51:x:10:ILE:HD12	51:x:10:ILE:O	2.20	0.41
1:1:774:G:N2	1:1:787:C:O2'	2.53	0.41
1:1:792:A:N3	1:1:2072:C:O2'	2.41	0.41
1:1:974:G:H2'	1:1:974:G:N3	2.34	0.41
1:1:1093:G:H21	1:1:1098:A:H62	1.68	0.41
1:1:2838:G:C4	1:1:2839:G:C8	3.08	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:131:A:O2'	2:2:262:A:N3	2.50	0.41
2:2:219:U:H2'	2:2:220:G:O4'	2.20	0.41
2:2:1012:A:N6	2:2:1018:G:O6	2.53	0.41
14:L:30:THR:O	14:L:31:GLY:C	2.63	0.41
17:O:13:ARG:NH1	55:O:201:HOH:O	2.52	0.41
22:T:6:ARG:NH1	22:T:42:GLU:OE1	2.52	0.41
32:e:44:ARG:N	32:e:45:PRO:HD2	2.34	0.41
37:j:121:ASN:OD1	37:j:122:VAL:HG13	2.20	0.41
37:j:135:VAL:O	37:j:139:THR:HG23	2.20	0.41
1:1:284:U:N3	1:1:285:G:N7	2.68	0.41
1:1:659:G:O2'	8:D:95:LYS:O	2.38	0.41
1:1:1118:C:H2'	1:1:1119:U:O4'	2.20	0.41
1:1:1900:A:H1'	1:1:1970:A:H2'	2.02	0.41
1:1:1917:U:O2	1:1:1917:U:O4'	2.38	0.41
1:1:2191:A:H2'	1:1:2192:U:O4'	2.19	0.41
1:1:2291:U:H2'	1:1:2292:U:C6	2.55	0.41
2:2:1399:C:H4'	2:2:1400:C:O5'	2.21	0.41
3:3:13:G:O2'	3:3:15:A:H2'	2.20	0.41
3:3:88:C:H4'	3:3:89:U:OP1	2.21	0.41
29:b:42:ILE:HG22	29:b:48:TYR:HB2	2.02	0.41
36:i:44:LYS:CE	55:i:306:HOH:O	2.67	0.41
36:i:64:TYR:HE1	36:i:99:ASN:HD22	1.67	0.41
36:i:131:ILE:N	36:i:131:ILE:HD12	2.36	0.41
44:q:87:VAL:O	44:q:87:VAL:HG13	2.19	0.41
48:u:44:SER:O	48:u:45:GLU:C	2.62	0.41
1:1:71:A:OP2	1:1:112:U:O2'	2.32	0.41
1:1:176:A:O2'	1:1:177:G:H5'	2.21	0.41
1:1:544:C:H2'	1:1:545:U:C1'	2.50	0.41
1:1:1223:G:N2	1:1:1226:A:OP2	2.44	0.41
1:1:1682:G:C4	1:1:1757:A:H1'	2.55	0.41
2:2:153:C:C2	2:2:154:U:C5	3.08	0.41
2:2:667:G:N2	47:t:48:ASP:OD2	2.51	0.41
8:D:145:ASP:HA	8:D:166:LYS:HB3	2.02	0.41
8:D:189:THR:HG22	8:D:190:ALA:N	2.36	0.41
11:G:133:GLN:HG2	11:G:139:PHE:CD2	2.56	0.41
14:L:77:ILE:HD13	14:L:108:ALA:HB1	2.02	0.41
15:M:36:VAL:HG13	24:V:82:TYR:CD2	2.54	0.41
17:O:34:HIS:O	17:O:36:TYR:CE2	2.73	0.41
1:1:67:U:C2	1:1:68:G:C8	3.09	0.41
1:1:894:U:H2'	1:1:895:U:O4'	2.21	0.41
1:1:1089:A:N3	55:1:3374:HOH:O	2.37	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:2815:C:C2	1:1:2816:G:C8	3.08	0.41
2:2:586:C:O2'	40:m:3:GLN:NE2	2.54	0.41
2:2:1120:C:C2	2:2:1121:U:C5	3.08	0.41
3:3:2:G:O6	3:3:119:A:N6	2.54	0.41
10:F:23:ILE:HD11	10:F:42:VAL:HG11	2.03	0.41
24:V:56:PHE:CE1	24:V:61:LEU:HD21	2.56	0.41
1:1:184:C:O2'	1:1:217:A:N3	2.49	0.41
1:1:277:G:H1'	1:1:361:G:H1	1.85	0.41
1:1:774:G:O2'	1:1:775:G:O4'	2.37	0.41
1:1:1171:G:H2'	1:1:1172:C:O4'	2.20	0.41
1:1:1182:G:H2'	1:1:1183:U:O4'	2.21	0.41
1:1:1329:U:H5''	1:1:1330:C:OP2	2.20	0.41
1:1:2170:A:H2'	1:1:2170:A:N3	2.36	0.41
1:1:2788:C:H2'	1:1:2789:C:C6	2.56	0.41
2:2:101:A:C2	2:2:102:G:C8	3.08	0.41
2:2:1523:G:H5''	43:p:124:LYS:HE2	2.03	0.41
5:5:31:C:H2'	5:5:32:A:O4'	2.21	0.41
6:B:30:ALA:N	6:B:31:PRO:CD	2.83	0.41
16:N:28:LEU:HD23	16:N:48:VAL:HG21	2.03	0.41
20:R:53:PHE:HD1	20:R:53:PHE:N	2.18	0.41
20:R:53:PHE:N	20:R:53:PHE:CD1	2.87	0.41
36:i:187:ARG:NH2	36:i:194:ILE:O	2.53	0.41
50:w:31:TYR:CG	50:w:54:LEU:HD21	2.55	0.41
1:1:421:C:O2'	1:1:422:A:P	2.78	0.41
1:1:481:G:O2'	1:1:507:A:N6	2.53	0.41
1:1:817:C:H2'	1:1:818:G:O4'	2.20	0.41
1:1:1495:A:N3	1:1:1578:U:O2'	2.50	0.41
1:1:1826:G:O2'	1:1:1971:U:OP2	2.35	0.41
2:2:62:U:OP1	2:2:385:C:O2'	2.38	0.41
2:2:147:G:H2'	2:2:148:G:C8	2.56	0.41
2:2:946:A:N3	2:2:1333:A:H2	2.19	0.41
2:2:1098:C:OP1	34:g:138:ARG:NH2	2.54	0.41
2:2:1356:G:H2'	2:2:1357:A:C8	2.56	0.41
2:2:1368:A:OP1	41:n:112:ARG:NH2	2.54	0.41
2:2:1464:U:C2	2:2:1465:A:C8	3.08	0.41
7:C:34:VAL:HA	7:C:50:VAL:HG12	2.03	0.41
34:g:79:VAL:HA	34:g:213:LEU:HD21	2.03	0.41
52:y:23:ARG:O	52:y:26:MET:HG3	2.21	0.41
1:1:136:G:H2'	1:1:137:U:O4'	2.20	0.41
1:1:242:G:O2'	1:1:243:U:O5'	2.37	0.41
1:1:639:U:H2'	1:1:640:C:C6	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:1005:C:O2'	12:J:30:THR:HG21	2.21	0.41
1:1:2204:G:H4'	6:B:149:LYS:HD3	2.02	0.41
1:1:2586:U:H2'	1:1:2587:A:O4'	2.21	0.41
1:1:2745:C:H2'	1:1:2746:U:C6	2.56	0.41
2:2:10:A:OP2	37:j:130:THR:OG1	2.36	0.41
2:2:152:A:C5	2:2:153:C:C6	3.09	0.41
2:2:352:C:H4'	2:2:354:G:OP1	2.21	0.41
2:2:768:A:C5	2:2:769:G:C8	3.08	0.41
9:E:107:VAL:N	9:E:108:PRO:CD	2.84	0.41
16:N:22:ARG:HG3	16:N:70:THR:HA	2.03	0.41
17:O:50:ALA:O	17:O:81:ARG:NH2	2.53	0.41
18:P:59:THR:HG22	18:P:72:VAL:HG22	2.02	0.41
21:S:59:GLU:HA	21:S:64:ALA:HB2	2.02	0.41
33:f:4:ARG:O	33:f:37:GLN:O	2.38	0.41
34:g:67:LEU:HD21	34:g:150:ILE:HG22	2.02	0.41
34:g:71:THR:O	34:g:72:LYS:HB2	2.21	0.41
36:i:16:THR:HG22	36:i:17:ASP:H	1.86	0.41
36:i:84:ASN:ND2	36:i:87:GLU:OE1	2.54	0.41
1:1:366:C:H2'	1:1:367:G:O4'	2.21	0.41
1:1:453:A:N3	1:1:457:A:O2'	2.53	0.41
1:1:898:C:O2'	1:1:899:A:P	2.77	0.41
1:1:1012:U:OP2	19:Q:69:ARG:NH1	2.54	0.41
1:1:1351:C:H2'	1:1:1352:U:O4'	2.21	0.41
1:1:1675:C:O2	7:C:133:THR:OG1	2.39	0.41
1:1:2720:U:C2	1:1:2721:A:C8	3.09	0.41
2:2:150:U:H2'	2:2:151:A:H8	1.86	0.41
2:2:712:A:H2'	2:2:713:G:O4'	2.21	0.41
2:2:1028:C:C2	55:2:1744:HOH:O	2.74	0.41
32:e:28:LEU:HD11	32:e:40:LYS:HA	2.02	0.41
35:h:80:GLY:O	35:h:84:GLU:OE1	2.39	0.41
35:h:120:THR:HG23	35:h:188:ALA:HB2	2.03	0.41
37:j:56:PRO:O	37:j:59:ILE:HG13	2.21	0.41
37:j:98:ALA:HB2	37:j:123:LEU:HD12	2.03	0.41
42:o:81:GLU:OE2	42:o:81:GLU:HA	2.21	0.41
49:v:60:ILE:HG22	49:v:72:TRP:CE3	2.56	0.41
1:1:760:G:H2'	1:1:761:A:O4'	2.21	0.40
1:1:2134:A:N6	1:1:2156:G:N3	2.69	0.40
1:1:2307:G:N1	9:E:38:GLY:O	2.54	0.40
1:1:2666:C:N4	10:F:108:PHE:O	2.55	0.40
2:2:574:A:HO2'	2:2:882:C:HO2'	1.56	0.40
7:C:77:ARG:NH2	7:C:200:ASP:OD1	2.55	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:S:29:VAL:HG13	21:S:55:ILE:HD11	2.04	0.40
53:z:7:GLU:C	55:z:102:HOH:O	2.63	0.40
53:z:39:LYS:N	53:z:40:PRO:HD2	2.37	0.40
1:1:171:U:C2	1:1:172:A:C8	3.09	0.40
1:1:475:C:H2'	1:1:476:G:O4'	2.21	0.40
1:1:669:G:C8	1:1:669:G:OP1	2.74	0.40
1:1:890:C:H2'	1:1:890:C:H6	1.73	0.40
1:1:1124:G:O2'	33:f:37:GLN:HG3	2.21	0.40
2:2:1073:U:C2	2:2:1074:G:C8	3.09	0.40
2:2:1133:G:H2'	2:2:1134:G:C8	2.56	0.40
6:B:68:ARG:O	6:B:188:ARG:NH1	2.54	0.40
10:F:55:ASP:OD2	10:F:55:ASP:N	2.54	0.40
13:K:91:SER:O	13:K:92:GLU:C	2.63	0.40
13:K:93:GLN:O	13:K:94:PRO:C	2.63	0.40
41:n:107:ALA:O	41:n:108:ARG:C	2.64	0.40
42:o:22:THR:HG21	42:o:39:PRO:HB3	2.02	0.40
1:1:324:A:N6	1:1:339:U:O4'	2.54	0.40
1:1:685:A:C8	1:1:773:U:C4	3.10	0.40
1:1:1328:A:C2	1:1:1330:C:C2	3.09	0.40
1:1:1667:G:O2'	1:1:1991:U:O4	2.36	0.40
1:1:1920:C:C4'	55:1:3546:HOH:O	2.51	0.40
1:1:2516:A:O2'	1:1:2517:C:H5'	2.21	0.40
2:2:1215:G:C2	2:2:1216:A:C8	3.09	0.40
9:E:116:LEU:N	9:E:116:LEU:HD12	2.36	0.40
10:F:46:ASP:O	10:F:47:ASN:HB2	2.22	0.40
34:g:53:LEU:HD22	34:g:219:THR:OG1	2.21	0.40
42:o:21:ALA:O	42:o:24:GLU:HG3	2.21	0.40
1:1:955:U:O2	1:1:955:U:O5'	2.40	0.40
1:1:1149:G:H2'	1:1:1150:C:C6	2.57	0.40
1:1:2655:G:C2'	1:1:2656:U:OP2	2.70	0.40
2:2:82:G:H2'	2:2:83:C:O4'	2.21	0.40
2:2:320:A:H2'	2:2:321:A:O4'	2.20	0.40
2:2:1375:A:O2'	39:l:101:ARG:NH2	2.54	0.40
2:2:1517:G:C6	2:2:1518:A:N7	2.90	0.40
3:3:55:U:H4'	9:E:23:SER:OG	2.20	0.40
16:N:49:GLU:HB2	16:N:50:PRO:HD3	2.04	0.40
39:l:29:LEU:HD22	39:l:42:VAL:HG23	2.03	0.40
1:1:306:U:H2'	1:1:307:G:O4'	2.22	0.40
1:1:1079:C:C2	1:1:1080:A:C8	3.09	0.40
2:2:207:C:H2'	2:2:208:U:O4'	2.21	0.40
2:2:565:U:OP2	2:2:566:G:O2'	2.34	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:640:A:H2'	2:2:641:U:O4'	2.22	0.40
9:E:116:LEU:HD13	9:E:175:PRO:CD	2.49	0.40
15:M:47:GLU:OE2	15:M:51:ARG:NE	2.55	0.40
20:R:49:ILE:HG22	20:R:54:VAL:HG22	2.04	0.40
34:g:33:ALA:HB2	34:g:39:ILE:CD1	2.52	0.40
34:g:56:LEU:HD23	34:g:59:ILE:HD11	2.02	0.40
42:o:84:VAL:CG1	42:o:85:ASP:N	2.84	0.40
45:r:2:ARG:NH2	45:r:5:GLY:O	2.55	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
6	B	269/273 (98%)	252 (94%)	17 (6%)	0	100	100
7	C	207/209 (99%)	198 (96%)	9 (4%)	0	100	100
8	D	199/201 (99%)	187 (94%)	12 (6%)	0	100	100
9	E	175/179 (98%)	166 (95%)	9 (5%)	0	100	100
10	F	174/177 (98%)	168 (97%)	6 (3%)	0	100	100
11	G	147/149 (99%)	133 (90%)	14 (10%)	0	100	100
12	J	140/142 (99%)	134 (96%)	6 (4%)	0	100	100
13	K	120/123 (98%)	107 (89%)	13 (11%)	0	100	100
14	L	141/144 (98%)	121 (86%)	19 (14%)	1 (1%)	19	49
15	M	134/136 (98%)	129 (96%)	4 (3%)	1 (1%)	19	49
16	N	118/127 (93%)	108 (92%)	10 (8%)	0	100	100
17	O	114/117 (97%)	110 (96%)	4 (4%)	0	100	100
18	P	112/115 (97%)	108 (96%)	4 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
19	Q	115/118 (98%)	112 (97%)	3 (3%)	0	100	100
20	R	101/103 (98%)	92 (91%)	8 (8%)	1 (1%)	13	40
21	S	108/110 (98%)	100 (93%)	7 (6%)	1 (1%)	14	43
22	T	91/100 (91%)	86 (94%)	5 (6%)	0	100	100
23	U	100/104 (96%)	89 (89%)	10 (10%)	1 (1%)	13	40
24	V	92/94 (98%)	92 (100%)	0	0	100	100
25	W	73/84 (87%)	73 (100%)	0	0	100	100
26	X	75/78 (96%)	71 (95%)	4 (5%)	0	100	100
27	Y	61/63 (97%)	58 (95%)	3 (5%)	0	100	100
28	Z	56/59 (95%)	56 (100%)	0	0	100	100
29	b	54/57 (95%)	52 (96%)	2 (4%)	0	100	100
30	c	48/55 (87%)	45 (94%)	3 (6%)	0	100	100
31	d	44/46 (96%)	43 (98%)	1 (2%)	0	100	100
32	e	62/65 (95%)	58 (94%)	4 (6%)	0	100	100
33	f	36/38 (95%)	30 (83%)	6 (17%)	0	100	100
34	g	216/241 (90%)	195 (90%)	21 (10%)	0	100	100
35	h	204/233 (88%)	201 (98%)	3 (2%)	0	100	100
36	i	203/206 (98%)	180 (89%)	23 (11%)	0	100	100
37	j	155/167 (93%)	140 (90%)	14 (9%)	1 (1%)	22	52
38	k	98/135 (73%)	83 (85%)	13 (13%)	2 (2%)	6	23
39	l	149/179 (83%)	139 (93%)	10 (7%)	0	100	100
40	m	127/130 (98%)	117 (92%)	10 (8%)	0	100	100
41	n	125/130 (96%)	105 (84%)	18 (14%)	2 (2%)	8	28
42	o	96/103 (93%)	82 (85%)	14 (15%)	0	100	100
43	p	114/129 (88%)	104 (91%)	10 (9%)	0	100	100
44	q	120/124 (97%)	109 (91%)	11 (9%)	0	100	100
45	r	112/118 (95%)	99 (88%)	9 (8%)	4 (4%)	3	12
46	s	99/102 (97%)	89 (90%)	10 (10%)	0	100	100
47	t	86/89 (97%)	78 (91%)	7 (8%)	1 (1%)	11	35
48	u	80/82 (98%)	71 (89%)	9 (11%)	0	100	100
49	v	78/84 (93%)	70 (90%)	8 (10%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
50	w	63/75 (84%)	57 (90%)	6 (10%)	0	100	100
51	x	77/92 (84%)	74 (96%)	3 (4%)	0	100	100
52	y	83/87 (95%)	80 (96%)	3 (4%)	0	100	100
53	z	63/71 (89%)	46 (73%)	14 (22%)	3 (5%)	2	7
All	All	5514/5843 (94%)	5097 (92%)	399 (7%)	18 (0%)	38	66

All (18) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
15	M	59	ARG
23	U	89	GLY
45	r	3	ILE
45	r	5	GLY
45	r	9	PRO
53	z	35	GLU
37	j	122	VAL
38	k	53	LYS
41	n	91	GLU
45	r	6	ILE
47	t	46	LYS
53	z	36	PHE
14	L	128	THR
38	k	95	ALA
53	z	37	TYR
41	n	90	ASP
21	S	64	ALA
20	R	54	VAL

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
6	B	216/218 (99%)	213 (99%)	3 (1%)	62	86
7	C	164/164 (100%)	163 (99%)	1 (1%)	84	95

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
8	D	165/165 (100%)	164 (99%)	1 (1%)	84	95
9	E	148/150 (99%)	143 (97%)	5 (3%)	32	67
10	F	137/138 (99%)	136 (99%)	1 (1%)	81	94
11	G	114/114 (100%)	109 (96%)	5 (4%)	24	57
12	J	116/116 (100%)	116 (100%)	0	100	100
13	K	103/104 (99%)	102 (99%)	1 (1%)	73	91
14	L	102/103 (99%)	102 (100%)	0	100	100
15	M	109/109 (100%)	108 (99%)	1 (1%)	75	92
16	N	100/103 (97%)	100 (100%)	0	100	100
17	O	86/87 (99%)	86 (100%)	0	100	100
18	P	99/100 (99%)	98 (99%)	1 (1%)	73	91
19	Q	89/90 (99%)	89 (100%)	0	100	100
20	R	84/84 (100%)	80 (95%)	4 (5%)	21	54
21	S	93/93 (100%)	90 (97%)	3 (3%)	34	69
22	T	80/84 (95%)	78 (98%)	2 (2%)	42	75
23	U	83/85 (98%)	82 (99%)	1 (1%)	67	89
24	V	78/78 (100%)	77 (99%)	1 (1%)	65	88
25	W	57/62 (92%)	56 (98%)	1 (2%)	54	82
26	X	67/68 (98%)	67 (100%)	0	100	100
27	Y	55/55 (100%)	55 (100%)	0	100	100
28	Z	48/49 (98%)	48 (100%)	0	100	100
29	b	47/48 (98%)	47 (100%)	0	100	100
30	c	45/49 (92%)	43 (96%)	2 (4%)	24	57
31	d	38/38 (100%)	37 (97%)	1 (3%)	41	74
32	e	51/52 (98%)	49 (96%)	2 (4%)	27	62
33	f	34/34 (100%)	33 (97%)	1 (3%)	37	72
34	g	180/199 (90%)	176 (98%)	4 (2%)	47	78
35	h	170/190 (90%)	165 (97%)	5 (3%)	37	72
36	i	172/173 (99%)	168 (98%)	4 (2%)	45	77
37	j	114/126 (90%)	111 (97%)	3 (3%)	41	74
38	k	87/116 (75%)	85 (98%)	2 (2%)	45	77

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
39	l	124/147 (84%)	123 (99%)	1 (1%)	79	93
40	m	104/105 (99%)	104 (100%)	0	100	100
41	n	105/107 (98%)	104 (99%)	1 (1%)	73	91
42	o	86/90 (96%)	85 (99%)	1 (1%)	67	89
43	p	89/99 (90%)	87 (98%)	2 (2%)	47	78
44	q	102/103 (99%)	95 (93%)	7 (7%)	13	37
45	r	92/96 (96%)	88 (96%)	4 (4%)	25	57
46	s	79/84 (94%)	76 (96%)	3 (4%)	28	63
47	t	76/77 (99%)	76 (100%)	0	100	100
48	u	65/65 (100%)	65 (100%)	0	100	100
49	v	74/78 (95%)	74 (100%)	0	100	100
50	w	48/65 (74%)	47 (98%)	1 (2%)	48	78
51	x	70/79 (89%)	69 (99%)	1 (1%)	62	86
52	y	65/66 (98%)	64 (98%)	1 (2%)	60	85
53	z	44/61 (72%)	42 (96%)	2 (4%)	23	56
All	All	4554/4766 (96%)	4475 (98%)	79 (2%)	56	83

All (79) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
6	B	48	ILE
6	B	69	ASN
6	B	252	LYS
7	C	35	THR
8	D	200	LEU
9	E	90	LEU
9	E	131	VAL
9	E	174	PHE
9	E	175	PRO
9	E	176	PHE
10	F	105	SER
11	G	60	GLU
11	G	121	VAL
11	G	122	LEU
11	G	139	PHE
11	G	146	VAL
13	K	58	LEU

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Mol	Chain	Res	Type
15	M	47	GLU
18	P	82	SER
20	R	22	LEU
20	R	37	GLU
20	R	53	PHE
20	R	102	SER
21	S	4	ILE
21	S	46	LEU
21	S	77	ASP
22	T	37	ASP
22	T	63	VAL
23	U	59	GLU
24	V	42	LEU
25	W	67	VAL
30	c	23	THR
30	c	45	HIS
31	d	46	LYS
32	e	28	LEU
32	e	31	ILE
33	f	17	VAL
34	g	63	LYS
34	g	85	SER
34	g	150	ILE
34	g	186	VAL
35	h	35	ASP
35	h	51	VAL
35	h	54	ILE
35	h	96	VAL
35	h	156	LEU
36	i	16	THR
36	i	54	LEU
36	i	98	ASP
36	i	124	VAL
37	j	45	VAL
37	j	123	LEU
37	j	152	VAL
38	k	30	THR
38	k	55	HIS
39	l	119	LEU
41	n	56	MET
42	o	101	SER
43	p	71	ASP

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Mol	Chain	Res	Type
43	p	100	ASN
44	q	29	GLN
44	q	43	LYS
44	q	44	LYS
44	q	64	THR
44	q	78	SER
44	q	102	LEU
44	q	119	VAL
45	r	3	ILE
45	r	6	ILE
45	r	7	ASN
45	r	101	THR
46	s	17	ASP
46	s	55	SER
46	s	84	VAL
50	w	28	LEU
51	x	3	SER
52	y	82	ILE
53	z	9	GLU
53	z	34	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (53) such sidechains are listed below:

Mol	Chain	Res	Type
6	B	45	ASN
6	B	69	ASN
6	B	85	ASN
6	B	89	ASN
6	B	114	GLN
6	B	133	ASN
6	B	242	HIS
7	C	36	GLN
7	C	49	GLN
7	C	164	GLN
7	C	173	GLN
10	F	114	HIS
10	F	115	GLN
11	G	28	ASN
11	G	119	ASN
12	J	40	HIS
12	J	47	HIS
16	N	9	GLN

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Mol	Chain	Res	Type
16	N	11	ASN
16	N	73	ASN
16	N	107	ASN
19	Q	51	GLN
19	Q	71	ASN
20	R	12	HIS
20	R	89	HIS
22	T	15	HIS
22	T	59	ASN
23	U	68	ASN
30	c	45	HIS
31	d	26	ASN
32	e	42	HIS
33	f	33	HIS
33	f	35	GLN
34	g	14	HIS
34	g	35	ASN
34	g	57	ASN
34	g	119	GLN
34	g	167	HIS
34	g	176	ASN
34	g	202	ASN
35	h	7	ASN
38	k	37	HIS
41	n	30	ASN
41	n	74	GLN
42	o	58	ASN
43	p	14	GLN
43	p	21	HIS
43	p	100	ASN
43	p	108	ASN
49	v	49	ASN
50	w	73	HIS
51	x	55	GLN
52	y	2	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	1	2898/2904 (99%)	482 (16%)	50 (1%)
2	2	1538/1540 (99%)	224 (14%)	19 (1%)

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
3	3	119/120 (99%)	13 (10%)	2 (1%)
4	4	8/18 (44%)	4 (50%)	1 (12%)
5	5	76/77 (98%)	22 (28%)	2 (2%)
All	All	4639/4659 (99%)	745 (16%)	74 (1%)

All (745) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	1	10	A
1	1	12	U
1	1	26	G
1	1	34	U
1	1	35	G
1	1	46	G
1	1	50	U
1	1	51	G
1	1	52	A
1	1	63	A
1	1	71	A
1	1	74	A
1	1	75	G
1	1	84	A
1	1	91	A
1	1	92	U
1	1	118	A
1	1	120	U
1	1	125	A
1	1	137	U
1	1	138	U
1	1	139	U
1	1	140	C
1	1	141	G
1	1	142	A
1	1	149	A
1	1	162	U
1	1	163	C
1	1	166	U
1	1	181	A
1	1	196	A
1	1	199	A
1	1	215	G
1	1	216	A

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Mol	Chain	Res	Type
1	1	218	A
1	1	219	A
1	1	221	A
1	1	222	A
1	1	228	C
1	1	242	G
1	1	243	U
1	1	248	G
1	1	249	C
1	1	255	A
1	1	265	A
1	1	266	G
1	1	276	U
1	1	277	G
1	1	278	A
1	1	281	C
1	1	294	A
1	1	311	A
1	1	323	C
1	1	324	A
1	1	329	G
1	1	330	A
1	1	361	G
1	1	362	A
1	1	367	G
1	1	371	A
1	1	372	G
1	1	373	U
1	1	386	G
1	1	387	U
1	1	389	G
1	1	396	G
1	1	404	A
1	1	406	G
1	1	411	G
1	1	412	A
1	1	417	C
1	1	422	A
1	1	424	G
1	1	451	U
1	1	455	C
1	1	457	A

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Mol	Chain	Res	Type
1	1	458	G
1	1	459	U
1	1	460	A
1	1	479	A
1	1	480	A
1	1	481	G
1	1	482	A
1	1	490	C
1	1	491	G
1	1	504	A
1	1	505	A
1	1	509	C
1	1	531	C
1	1	532	A
1	1	534	U
1	1	544	C
1	1	545	U
1	1	547	A
1	1	549	G
1	1	550	C
1	1	563	A
1	1	573	U
1	1	574	A
1	1	575	A
1	1	603	A
1	1	614	A
1	1	616	A
1	1	622	G
1	1	627	A
1	1	637	A
1	1	645	C
1	1	646	U
1	1	647	G
1	1	654	A
1	1	655	A
1	1	669	G
1	1	685	A
1	1	686	U
1	1	694	U
1	1	695	G
1	1	704	G
1	1	726	G

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Mol	Chain	Res	Type
1	1	729	G
1	1	730	A
1	1	747	C
1	1	752	A
1	1	753	A
1	1	757	G
1	1	764	A
1	1	775	G
1	1	776	G
1	1	782	A
1	1	784	G
1	1	785	G
1	1	805	G
1	1	812	C
1	1	819	A
1	1	827	U
1	1	828	U
1	1	830	G
1	1	845	A
1	1	846	U
1	1	847	U
1	1	858	G
1	1	859	G
1	1	860	U
1	1	869	G
1	1	878	A
1	1	884	U
1	1	885	C
1	1	891	G
1	1	892	A
1	1	896	A
1	1	897	C
1	1	899	A
1	1	900	A
1	1	901	C
1	1	907	G
1	1	910	A
1	1	932	U
1	1	941	A
1	1	945	A
1	1	946	C
1	1	953	G

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Mol	Chain	Res	Type
1	1	961	C
1	1	973	A
1	1	974	G
1	1	983	A
1	1	993	G
1	1	995	C
1	1	996	A
1	1	999	U
1	1	1012	U
1	1	1013	C
1	1	1021	A
1	1	1023	U
1	1	1026	G
1	1	1027	A
1	1	1033	U
1	1	1045	C
1	1	1046	A
1	1	1047	G
1	1	1057	A
1	1	1059	G
1	1	1060	U
1	1	1061	U
1	1	1062	G
1	1	1064	C
1	1	1065	U
1	1	1066	U
1	1	1069	A
1	1	1070	A
1	1	1071	G
1	1	1072	C
1	1	1075	C
1	1	1076	C
1	1	1079	C
1	1	1081	U
1	1	1083	U
1	1	1084	A
1	1	1088	A
1	1	1096	A
1	1	1104	C
1	1	1106	G
1	1	1111	A
1	1	1112	G

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Mol	Chain	Res	Type
1	1	1119	U
1	1	1130	U
1	1	1131	G
1	1	1132	U
1	1	1133	A
1	1	1135	C
1	1	1141	U
1	1	1142	A
1	1	1171	G
1	1	1172	C
1	1	1174	U
1	1	1176	U
1	1	1177	G
1	1	1179	G
1	1	1180	U
1	1	1211	C
1	1	1212	G
1	1	1225	G
1	1	1237	A
1	1	1238	G
1	1	1250	G
1	1	1251	C
1	1	1253	A
1	1	1256	G
1	1	1271	G
1	1	1272	A
1	1	1273	U
1	1	1300	G
1	1	1301	A
1	1	1306	C
1	1	1321	A
1	1	1325	U
1	1	1329	U
1	1	1330	C
1	1	1341	G
1	1	1345	C
1	1	1352	U
1	1	1365	A
1	1	1368	G
1	1	1378	A
1	1	1379	U
1	1	1383	A

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Mol	Chain	Res	Type
1	1	1396	U
1	1	1397	U
1	1	1416	G
1	1	1419	A
1	1	1420	A
1	1	1421	G
1	1	1428	C
1	1	1437	C
1	1	1454	C
1	1	1456	G
1	1	1459	G
1	1	1461	C
1	1	1475	G
1	1	1482	G
1	1	1490	A
1	1	1491	G
1	1	1504	A
1	1	1508	A
1	1	1509	A
1	1	1515	A
1	1	1524	G
1	1	1532	A
1	1	1533	C
1	1	1535	A
1	1	1536	C
1	1	1555	G
1	1	1559	U
1	1	1560	G
1	1	1569	A
1	1	1578	U
1	1	1584	U
1	1	1585	C
1	1	1607	C
1	1	1611	C
1	1	1646	C
1	1	1647	U
1	1	1648	U
1	1	1670	C
1	1	1674	G
1	1	1677	A
1	1	1715	G
1	1	1729	U

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Mol	Chain	Res	Type
1	1	1730	C
1	1	1735	A
1	1	1738	G
1	1	1758	U
1	1	1764	C
1	1	1773	A
1	1	1776	G
1	1	1780	A
1	1	1781	U
1	1	1782	U
1	1	1784	A
1	1	1791	A
1	1	1800	C
1	1	1801	A
1	1	1808	A
1	1	1816	C
1	1	1829	A
1	1	1833	C
1	1	1848	A
1	1	1858	A
1	1	1859	U
1	1	1871	A
1	1	1901	A
1	1	1906	G
1	1	1907	G
1	1	1913	A
1	1	1914	C
1	1	1917	U
1	1	1925	C
1	1	1926	U
1	1	1930	G
1	1	1931	U
1	1	1937	A
1	1	1938	A
1	1	1940	U
1	1	1941	C
1	1	1955	U
1	1	1960	A
1	1	1967	C
1	1	1970	A
1	1	1971	U
1	1	1972	G

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Mol	Chain	Res	Type
1	1	1991	U
1	1	1993	U
1	1	1997	C
1	1	2022	U
1	1	2023	C
1	1	2031	A
1	1	2033	A
1	1	2043	C
1	1	2052	A
1	1	2055	C
1	1	2056	G
1	1	2060	A
1	1	2061	G
1	1	2062	A
1	1	2069	G
1	1	2096	C
1	1	2100	G
1	1	2108	A
1	1	2110	G
1	1	2111	U
1	1	2112	G
1	1	2113	U
1	1	2118	U
1	1	2119	A
1	1	2126	A
1	1	2131	U
1	1	2132	U
1	1	2133	G
1	1	2136	G
1	1	2145	C
1	1	2159	G
1	1	2162	G
1	1	2164	C
1	1	2166	U
1	1	2167	U
1	1	2169	A
1	1	2170	A
1	1	2172	U
1	1	2173	A
1	1	2189	U
1	1	2192	U
1	1	2195	U

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Mol	Chain	Res	Type
1	1	2198	A
1	1	2199	A
1	1	2204	G
1	1	2211	A
1	1	2213	U
1	1	2225	A
1	1	2226	C
1	1	2238	G
1	1	2239	G
1	1	2250	G
1	1	2251	G
1	1	2258	C
1	1	2279	G
1	1	2283	C
1	1	2286	G
1	1	2287	A
1	1	2288	A
1	1	2294	G
1	1	2296	U
1	1	2305	U
1	1	2309	A
1	1	2320	U
1	1	2325	G
1	1	2327	A
1	1	2334	U
1	1	2345	G
1	1	2347	C
1	1	2350	C
1	1	2354	C
1	1	2361	G
1	1	2383	G
1	1	2385	C
1	1	2392	A
1	1	2402	U
1	1	2406	A
1	1	2407	A
1	1	2423	U
1	1	2424	C
1	1	2425	A
1	1	2428	G
1	1	2429	G
1	1	2430	A

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Mol	Chain	Res	Type
1	1	2435	A
1	1	2441	U
1	1	2448	A
1	1	2475	C
1	1	2476	A
1	1	2497	A
1	1	2502	G
1	1	2503	A
1	1	2504	U
1	1	2506	U
1	1	2513	A
1	1	2518	A
1	1	2520	C
1	1	2529	G
1	1	2535	G
1	1	2547	A
1	1	2554	U
1	1	2567	G
1	1	2573	C
1	1	2574	G
1	1	2579	C
1	1	2582	G
1	1	2585	U
1	1	2586	U
1	1	2603	G
1	1	2609	U
1	1	2610	C
1	1	2613	U
1	1	2629	U
1	1	2630	G
1	1	2645	G
1	1	2646	C
1	1	2655	G
1	1	2656	U
1	1	2682	A
1	1	2689	U
1	1	2690	U
1	1	2714	G
1	1	2718	G
1	1	2722	G
1	1	2726	A
1	1	2733	A

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Mol	Chain	Res	Type
1	1	2739	U
1	1	2744	G
1	1	2748	A
1	1	2764	A
1	1	2765	A
1	1	2778	A
1	1	2779	U
1	1	2791	G
1	1	2794	C
1	1	2797	U
1	1	2799	A
1	1	2800	A
1	1	2807	U
1	1	2808	G
1	1	2809	A
1	1	2818	U
1	1	2820	A
1	1	2832	U
1	1	2833	U
1	1	2834	G
1	1	2849	U
1	1	2867	G
1	1	2868	A
1	1	2873	A
1	1	2880	C
1	1	2883	A
1	1	2894	G
1	1	2902	C
2	2	7	A
2	2	9	G
2	2	22	G
2	2	32	A
2	2	39	G
2	2	47	C
2	2	48	C
2	2	51	A
2	2	71	A
2	2	82	G
2	2	86	G
2	2	87	C
2	2	94	G
2	2	121	U

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Mol	Chain	Res	Type
2	2	130	A
2	2	174	A
2	2	183	C
2	2	184	G
2	2	197	A
2	2	199	A
2	2	209	U
2	2	210	C
2	2	211	G
2	2	212	G
2	2	214	C
2	2	215	C
2	2	226	G
2	2	240	G
2	2	245	U
2	2	247	G
2	2	251	G
2	2	253	A
2	2	266	G
2	2	267	C
2	2	269	C
2	2	280	C
2	2	281	G
2	2	289	G
2	2	306	A
2	2	328	C
2	2	329	A
2	2	330	C
2	2	345	C
2	2	346	G
2	2	352	C
2	2	354	G
2	2	355	C
2	2	367	U
2	2	372	C
2	2	373	A
2	2	392	C
2	2	397	A
2	2	406	G
2	2	412	A
2	2	413	G
2	2	428	G

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Mol	Chain	Res	Type
2	2	429	U
2	2	439	U
2	2	460	A
2	2	467	U
2	2	479	U
2	2	481	G
2	2	482	A
2	2	484	G
2	2	486	U
2	2	496	A
2	2	497	G
2	2	509	A
2	2	511	C
2	2	516	U
2	2	517	G
2	2	521	G
2	2	527	G
2	2	531	U
2	2	532	A
2	2	547	A
2	2	559	A
2	2	561	U
2	2	564	C
2	2	572	A
2	2	573	A
2	2	575	G
2	2	576	C
2	2	577	G
2	2	596	A
2	2	633	G
2	2	642	A
2	2	650	G
2	2	661	G
2	2	665	A
2	2	701	U
2	2	703	G
2	2	713	G
2	2	723	U
2	2	724	G
2	2	731	G
2	2	755	G
2	2	777	A

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Mol	Chain	Res	Type
2	2	815	A
2	2	817	C
2	2	818	G
2	2	819	A
2	2	828	U
2	2	832	G
2	2	843	U
2	2	844	G
2	2	846	G
2	2	858	G
2	2	871	U
2	2	872	A
2	2	890	G
2	2	902	G
2	2	914	A
2	2	926	G
2	2	934	C
2	2	935	A
2	2	958	A
2	2	960	U
2	2	961	U
2	2	969	A
2	2	975	A
2	2	976	G
2	2	977	A
2	2	992	U
2	2	993	G
2	2	994	A
2	2	1004	A
2	2	1015	G
2	2	1020	G
2	2	1022	A
2	2	1026	G
2	2	1028	C
2	2	1030	U
2	2	1031	C
2	2	1033	G
2	2	1035	A
2	2	1041	G
2	2	1053	G
2	2	1056	U
2	2	1065	U

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Mol	Chain	Res	Type
2	2	1085	U
2	2	1094	G
2	2	1099	G
2	2	1101	A
2	2	1124	G
2	2	1125	U
2	2	1126	U
2	2	1130	A
2	2	1137	C
2	2	1138	G
2	2	1139	G
2	2	1140	C
2	2	1152	A
2	2	1158	C
2	2	1159	U
2	2	1168	U
2	2	1183	U
2	2	1184	G
2	2	1191	A
2	2	1196	A
2	2	1201	A
2	2	1202	U
2	2	1208	C
2	2	1212	U
2	2	1213	A
2	2	1225	A
2	2	1227	A
2	2	1228	C
2	2	1236	A
2	2	1238	A
2	2	1240	U
2	2	1241	G
2	2	1253	G
2	2	1256	A
2	2	1258	G
2	2	1260	G
2	2	1275	A
2	2	1278	G
2	2	1280	A
2	2	1282	C
2	2	1287	A
2	2	1297	G

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Mol	Chain	Res	Type
2	2	1298	U
2	2	1300	G
2	2	1301	U
2	2	1302	C
2	2	1303	C
2	2	1305	G
2	2	1306	A
2	2	1317	C
2	2	1331	G
2	2	1332	A
2	2	1346	A
2	2	1348	U
2	2	1363	A
2	2	1364	U
2	2	1381	U
2	2	1395	C
2	2	1396	A
2	2	1397	C
2	2	1398	A
2	2	1400	C
2	2	1433	A
2	2	1446	A
2	2	1448	C
2	2	1452	C
2	2	1455	G
2	2	1492	A
2	2	1493	A
2	2	1497	G
2	2	1499	A
2	2	1502	A
2	2	1503	A
2	2	1506	U
2	2	1517	G
2	2	1519	A
2	2	1520	C
2	2	1529	G
2	2	1530	G
2	2	1533	C
2	2	1534	A
2	2	1535	C
2	2	1536	C
2	2	1539	C

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Mol	Chain	Res	Type
3	3	12	C
3	3	13	G
3	3	35	C
3	3	41	G
3	3	44	G
3	3	45	A
3	3	55	U
3	3	67	G
3	3	88	C
3	3	89	U
3	3	90	C
3	3	91	C
3	3	109	A
4	4	15	C
4	4	17	C
4	4	18	G
4	4	21	A
5	5	2	G
5	5	3	G
5	5	4	C
5	5	5	A
5	5	6	C
5	5	9	A
5	5	17	C
5	5	17(A)	U
5	5	18	G
5	5	19	G
5	5	20	U
5	5	21	A
5	5	36	G
5	5	41	C
5	5	44	G
5	5	45	G
5	5	47	U
5	5	54	U
5	5	56	C
5	5	57	A
5	5	60	U
5	5	76	A

All (74) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	1	51	G
1	1	91	A
1	1	140	C
1	1	227	A
1	1	242	G
1	1	310	A
1	1	372	G
1	1	421	C
1	1	458	G
1	1	479	A
1	1	490	C
1	1	546	U
1	1	548	G
1	1	549	G
1	1	615	U
1	1	752	A
1	1	858	G
1	1	859	G
1	1	884	U
1	1	898	C
1	1	1020	A
1	1	1022	G
1	1	1070	A
1	1	1111	A
1	1	1130	U
1	1	1141	U
1	1	1224	U
1	1	1328	A
1	1	1378	A
1	1	1396	U
1	1	1490	A
1	1	1847	G
1	1	1857	G
1	1	1900	A
1	1	1930	G
1	1	1940	U
1	1	2168	G
1	1	2194	U
1	1	2326	C
1	1	2333	A
1	1	2391	G
1	1	2505	G
1	1	2566	A

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Mol	Chain	Res	Type
1	1	2629	U
1	1	2645	G
1	1	2655	G
1	1	2725	A
1	1	2808	G
1	1	2867	G
1	1	2893	A
2	2	70	U
2	2	86	G
2	2	213	G
2	2	428	G
2	2	438	U
2	2	960	U
2	2	1124	G
2	2	1125	U
2	2	1151	A
2	2	1182	G
2	2	1190	G
2	2	1201	A
2	2	1297	G
2	2	1300	G
2	2	1301	U
2	2	1305	G
2	2	1347	G
2	2	1399	C
2	2	1432	G
3	3	66	A
3	3	88	C
4	4	17	C
5	5	56	C
5	5	59	A

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

1 non-standard protein/DNA/RNA residue is modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
44	0TD	q	89	44	8,9,10	1.44	0	6,11,13	2.65	3 (50%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
44	0TD	q	89	44	-	5/7/12/14	-

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
44	q	89	0TD	OD2-CG-CB	3.91	121.61	113.15
44	q	89	0TD	CSB-SB-CB	3.74	109.08	102.36
44	q	89	0TD	OD1-CG-CB	-2.62	116.96	122.44

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
44	q	89	0TD	CA-CB-SB-CSB
44	q	89	0TD	CA-CB-CG-OD1
44	q	89	0TD	SB-CB-CG-OD1
44	q	89	0TD	CA-CB-CG-OD2
44	q	89	0TD	CG-CB-SB-CSB

There are no ring outliers.

1 monomer is involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
44	q	89	0TD	5	0

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 287 ligands modelled in this entry, 287 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

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

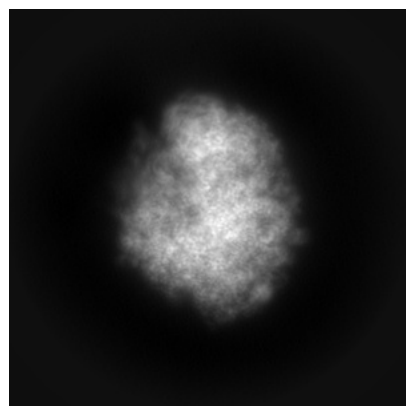
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-42721. These allow visual inspection of the internal detail of the map and identification of artifacts.

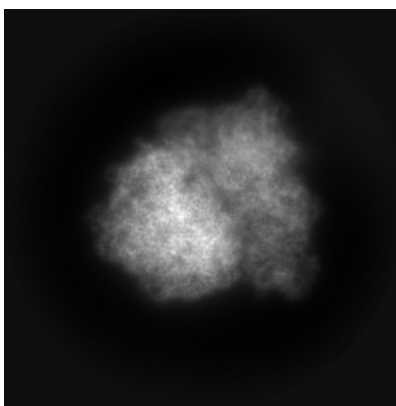
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

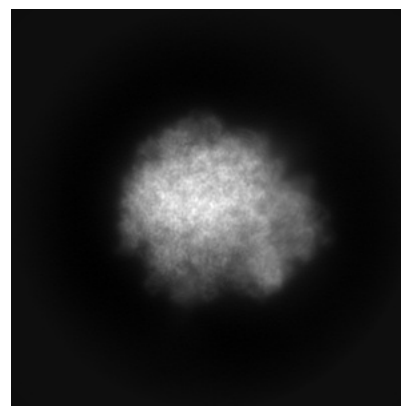
6.1.1 Primary map



X

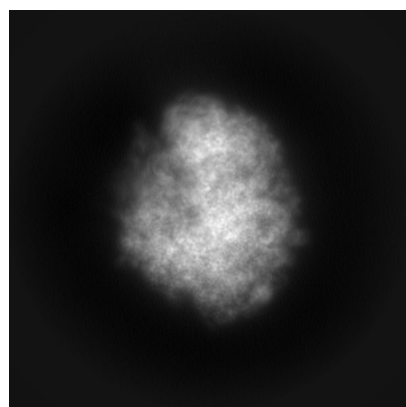


Y

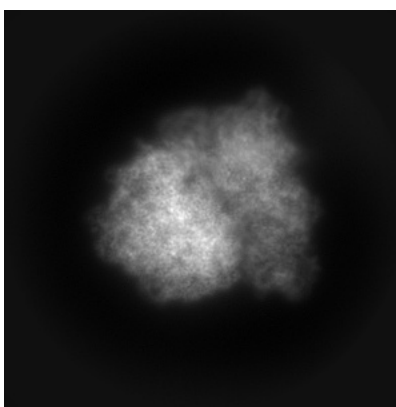


Z

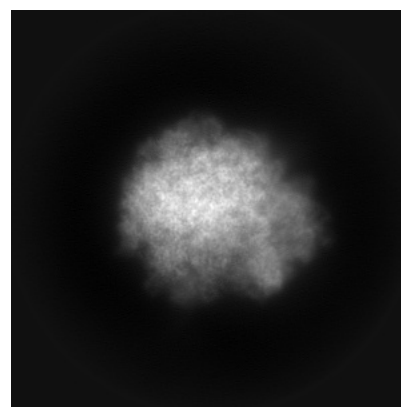
6.1.2 Raw map



X



Y

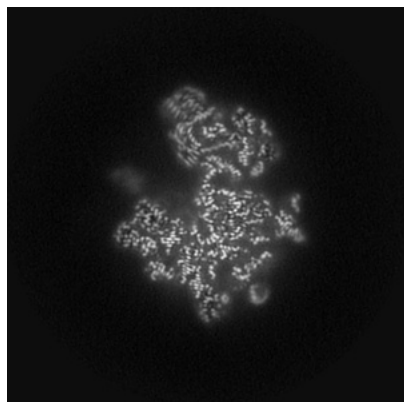


Z

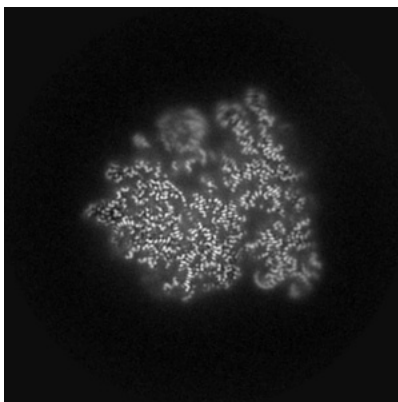
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

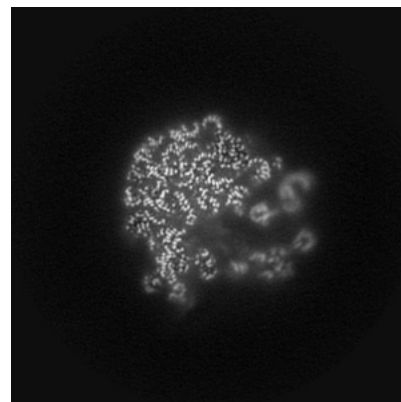
6.2.1 Primary map



X Index: 200

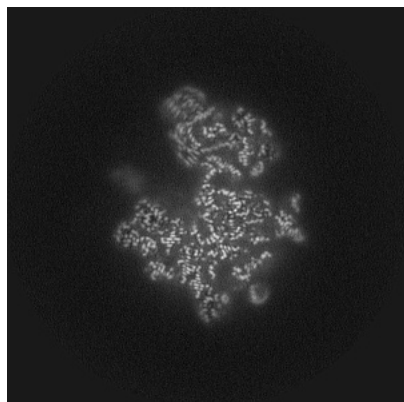


Y Index: 200

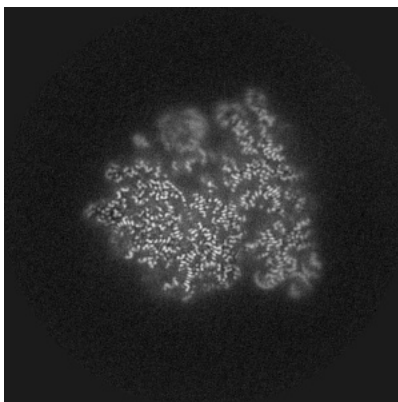


Z Index: 200

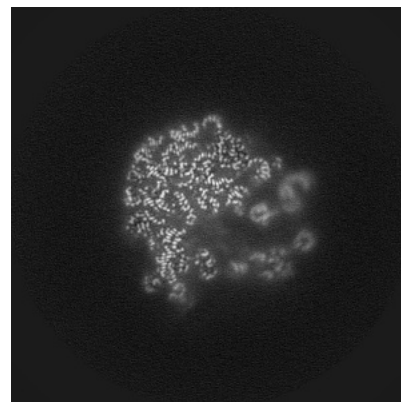
6.2.2 Raw map



X Index: 200



Y Index: 200

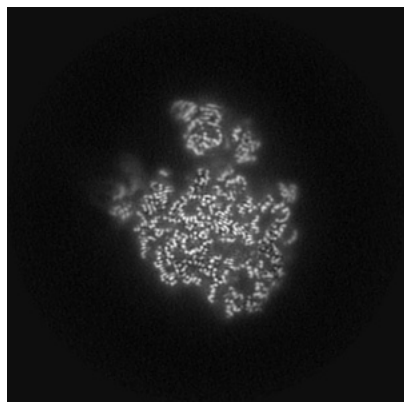


Z Index: 200

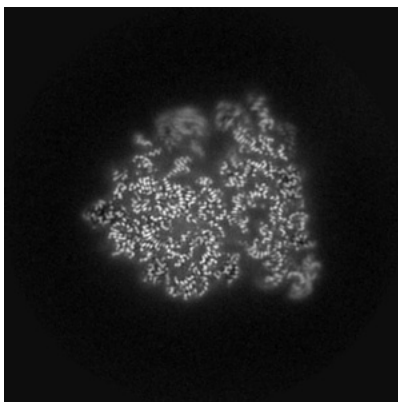
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

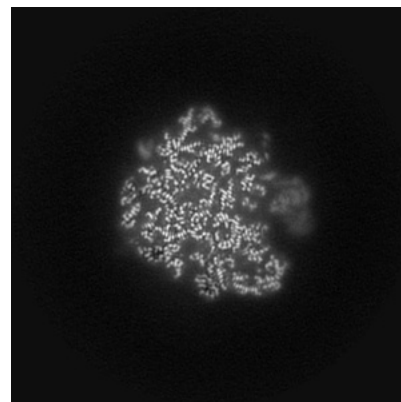
6.3.1 Primary map



X Index: 169

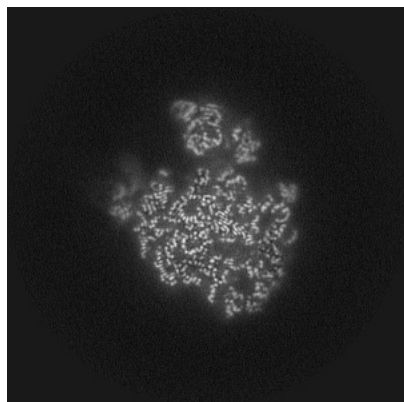


Y Index: 205

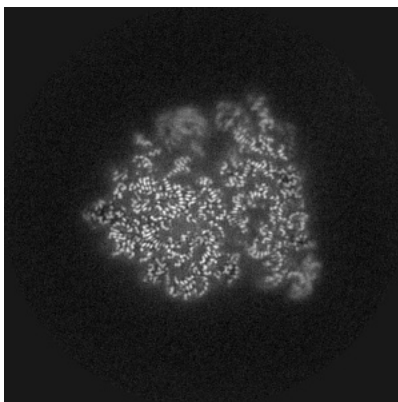


Z Index: 169

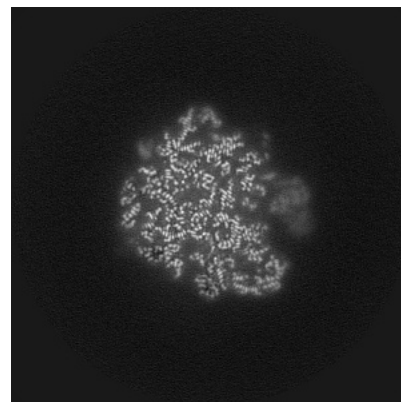
6.3.2 Raw map



X Index: 169



Y Index: 205

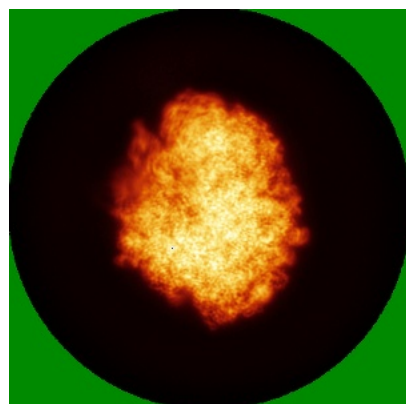


Z Index: 169

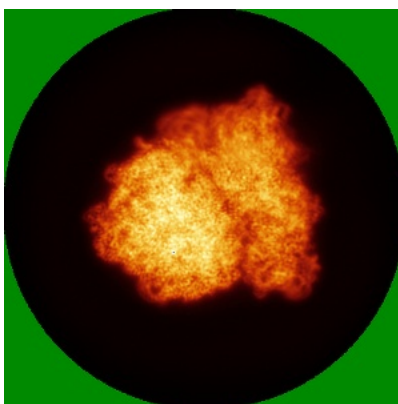
The images above show the largest variance slices of the map in three orthogonal directions.

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

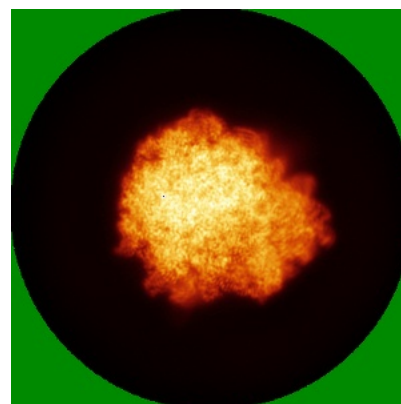
6.4.1 Primary map



X

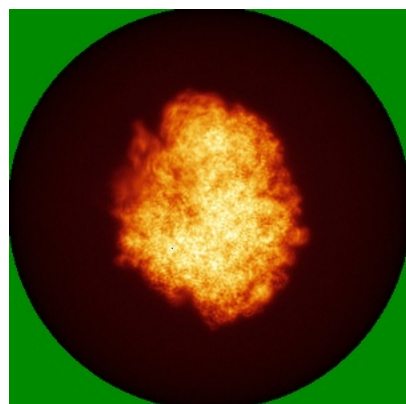


Y

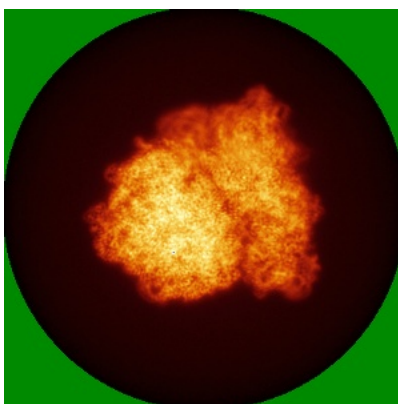


Z

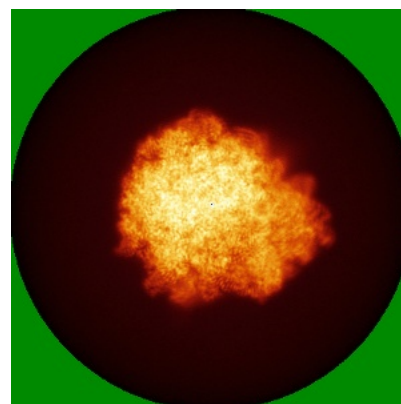
6.4.2 Raw map



X



Y

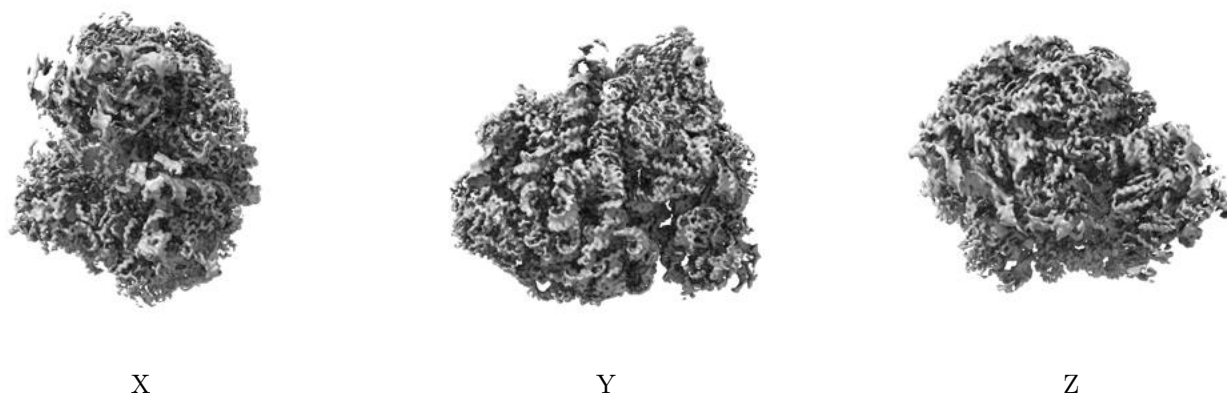


Z

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.

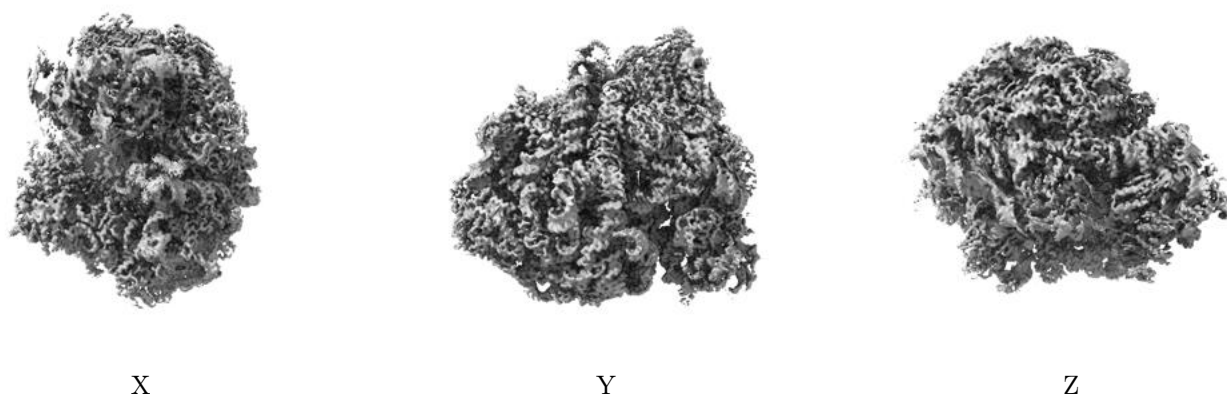
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.0198. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

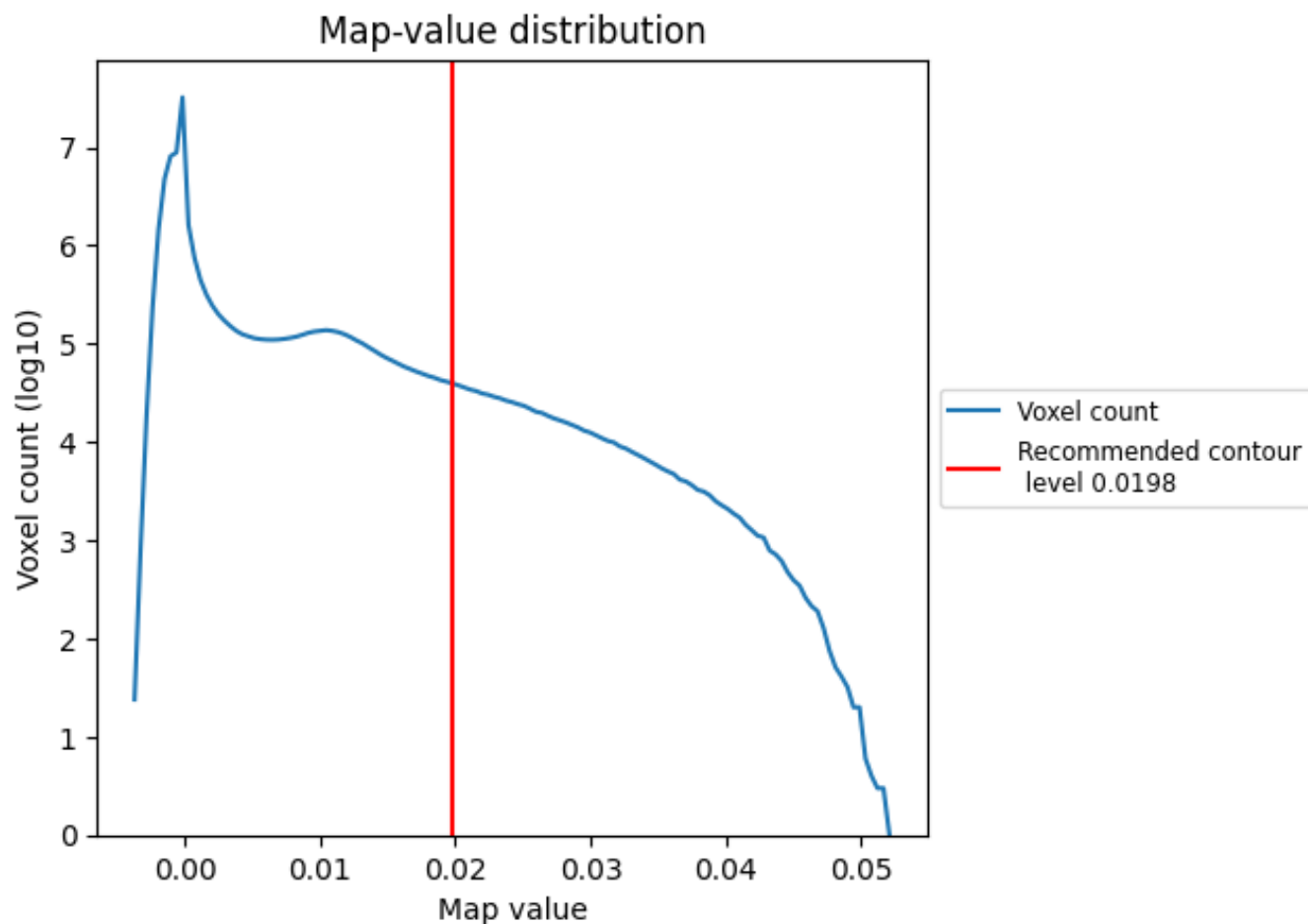
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

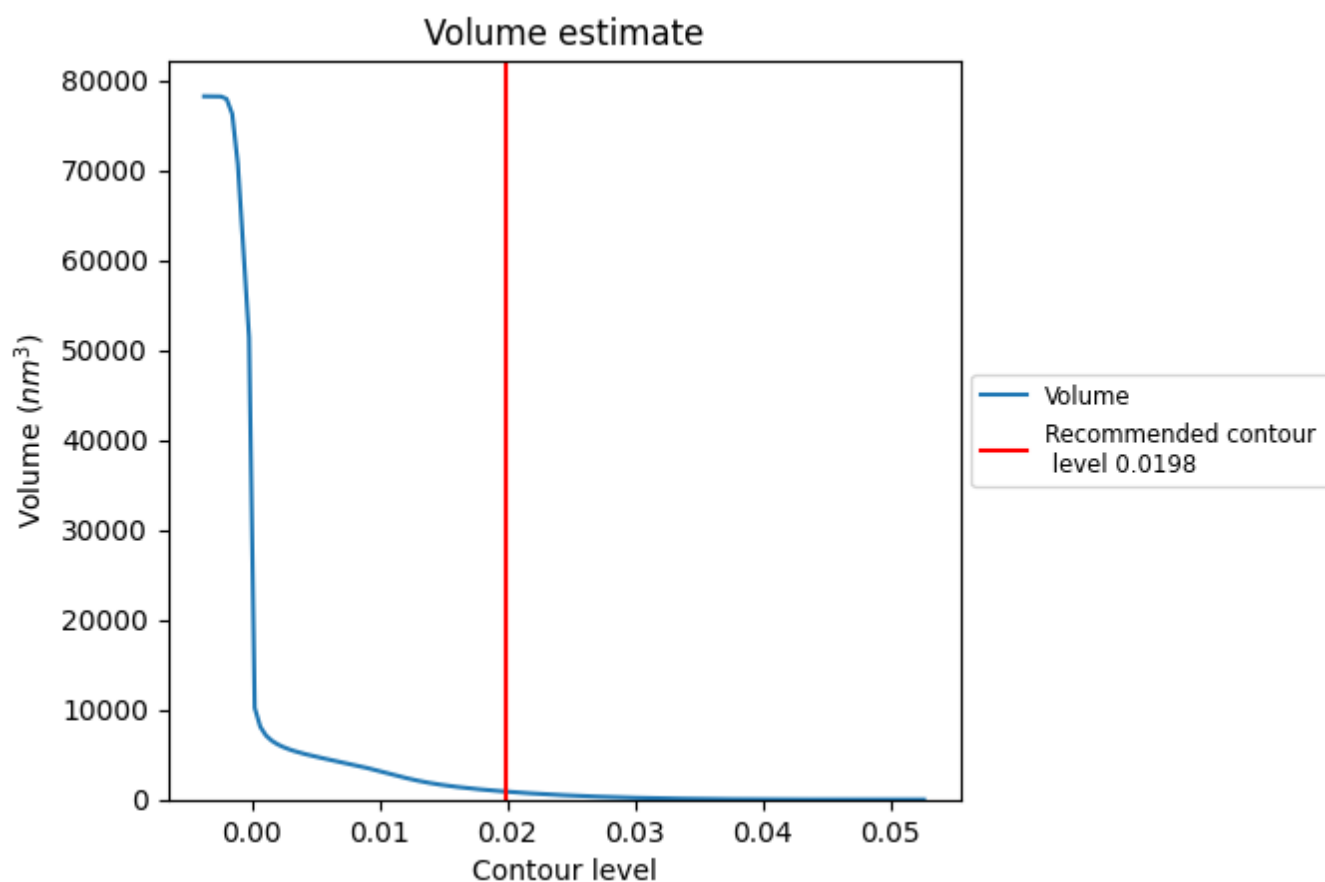
This section contains the results of statistical analysis of the map.

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.

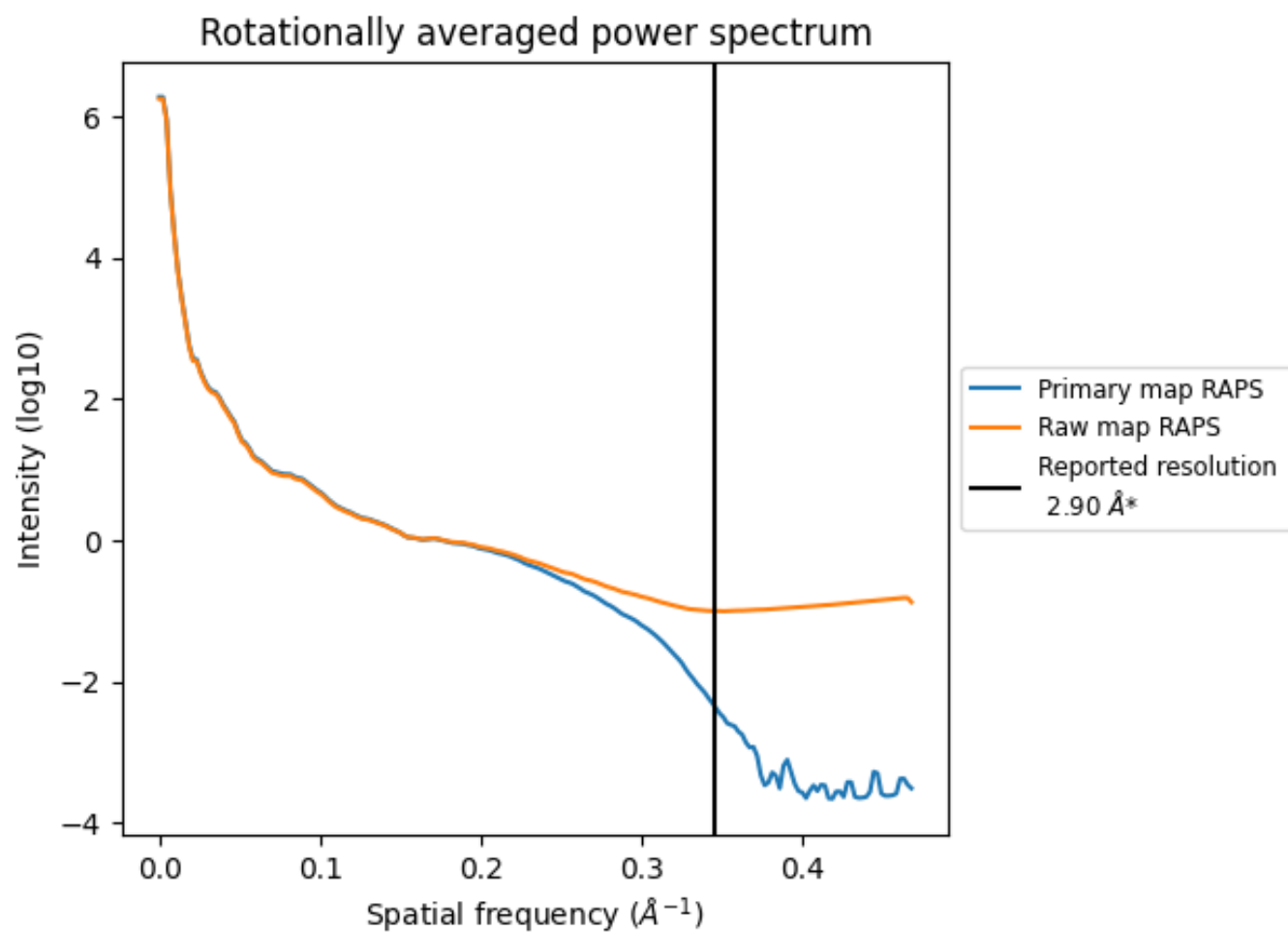
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 895 nm³; this corresponds to an approximate mass of 809 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 ⓘ

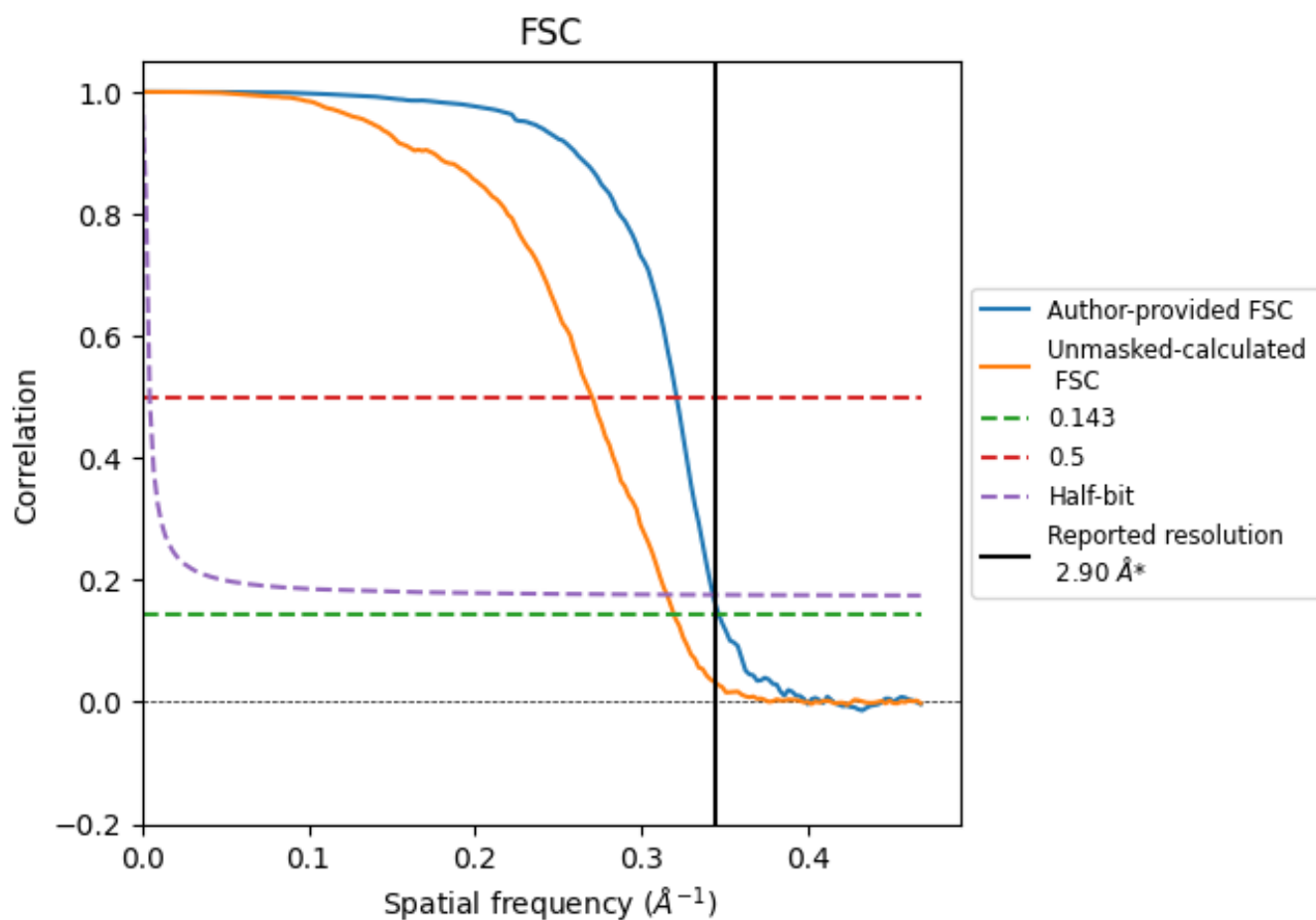


*Reported resolution corresponds to spatial frequency of 0.345 Å⁻¹

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.345 \AA^{-1}

8.2 Resolution estimates [i](#)

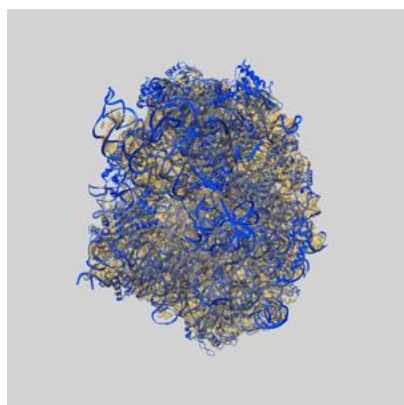
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.90	-	-
Author-provided FSC curve	2.89	3.12	2.92
Unmasked-calculated*	3.13	3.70	3.17

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

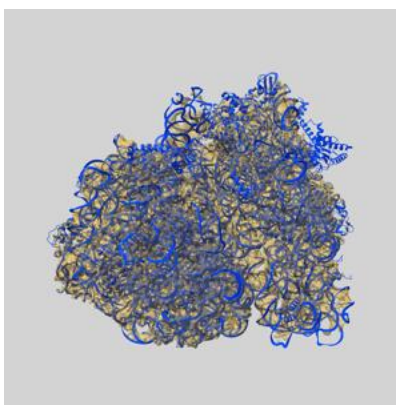
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-42721 and PDB model 8UXB. Per-residue inclusion information can be found in section [3](#) on page [16](#).

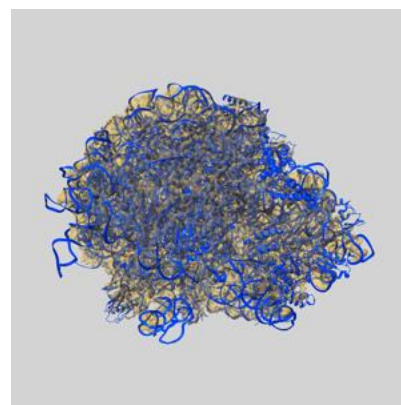
9.1 Map-model overlay [i](#)



X



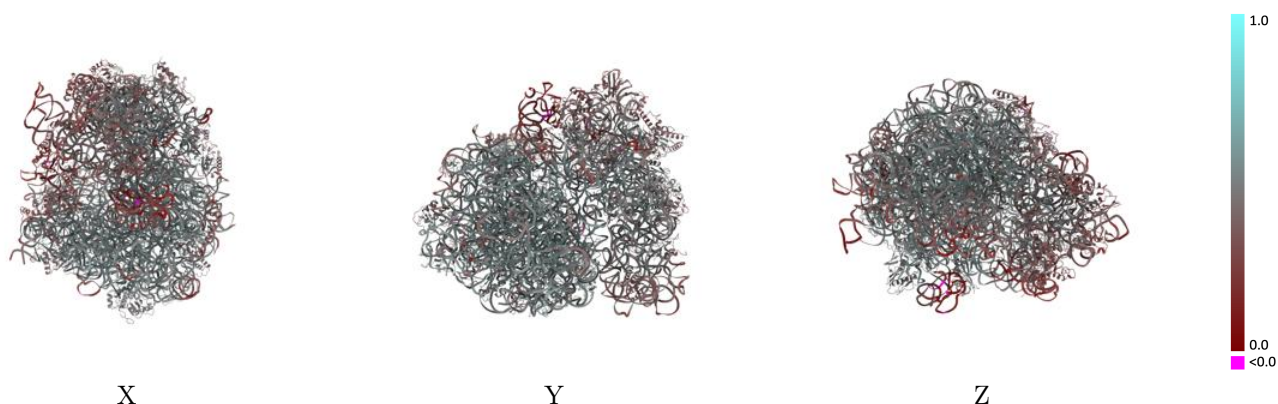
Y



Z

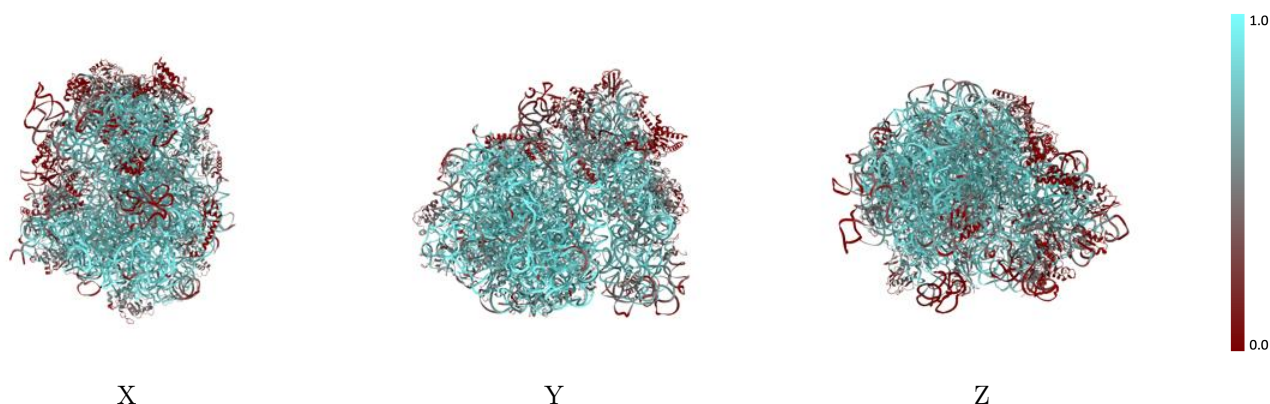
The images above show the 3D surface view of the map at the recommended contour level 0.0198 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



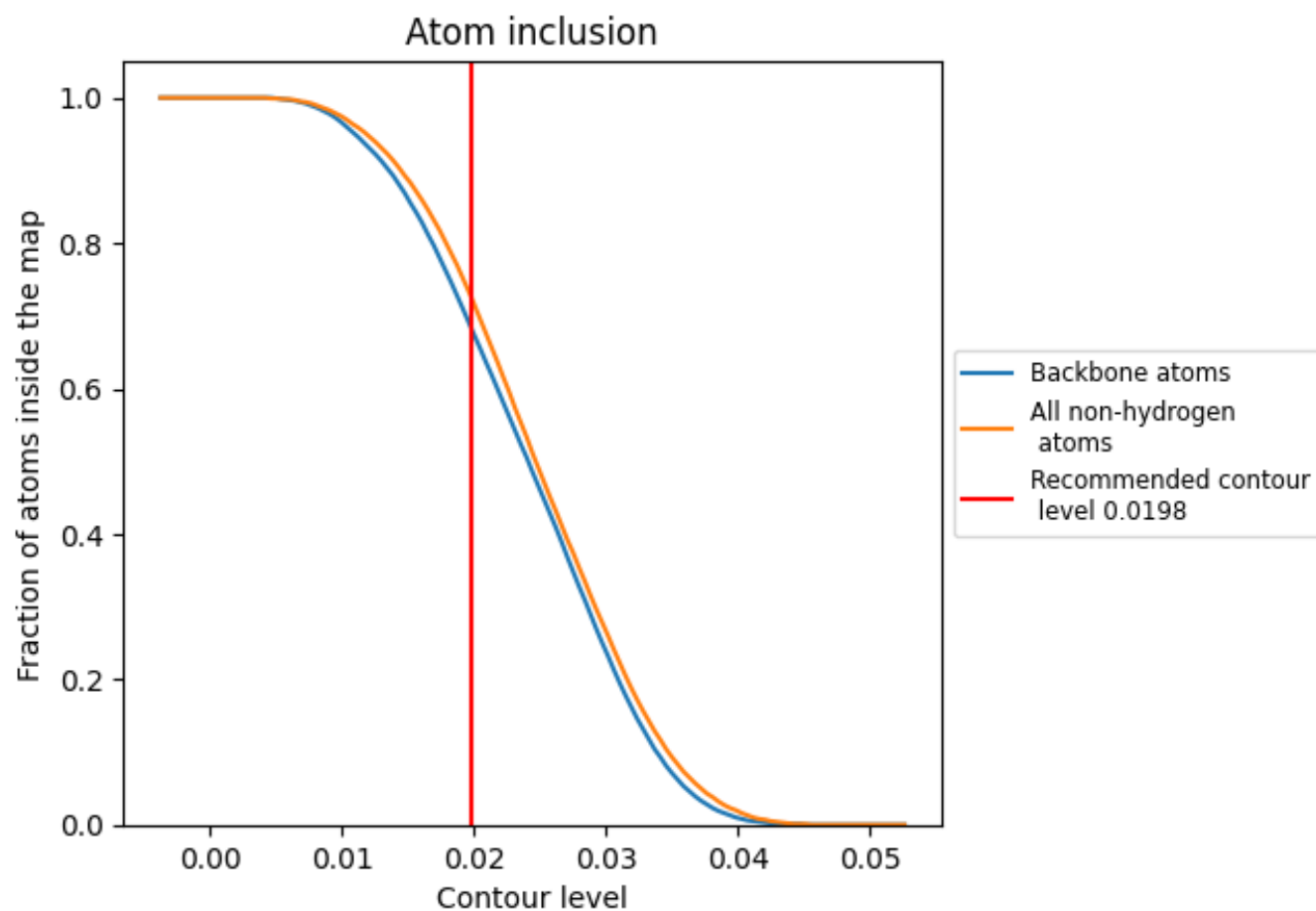
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0198).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 68% of all backbone atoms, 72% 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 (0.0198) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7250	 0.4680
1	 0.8650	 0.4980
2	 0.7730	 0.4420
3	 0.7780	 0.4760
4	 0.6220	 0.4620
5	 0.7790	 0.3930
B	 0.7790	 0.5390
C	 0.6850	 0.5340
D	 0.5660	 0.4970
E	 0.2540	 0.3400
F	 0.3620	 0.4640
G	 0.0500	 0.3370
J	 0.6960	 0.5170
K	 0.7040	 0.5160
L	 0.6460	 0.5060
M	 0.7050	 0.5220
N	 0.7290	 0.5250
O	 0.4540	 0.4560
P	 0.6060	 0.5040
Q	 0.7580	 0.5260
R	 0.5670	 0.5040
S	 0.6850	 0.5110
T	 0.5720	 0.4880
U	 0.4380	 0.4920
V	 0.5140	 0.4940
W	 0.7210	 0.5320
X	 0.7120	 0.5040
Y	 0.4610	 0.4200
Z	 0.6250	 0.5200
b	 0.7060	 0.5090
c	 0.6230	 0.4980
d	 0.8730	 0.5120
e	 0.8210	 0.5460
f	 0.7400	 0.5080
g	 0.0010	 0.3740



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Chain	Atom inclusion	Q-score
h	 0.3480	 0.4090
i	 0.2520	 0.3540
j	 0.5760	 0.4570
k	 0.3190	 0.3790
l	 0.1330	 0.3040
m	 0.5200	 0.4890
n	 0.2410	 0.3470
o	 0.2500	 0.3740
p	 0.5690	 0.4620
q	 0.5950	 0.4720
r	 0.1840	 0.3140
s	 0.3750	 0.3640
t	 0.5510	 0.4480
u	 0.5090	 0.4450
v	 0.4890	 0.4530
w	 0.4660	 0.4350
x	 0.1920	 0.2980
y	 0.4650	 0.3560
z	 0.3420	 0.3170