



Full wwPDB EM Validation Report ⓘ

Mar 24, 2026 – 03:51 AM UTC

PDB ID : 6ENJ / pdb_00006enj
EMDB ID : EMD-3899
Title : Polyproline-stalled ribosome in the presence of A+P site tRNA and elongation-factor P (EF-P)
Authors : Huter, P.; Wilson, D.N.
Deposited on : 2017-10-05
Resolution : 3.70 Å(reported)

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

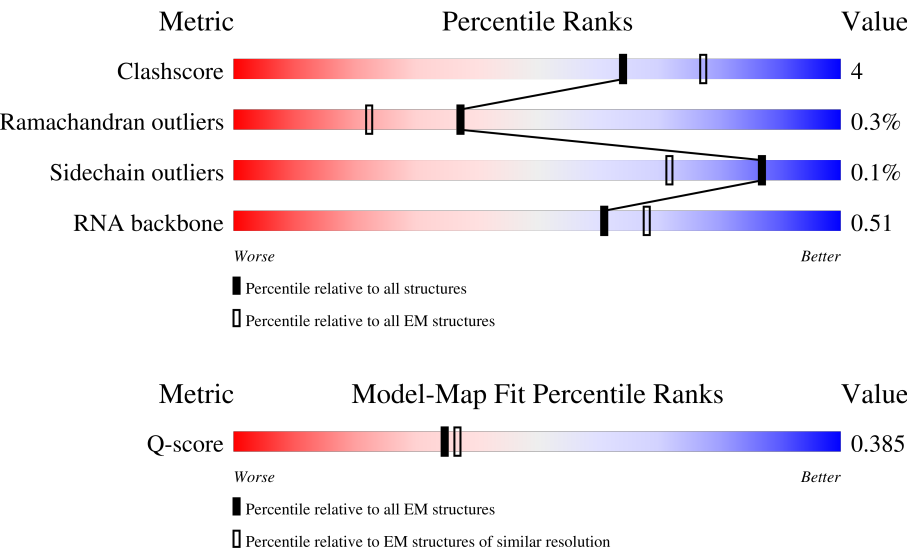
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDb archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance

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

The reported resolution of this entry is 3.70 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	11569 (3.20 - 4.20)

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

Mol	Chain	Length	Quality of chain
1	A	2903	14% 72% 24% ••
2	B	120	12% 76% 23% •
3	C	271	21% 83% 17%

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Mol	Chain	Length	Quality of chain
4	D	209	
5	E	201	
6	F	177	
7	G	176	
8	J	142	
9	K	122	
10	L	143	
11	M	136	
12	N	120	
13	O	116	
14	P	114	
15	Q	117	
16	R	103	
17	S	110	
18	T	93	
19	U	102	
20	V	94	
21	W	84	
22	X	77	
23	Y	63	
24	Z	58	
25	0	56	
26	1	50	
27	2	46	
28	3	64	

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Mol	Chain	Length	Quality of chain
29	4	38	
30	6	66	
31	a	1539	
32	b	218	
33	c	206	
34	d	205	
35	e	157	
36	f	100	
37	g	151	
38	h	129	
39	i	127	
40	j	98	
41	k	116	
42	l	123	
43	m	114	
44	n	101	
45	o	88	
46	p	82	
47	q	80	
48	r	65	
49	s	79	
50	t	85	
51	u	65	
52	w	188	
53	v	9	

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Mol	Chain	Length	Quality of chain
54	9	77	68% 32% 53% 13%
54	x	77	31% 68% 23% 9%
55	7	224	99% 89% 11%

2 Entry composition

There are 56 unique types of molecules in this entry. The entry contains 147111 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	A	2871	Total	C	N	O	P	0	0
			61641	27498	11350	19922	2871		

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	747	C	U	conflict	GB 802133627
A	1847	G	A	conflict	GB 802133627
A	2069	A	G	conflict	GB 802133627
A	2104	U	C	conflict	GB 802133627

- Molecule 2 is a RNA chain called 5S Ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	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
B	120	A	U	conflict	GB 1213441078

- Molecule 3 is a protein called 50S ribosomal protein L2.

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

- Molecule 4 is a protein called 50S ribosomal protein L3.

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

- Molecule 5 is a protein called 50S ribosomal protein L4.

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

- Molecule 6 is a protein called 50S ribosomal protein L5.

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

- Molecule 7 is a protein called 50S ribosomal protein L6.

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

- Molecule 8 is a protein called 50S ribosomal protein L13.

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

- Molecule 9 is a protein called 50S ribosomal protein L14.

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

- Molecule 10 is a protein called 50S ribosomal protein L15.

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

- Molecule 11 is a protein called 50S ribosomal protein L16.

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

- Molecule 12 is a protein called 50S ribosomal protein L17.

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

- Molecule 13 is a protein called 50S ribosomal protein L18.

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

- Molecule 14 is a protein called 50S ribosomal protein L19.

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

- Molecule 15 is a protein called 50S ribosomal protein L20.

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

- Molecule 16 is a protein called 50S ribosomal protein L21.

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

- Molecule 17 is a protein called 50S ribosomal protein L22.

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

- Molecule 18 is a protein called 50S ribosomal protein L23.

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

- Molecule 19 is a protein called 50S ribosomal protein L24.

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

- Molecule 20 is a protein called 50S ribosomal protein L25.

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

- Molecule 21 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms				AltConf	Trace
21	W	84	Total	C	N	O	S	
			637	394	129	113	1	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
W	6	GLY	ALA	conflict	UNP P0A7L8
W	7	LEU	GLY	conflict	UNP P0A7L8

- Molecule 22 is a protein called 50S ribosomal protein L28.

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

- Molecule 23 is a protein called 50S ribosomal protein L29.

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

- Molecule 24 is a protein called 50S ribosomal protein L30.

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

- Molecule 25 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	0	56	Total	C	N	O	S	0	0
			444	269	94	80	1		

- Molecule 26 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	1	50	Total	C	N	O		0	0
			409	263	75	71			

- Molecule 27 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	2	46	Total	C	N	O	S	0	0
			377	228	90	57	2		

- Molecule 28 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	3	64	Total	C	N	O	S	0	0
			504	323	105	74	2		

- Molecule 29 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	4	38	Total	C	N	O	S	0	0
			302	185	65	48	4		

- Molecule 30 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	6	66	Total	C	N	O	S	0	0
			522	323	99	94	6		

- Molecule 31 is a RNA chain called 16S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	a	1539	Total	C	N	O	P	0	0
			33016	14725	6052	10700	1539		

- Molecule 32 is a protein called 30S ribosomal protein S2.

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

- Molecule 33 is a protein called 30S ribosomal protein S3.

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

- Molecule 34 is a protein called 30S ribosomal protein S4.

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

- Molecule 35 is a protein called 30S ribosomal protein S5.

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

- Molecule 36 is a protein called 30S ribosomal protein S6.

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

- Molecule 37 is a protein called 30S ribosomal protein S7.

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

- Molecule 38 is a protein called 30S ribosomal protein S8.

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

- Molecule 39 is a protein called 30S ribosomal protein S9.

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

- Molecule 40 is a protein called 30S ribosomal protein S10.

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

- Molecule 41 is a protein called 30S ribosomal protein S11.

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

- Molecule 42 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	l	123	Total	C	N	O	S	0	0
			955	590	196	165	4		

- Molecule 43 is a protein called 30S ribosomal protein S13.

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

- Molecule 44 is a protein called 30S ribosomal protein S14.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	n	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
n	35	ALA	-	insertion	UNP P0AG59

- Molecule 45 is a protein called 30S ribosomal protein S15.

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

- Molecule 46 is a protein called 30S ribosomal protein S16.

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

- Molecule 47 is a protein called 30S ribosomal protein S17.

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

- Molecule 48 is a protein called 30S ribosomal protein S18.

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

- Molecule 49 is a protein called 30S ribosomal protein S19.

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

- Molecule 50 is a protein called 30S ribosomal protein S20.

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

- Molecule 51 is a protein called 30S ribosomal protein S21.

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

- Molecule 52 is a protein called Elongation factor P.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	w	188	Total	C	N	O	S	0	0
			1461	928	242	286	5		

- Molecule 53 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	v	9	Total	C	N	O	P	0	0
			189	84	33	63	9		

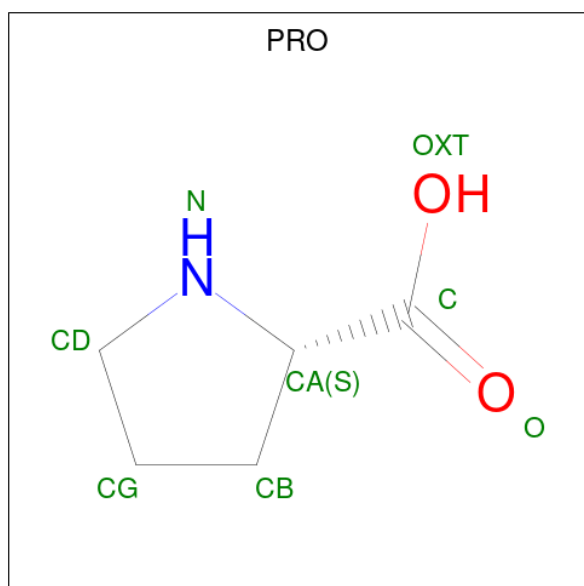
- Molecule 54 is a RNA chain called Proline tRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	x	77	Total	C	N	O	P	0	0
			1646	733	295	541	77		
54	9	77	Total	C	N	O	P	0	0
			1646	733	295	541	77		

- Molecule 55 is a protein called 50S ribosomal protein L1.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	7	224	Total	C	N	O	S	0	0
			1663	1039	303	315	6		

- Molecule 56 is PROLINE (CCD ID: PRO) (formula: $C_5H_9NO_2$).

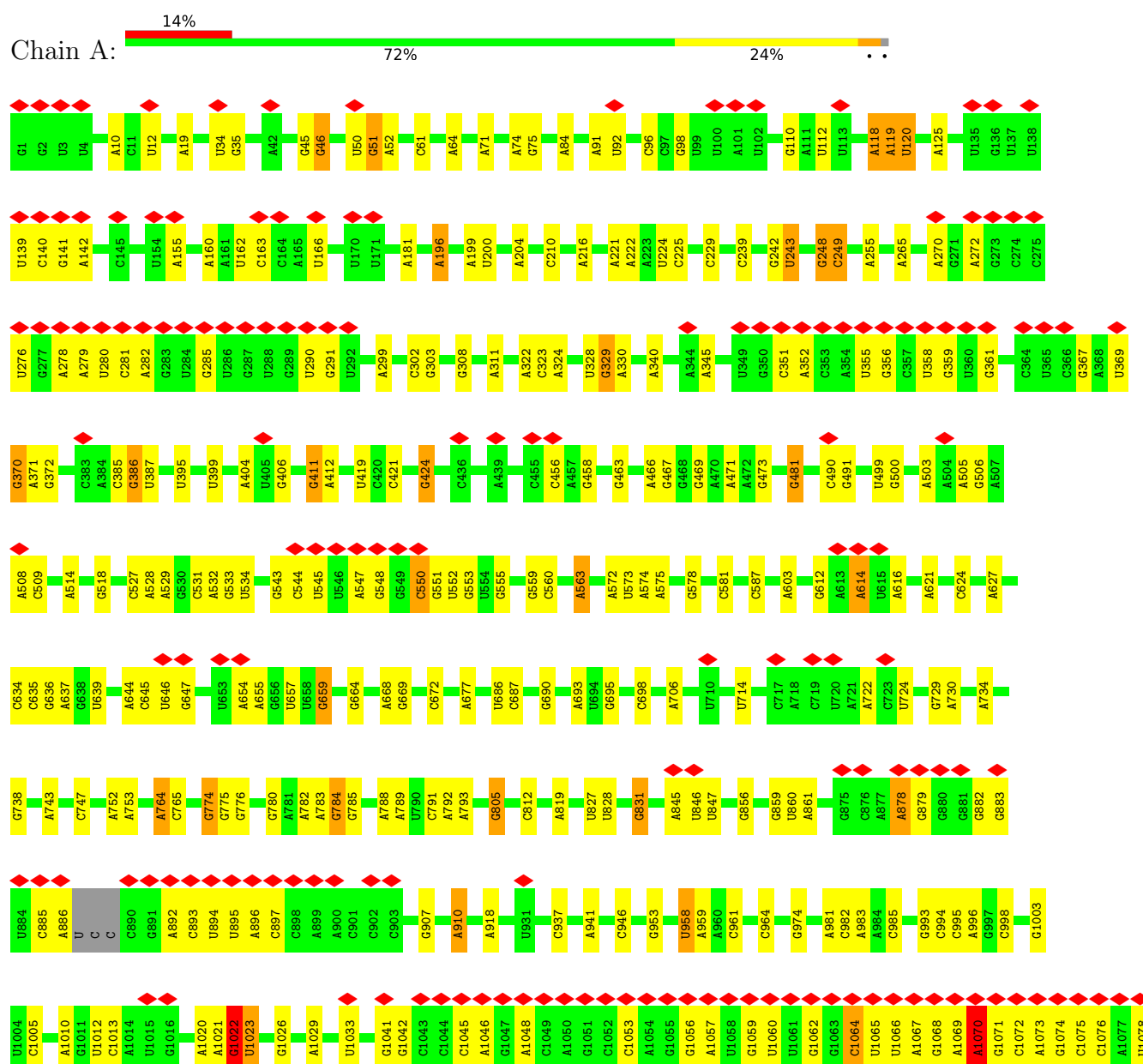


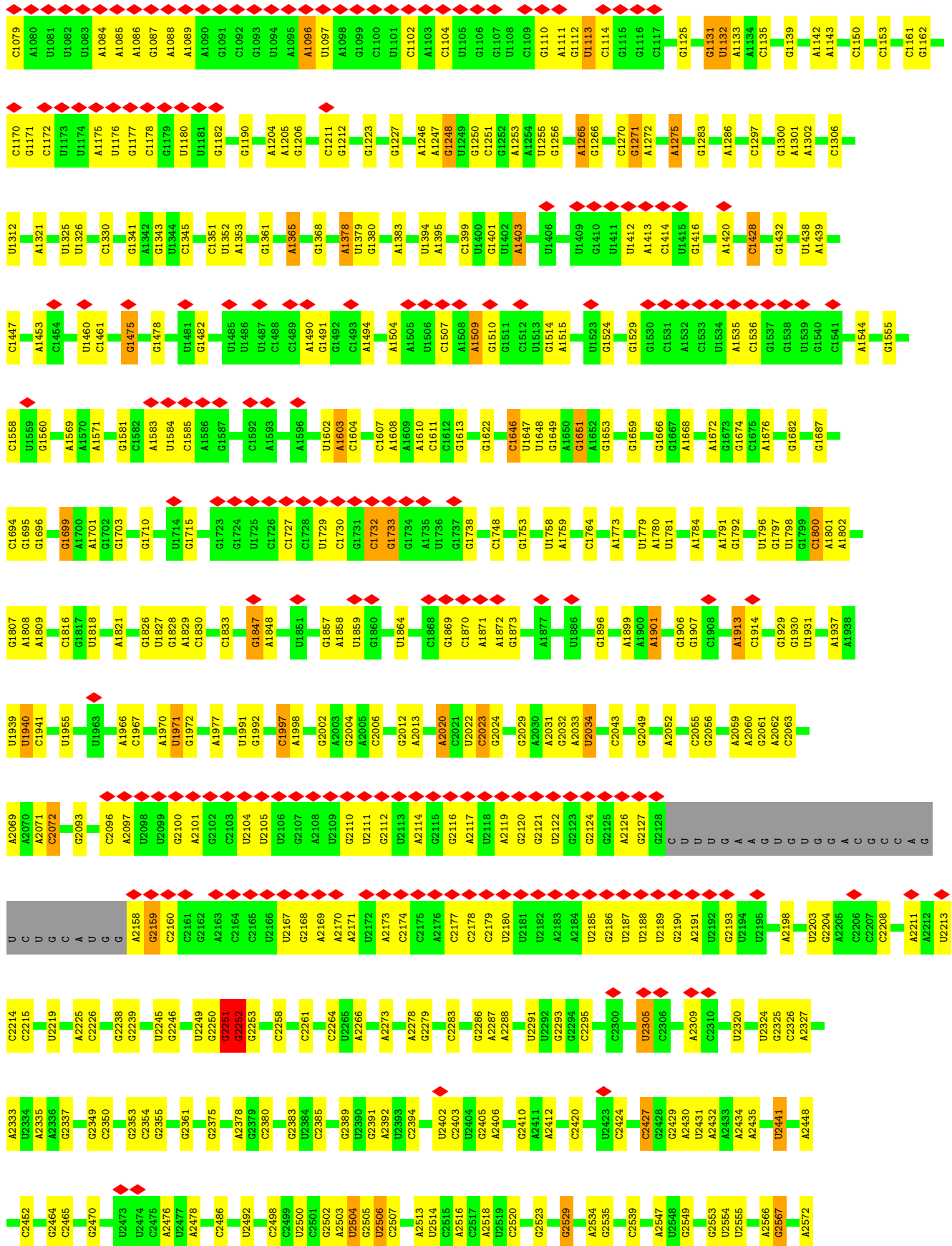
Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
56	9	1	7	5	1	1	0

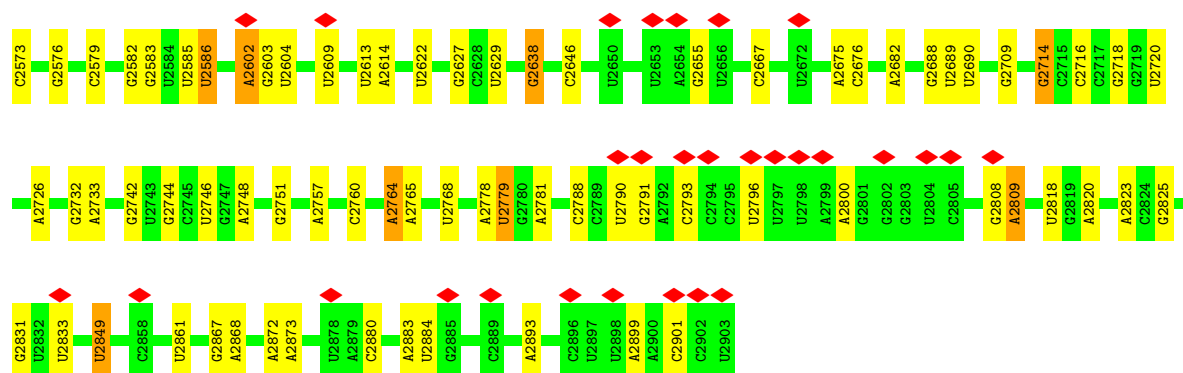
3 Residue-property plots

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.

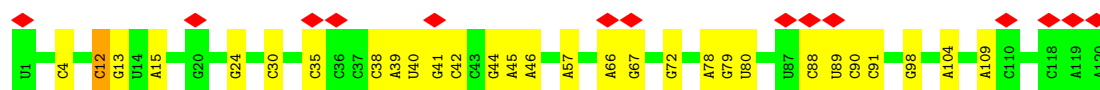
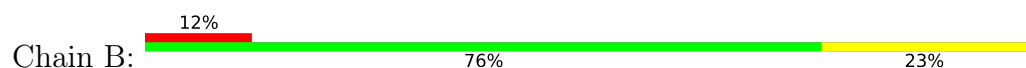
• Molecule 1: 23S Ribosomal RNA



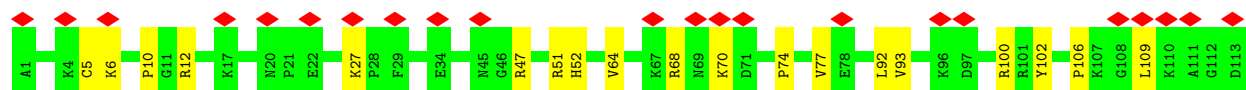
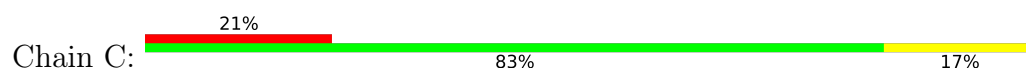




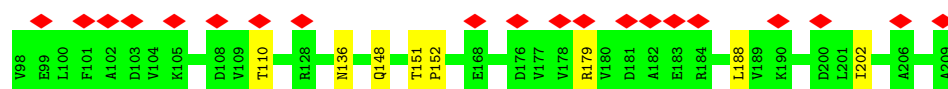
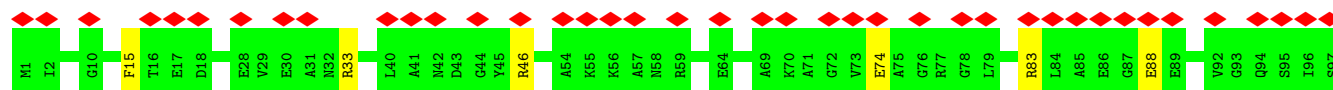
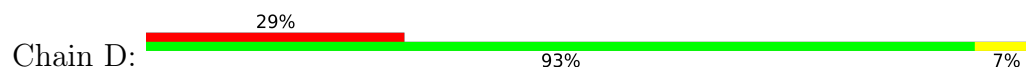
- Molecule 2: 5S Ribosomal RNA



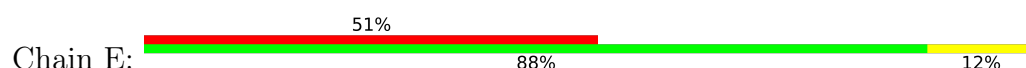
- Molecule 3: 50S ribosomal protein L2

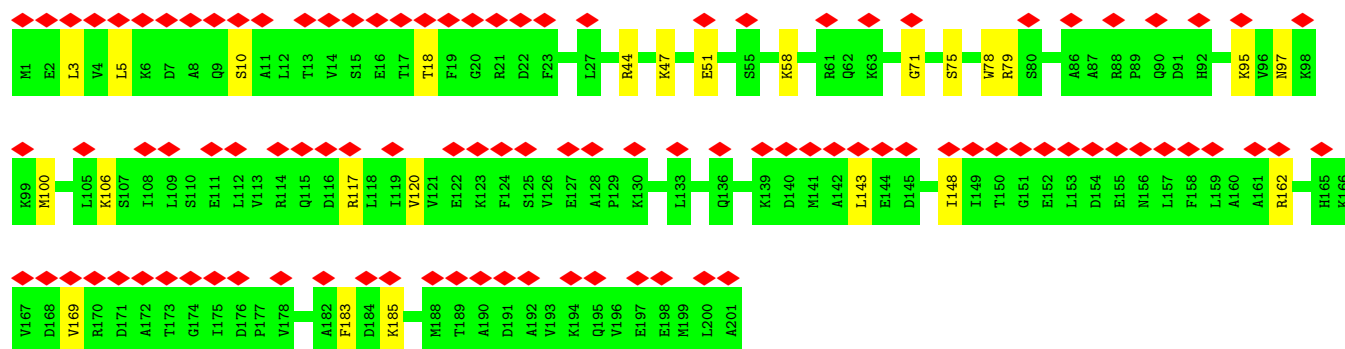


- Molecule 4: 50S ribosomal protein L3

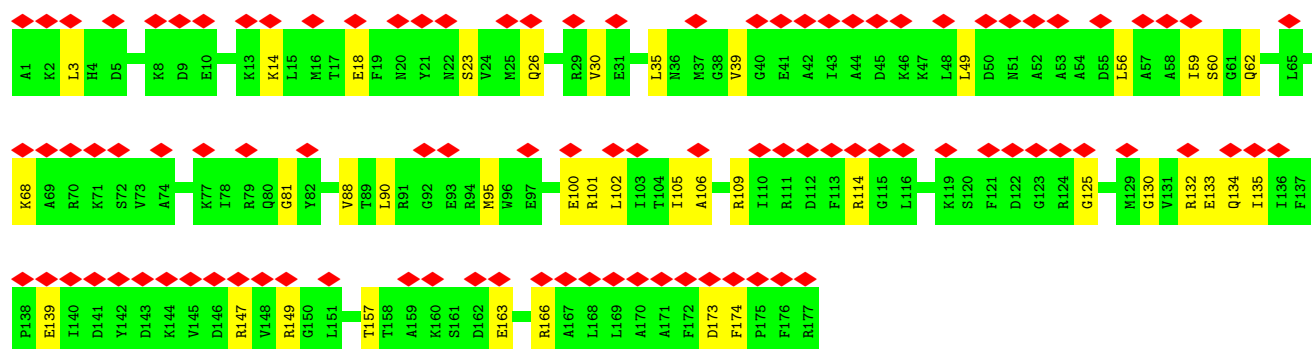
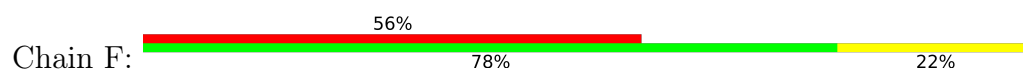


- Molecule 5: 50S ribosomal protein L4

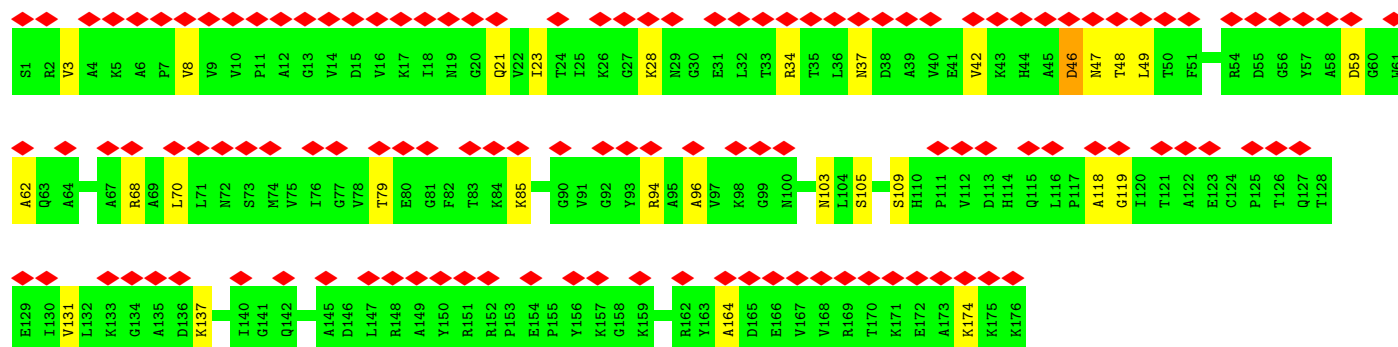
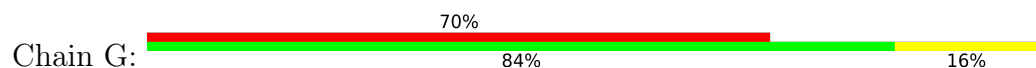




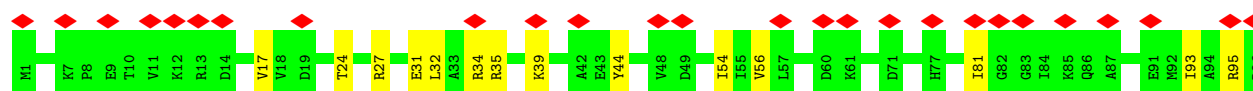
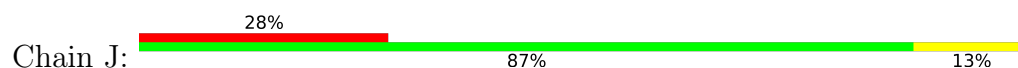
• Molecule 6: 50S ribosomal protein L5

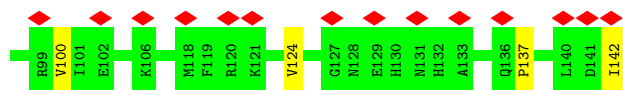


• Molecule 7: 50S ribosomal protein L6

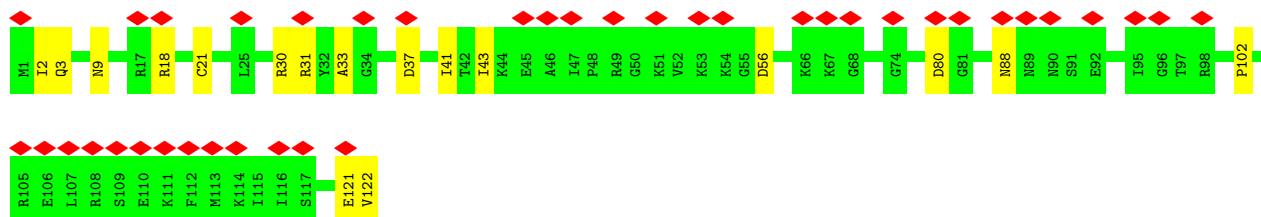
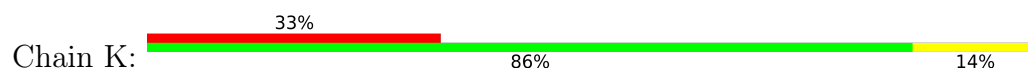


• Molecule 8: 50S ribosomal protein L13

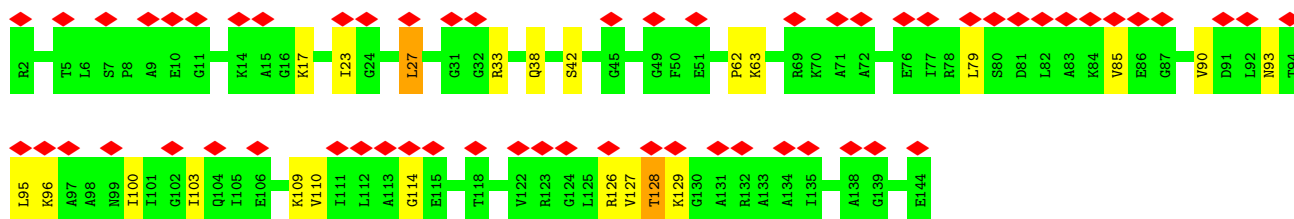
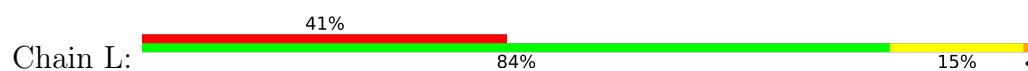




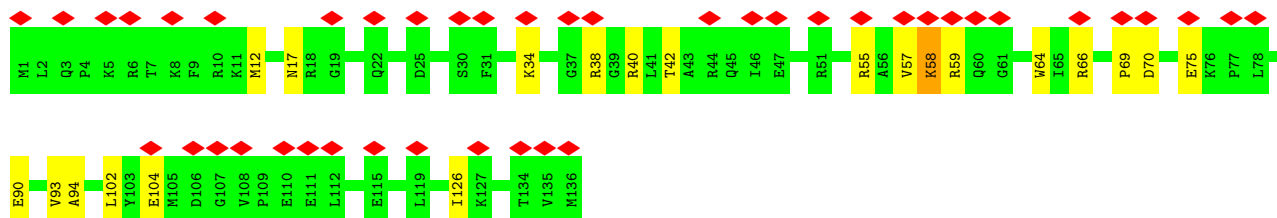
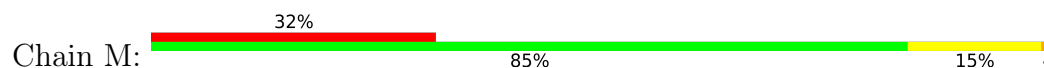
- Molecule 9: 50S ribosomal protein L14



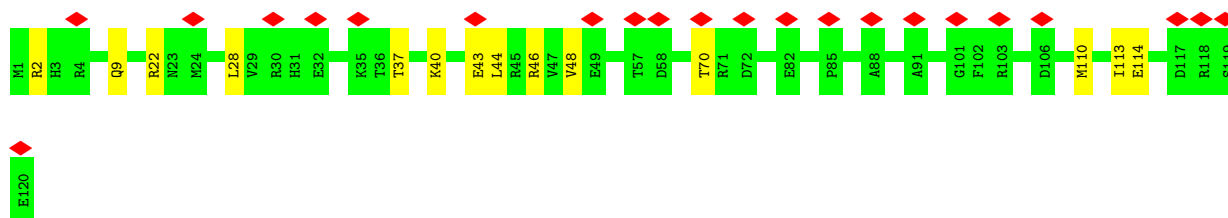
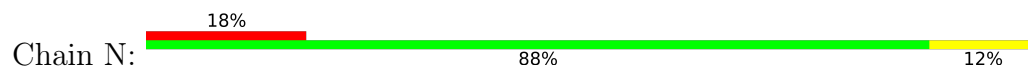
- Molecule 10: 50S ribosomal protein L15



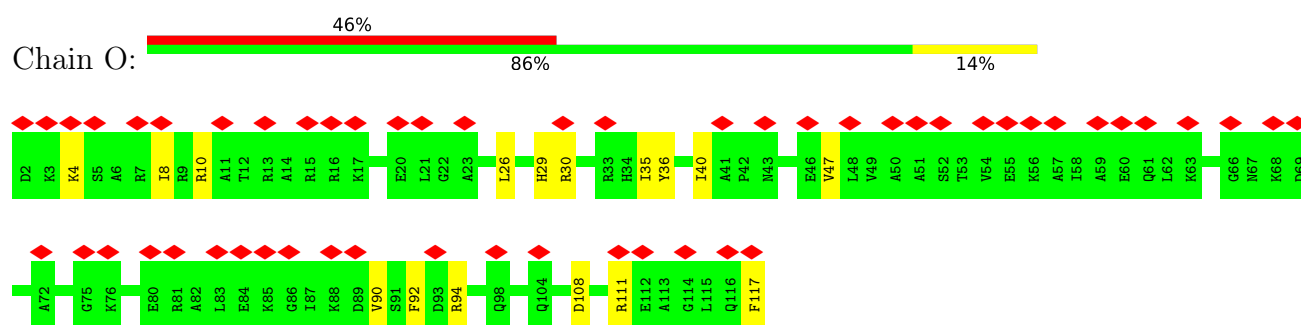
- Molecule 11: 50S ribosomal protein L16



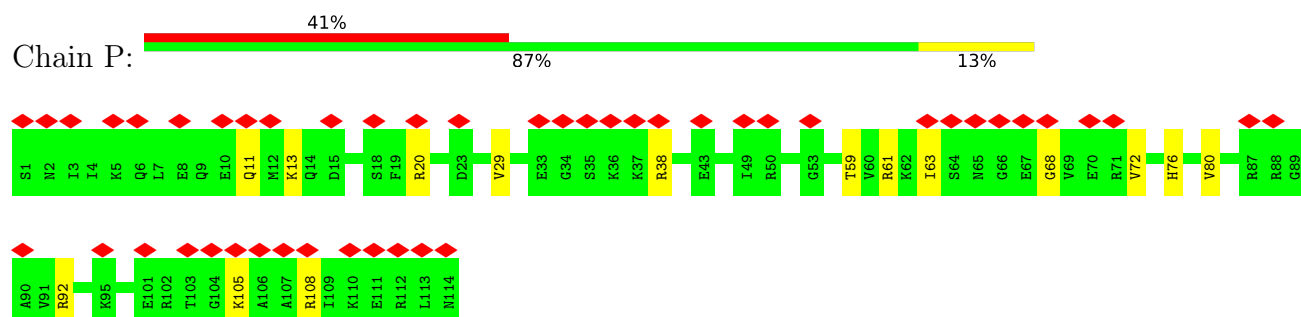
- Molecule 12: 50S ribosomal protein L17



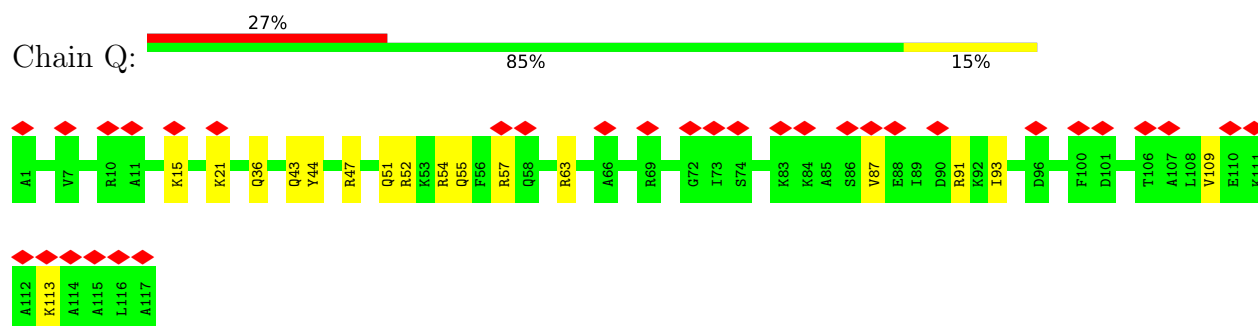
- Molecule 13: 50S ribosomal protein L18



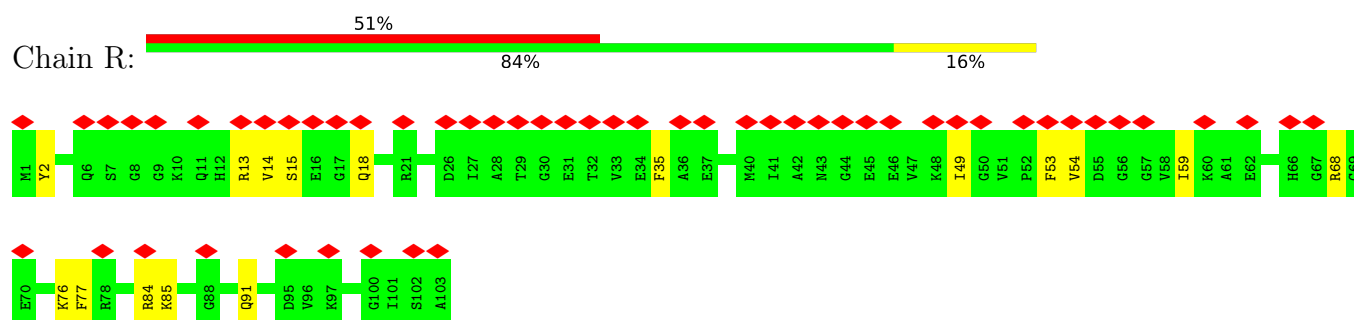
• Molecule 14: 50S ribosomal protein L19



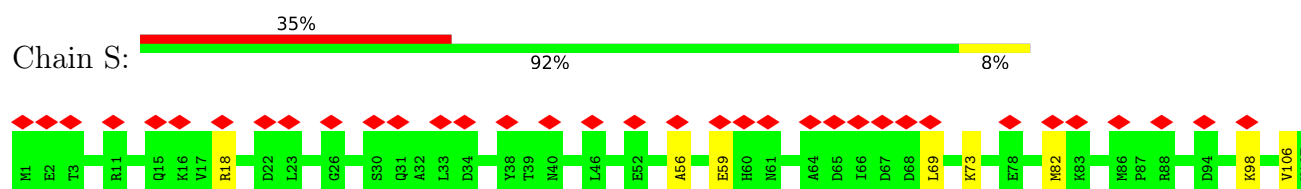
• Molecule 15: 50S ribosomal protein L20



• Molecule 16: 50S ribosomal protein L21

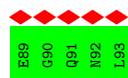
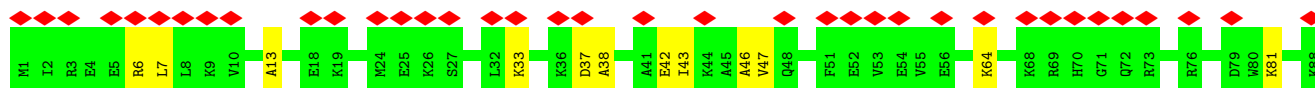
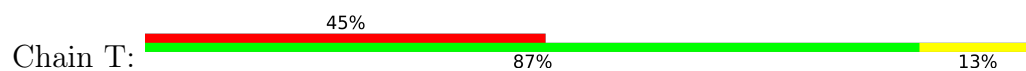


• Molecule 17: 50S ribosomal protein L22

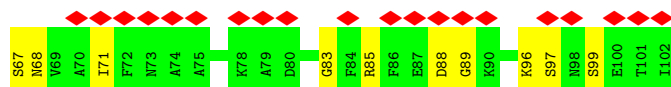
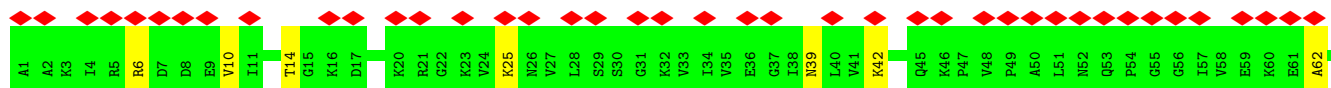
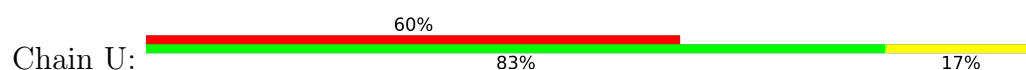




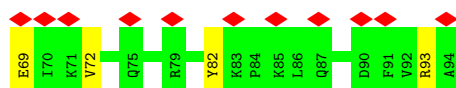
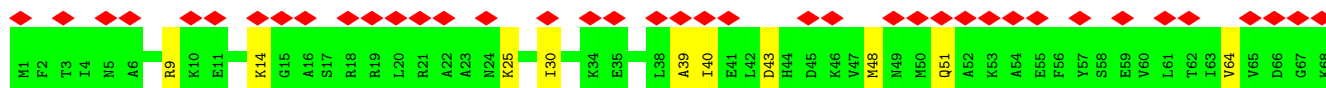
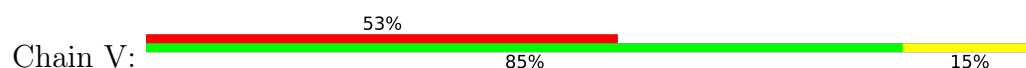
- Molecule 18: 50S ribosomal protein L23



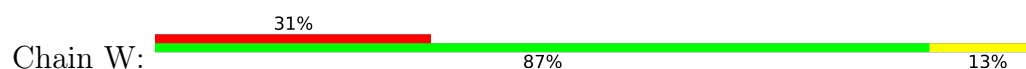
- Molecule 19: 50S ribosomal protein L24



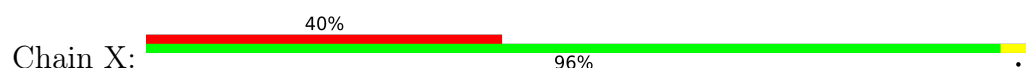
- Molecule 20: 50S ribosomal protein L25

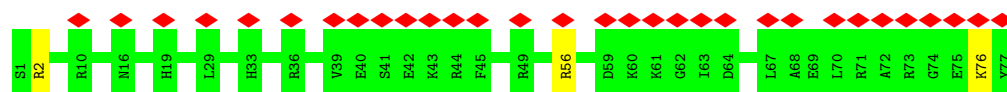


- Molecule 21: 50S ribosomal protein L27

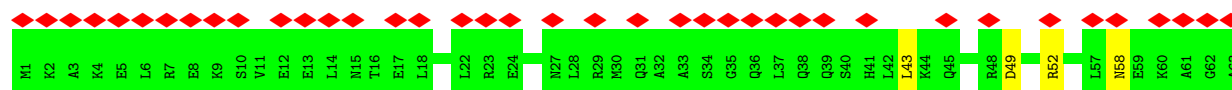


- Molecule 22: 50S ribosomal protein L28

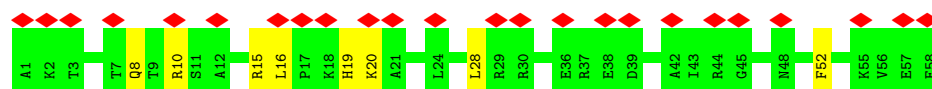
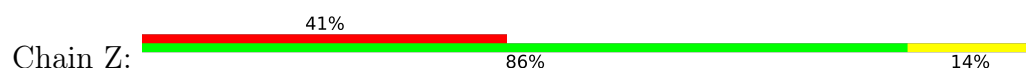




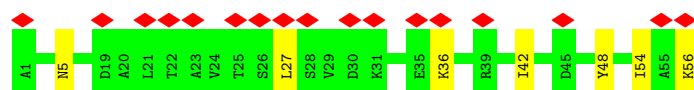
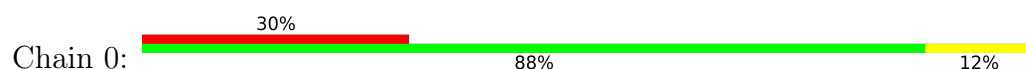
- Molecule 23: 50S ribosomal protein L29



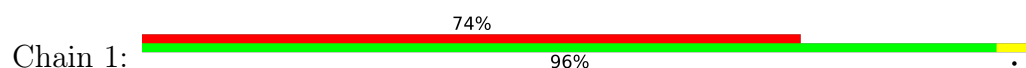
- Molecule 24: 50S ribosomal protein L30



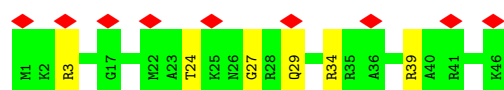
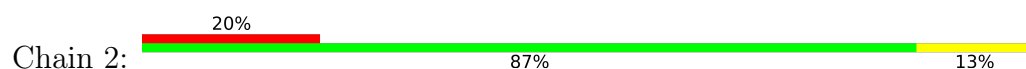
- Molecule 25: 50S ribosomal protein L32



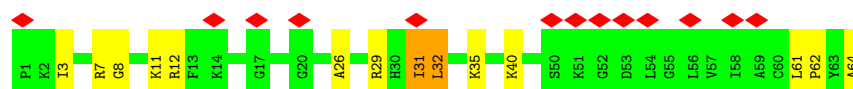
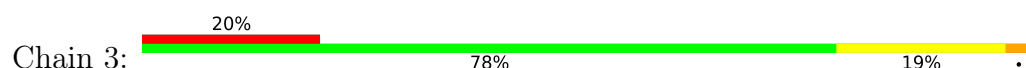
- Molecule 26: 50S ribosomal protein L33



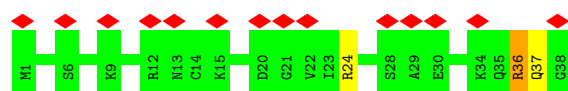
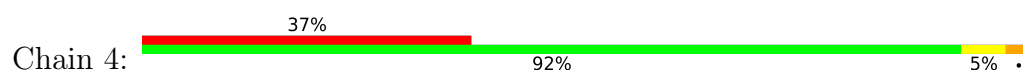
- Molecule 27: 50S ribosomal protein L34



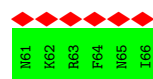
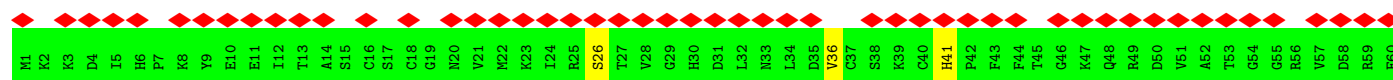
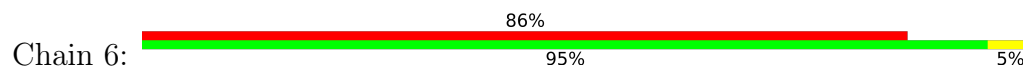
- Molecule 28: 50S ribosomal protein L35



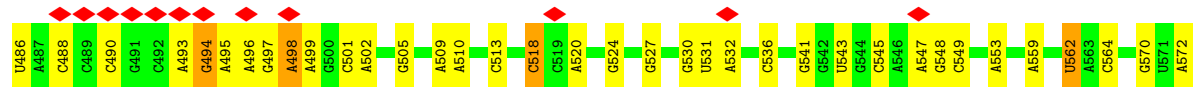
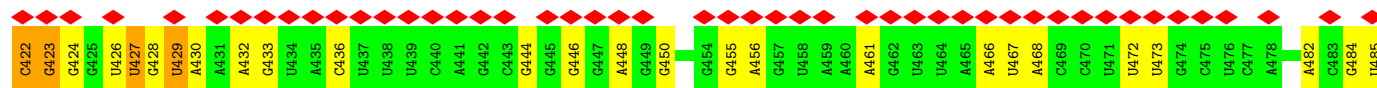
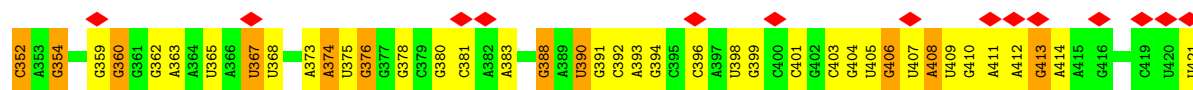
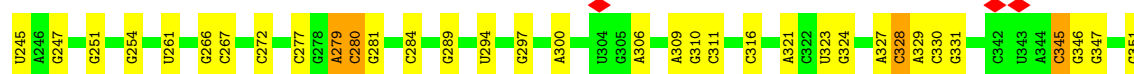
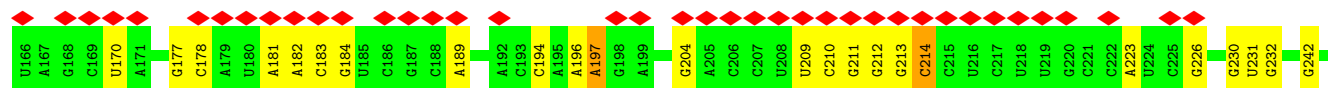
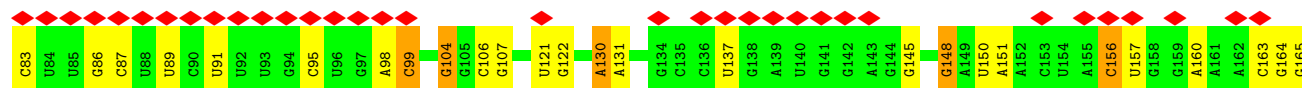
- Molecule 29: 50S ribosomal protein L36

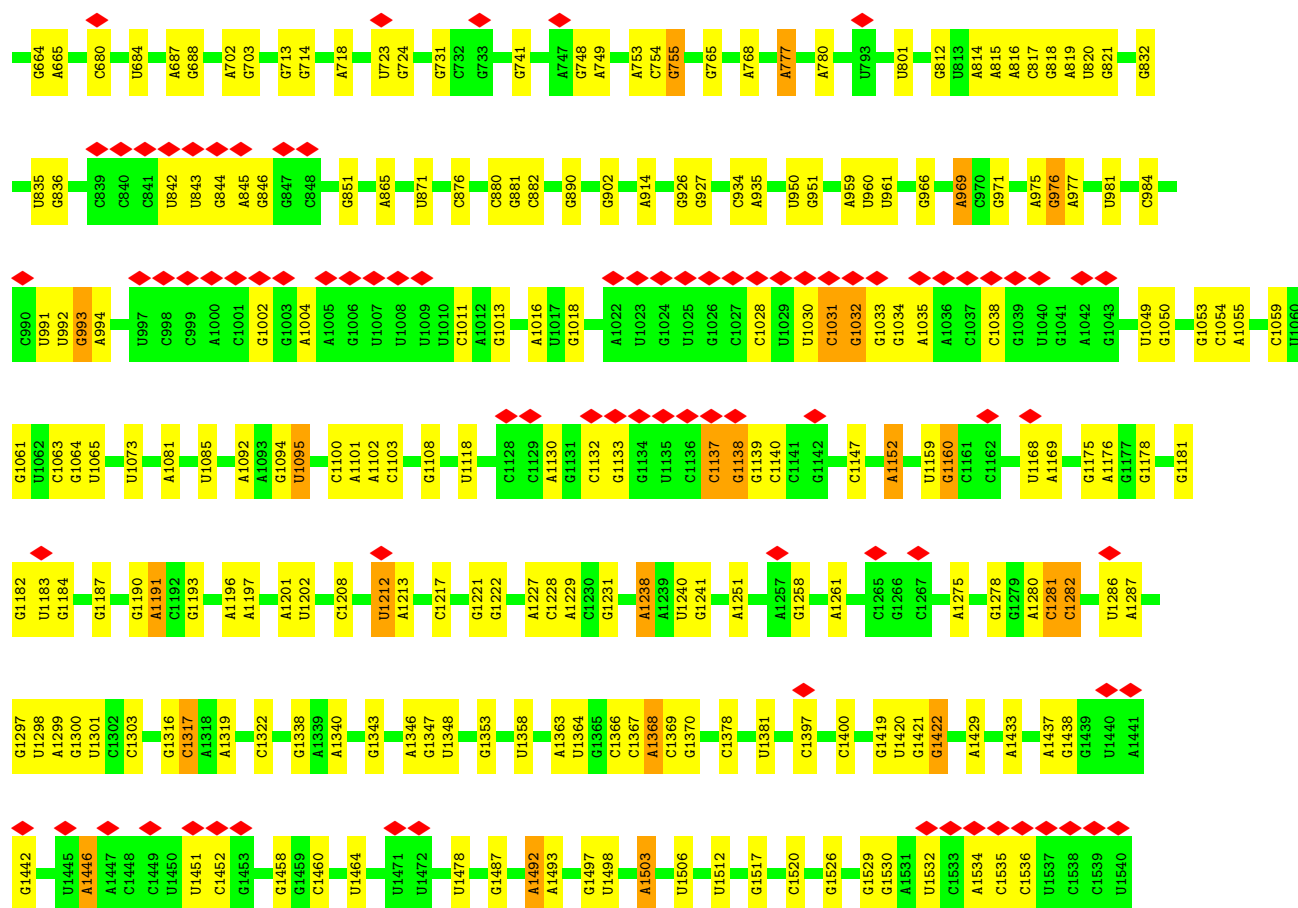


• Molecule 30: 50S ribosomal protein L31

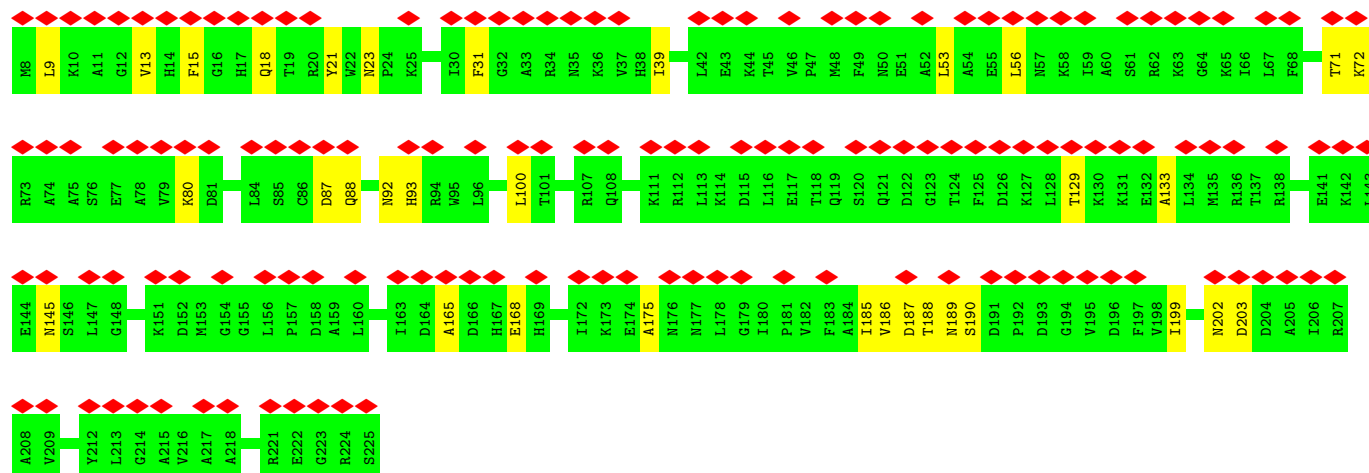
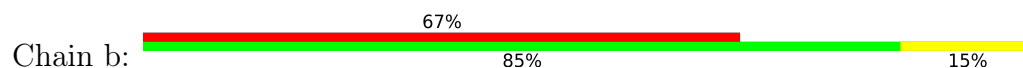


• Molecule 31: 16S ribosomal RNA

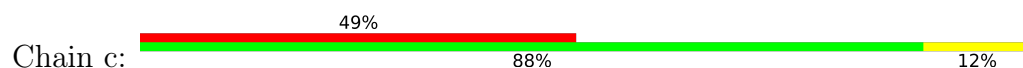


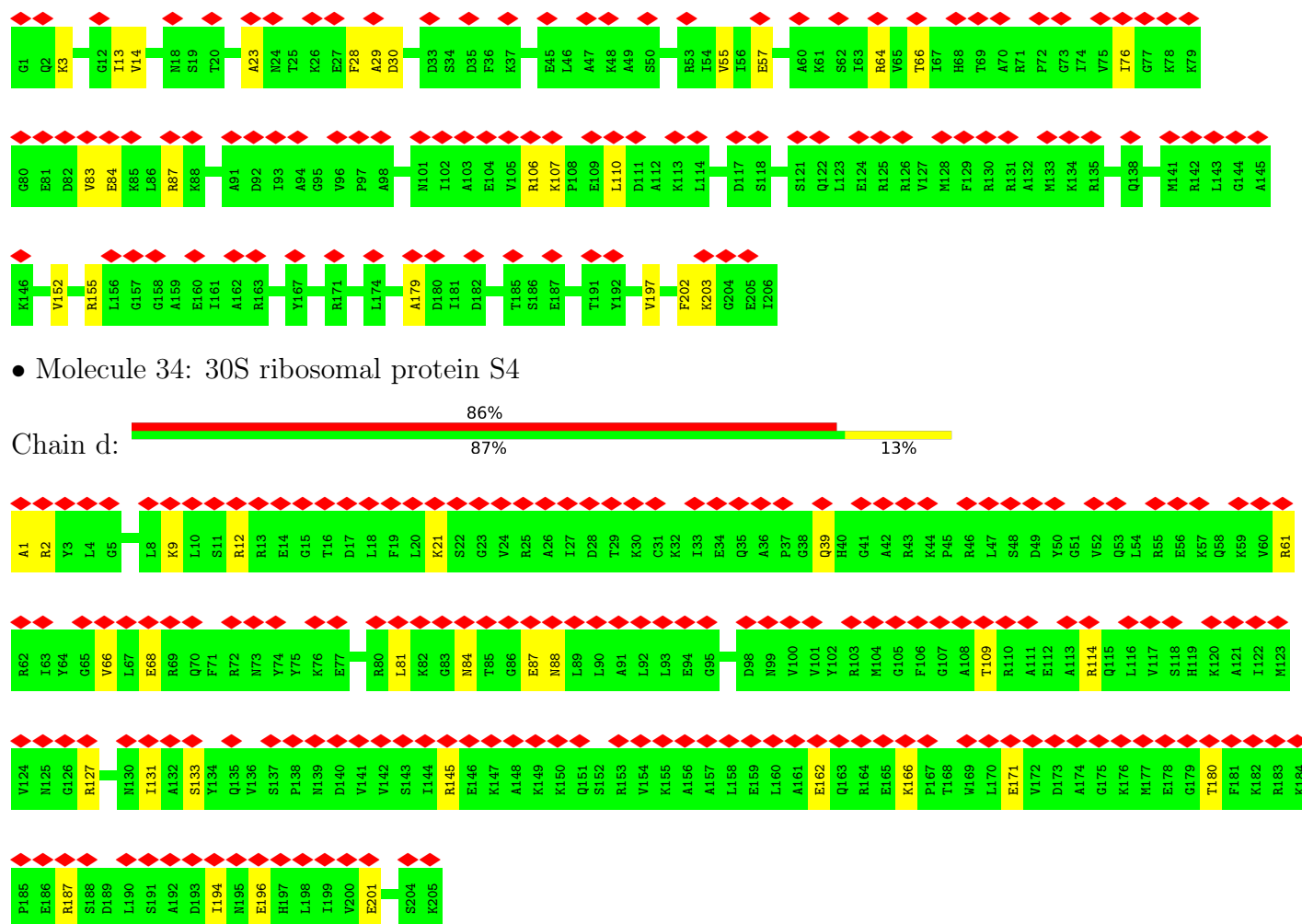


• Molecule 32: 30S ribosomal protein S2

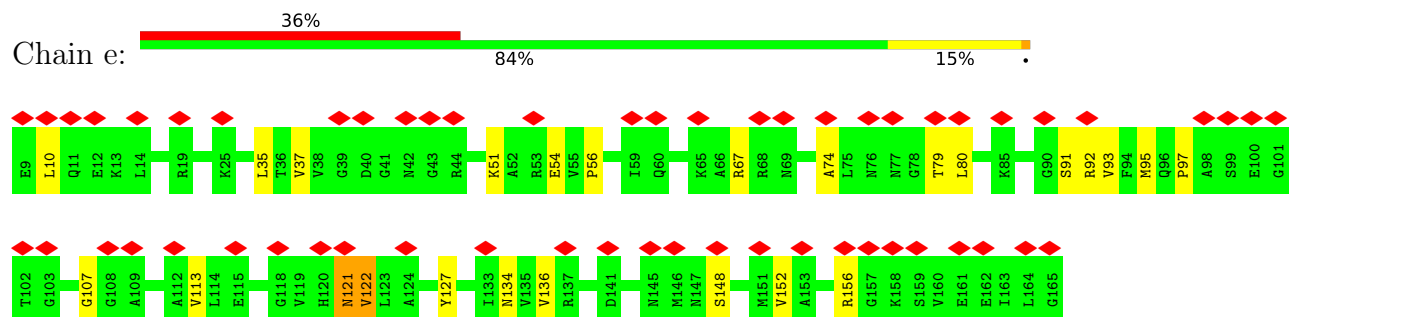


• Molecule 33: 30S ribosomal protein S3

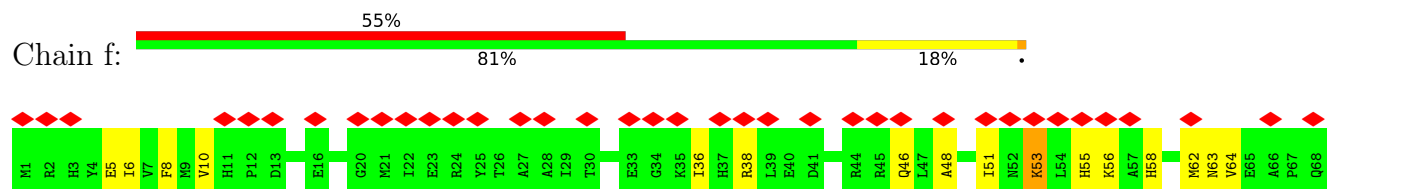


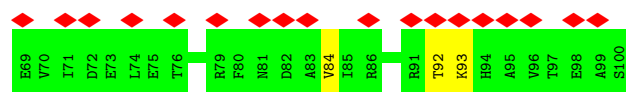


• Molecule 35: 30S ribosomal protein S5

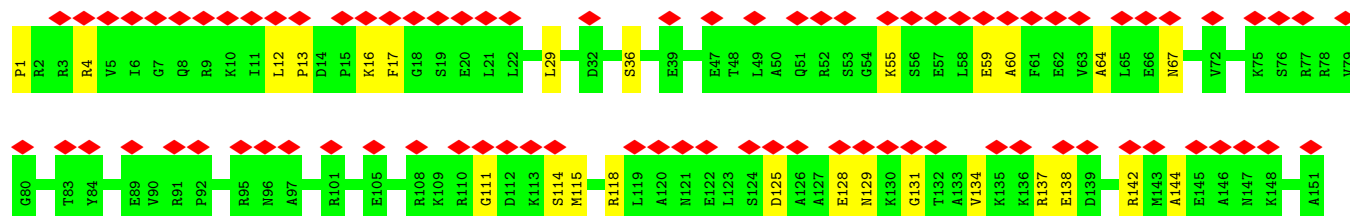
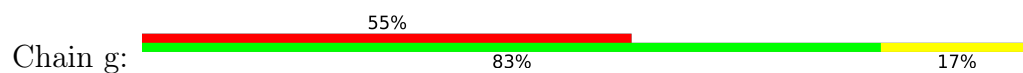


• Molecule 36: 30S ribosomal protein S6

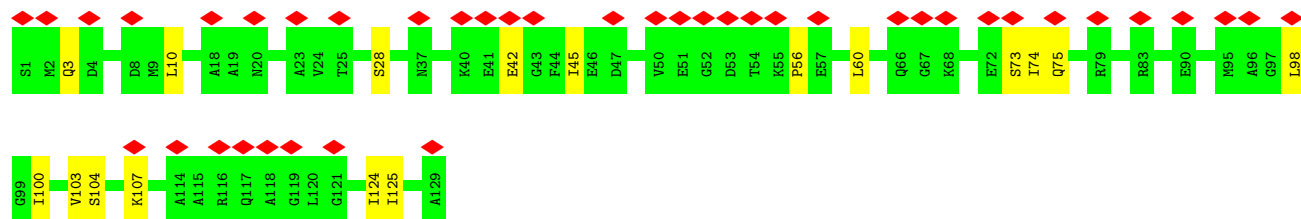
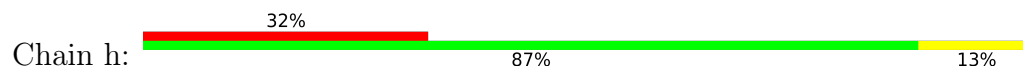




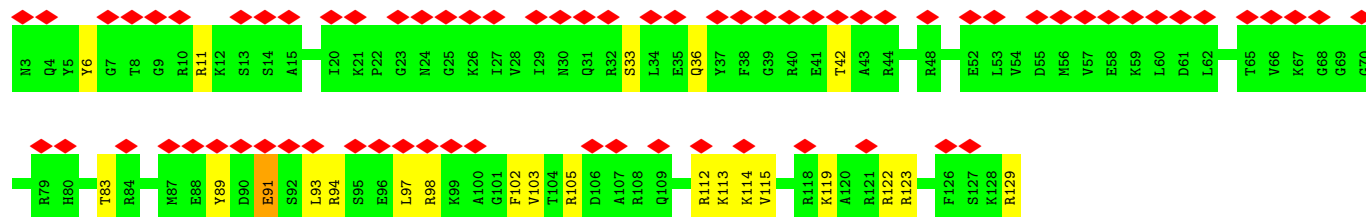
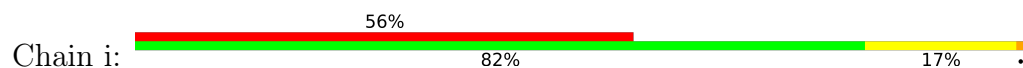
- Molecule 37: 30S ribosomal protein S7



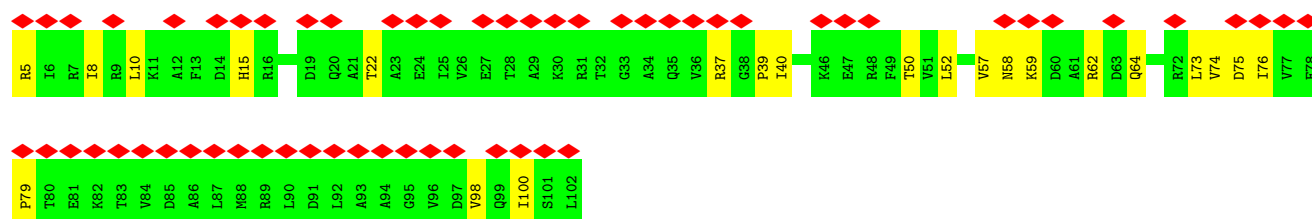
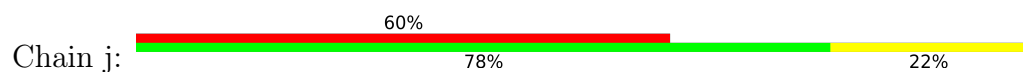
- Molecule 38: 30S ribosomal protein S8



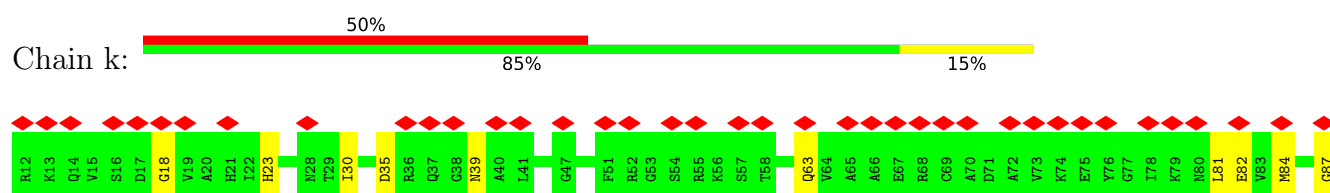
- Molecule 39: 30S ribosomal protein S9



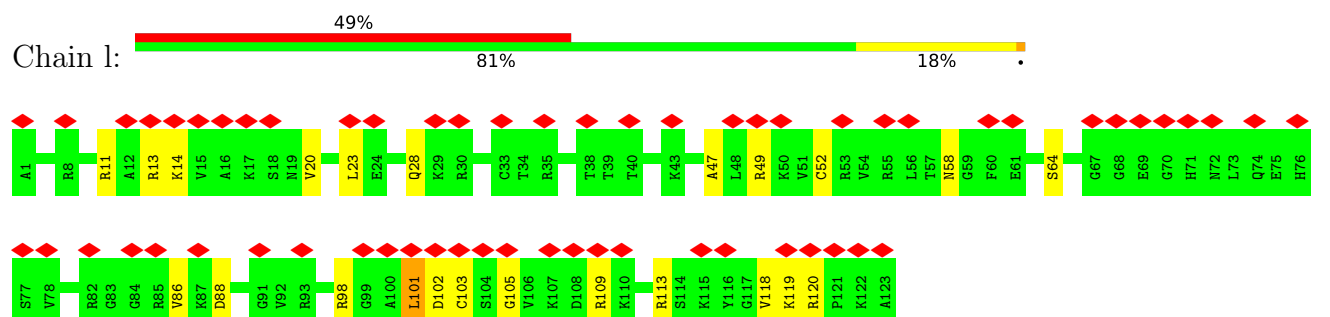
- Molecule 40: 30S ribosomal protein S10



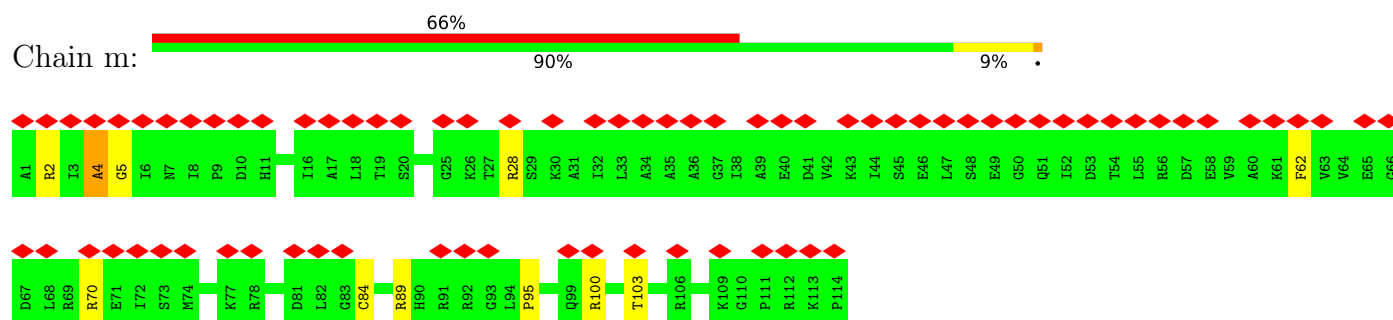
- Molecule 41: 30S ribosomal protein S11



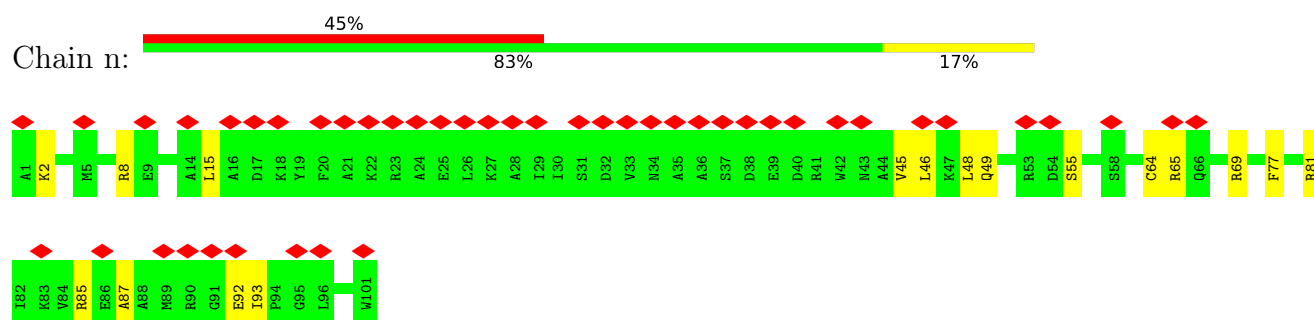
• Molecule 42: 30S ribosomal protein S12



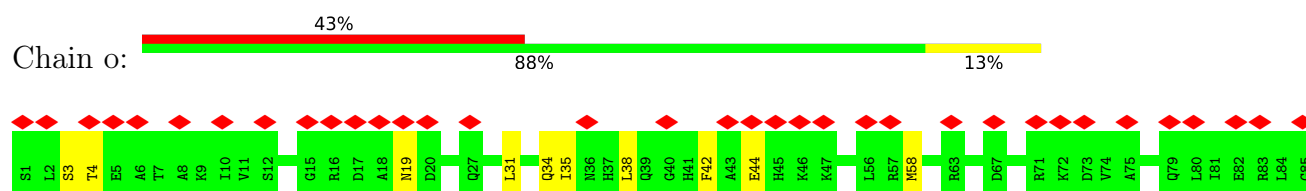
• Molecule 43: 30S ribosomal protein S13



• Molecule 44: 30S ribosomal protein S14

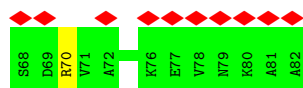
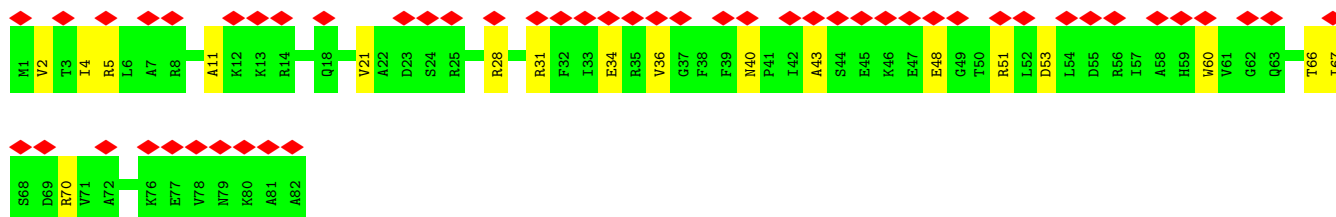
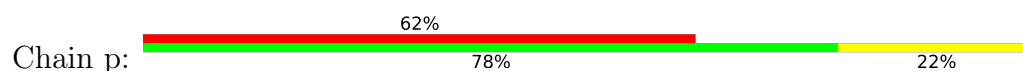


• Molecule 45: 30S ribosomal protein S15

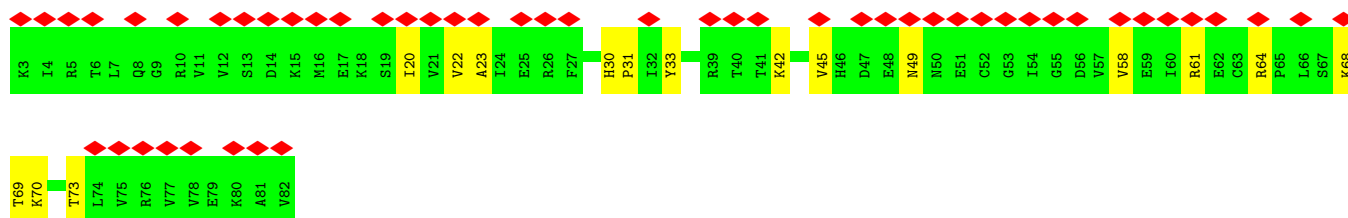
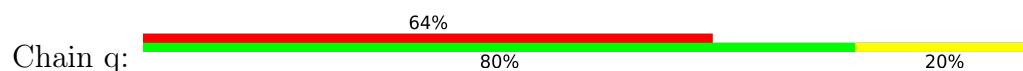




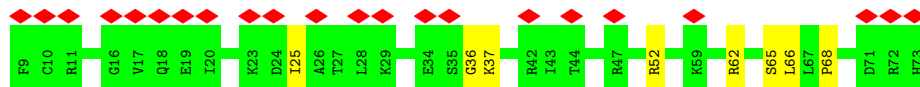
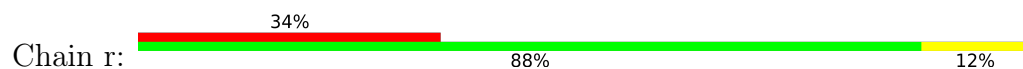
• Molecule 46: 30S ribosomal protein S16



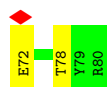
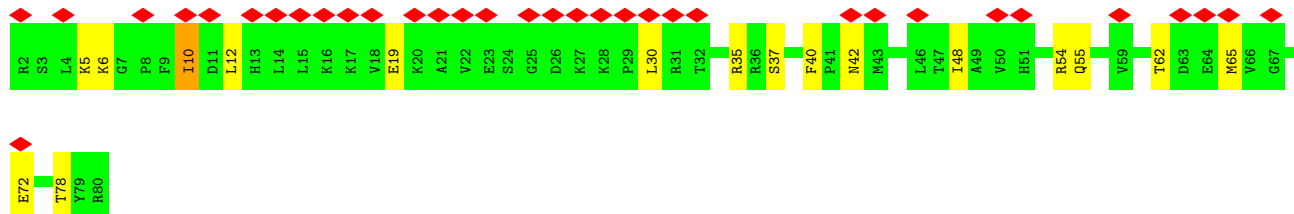
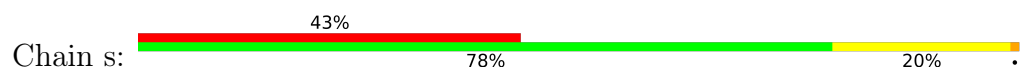
• Molecule 47: 30S ribosomal protein S17



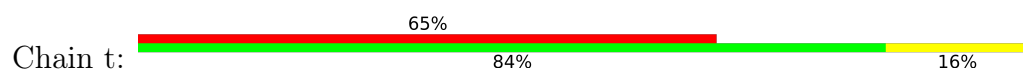
• Molecule 48: 30S ribosomal protein S18

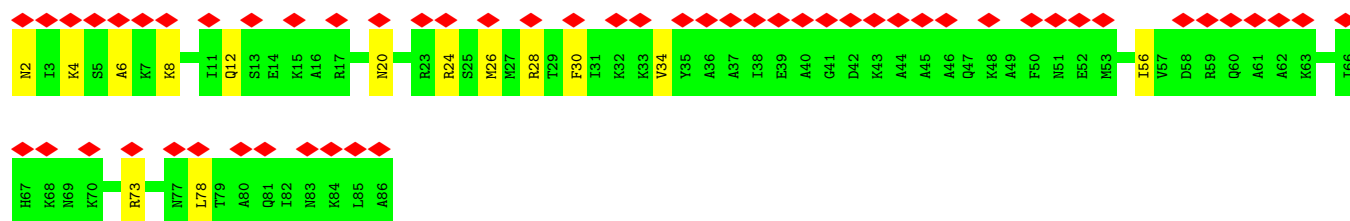


• Molecule 49: 30S ribosomal protein S19

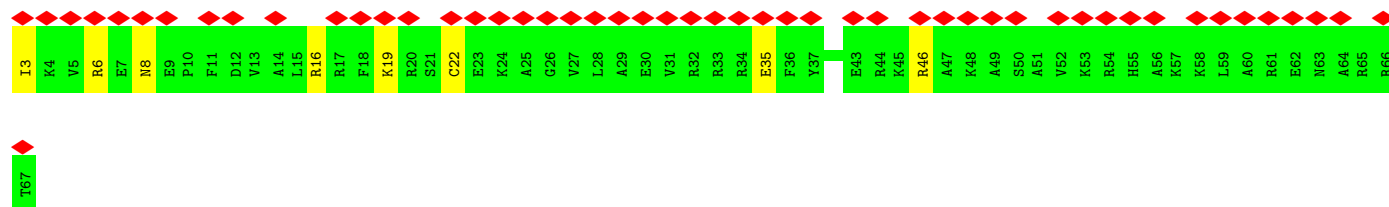
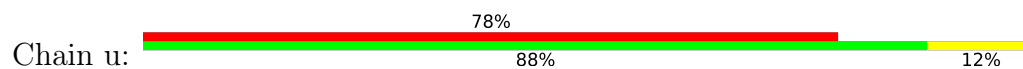


• Molecule 50: 30S ribosomal protein S20

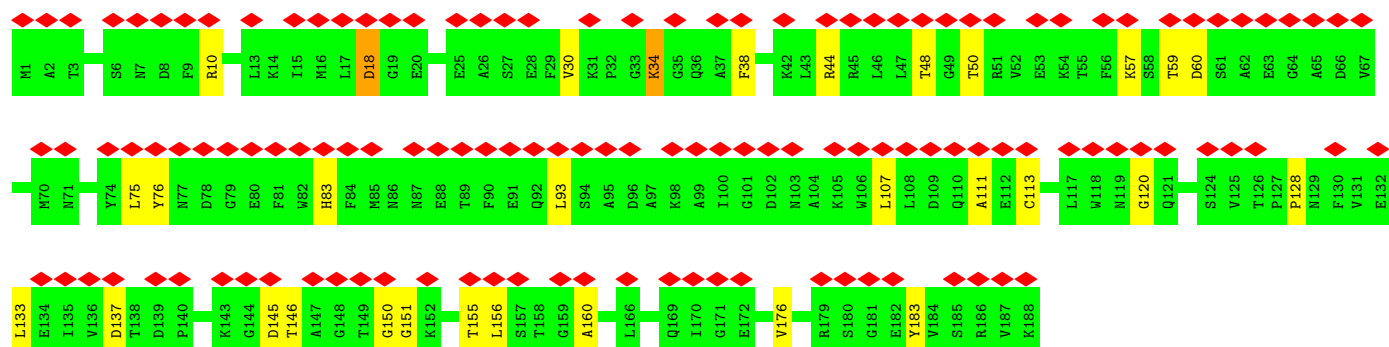
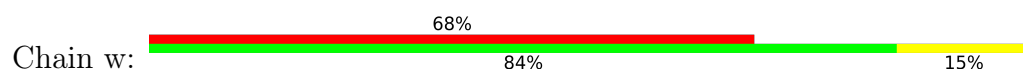




• Molecule 51: 30S ribosomal protein S21



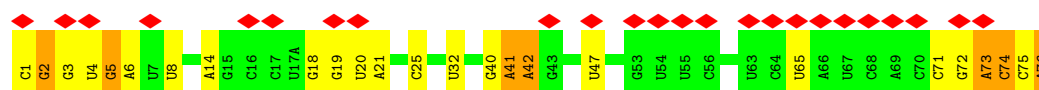
• Molecule 52: Elongation factor P



• Molecule 53: mRNA

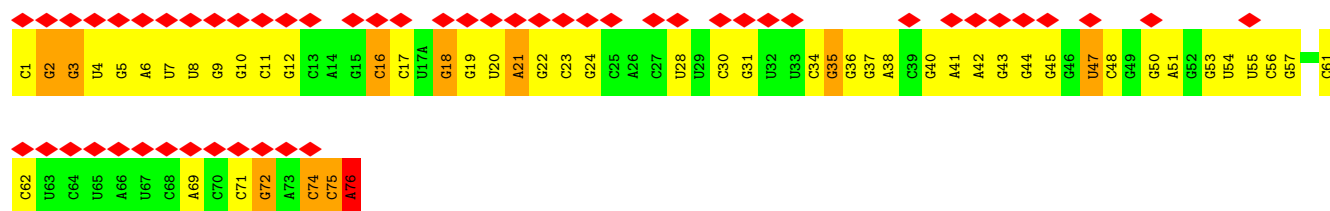


• Molecule 54: Proline tRNA

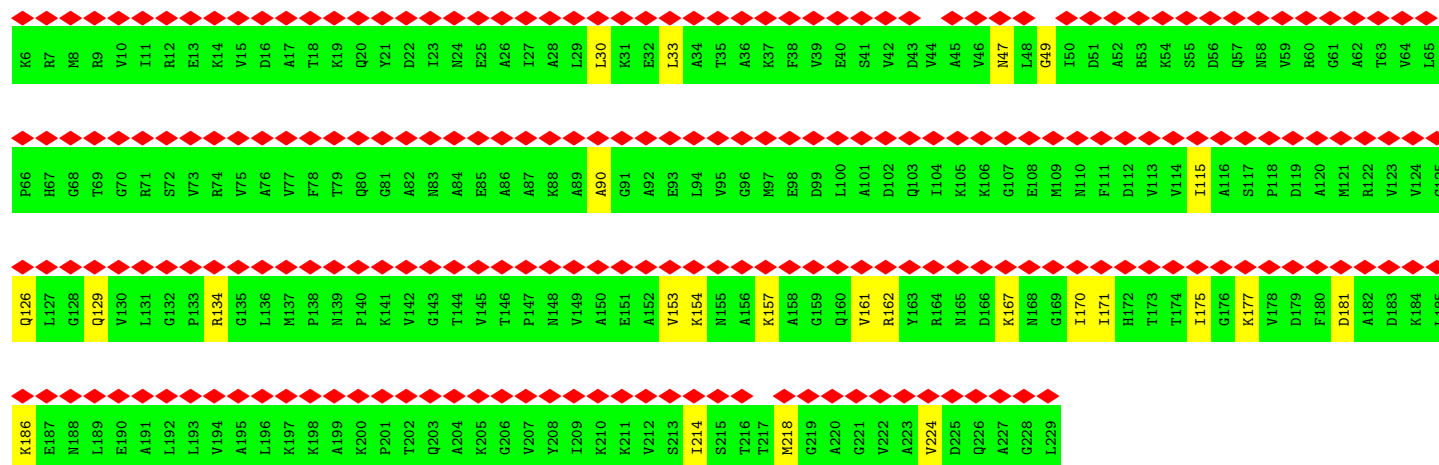
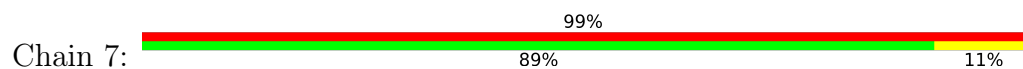


• Molecule 54: Proline tRNA





● Molecule 55: 50S ribosomal protein L1



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	21655	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	28	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	FEI FALCON II (4k x 4k)	Depositor
Maximum map value	0.443	Depositor
Minimum map value	-0.298	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.018	Depositor
Recommended contour level	0.0963	Depositor
Map size (Å)	390.24, 390.24, 390.24	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.084, 1.084, 1.084	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.11	2/69039 (0.0%)	0.24	7/107701 (0.0%)
2	B	0.10	0/2876	0.24	0/4483
3	C	0.18	0/2121	0.49	0/2852
4	D	0.17	0/1586	0.47	0/2134
5	E	0.14	0/1571	0.41	0/2113
6	F	0.22	0/1434	0.54	0/1926
7	G	0.17	0/1343	0.39	0/1816
8	J	0.14	0/1152	0.42	0/1551
9	K	0.19	0/947	0.53	0/1268
10	L	0.19	0/1054	0.60	2/1403 (0.1%)
11	M	0.18	0/1093	0.55	0/1460
12	N	0.20	0/973	0.59	0/1301
13	O	0.16	0/902	0.45	0/1209
14	P	0.15	0/929	0.42	0/1242
15	Q	0.15	0/960	0.40	0/1278
16	R	0.16	0/829	0.48	0/1107
17	S	0.15	0/864	0.45	0/1156
18	T	0.15	0/744	0.57	1/994 (0.1%)
19	U	0.22	0/787	0.57	0/1051
20	V	0.14	0/766	0.40	0/1025
21	W	0.72	1/645 (0.2%)	0.60	1/852 (0.1%)
22	X	0.14	0/635	0.41	0/848
23	Y	0.11	0/510	0.38	0/677
24	Z	0.15	0/453	0.40	0/605
25	0	0.16	0/450	0.48	0/599
26	1	0.16	0/416	0.45	0/554
27	2	0.14	0/380	0.46	0/498
28	3	0.30	0/513	0.66	0/676
29	4	0.19	0/303	0.63	2/397 (0.5%)
30	6	0.16	0/531	0.45	0/709
31	a	0.10	0/36967	0.23	0/57666
32	b	0.18	0/1735	0.49	0/2338

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	c	0.18	0/1651	0.48	0/2225
34	d	0.21	0/1665	0.62	0/2227
35	e	0.20	0/1154	0.62	2/1554 (0.1%)
36	f	0.24	0/835	0.68	0/1128
37	g	0.19	0/1195	0.61	5/1602 (0.3%)
38	h	0.18	0/989	0.49	0/1326
39	i	0.21	0/1034	0.63	2/1375 (0.1%)
40	j	0.24	0/796	0.66	0/1077
41	k	0.19	0/885	0.51	0/1195
42	l	0.23	0/969	0.64	0/1300
43	m	0.18	0/892	0.63	0/1193
44	n	0.16	0/811	0.47	0/1081
45	o	0.16	0/722	0.50	2/964 (0.2%)
46	p	0.21	0/659	0.53	0/884
47	q	0.24	0/657	0.63	3/881 (0.3%)
48	r	0.17	0/511	0.56	0/689
49	s	0.18	0/652	0.46	0/877
50	t	0.17	0/671	0.49	0/888
51	u	0.31	0/500	0.76	2/668 (0.3%)
52	w	0.24	0/1470	0.70	7/1992 (0.4%)
53	v	0.25	0/209	0.47	0/323
54	9	0.42	1/1839 (0.1%)	0.59	2/2866 (0.1%)
54	x	0.17	0/1838	0.39	0/2862
55	7	0.16	0/1672	0.44	0/2244
All	All	0.15	4/159784 (0.0%)	0.35	38/238910 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
6	F	0	2
7	G	0	2
9	K	0	1
11	M	0	2
16	R	0	1
19	U	0	2
32	b	0	2
36	f	0	1
40	j	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
42	l	0	1
43	m	0	1
47	q	0	1
52	w	0	2
All	All	0	20

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	W	10	THR	C-N	-15.36	1.10	1.33
54	9	76	A	C3'-O3'	-9.87	1.27	1.42
1	A	2252	G	O3'-P	-9.24	1.47	1.61
1	A	2252	G	C3'-O3'	-5.34	1.34	1.42

All (38) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	2252	G	C2'-C3'-O3'	-12.74	94.59	113.70
54	9	76	A	C2'-C3'-O3'	-10.74	97.58	113.70
1	A	2252	G	C3'-C2'-O2'	9.06	124.28	110.70
1	A	2251	G	C1'-C2'-O2'	-7.86	96.61	108.40
1	A	2251	G	C2'-C3'-O3'	6.99	124.19	113.70
1	A	2251	G	N9-C1'-C2'	6.70	122.05	112.00
18	T	47	VAL	N-CA-C	-6.49	106.47	112.96
37	g	64	ALA	N-CA-C	-5.97	105.56	114.64
52	w	48	THR	CA-C-N	5.90	132.33	121.70
52	w	48	THR	C-N-CA	5.90	132.33	121.70
35	e	121	ASN	CA-C-N	5.88	132.55	121.97
35	e	121	ASN	C-N-CA	5.88	132.55	121.97
52	w	18	ASP	CA-C-N	5.85	132.22	121.70
52	w	18	ASP	C-N-CA	5.85	132.22	121.70
47	q	68	LYS	CA-C-N	5.67	129.76	121.31
47	q	68	LYS	C-N-CA	5.67	129.76	121.31
52	w	145	ASP	CA-C-N	5.64	131.85	121.70
52	w	145	ASP	C-N-CA	5.64	131.85	121.70
52	w	18	ASP	N-CA-C	5.47	121.83	113.51
29	4	36	ARG	CA-C-N	5.42	131.88	121.54
29	4	36	ARG	C-N-CA	5.42	131.88	121.54
45	o	44	GLU	CA-C-N	5.18	131.44	121.54
45	o	44	GLU	C-N-CA	5.18	131.44	121.54
47	q	49	ASN	N-CA-C	5.18	117.98	110.42
51	u	35	GLU	CA-C-N	5.17	131.42	121.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
51	u	35	GLU	C-N-CA	5.17	131.42	121.54
39	i	119	LYS	CA-C-N	5.12	131.33	121.54
39	i	119	LYS	C-N-CA	5.12	131.33	121.54
1	A	1070	A	P-O3'-C3'	5.08	127.83	120.20
37	g	128	GLU	CA-C-N	5.08	131.24	121.54
37	g	128	GLU	C-N-CA	5.08	131.24	121.54
1	A	1022	G	P-O3'-C3'	5.06	127.79	120.20
10	L	93	ASN	CA-C-N	5.03	131.14	121.54
10	L	93	ASN	C-N-CA	5.03	131.14	121.54
21	W	10	THR	O-C-N	5.01	129.70	123.28
54	9	3	G	P-O3'-C3'	5.00	127.71	120.20
37	g	144	ALA	CA-C-N	5.00	131.09	121.54
37	g	144	ALA	C-N-CA	5.00	131.09	121.54

There are no chirality outliers.

All (20) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	2252	G	Sidechain
6	F	173	ASP	Peptide
6	F	174	PHE	Peptide
7	G	118	ALA	Peptide
7	G	46	ASP	Peptide
9	K	88	ASN	Peptide
11	M	57	VAL	Peptide
11	M	58	LYS	Peptide
16	R	53	PHE	Peptide
19	U	88	ASP	Peptide
19	U	97	SER	Peptide
32	b	15	PHE	Peptide
32	b	18	GLN	Peptide
36	f	53	LYS	Peptide
40	j	57	VAL	Peptide
42	l	101	LEU	Peptide
43	m	4	ALA	Peptide
47	q	69	THR	Peptide
52	w	120	GLY	Peptide
52	w	18	ASP	Peptide

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	61641	0	31003	271	0
2	B	2572	0	1302	15	0
3	C	2082	0	2157	32	0
4	D	1565	0	1616	9	0
5	E	1552	0	1619	14	0
6	F	1410	0	1447	23	0
7	G	1323	0	1374	16	0
8	J	1129	0	1162	11	0
9	K	938	0	1012	10	0
10	L	1045	0	1117	17	0
11	M	1074	0	1157	12	0
12	N	960	0	1000	10	0
13	O	892	0	923	9	0
14	P	917	0	965	11	0
15	Q	947	0	1022	15	0
16	R	816	0	839	10	0
17	S	857	0	922	5	0
18	T	738	0	807	8	0
19	U	779	0	834	8	0
20	V	753	0	780	8	0
21	W	637	0	658	17	0
22	X	625	0	655	3	0
23	Y	509	0	543	3	0
24	Z	449	0	491	4	0
25	0	444	0	461	5	0
26	1	409	0	440	1	0
27	2	377	0	418	5	0
28	3	504	0	574	11	0
29	4	302	0	343	3	0
30	6	522	0	522	2	0
31	a	33016	0	16617	169	0
32	b	1704	0	1732	17	0
33	c	1624	0	1699	14	0
34	d	1643	0	1710	22	0
35	e	1141	0	1170	16	0
36	f	817	0	808	11	0
37	g	1181	0	1240	13	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
38	h	979	0	1034	11	0
39	i	1022	0	1070	18	0
40	j	786	0	828	19	0
41	k	869	0	878	10	0
42	l	955	0	1019	15	0
43	m	883	0	944	7	0
44	n	799	0	841	13	0
45	o	714	0	737	7	0
46	p	649	0	666	12	0
47	q	648	0	691	7	0
48	r	504	0	502	7	0
49	s	637	0	665	11	0
50	t	665	0	714	10	0
51	u	495	0	486	5	0
52	w	1461	0	1421	17	0
53	v	189	0	100	9	0
54	9	1646	0	831	60	0
54	x	1646	0	831	50	0
55	7	1663	0	1740	18	0
56	9	7	0	7	3	0
All	All	147111	0	99144	895	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 4.

All (895) 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:A:2555:U:N3	54:9:74:C:C5	1.73	1.55
54:x:1:C:N3	54:x:72:G:N2	1.61	1.47
54:x:1:C:N4	54:x:72:G:H1	0.99	1.42
1:A:2251:G:N1	54:x:75:C:N3	1.73	1.35
1:A:2555:U:C2	54:9:74:C:C4	2.17	1.33
1:A:2555:U:N3	54:9:74:C:C4	2.01	1.27
31:a:530:G:C1'	54:9:35:G:O2'	1.87	1.21
1:A:2555:U:C4	54:9:74:C:C5	2.31	1.18
1:A:2555:U:C2	54:9:74:C:N4	2.13	1.15
54:x:75:C:H41	54:x:76:A:N6	1.44	1.13
2:B:12:C:H42	21:W:74:PRO:HD3	0.96	1.09
31:a:530:G:H1'	54:9:35:G:O2'	0.93	1.08
1:A:2252:G:H2'	1:A:2253:G:O5'	1.50	1.05

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
54:x:75:C:C5	54:x:76:A:C6	2.47	1.02
1:A:2251:G:N2	54:x:75:C:O2	1.91	1.01
54:x:1:C:C2	54:x:72:G:N2	2.29	0.99
2:B:12:C:N4	21:W:74:PRO:HD3	1.76	0.99
54:x:75:C:N4	54:x:76:A:C6	2.32	0.98
1:A:2555:U:O2	54:9:74:C:C4	2.17	0.97
54:x:75:C:C4	54:x:76:A:C6	2.54	0.95
1:A:2252:G:O2'	1:A:2253:G:H5'	1.66	0.95
1:A:2252:G:H2'	1:A:2253:G:C5'	1.97	0.93
54:x:75:C:C4	54:x:76:A:N1	2.36	0.93
2:B:12:C:H42	21:W:74:PRO:CD	1.82	0.93
54:x:1:C:N4	54:x:72:G:N1	1.73	0.92
54:x:1:C:N3	54:x:72:G:C2	2.38	0.92
54:x:40:G:O3'	54:x:41:A:P	2.28	0.92
54:x:75:C:N4	54:x:76:A:N1	2.17	0.92
54:9:74:C:H2'	54:9:75:C:H5'	1.52	0.91
54:x:75:C:H41	54:x:76:A:H61	1.15	0.91
54:x:73:A:O2'	54:x:74:C:OP1	1.88	0.90
1:A:2452:C:O4'	56:9:101:PRO:HG3	1.71	0.89
54:x:75:C:N4	54:x:76:A:N6	2.18	0.89
54:x:75:C:C5	54:x:76:A:C5	2.62	0.88
1:A:2252:G:N3	1:A:2253:G:C1'	2.39	0.85
1:A:2252:G:N2	54:x:74:C:O2	2.10	0.85
1:A:2555:U:C4	54:9:74:C:H5	1.84	0.85
31:a:530:G:H1'	54:9:35:G:HO2'	1.38	0.83
1:A:2252:G:C2	1:A:2253:G:C4	2.67	0.82
31:a:530:G:N1	54:9:35:G:N2	2.28	0.82
54:x:73:A:O2'	54:x:74:C:P	2.37	0.82
1:A:2252:G:C2	1:A:2253:G:H1'	2.14	0.82
52:w:146:THR:O	53:v:14:C:O2	1.98	0.80
1:A:2252:G:C4	1:A:2253:G:C8	2.69	0.79
1:A:2252:G:N2	1:A:2253:G:H1'	1.98	0.78
1:A:2251:G:C6	54:x:75:C:N3	2.55	0.74
31:a:530:G:H1	54:9:35:G:H21	1.36	0.73
1:A:2252:G:C2'	1:A:2253:G:C5'	2.67	0.72
1:A:2555:U:O2	54:9:74:C:N3	2.21	0.72
1:A:2252:G:C2	1:A:2253:G:N9	2.59	0.71
1:A:2261:C:OP1	21:W:19:LYS:NZ	2.19	0.70
53:v:21:G:O6	54:9:35:G:O6	2.09	0.70
37:g:111:GLY:HA2	37:g:118:ARG:HD3	1.74	0.70
1:A:2252:G:C2	1:A:2253:G:C1'	2.74	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
49:s:5:LYS:HG3	49:s:6:LYS:HG2	1.74	0.69
31:a:1054:C:O2'	54:9:34:C:H4'	1.92	0.69
54:x:2:G:O6	54:x:72:G:C6	2.46	0.69
31:a:156:C:H42	31:a:165:G:H22	1.41	0.68
1:A:2252:G:N3	1:A:2253:G:H1'	2.06	0.68
1:A:2252:G:N1	1:A:2253:G:C4	2.63	0.67
1:A:2555:U:O4	54:9:74:C:C5	2.47	0.67
1:A:910:A:H62	11:M:12:MET:HA	1.61	0.66
31:a:530:G:N2	54:9:36:G:O4'	2.29	0.66
6:F:62:GLN:HE22	6:F:90:LEU:HB3	1.61	0.65
54:x:1:C:N4	54:x:72:G:C6	2.42	0.65
41:k:87:GLY:H	41:k:113:THR:HG22	1.62	0.65
1:A:2452:C:C1'	56:9:101:PRO:HG3	2.26	0.65
1:A:2252:G:N3	1:A:2253:G:N9	2.45	0.65
42:l:23:LEU:HB2	42:l:58:ASN:HD22	1.62	0.64
1:A:1913:A:N6	54:9:38:A:H4'	2.12	0.64
35:e:10:LEU:HD22	35:e:67:ARG:HH22	1.61	0.64
1:A:2553:G:H1	54:9:75:C:H42	1.45	0.64
54:x:72:G:H1'	54:x:73:A:H5'	1.80	0.64
1:A:1171:G:N2	1:A:1178:C:N3	2.46	0.63
1:A:559:G:N3	15:Q:55:GLN:NE2	2.46	0.63
33:c:106:ARG:HG3	33:c:107:LYS:HG3	1.80	0.62
10:L:109:LYS:HD2	10:L:126:ARG:HH11	1.63	0.62
34:d:187:ARG:HE	34:d:196:GLU:HB3	1.65	0.62
1:A:2252:G:C6	1:A:2253:G:C5	2.87	0.62
18:T:13:ALA:HB3	18:T:33:LYS:HD3	1.82	0.62
1:A:2252:G:C2'	1:A:2253:G:H5'	2.29	0.62
31:a:959:A:HO2'	31:a:984:C:HO2'	1.48	0.61
21:W:21:LEU:HD21	21:W:41:ARG:HH21	1.65	0.61
53:v:19:C:C2	54:9:37:G:N2	2.69	0.61
36:f:10:VAL:HB	36:f:58:HIS:HB3	1.82	0.61
10:L:23:ILE:HD13	16:R:84:ARG:HH22	1.66	0.61
31:a:664:G:H22	31:a:741:G:H1	1.48	0.61
47:q:30:HIS:HD2	47:q:33:TYR:H	1.48	0.61
31:a:45:G:H1	31:a:396:C:H42	1.48	0.61
2:B:12:C:N4	21:W:74:PRO:CD	2.52	0.61
4:D:33:ARG:HH22	4:D:74:GLU:HB3	1.67	0.60
39:i:33:SER:H	39:i:36:GLN:HE21	1.46	0.60
31:a:409:U:H3	31:a:433:G:H1	1.48	0.60
6:F:134:GLN:NE2	6:F:149:ARG:O	2.35	0.60
13:O:40:ILE:HG12	13:O:47:VAL:HG12	1.84	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1759:A:HO2'	1:A:2714:G:HO2'	1.50	0.59
3:C:143:VAL:HB	3:C:153:LEU:HB2	1.83	0.59
10:L:79:LEU:HD12	10:L:114:GLY:H	1.67	0.59
54:9:7:U:OP1	54:9:16:C:N4	2.34	0.59
1:A:2555:U:O2	54:9:74:C:N4	2.28	0.59
54:x:75:C:H5	54:x:76:A:C6	2.18	0.59
1:A:1153:C:OP1	15:Q:91:ARG:NH2	2.34	0.59
1:A:2252:G:O2'	1:A:2253:G:C5'	2.46	0.59
1:A:1270:C:H5''	1:A:1271:G:H5'	1.84	0.59
36:f:46:GLN:HA	36:f:56:LYS:HG2	1.85	0.59
1:A:1727:C:H42	1:A:1733:G:H1	1.51	0.59
31:a:1050:G:H1	31:a:1208:C:H42	1.49	0.59
40:j:8:ILE:HG12	40:j:100:ILE:HG22	1.82	0.59
31:a:1059:C:H4'	44:n:85:ARG:HH22	1.68	0.59
31:a:405:U:O4	34:d:1:ALA:N	2.36	0.58
33:c:84:GLU:HG3	33:c:87:ARG:HH12	1.68	0.58
31:a:1222:G:OP2	31:a:1322:C:N4	2.36	0.58
36:f:48:ALA:H	48:r:65:SER:HG	1.51	0.58
1:A:2452:C:O4'	56:9:101:PRO:CG	2.49	0.58
54:9:21:A:N6	54:9:47:U:O2'	2.36	0.58
39:i:122:ARG:NH1	39:i:123:ARG:O	2.37	0.58
55:7:177:LYS:HB2	55:7:186:LYS:HE2	1.85	0.58
31:a:104:G:N7	50:t:8:LYS:NZ	2.51	0.58
32:b:31:PHE:HB2	32:b:39:ILE:HB	1.85	0.58
49:s:19:GLU:OE2	49:s:42:ASN:ND2	2.37	0.58
54:9:74:C:H2'	54:9:75:C:C5'	2.30	0.58
31:a:1137:C:O2'	31:a:1138:G:N2	2.37	0.58
1:A:636:G:N7	10:L:109:LYS:NZ	2.52	0.58
1:A:1779:U:OP2	1:A:1784:A:N6	2.36	0.58
33:c:30:ASP:HA	44:n:65:ARG:HH12	1.69	0.58
54:x:1:C:C4	54:x:72:G:N1	2.44	0.58
35:e:92:ARG:HB2	35:e:127:TYR:HB2	1.85	0.57
39:i:83:THR:HG21	39:i:102:PHE:HB3	1.85	0.57
39:i:91:GLU:HA	39:i:94:ARG:HB2	1.84	0.57
1:A:1753:G:H5''	14:P:92:ARG:HD3	1.86	0.57
5:E:58:LYS:HG2	5:E:71:GLY:HA2	1.86	0.57
31:a:1016:A:HO2'	31:a:1217:C:HO2'	1.52	0.57
34:d:84:ASN:O	34:d:88:ASN:ND2	2.37	0.57
40:j:52:LEU:HD21	40:j:59:LYS:HD3	1.85	0.57
4:D:148:GLN:HB2	4:D:152:PRO:HG2	1.85	0.57
31:a:393:A:H2'	31:a:394:G:H8	1.68	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:d:61:ARG:HG3	34:d:66:VAL:HB	1.86	0.57
7:G:23:ILE:HD11	7:G:42:VAL:HG11	1.86	0.57
1:A:2553:G:H1	54:9:75:C:N4	2.02	0.57
31:a:1073:U:H3	31:a:1102:A:H61	1.53	0.57
49:s:62:THR:H	49:s:65:MET:HE3	1.69	0.57
1:A:1475:G:O2'	1:A:1732:C:N4	2.38	0.57
1:A:1478:G:O6	1:A:1514:G:N2	2.38	0.56
1:A:2020:A:N7	25:0:5:ASN:ND2	2.51	0.56
39:i:89:TYR:HB3	39:i:93:LEU:HD12	1.86	0.56
1:A:2688:G:N1	1:A:2720:U:OP2	2.37	0.56
46:p:48:GLU:HG2	46:p:51:ARG:HE	1.69	0.56
55:7:214:ILE:HG12	55:7:224:VAL:HA	1.86	0.56
1:A:2252:G:C2'	1:A:2253:G:O5'	2.37	0.56
31:a:8:A:N6	34:d:201:GLU:O	2.38	0.56
40:j:40:ILE:HB	40:j:73:LEU:HB2	1.87	0.56
42:l:86:VAL:HG23	42:l:88:ASP:H	1.69	0.56
3:C:257:ARG:HH21	3:C:266:ILE:HD12	1.71	0.56
9:K:102:PRO:HB3	9:K:121:GLU:HB3	1.87	0.56
20:V:64:VAL:HG22	20:V:69:GLU:HG2	1.87	0.56
24:Z:8:GLN:HB2	24:Z:28:LEU:HD13	1.87	0.56
31:a:1152:A:H5'	40:j:15:HIS:HB2	1.88	0.56
1:A:2420:C:N4	28:3:29:ARG:O	2.38	0.56
11:M:66:ARG:NH1	11:M:104:GLU:OE2	2.38	0.56
31:a:951:G:OP2	43:m:100:ARG:NH2	2.39	0.56
13:O:29:HIS:HB3	13:O:36:TYR:HB2	1.88	0.56
17:S:82:MET:HB2	17:S:98:LYS:HB2	1.87	0.56
31:a:78:A:H61	31:a:91:U:H3	1.54	0.56
49:s:10:ILE:HG22	49:s:37:SER:HB2	1.87	0.56
31:a:403:C:H5'	34:d:131:ILE:HG23	1.88	0.56
3:C:51:ARG:HH22	3:C:246:PRO:HG2	1.71	0.55
42:l:13:ARG:NH1	42:l:14:LYS:O	2.39	0.55
1:A:910:A:N3	1:A:2264:C:O2'	2.36	0.55
6:F:14:LYS:NZ	6:F:18:GLU:OE2	2.39	0.55
31:a:261:U:OP2	50:t:73:ARG:NH2	2.40	0.55
31:a:1081:A:OP2	35:e:51:LYS:NZ	2.39	0.55
31:a:1316:G:N1	31:a:1319:A:OP2	2.37	0.55
46:p:40:ASN:HB3	46:p:43:ALA:HB2	1.86	0.55
54:x:75:C:H5	54:x:76:A:C5	2.20	0.55
20:V:48:MET:SD	20:V:51:GLN:NE2	2.79	0.55
1:A:2788:C:O2'	1:A:2809:A:N3	2.38	0.55
10:L:17:LYS:HE3	10:L:27:LEU:HD22	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:T:6:ARG:NH2	18:T:37:ASP:OD2	2.39	0.55
31:a:375:U:O2'	46:p:28:ARG:NH1	2.40	0.55
32:b:23:ASN:HB2	32:b:189:ASN:HA	1.88	0.55
40:j:52:LEU:HB2	44:n:81:ARG:HD2	1.89	0.55
1:A:514:A:N3	1:A:581:C:O2'	2.37	0.55
21:W:4:LYS:HB3	54:x:74:C:H41	1.71	0.55
31:a:413:G:N2	31:a:428:G:O2'	2.40	0.55
31:a:530:G:C6	54:9:35:G:N2	2.75	0.55
42:l:98:ARG:NH2	42:l:105:GLY:O	2.40	0.55
1:A:644:A:H61	1:A:2349:G:H21	1.53	0.55
12:N:28:LEU:HD23	12:N:48:VAL:HG21	1.89	0.55
31:a:1191:A:H5''	33:c:3:LYS:HE3	1.89	0.55
18:T:6:ARG:NH1	18:T:42:GLU:OE1	2.40	0.54
39:i:11:ARG:HA	39:i:105:ARG:HH12	1.71	0.54
41:k:84:MET:SD	41:k:110:THR:OG1	2.65	0.54
31:a:618:C:N4	31:a:621:A:OP2	2.40	0.54
31:a:574:A:HO2'	31:a:882:C:HO2'	1.55	0.54
10:L:62:PRO:HD3	28:3:26:ALA:HB2	1.89	0.54
1:A:340:A:O2'	5:E:162:ARG:NH1	2.40	0.54
36:f:6:ILE:HB	36:f:62:MET:HB2	1.88	0.54
3:C:154:ALA:HB2	3:C:161:VAL:HG23	1.90	0.54
34:d:61:ARG:NH1	34:d:68:GLU:OE1	2.41	0.54
14:P:38:ARG:NH2	31:a:345:C:OP1	2.41	0.54
31:a:1532:U:O4	51:u:46:ARG:NH1	2.41	0.54
33:c:179:ALA:HB1	33:c:202:PHE:HE1	1.73	0.54
38:h:103:VAL:HA	38:h:124:ILE:HA	1.88	0.54
10:L:95:LEU:HD22	10:L:100:ILE:HD11	1.88	0.53
31:a:1343:G:H4'	39:i:123:ARG:HB2	1.89	0.53
15:Q:43:GLN:HE21	16:R:77:PHE:HB3	1.72	0.53
28:3:32:LEU:HD23	28:3:35:LYS:HD2	1.89	0.53
38:h:28:SER:HB3	38:h:56:PRO:HB2	1.89	0.53
9:K:43:ILE:HD12	9:K:56:ASP:HB2	1.90	0.53
31:a:375:U:OP1	46:p:70:ARG:NH1	2.37	0.53
31:a:617:G:O6	31:a:623:C:N4	2.40	0.53
31:a:1367:C:OP2	39:i:113:LYS:NZ	2.41	0.53
54:x:75:C:N4	54:x:76:A:H61	1.90	0.53
8:J:32:LEU:HD22	8:J:54:ILE:HG21	1.91	0.53
21:W:37:ILE:HG22	21:W:38:VAL:HG23	1.90	0.53
33:c:57:GLU:OE1	33:c:64:ARG:NH2	2.39	0.53
1:A:774:G:H5''	3:C:47:ARG:HH21	1.72	0.53
1:A:2676:C:OP1	9:K:31:ARG:NH2	2.42	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:64:VAL:HA	3:C:102:TYR:HB2	1.90	0.53
27:2:24:THR:HG23	27:2:27:GLY:H	1.73	0.53
31:a:1368:A:OP1	40:j:64:GLN:NE2	2.41	0.53
39:i:94:ARG:HA	39:i:97:LEU:HB3	1.90	0.53
41:k:92:ARG:NH2	41:k:111:ASP:OD1	2.41	0.53
1:A:2063:C:O2'	52:w:34:KEO:N03	2.42	0.53
19:U:85:ARG:NH1	19:U:99:SER:OG	2.42	0.53
1:A:563:A:N3	15:Q:36:GLN:NE2	2.56	0.53
3:C:151:GLY:O	3:C:155:ARG:NH1	2.42	0.53
7:G:94:ARG:HB2	7:G:105:SER:HB2	1.91	0.53
31:a:530:G:N2	54:9:36:G:C1'	2.71	0.53
31:a:755:G:H21	38:h:3:GLN:HE22	1.57	0.53
31:a:969:A:OP2	40:j:58:ASN:ND2	2.42	0.53
33:c:76:ILE:HA	33:c:83:VAL:HG23	1.91	0.53
44:n:15:LEU:HD23	44:n:55:SER:HB3	1.91	0.53
5:E:117:ARG:NH2	5:E:183:PHE:O	2.42	0.53
1:A:714:U:OP2	45:o:88:ARG:NH2	2.41	0.53
3:C:77:VAL:HG22	3:C:93:VAL:HG22	1.91	0.53
9:K:9:ASN:OD1	9:K:18:ARG:NH1	2.42	0.53
31:a:374:A:N6	31:a:390:U:O2'	2.41	0.52
31:a:553:A:H5''	42:l:20:VAL:HG21	1.92	0.52
1:A:200:U:O2	1:A:386:G:N2	2.43	0.52
1:A:1131:G:N2	1:A:1132:U:O4	2.41	0.52
1:A:1791:A:N6	1:A:1828:G:O2'	2.42	0.52
24:Z:10:ARG:NH2	24:Z:52:PHE:O	2.42	0.52
31:a:362:G:N2	31:a:365:U:OP2	2.42	0.52
31:a:993:G:O2'	31:a:994:A:N7	2.42	0.52
1:A:2252:G:C5	1:A:2253:G:C8	2.96	0.52
1:A:2746:U:H5''	7:G:137:LYS:HE2	1.90	0.52
31:a:780:A:N6	31:a:801:U:OP2	2.41	0.52
31:a:1011:C:H42	31:a:1018:G:H1	1.57	0.52
1:A:776:G:H22	1:A:2072:C:H5'	1.73	0.52
31:a:501:C:OP1	42:l:113:ARG:NH1	2.43	0.52
31:a:1063:C:H42	31:a:1193:G:H1	1.58	0.52
43:m:89:ARG:NE	43:m:95:PRO:O	2.39	0.52
54:9:9:G:O2'	54:9:10:G:N7	2.41	0.52
1:A:1042:G:H1	1:A:1113:U:H3	1.57	0.52
1:A:2252:G:H21	1:A:2253:G:H1'	1.73	0.52
10:L:109:LYS:HG2	10:L:126:ARG:HB3	1.92	0.52
12:N:22:ARG:HG3	12:N:70:THR:HA	1.91	0.52
48:r:36:GLY:O	48:r:62:ARG:NH2	2.42	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:249:C:O2	28:3:11:LYS:NZ	2.42	0.52
1:A:1275:A:OP2	1:A:1646:C:N4	2.42	0.52
1:A:2266:A:N6	1:A:2273:A:OP2	2.42	0.52
31:a:71:A:N1	31:a:99:C:O2'	2.43	0.52
37:g:29:LEU:HD11	37:g:115:MET:HE2	1.91	0.52
1:A:2667:C:N3	7:G:109:SER:OG	2.42	0.52
31:a:254:G:H1	31:a:272:C:H42	1.58	0.52
16:R:76:LYS:HB2	16:R:85:LYS:HB3	1.92	0.52
30:6:36:VAL:HG21	30:6:41:HIS:HD2	1.74	0.52
32:b:71:THR:OG1	32:b:168:GLU:OE2	2.28	0.52
31:a:1367:C:H4'	40:j:50:THR:HG21	1.92	0.52
54:9:30:C:H2'	54:9:31:G:H8	1.74	0.52
1:A:2124:G:N2	55:7:218:MET:O	2.42	0.51
1:A:2251:G:O6	54:x:76:A:N1	2.43	0.51
1:A:775:G:H4'	1:A:776:G:H5'	1.91	0.51
1:A:805:G:H5''	10:L:38:GLN:HG3	1.92	0.51
3:C:68:ARG:O	3:C:188:ARG:NH1	2.43	0.51
44:n:45:VAL:O	44:n:49:GLN:NE2	2.44	0.51
54:x:72:G:O2'	54:x:73:A:O5'	2.22	0.51
3:C:268:ARG:NH2	31:a:680:C:O2'	2.43	0.51
31:a:429:U:O2'	34:d:21:LYS:NZ	2.44	0.51
54:9:1:C:N4	54:9:2:G:O6	2.43	0.51
1:A:883:G:H1	1:A:893:C:H42	1.57	0.51
12:N:44:LEU:HD23	12:N:113:ILE:HD13	1.91	0.51
31:a:297:G:N2	31:a:300:A:OP2	2.43	0.51
40:j:5:ARG:HG2	40:j:79:PRO:HB3	1.93	0.51
2:B:12:C:N3	21:W:74:PRO:N	2.58	0.51
39:i:112:ARG:NH2	40:j:64:GLN:OE1	2.43	0.51
41:k:23:HIS:HB3	41:k:30:ILE:HG23	1.92	0.51
46:p:4:ILE:HG12	46:p:21:VAL:HG22	1.92	0.51
1:A:958:U:OP1	11:M:40:ARG:NH1	2.43	0.51
7:G:21:GLN:NE2	7:G:37:ASN:O	2.43	0.51
43:m:28:ARG:HH21	43:m:62:PHE:HB2	1.75	0.51
1:A:1827:U:OP2	3:C:220:ARG:NH1	2.43	0.51
31:a:530:G:O2'	54:9:35:G:H1'	2.11	0.51
54:x:75:C:C4	54:x:76:A:C2	2.98	0.51
1:A:210:C:OP1	27:2:29:GLN:NE2	2.43	0.51
1:A:574:A:N6	1:A:2034:U:OP1	2.44	0.51
15:Q:109:VAL:HG12	15:Q:113:LYS:HE2	1.93	0.51
40:j:22:THR:HG21	40:j:39:PRO:HB3	1.93	0.51
1:A:527:C:N4	1:A:2779:U:OP2	2.44	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:V:25:LYS:HG2	20:V:43:ASP:HA	1.92	0.51
31:a:196:A:H2'	31:a:197:A:H2'	1.92	0.51
31:a:367:U:O4'	31:a:394:G:N2	2.44	0.51
48:r:25:ILE:HG21	48:r:66:LEU:HB3	1.92	0.51
55:7:47:ASN:HB3	55:7:170:ILE:HG22	1.93	0.51
1:A:481:G:O2'	1:A:506:G:N2	2.44	0.51
31:a:426:U:H4'	34:d:39:GLN:HG3	1.93	0.51
35:e:79:THR:HA	35:e:121:ASN:HD22	1.75	0.51
8:J:56:VAL:HB	8:J:124:VAL:HG12	1.93	0.50
13:O:108:ASP:OD1	13:O:111:ARG:NH1	2.43	0.50
21:W:21:LEU:HD11	21:W:41:ARG:HE	1.76	0.50
54:x:2:G:O6	54:x:72:G:O6	2.29	0.50
1:A:119:A:H4'	1:A:120:U:H5'	1.93	0.50
1:A:2169:A:N3	55:7:134:ARG:NH1	2.59	0.50
7:G:59:ASP:HB2	7:G:62:ALA:HB3	1.94	0.50
31:a:151:A:H62	31:a:170:U:H3	1.59	0.50
31:a:323:U:OP1	50:t:20:ASN:ND2	2.44	0.50
40:j:37:ARG:HB2	40:j:75:ASP:HB2	1.93	0.50
45:o:34:GLN:HB3	45:o:58:MET:HE1	1.92	0.50
32:b:100:LEU:HD13	32:b:175:ALA:HB2	1.92	0.50
1:A:2158:A:OP1	1:A:2159:G:N2	2.44	0.50
32:b:21:TYR:HE2	32:b:189:ASN:HD22	1.58	0.50
35:e:54:GLU:HG2	35:e:56:PRO:HD2	1.93	0.50
36:f:92:THR:OG1	36:f:93:LYS:N	2.43	0.50
24:Z:16:LEU:HB2	24:Z:19:HIS:HD2	1.77	0.50
35:e:91:SER:HB3	35:e:93:VAL:HG23	1.94	0.50
41:k:63:GLN:HG3	41:k:98:ALA:HB2	1.93	0.50
54:9:71:C:H2'	54:9:72:G:C8	2.47	0.50
1:A:518:G:OP1	17:S:18:ARG:NH1	2.44	0.50
1:A:918:A:N3	2:B:80:U:O2'	2.42	0.50
1:A:2305:U:O2'	6:F:132:ARG:NH2	2.45	0.50
38:h:45:ILE:HG21	38:h:60:LEU:HD22	1.93	0.50
54:9:11:C:H2'	54:9:12:G:H8	1.76	0.50
54:9:18:G:H22	54:9:55:U:H6	1.59	0.50
1:A:1056:G:N1	1:A:1102:C:OP2	2.45	0.50
1:A:1378:A:O2'	1:A:1380:G:OP2	2.30	0.50
1:A:1913:A:C6	54:9:38:A:H4'	2.46	0.50
1:A:2245:U:H5''	1:A:2246:G:H5'	1.92	0.50
44:n:46:LEU:HA	49:s:12:LEU:HD21	1.93	0.50
1:A:729:G:N2	3:C:10:PRO:O	2.45	0.50
1:A:1607:C:N4	1:A:1622:G:OP2	2.43	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:85:LYS:HB3	7:G:164:ALA:HB2	1.94	0.50
19:U:10:VAL:HA	19:U:71:ILE:HA	1.94	0.50
28:3:8:GLY:O	28:3:12:ARG:NH2	2.43	0.50
31:a:562:U:H1'	42:l:11:ARG:HD2	1.93	0.50
1:A:788:A:OP1	1:A:791:C:N4	2.42	0.49
1:A:706:A:OP1	3:C:6:LYS:NZ	2.43	0.49
15:Q:51:GLN:HG2	15:Q:54:ARG:HD2	1.94	0.49
21:W:4:LYS:HD3	54:x:74:C:H42	1.77	0.49
1:A:2742:G:OP2	29:4:24:ARG:NH1	2.43	0.49
31:a:213:G:OP2	31:a:214:C:N4	2.45	0.49
31:a:406:G:N7	31:a:495:A:O2'	2.45	0.49
31:a:1221:G:OP1	49:s:35:ARG:NH1	2.45	0.49
35:e:74:ALA:HB1	35:e:148:SER:HB3	1.95	0.49
1:A:1283:G:N1	1:A:1286:A:OP2	2.43	0.49
1:A:2523:G:HO2'	1:A:2764:A:HO2'	1.53	0.49
1:A:2709:G:H5'	12:N:22:ARG:HH22	1.78	0.49
6:F:109:ARG:HH22	43:m:2:ARG:HD3	1.78	0.49
10:L:110:VAL:HB	10:L:127:VAL:HG22	1.93	0.49
31:a:324:G:N2	31:a:327:A:OP2	2.44	0.49
1:A:729:G:OP2	3:C:206:LYS:NZ	2.46	0.49
1:A:2168:G:N1	1:A:2171:A:OP2	2.45	0.49
31:a:408:A:OP1	34:d:109:THR:OG1	2.30	0.49
32:b:87:ASP:OD1	32:b:88:GLN:NE2	2.46	0.49
34:d:162:GLU:HA	34:d:166:LYS:HD3	1.94	0.49
49:s:54:ARG:HG3	49:s:55:GLN:HG2	1.95	0.49
1:A:1086:A:O2'	1:A:1087:G:N7	2.44	0.49
1:A:1687:G:H21	1:A:1701:A:H62	1.59	0.49
1:A:1827:U:H5	3:C:220:ARG:HD3	1.78	0.49
31:a:130:A:OP1	47:q:64:ARG:NH1	2.46	0.49
52:w:75:LEU:HD12	52:w:76:TYR:HB2	1.95	0.49
1:A:2646:C:N4	1:A:2675:A:N1	2.60	0.49
4:D:15:PHE:H	14:P:11:GLN:HE22	1.60	0.49
31:a:1442:G:H1	31:a:1460:C:H42	1.61	0.49
42:l:23:LEU:HD22	42:l:58:ASN:HB3	1.95	0.48
1:A:1265:A:H61	1:A:2013:A:H5''	1.78	0.48
1:A:2006:C:O2'	1:A:2823:A:N3	2.44	0.48
1:A:2032:G:N2	4:D:151:THR:OG1	2.46	0.48
31:a:545:C:OP2	34:d:61:ARG:NH2	2.46	0.48
33:c:152:VAL:HG12	33:c:197:VAL:HG22	1.95	0.48
37:g:138:GLU:O	37:g:142:ARG:N	2.45	0.48
54:x:72:G:N3	54:x:73:A:C8	2.81	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
55:7:153:VAL:HG13	55:7:157:LYS:HD2	1.95	0.48
31:a:43:C:H5'	46:p:11:ALA:HB1	1.94	0.48
31:a:376:G:H5'	46:p:5:ARG:HB2	1.93	0.48
35:e:97:PRO:HA	35:e:122:VAL:HG12	1.95	0.48
40:j:8:ILE:HB	40:j:74:VAL:HB	1.94	0.48
46:p:36:VAL:HG21	46:p:53:ASP:HB2	1.94	0.48
54:x:73:A:H4'	54:x:74:C:OP2	2.13	0.48
1:A:1796:U:H2'	1:A:1797:G:H8	1.79	0.48
7:G:34:ARG:HE	7:G:70:LEU:HD13	1.77	0.48
31:a:54:C:H2'	31:a:352:C:H41	1.77	0.48
31:a:1013:G:N2	31:a:1016:A:OP2	2.46	0.48
1:A:587:C:O2	10:L:33:ARG:NH1	2.46	0.48
1:A:964:C:O2'	1:A:2273:A:N3	2.43	0.48
1:A:2375:G:N2	1:A:2378:A:OP2	2.46	0.48
3:C:167:ASP:HB3	3:C:170:TYR:HB2	1.96	0.48
6:F:23:SER:HB3	6:F:26:GLN:HG3	1.94	0.48
26:1:4:ILE:HG23	26:1:27:ARG:HH21	1.79	0.48
42:l:52:CYS:SG	42:l:64:SER:OG	2.71	0.48
1:A:878:A:H3'	1:A:879:G:H8	1.77	0.48
1:A:2324:U:O2'	1:A:2337:G:OP1	2.32	0.48
12:N:43:GLU:OE2	12:N:46:ARG:NH2	2.46	0.48
31:a:405:U:O2	31:a:498:A:O2'	2.28	0.48
31:a:1049:U:H2'	44:n:2:LYS:HD3	1.95	0.48
1:A:560:C:O2'	15:Q:47:ARG:NH2	2.47	0.48
14:P:29:VAL:HG22	14:P:80:VAL:HG12	1.95	0.48
1:A:64:A:N1	1:A:91:A:N6	2.61	0.48
1:A:385:C:H42	1:A:411:G:H1	1.62	0.48
3:C:92:LEU:HD11	3:C:100:ARG:HB3	1.95	0.48
31:a:331:G:O3'	50:t:2:ASN:ND2	2.46	0.48
31:a:1061:G:O2'	40:j:58:ASN:ND2	2.47	0.48
16:R:35:PHE:HB2	16:R:59:ILE:HB	1.96	0.48
31:a:765:G:N1	31:a:812:G:O2'	2.43	0.48
32:b:187:ASP:OD1	32:b:188:THR:N	2.47	0.48
53:v:20:C:C2	54:9:36:G:N2	2.82	0.48
2:B:91:C:OP1	11:M:38:ARG:NH2	2.47	0.47
52:w:137:ASP:HB2	52:w:155:THR:HB	1.95	0.47
55:7:162:ARG:NH1	55:7:175:ILE:O	2.47	0.47
3:C:106:PRO:HD2	3:C:109:LEU:HD22	1.96	0.47
34:d:2:ARG:HE	34:d:114:ARG:HE	1.61	0.47
36:f:5:GLU:HA	36:f:63:ASN:HA	1.95	0.47
39:i:98:ARG:HG3	39:i:103:VAL:HG21	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1653:G:H3'	12:N:2:ARG:HG2	1.96	0.47
6:F:3:LEU:HD21	6:F:100:GLU:HA	1.96	0.47
7:G:85:LYS:HG3	7:G:131:VAL:HG22	1.95	0.47
1:A:499:U:H5''	19:U:42:LYS:HE2	1.96	0.47
1:A:793:A:OP2	1:A:2071:A:O2'	2.31	0.47
8:J:35:ARG:HB2	8:J:54:ILE:HD11	1.97	0.47
13:O:30:ARG:HA	13:O:35:ILE:HG13	1.96	0.47
31:a:835:U:OP1	48:r:52:ARG:NH2	2.43	0.47
31:a:279:A:H5''	31:a:280:C:H3'	1.96	0.47
55:7:157:LYS:HG2	55:7:161:VAL:HG21	1.96	0.47
1:A:690:G:O2'	1:A:780:G:OP1	2.28	0.47
1:A:2295:C:OP1	13:O:10:ARG:NH1	2.47	0.47
5:E:18:THR:HA	5:E:106:LYS:HE3	1.95	0.47
6:F:35:LEU:HB2	6:F:88:VAL:HB	1.95	0.47
8:J:93:ILE:HD13	8:J:100:VAL:HG21	1.96	0.47
11:M:34:LYS:HD3	20:V:82:TYR:HA	1.95	0.47
55:7:181:ASP:HB2	55:7:186:LYS:HE3	1.96	0.47
1:A:659:G:O2'	5:E:95:LYS:O	2.32	0.47
4:D:46:ARG:NH2	4:D:88:GLU:O	2.47	0.47
31:a:427:U:O2'	31:a:541:G:OP1	2.33	0.47
31:a:1458:G:H5'	50:t:26:MET:HB3	1.96	0.47
54:x:1:C:N4	54:x:2:G:O6	2.48	0.47
54:x:2:G:O6	54:x:72:G:N1	2.46	0.47
1:A:1864:U:OP1	1:A:2410:G:O2'	2.32	0.47
31:a:444:G:H1	31:a:490:C:H42	1.62	0.47
1:A:299:A:N1	1:A:322:A:O2'	2.46	0.47
1:A:2464:G:H1	1:A:2486:C:H42	1.61	0.47
6:F:147:ARG:HG3	6:F:149:ARG:H	1.80	0.47
9:K:30:ARG:NH2	9:K:37:ASP:OD2	2.40	0.47
11:M:102:LEU:HD11	11:M:126:ILE:HD11	1.96	0.47
14:P:105:LYS:O	14:P:108:ARG:NH2	2.48	0.47
31:a:518:C:O2'	31:a:1492:A:N6	2.48	0.47
54:9:71:C:H2'	54:9:72:G:H8	1.78	0.47
1:A:466:A:OP1	27:2:34:ARG:NH1	2.40	0.47
1:A:882:G:H1	1:A:894:U:H3	1.63	0.47
1:A:1779:U:H5''	1:A:1780:A:H5''	1.97	0.47
1:A:2405:G:O2'	1:A:2412:A:N6	2.48	0.47
1:A:2553:G:C6	54:9:75:C:N4	2.83	0.47
31:a:1095:U:OP1	31:a:1108:G:N2	2.48	0.47
52:w:150:GLY:HA2	52:w:151:GLY:HA3	1.63	0.47
29:4:36:ARG:HG2	29:4:37:GLN:H	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:a:1002:G:H1	31:a:1038:C:H42	1.61	0.46
31:a:1338:G:O2'	54:x:42:A:OP1	2.30	0.46
32:b:53:LEU:HD23	32:b:56:LEU:HD12	1.97	0.46
37:g:12:LEU:HD12	37:g:13:PRO:HD2	1.98	0.46
38:h:104:SER:HB2	38:h:125:ILE:HD11	1.97	0.46
1:A:355:U:H2'	1:A:356:G:H8	1.79	0.46
1:A:1361:G:HO2'	1:A:2215:C:HO2'	1.56	0.46
1:A:1682:G:OP2	1:A:1699:G:N2	2.45	0.46
1:A:2394:C:H5''	10:L:63:LYS:HE3	1.97	0.46
4:D:110:THR:HB	4:D:202:ILE:HB	1.96	0.46
31:a:242:G:H1	31:a:284:C:H42	1.62	0.46
31:a:927:G:O2'	31:a:1503:A:N7	2.42	0.46
37:g:55:LYS:HB3	37:g:59:GLU:HG3	1.97	0.46
42:l:113:ARG:HH12	42:l:120:ARG:HH11	1.62	0.46
48:r:37:LYS:NZ	51:u:22:CYS:SG	2.88	0.46
52:w:44:ARG:NH1	52:w:50:THR:O	2.43	0.46
1:A:1068:G:N2	1:A:1096:A:O4'	2.48	0.46
1:A:1161:C:H2'	1:A:1162:G:H8	1.79	0.46
1:A:2539:C:O2'	29:4:36:ARG:NH1	2.48	0.46
31:a:749:A:O2'	45:o:19:ASN:OD1	2.33	0.46
54:x:72:G:H1'	54:x:73:A:C5'	2.45	0.46
54:x:75:C:OP1	54:x:76:A:OP2	2.34	0.46
1:A:469:G:O6	27:2:39:ARG:NH2	2.48	0.46
1:A:1827:U:H5'	1:A:1971:U:H4'	1.98	0.46
6:F:114:ARG:HH11	43:m:70:ARG:HD2	1.79	0.46
8:J:24:THR:HB	8:J:27:ARG:HB2	1.97	0.46
41:k:111:ASP:HB3	51:u:3:ILE:HA	1.96	0.46
53:v:21:G:O6	54:9:35:G:C6	2.68	0.46
11:M:55:ARG:HH12	54:9:53:G:H4'	1.80	0.46
31:a:1054:C:C2	54:9:34:C:H1'	2.51	0.46
34:d:9:LYS:HG3	34:d:12:ARG:HH21	1.81	0.46
34:d:84:ASN:ND2	34:d:87:GLU:OE1	2.49	0.46
36:f:48:ALA:HB1	48:r:68:PRO:HG3	1.97	0.46
1:A:1064:C:O2'	1:A:1074:G:N2	2.49	0.46
1:A:2258:C:O2'	1:A:2427:C:OP2	2.34	0.46
1:A:2638:G:OP2	4:D:83:ARG:NH2	2.46	0.46
1:A:280:U:O4	1:A:361:G:N2	2.48	0.46
1:A:1048:A:OP2	1:A:1110:G:N2	2.41	0.46
33:c:23:ALA:HB3	33:c:28:PHE:HD1	1.81	0.46
49:s:54:ARG:HH22	49:s:78:THR:HG21	1.81	0.46
1:A:281:C:H2'	1:A:282:A:H8	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:500:G:N1	1:A:503:A:OP2	2.47	0.46
1:A:1792:G:O2'	1:A:1830:C:OP1	2.34	0.46
1:A:1807:G:OP1	3:C:47:ARG:NH1	2.49	0.46
1:A:2579:C:O2'	4:D:136:ASN:OD1	2.34	0.46
2:B:12:C:N3	21:W:73:GLY:C	2.73	0.46
31:a:1420:U:H2'	31:a:1421:G:H8	1.81	0.46
17:S:56:ALA:HA	17:S:59:GLU:HG2	1.98	0.46
19:U:83:GLY:HA3	19:U:96:LYS:HE3	1.98	0.46
37:g:55:LYS:HB2	37:g:60:ALA:HB2	1.97	0.46
40:j:5:ARG:N	40:j:76:ILE:O	2.49	0.46
51:u:6:ARG:HH21	51:u:8:ASN:HD21	1.64	0.46
11:M:42:THR:HG22	11:M:93:VAL:HG12	1.99	0.45
13:O:90:VAL:HG23	13:O:117:PHE:HB3	1.98	0.45
31:a:311:C:OP1	46:p:31:ARG:NH1	2.49	0.45
31:a:619:U:H5'	34:d:127:ARG:HH21	1.81	0.45
31:a:816:A:OP1	31:a:1526:G:O2'	2.32	0.45
52:w:111:ALA:HB1	52:w:128:PRO:HG2	1.97	0.45
54:9:11:C:H2'	54:9:12:G:C8	2.51	0.45
9:K:121:GLU:HG2	9:K:122:VAL:HG23	1.98	0.45
25:0:42:ILE:HG22	25:0:48:TYR:HB2	1.98	0.45
31:a:613:C:N4	31:a:627:G:O6	2.49	0.45
31:a:1366:C:O2'	40:j:62:ARG:NH2	2.50	0.45
1:A:1447:C:O2'	1:A:1544:A:N3	2.46	0.45
1:A:2883:A:OP1	25:0:48:TYR:OH	2.34	0.45
10:L:85:VAL:HG21	10:L:90:VAL:HG22	1.98	0.45
31:a:1100:C:N4	31:a:1103:C:OP1	2.50	0.45
32:b:80:LYS:HB2	32:b:92:ASN:HD22	1.82	0.45
1:A:2002:G:OP2	12:N:9:GLN:NE2	2.49	0.45
3:C:140:VAL:HG12	3:C:191:LEU:HD23	1.97	0.45
4:D:179:ARG:HB3	4:D:188:LEU:HD12	1.97	0.45
31:a:640:A:O2'	38:h:107:LYS:NZ	2.41	0.45
37:g:1:PRO:HG2	37:g:4:ARG:HB2	1.98	0.45
40:j:10:LEU:HB3	40:j:98:VAL:HG23	1.97	0.45
47:q:61:ARG:HH12	47:q:73:THR:HB	1.82	0.45
51:u:16:ARG:HB2	51:u:19:LYS:HD3	1.98	0.45
52:w:10:ARG:NE	54:x:5:G:OP1	2.49	0.45
1:A:370:G:O2'	1:A:424:G:OP1	2.34	0.45
1:A:994:C:OP1	15:Q:52:ARG:NH2	2.49	0.45
1:A:2333:A:H5'	1:A:2335:A:H1'	1.98	0.45
5:E:143:LEU:HD22	5:E:185:LYS:HG3	1.99	0.45
31:a:36:C:H5'	42:l:119:LYS:HA	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:a:59:A:H3'	31:a:331:G:H22	1.80	0.45
34:d:171:GLU:HB3	34:d:180:THR:HB	1.98	0.45
50:t:34:VAL:HG11	50:t:78:LEU:HD21	1.99	0.45
1:A:1297:C:O2'	1:A:1302:A:N1	2.48	0.45
1:A:1602:U:OP2	18:T:64:LYS:NZ	2.47	0.45
3:C:5:CYS:SG	3:C:12:ARG:NH2	2.90	0.45
3:C:74:PRO:HB3	3:C:114:GLN:HE21	1.80	0.45
7:G:96:ALA:HB3	7:G:103:ASN:HB3	1.99	0.45
31:a:530:G:N2	54:9:36:G:H1'	2.31	0.45
33:c:55:VAL:HB	33:c:66:THR:HB	1.97	0.45
35:e:156:ARG:NH2	38:h:42:GLU:OE2	2.41	0.45
1:A:463:G:N2	1:A:466:A:OP2	2.39	0.45
1:A:1223:G:OP1	16:R:68:ARG:NH2	2.50	0.45
1:A:1613:G:H4'	27:2:3:ARG:HE	1.82	0.45
1:A:2514:U:H5''	8:J:81:ILE:HD11	1.99	0.45
10:L:96:LYS:HE3	10:L:103:ILE:HA	1.99	0.45
11:M:17:ASN:O	11:M:38:ARG:NH1	2.47	0.45
21:W:23:VAL:HG22	21:W:38:VAL:HG22	1.98	0.45
31:a:410:G:N3	31:a:433:G:N2	2.64	0.45
31:a:1118:U:H5'	39:i:105:ARG:HG3	1.98	0.45
1:A:45:G:H5''	1:A:46:G:H5'	1.97	0.45
1:A:1696:G:N2	1:A:1977:A:O2'	2.40	0.45
1:A:1710:G:H1	1:A:1748:C:H42	1.65	0.45
31:a:363:A:H1'	42:l:28:GLN:HB2	1.99	0.45
46:p:2:VAL:O	46:p:66:THR:OG1	2.32	0.45
1:A:693:A:O2'	1:A:1353:A:N3	2.46	0.45
1:A:784:G:O4'	3:C:225:ASN:ND2	2.50	0.45
37:g:125:ASP:HB3	37:g:131:GLY:HA3	1.99	0.45
43:m:84:CYS:HB2	49:s:72:GLU:HB3	1.99	0.45
2:B:12:C:N3	21:W:74:PRO:CA	2.79	0.45
2:B:79:G:N7	20:V:14:LYS:NZ	2.64	0.45
3:C:70:LYS:O	3:C:117:SER:OG	2.35	0.45
6:F:163:GLU:OE1	6:F:166:ARG:NH1	2.50	0.45
42:l:101:LEU:O	42:l:103:CYS:N	2.50	0.45
54:9:9:G:O2'	54:9:45:G:N2	2.49	0.45
1:A:764:A:N3	3:C:211:ARG:NH1	2.66	0.44
1:A:1997:C:H2'	1:A:1998:A:H8	1.81	0.44
1:A:2251:G:N2	54:x:75:C:C2	2.74	0.44
2:B:78:A:H62	2:B:98:G:H21	1.65	0.44
8:J:17:VAL:HG23	8:J:137:PRO:HB2	1.98	0.44
18:T:37:ASP:OD1	18:T:37:ASP:N	2.46	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:a:501:C:O2	31:a:549:C:O2'	2.35	0.44
31:a:1178:G:N2	31:a:1181:G:OP2	2.51	0.44
32:b:72:LYS:NZ	32:b:203:ASP:OD2	2.50	0.44
36:f:36:ILE:HA	36:f:64:VAL:HG23	2.00	0.44
52:w:59:THR:HA	52:w:60:ASP:HA	1.73	0.44
1:A:1438:U:H2'	1:A:1439:A:H8	1.81	0.44
1:A:1899:A:H4'	1:A:1901:A:H5''	1.99	0.44
31:a:354:G:N2	31:a:388:G:O2'	2.47	0.44
31:a:410:G:H21	31:a:432:A:H62	1.64	0.44
52:w:75:LEU:HB2	55:7:129:GLN:HB3	1.99	0.44
1:A:572:A:H61	1:A:2029:G:H21	1.66	0.44
1:A:1227:G:OP2	15:Q:15:LYS:NZ	2.48	0.44
1:A:1343:G:O6	1:A:1403:A:N6	2.50	0.44
1:A:2251:G:N1	54:x:75:C:C4	2.66	0.44
1:A:2441:U:OP2	1:A:2586:U:O2'	2.34	0.44
31:a:68:G:H21	31:a:151:A:H2	1.65	0.44
31:a:422:C:O2'	31:a:423:G:N2	2.50	0.44
31:a:570:G:O6	31:a:865:A:N6	2.50	0.44
47:q:23:ALA:HA	47:q:42:LYS:HA	1.99	0.44
1:A:2252:G:C4	1:A:2253:G:N9	2.85	0.44
3:C:184:GLU:HG3	3:C:186:ASP:H	1.82	0.44
6:F:30:VAL:HG13	6:F:95:MET:HE1	1.98	0.44
7:G:46:ASP:O	7:G:48:THR:N	2.50	0.44
18:T:7:LEU:HD22	18:T:46:ALA:HB2	1.99	0.44
31:a:991:U:O4	31:a:1212:U:O2'	2.30	0.44
31:a:1281:C:H5''	31:a:1282:C:H5	1.82	0.44
37:g:67:ASN:O	37:g:137:ARG:NE	2.50	0.44
50:t:8:LYS:O	50:t:12:GLN:N	2.41	0.44
52:w:83:HIS:ND1	52:w:93:LEU:O	2.42	0.44
54:9:23:C:H2'	54:9:24:G:C8	2.52	0.44
1:A:270:A:N1	1:A:369:U:O2'	2.47	0.44
1:A:2023:C:H2'	1:A:2024:G:H8	1.82	0.44
1:A:2831:G:N2	1:A:2884:U:OP2	2.51	0.44
7:G:28:LYS:HE3	7:G:79:THR:HG23	1.99	0.44
31:a:46:G:O2'	31:a:365:U:O2	2.36	0.44
46:p:34:GLU:OE2	46:p:60:TRP:NE1	2.43	0.44
55:7:30:LEU:HD23	55:7:33:LEU:HD12	1.98	0.44
54:9:9:G:H2'	54:9:11:C:H41	1.83	0.44
1:A:1651:G:OP2	12:N:40:LYS:NZ	2.50	0.44
1:A:2576:G:O2'	1:A:2579:C:OP2	2.29	0.44
19:U:6:ARG:NH2	19:U:25:LYS:O	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
45:o:31:LEU:HD22	45:o:58:MET:HB2	1.99	0.44
55:7:167:LYS:HD2	55:7:171:ILE:HB	2.00	0.44
54:9:23:C:H2'	54:9:24:G:H8	1.83	0.44
1:A:1394:U:H4'	1:A:1603:A:H4'	1.99	0.44
1:A:1798:U:OP2	3:C:270:ARG:NH2	2.40	0.44
1:A:2291:U:OP1	1:A:2380:C:O2'	2.32	0.44
6:F:59:ILE:O	6:F:101:ARG:NH1	2.50	0.44
15:Q:87:VAL:HG13	16:R:49:ILE:HD11	1.99	0.44
31:a:9:G:H5'	35:e:107:GLY:HA3	2.00	0.44
31:a:231:U:H2'	31:a:232:G:H8	1.82	0.44
36:f:51:ILE:HD11	48:r:65:SER:HB2	1.99	0.44
54:9:43:G:H2'	54:9:44:G:C8	2.53	0.44
1:A:1428:C:OP2	3:C:27:LYS:NZ	2.49	0.44
16:R:14:VAL:HG23	16:R:18:GLN:HE21	1.82	0.44
17:S:73:LYS:HB2	17:S:106:VAL:HB	2.00	0.44
31:a:880:C:H2'	31:a:881:G:H8	1.83	0.44
36:f:38:ARG:HB2	36:f:63:ASN:HB3	2.00	0.44
5:E:3:LEU:HD13	5:E:120:VAL:HG21	1.99	0.43
9:K:80:ASP:OD2	14:P:61:ARG:NH1	2.43	0.43
31:a:596:A:H61	31:a:644:U:H3	1.66	0.43
31:a:1422:G:H1	31:a:1478:U:H3	1.64	0.43
39:i:129:ARG:NH1	54:x:32:U:OP2	2.50	0.43
41:k:82:GLU:HG3	41:k:107:THR:HB	2.00	0.43
44:n:77:PHE:HE1	44:n:93:ILE:HG21	1.83	0.43
1:A:1604:C:O2'	1:A:1610:A:N1	2.42	0.43
1:A:1668:A:H61	1:A:1676:A:H61	1.66	0.43
31:a:1238:A:N7	31:a:1299:A:N6	2.66	0.43
45:o:35:ILE:HG13	45:o:58:MET:HE2	2.00	0.43
45:o:38:LEU:HD23	45:o:42:PHE:HE2	1.83	0.43
50:t:24:ARG:HG2	50:t:28:ARG:HH21	1.83	0.43
24:Z:15:ARG:O	24:Z:20:LYS:NZ	2.51	0.43
31:a:106:C:H2'	31:a:107:G:H8	1.82	0.43
44:n:87:ALA:HB1	44:n:92:GLU:HB2	2.00	0.43
54:x:72:G:N3	54:x:73:A:H8	2.16	0.43
1:A:19:A:H5''	15:Q:21:LYS:HG2	2.00	0.43
5:E:5:LEU:HD13	5:E:10:SER:HB3	2.00	0.43
6:F:56:LEU:HD13	6:F:88:VAL:HG23	2.00	0.43
28:3:3:ILE:HG21	28:3:62:PRO:HG2	2.01	0.43
31:a:1160:G:N7	31:a:1182:G:N2	2.66	0.43
32:b:165:ALA:HB3	32:b:190:SER:HB3	2.00	0.43
47:q:22:VAL:HG11	47:q:58:VAL:HG11	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:J:31:GLU:HG2	8:J:142:ILE:HG12	2.01	0.43
11:M:64:TRP:HB2	11:M:104:GLU:HB2	2.00	0.43
31:a:1064:G:O2'	31:a:1190:G:N2	2.43	0.43
32:b:202:ASN:HD22	32:b:203:ASP:H	1.66	0.43
42:l:47:ALA:HB3	42:l:49:ARG:HE	1.82	0.43
53:v:21:G:C6	54:9:35:G:C6	3.06	0.43
1:A:328:U:O2'	19:U:67:SER:OG	2.37	0.43
1:A:743:A:O2'	1:A:1659:G:OP1	2.34	0.43
1:A:2602:A:C2	54:9:76:A:N7	2.87	0.43
2:B:72:G:H21	2:B:104:A:H62	1.67	0.43
5:E:97:ASN:ND2	5:E:100:MET:SD	2.90	0.43
41:k:18:GLY:HA2	41:k:35:ASP:HA	1.99	0.43
1:A:698:C:O2'	1:A:734:A:N6	2.46	0.43
1:A:764:A:H5''	3:C:208:GLY:HA3	2.00	0.43
1:A:2529:G:H4'	7:G:174:LYS:HG3	2.01	0.43
14:P:108:ARG:NH1	31:a:1464:U:OP2	2.52	0.43
19:U:14:THR:OG1	19:U:68:ASN:ND2	2.52	0.43
21:W:4:LYS:HD3	54:x:74:C:N4	2.34	0.43
31:a:1055:A:N3	33:c:155:ARG:NH1	2.66	0.43
31:a:1251:A:N3	31:a:1369:C:O2'	2.46	0.43
35:e:152:VAL:HG21	38:h:98:LEU:HB2	2.01	0.43
53:v:13:C:H2'	53:v:14:C:H5'	2.01	0.43
1:A:243:U:OP1	28:3:7:ARG:NH1	2.52	0.43
1:A:308:G:H21	1:A:329:G:H21	1.67	0.43
31:a:1317:C:H4'	44:n:48:LEU:HD21	2.00	0.43
1:A:61:C:H5''	23:Y:43:LEU:HD22	2.01	0.43
1:A:112:U:H5'	23:Y:58:ASN:HD21	1.84	0.43
1:A:249:C:O5'	1:A:2394:C:O2'	2.36	0.43
1:A:1351:C:O2'	1:A:1571:A:N3	2.46	0.43
1:A:1826:G:O2'	1:A:1971:U:OP2	2.28	0.43
1:A:2516:A:N6	1:A:2567:G:O6	2.51	0.43
6:F:101:ARG:HG3	6:F:105:ILE:HD11	2.01	0.43
10:L:128:THR:OG1	10:L:129:LYS:N	2.52	0.43
14:P:63:ILE:HA	14:P:68:GLY:HA2	2.01	0.43
18:T:38:ALA:HB3	18:T:81:LYS:HD2	2.00	0.43
54:x:73:A:N3	54:x:73:A:H2'	2.33	0.43
55:7:90:ALA:HB1	55:7:154:LYS:HB2	2.01	0.43
1:A:534:U:O2'	15:Q:44:TYR:O	2.36	0.43
1:A:635:C:O2'	1:A:639:U:OP1	2.36	0.43
1:A:998:C:OP2	15:Q:57:ARG:NH2	2.52	0.43
1:A:1847:G:H21	1:A:1848:A:H62	1.66	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:12:C:N3	21:W:74:PRO:HA	2.33	0.43
12:N:28:LEU:HD11	12:N:114:GLU:HA	2.01	0.43
34:d:81:LEU:HD12	34:d:88:ASN:HB3	2.00	0.43
53:v:19:C:N3	54:9:37:G:C2	2.87	0.43
1:A:358:U:H2'	1:A:359:G:H8	1.84	0.42
1:A:1412:U:H2'	1:A:1413:A:H8	1.83	0.42
1:A:2431:U:N3	1:A:2434:A:OP2	2.41	0.42
31:a:455:G:H3'	31:a:456:A:H8	1.84	0.42
32:b:185:ILE:HA	32:b:199:ILE:HB	2.01	0.42
1:A:248:G:O2'	1:A:2432:A:OP1	2.37	0.42
1:A:552:U:H2'	1:A:553:G:H8	1.84	0.42
1:A:1022:G:N2	1:A:1023:U:O4	2.50	0.42
5:E:75:SER:HB3	5:E:78:TRP:CD1	2.54	0.42
6:F:139:GLU:OE2	30:6:26:SER:OG	2.37	0.42
11:M:69:PRO:HA	11:M:94:ALA:HB2	2.00	0.42
14:P:59:THR:HG22	14:P:72:VAL:HG12	2.01	0.42
31:a:541:G:O2'	34:d:39:GLN:OE1	2.34	0.42
33:c:110:LEU:HD13	33:c:203:LYS:HE2	2.00	0.42
35:e:37:VAL:HG11	35:e:113:VAL:HA	2.02	0.42
54:9:50:G:H2'	54:9:51:A:C8	2.54	0.42
1:A:1266:G:O2'	1:A:2012:G:O6	2.34	0.42
1:A:1361:G:OP1	22:X:76:LYS:NZ	2.45	0.42
6:F:133:GLU:HB3	6:F:135:ILE:HG13	2.01	0.42
25:0:54:ILE:HG23	25:0:56:LYS:H	1.85	0.42
31:a:50:A:O2'	31:a:360:G:N2	2.52	0.42
31:a:601:G:H1	31:a:637:C:H42	1.67	0.42
31:a:714:G:N2	31:a:777:A:N3	2.63	0.42
1:A:1940:U:OP1	1:A:2603:G:N2	2.52	0.42
28:3:31:ILE:H	28:3:31:ILE:HG13	1.47	0.42
52:w:176:VAL:HG12	52:w:183:TYR:HA	2.02	0.42
31:a:599:C:H2'	31:a:600:A:H8	1.84	0.42
31:a:842:U:O2'	31:a:845:A:OP1	2.33	0.42
31:a:1187:G:H5'	39:i:114:LYS:HE3	2.01	0.42
35:e:80:LEU:HD22	35:e:122:VAL:HG11	2.01	0.42
52:w:113:CYS:HB3	52:w:128:PRO:HD3	2.01	0.42
1:A:471:A:OP1	5:E:79:ARG:NH1	2.41	0.42
20:V:9:ARG:HD3	20:V:39:ALA:HB1	2.00	0.42
31:a:530:G:H21	54:9:36:G:C4'	2.33	0.42
1:A:196:A:H61	1:A:831:G:H21	1.68	0.42
1:A:1807:G:O2'	1:A:1809:A:N6	2.52	0.42
1:A:2622:U:O2'	1:A:2825:G:N7	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:U:39:ASN:HB3	19:U:62:ALA:HB3	2.01	0.42
31:a:684:U:H1'	41:k:39:ASN:HB2	2.02	0.42
36:f:8:PHE:HB2	36:f:84:VAL:HG13	2.01	0.42
1:A:861:A:N3	2:B:79:G:O2'	2.53	0.42
1:A:1003:G:O2'	1:A:1010:A:N1	2.50	0.42
1:A:2124:G:H2'	55:7:218:MET:HE1	2.01	0.42
1:A:2602:A:C2	54:9:76:A:C8	3.07	0.42
2:B:39:A:O2'	2:B:46:A:N1	2.53	0.42
5:E:47:LYS:HB2	5:E:51:GLU:HB2	2.01	0.42
7:G:8:VAL:HB	7:G:49:LEU:HB2	2.02	0.42
7:G:96:ALA:O	7:G:103:ASN:N	2.50	0.42
12:N:37:THR:HG22	12:N:110:MET:HE1	2.00	0.42
15:Q:93:ILE:HD12	16:R:13:ARG:HB2	2.02	0.42
31:a:145:G:N2	31:a:178:C:N3	2.67	0.42
41:k:81:LEU:HD11	41:k:99:LEU:HD23	2.00	0.42
49:s:10:ILE:HG12	49:s:40:PHE:HE2	1.84	0.42
1:A:1939:U:OP1	1:A:2604:U:O2'	2.38	0.42
1:A:2646:C:OP2	1:A:2732:G:O2'	2.31	0.42
1:A:2768:U:O2'	8:J:95:ARG:NH2	2.53	0.42
28:3:32:LEU:HB3	28:3:40:LYS:HD3	2.01	0.42
31:a:1054:C:O2'	54:9:34:C:C4'	2.66	0.42
35:e:80:LEU:HD21	35:e:95:MET:HE2	2.01	0.42
52:w:156:LEU:HD23	52:w:160:ALA:HB3	2.02	0.42
55:7:49:GLY:HA2	55:7:170:ILE:HG23	2.02	0.42
1:A:672:C:H5	10:L:42:SER:HB2	1.84	0.42
1:A:2252:G:N3	1:A:2253:G:O4'	2.52	0.42
8:J:34:ARG:HG3	8:J:39:LYS:HB2	2.01	0.42
31:a:490:C:OP1	34:d:145:ARG:NH2	2.53	0.42
31:a:1031:C:OP1	31:a:1032:G:N1	2.53	0.42
34:d:187:ARG:NH2	34:d:194:ILE:O	2.53	0.42
40:j:52:LEU:HD23	40:j:62:ARG:HG2	2.02	0.42
1:A:224:U:O4	1:A:419:U:O2'	2.38	0.41
1:A:302:C:H2'	1:A:303:G:H8	1.85	0.41
1:A:1068:G:O2'	1:A:1070:A:N6	2.52	0.41
6:F:125:GLY:O	6:F:157:THR:OG1	2.35	0.41
10:L:62:PRO:HB2	28:3:29:ARG:HH11	1.85	0.41
18:T:38:ALA:HB1	18:T:43:ILE:HD11	2.01	0.41
20:V:72:VAL:HG12	20:V:93:ARG:HA	2.01	0.41
31:a:1229:A:N6	43:m:103:THR:OG1	2.53	0.41
37:g:16:LYS:HG2	37:g:17:PHE:H	1.85	0.41
38:h:73:SER:HG	38:h:75:GLN:HE22	1.65	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
47:q:30:HIS:HA	47:q:31:PRO:HD3	1.93	0.41
1:A:2553:G:N1	54:9:75:C:N4	2.65	0.41
3:C:77:VAL:HG21	3:C:109:LEU:HD11	2.02	0.41
3:C:210:ALA:HB1	3:C:215:VAL:HB	2.01	0.41
9:K:21:CYS:HA	9:K:41:ILE:HG22	2.02	0.41
11:M:75:GLU:HB3	11:M:90:GLU:HG3	2.02	0.41
31:a:768:A:N3	31:a:1512:U:O2'	2.52	0.41
32:b:186:VAL:HB	32:b:190:SER:HB2	2.01	0.41
37:g:129:ASN:HA	37:g:134:VAL:HG11	2.02	0.41
52:w:30:VAL:HA	54:x:71:C:O2'	2.20	0.41
1:A:612:G:N2	1:A:614:A:O2'	2.53	0.41
1:A:2252:G:N1	54:x:74:C:N3	2.58	0.41
1:A:2293:G:OP1	13:O:94:ARG:NH1	2.53	0.41
14:P:13:LYS:HE3	14:P:76:HIS:HA	2.01	0.41
25:0:27:LEU:HD23	25:0:36:LYS:HB3	2.02	0.41
32:b:93:HIS:CG	32:b:145:ASN:HB2	2.55	0.41
35:e:35:LEU:HD11	35:e:136:VAL:HG11	2.00	0.41
38:h:10:LEU:HD22	38:h:74:ILE:HD11	2.01	0.41
47:q:20:ILE:HG23	47:q:45:VAL:HB	2.02	0.41
1:A:51:G:H21	1:A:118:A:H62	1.67	0.41
1:A:399:U:OP2	22:X:56:ARG:NH1	2.53	0.41
1:A:1041:G:H1	1:A:1114:C:H42	1.67	0.41
1:A:2355:G:O2'	21:W:24:LYS:HE2	2.21	0.41
6:F:102:LEU:HA	6:F:106:ALA:HB3	2.02	0.41
13:O:4:LYS:HE2	13:O:8:ILE:HD11	2.02	0.41
31:a:19:A:OP1	35:e:134:ASN:ND2	2.51	0.41
31:a:148:G:H21	31:a:1446:A:H2	1.68	0.41
31:a:1175:G:H2'	31:a:1176:A:H8	1.86	0.41
46:p:4:ILE:HD12	46:p:67:ILE:HG13	2.03	0.41
1:A:2506:U:H5	1:A:2583:G:H1	1.68	0.41
31:a:1498:U:C2	53:v:17:C:H5''	2.56	0.41
33:c:13:ILE:HG22	33:c:14:VAL:HG23	2.03	0.41
38:h:42:GLU:HG2	38:h:100:ILE:HG12	2.02	0.41
55:7:115:ILE:HD12	55:7:154:LYS:HE2	2.03	0.41
55:7:126:GLN:HA	55:7:129:GLN:HE21	1.84	0.41
1:A:351:C:H2'	1:A:352:A:H8	1.85	0.41
1:A:993:G:H1'	16:R:91:GLN:HE21	1.85	0.41
5:E:148:ILE:HB	5:E:169:VAL:HG22	2.02	0.41
6:F:68:LYS:HB3	6:F:81:GLY:HA2	2.03	0.41
9:K:2:ILE:HB	9:K:33:ALA:HB3	2.01	0.41
31:a:981:U:OP1	44:n:8:ARG:NH1	2.41	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:g:36:SER:HA	39:i:42:THR:HG21	2.01	0.41
1:A:1248:G:OP1	5:E:44:ARG:NH1	2.48	0.41
1:A:2627:G:O2'	1:A:2781:A:N1	2.52	0.41
20:V:30:ILE:HG13	20:V:40:ILE:HG13	2.02	0.41
31:a:294:U:OP1	31:a:610:U:O2'	2.38	0.41
1:A:2252:G:C2	1:A:2253:G:N3	2.87	0.41
16:R:2:TYR:HA	16:R:15:SER:HA	2.03	0.41
31:a:1147:C:O2'	39:i:6:TYR:OH	2.33	0.41
31:a:1240:U:OP2	37:g:114:SER:OG	2.39	0.41
33:c:29:ALA:O	44:n:65:ARG:NH1	2.54	0.41
1:A:290:U:H2'	1:A:291:G:H8	1.86	0.41
1:A:981:A:OP2	1:A:982:C:N4	2.54	0.41
1:A:1365:A:OP1	22:X:2:ARG:NH1	2.48	0.41
1:A:1666:G:H1'	9:K:3:GLN:HE21	1.86	0.41
1:A:2122:U:H1'	55:7:167:LYS:HE2	2.03	0.41
1:A:2505:G:O2'	1:A:2506:U:O2	2.29	0.41
17:S:69:LEU:HA	17:S:109:ASP:HA	2.02	0.41
31:a:1437:A:H2'	31:a:1438:G:H8	1.86	0.41
1:A:2500:U:O2'	1:A:2504:U:OP1	2.37	0.41
6:F:39:VAL:HG11	6:F:49:LEU:HD13	2.02	0.41
31:a:328:C:H4'	31:a:329:A:H5'	2.03	0.41
31:a:373:A:H61	31:a:391:G:H1'	1.86	0.41
1:A:160:A:N3	1:A:2208:C:O2'	2.54	0.40
1:A:578:G:OP1	1:A:1255:U:O2'	2.31	0.40
1:A:1029:A:N6	1:A:1125:G:O2'	2.54	0.40
1:A:1509:A:H2'	1:A:1510:G:C8	2.57	0.40
1:A:1800:C:N4	1:A:1818:U:O2'	2.54	0.40
1:A:2849:U:O4	14:P:20:ARG:NH2	2.54	0.40
31:a:530:G:O2'	54:9:35:G:C1'	2.69	0.40
31:a:530:G:C2'	54:9:35:G:O2'	2.64	0.40
39:i:115:VAL:HG23	40:j:62:ARG:HH11	1.86	0.40
1:A:550:C:N4	1:A:551:G:O6	2.55	0.40
6:F:56:LEU:O	6:F:60:SER:OG	2.36	0.40
31:a:591:U:H2'	31:a:592:G:H8	1.86	0.40
31:a:950:U:H3	31:a:1231:G:H1	1.69	0.40
32:b:9:LEU:HD21	32:b:13:VAL:HG22	2.04	0.40
42:l:109:ARG:HB2	42:l:118:VAL:HG21	2.01	0.40
1:A:624:C:O2'	1:A:657:U:OP1	2.38	0.40
1:A:1818:U:H4'	1:A:1821:A:H1'	2.03	0.40
8:J:44:TYR:O	15:Q:63:ARG:NE	2.54	0.40
31:a:502:A:H61	31:a:543:U:H3	1.69	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:d:131:ILE:HG22	34:d:133:SER:H	1.86	0.40
52:w:133:LEU:HD13	52:w:156:LEU:HD21	2.03	0.40
1:A:290:U:H2'	1:A:291:G:C8	2.56	0.40
13:O:26:LEU:HD23	13:O:92:PHE:HD1	1.86	0.40
28:3:61:LEU:HD13	28:3:64:ALA:HB3	2.03	0.40
31:a:1368:A:H5''	39:i:113:LYS:HB3	2.02	0.40
32:b:129:THR:O	32:b:133:ALA:N	2.49	0.40
44:n:64:CYS:HB3	44:n:69:ARG:H	1.86	0.40
52:w:38:PHE:HB3	52:w:57:LYS:HD3	2.04	0.40
54:9:18:G:O2'	54:9:57:G:N2	2.38	0.40
1:A:2305:U:H5''	6:F:130:GLY:HA3	2.03	0.40
3:C:52:HIS:CE1	3:C:218:THR:HA	2.57	0.40
7:G:3:VAL:HG12	7:G:68:ARG:HD2	2.03	0.40
23:Y:49:ASP:OD1	23:Y:52:ARG:NH2	2.55	0.40
31:a:309:A:H2'	31:a:310:G:H8	1.86	0.40
31:a:493:A:H62	31:a:494:G:H21	1.68	0.40
31:a:976:G:OP2	31:a:1358:U:O2'	2.39	0.40
45:o:3:SER:OG	45:o:4:THR:N	2.54	0.40
49:s:30:LEU:HB2	49:s:48:ILE:HG22	2.03	0.40
50:t:4:LYS:HG3	50:t:6:ALA:H	1.87	0.40
50:t:30:PHE:HD2	50:t:56:ILE:HG21	1.86	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	C	269/271 (99%)	251 (93%)	18 (7%)	0	100	100
4	D	207/209 (99%)	196 (95%)	11 (5%)	0	100	100
5	E	199/201 (99%)	188 (94%)	11 (6%)	0	100	100
6	F	175/177 (99%)	164 (94%)	11 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
7	G	174/176 (99%)	163 (94%)	9 (5%)	2 (1%)	11	42
8	J	140/142 (99%)	132 (94%)	8 (6%)	0	100	100
9	K	120/122 (98%)	104 (87%)	16 (13%)	0	100	100
10	L	141/143 (99%)	126 (89%)	14 (10%)	1 (1%)	18	50
11	M	134/136 (98%)	126 (94%)	5 (4%)	3 (2%)	5	31
12	N	118/120 (98%)	109 (92%)	9 (8%)	0	100	100
13	O	114/116 (98%)	109 (96%)	5 (4%)	0	100	100
14	P	112/114 (98%)	105 (94%)	7 (6%)	0	100	100
15	Q	115/117 (98%)	113 (98%)	2 (2%)	0	100	100
16	R	101/103 (98%)	91 (90%)	9 (9%)	1 (1%)	12	43
17	S	108/110 (98%)	102 (94%)	6 (6%)	0	100	100
18	T	91/93 (98%)	81 (89%)	10 (11%)	0	100	100
19	U	100/102 (98%)	86 (86%)	13 (13%)	1 (1%)	12	43
20	V	92/94 (98%)	91 (99%)	1 (1%)	0	100	100
21	W	82/84 (98%)	78 (95%)	4 (5%)	0	100	100
22	X	75/77 (97%)	72 (96%)	3 (4%)	0	100	100
23	Y	61/63 (97%)	61 (100%)	0	0	100	100
24	Z	56/58 (97%)	56 (100%)	0	0	100	100
25	0	54/56 (96%)	54 (100%)	0	0	100	100
26	1	48/50 (96%)	47 (98%)	1 (2%)	0	100	100
27	2	44/46 (96%)	43 (98%)	1 (2%)	0	100	100
28	3	62/64 (97%)	56 (90%)	4 (6%)	2 (3%)	3	25
29	4	36/38 (95%)	31 (86%)	5 (14%)	0	100	100
30	6	64/66 (97%)	55 (86%)	9 (14%)	0	100	100
32	b	216/218 (99%)	197 (91%)	19 (9%)	0	100	100
33	c	204/206 (99%)	195 (96%)	9 (4%)	0	100	100
34	d	203/205 (99%)	178 (88%)	25 (12%)	0	100	100
35	e	155/157 (99%)	139 (90%)	15 (10%)	1 (1%)	21	52
36	f	98/100 (98%)	81 (83%)	15 (15%)	2 (2%)	6	32
37	g	149/151 (99%)	134 (90%)	15 (10%)	0	100	100
38	h	127/129 (98%)	121 (95%)	6 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
39	i	125/127 (98%)	105 (84%)	19 (15%)	1 (1%)	16	48
40	j	96/98 (98%)	81 (84%)	15 (16%)	0	100	100
41	k	114/116 (98%)	101 (89%)	13 (11%)	0	100	100
42	l	121/123 (98%)	94 (78%)	26 (22%)	1 (1%)	16	48
43	m	112/114 (98%)	101 (90%)	9 (8%)	2 (2%)	6	34
44	n	99/101 (98%)	90 (91%)	9 (9%)	0	100	100
45	o	86/88 (98%)	79 (92%)	7 (8%)	0	100	100
46	p	80/82 (98%)	68 (85%)	12 (15%)	0	100	100
47	q	78/80 (98%)	66 (85%)	11 (14%)	1 (1%)	9	38
48	r	63/65 (97%)	56 (89%)	7 (11%)	0	100	100
49	s	77/79 (98%)	71 (92%)	6 (8%)	0	100	100
50	t	83/85 (98%)	80 (96%)	3 (4%)	0	100	100
51	u	63/65 (97%)	50 (79%)	13 (21%)	0	100	100
52	w	185/188 (98%)	161 (87%)	24 (13%)	0	100	100
55	7	210/224 (94%)	189 (90%)	21 (10%)	0	100	100
All	All	5836/5949 (98%)	5327 (91%)	491 (8%)	18 (0%)	37	65

All (18) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
28	3	31	ILE
7	G	47	ASN
11	M	59	ARG
28	3	32	LEU
36	f	55	HIS
47	q	70	LYS
11	M	58	LYS
42	l	102	ASP
43	m	4	ALA
19	U	89	GLY
36	f	53	LYS
43	m	5	GLY
10	L	128	THR
11	M	70	ASP
39	i	91	GLU
35	e	122	VAL
7	G	119	GLY

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Mol	Chain	Res	Type
16	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	
3	C	216/216 (100%)	216 (100%)	0	100	100
4	D	164/164 (100%)	164 (100%)	0	100	100
5	E	165/165 (100%)	165 (100%)	0	100	100
6	F	148/148 (100%)	148 (100%)	0	100	100
7	G	137/137 (100%)	137 (100%)	0	100	100
8	J	116/116 (100%)	116 (100%)	0	100	100
9	K	103/103 (100%)	103 (100%)	0	100	100
10	L	102/102 (100%)	101 (99%)	1 (1%)	68	74
11	M	109/109 (100%)	109 (100%)	0	100	100
12	N	100/100 (100%)	100 (100%)	0	100	100
13	O	86/86 (100%)	86 (100%)	0	100	100
14	P	99/99 (100%)	99 (100%)	0	100	100
15	Q	89/89 (100%)	89 (100%)	0	100	100
16	R	84/84 (100%)	84 (100%)	0	100	100
17	S	93/93 (100%)	93 (100%)	0	100	100
18	T	80/80 (100%)	80 (100%)	0	100	100
19	U	83/83 (100%)	83 (100%)	0	100	100
20	V	78/78 (100%)	78 (100%)	0	100	100
21	W	63/63 (100%)	63 (100%)	0	100	100
22	X	67/67 (100%)	67 (100%)	0	100	100
23	Y	55/55 (100%)	55 (100%)	0	100	100
24	Z	48/48 (100%)	48 (100%)	0	100	100
25	0	47/47 (100%)	47 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
26	1	45/45 (100%)	45 (100%)	0	100	100
27	2	38/38 (100%)	38 (100%)	0	100	100
28	3	51/51 (100%)	51 (100%)	0	100	100
29	4	34/34 (100%)	34 (100%)	0	100	100
30	6	59/59 (100%)	59 (100%)	0	100	100
32	b	180/180 (100%)	180 (100%)	0	100	100
33	c	170/170 (100%)	170 (100%)	0	100	100
34	d	172/172 (100%)	172 (100%)	0	100	100
35	e	114/119 (96%)	114 (100%)	0	100	100
36	f	87/87 (100%)	87 (100%)	0	100	100
37	g	124/124 (100%)	124 (100%)	0	100	100
38	h	104/104 (100%)	104 (100%)	0	100	100
39	i	105/105 (100%)	105 (100%)	0	100	100
40	j	86/86 (100%)	86 (100%)	0	100	100
41	k	89/89 (100%)	89 (100%)	0	100	100
42	l	103/103 (100%)	103 (100%)	0	100	100
43	m	92/92 (100%)	92 (100%)	0	100	100
44	n	79/83 (95%)	79 (100%)	0	100	100
45	o	76/76 (100%)	76 (100%)	0	100	100
46	p	65/65 (100%)	65 (100%)	0	100	100
47	q	74/74 (100%)	74 (100%)	0	100	100
48	r	48/56 (86%)	48 (100%)	0	100	100
49	s	70/70 (100%)	69 (99%)	1 (1%)	59	70
50	t	65/65 (100%)	65 (100%)	0	100	100
51	u	44/55 (80%)	44 (100%)	0	100	100
52	w	154/154 (100%)	153 (99%)	1 (1%)	78	79
55	7	173/173 (100%)	173 (100%)	0	100	100
All	All	4833/4861 (99%)	4830 (100%)	3 (0%)	87	88

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
10	L	27	LEU

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Mol	Chain	Res	Type
49	s	10	ILE
52	w	107	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (68) such sidechains are listed below:

Mol	Chain	Res	Type
3	C	36	ASN
3	C	85	ASN
3	C	114	GLN
3	C	116	GLN
3	C	250	GLN
4	D	164	GLN
4	D	173	GLN
5	E	156	ASN
7	G	63	GLN
7	G	115	GLN
7	G	138	GLN
8	J	40	HIS
8	J	58	ASN
8	J	86	GLN
9	K	3	GLN
9	K	5	GLN
9	K	29	HIS
12	N	9	GLN
13	O	29	HIS
13	O	34	HIS
13	O	38	GLN
13	O	98	GLN
14	P	11	GLN
14	P	55	HIS
15	Q	43	GLN
15	Q	51	GLN
15	Q	58	GLN
15	Q	71	ASN
16	R	6	GLN
16	R	18	GLN
16	R	43	ASN
17	S	7	HIS
17	S	9	HIS
17	S	57	ASN
21	W	12	ASN
21	W	46	HIS

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Mol	Chain	Res	Type
22	X	35	HIS
23	Y	58	ASN
24	Z	19	HIS
26	1	45	HIS
29	4	37	GLN
30	6	41	HIS
32	b	23	ASN
32	b	35	ASN
32	b	38	HIS
32	b	169	HIS
32	b	202	ASN
33	c	122	GLN
33	c	184	ASN
34	d	35	GLN
34	d	125	ASN
34	d	130	ASN
35	e	69	ASN
35	e	120	HIS
35	e	121	ASN
38	h	3	GLN
38	h	15	ASN
38	h	66	GLN
39	i	36	GLN
40	j	58	ASN
41	k	108	ASN
41	k	118	ASN
42	l	95	HIS
45	o	45	HIS
47	q	30	HIS
49	s	13	HIS
49	s	55	GLN
49	s	68	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	2868/2903 (98%)	504 (17%)	23 (0%)
2	B	119/120 (99%)	20 (16%)	1 (0%)
31	a	1538/1539 (99%)	304 (19%)	0
53	v	8/9 (88%)	3 (37%)	0
54	9	76/77 (98%)	27 (35%)	4 (5%)

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
54	x	76/77 (98%)	19 (25%)	0
All	All	4685/4725 (99%)	877 (18%)	28 (0%)

All (877) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	10	A
1	A	12	U
1	A	34	U
1	A	35	G
1	A	46	G
1	A	50	U
1	A	51	G
1	A	52	A
1	A	71	A
1	A	74	A
1	A	75	G
1	A	84	A
1	A	92	U
1	A	96	C
1	A	98	G
1	A	110	G
1	A	118	A
1	A	119	A
1	A	120	U
1	A	125	A
1	A	139	U
1	A	140	C
1	A	141	G
1	A	142	A
1	A	155	A
1	A	162	U
1	A	163	C
1	A	166	U
1	A	181	A
1	A	196	A
1	A	199	A
1	A	204	A
1	A	216	A
1	A	221	A
1	A	222	A
1	A	225	C

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Mol	Chain	Res	Type
1	A	229	C
1	A	239	C
1	A	242	G
1	A	243	U
1	A	248	G
1	A	249	C
1	A	255	A
1	A	265	A
1	A	272	A
1	A	276	U
1	A	278	A
1	A	279	A
1	A	285	G
1	A	311	A
1	A	323	C
1	A	324	A
1	A	329	G
1	A	330	A
1	A	345	A
1	A	367	G
1	A	370	G
1	A	371	A
1	A	372	G
1	A	386	G
1	A	387	U
1	A	395	U
1	A	404	A
1	A	406	G
1	A	411	G
1	A	412	A
1	A	421	C
1	A	424	G
1	A	456	C
1	A	458	G
1	A	467	G
1	A	473	G
1	A	481	G
1	A	491	G
1	A	505	A
1	A	508	A
1	A	509	C
1	A	528	A

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Mol	Chain	Res	Type
1	A	529	A
1	A	531	C
1	A	532	A
1	A	533	G
1	A	543	G
1	A	544	C
1	A	545	U
1	A	547	A
1	A	548	G
1	A	550	C
1	A	555	G
1	A	563	A
1	A	573	U
1	A	575	A
1	A	603	A
1	A	614	A
1	A	616	A
1	A	621	A
1	A	627	A
1	A	634	C
1	A	637	A
1	A	645	C
1	A	646	U
1	A	647	G
1	A	654	A
1	A	655	A
1	A	659	G
1	A	664	G
1	A	668	A
1	A	669	G
1	A	677	A
1	A	686	U
1	A	687	C
1	A	695	G
1	A	722	A
1	A	724	U
1	A	730	A
1	A	738	G
1	A	747	C
1	A	752	A
1	A	753	A
1	A	764	A

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Mol	Chain	Res	Type
1	A	765	C
1	A	774	G
1	A	782	A
1	A	783	A
1	A	784	G
1	A	785	G
1	A	789	A
1	A	792	A
1	A	805	G
1	A	812	C
1	A	819	A
1	A	827	U
1	A	828	U
1	A	831	G
1	A	845	A
1	A	846	U
1	A	847	U
1	A	856	G
1	A	859	G
1	A	860	U
1	A	878	A
1	A	885	C
1	A	886	A
1	A	892	A
1	A	895	U
1	A	896	A
1	A	897	C
1	A	907	G
1	A	910	A
1	A	937	C
1	A	941	A
1	A	946	C
1	A	953	G
1	A	958	U
1	A	959	A
1	A	961	C
1	A	974	G
1	A	983	A
1	A	985	C
1	A	995	C
1	A	996	A
1	A	1005	C

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Mol	Chain	Res	Type
1	A	1012	U
1	A	1013	C
1	A	1021	A
1	A	1022	G
1	A	1023	U
1	A	1026	G
1	A	1033	U
1	A	1045	C
1	A	1046	A
1	A	1053	C
1	A	1057	A
1	A	1059	G
1	A	1060	U
1	A	1062	G
1	A	1064	C
1	A	1065	U
1	A	1066	U
1	A	1067	A
1	A	1069	A
1	A	1070	A
1	A	1071	G
1	A	1072	C
1	A	1073	A
1	A	1075	C
1	A	1076	C
1	A	1078	U
1	A	1079	C
1	A	1084	A
1	A	1085	A
1	A	1088	A
1	A	1089	A
1	A	1096	A
1	A	1097	U
1	A	1104	C
1	A	1111	A
1	A	1112	G
1	A	1113	U
1	A	1131	G
1	A	1132	U
1	A	1133	A
1	A	1135	C
1	A	1139	G

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Mol	Chain	Res	Type
1	A	1142	A
1	A	1143	A
1	A	1150	C
1	A	1170	C
1	A	1172	C
1	A	1175	A
1	A	1176	U
1	A	1177	G
1	A	1180	U
1	A	1204	A
1	A	1205	A
1	A	1206	G
1	A	1211	C
1	A	1212	G
1	A	1246	A
1	A	1247	A
1	A	1248	G
1	A	1250	G
1	A	1251	C
1	A	1253	A
1	A	1256	G
1	A	1265	A
1	A	1271	G
1	A	1272	A
1	A	1275	A
1	A	1300	G
1	A	1301	A
1	A	1306	C
1	A	1312	U
1	A	1321	A
1	A	1325	U
1	A	1326	U
1	A	1330	C
1	A	1341	G
1	A	1345	C
1	A	1352	U
1	A	1365	A
1	A	1368	G
1	A	1378	A
1	A	1379	U
1	A	1383	A
1	A	1395	A

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Mol	Chain	Res	Type
1	A	1401	G
1	A	1403	A
1	A	1414	C
1	A	1416	G
1	A	1420	A
1	A	1428	C
1	A	1453	A
1	A	1460	U
1	A	1461	C
1	A	1475	G
1	A	1482	G
1	A	1490	A
1	A	1491	G
1	A	1494	A
1	A	1504	A
1	A	1507	C
1	A	1509	A
1	A	1515	A
1	A	1524	G
1	A	1529	G
1	A	1535	A
1	A	1536	C
1	A	1555	G
1	A	1558	C
1	A	1560	G
1	A	1569	A
1	A	1581	G
1	A	1583	A
1	A	1584	U
1	A	1585	C
1	A	1603	A
1	A	1608	A
1	A	1611	C
1	A	1646	C
1	A	1647	U
1	A	1648	U
1	A	1649	G
1	A	1651	G
1	A	1672	A
1	A	1674	G
1	A	1694	C
1	A	1695	G

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Mol	Chain	Res	Type
1	A	1699	G
1	A	1703	G
1	A	1715	G
1	A	1729	U
1	A	1730	C
1	A	1732	C
1	A	1733	G
1	A	1738	G
1	A	1758	U
1	A	1764	C
1	A	1773	A
1	A	1781	U
1	A	1800	C
1	A	1801	A
1	A	1802	A
1	A	1808	A
1	A	1816	C
1	A	1829	A
1	A	1833	C
1	A	1847	G
1	A	1857	G
1	A	1858	A
1	A	1859	U
1	A	1869	G
1	A	1870	C
1	A	1871	A
1	A	1872	A
1	A	1873	G
1	A	1896	G
1	A	1901	A
1	A	1906	G
1	A	1907	G
1	A	1913	A
1	A	1914	C
1	A	1929	G
1	A	1930	G
1	A	1931	U
1	A	1937	A
1	A	1940	U
1	A	1941	C
1	A	1955	U
1	A	1966	A

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Mol	Chain	Res	Type
1	A	1967	C
1	A	1970	A
1	A	1971	U
1	A	1972	G
1	A	1991	U
1	A	1992	G
1	A	1997	C
1	A	2004	G
1	A	2020	A
1	A	2022	U
1	A	2023	C
1	A	2031	A
1	A	2033	A
1	A	2034	U
1	A	2043	C
1	A	2049	G
1	A	2052	A
1	A	2055	C
1	A	2056	G
1	A	2059	A
1	A	2060	A
1	A	2061	G
1	A	2062	A
1	A	2069	A
1	A	2072	C
1	A	2093	G
1	A	2096	C
1	A	2097	A
1	A	2100	G
1	A	2101	A
1	A	2104	U
1	A	2105	U
1	A	2110	G
1	A	2111	U
1	A	2112	G
1	A	2114	A
1	A	2116	G
1	A	2117	A
1	A	2119	A
1	A	2120	G
1	A	2121	G
1	A	2126	A

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Mol	Chain	Res	Type
1	A	2127	G
1	A	2159	G
1	A	2160	C
1	A	2167	U
1	A	2170	A
1	A	2173	A
1	A	2174	C
1	A	2177	C
1	A	2178	C
1	A	2179	C
1	A	2180	U
1	A	2185	U
1	A	2186	G
1	A	2187	U
1	A	2188	U
1	A	2189	U
1	A	2190	G
1	A	2191	A
1	A	2193	G
1	A	2198	A
1	A	2203	U
1	A	2204	G
1	A	2211	A
1	A	2213	U
1	A	2214	C
1	A	2219	U
1	A	2225	A
1	A	2226	C
1	A	2238	G
1	A	2239	G
1	A	2249	U
1	A	2250	G
1	A	2251	G
1	A	2252	G
1	A	2278	A
1	A	2279	G
1	A	2283	C
1	A	2287	A
1	A	2288	A
1	A	2305	U
1	A	2309	A
1	A	2320	U

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Mol	Chain	Res	Type
1	A	2325	G
1	A	2327	A
1	A	2350	C
1	A	2353	G
1	A	2354	C
1	A	2361	G
1	A	2383	G
1	A	2385	C
1	A	2389	G
1	A	2392	A
1	A	2402	U
1	A	2403	C
1	A	2406	A
1	A	2424	C
1	A	2427	C
1	A	2429	G
1	A	2430	A
1	A	2435	A
1	A	2441	U
1	A	2448	A
1	A	2465	C
1	A	2470	G
1	A	2476	A
1	A	2478	A
1	A	2492	U
1	A	2498	C
1	A	2502	G
1	A	2503	A
1	A	2504	U
1	A	2506	U
1	A	2507	C
1	A	2513	A
1	A	2518	A
1	A	2520	C
1	A	2529	G
1	A	2534	A
1	A	2535	G
1	A	2547	A
1	A	2549	G
1	A	2554	U
1	A	2567	G
1	A	2572	A

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Mol	Chain	Res	Type
1	A	2573	C
1	A	2582	G
1	A	2585	U
1	A	2586	U
1	A	2602	A
1	A	2609	U
1	A	2613	U
1	A	2614	A
1	A	2629	U
1	A	2638	G
1	A	2655	G
1	A	2682	A
1	A	2689	U
1	A	2690	U
1	A	2714	G
1	A	2716	C
1	A	2718	G
1	A	2726	A
1	A	2733	A
1	A	2744	G
1	A	2748	A
1	A	2751	G
1	A	2757	A
1	A	2760	C
1	A	2764	A
1	A	2765	A
1	A	2778	A
1	A	2779	U
1	A	2790	U
1	A	2791	G
1	A	2793	C
1	A	2796	U
1	A	2800	A
1	A	2808	G
1	A	2809	A
1	A	2818	U
1	A	2820	A
1	A	2833	U
1	A	2849	U
1	A	2861	U
1	A	2867	G
1	A	2868	A

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Mol	Chain	Res	Type
1	A	2872	A
1	A	2873	A
1	A	2880	C
1	A	2893	A
1	A	2899	A
1	A	2901	C
2	B	4	C
2	B	12	C
2	B	13	G
2	B	15	A
2	B	24	G
2	B	30	C
2	B	35	C
2	B	38	C
2	B	40	U
2	B	41	G
2	B	42	C
2	B	44	G
2	B	45	A
2	B	57	A
2	B	66	A
2	B	67	G
2	B	88	C
2	B	89	U
2	B	90	C
2	B	109	A
31	a	4	U
31	a	6	G
31	a	7	A
31	a	8	A
31	a	9	G
31	a	22	G
31	a	32	A
31	a	36	C
31	a	37	U
31	a	39	G
31	a	41	G
31	a	47	C
31	a	49	U
31	a	51	A
31	a	55	A
31	a	56	U

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Mol	Chain	Res	Type
31	a	58	C
31	a	62	U
31	a	64	G
31	a	65	A
31	a	66	A
31	a	68	G
31	a	70	U
31	a	71	A
31	a	72	A
31	a	74	A
31	a	80	A
31	a	81	A
31	a	83	C
31	a	86	G
31	a	87	C
31	a	89	U
31	a	95	C
31	a	98	A
31	a	99	C
31	a	104	G
31	a	121	U
31	a	122	G
31	a	130	A
31	a	131	A
31	a	137	U
31	a	148	G
31	a	150	U
31	a	156	C
31	a	157	U
31	a	160	A
31	a	163	C
31	a	164	G
31	a	177	G
31	a	181	A
31	a	182	A
31	a	183	C
31	a	184	G
31	a	189	A
31	a	194	C
31	a	197	A
31	a	204	G
31	a	209	U

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Mol	Chain	Res	Type
31	a	210	C
31	a	211	G
31	a	212	G
31	a	214	C
31	a	223	A
31	a	226	G
31	a	230	G
31	a	245	U
31	a	247	G
31	a	251	G
31	a	266	G
31	a	267	C
31	a	277	C
31	a	279	A
31	a	280	C
31	a	281	G
31	a	289	G
31	a	306	A
31	a	316	C
31	a	321	A
31	a	328	C
31	a	330	C
31	a	345	C
31	a	346	G
31	a	347	G
31	a	351	G
31	a	352	C
31	a	354	G
31	a	359	G
31	a	360	G
31	a	367	U
31	a	368	U
31	a	374	A
31	a	376	G
31	a	378	G
31	a	380	G
31	a	381	C
31	a	383	A
31	a	388	G
31	a	390	U
31	a	392	C
31	a	398	U

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Mol	Chain	Res	Type
31	a	399	G
31	a	401	C
31	a	404	G
31	a	406	G
31	a	407	U
31	a	408	A
31	a	411	A
31	a	412	A
31	a	413	G
31	a	414	A
31	a	421	U
31	a	422	C
31	a	423	G
31	a	424	G
31	a	427	U
31	a	429	U
31	a	430	A
31	a	436	C
31	a	446	G
31	a	448	A
31	a	450	G
31	a	461	A
31	a	466	A
31	a	467	U
31	a	468	A
31	a	472	U
31	a	473	U
31	a	482	A
31	a	484	G
31	a	485	U
31	a	486	U
31	a	488	C
31	a	494	G
31	a	496	A
31	a	497	G
31	a	498	A
31	a	499	A
31	a	505	G
31	a	509	A
31	a	510	A
31	a	513	C
31	a	518	C

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Mol	Chain	Res	Type
31	a	520	A
31	a	524	G
31	a	527	G
31	a	531	U
31	a	532	A
31	a	536	C
31	a	547	A
31	a	548	G
31	a	559	A
31	a	562	U
31	a	564	C
31	a	572	A
31	a	573	A
31	a	575	G
31	a	576	C
31	a	577	G
31	a	579	A
31	a	604	G
31	a	607	A
31	a	617	G
31	a	620	C
31	a	623	C
31	a	633	G
31	a	636	U
31	a	642	A
31	a	650	G
31	a	656	G
31	a	661	G
31	a	665	A
31	a	687	A
31	a	688	G
31	a	702	A
31	a	703	G
31	a	713	G
31	a	718	A
31	a	723	U
31	a	724	G
31	a	731	G
31	a	748	G
31	a	753	A
31	a	754	C
31	a	755	G

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Mol	Chain	Res	Type
31	a	777	A
31	a	814	A
31	a	815	A
31	a	817	C
31	a	818	G
31	a	819	A
31	a	820	U
31	a	821	G
31	a	832	G
31	a	836	G
31	a	843	U
31	a	844	G
31	a	846	G
31	a	851	G
31	a	871	U
31	a	876	C
31	a	890	G
31	a	902	G
31	a	914	A
31	a	926	G
31	a	934	C
31	a	935	A
31	a	960	U
31	a	961	U
31	a	966	G
31	a	969	A
31	a	971	G
31	a	975	A
31	a	976	G
31	a	977	A
31	a	992	U
31	a	993	G
31	a	1004	A
31	a	1028	C
31	a	1030	U
31	a	1031	C
31	a	1032	G
31	a	1033	G
31	a	1034	G
31	a	1035	A
31	a	1053	G
31	a	1065	U

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Mol	Chain	Res	Type
31	a	1085	U
31	a	1092	A
31	a	1094	G
31	a	1095	U
31	a	1101	A
31	a	1130	A
31	a	1132	C
31	a	1133	G
31	a	1137	C
31	a	1138	G
31	a	1139	G
31	a	1140	C
31	a	1152	A
31	a	1159	U
31	a	1160	G
31	a	1168	U
31	a	1169	A
31	a	1183	U
31	a	1184	G
31	a	1191	A
31	a	1196	A
31	a	1197	A
31	a	1201	A
31	a	1202	U
31	a	1212	U
31	a	1213	A
31	a	1227	A
31	a	1228	C
31	a	1238	A
31	a	1241	G
31	a	1258	G
31	a	1261	A
31	a	1275	A
31	a	1278	G
31	a	1280	A
31	a	1281	C
31	a	1282	C
31	a	1286	U
31	a	1287	A
31	a	1297	G
31	a	1298	U
31	a	1300	G

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Mol	Chain	Res	Type
31	a	1301	U
31	a	1303	C
31	a	1317	C
31	a	1340	A
31	a	1346	A
31	a	1347	G
31	a	1348	U
31	a	1353	G
31	a	1363	A
31	a	1364	U
31	a	1368	A
31	a	1370	G
31	a	1378	C
31	a	1381	U
31	a	1397	C
31	a	1400	C
31	a	1419	G
31	a	1422	G
31	a	1429	A
31	a	1433	A
31	a	1446	A
31	a	1451	U
31	a	1452	C
31	a	1487	G
31	a	1492	A
31	a	1493	A
31	a	1497	G
31	a	1503	A
31	a	1506	U
31	a	1517	G
31	a	1520	C
31	a	1529	G
31	a	1530	G
31	a	1534	A
31	a	1535	C
31	a	1536	C
53	v	17	C
53	v	18	G
53	v	21	G
54	x	2	G
54	x	3	G
54	x	4	U

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Mol	Chain	Res	Type
54	x	5	G
54	x	6	A
54	x	8	U
54	x	14	A
54	x	18	G
54	x	19	G
54	x	20	U
54	x	21	A
54	x	25	C
54	x	41	A
54	x	42	A
54	x	47	U
54	x	65	U
54	x	73	A
54	x	74	C
54	x	76	A
54	9	3	G
54	9	4	U
54	9	5	G
54	9	6	A
54	9	8	U
54	9	16	C
54	9	17	C
54	9	18	G
54	9	19	G
54	9	20	U
54	9	21	A
54	9	22	G
54	9	28	U
54	9	35	G
54	9	40	G
54	9	42	A
54	9	47	U
54	9	48	C
54	9	54	U
54	9	56	C
54	9	61	C
54	9	62	C
54	9	69	A
54	9	72	G
54	9	74	C
54	9	75	C

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Mol	Chain	Res	Type
54	9	76	A

All (28) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	51	G
1	A	242	G
1	A	490	C
1	A	859	G
1	A	1020	A
1	A	1022	G
1	A	1070	A
1	A	1111	A
1	A	1182	G
1	A	1190	G
1	A	1300	G
1	A	1378	A
1	A	1399	C
1	A	1432	G
1	A	1930	G
1	A	1940	U
1	A	2190	G
1	A	2251	G
1	A	2286	G
1	A	2326	C
1	A	2391	G
1	A	2566	A
1	A	2808	G
2	B	66	A
54	9	2	G
54	9	3	G
54	9	19	G
54	9	41	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	$\# Z > 2$
52	KEO	w	34	52	16,18,19	1.45	2 (12%)	15,21,23	1.17	1 (6%)

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
52	KEO	w	34	52	-	10/19/20/22	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
52	w	34	KEO	C05-NZ	5.17	1.45	1.33
52	w	34	KEO	O02-C05	-2.18	1.18	1.23

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
52	w	34	KEO	C06-C05-NZ	2.66	120.08	115.97

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
52	w	34	KEO	O-C-CA-CB
52	w	34	KEO	N-CA-CB-CG
52	w	34	KEO	C-CA-CB-CG
52	w	34	KEO	CG-CD-CE-NZ
52	w	34	KEO	C06-C07-C08-C09
52	w	34	KEO	N02-C07-C08-C09
52	w	34	KEO	C06-C05-NZ-CE
52	w	34	KEO	O02-C05-NZ-CE
52	w	34	KEO	C05-C06-C07-C08
52	w	34	KEO	C05-C06-C07-N02

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
52	w	34	KEO	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

1 ligand 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	$\# Z > 2$
56	PRO	9	101	54	6,7,8	0.78	0	7,8,10	1.60	1 (14%)

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
56	PRO	9	101	54	-	0/0/9/11	0/1/1/1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
56	9	101	PRO	O-C-CA	-3.39	116.04	124.77

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
56	9	101	PRO	3	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
55	7	6
54	x	1
21	W	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	7	66:PRO	C	67:HIS	N	6.78
1	7	138:PRO	C	139:ASN	N	6.13
1	7	201:PRO	C	202:THR	N	4.61
1	7	133:PRO	C	134:ARG	N	3.99
1	7	140:PRO	C	141:LYS	N	3.47
1	7	118:PRO	C	119:ASP	N	3.31
1	x	40:G	O3'	41:A	P	2.28
1	W	10:THR	C	11:ARG	N	1.11

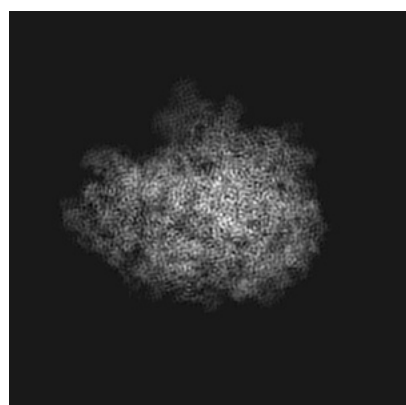
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-3899. These allow visual inspection of the internal detail of the map and identification of artifacts.

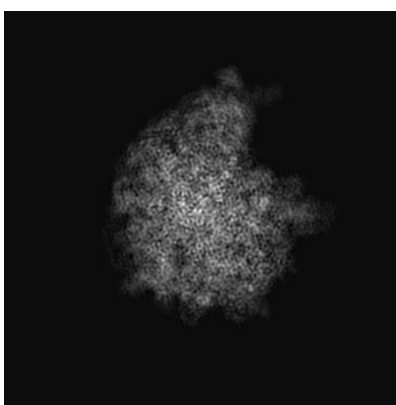
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

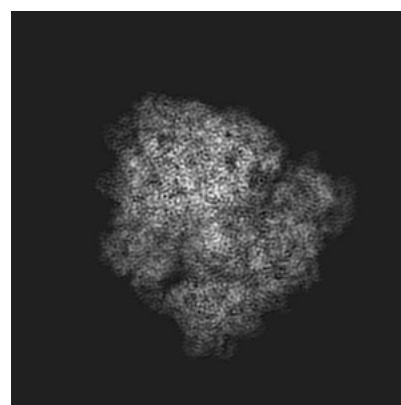
6.1.1 Primary map



X



Y

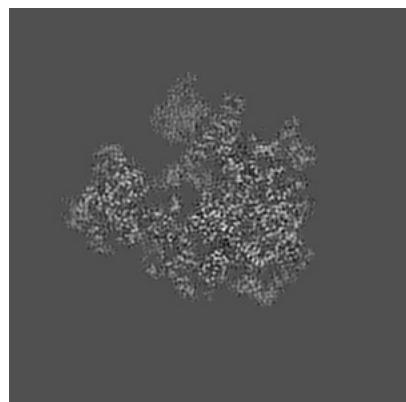


Z

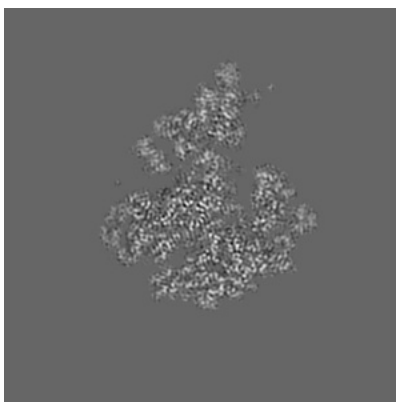
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

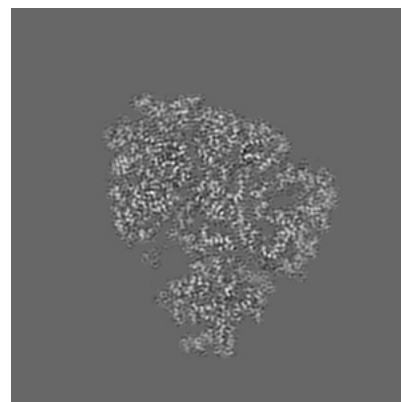
6.2.1 Primary map



X Index: 180



Y Index: 180

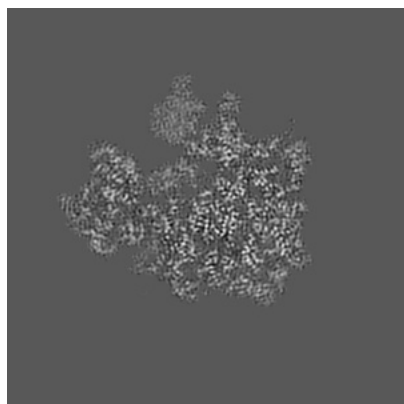


Z Index: 180

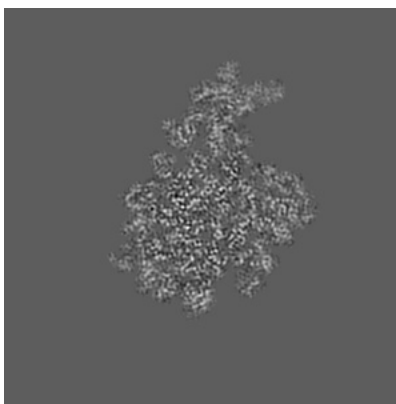
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

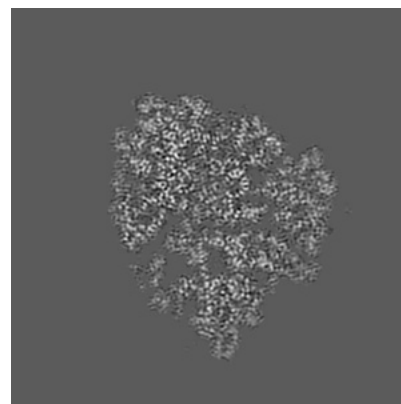
6.3.1 Primary map



X Index: 184



Y Index: 192

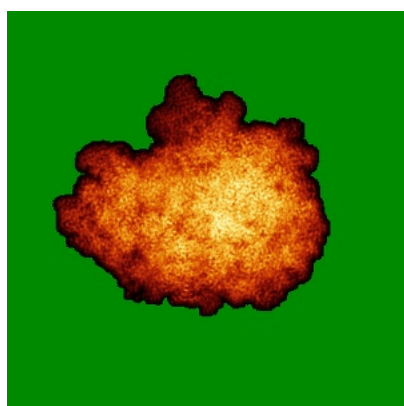


Z Index: 186

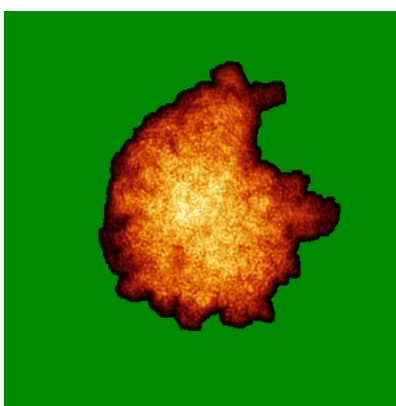
The images above show the largest variance slices of the map in three orthogonal directions.

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

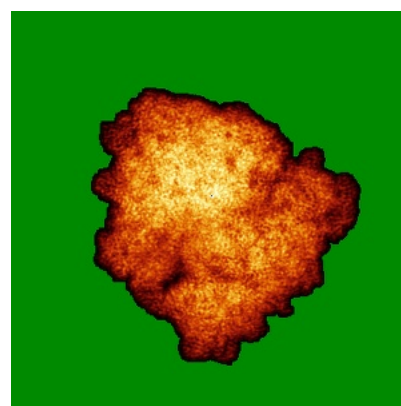
6.4.1 Primary map



X



Y

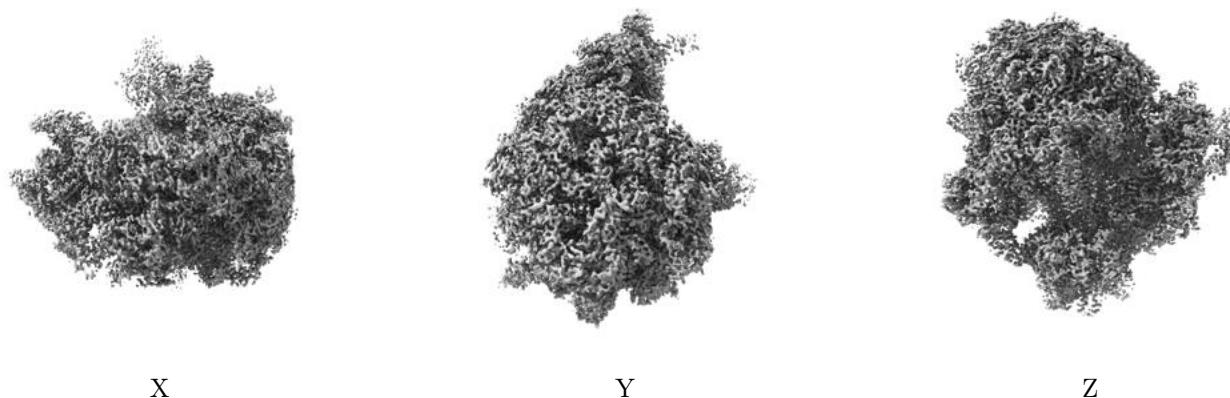


Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.0963. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

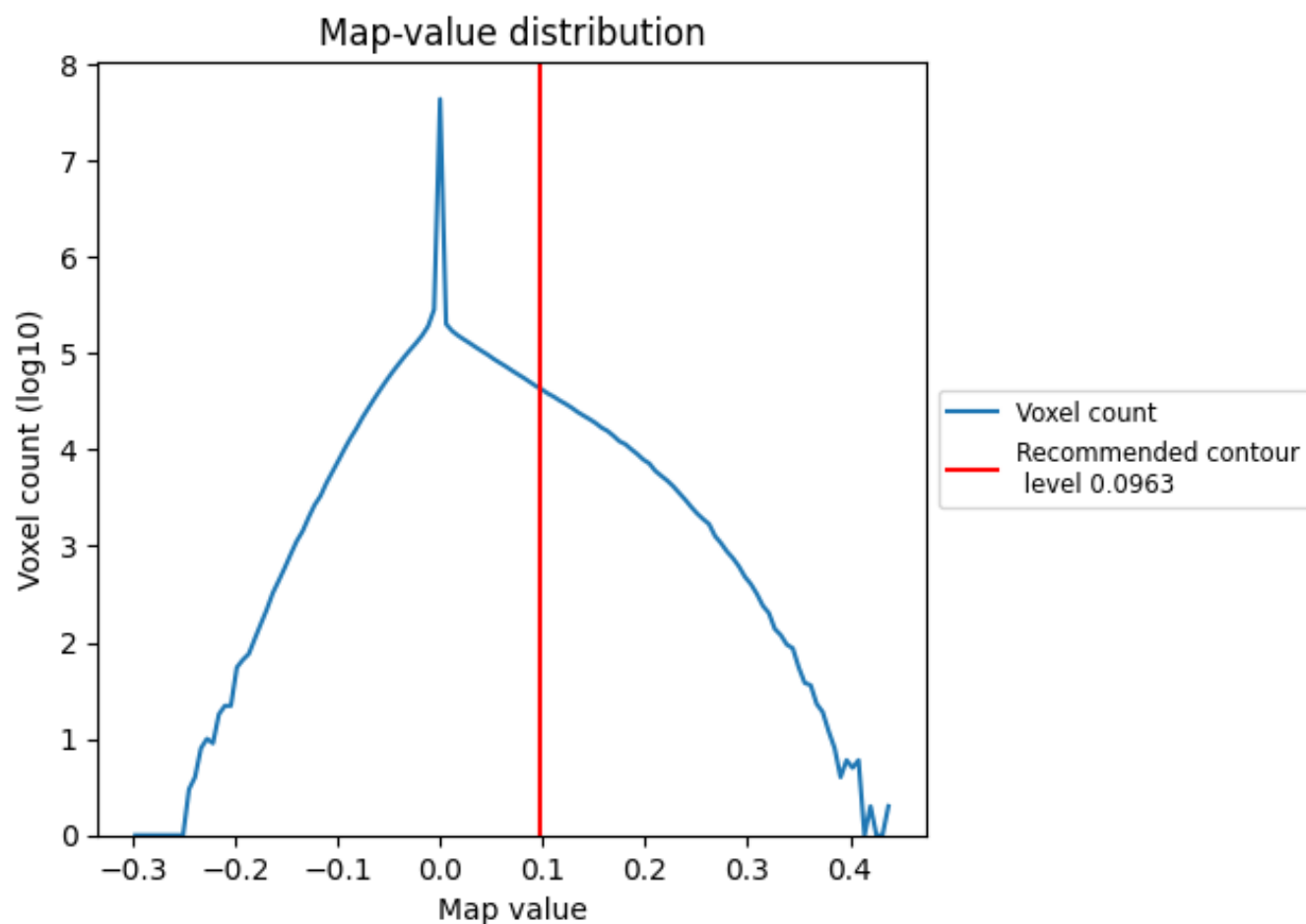
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

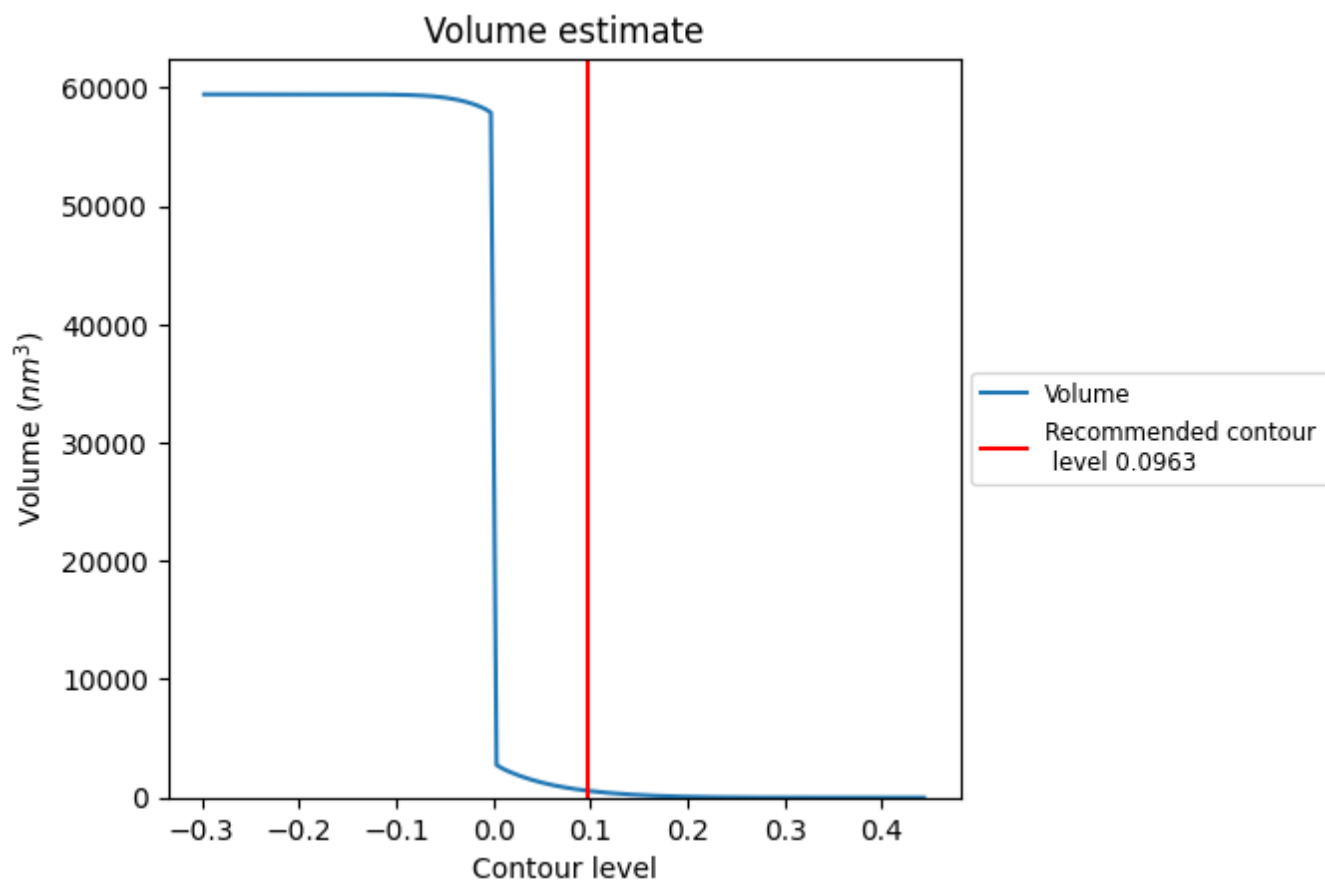
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

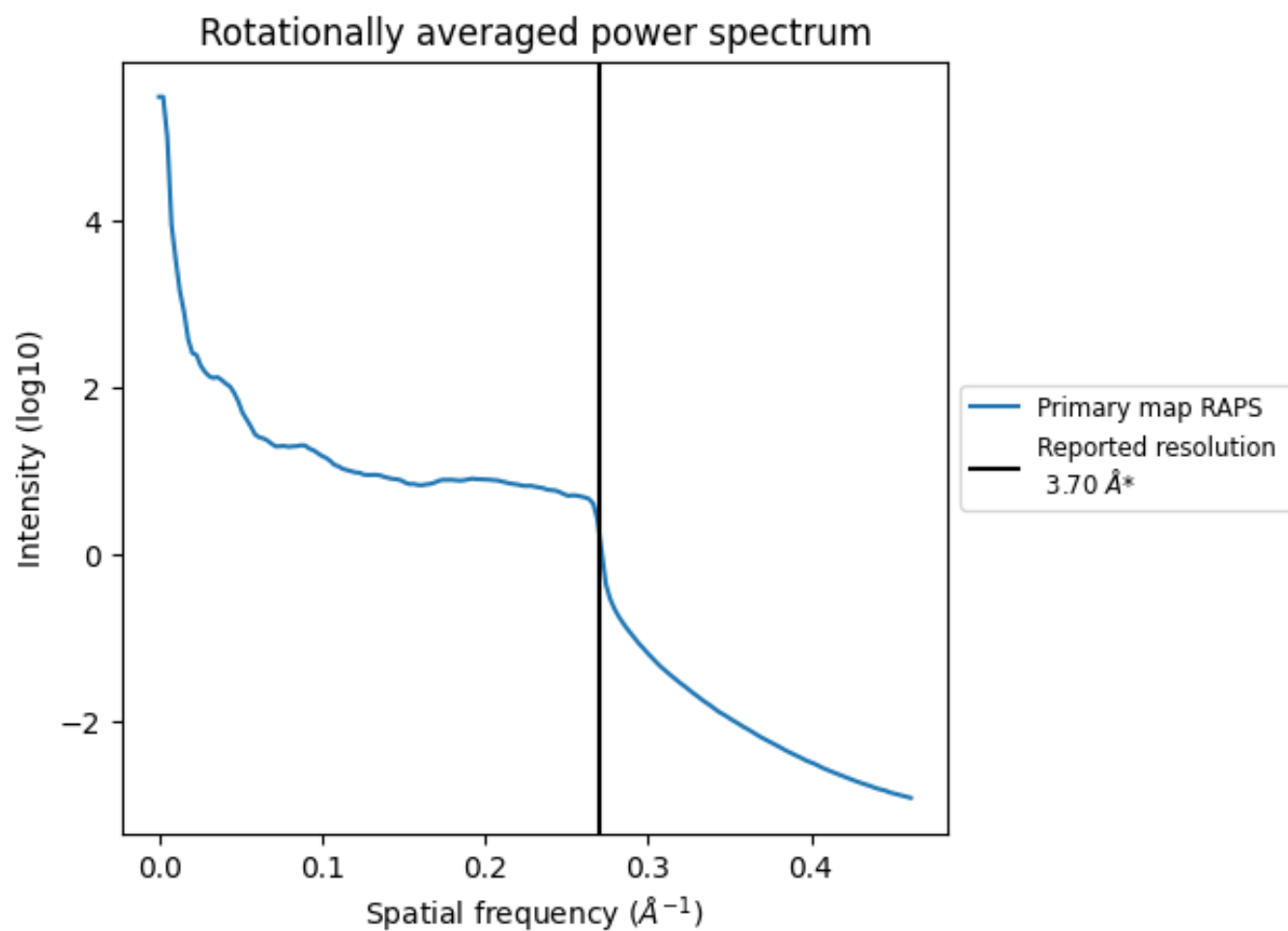
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 584 nm³; this corresponds to an approximate mass of 528 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ



*Reported resolution corresponds to spatial frequency of 0.270 Å⁻¹

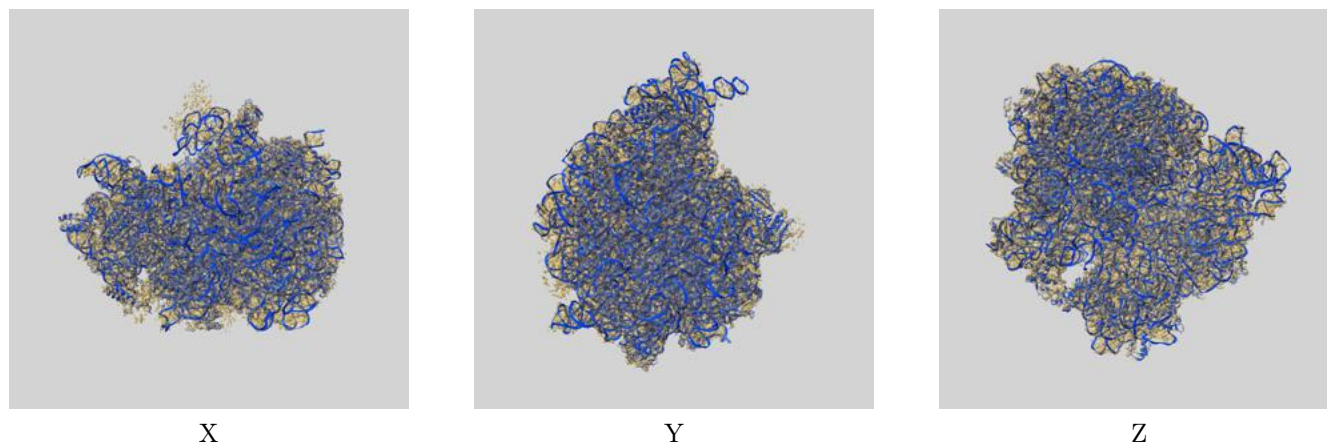
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

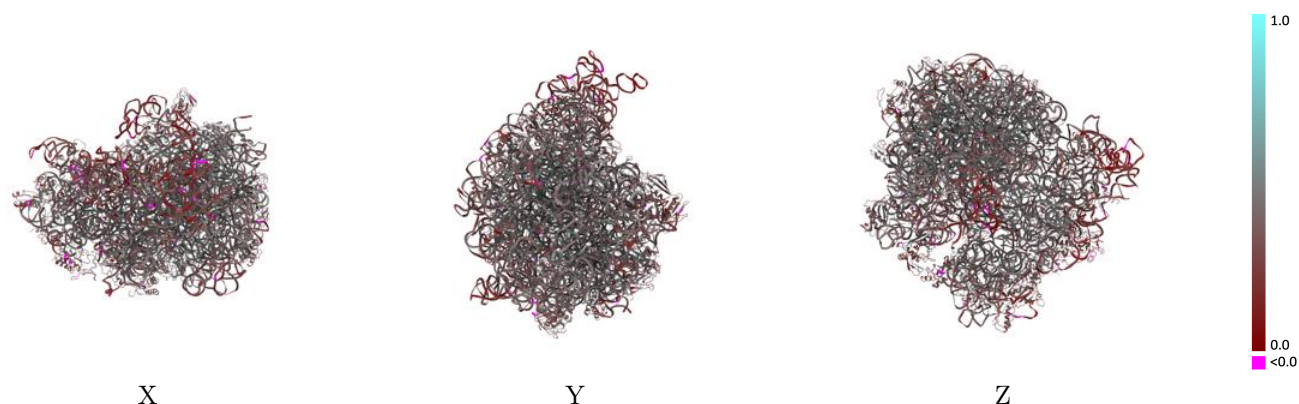
This section contains information regarding the fit between EMDB map EMD-3899 and PDB model 6ENJ. Per-residue inclusion information can be found in [section 3](#) on [page 16](#).

9.1 Map-model overlay [i](#)



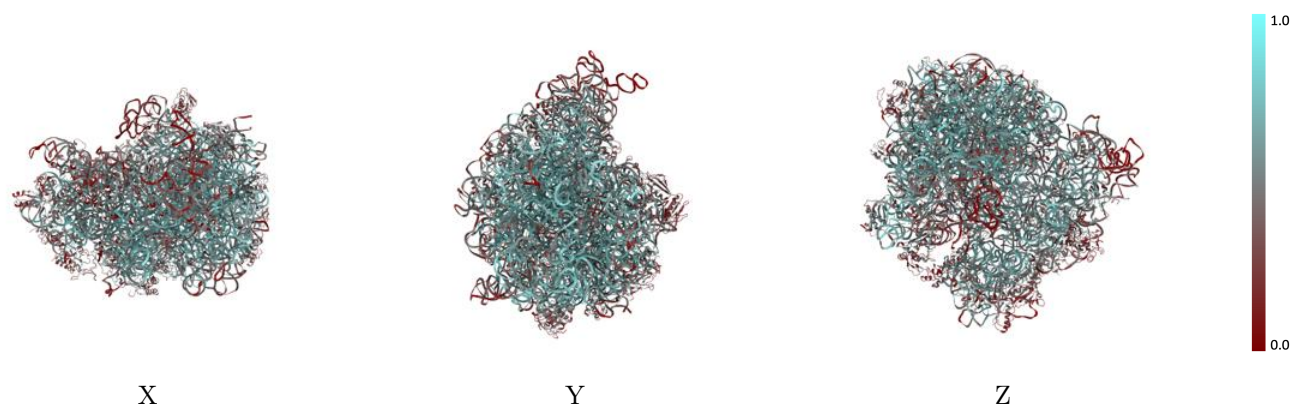
The images above show the 3D surface view of the map at the recommended contour level 0.0963 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



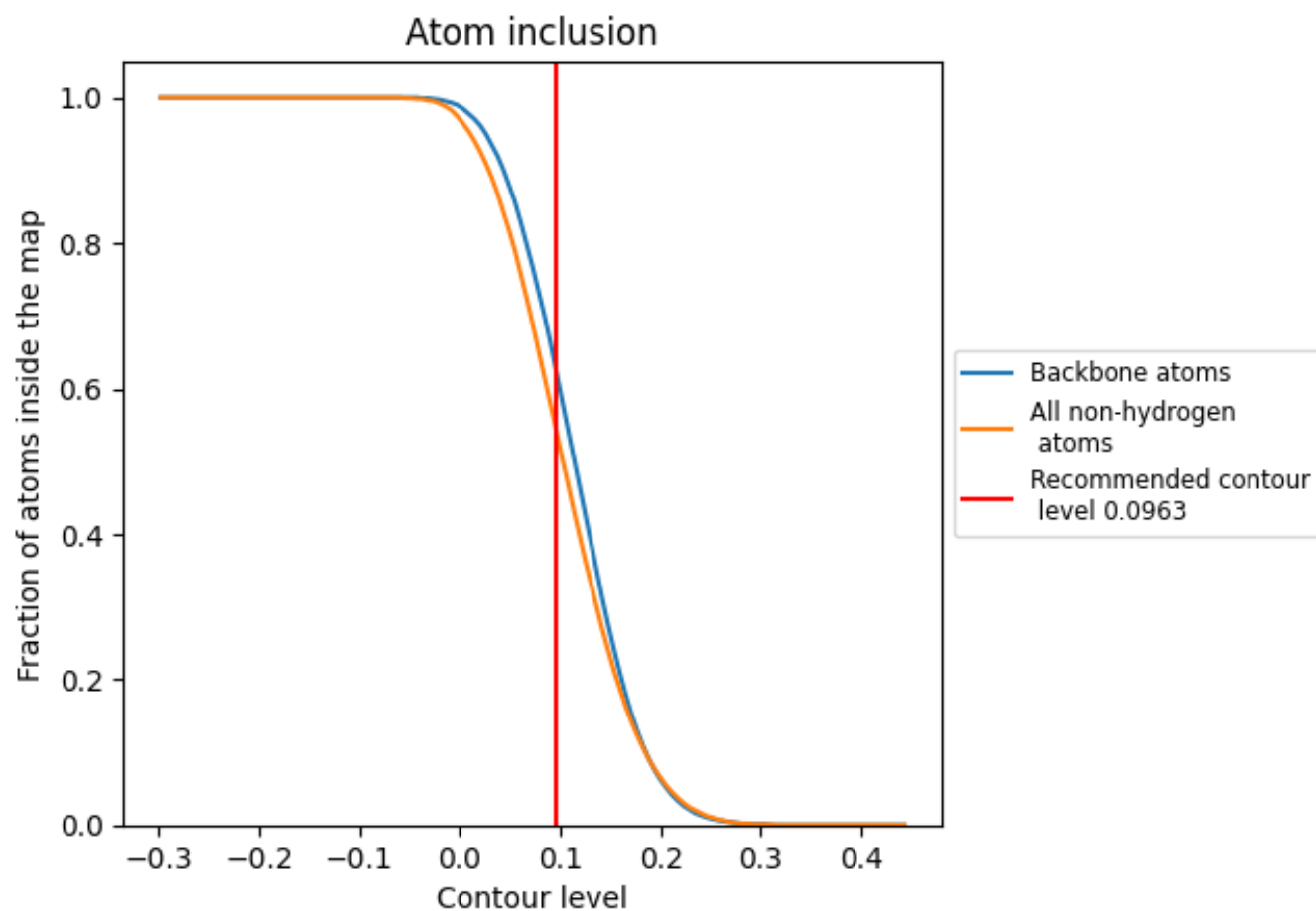
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0963).

9.4 Atom inclusion [i](#)



At the recommended contour level, 62% of all backbone atoms, 54% 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 (0.0963) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.5430	 0.3850
0	 0.4650	 0.4000
1	 0.3290	 0.3700
2	 0.6030	 0.4330
3	 0.5360	 0.4250
4	 0.4620	 0.3920
6	 0.1960	 0.2460
7	 0.0490	 0.1530
9	 0.3070	 0.2590
A	 0.6330	 0.4120
B	 0.6000	 0.3980
C	 0.5510	 0.4370
D	 0.4940	 0.4280
E	 0.3980	 0.3700
F	 0.3770	 0.3340
G	 0.2930	 0.3220
J	 0.5060	 0.4040
K	 0.4670	 0.4040
L	 0.4600	 0.3990
M	 0.4870	 0.4220
N	 0.5380	 0.4050
O	 0.4380	 0.3740
P	 0.4580	 0.4050
Q	 0.5270	 0.4210
R	 0.3860	 0.3780
S	 0.4630	 0.4090
T	 0.4070	 0.3750
U	 0.3560	 0.3410
V	 0.3890	 0.3820
W	 0.4960	 0.4170
X	 0.4590	 0.3960
Y	 0.3560	 0.3190
Z	 0.4740	 0.4020
a	 0.5840	 0.3820
b	 0.3160	 0.3070



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Chain	Atom inclusion	Q-score
c	 0.4280	 0.3800
d	 0.1990	 0.2200
e	 0.4590	 0.3680
f	 0.3780	 0.3300
g	 0.3670	 0.3500
h	 0.4830	 0.3900
i	 0.3870	 0.3500
j	 0.3570	 0.3240
k	 0.4010	 0.3700
l	 0.3970	 0.3500
m	 0.3640	 0.3390
n	 0.4240	 0.3680
o	 0.4330	 0.3740
p	 0.3140	 0.2770
q	 0.3530	 0.3080
r	 0.4620	 0.3750
s	 0.4250	 0.3750
t	 0.3540	 0.3000
u	 0.2480	 0.2700
v	 0.6510	 0.4300
w	 0.3050	 0.3380
x	 0.4760	 0.3570