



Full wwPDB EM Validation Report ⓘ

Mar 24, 2026 – 07:45 PM UTC

PDB ID : 6GXP / pdb_00006gxp
EMDB ID : EMD-0083
Title : Cryo-EM structure of a rotated E. coli 70S ribosome in complex with RF3-GDPCP(RF3-only)
Authors : Graf, M.; Huter, P.; Maracci, C.; Peterek, M.; Rodnina, M.V.; Wilson, D.N.
Deposited on : 2018-06-27
Resolution : 4.40 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
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
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

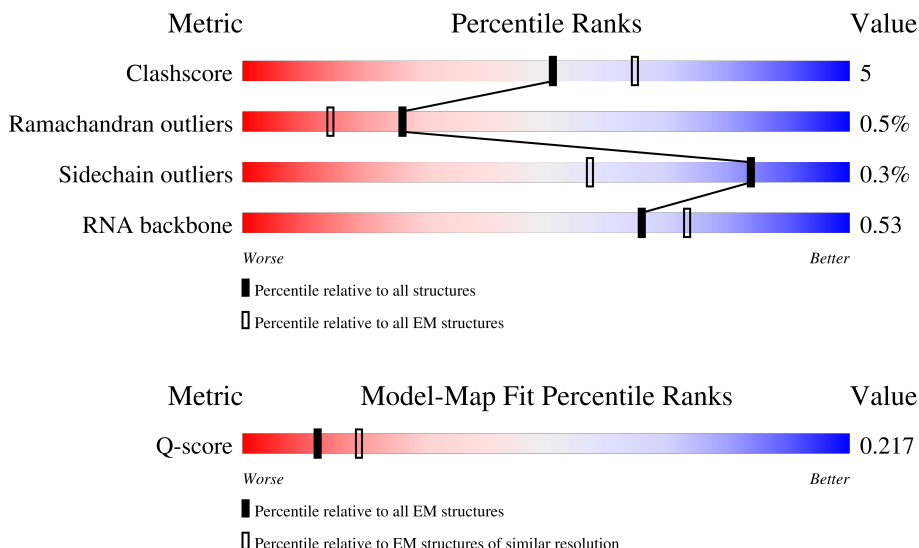
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.40 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	3132 (3.91 - 4.90)

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	10% 65% 31% .
2	B	120	8% 62% 36% .
3	C	271	70% 82% 18%

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Mol	Chain	Length	Quality of chain
4	D	209	56% 86% 14%
5	E	201	57% 86% 14%
6	F	177	72% 81% 19%
7	G	176	56% 90% 9%
8	H	149	86% 83% 17%
9	I	141	99% 87% 13%
10	J	142	50% 88% 12%
11	K	122	73% 79% 21%
12	L	143	63% 86% 13%
13	M	136	71% 85% 15%
14	N	120	48% 86% 14%
15	O	116	48% 91% 9%
16	P	114	65% 86% 14%
17	Q	117	45% 91% 9%
18	R	103	57% 84% 16%
19	S	110	71% 88% 12%
20	T	93	53% 80% 20%
21	U	102	52% 89% 11%
22	V	94	46% 84% 16%
23	W	75	68% 93% 7%
24	X	77	56% 88% 12%
25	Y	63	33% 84% 16%
26	Z	58	62% 84% 16%
27	0	56	68% 88% 12%
28	1	50	80% 92% 8%

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Mol	Chain	Length	Quality of chain
29	2	46	
30	3	64	
31	4	38	
32	5	131	
33	a	1539	
34	b	218	
35	c	206	
36	d	205	
37	e	157	
38	f	100	
39	g	151	
40	h	129	
41	i	127	
42	j	98	
43	k	112	
44	l	123	
45	m	114	
46	n	101	
47	o	88	
48	p	82	
49	q	80	
50	r	65	
51	s	79	
52	t	85	
53	u	65	

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Mol	Chain	Length	Quality of chain
54	w	529	91% 74% 18% • 6%
55	z	14	100% 57% 43%

2 Entry composition

There are 56 unique types of molecules in this entry. The entry contains 147637 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	2896	Total	C	N	O	P	0	0
			62177	27736	11444	20101	2896		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	747	C	U	conflict	GB 1063812051
A	1847	G	A	conflict	GB 1063812051

- 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 1373146531

- 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 L9.

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

- Molecule 9 is a protein called 50S ribosomal protein L11.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	141	Total	C	N	O	S	0	0
			1032	651	179	196	6		

- Molecule 10 is a protein called 50S ribosomal protein L13.

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

- Molecule 11 is a protein called 50S ribosomal protein L14.

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

- Molecule 12 is a protein called 50S ribosomal protein L15.

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

- Molecule 13 is a protein called 50S ribosomal protein L16.

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

- Molecule 14 is a protein called 50S ribosomal protein L17.

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

- Molecule 15 is a protein called 50S ribosomal protein L18.

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

- Molecule 16 is a protein called 50S ribosomal protein L19.

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

- Molecule 17 is a protein called 50S ribosomal protein L20.

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

- Molecule 18 is a protein called 50S ribosomal protein L21.

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

- Molecule 19 is a protein called 50S ribosomal protein L22.

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

- Molecule 20 is a protein called 50S ribosomal protein L23.

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

- Molecule 21 is a protein called 50S ribosomal protein L24.

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

- Molecule 22 is a protein called 50S ribosomal protein L25.

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

- Molecule 23 is a protein called 50S ribosomal protein L27.

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

- Molecule 24 is a protein called 50S ribosomal protein L28.

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

- Molecule 25 is a protein called 50S ribosomal protein L29.

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

- Molecule 26 is a protein called 50S ribosomal protein L30.

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

- Molecule 27 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	0	56	Total	C	N	O	S	0	0
			444	269	94	80	1		

- Molecule 28 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	1	50	Total	C	N	O	S	0	0
			409	263	75	71			

- Molecule 29 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	2	46	Total	C	N	O	S	0	0
			377	228	90	57	2		

- Molecule 30 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	3	64	Total	C	N	O	S	0	0
			504	323	105	74	2		

- Molecule 31 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	4	38	Total	C	N	O	S	0	0
			302	185	65	48	4		

- Molecule 32 is a protein called 50S ribosomal protein L10.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	5	131	Total	C	N	O	S	0	0
			988	625	175	183	5		

- Molecule 33 is a RNA chain called 16S ribosomal RNA.

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
43	k	112	Total	C	N	O	S	0	0
			829	511	161	154	3		

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
46	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 47 is a protein called 30S ribosomal protein S15.

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

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

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

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

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

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

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

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

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

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

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

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

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

- Molecule 54 is a protein called Peptide chain release factor RF3.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	w	499	Total	C	N	O	S	0	0
			3943	2498	680	745	20		

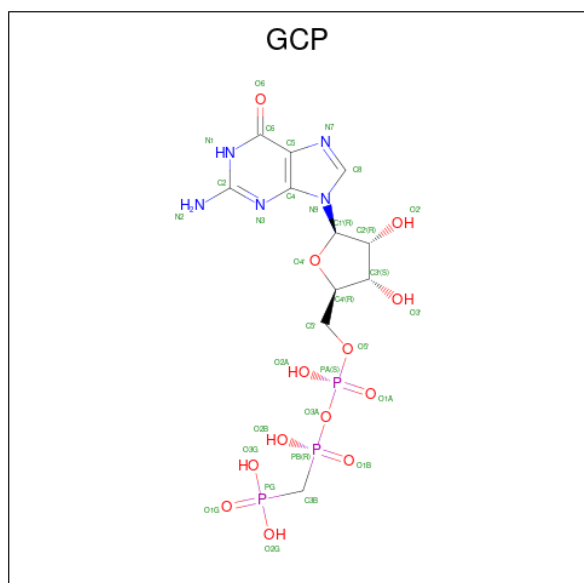
- Molecule 55 is a protein called Apidaecin.

Mol	Chain	Residues	Atoms				AltConf	Trace
55	z	14	Total	C	N	O	0	0
			120	80	25	15		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
z	10	ARG	GLN	conflict	UNP Q8WSY8

- Molecule 56 is PHOSPHOMETHYLPHOSPHONIC ACID GUANYLATE ESTER (CCD ID: GCP) (formula: $C_{11}H_{18}N_5O_{13}P_3$).

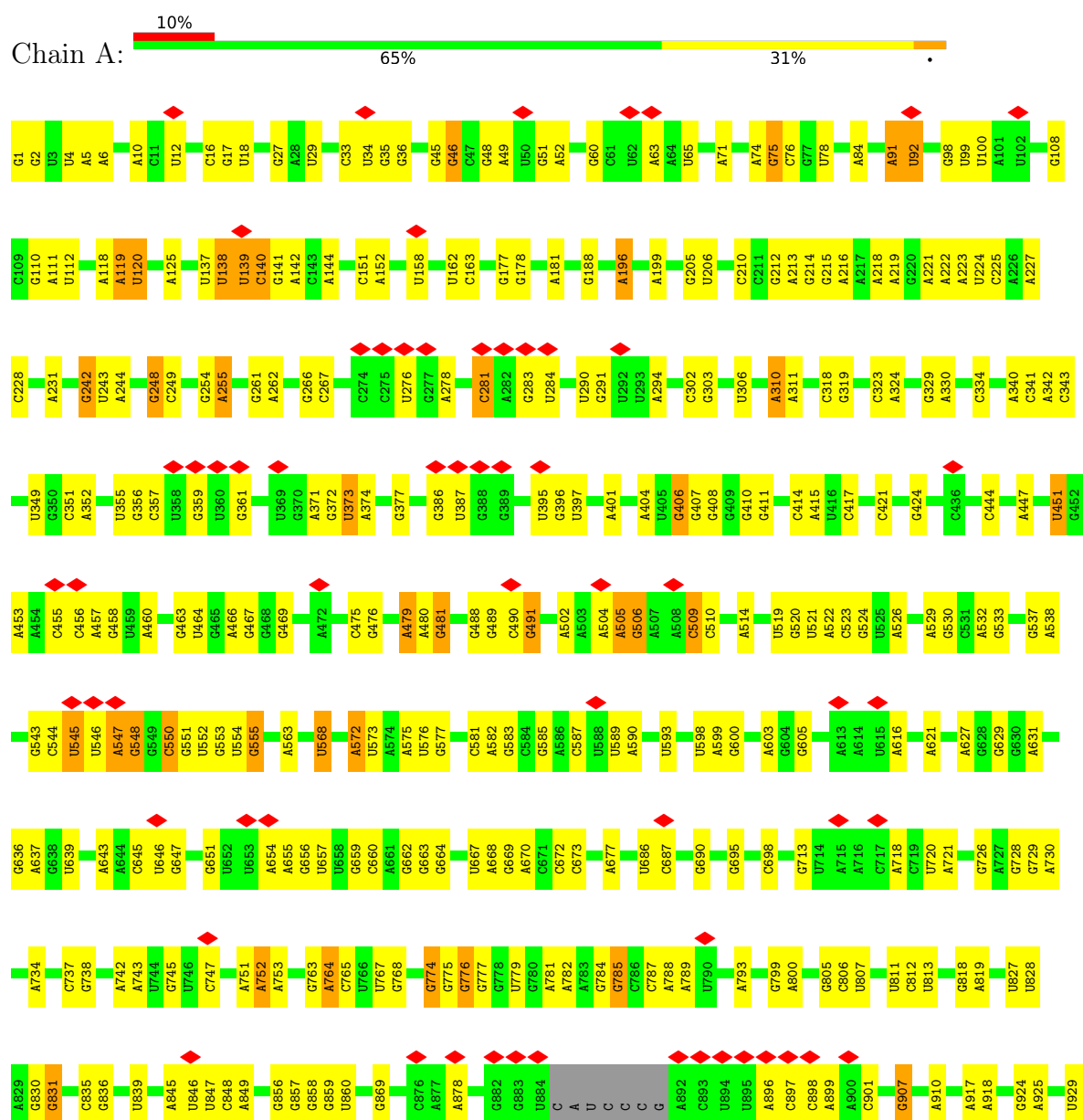


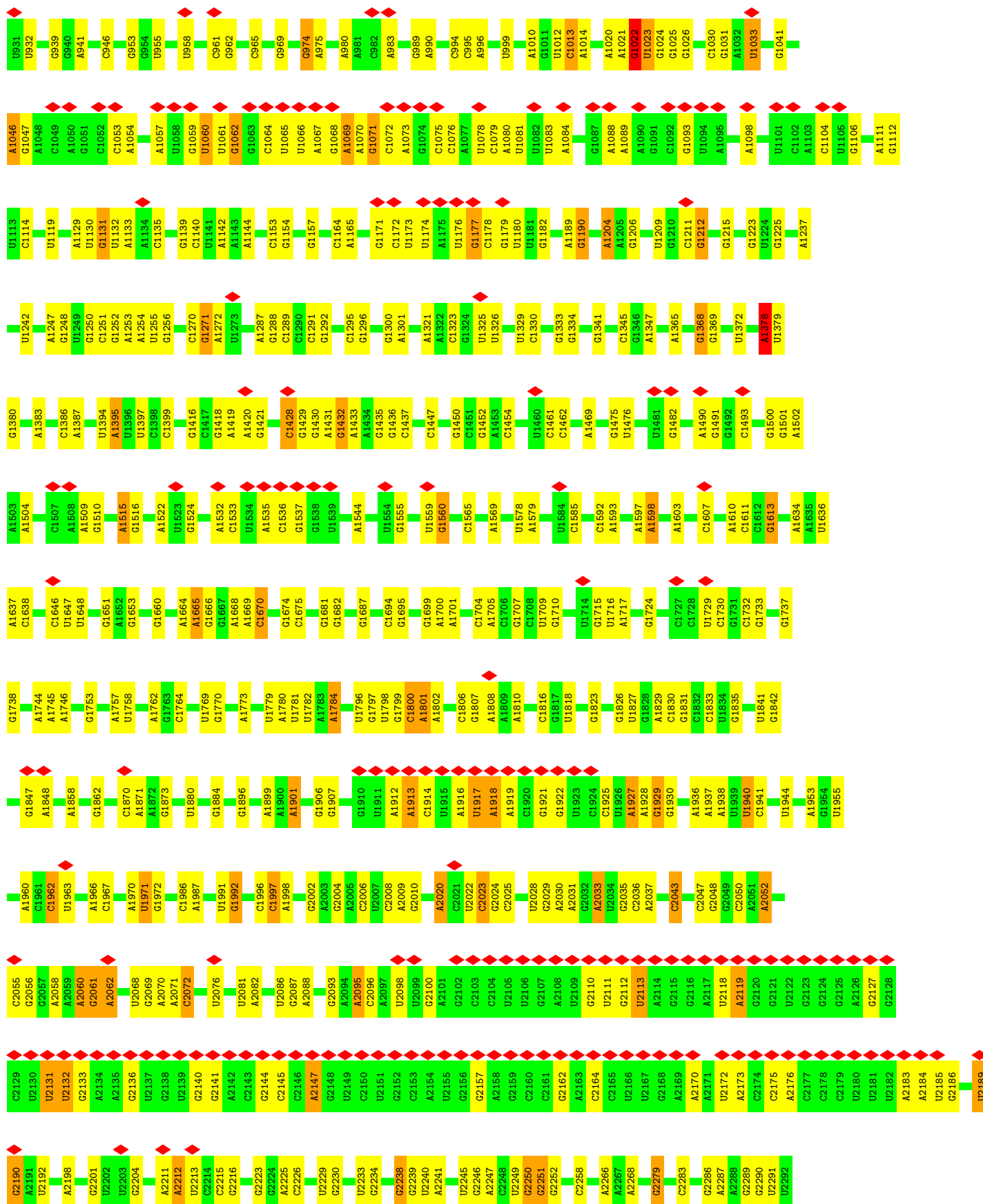
Mol	Chain	Residues	Atoms					AltConf
56	w	1	Total	C	N	O	P	0
			32	11	5	13	3	

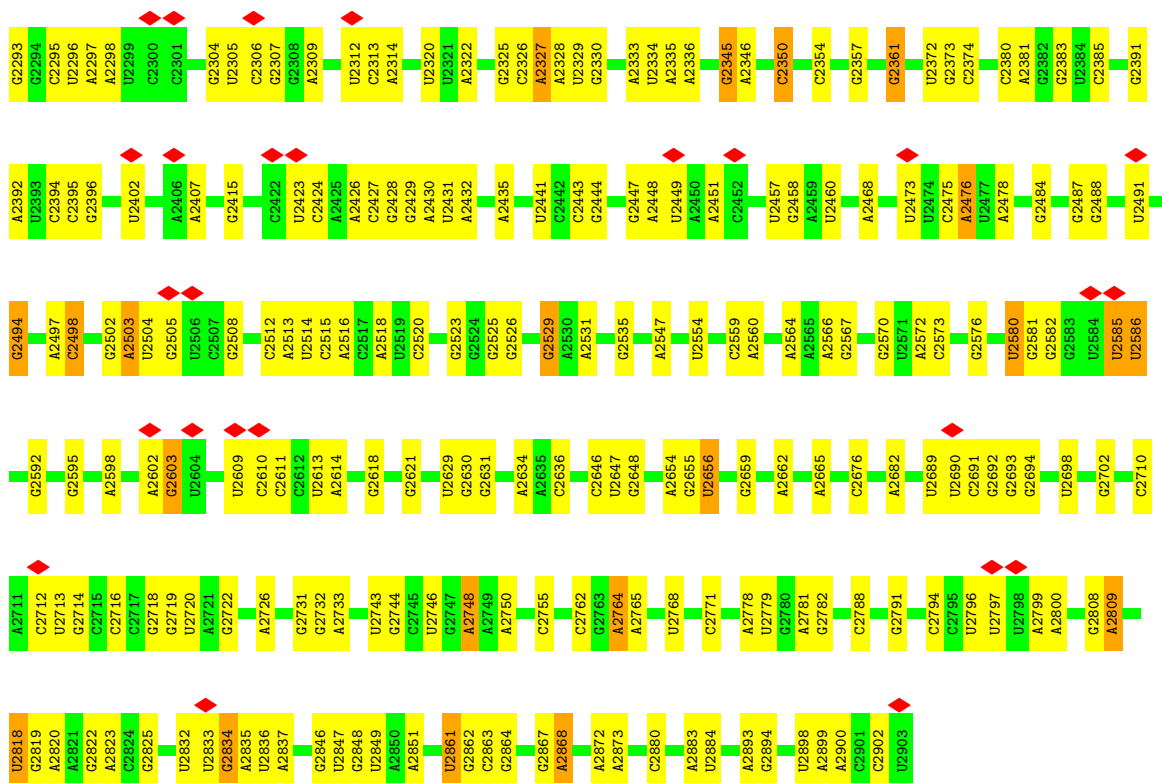
3 Residue-property plots

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.

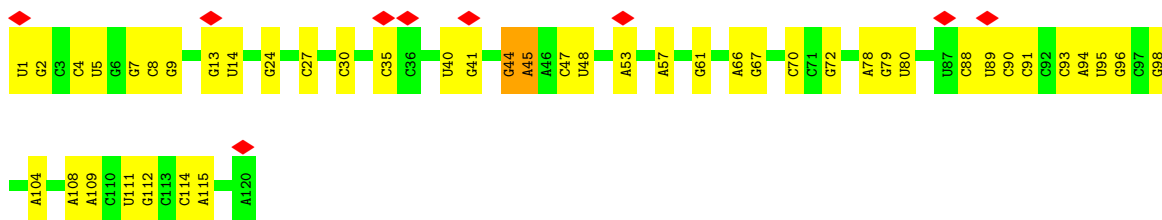
• Molecule 1: 23S ribosomal RNA



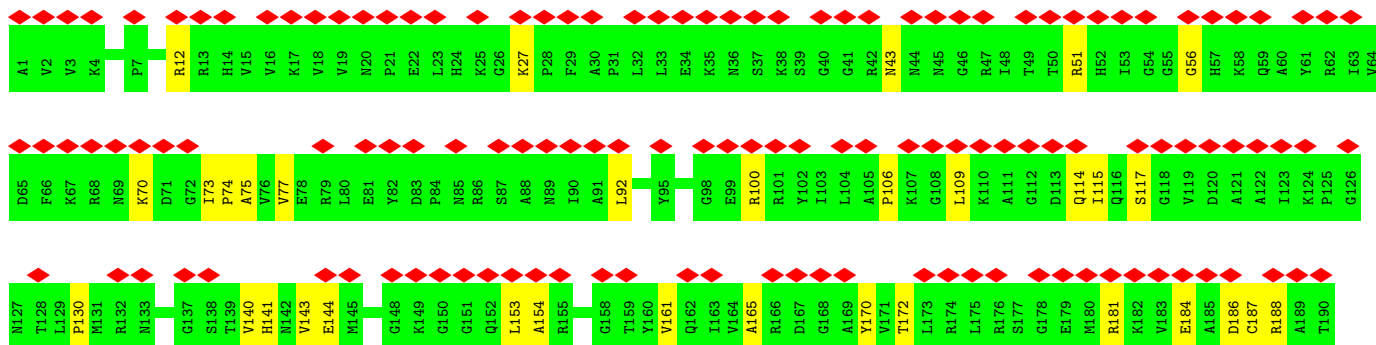
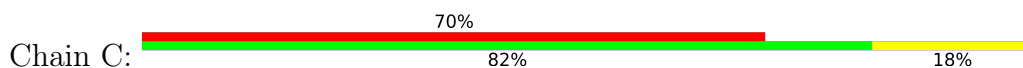




• Molecule 2: 5S ribosomal RNA

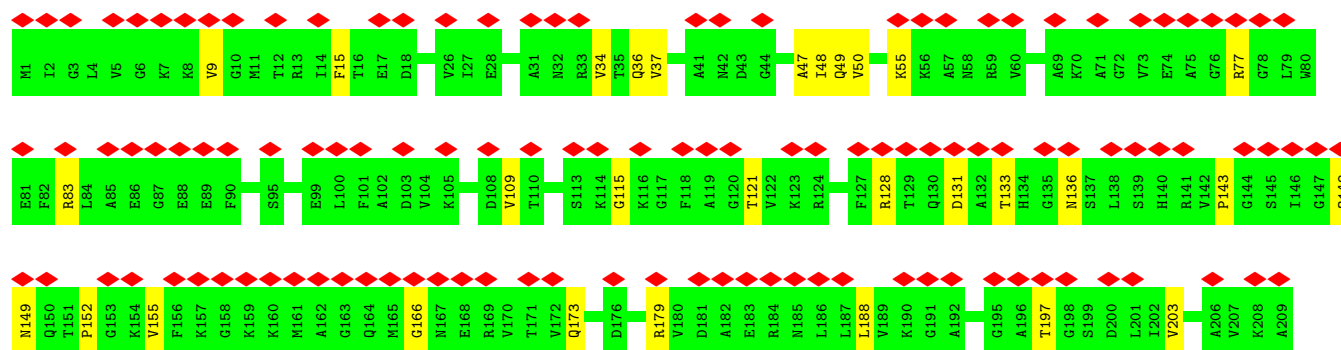
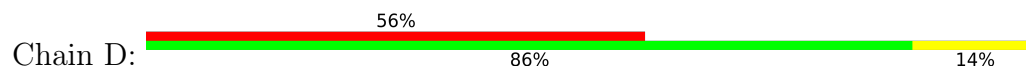


• Molecule 3: 50S ribosomal protein L2

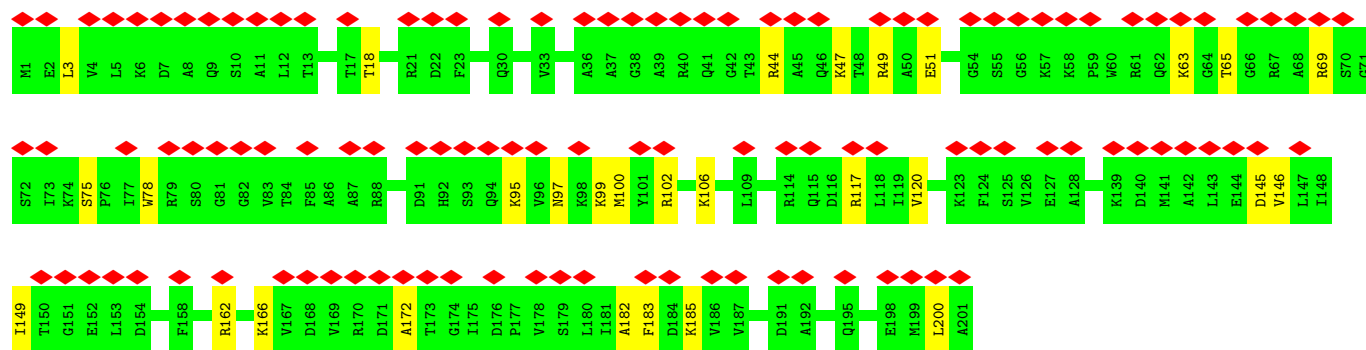
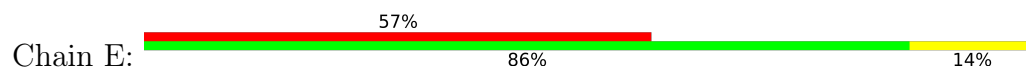




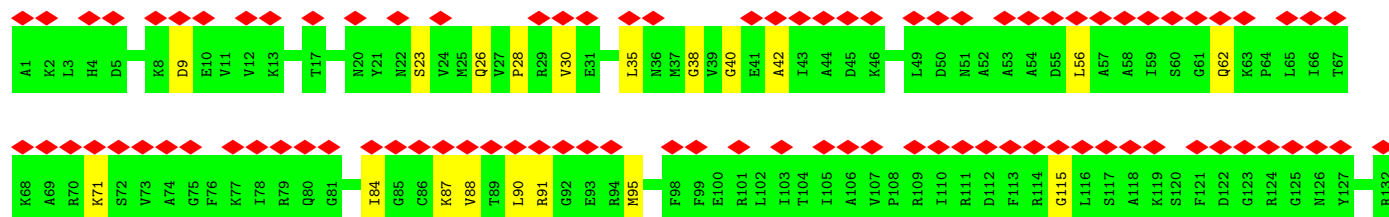
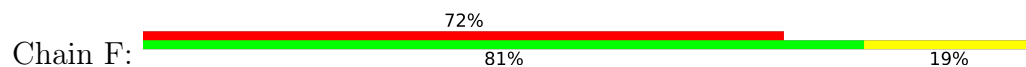
• Molecule 4: 50S ribosomal protein L3



• Molecule 5: 50S ribosomal protein L4

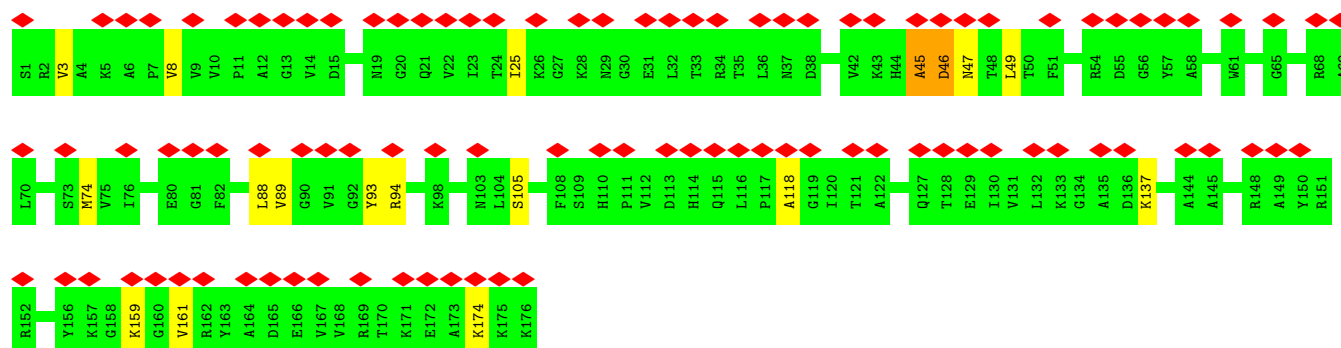
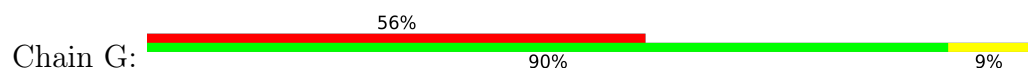


• Molecule 6: 50S ribosomal protein L5

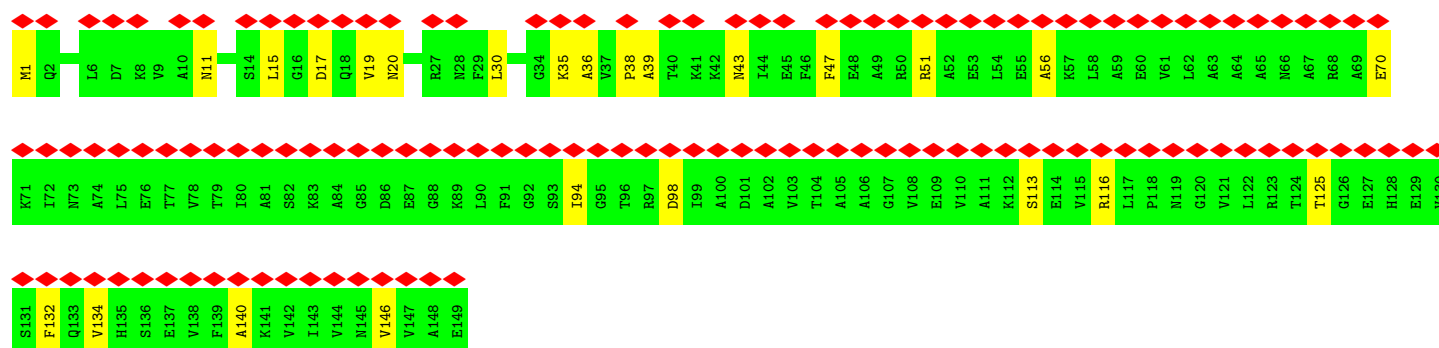
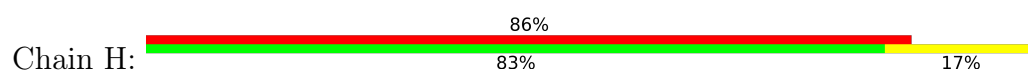




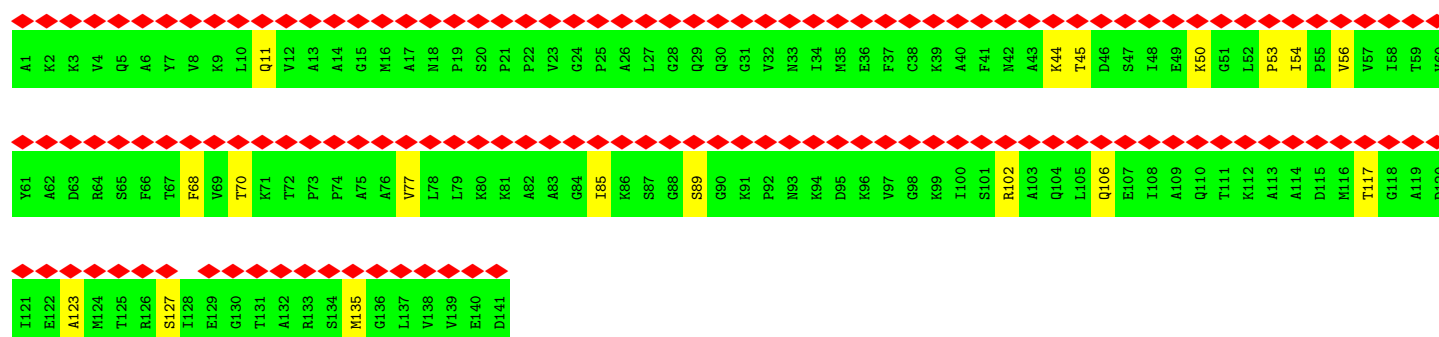
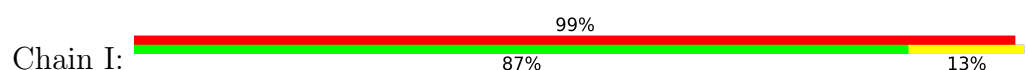
• Molecule 7: 50S ribosomal protein L6



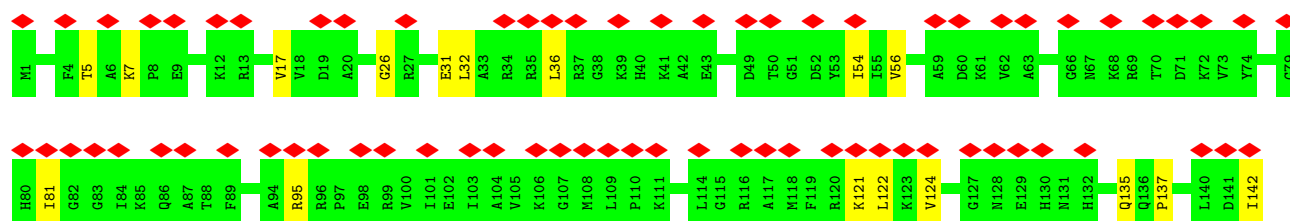
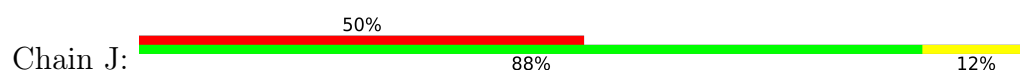
• Molecule 8: 50S ribosomal protein L9



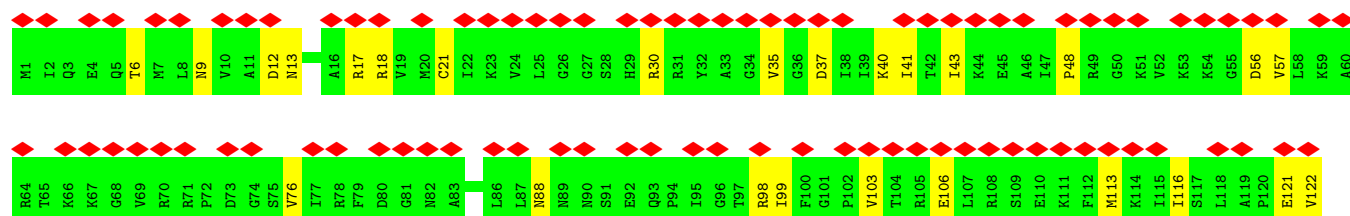
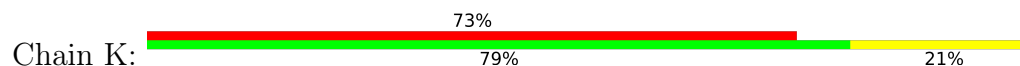
• Molecule 9: 50S ribosomal protein L11



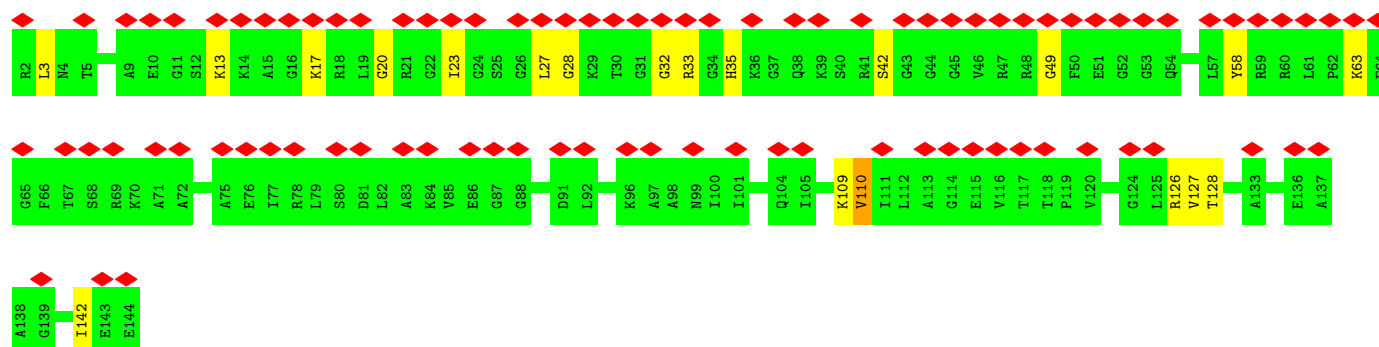
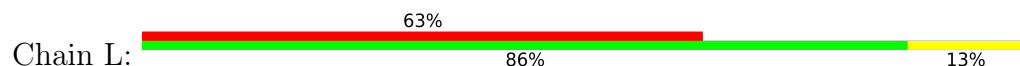
• Molecule 10: 50S ribosomal protein L13



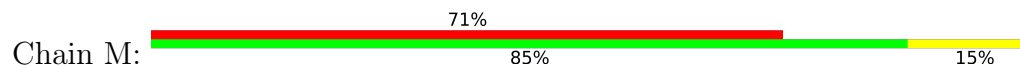
- Molecule 11: 50S ribosomal protein L14



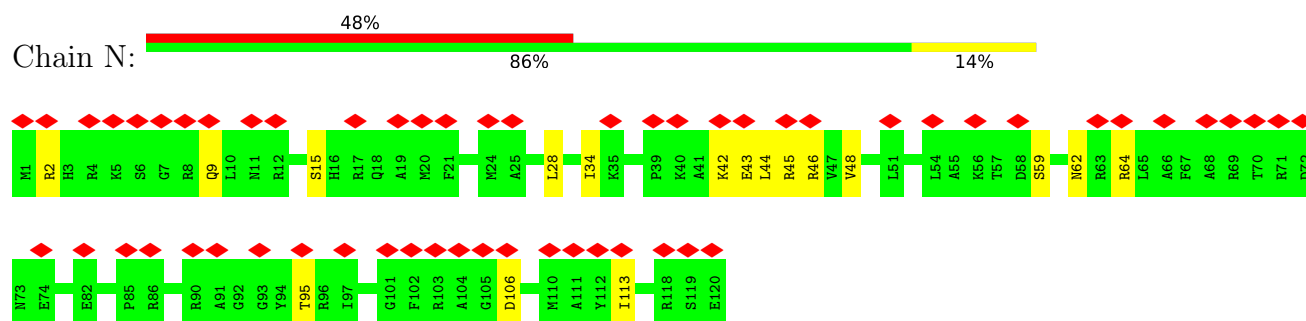
- Molecule 12: 50S ribosomal protein L15



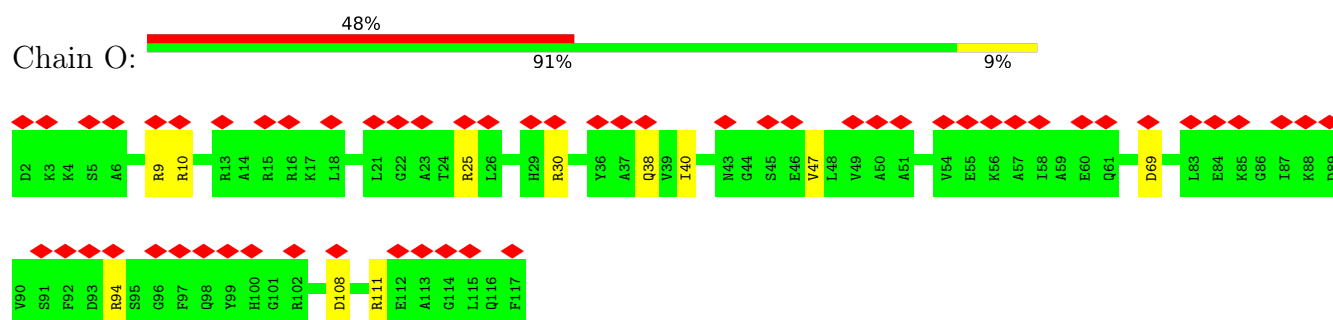
- Molecule 13: 50S ribosomal protein L16



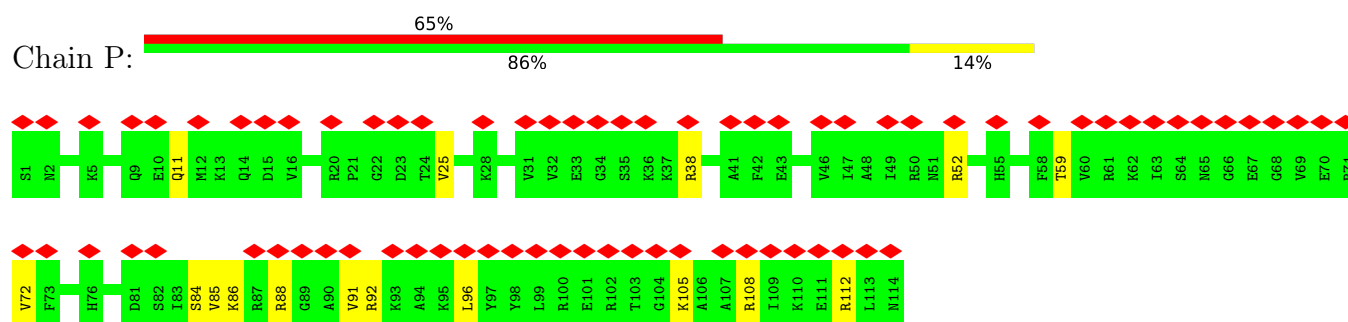
- Molecule 14: 50S ribosomal protein L17



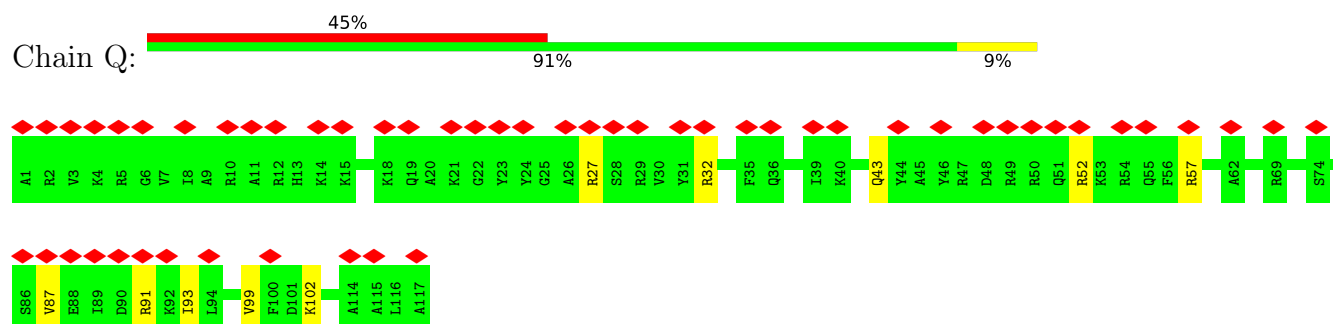
- Molecule 15: 50S ribosomal protein L18



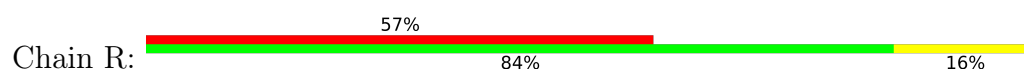
- Molecule 16: 50S ribosomal protein L19

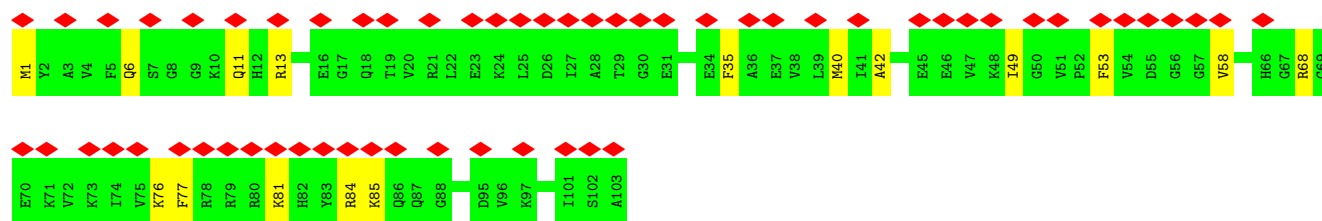


- Molecule 17: 50S ribosomal protein L20

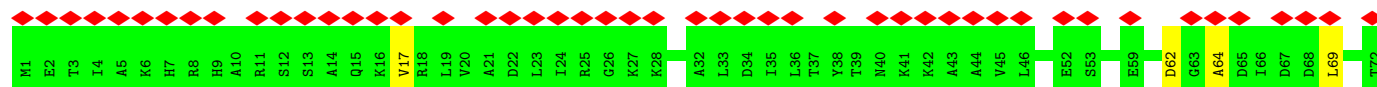
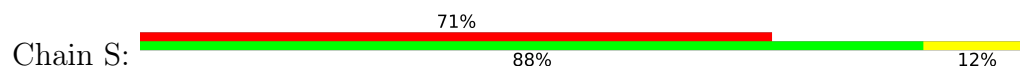


- Molecule 18: 50S ribosomal protein L21

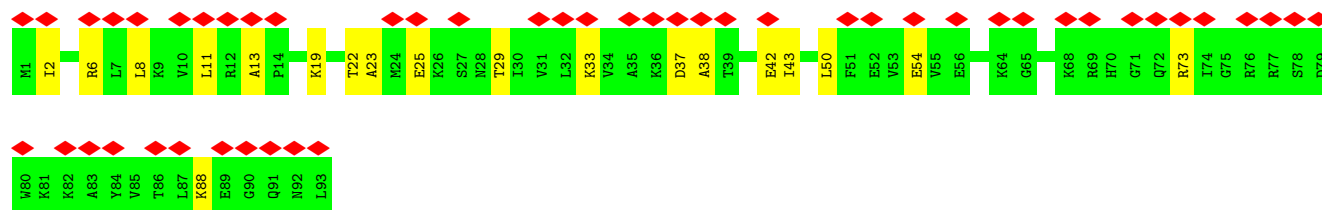
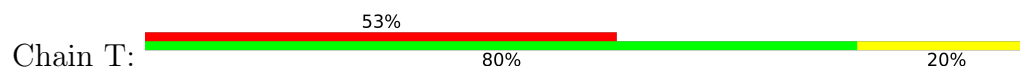




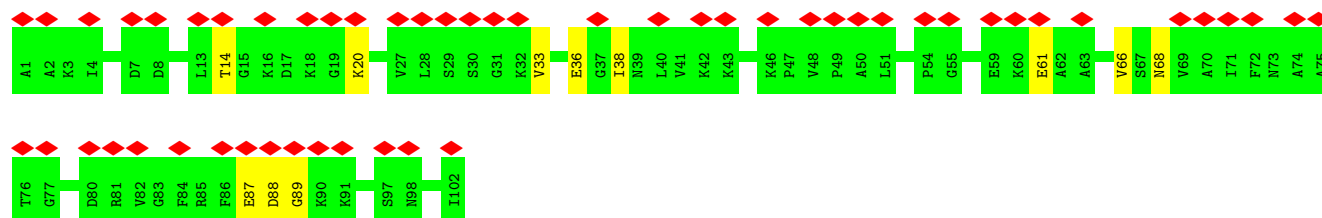
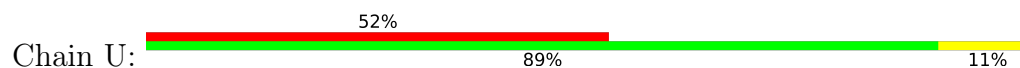
• Molecule 19: 50S ribosomal protein L22



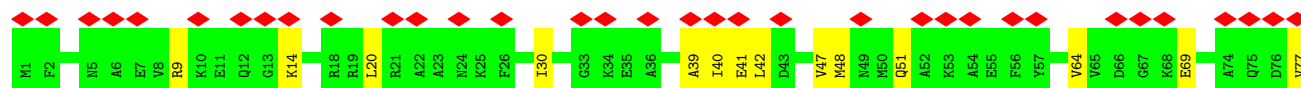
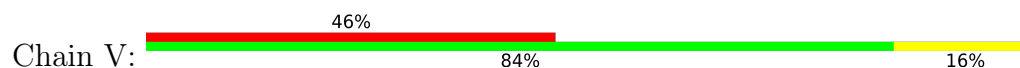
• Molecule 20: 50S ribosomal protein L23

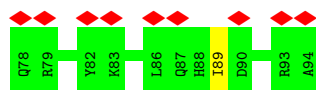


• Molecule 21: 50S ribosomal protein L24

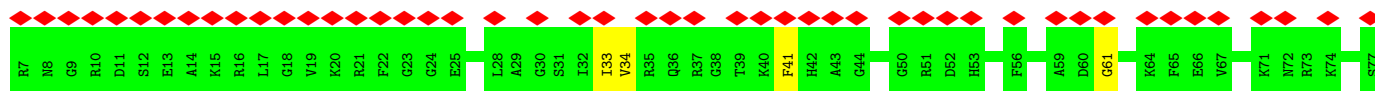


• Molecule 22: 50S ribosomal protein L25

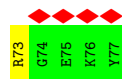
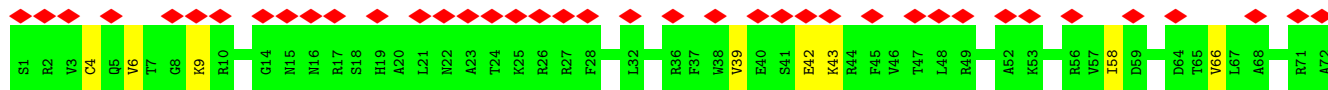
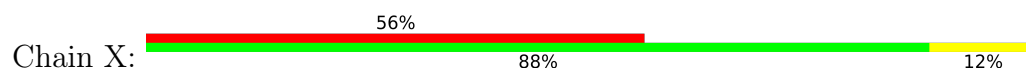




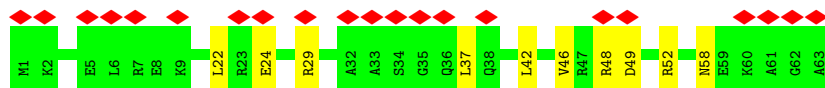
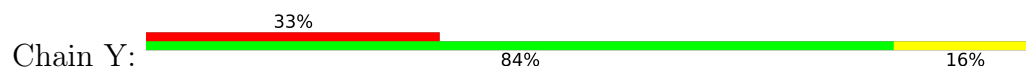
- Molecule 23: 50S ribosomal protein L27



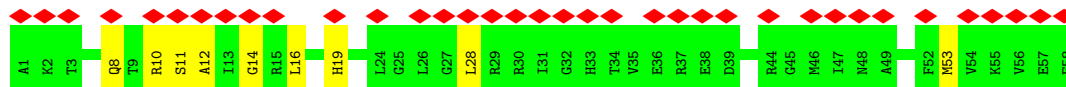
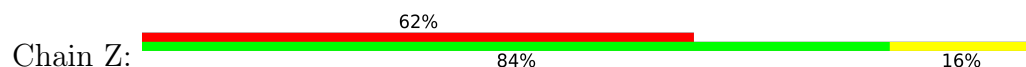
- Molecule 24: 50S ribosomal protein L28



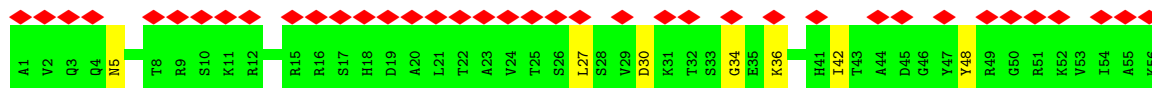
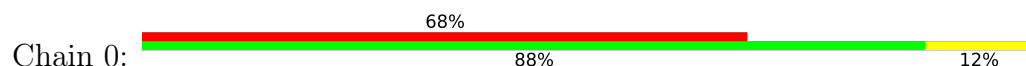
- Molecule 25: 50S ribosomal protein L29



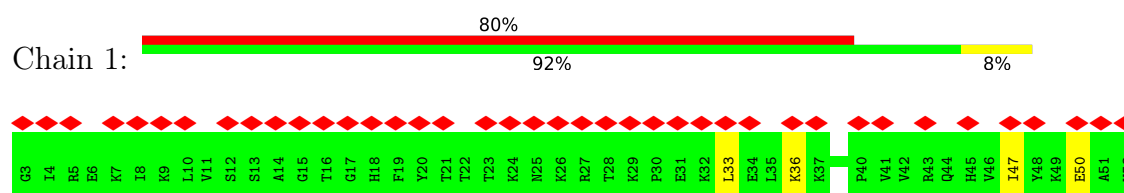
- Molecule 26: 50S ribosomal protein L30



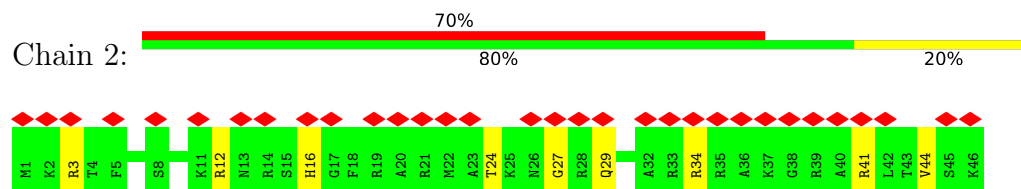
- Molecule 27: 50S ribosomal protein L32



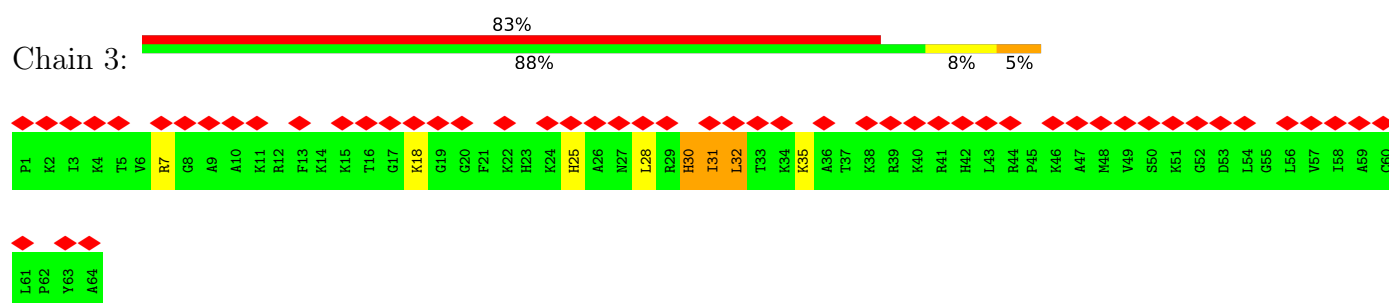
- Molecule 28: 50S ribosomal protein L33



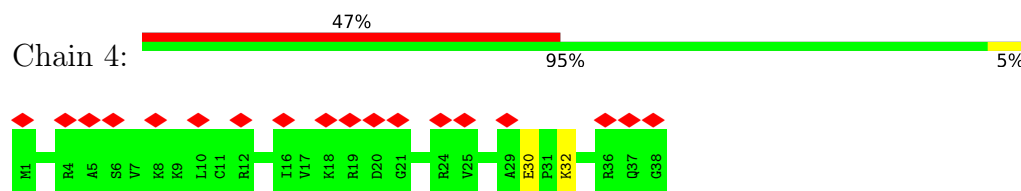
- Molecule 29: 50S ribosomal protein L34



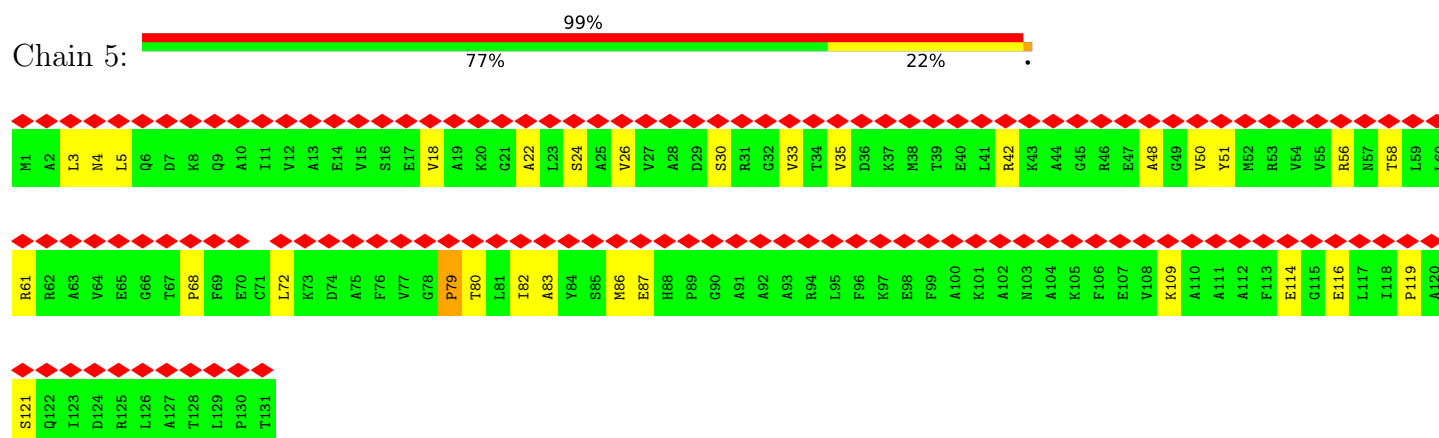
- Molecule 30: 50S ribosomal protein L35



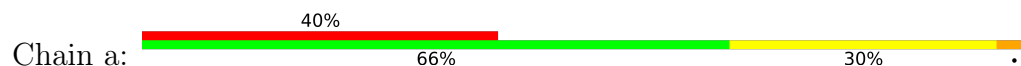
- Molecule 31: 50S ribosomal protein L36

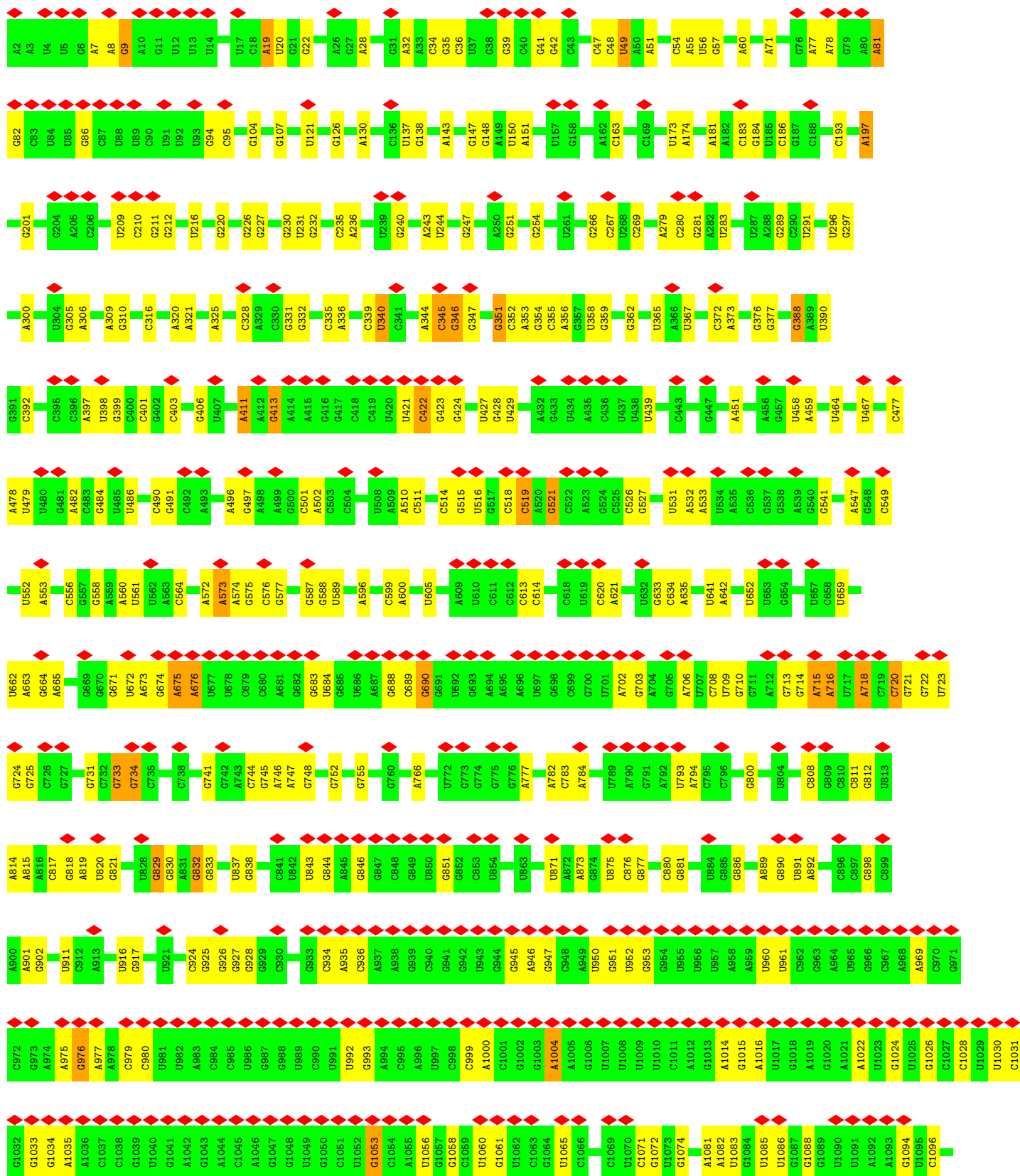


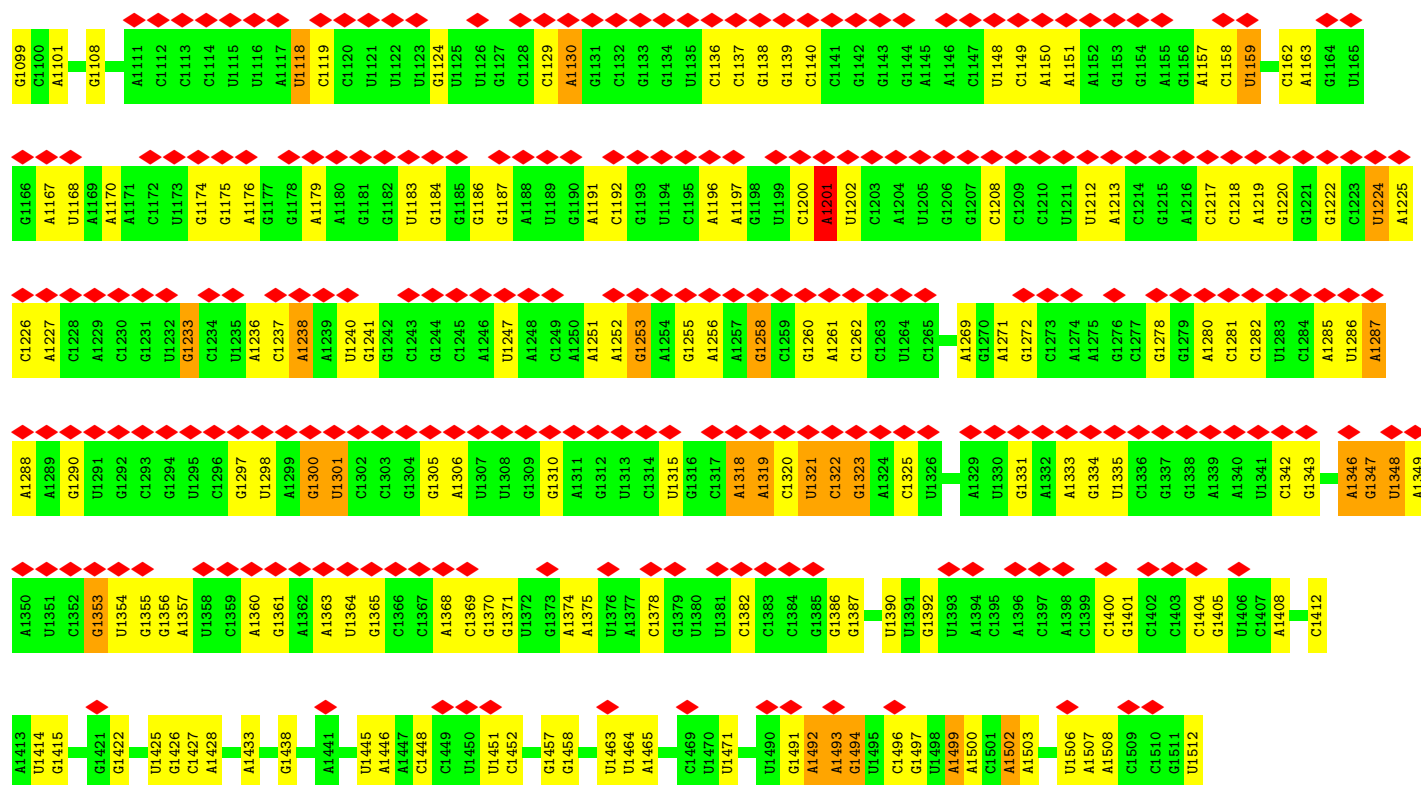
- Molecule 32: 50S ribosomal protein L10



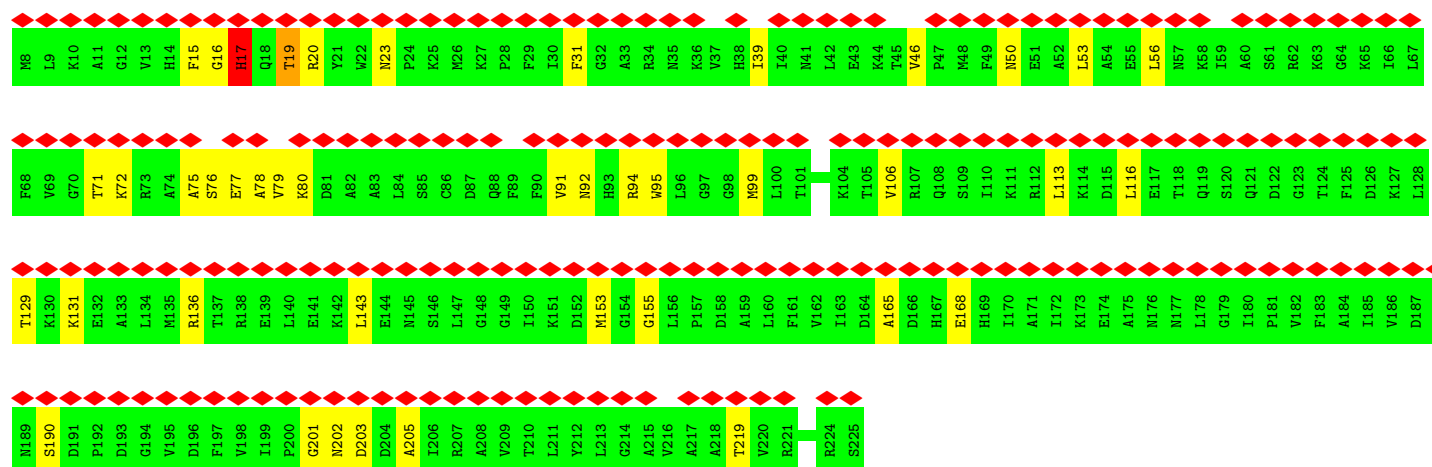
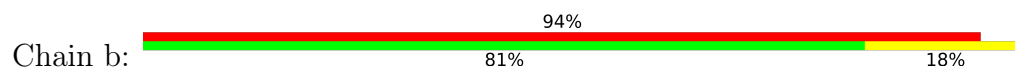
- Molecule 33: 16S ribosomal RNA



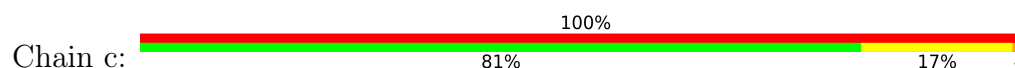


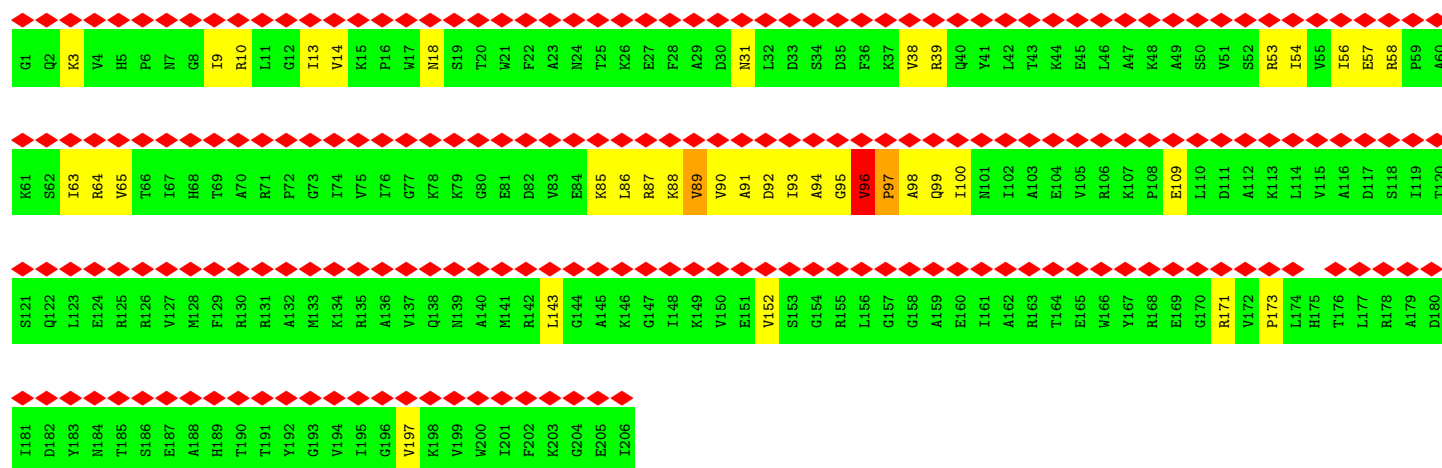


• Molecule 34: 30S ribosomal protein S2

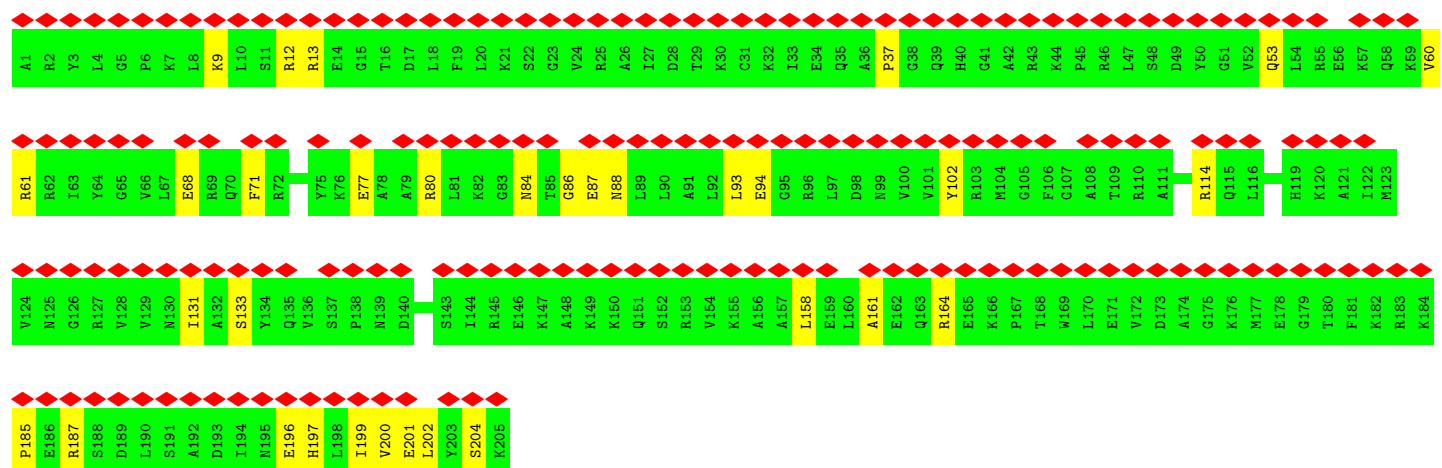
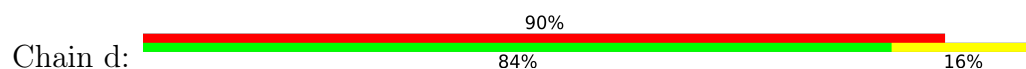


• Molecule 35: 30S ribosomal protein S3

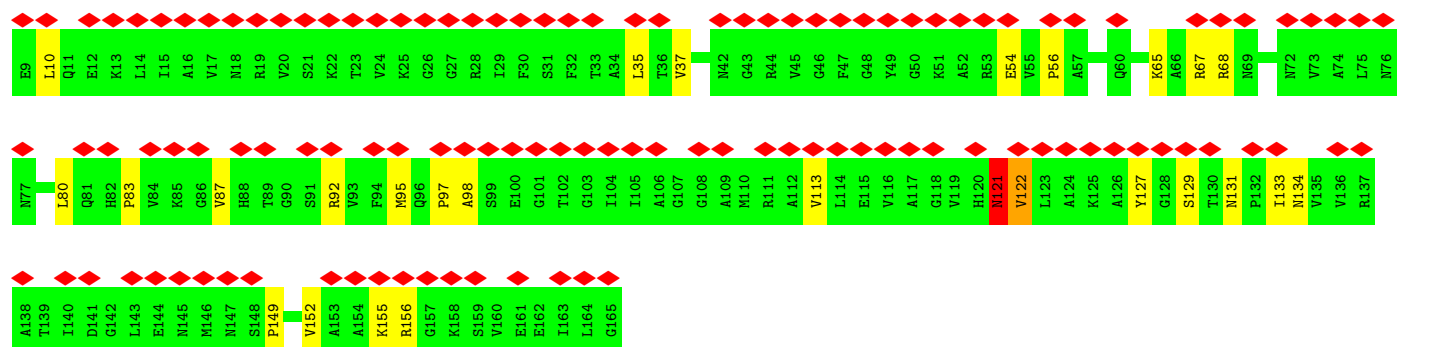
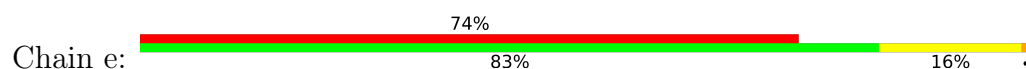




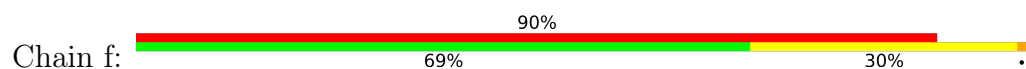
• Molecule 36: 30S ribosomal protein S4

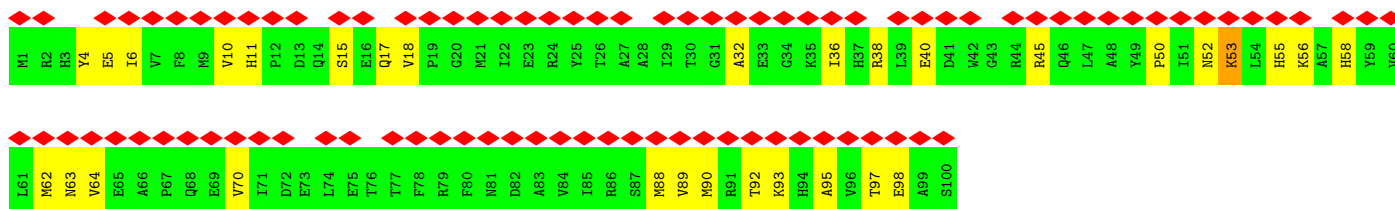


• Molecule 37: 30S ribosomal protein S5

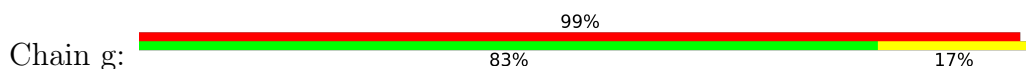


• Molecule 38: 30S ribosomal protein S6

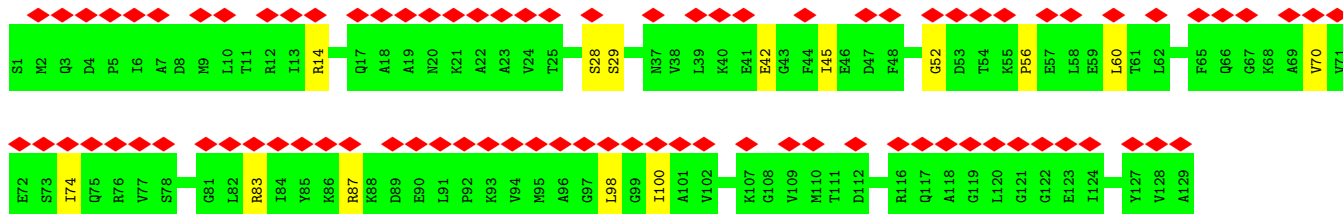
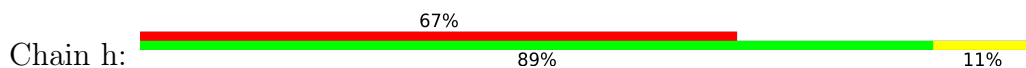




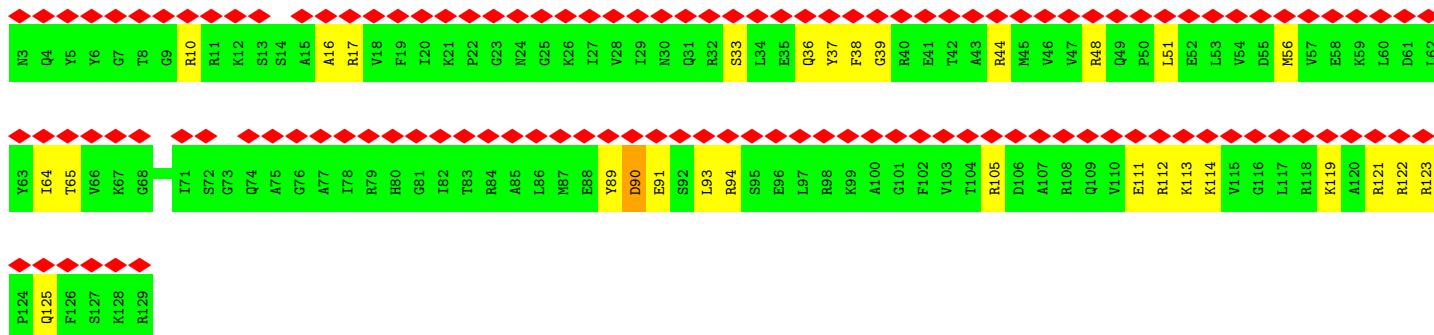
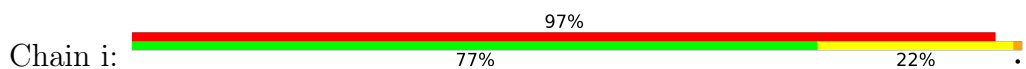
• Molecule 39: 30S ribosomal protein S7



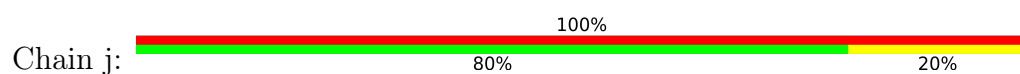
• Molecule 40: 30S ribosomal protein S8



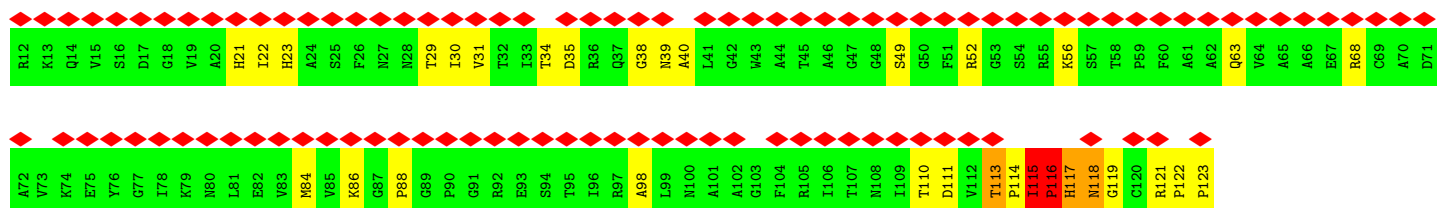
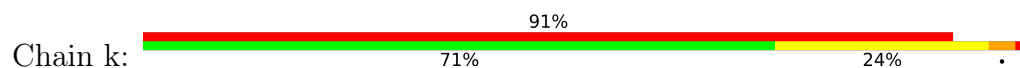
• Molecule 41: 30S ribosomal protein S9



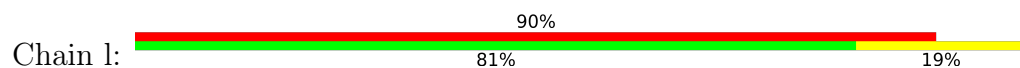
• Molecule 42: 30S ribosomal protein S10



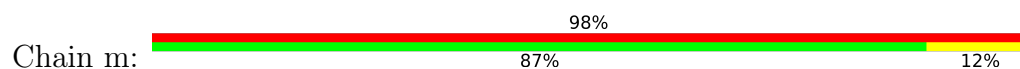
• Molecule 43: 30S ribosomal protein S11



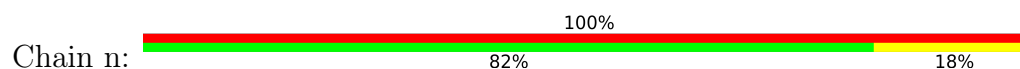
• Molecule 44: 30S ribosomal protein S12



• Molecule 45: 30S ribosomal protein S13

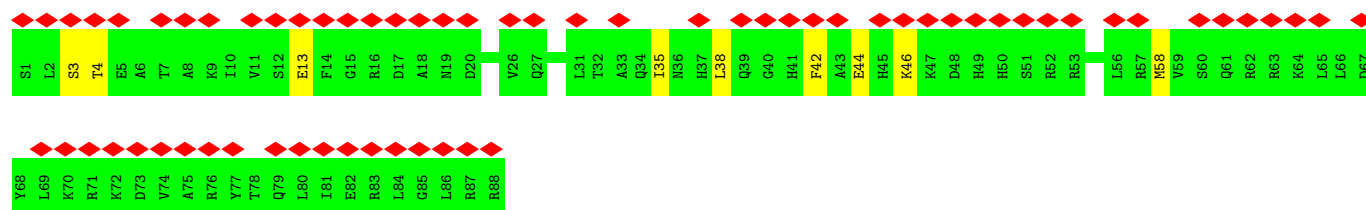
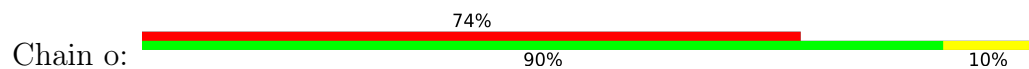


• Molecule 46: 30S ribosomal protein S14

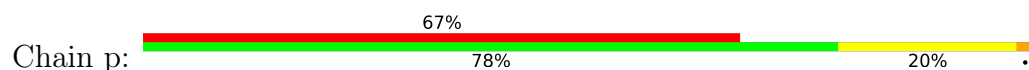




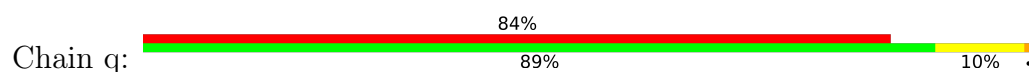
• Molecule 47: 30S ribosomal protein S15



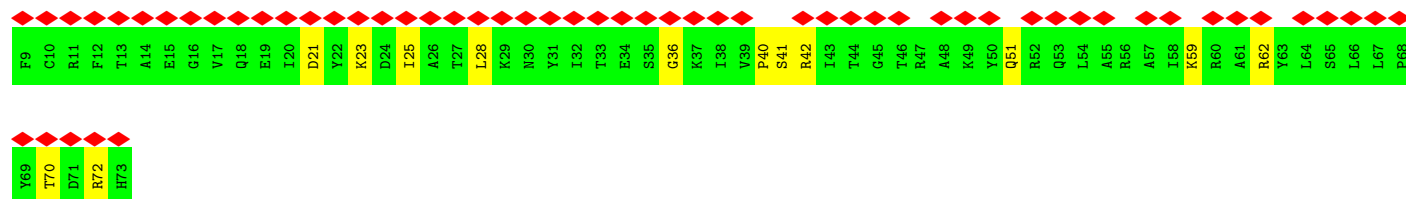
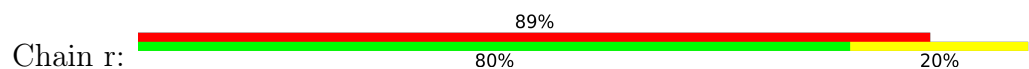
• Molecule 48: 30S ribosomal protein S16



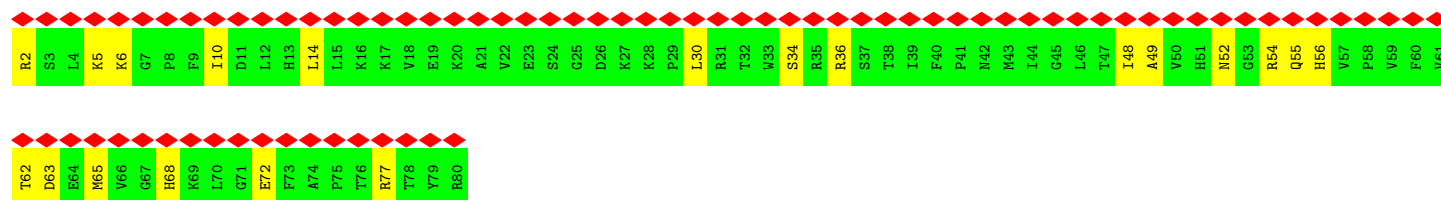
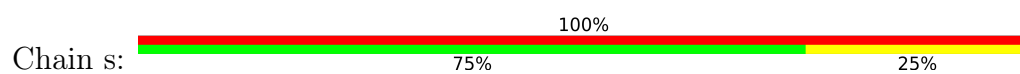
• Molecule 49: 30S ribosomal protein S17



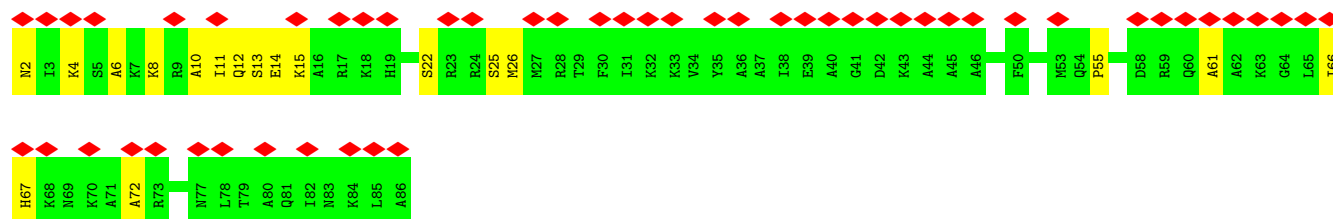
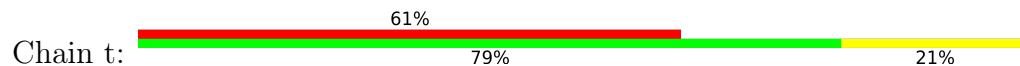
• Molecule 50: 30S ribosomal protein S18



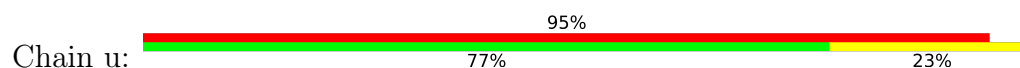
• Molecule 51: 30S ribosomal protein S19



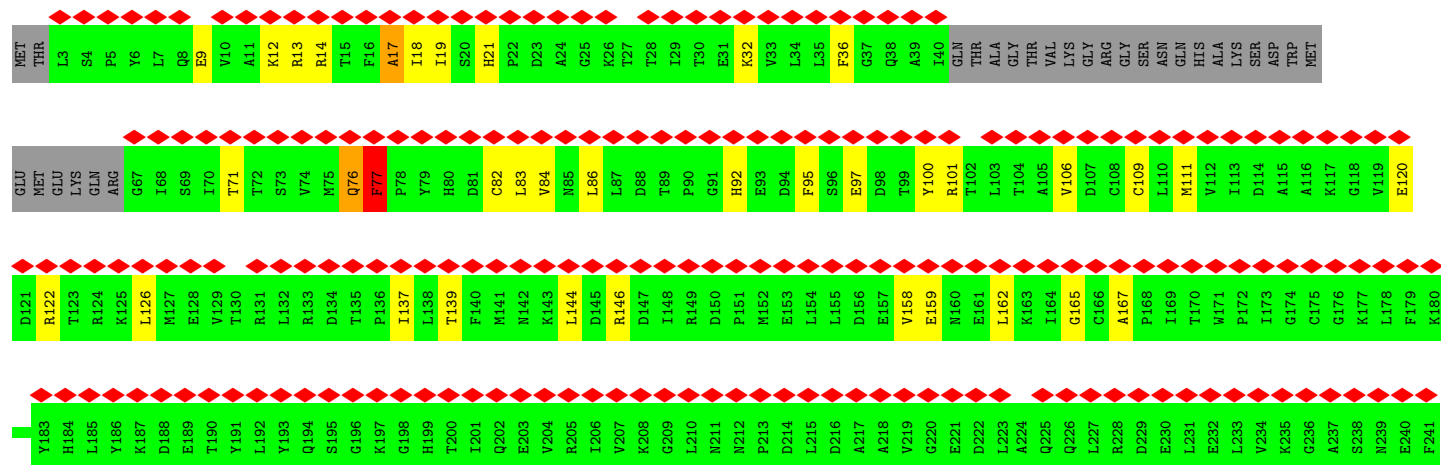
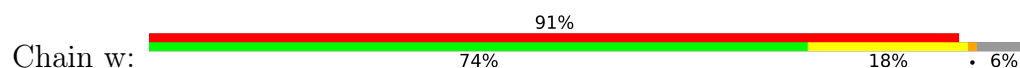
• Molecule 52: 30S ribosomal protein S20



• Molecule 53: 30S ribosomal protein S21



• Molecule 54: Peptide chain release factor RF3



- Molecule 55: Apidaecin



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	30535	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 ($e^-/\text{\AA}^2$)	45.9	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	0.106	Depositor
Minimum map value	-0.050	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.008	Depositor
Recommended contour level	0.035	Depositor
Map size (Å)	381.96, 381.96, 381.96	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.061, 1.061, 1.061	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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	0.15	0/69638	0.33	3/108636 (0.0%)
2	B	0.18	0/2876	0.38	0/4483
3	C	0.20	0/2121	0.52	0/2852
4	D	0.20	0/1586	0.52	0/2134
5	E	0.19	0/1571	0.50	0/2113
6	F	0.23	0/1434	0.63	1/1926 (0.1%)
7	G	0.21	0/1343	0.57	2/1816 (0.1%)
8	H	0.19	0/1122	0.50	0/1515
9	I	0.24	0/1046	0.60	0/1410
10	J	0.18	0/1152	0.45	0/1551
11	K	0.22	0/947	0.62	0/1268
12	L	0.23	0/1054	0.68	4/1403 (0.3%)
13	M	0.25	0/1093	0.70	3/1460 (0.2%)
14	N	0.24	0/973	0.66	0/1301
15	O	0.20	0/902	0.49	0/1209
16	P	0.21	0/929	0.53	0/1242
17	Q	0.20	0/960	0.52	0/1278
18	R	0.20	0/829	0.54	0/1107
19	S	0.21	0/864	0.57	0/1156
20	T	0.20	0/744	0.58	0/994
21	U	0.27	0/787	0.73	2/1051 (0.2%)
22	V	0.19	0/766	0.50	0/1025
23	W	0.17	0/582	0.47	0/769
24	X	0.17	0/635	0.47	0/848
25	Y	0.16	0/510	0.49	0/677
26	Z	0.18	0/453	0.45	0/605
27	0	0.18	0/450	0.51	0/599
28	1	0.20	0/416	0.55	0/554
29	2	0.17	0/380	0.46	0/498
30	3	0.23	0/513	0.69	2/676 (0.3%)
31	4	0.28	0/303	0.67	0/397
32	5	0.28	0/1001	0.82	4/1350 (0.3%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	a	0.16	1/36965 (0.0%)	0.33	2/57658 (0.0%)
34	b	0.25	0/1735	0.67	4/2338 (0.2%)
35	c	0.23	0/1651	0.64	2/2225 (0.1%)
36	d	0.22	0/1665	0.64	0/2227
37	e	0.23	0/1154	0.71	2/1554 (0.1%)
38	f	0.35	0/835	0.84	2/1128 (0.2%)
39	g	0.24	0/1195	0.68	3/1602 (0.2%)
40	h	0.23	0/989	0.61	0/1326
41	i	0.26	0/1034	0.76	0/1375
42	j	0.29	0/796	0.76	0/1077
43	k	0.64	3/845 (0.4%)	1.03	8/1145 (0.7%)
44	l	0.27	0/969	0.72	0/1300
45	m	0.27	0/892	0.68	0/1193
46	n	0.20	0/811	0.56	0/1081
47	o	0.21	0/722	0.64	3/964 (0.3%)
48	p	0.22	0/659	0.62	3/884 (0.3%)
49	q	0.28	0/657	0.74	2/881 (0.2%)
50	r	0.23	0/511	0.70	0/689
51	s	0.22	0/652	0.59	0/877
52	t	0.25	0/671	0.66	2/888 (0.2%)
53	u	0.33	0/500	0.93	4/668 (0.6%)
54	w	0.26	0/4016	0.74	14/5428 (0.3%)
55	z	0.22	0/127	0.61	0/175
All	All	0.19	4/160031 (0.0%)	0.44	72/238586 (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
6	F	0	2
7	G	0	3
11	K	0	1
13	M	0	1
18	R	0	1
21	U	0	1
30	3	0	1
32	5	0	1
34	b	0	2
37	e	0	1
38	f	0	2

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Mol	Chain	#Chirality outliers	#Planarity outliers
39	g	0	1
41	i	0	2
44	l	0	1
45	m	0	1
48	p	0	1
49	q	0	1
54	w	0	3
All	All	0	26

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
43	k	115	ILE	C-N	-9.55	1.22	1.33
43	k	116	PRO	CA-CB	-8.10	1.42	1.53
33	a	716	A	Cl'-N9	7.83	1.59	1.48
43	k	113	THR	C-O	7.19	1.33	1.24

All (72) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
43	k	116	PRO	N-CA-C	14.27	132.40	113.84
43	k	115	ILE	CA-C-N	-9.51	109.86	119.56
43	k	115	ILE	C-N-CA	-9.51	109.86	119.56
35	c	95	GLY	N-CA-C	-8.83	103.13	115.32
54	w	77	PHE	N-CA-C	7.66	126.74	109.81
39	g	64	ALA	N-CA-C	-7.52	105.28	114.75
43	k	116	PRO	N-CA-CB	-7.38	96.10	103.48
35	c	96	VAL	N-CA-C	7.31	124.68	108.88
54	w	17	ALA	N-CA-C	7.20	120.18	111.40
54	w	314	ARG	CA-C-N	7.17	134.88	121.97
54	w	314	ARG	C-N-CA	7.17	134.88	121.97
43	k	115	ILE	N-CA-CB	6.91	120.89	111.21
7	G	45	ALA	CA-C-N	6.69	134.32	121.54
7	G	45	ALA	C-N-CA	6.69	134.32	121.54
37	e	121	ASN	CA-C-N	6.45	133.57	121.97
37	e	121	ASN	C-N-CA	6.45	133.57	121.97
21	U	87	GLU	CA-C-N	6.31	130.71	121.31
21	U	87	GLU	C-N-CA	6.31	130.71	121.31
54	w	503	TYR	CA-C-N	6.28	133.27	121.97
54	w	503	TYR	C-N-CA	6.28	133.27	121.97
54	w	315	VAL	CB-CA-C	-6.27	101.01	111.29
43	k	113	THR	N-CA-C	6.26	119.60	110.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	w	17	ALA	CA-C-N	6.26	133.25	121.97
54	w	17	ALA	C-N-CA	6.26	133.25	121.97
34	b	19	THR	N-CA-C	6.21	116.27	108.45
13	M	96	ILE	CA-C-N	6.19	134.10	121.48
13	M	96	ILE	C-N-CA	6.19	134.10	121.48
43	k	115	ILE	CB-CA-C	6.18	122.62	111.36
34	b	17	HIS	CA-C-N	6.09	130.88	121.19
34	b	17	HIS	C-N-CA	6.09	130.88	121.19
54	w	76	GLN	O-C-N	6.07	128.32	122.07
13	M	53	MET	N-CA-C	-5.91	107.88	114.62
53	u	23	GLU	CA-C-N	5.91	128.47	120.38
53	u	23	GLU	C-N-CA	5.91	128.47	120.38
49	q	68	LYS	CA-C-N	5.85	132.72	121.54
49	q	68	LYS	C-N-CA	5.85	132.72	121.54
12	L	35	HIS	CA-C-N	5.81	129.36	120.82
12	L	35	HIS	C-N-CA	5.81	129.36	120.82
43	k	117	HIS	N-CA-C	-5.66	103.60	111.52
12	L	110	VAL	CA-C-N	5.57	128.18	120.49
12	L	110	VAL	C-N-CA	5.57	128.18	120.49
34	b	201	GLY	N-CA-C	5.54	119.79	111.42
47	o	13	GLU	N-CA-C	-5.46	108.39	114.62
30	3	30	HIS	CA-C-N	5.35	131.59	121.97
30	3	30	HIS	C-N-CA	5.35	131.59	121.97
53	u	35	GLU	CA-C-N	5.29	131.64	121.54
53	u	35	GLU	C-N-CA	5.29	131.64	121.54
1	A	1378	A	P-O3'-C3'	5.29	128.13	120.20
54	w	313	ASP	O-C-N	5.23	129.55	122.59
48	p	78	VAL	CA-C-N	5.23	129.10	121.31
48	p	78	VAL	C-N-CA	5.23	129.10	121.31
6	F	176	PHE	N-CA-C	5.19	116.98	110.91
39	g	128	GLU	CA-C-N	5.18	129.77	122.46
39	g	128	GLU	C-N-CA	5.18	129.77	122.46
32	5	50	VAL	CA-C-N	5.17	127.93	120.38
32	5	50	VAL	C-N-CA	5.17	127.93	120.38
54	w	315	VAL	CA-C-N	-5.16	115.52	122.95
54	w	315	VAL	C-N-CA	-5.16	115.52	122.95
52	t	67	HIS	CA-C-N	5.13	129.62	122.08
52	t	67	HIS	C-N-CA	5.13	129.62	122.08
38	f	17	GLN	CA-C-N	5.13	124.43	120.33
38	f	17	GLN	C-N-CA	5.13	124.43	120.33
47	o	44	GLU	CA-C-N	5.11	131.29	121.54
47	o	44	GLU	C-N-CA	5.11	131.29	121.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	a	1201	A	P-O3'-C3'	5.09	127.84	120.20
32	5	79	PRO	CA-C-N	5.07	128.27	120.82
32	5	79	PRO	C-N-CA	5.07	128.27	120.82
1	A	1022	G	P-O3'-C3'	5.06	127.79	120.20
1	A	752	A	P-O3'-C3'	5.05	127.77	120.20
33	a	1297	G	P-O3'-C3'	5.02	127.73	120.20
48	p	79	ASN	N-CA-C	5.01	117.36	110.35
54	w	314	ARG	O-C-N	5.01	129.25	122.59

There are no chirality outliers.

All (26) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
30	3	30	HIS	Peptide
32	5	80	THR	Peptide
6	F	173	ASP	Peptide
6	F	174	PHE	Peptide
7	G	118	ALA	Peptide
7	G	45	ALA	Peptide
7	G	46	ASP	Peptide
11	K	88	ASN	Peptide
13	M	57	VAL	Peptide
18	R	53	PHE	Peptide
21	U	88	ASP	Peptide
34	b	15	PHE	Peptide
34	b	16	GLY	Peptide
37	e	121	ASN	Peptide
38	f	52	ASN	Peptide
38	f	95	ALA	Peptide
39	g	29	LEU	Peptide
41	i	56	MET	Peptide
41	i	90	ASP	Peptide
44	l	101	LEU	Peptide
45	m	4	ALA	Peptide
48	p	44	SER	Peptide
49	q	68	LYS	Peptide
54	w	398	PHE	Peptide
54	w	470	THR	Peptide
54	w	502	ALA	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	62177	0	31271	464	0
2	B	2572	0	1302	22	0
3	C	2082	0	2157	32	0
4	D	1565	0	1616	18	0
5	E	1552	0	1619	23	0
6	F	1410	0	1447	21	0
7	G	1323	0	1374	8	0
8	H	1111	0	1148	14	0
9	I	1032	0	1088	11	0
10	J	1129	0	1162	12	0
11	K	938	0	1012	16	0
12	L	1045	0	1117	13	0
13	M	1074	0	1157	9	0
14	N	960	0	1000	12	0
15	O	892	0	923	9	0
16	P	917	0	965	12	0
17	Q	947	0	1022	9	0
18	R	816	0	839	12	0
19	S	857	0	922	8	0
20	T	738	0	807	14	0
21	U	779	0	834	4	0
22	V	753	0	780	8	0
23	W	575	0	592	3	0
24	X	625	0	655	8	0
25	Y	509	0	543	9	0
26	Z	449	0	491	5	0
27	0	444	0	461	5	0
28	1	409	0	440	2	0
29	2	377	0	418	7	0
30	3	504	0	574	6	0
31	4	302	0	343	1	0
32	5	988	0	1025	15	0
33	a	33016	0	16619	298	0
34	b	1704	0	1732	25	0
35	c	1624	0	1699	50	0
36	d	1643	0	1710	21	0
37	e	1141	0	1170	16	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
38	f	817	0	808	15	0
39	g	1181	0	1240	11	0
40	h	979	0	1034	13	0
41	i	1022	0	1070	20	0
42	j	786	0	828	12	0
43	k	829	0	826	81	0
44	l	955	0	1019	16	0
45	m	883	0	944	11	0
46	n	799	0	841	13	0
47	o	714	0	737	4	0
48	p	649	0	666	10	0
49	q	648	0	691	4	0
50	r	504	0	502	11	0
51	s	637	0	665	13	0
52	t	665	0	714	11	0
53	u	495	0	486	23	0
54	w	3943	0	3934	67	0
55	z	120	0	128	32	0
56	w	32	0	13	0	0
All	All	147637	0	101180	1302	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

All (1302) 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)
43:k:121:ARG:CD	53:u:31:VAL:HG22	1.54	1.36
1:A:1913:A:N7	33:a:1494:G:C8	2.05	1.25
1:A:1913:A:C8	33:a:1494:G:C8	2.27	1.23
43:k:123:PRO:C	53:u:33:ARG:HA	1.64	1.20
35:c:91:ALA:HB2	35:c:98:ALA:CB	1.73	1.19
1:A:1913:A:N7	33:a:1494:G:N7	1.94	1.15
33:a:676:A:OP2	43:k:113:THR:O	1.61	1.15
33:a:716:A:C6	43:k:118:ASN:HB2	1.83	1.14
43:k:122:PRO:HB2	43:k:123:PRO:HD2	1.33	1.10
1:A:2586:U:H5'	55:z:18:LEU:HD13	1.25	1.09
33:a:716:A:C4	43:k:118:ASN:ND2	2.23	1.07
35:c:91:ALA:CB	35:c:98:ALA:HB2	1.84	1.07
43:k:121:ARG:HD2	53:u:31:VAL:CG2	1.85	1.06
33:a:716:A:C5	43:k:118:ASN:CG	2.34	1.05

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2585:U:C2'	55:z:18:LEU:CB	2.34	1.05
1:A:2585:U:C2'	55:z:18:LEU:HB2	1.87	1.05
43:k:121:ARG:CD	53:u:31:VAL:CG2	2.34	1.05
1:A:2585:U:O2'	55:z:18:LEU:HB3	1.57	1.04
1:A:2585:U:H2'	55:z:18:LEU:HB2	1.33	1.04
35:c:91:ALA:HB2	35:c:98:ALA:HB2	1.37	1.03
1:A:2585:U:H2'	55:z:18:LEU:CB	1.90	1.02
1:A:2585:U:H1'	55:z:18:LEU:O	1.60	1.02
43:k:121:ARG:HD3	53:u:31:VAL:HG22	1.40	1.01
35:c:91:ALA:CA	35:c:98:ALA:HB2	1.89	1.01
43:k:121:ARG:HD2	53:u:31:VAL:HG22	1.39	1.00
33:a:1238:A:H62	33:a:1301:U:H3	1.00	1.00
43:k:122:PRO:HB2	43:k:123:PRO:CD	1.93	0.98
43:k:123:PRO:HA	53:u:34:ARG:H	1.27	0.98
1:A:593:U:H3	1:A:664:G:H1	1.12	0.97
33:a:1247:U:H3	33:a:1290:G:H1	1.10	0.95
54:w:314:ARG:HH12	54:w:418:GLN:HA	1.28	0.95
1:A:1476:U:H3	1:A:1515:A:H62	0.99	0.94
1:A:545:U:H3	1:A:548:G:H1	1.02	0.94
54:w:17:ALA:HB2	54:w:106:VAL:HG21	1.50	0.94
1:A:2585:U:H1'	55:z:18:LEU:C	1.92	0.94
1:A:2451:A:C2	55:z:17:ARG:NH2	2.36	0.93
35:c:87:ARG:O	35:c:91:ALA:N	2.01	0.93
1:A:2475:C:H42	1:A:2529:G:N2	1.67	0.92
33:a:716:A:C6	43:k:118:ASN:CB	2.53	0.91
1:A:306:U:H3	1:A:310:A:H62	0.96	0.91
33:a:782:A:H62	33:a:800:G:H21	1.18	0.91
1:A:2028:U:H3	1:A:2033:A:H62	1.12	0.90
1:A:2585:U:C2'	55:z:18:LEU:HB3	2.00	0.90
33:a:1238:A:N6	33:a:1301:U:H3	1.68	0.90
1:A:1433:A:H61	1:A:1560:G:H1	1.15	0.89
33:a:1445:U:H3	33:a:1457:G:H1	1.21	0.88
5:E:65:THR:HG22	55:z:8:ILE:HG21	1.56	0.87
33:a:886:G:H1	33:a:911:U:H3	1.22	0.87
1:A:2457:U:H5	1:A:2494:G:H1	0.92	0.87
35:c:86:LEU:O	35:c:90:VAL:HG23	1.73	0.87
33:a:1074:G:H1	33:a:1083:U:H3	1.23	0.86
33:a:716:A:C2	43:k:118:ASN:HA	2.11	0.85
1:A:1912:A:O2'	33:a:1494:G:N3	2.10	0.85
33:a:715:A:C6	43:k:118:ASN:ND2	2.45	0.84
43:k:123:PRO:C	53:u:33:ARG:CA	2.49	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:306:U:H3	1:A:310:A:N6	1.75	0.83
1:A:1913:A:O2'	33:a:1408:A:H2	1.62	0.83
1:A:2475:C:H42	1:A:2529:G:H22	1.23	0.82
35:c:91:ALA:HA	35:c:98:ALA:HB2	1.60	0.81
33:a:715:A:N6	43:k:118:ASN:O	2.14	0.80
35:c:91:ALA:HB2	35:c:98:ALA:HB3	1.62	0.80
33:a:716:A:N1	43:k:118:ASN:HB2	1.98	0.79
1:A:2475:C:N4	1:A:2529:G:H22	1.81	0.78
1:A:2611:C:C5	55:z:12:ARG:NH1	2.51	0.78
35:c:99:GLN:O	35:c:100:ILE:HG23	1.84	0.77
43:k:123:PRO:CA	53:u:34:ARG:H	1.96	0.77
1:A:2457:U:H5	1:A:2494:G:N1	1.77	0.77
35:c:87:ARG:HD2	35:c:98:ALA:O	1.84	0.77
33:a:716:A:C6	43:k:118:ASN:CG	2.62	0.76
1:A:1916:A:N6	33:a:1408:A:O2'	2.17	0.76
35:c:63:ILE:HG21	35:c:94:ALA:HB1	1.67	0.76
1:A:1913:A:O2'	33:a:1408:A:C2	2.38	0.76
33:a:675:A:H3'	43:k:115:ILE:HG13	1.66	0.75
33:a:676:A:H8	43:k:114:PRO:O	1.69	0.75
33:a:715:A:N6	43:k:118:ASN:CG	2.44	0.75
1:A:600:G:H1	1:A:657:U:H3	1.33	0.75
33:a:1438:G:H1	33:a:1463:U:H3	1.34	0.75
1:A:2611:C:H5	55:z:12:ARG:HH11	1.34	0.75
43:k:121:ARG:NE	53:u:31:VAL:HG22	2.02	0.75
43:k:115:ILE:HG22	43:k:116:PRO:HD3	1.70	0.74
35:c:63:ILE:H	35:c:97:PRO:HG2	1.51	0.74
33:a:927:G:H1	33:a:1390:U:H3	1.37	0.73
11:K:13:ASN:ND2	33:a:339:C:OP2	2.22	0.72
33:a:54:C:O2	54:w:310:LYS:NZ	2.21	0.72
1:A:78:U:H3	1:A:108:G:H1	1.36	0.72
35:c:91:ALA:CB	35:c:98:ALA:CB	2.51	0.72
43:k:121:ARG:HD2	53:u:31:VAL:HG23	1.70	0.72
1:A:2514:U:H3	1:A:2570:G:H1	1.38	0.71
16:P:105:LYS:NZ	33:a:1464:U:OP2	2.22	0.71
33:a:676:A:C8	43:k:114:PRO:O	2.42	0.71
23:W:61:GLY:HA3	23:W:79:GLU:O	1.90	0.71
44:l:122:LYS:HD3	54:w:490:GLU:HB2	1.73	0.70
33:a:782:A:H62	33:a:800:G:N2	1.87	0.70
35:c:99:GLN:O	35:c:100:ILE:CG2	2.40	0.70
1:A:377:G:H1	1:A:397:U:H3	1.40	0.70
1:A:2585:U:C1'	55:z:18:LEU:HB2	2.21	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2058:A:H2	55:z:12:ARG:HD2	1.57	0.69
1:A:955:U:C5	1:A:962:G:N1	2.59	0.69
39:g:111:GLY:HA2	39:g:118:ARG:HD3	1.74	0.69
33:a:716:A:C4	43:k:118:ASN:CG	2.67	0.68
33:a:716:A:N6	43:k:118:ASN:HB2	2.08	0.68
42:j:42:LEU:HD11	42:j:73:LEU:HG	1.75	0.68
1:A:1912:A:N7	1:A:1917:U:O4	2.27	0.68
2:B:78:A:H62	2:B:98:G:H21	1.39	0.68
1:A:244:A:H62	1:A:254:G:H21	1.41	0.68
1:A:1912:A:H1'	33:a:1494:G:H21	1.57	0.68
35:c:87:ARG:HG2	35:c:98:ALA:CB	2.24	0.68
1:A:751:A:C2	55:z:7:TYR:CE1	2.81	0.67
51:s:5:LYS:HG3	51:s:6:LYS:HG2	1.76	0.67
38:f:4:TYR:O	38:f:63:ASN:HA	1.94	0.67
1:A:2585:U:C2	55:z:18:LEU:C	2.73	0.67
54:w:295:LYS:HG2	54:w:381:GLN:HB2	1.77	0.67
1:A:196:A:H61	1:A:831:G:H21	1.43	0.67
1:A:2457:U:O4	1:A:2494:G:O6	2.13	0.67
1:A:1687:G:H21	1:A:1701:A:H62	1.43	0.67
35:c:87:ARG:CG	35:c:98:ALA:HB1	2.24	0.67
1:A:1476:U:H3	1:A:1515:A:N6	1.84	0.66
16:P:59:THR:HG22	16:P:72:VAL:HG12	1.78	0.66
43:k:122:PRO:CB	43:k:123:PRO:CD	2.68	0.66
48:p:4:ILE:HG12	48:p:21:VAL:HG22	1.78	0.66
38:f:45:ARG:O	38:f:56:LYS:HA	1.95	0.66
1:A:2585:U:C6	55:z:18:LEU:HB2	2.30	0.66
35:c:63:ILE:HG22	35:c:97:PRO:HG2	1.78	0.65
33:a:675:A:H3'	43:k:115:ILE:CG1	2.26	0.65
33:a:675:A:H5''	43:k:114:PRO:HA	1.78	0.65
33:a:716:A:C5	43:k:118:ASN:OD1	2.49	0.65
1:A:1418:G:N2	1:A:1579:A:N7	2.45	0.65
1:A:1913:A:C8	33:a:1494:G:N9	2.65	0.65
33:a:230:G:H5''	48:p:31:ARG:HH21	1.62	0.64
33:a:599:C:H5''	40:h:87:ARG:HA	1.80	0.64
1:A:2656:U:N3	1:A:2665:A:C8	2.61	0.64
1:A:1666:G:H4'	11:K:6:THR:HG23	1.80	0.64
33:a:516:U:O4	33:a:533:A:N7	2.30	0.64
33:a:1238:A:N7	33:a:1301:U:O4	2.31	0.63
6:F:62:GLN:HE22	6:F:90:LEU:HB3	1.64	0.63
33:a:875:U:O2'	40:h:14:ARG:NH1	2.31	0.63
14:N:28:LEU:HD23	14:N:48:VAL:HG21	1.81	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
43:k:123:PRO:HA	53:u:34:ARG:N	2.09	0.63
1:A:955:U:H5	1:A:962:G:H1	1.43	0.63
34:b:165:ALA:HB3	34:b:190:SER:HB3	1.81	0.63
3:C:143:VAL:HB	3:C:153:LEU:HB2	1.80	0.63
5:E:146:VAL:HG12	5:E:185:LYS:HB2	1.81	0.62
33:a:1148:U:OP1	41:i:10:ARG:NH2	2.31	0.62
1:A:818:G:H21	1:A:1189:A:H62	1.44	0.62
12:L:109:LYS:HD2	12:L:126:ARG:HH11	1.64	0.62
37:e:156:ARG:NH1	40:h:98:LEU:O	2.33	0.62
1:A:281:C:H42	1:A:359:G:H1	1.47	0.62
1:A:2451:A:N1	55:z:17:ARG:NH2	2.40	0.62
11:K:17:ARG:HH12	33:a:1471:U:H5''	1.64	0.62
1:A:1093:G:H21	1:A:1098:A:H62	1.48	0.62
1:A:2062:A:H62	1:A:2503:A:H62	1.45	0.62
51:s:30:LEU:HB2	51:s:48:ILE:HG22	1.81	0.62
2:B:78:A:H62	2:B:98:G:N2	1.97	0.62
43:k:121:ARG:NE	53:u:31:VAL:CG2	2.60	0.62
1:A:955:U:H5	1:A:962:G:N1	1.97	0.62
1:A:2586:U:H5'	55:z:18:LEU:CD1	2.17	0.62
35:c:86:LEU:O	35:c:90:VAL:CG2	2.46	0.62
1:A:2508:G:C6	1:A:2580:U:O4	2.53	0.61
1:A:1862:G:H1	1:A:1880:U:H3	1.46	0.61
11:K:98:ARG:NH2	33:a:340:U:O4	2.33	0.61
34:b:31:PHE:HB2	34:b:39:ILE:HB	1.83	0.61
42:j:7:ARG:HB3	42:j:101:SER:HB2	1.83	0.61
1:A:1081:U:H4'	9:I:123:ALA:HB1	1.81	0.61
1:A:2585:U:C1'	55:z:18:LEU:C	2.72	0.61
1:A:629:G:N3	1:A:639:U:O2'	2.33	0.61
38:f:5:GLU:HB2	38:f:90:MET:HB2	1.83	0.61
33:a:715:A:N1	43:k:118:ASN:ND2	2.49	0.60
1:A:2585:U:C1'	55:z:18:LEU:CB	2.78	0.60
33:a:55:A:C6	54:w:311:HIS:CE1	2.89	0.60
1:A:839:U:H3	1:A:939:G:H1	1.48	0.60
1:A:1799:G:O2'	3:C:181:ARG:NH1	2.34	0.60
43:k:123:PRO:C	53:u:34:ARG:H	2.09	0.60
33:a:715:A:C6	43:k:118:ASN:O	2.54	0.60
54:w:314:ARG:HH12	54:w:418:GLN:CA	2.08	0.60
1:A:955:U:O4	1:A:962:G:O6	2.20	0.60
29:2:34:ARG:NH2	29:2:41:ARG:O	2.34	0.60
1:A:306:U:O4	1:A:310:A:N7	2.35	0.60
1:A:1433:A:N6	1:A:1560:G:H1	1.93	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:34:VAL:HA	4:D:50:VAL:HG12	1.84	0.60
19:S:82:MET:HB2	19:S:98:LYS:HB2	1.84	0.60
33:a:321:A:H61	33:a:332:G:H1	1.49	0.60
36:d:94:GLU:HG2	36:d:185:PRO:HG2	1.84	0.60
33:a:227:G:O2'	48:p:63:GLN:NE2	2.35	0.60
33:a:1349:A:OP2	41:i:119:LYS:NZ	2.34	0.60
1:A:585:G:H21	1:A:1254:A:H62	1.50	0.60
43:k:115:ILE:CG2	43:k:116:PRO:HD3	2.32	0.60
1:A:1060:U:H5'	1:A:1062:G:H5'	1.84	0.60
3:C:51:ARG:HH22	3:C:246:PRO:HG2	1.67	0.59
5:E:117:ARG:NH2	5:E:183:PHE:O	2.35	0.59
22:V:64:VAL:HG22	22:V:69:GLU:HG2	1.83	0.59
35:c:85:LYS:O	35:c:89:VAL:HG22	2.02	0.59
33:a:1222:G:OP2	33:a:1322:C:N4	2.36	0.59
1:A:1046:A:H62	32:5:4:ASN:HD21	1.47	0.59
35:c:88:LYS:HA	35:c:91:ALA:HB3	1.83	0.59
1:A:585:G:H21	1:A:1254:A:N6	2.00	0.59
8:H:39:ALA:HA	8:H:43:ASN:HB2	1.85	0.59
51:s:68:HIS:HB3	51:s:72:GLU:HG3	1.85	0.59
1:A:488:G:H22	1:A:491:G:H5''	1.66	0.59
33:a:1288:A:H61	33:a:1371:G:H1'	1.68	0.59
4:D:179:ARG:HB3	4:D:188:LEU:HD12	1.84	0.59
33:a:725:G:OP1	33:a:833:G:N2	2.36	0.59
1:A:1041:G:H1	1:A:1114:C:H42	1.50	0.59
35:c:87:ARG:HG2	35:c:98:ALA:HB3	1.85	0.59
54:w:315:VAL:HG21	54:w:317:PHE:CE2	2.37	0.59
1:A:2185:U:H2'	1:A:2186:G:H8	1.68	0.59
1:A:1798:U:H5''	3:C:257:ARG:HB2	1.84	0.58
33:a:715:A:C6	43:k:118:ASN:CG	2.81	0.58
35:c:87:ARG:O	35:c:91:ALA:CB	2.51	0.58
38:f:6:ILE:HG12	38:f:89:VAL:HG22	1.85	0.58
33:a:980:C:O2'	46:n:12:ARG:NH2	2.36	0.58
35:c:89:VAL:O	35:c:93:ILE:HG12	2.02	0.58
54:w:488:LYS:HE2	54:w:517:ARG:HH21	1.68	0.58
1:A:2508:G:O6	1:A:2580:U:O4	2.22	0.58
54:w:312:ARG:C	54:w:314:ARG:H	2.11	0.58
30:3:32:LEU:HD23	30:3:35:LYS:HD2	1.85	0.58
33:a:1200:C:H5''	33:a:1201:A:H3'	1.86	0.58
1:A:2296:U:OP2	15:O:9:ARG:NH2	2.37	0.58
40:h:42:GLU:HG2	40:h:100:ILE:HG12	1.85	0.58
54:w:14:ARG:HB2	54:w:84:VAL:HG22	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1252:G:N2	17:Q:32:ARG:O	2.37	0.58
35:c:87:ARG:HG3	35:c:98:ALA:HB1	1.85	0.58
32:5:58:THR:HG21	32:5:82:ILE:H	1.68	0.58
38:f:32:ALA:HB2	38:f:70:VAL:HG11	1.86	0.58
39:g:75:LYS:HE3	39:g:88:VAL:HG11	1.86	0.58
41:i:10:ARG:O	41:i:105:ARG:NH2	2.37	0.58
1:A:2656:U:O2	1:A:2665:A:N7	2.37	0.57
2:B:79:G:N7	22:V:14:LYS:NZ	2.52	0.57
24:X:6:VAL:HG21	24:X:58:ILE:HD11	1.86	0.57
33:a:676:A:C5	43:k:116:PRO:HA	2.39	0.57
35:c:87:ARG:CG	35:c:98:ALA:CB	2.80	0.57
37:e:80:LEU:HD13	37:e:122:VAL:HG21	1.86	0.57
1:A:2515:C:H2'	1:A:2516:A:H8	1.69	0.57
35:c:99:GLN:C	35:c:100:ILE:HG23	2.29	0.57
3:C:92:LEU:HD11	3:C:100:ARG:HB3	1.85	0.57
54:w:21:HIS:HA	54:w:122:ARG:HG2	1.85	0.57
52:t:11:ILE:O	52:t:14:GLU:HB2	2.04	0.57
1:A:907:G:N2	13:M:70:ASP:OD2	2.38	0.57
1:A:2061:G:OP1	5:E:63:LYS:NZ	2.36	0.57
20:T:23:ALA:HB1	20:T:29:THR:HB	1.86	0.57
1:A:538:A:H4'	10:J:7:LYS:HG2	1.86	0.57
1:A:2279:G:HO2'	1:A:2327:A:HO2'	1.51	0.57
2:B:72:G:H21	2:B:104:A:H62	1.52	0.57
18:R:35:PHE:O	18:R:58:VAL:HA	2.04	0.57
45:m:85:TYR:OH	45:m:89:ARG:NH1	2.38	0.57
54:w:92:HIS:HB2	54:w:95:PHE:HB2	1.86	0.57
1:A:1992:G:N2	1:A:1996:C:O2'	2.36	0.57
1:A:2028:U:H3	1:A:2033:A:N6	1.92	0.57
12:L:23:ILE:HD13	18:R:84:ARG:HH22	1.70	0.57
43:k:84:MET:SD	43:k:110:THR:OG1	2.63	0.57
47:o:38:LEU:HD23	47:o:42:PHE:HE2	1.70	0.57
42:j:8:ILE:HG12	42:j:100:ILE:HG22	1.87	0.57
1:A:318:C:H2'	1:A:319:G:H8	1.70	0.57
1:A:1986:C:H2'	1:A:1987:A:H8	1.70	0.57
13:M:40:ARG:HH11	13:M:93:VAL:HG11	1.70	0.57
33:a:672:U:O2	33:a:734:G:O6	2.22	0.57
33:a:1219:A:OP1	46:n:53:ARG:NH1	2.38	0.57
1:A:849:A:H61	1:A:929:U:H3	1.53	0.57
29:2:24:THR:HG23	29:2:27:GLY:H	1.69	0.57
33:a:358:U:H2'	33:a:359:G:H8	1.70	0.56
33:a:716:A:N1	43:k:118:ASN:CB	2.62	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:a:718:A:OP2	33:a:720:C:N4	2.38	0.56
33:a:1271:A:O2'	51:s:5:LYS:NZ	2.38	0.56
1:A:605:G:H1'	1:A:657:U:H1'	1.88	0.56
3:C:70:LYS:HB3	3:C:73:ILE:HD12	1.87	0.56
27:0:30:ASP:HB3	27:0:34:GLY:H	1.70	0.56
33:a:837:U:H2'	33:a:838:G:H8	1.71	0.56
50:r:36:GLY:O	50:r:62:ARG:NH2	2.39	0.56
1:A:1668:A:N3	1:A:1670:C:N4	2.54	0.56
1:A:2028:U:O4	1:A:2033:A:N7	2.38	0.56
7:G:94:ARG:HB2	7:G:105:SER:HB2	1.87	0.56
21:U:33:VAL:HG13	21:U:66:VAL:HG22	1.87	0.56
33:a:20:U:O2'	33:a:573:A:N6	2.37	0.56
33:a:675:A:C3'	43:k:115:ILE:HG13	2.35	0.56
33:a:716:A:N3	43:k:118:ASN:ND2	2.54	0.56
33:a:1086:U:H3	33:a:1099:G:H1	1.53	0.56
1:A:647:G:N2	1:A:2350:C:O2'	2.38	0.56
23:W:33:ILE:HG22	23:W:34:VAL:HG23	1.88	0.56
1:A:1476:U:O4	1:A:1515:A:N7	2.39	0.56
1:A:2291:U:H1'	1:A:2374:C:H1'	1.88	0.56
4:D:15:PHE:H	16:P:11:GLN:HE22	1.53	0.56
17:Q:43:GLN:HE21	18:R:77:PHE:HB3	1.71	0.56
33:a:55:A:C5	54:w:311:HIS:HE1	2.23	0.56
36:d:61:ARG:NH1	36:d:68:GLU:OE1	2.38	0.56
1:A:2394:C:H5''	12:L:63:LYS:HE3	1.87	0.56
1:A:2893:A:H5''	1:A:2894:G:H5'	1.88	0.56
33:a:672:U:H2'	33:a:673:A:H8	1.71	0.56
38:f:38:ARG:NH2	38:f:40:GLU:OE1	2.39	0.56
1:A:698:C:O2'	1:A:734:A:N6	2.36	0.56
1:A:1450:G:H21	1:A:1452:G:H1	1.54	0.56
1:A:2692:G:H1'	1:A:2847:U:H1'	1.87	0.56
26:Z:8:GLN:HB2	26:Z:28:LEU:HD13	1.88	0.56
39:g:68:VAL:HG23	39:g:99:ALA:HB1	1.87	0.56
6:F:23:SER:HB3	6:F:26:GLN:HG3	1.87	0.56
5:E:65:THR:CG2	55:z:8:ILE:HD13	2.36	0.56
24:X:39:VAL:HG12	24:X:42:GLU:H	1.70	0.56
48:p:40:ASN:HB3	48:p:43:ALA:HB2	1.87	0.56
22:V:42:LEU:HD13	22:V:47:VAL:HG21	1.87	0.56
36:d:13:ARG:HA	36:d:37:PRO:HB3	1.88	0.56
1:A:514:A:N3	1:A:581:C:O2'	2.36	0.55
1:A:2585:U:N1	55:z:18:LEU:HB2	2.20	0.55
1:A:2748:A:H5'	7:G:3:VAL:HG21	1.87	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:X:58:ILE:HG12	24:X:66:VAL:HG21	1.87	0.55
33:a:716:A:N7	43:k:118:ASN:OD1	2.38	0.55
35:c:90:VAL:O	35:c:94:ALA:HB2	2.06	0.55
15:O:40:ILE:HG12	15:O:47:VAL:HG12	1.88	0.55
39:g:46:LEU:HD23	39:g:57:GLU:HB3	1.87	0.55
54:w:326:GLU:HB2	54:w:329:MET:HB2	1.88	0.55
1:A:962:G:O2'	1:A:2250:G:N2	2.39	0.55
7:G:88:LEU:HG	7:G:161:VAL:HG22	1.87	0.55
33:a:676:A:OP2	43:k:113:THR:C	2.45	0.55
35:c:39:ARG:HG3	35:c:54:ILE:HD11	1.89	0.55
44:l:49:ARG:HB3	44:l:65:TYR:HE1	1.71	0.55
54:w:14:ARG:NH1	54:w:82:CYS:SG	2.79	0.55
1:A:460:A:H62	1:A:469:G:H21	1.54	0.55
9:I:11:GLN:NE2	9:I:54:ILE:O	2.39	0.55
24:X:39:VAL:O	24:X:43:LYS:N	2.39	0.55
1:A:2720:U:OP1	16:P:52:ARG:NH2	2.40	0.55
33:a:1414:U:H2'	33:a:1415:G:H8	1.72	0.55
34:b:19:THR:OG1	34:b:20:ARG:N	2.38	0.55
45:m:76:ILE:HG22	45:m:80:MET:HE2	1.88	0.55
1:A:589:U:H2'	1:A:590:A:H8	1.72	0.55
1:A:1500:G:H4'	3:C:100:ARG:HH12	1.71	0.55
2:B:30:C:H1'	2:B:57:A:H61	1.72	0.55
49:q:30:HIS:HD2	49:q:33:TYR:H	1.53	0.55
1:A:45:G:H5''	1:A:46:G:H5'	1.88	0.55
1:A:1069:A:N7	1:A:1073:A:N6	2.55	0.55
33:a:1318:A:H1'	51:s:36:ARG:HB2	1.87	0.55
35:c:87:ARG:O	35:c:98:ALA:HB1	2.07	0.55
1:A:1925:C:H42	1:A:1929:G:H22	1.54	0.55
33:a:254:G:N2	49:q:17:GLU:OE1	2.40	0.55
33:a:1321:U:H3'	33:a:1322:C:H2'	1.89	0.55
35:c:63:ILE:CG2	35:c:94:ALA:HB1	2.37	0.55
1:A:605:G:N3	1:A:657:U:O2'	2.38	0.55
1:A:1204:A:N6	1:A:1242:U:O4	2.40	0.55
5:E:65:THR:HG22	55:z:8:ILE:HD13	1.88	0.55
36:d:77:GLU:OE2	36:d:80:ARG:NH1	2.40	0.55
4:D:148:GLN:HB2	4:D:152:PRO:HG2	1.89	0.54
54:w:306:ASN:ND2	54:w:312:ARG:O	2.40	0.54
1:A:1270:C:H5''	1:A:1271:G:H5'	1.89	0.54
1:A:2306:C:N4	6:F:38:GLY:O	2.40	0.54
1:A:587:C:O2	12:L:33:ARG:NH1	2.41	0.54
1:A:2585:U:O2	55:z:18:LEU:C	2.50	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:5:22:ALA:HB3	32:5:87:GLU:HB2	1.88	0.54
46:n:15:LEU:HD23	46:n:55:SER:HB3	1.89	0.54
1:A:1798:U:OP2	3:C:270:ARG:NH2	2.40	0.54
1:A:1800:C:N4	1:A:1818:U:O2'	2.41	0.54
33:a:514:C:H2'	33:a:515:G:H8	1.72	0.54
33:a:659:U:H3	33:a:747:A:H61	1.56	0.54
34:b:71:THR:OG1	34:b:168:GLU:OE2	2.24	0.54
35:c:57:GLU:OE1	35:c:64:ARG:NH2	2.36	0.54
35:c:171:ARG:HG2	35:c:173:PRO:HD3	1.90	0.54
42:j:55:PRO:HA	46:n:81:ARG:HH22	1.72	0.54
8:H:15:LEU:HD21	8:H:56:ALA:HB1	1.89	0.54
18:R:40:MET:HE3	18:R:42:ALA:HB2	1.89	0.54
33:a:927:G:H21	33:a:1532:U:H5''	1.73	0.54
43:k:86:LYS:NZ	43:k:113:THR:HG23	2.23	0.54
1:A:533:G:O5'	17:Q:27:ARG:NH1	2.41	0.54
1:A:538:A:N6	1:A:555:G:O2'	2.41	0.54
1:A:807:U:O2'	1:A:2060:A:N1	2.40	0.54
1:A:1154:G:OP2	17:Q:57:ARG:NH1	2.41	0.54
11:K:43:ILE:HD12	11:K:56:ASP:HB2	1.90	0.54
15:O:108:ASP:OD1	15:O:111:ARG:NH1	2.40	0.54
35:c:87:ARG:HG2	35:c:98:ALA:HB1	1.87	0.54
33:a:56:U:H2'	33:a:57:G:H8	1.73	0.54
33:a:1159:U:OP1	34:b:131:LYS:NZ	2.41	0.54
38:f:6:ILE:HA	38:f:88:MET:O	2.08	0.54
1:A:2320:U:O2'	1:A:2322:A:N6	2.40	0.54
11:K:40:LYS:HE3	11:K:57:VAL:HG12	1.90	0.54
33:a:1179:A:H4'	41:i:105:ARG:H	1.73	0.54
37:e:156:ARG:HD3	40:h:42:GLU:HG3	1.90	0.54
1:A:1288:G:OP2	1:A:1288:G:N2	2.40	0.54
1:A:1916:A:N6	33:a:1408:A:HO2'	2.03	0.54
1:A:2581:G:N2	1:A:2581:G:OP2	2.38	0.54
1:A:2861:U:H2'	1:A:2862:G:H8	1.73	0.54
11:K:48:PRO:HG3	33:a:1422:G:H5'	1.90	0.54
1:A:550:C:H2'	1:A:551:G:H8	1.73	0.54
3:C:165:ALA:HB3	3:C:172:THR:HB	1.90	0.54
20:T:13:ALA:HB3	20:T:33:LYS:HD3	1.89	0.54
1:A:1724:G:O6	1:A:1737:G:N2	2.41	0.53
1:A:1806:C:H1'	3:C:43:ASN:HD21	1.73	0.53
8:H:1:MET:N	8:H:20:ASN:OD1	2.41	0.53
27:O:27:LEU:HD23	27:O:36:LYS:HB3	1.89	0.53
33:a:689:C:OP2	43:k:52:ARG:NH1	2.40	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:134:GLN:NE2	6:F:149:ARG:O	2.42	0.53
33:a:782:A:N6	33:a:800:G:H21	1.98	0.53
33:a:1271:A:H2'	33:a:1272:G:H8	1.74	0.53
53:u:16:ARG:HH21	53:u:19:LYS:HG2	1.74	0.53
5:E:18:THR:HA	5:E:106:LYS:HE3	1.90	0.53
11:K:113:MET:SD	33:a:345:C:N4	2.81	0.53
33:a:231:U:H2'	33:a:232:G:H8	1.73	0.53
41:i:33:SER:H	41:i:36:GLN:HE21	1.55	0.53
1:A:1153:C:OP1	17:Q:91:ARG:NH2	2.41	0.53
11:K:9:ASN:OD1	11:K:18:ARG:NH1	2.42	0.53
33:a:722:G:H4'	53:u:48:LYS:HE3	1.90	0.53
33:a:829:G:H2'	33:a:830:G:H8	1.73	0.53
33:a:1217:C:OP1	46:n:8:ARG:NH2	2.42	0.53
26:Z:10:ARG:HB2	26:Z:53:MET:HB2	1.90	0.53
33:a:1252:A:H61	33:a:1285:A:H61	1.57	0.53
36:d:102:TYR:O	36:d:164:ARG:NH1	2.38	0.53
8:H:30:LEU:HB3	8:H:36:ALA:HB3	1.90	0.53
11:K:12:ASP:HB3	11:K:99:ILE:HG12	1.91	0.53
33:a:521:G:O6	44:l:49:ARG:NH2	2.40	0.53
41:i:122:ARG:NH1	41:i:123:ARG:O	2.42	0.53
1:A:444:C:OP2	5:E:44:ARG:NH2	2.41	0.53
1:A:2229:U:H2'	1:A:2230:G:H8	1.73	0.53
33:a:297:G:N2	33:a:300:A:OP2	2.40	0.53
33:a:664:G:H22	33:a:741:G:H1	1.57	0.53
33:a:916:U:H2'	33:a:917:G:H8	1.74	0.53
1:A:2505:G:H2'	1:A:2576:G:H1	1.74	0.53
33:a:216:U:H4'	33:a:464:U:H4'	1.91	0.53
43:k:22:ILE:HG12	43:k:31:VAL:HG22	1.91	0.53
33:a:951:G:OP2	45:m:100:ARG:NH2	2.41	0.53
54:w:32:LYS:HD2	54:w:262:ASN:HA	1.90	0.53
1:A:1913:A:H8	33:a:1494:G:N9	2.06	0.53
2:B:48:U:OP2	15:O:30:ARG:NH2	2.42	0.53
35:c:152:VAL:HG12	35:c:197:VAL:HG22	1.91	0.53
8:H:132:PHE:H	8:H:140:ALA:HB3	1.73	0.52
33:a:373:A:O2'	33:a:451:A:N7	2.41	0.52
43:k:114:PRO:CB	43:k:117:HIS:NE2	2.71	0.52
54:w:298:GLY:HA2	54:w:319:ARG:H	1.73	0.52
1:A:177:G:H3'	1:A:178:G:H8	1.73	0.52
1:A:1428:C:OP2	3:C:27:LYS:NZ	2.42	0.52
4:D:131:ASP:O	4:D:136:ASN:ND2	2.39	0.52
3:C:106:PRO:HD2	3:C:109:LEU:HD22	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:102:ARG:NH1	5:E:200:LEU:O	2.43	0.52
34:b:202:ASN:HD21	34:b:205:ALA:H	1.58	0.52
37:e:54:GLU:HG2	37:e:56:PRO:HD2	1.89	0.52
42:j:45:ARG:HB2	42:j:69:THR:HB	1.92	0.52
1:A:1753:G:H5''	16:P:92:ARG:HD3	1.90	0.52
1:A:2692:G:N3	1:A:2847:U:O2'	2.40	0.52
24:X:4:CYS:HB3	24:X:9:LYS:H	1.74	0.52
32:5:3:LEU:HD12	32:5:5:LEU:H	1.75	0.52
1:A:119:A:H4'	1:A:120:U:H5'	1.91	0.52
1:A:144:A:H4'	20:T:2:ILE:HD11	1.91	0.52
1:A:2743:U:OP2	1:A:2755:C:N4	2.43	0.52
1:A:2081:U:H2'	1:A:2082:A:H8	1.75	0.52
14:N:44:LEU:HD23	14:N:113:ILE:HD13	1.91	0.52
33:a:362:G:N2	33:a:365:U:OP2	2.43	0.52
33:a:766:A:OP2	33:a:812:G:N2	2.43	0.52
37:e:10:LEU:HD22	37:e:67:ARG:HH22	1.75	0.52
1:A:958:U:OP2	13:M:14:LYS:NZ	2.43	0.52
1:A:2848:G:O2'	1:A:2868:A:N6	2.43	0.52
22:V:9:ARG:HD3	22:V:39:ALA:HB1	1.91	0.52
33:a:1370:G:H2'	33:a:1371:G:H8	1.75	0.52
43:k:23:HIS:HB3	43:k:30:ILE:HG22	1.92	0.52
48:p:7:ALA:HB3	48:p:18:GLN:HB2	1.92	0.52
54:w:76:GLN:OE1	54:w:83:LEU:HB3	2.10	0.52
54:w:77:PHE:HE2	54:w:86:LEU:HG	1.74	0.52
1:A:111:A:O2'	25:Y:58:ASN:ND2	2.43	0.52
1:A:475:C:H4'	1:A:510:C:H5'	1.90	0.52
1:A:523:C:O2	1:A:554:U:O2'	2.28	0.52
1:A:605:G:OP1	5:E:99:LYS:NZ	2.43	0.52
1:A:1899:A:H4'	1:A:1901:A:H5''	1.91	0.52
1:A:2523:G:HO2'	1:A:2764:A:HO2'	1.58	0.52
1:A:2746:U:H5''	7:G:137:LYS:HE2	1.92	0.52
33:a:335:C:H2'	33:a:336:A:H8	1.75	0.52
1:A:112:U:H5'	25:Y:58:ASN:HD21	1.75	0.52
1:A:1223:G:OP1	18:R:68:ARG:NH2	2.43	0.52
11:K:30:ARG:NH2	11:K:37:ASP:OD2	2.42	0.52
13:M:66:ARG:NH1	13:M:104:GLU:OE2	2.43	0.52
33:a:880:C:OP1	44:l:8:ARG:NH1	2.43	0.52
33:a:1237:C:O2'	33:a:1300:G:N2	2.43	0.52
1:A:576:U:H2'	1:A:577:G:C8	2.45	0.51
1:A:720:U:H2'	1:A:721:A:H8	1.75	0.51
12:L:127:VAL:HG21	12:L:142:ILE:HD13	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:5:26:VAL:HG21	32:5:114:GLU:HG2	1.92	0.51
33:a:1464:U:H2'	33:a:1465:A:H8	1.75	0.51
46:n:26:LEU:HA	46:n:30:ILE:HD12	1.92	0.51
1:A:835:C:H2'	1:A:836:G:H8	1.74	0.51
10:J:17:VAL:HG23	10:J:137:PRO:HB2	1.92	0.51
10:J:56:VAL:HB	10:J:124:VAL:HG12	1.91	0.51
33:a:1492:A:O2'	33:a:1493:A:O4'	2.28	0.51
41:i:91:GLU:OE2	41:i:94:ARG:NH1	2.44	0.51
1:A:291:G:H1	1:A:349:U:H3	1.58	0.51
1:A:407:G:H2'	1:A:408:G:H8	1.75	0.51
1:A:1953:A:O2'	1:A:2559:C:O2	2.27	0.51
25:Y:49:ASP:OD1	25:Y:52:ARG:NH2	2.44	0.51
2:B:5:U:OP1	2:B:61:G:O2'	2.29	0.51
33:a:613:C:OP1	36:d:80:ARG:NE	2.37	0.51
34:b:53:LEU:HB3	34:b:219:THR:HG21	1.92	0.51
41:i:39:GLY:HA2	41:i:44:ARG:HB2	1.92	0.51
1:A:660:C:O2'	12:L:13:LYS:NZ	2.42	0.51
20:T:6:ARG:NH2	20:T:37:ASP:OD2	2.44	0.51
21:U:36:GLU:HA	21:U:61:GLU:HG2	1.92	0.51
33:a:683:G:H21	43:k:39:ASN:HA	1.76	0.51
36:d:9:LYS:HA	36:d:12:ARG:HE	1.74	0.51
39:g:87:PRO:HG3	39:g:148:LYS:HA	1.92	0.51
50:r:70:THR:HG23	50:r:72:ARG:H	1.76	0.51
1:A:1013:C:H2'	1:A:1014:A:H8	1.74	0.51
35:c:87:ARG:O	35:c:91:ALA:HB2	2.09	0.51
38:f:36:ILE:HA	38:f:64:VAL:HG23	1.93	0.51
46:n:64:CYS:HB3	46:n:68:GLY:H	1.76	0.51
1:A:590:A:H61	1:A:667:U:H3	1.59	0.51
1:A:924:G:H2'	1:A:925:A:H8	1.75	0.51
1:A:2693:G:H2'	1:A:2694:G:H8	1.75	0.51
8:H:38:PRO:O	8:H:43:ASN:ND2	2.41	0.51
33:a:291:U:H3'	33:a:305:G:H22	1.75	0.51
33:a:722:G:H22	33:a:733:G:H1	1.58	0.51
33:a:1323:G:N2	33:a:1361:G:O2'	2.43	0.51
1:A:99:U:H5''	1:A:100:U:H5'	1.91	0.51
8:H:47:PHE:HA	8:H:51:ARG:HB2	1.91	0.51
13:M:75:GLU:HB3	13:M:90:GLU:HG3	1.92	0.51
1:A:737:C:N4	1:A:738:G:O6	2.44	0.51
33:a:976:G:OP1	46:n:71:HIS:ND1	2.43	0.51
37:e:149:PRO:HA	37:e:152:VAL:HG22	1.93	0.51
1:A:2586:U:C5'	55:z:18:LEU:HD13	2.17	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2656:U:C2	1:A:2665:A:N7	2.78	0.51
20:T:8:LEU:HA	20:T:50:LEU:HD21	1.93	0.51
33:a:589:U:H5'	40:h:29:SER:HB2	1.93	0.51
33:a:1238:A:N6	33:a:1301:U:N3	2.41	0.51
43:k:34:THR:HA	43:k:40:ALA:HA	1.93	0.51
1:A:1779:U:OP2	1:A:1784:A:N6	2.43	0.50
1:A:1966:A:N3	1:A:2592:G:O2'	2.41	0.50
1:A:2233:U:H2'	1:A:2234:G:H8	1.76	0.50
33:a:1315:U:O2'	33:a:1360:A:N3	2.42	0.50
54:w:14:ARG:HD3	54:w:276:ALA:HB3	1.92	0.50
34:b:99:MET:HA	34:b:106:VAL:HG21	1.93	0.50
41:i:89:TYR:HB3	41:i:93:LEU:HD12	1.92	0.50
1:A:481:G:O2'	1:A:506:G:N2	2.44	0.50
1:A:751:A:C2	55:z:7:TYR:CZ	2.98	0.50
1:A:2585:U:H2'	55:z:18:LEU:CD1	2.42	0.50
32:5:68:PRO:HA	32:5:72:LEU:HG	1.93	0.50
1:A:2023:C:H2'	1:A:2024:G:H8	1.76	0.50
1:A:2659:G:N2	1:A:2662:A:OP2	2.43	0.50
33:a:950:U:OP2	45:m:100:ARG:NE	2.43	0.50
35:c:65:VAL:HB	35:c:100:ILE:HG22	1.94	0.50
1:A:2291:U:O2'	1:A:2374:C:O2	2.30	0.50
1:A:2768:U:O2'	10:J:95:ARG:NH2	2.45	0.50
1:A:2008:C:H2'	1:A:2009:A:H8	1.75	0.50
33:a:49:U:H3	33:a:362:G:H1'	1.77	0.50
33:a:744:C:H2'	33:a:745:G:H8	1.76	0.50
33:a:952:U:H2'	33:a:953:G:H8	1.76	0.50
49:q:63:CYS:SG	49:q:73:THR:OG1	2.60	0.50
1:A:673:C:OP1	5:E:49:ARG:NH2	2.44	0.50
6:F:35:LEU:HB2	6:F:88:VAL:HB	1.93	0.50
1:A:2258:C:O2'	1:A:2427:C:OP2	2.29	0.50
6:F:163:GLU:OE1	6:F:166:ARG:NH1	2.45	0.50
7:G:8:VAL:HB	7:G:49:LEU:HB2	1.94	0.50
33:a:1186:G:H2'	33:a:1187:G:H8	1.76	0.50
35:c:87:ARG:O	35:c:98:ALA:CB	2.60	0.50
44:l:109:ARG:HB2	44:l:118:VAL:HG21	1.94	0.50
4:D:55:LYS:HE2	4:D:77:ARG:HA	1.94	0.50
32:5:119:PRO:HG2	32:5:121:SER:HB2	1.94	0.50
33:a:1425:U:H2'	33:a:1426:G:H8	1.76	0.50
43:k:115:ILE:CB	43:k:116:PRO:CD	2.90	0.50
1:A:463:G:N2	1:A:466:A:OP2	2.35	0.49
18:R:76:LYS:HB2	18:R:85:LYS:HB3	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:a:36:C:H5''	44:l:119:LYS:HG2	1.93	0.49
44:l:36:VAL:HG21	44:l:73:LEU:HB3	1.94	0.49
54:w:158:VAL:HG13	54:w:162:LEU:HD12	1.94	0.49
1:A:451:U:O2	1:A:453:A:N6	2.45	0.49
1:A:2113:U:O4	1:A:2119:A:N6	2.45	0.49
3:C:77:VAL:HG21	3:C:109:LEU:HD11	1.92	0.49
33:a:54:C:OP1	33:a:351:G:N2	2.43	0.49
54:w:36:PHE:HB3	54:w:269:LEU:HD11	1.93	0.49
1:A:476:G:N1	1:A:479:A:OP2	2.40	0.49
1:A:629:G:H1'	1:A:639:U:H1'	1.93	0.49
1:A:1080:A:H1'	9:I:127:SER:HA	1.94	0.49
1:A:2058:A:C2	55:z:12:ARG:HD2	2.42	0.49
2:B:7:G:O2'	15:O:38:GLN:NE2	2.45	0.49
3:C:140:VAL:HG12	3:C:191:LEU:HD23	1.94	0.49
7:G:88:LEU:HD23	7:G:93:TYR:HB3	1.94	0.49
33:a:28:A:O2'	33:a:296:U:OP1	2.30	0.49
33:a:1253:G:OP1	42:j:48:ARG:NH1	2.46	0.49
33:a:1348:U:H4'	41:i:121:ARG:HG3	1.95	0.49
1:A:537:G:H22	1:A:555:G:H2'	1.77	0.49
1:A:1323:C:OP1	19:S:98:LYS:NZ	2.44	0.49
9:I:44:LYS:HG2	9:I:70:THR:HG21	1.95	0.49
9:I:45:THR:HG22	9:I:50:LYS:HG2	1.94	0.49
33:a:734:G:H21	50:r:59:LYS:HB3	1.76	0.49
33:a:745:G:OP1	33:a:851:G:O2'	2.31	0.49
33:a:1218:C:H2'	33:a:1219:A:H8	1.77	0.49
1:A:585:G:N2	1:A:1254:A:H62	2.10	0.49
33:a:1445:U:O2	33:a:1457:G:N2	2.37	0.49
54:w:101:ARG:HH21	54:w:302:LYS:HG3	1.77	0.49
1:A:48:G:N2	1:A:177:G:OP2	2.44	0.49
1:A:177:G:OP2	1:A:177:G:N2	2.36	0.49
1:A:1173:U:O2'	1:A:1177:G:N2	2.41	0.49
1:A:1378:A:O2'	1:A:1380:G:OP2	2.31	0.49
6:F:152:ASP:N	6:F:152:ASP:OD1	2.45	0.49
14:N:43:GLU:OE2	14:N:46:ARG:NH2	2.45	0.49
48:p:18:GLN:HE22	48:p:35:ARG:HH21	1.59	0.49
3:C:184:GLU:HG3	3:C:186:ASP:H	1.78	0.49
12:L:17:LYS:HE3	12:L:27:LEU:HD22	1.94	0.49
19:S:73:LYS:HB2	19:S:106:VAL:HB	1.93	0.49
33:a:1175:G:H2'	33:a:1176:A:H8	1.78	0.49
1:A:918:A:N3	2:B:80:U:O2'	2.42	0.49
37:e:37:VAL:HG11	37:e:113:VAL:HG23	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
41:i:48:ARG:HA	41:i:51:LEU:HD12	1.94	0.49
46:n:89:MET:HE1	46:n:98:LYS:HD2	1.95	0.49
1:A:776:G:H22	1:A:2072:C:H5'	1.78	0.49
1:A:1447:C:O2'	1:A:1544:A:N3	2.39	0.49
18:R:1:MET:N	18:R:42:ALA:O	2.37	0.49
1:A:1024:G:O2'	1:A:1144:A:O2'	2.30	0.49
1:A:2788:C:O2'	1:A:2809:A:N3	2.42	0.49
2:B:95:U:H2'	2:B:96:G:H8	1.78	0.49
3:C:243:PRO:O	3:C:250:GLN:NE2	2.45	0.49
33:a:243:A:H4'	33:a:244:U:H3'	1.95	0.49
34:b:116:LEU:HG	34:b:136:ARG:HH21	1.78	0.49
40:h:14:ARG:NH2	40:h:74:ILE:O	2.45	0.49
43:k:114:PRO:HB2	43:k:117:HIS:NE2	2.27	0.49
54:w:395:PRO:HA	54:w:441:VAL:HA	1.95	0.49
1:A:1913:A:C8	33:a:1494:G:N7	2.60	0.48
3:C:141:HIS:ND1	3:C:192:GLY:O	2.41	0.48
14:N:28:LEU:HD13	14:N:34:ILE:HG12	1.94	0.48
33:a:1004:A:H3'	33:a:1024:G:H22	1.78	0.48
34:b:202:ASN:HD22	34:b:203:ASP:N	2.10	0.48
1:A:1807:G:N2	1:A:1810:A:OP2	2.45	0.48
6:F:9:ASP:OD1	6:F:9:ASP:N	2.43	0.48
31:4:30:GLU:HG3	31:4:32:LYS:H	1.78	0.48
33:a:201:G:H1	33:a:216:U:H3	1.61	0.48
33:a:1081:A:H2'	33:a:1082:A:H8	1.78	0.48
33:a:1096:C:O2	33:a:1170:A:O2'	2.31	0.48
33:a:1251:A:N3	33:a:1369:C:O2'	2.41	0.48
43:k:63:GLN:HG3	43:k:98:ALA:HB2	1.94	0.48
1:A:6:A:N3	10:J:135:GLN:NE2	2.61	0.48
1:A:2345:G:H4'	1:A:2346:A:H3'	1.94	0.48
3:C:130:PRO:HA	3:C:188:ARG:HA	1.96	0.48
13:M:35:ALA:O	13:M:99:GLY:N	2.43	0.48
33:a:1321:U:O2'	51:s:77:ARG:NH1	2.47	0.48
34:b:153:MET:HG2	34:b:155:GLY:H	1.78	0.48
38:f:11:HIS:O	38:f:15:SER:N	2.47	0.48
53:u:16:ARG:HB2	53:u:19:LYS:HD3	1.96	0.48
1:A:242:G:N2	1:A:255:A:OP2	2.45	0.48
1:A:1432:G:H2'	1:A:1433:A:H8	1.78	0.48
1:A:2851:A:O2'	14:N:64:ARG:NH2	2.46	0.48
33:a:715:A:N1	43:k:118:ASN:O	2.47	0.48
33:a:1053:G:N2	33:a:1058:G:O6	2.46	0.48
54:w:331:LEU:HD12	54:w:342:ILE:HD12	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1022:G:N2	1:A:1023:U:O4	2.46	0.48
1:A:1326:U:H5'	1:A:2010:G:H21	1.79	0.48
1:A:1469:A:OP2	1:A:1522:A:N6	2.47	0.48
2:B:114:C:H2'	2:B:115:A:H8	1.77	0.48
6:F:56:LEU:HD13	6:F:88:VAL:HG23	1.96	0.48
33:a:1129:C:O2'	33:a:1130:A:O4'	2.31	0.48
1:A:91:A:O2'	1:A:92:U:O4'	2.31	0.48
1:A:774:G:N2	1:A:787:C:O2'	2.46	0.48
1:A:2076:U:OP2	1:A:2238:G:N2	2.45	0.48
5:E:97:ASN:ND2	5:E:100:MET:SD	2.86	0.48
33:a:137:U:H2'	33:a:138:G:H8	1.79	0.48
33:a:721:G:OP2	50:r:41:SER:OG	2.30	0.48
33:a:1060:U:H2'	33:a:1061:G:H8	1.78	0.48
51:s:62:THR:H	51:s:65:MET:HE3	1.79	0.48
1:A:659:G:O2'	5:E:95:LYS:O	2.31	0.48
1:A:1129:A:O2'	1:A:2515:C:O2	2.31	0.48
1:A:1919:A:O2'	33:a:1517:G:H1'	2.13	0.48
33:a:309:A:H2'	33:a:310:G:H8	1.79	0.48
1:A:545:U:O2	1:A:548:G:N2	2.40	0.48
1:A:1682:G:OP2	1:A:1699:G:N2	2.45	0.48
33:a:235:C:H2'	33:a:236:A:H8	1.79	0.48
33:a:1458:G:H5'	52:t:26:MET:HB3	1.95	0.48
52:t:22:SER:O	52:t:25:SER:HB3	2.13	0.48
1:A:290:U:H2'	1:A:291:G:H8	1.79	0.48
1:A:793:A:OP2	1:A:2071:A:O2'	2.28	0.48
1:A:1613:G:H4'	29:2:3:ARG:HE	1.78	0.48
1:A:2618:G:H21	4:D:155:VAL:HG21	1.78	0.48
1:A:2822:G:O2'	1:A:2825:G:N1	2.40	0.48
8:H:94:ILE:HG23	8:H:98:ASP:HB2	1.95	0.48
11:K:35:VAL:HG11	11:K:106:GLU:HB2	1.95	0.48
21:U:14:THR:OG1	21:U:68:ASN:ND2	2.44	0.48
33:a:708:C:H5'	43:k:21:HIS:CD2	2.49	0.48
33:a:1119:C:OP2	41:i:10:ARG:NH1	2.47	0.48
33:a:1386:G:H2'	33:a:1387:G:H8	1.79	0.48
46:n:69:ARG:NH1	46:n:71:HIS:O	2.46	0.48
54:w:257:GLY:HA3	54:w:264:GLY:HA3	1.96	0.48
1:A:227:A:H61	1:A:410:G:H21	1.60	0.48
1:A:355:U:H2'	1:A:356:G:H8	1.79	0.48
1:A:2002:G:OP2	14:N:9:GLN:NE2	2.47	0.48
35:c:87:ARG:HG3	35:c:98:ALA:C	2.38	0.48
2:B:1:U:H2'	2:B:2:G:H8	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:36:GLN:OE1	4:D:49:GLN:NE2	2.47	0.47
52:t:61:ALA:HA	52:t:66:ILE:HB	1.95	0.47
1:A:196:A:N6	1:A:831:G:H21	2.10	0.47
1:A:806:C:O2	1:A:2444:G:O2'	2.32	0.47
1:A:1796:U:H3	1:A:1823:G:H1	1.62	0.47
17:Q:87:VAL:HG13	18:R:49:ILE:HD11	1.96	0.47
29:2:12:ARG:HE	29:2:44:VAL:HG21	1.78	0.47
33:a:1071:C:H2'	33:a:1072:G:H8	1.79	0.47
54:w:314:ARG:NH1	54:w:418:GLN:HA	2.11	0.47
54:w:333:GLN:O	54:w:337:ALA:N	2.47	0.47
1:A:1046:A:H4'	32:5:61:ARG:HB3	1.96	0.47
1:A:1190:G:H5''	12:L:32:GLY:HA2	1.96	0.47
1:A:1394:U:O2	20:T:19:LYS:NZ	2.40	0.47
1:A:2647:U:H2'	1:A:2648:G:H8	1.79	0.47
33:a:55:A:C5	54:w:311:HIS:CE1	3.02	0.47
33:a:403:C:OP1	36:d:114:ARG:NH2	2.47	0.47
34:b:75:ALA:O	34:b:79:VAL:N	2.45	0.47
40:h:52:GLY:HA3	40:h:56:PRO:HA	1.96	0.47
1:A:213:A:H2'	1:A:214:G:C8	2.50	0.47
1:A:1913:A:H61	33:a:1492:A:H1'	1.77	0.47
10:J:36:LEU:HD22	10:J:121:LYS:HB2	1.94	0.47
33:a:1224:U:O2'	33:a:1322:C:OP1	2.30	0.47
1:A:519:U:H2'	1:A:520:G:H8	1.79	0.47
1:A:582:A:H2'	1:A:583:G:H8	1.80	0.47
1:A:2052:A:O2'	4:D:149:ASN:O	2.33	0.47
5:E:75:SER:HB3	5:E:78:TRP:HD1	1.78	0.47
20:T:38:ALA:HB1	20:T:43:ILE:HD11	1.95	0.47
38:f:15:SER:HA	38:f:18:VAL:HG23	1.96	0.47
41:i:16:ALA:HA	41:i:65:THR:O	2.13	0.47
45:m:106:ARG:HH21	45:m:112:ARG:HE	1.61	0.47
50:r:21:ASP:OD2	50:r:23:LYS:NZ	2.46	0.47
1:A:1429:G:H2'	1:A:1430:G:H8	1.79	0.47
1:A:1917:U:H3'	1:A:1918:A:H8	1.80	0.47
16:P:25:VAL:HG22	16:P:85:VAL:HG22	1.96	0.47
16:P:84:SER:OG	16:P:86:LYS:NZ	2.48	0.47
1:A:76:C:OP1	25:Y:48:ARG:NH1	2.48	0.47
1:A:764:A:N3	3:C:211:ARG:NH1	2.63	0.47
1:A:1333:G:H2'	1:A:1334:G:H8	1.80	0.47
1:A:2295:C:OP1	15:O:10:ARG:NH1	2.42	0.47
1:A:2512:C:OP2	4:D:128:ARG:NH2	2.47	0.47
3:C:267:VAL:HG12	3:C:268:ARG:HG2	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:a:104:G:N7	52:t:8:LYS:NZ	2.60	0.47
35:c:18:ASN:OD1	35:c:53:ARG:NH2	2.47	0.47
40:h:28:SER:HB3	40:h:56:PRO:HB2	1.96	0.47
43:k:115:ILE:HB	43:k:116:PRO:CD	2.45	0.47
44:l:122:LYS:HE3	54:w:486:LYS:HB3	1.95	0.47
54:w:488:LYS:HB2	54:w:517:ARG:HH21	1.80	0.47
1:A:302:C:H2'	1:A:303:G:H8	1.79	0.47
1:A:1936:A:OP2	1:A:1962:C:N4	2.41	0.47
32:5:30:SER:HB3	32:5:109:LYS:HD2	1.97	0.47
33:a:684:U:H1'	43:k:40:ALA:HB3	1.97	0.47
1:A:33:C:O2	1:A:447:A:N6	2.48	0.47
1:A:1291:C:H2'	1:A:1292:G:H8	1.80	0.47
1:A:1830:C:H2'	1:A:1831:G:H8	1.80	0.47
1:A:2245:U:H5''	1:A:2246:G:H5'	1.95	0.47
1:A:2458:G:O2'	1:A:2460:U:O4	2.33	0.47
33:a:1261:A:H5''	33:a:1262:C:H5	1.79	0.47
1:A:244:A:OP2	30:3:7:ARG:NH1	2.45	0.47
1:A:537:G:H4'	10:J:5:THR:HG21	1.96	0.47
1:A:1071:G:N2	1:A:1089:A:O2'	2.44	0.47
1:A:2223:G:OP1	3:C:170:TYR:OH	2.33	0.47
5:E:182:ALA:HB2	12:L:3:LEU:HD22	1.97	0.47
42:j:52:LEU:HD23	42:j:62:ARG:HG2	1.95	0.47
43:k:118:ASN:ND2	43:k:118:ASN:C	2.73	0.47
1:A:139:U:O2'	1:A:140:C:O2	2.32	0.46
1:A:351:C:H2'	1:A:352:A:H8	1.80	0.46
1:A:779:U:O2	1:A:785:G:O6	2.33	0.46
5:E:3:LEU:HD13	5:E:120:VAL:HG21	1.96	0.46
36:d:158:LEU:O	36:d:161:ALA:HB3	2.16	0.46
1:A:781:A:OP1	3:C:216:ARG:NH2	2.46	0.46
1:A:2611:C:H5	55:z:12:ARG:NH1	2.04	0.46
33:a:552:U:H2'	33:a:553:A:H8	1.80	0.46
35:c:109:GLU:HB2	35:c:143:LEU:HD13	1.97	0.46
1:A:283:G:H1	1:A:357:C:H42	1.62	0.46
1:A:767:U:H2'	1:A:768:G:H8	1.80	0.46
1:A:1368:G:H2'	1:A:1369:G:H8	1.80	0.46
1:A:1940:U:OP1	1:A:2603:G:N2	2.48	0.46
9:I:102:ARG:NH1	9:I:106:GLN:OE1	2.48	0.46
33:a:150:U:H2'	33:a:151:A:H8	1.79	0.46
33:a:652:U:O4	33:a:752:G:O2'	2.30	0.46
33:a:829:G:H2'	33:a:830:G:C8	2.51	0.46
33:a:1405:G:O2'	33:a:1518:A:O2'	2.26	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:e:92:ARG:HB2	37:e:127:TYR:HB2	1.98	0.46
54:w:9:GLU:HG2	54:w:12:LYS:HD2	1.97	0.46
54:w:430:PRO:HD2	54:w:436:LEU:HD23	1.97	0.46
1:A:2047:C:H2'	1:A:2048:G:H8	1.81	0.46
33:a:19:A:OP1	37:e:129:SER:OG	2.29	0.46
33:a:745:G:H2'	33:a:746:A:H8	1.81	0.46
33:a:1150:A:H2'	33:a:1151:A:H8	1.79	0.46
45:m:15:VAL:HG23	45:m:16:ILE:HD12	1.97	0.46
54:w:312:ARG:HG2	54:w:313:ASP:H	1.80	0.46
54:w:329:MET:HE3	54:w:381:GLN:HE21	1.80	0.46
1:A:848:C:H2'	1:A:849:A:H8	1.81	0.46
1:A:1171:G:N2	1:A:1179:G:N7	2.63	0.46
5:E:149:ILE:HD11	5:E:172:ALA:HA	1.98	0.46
6:F:140:ILE:HG22	6:F:142:TYR:H	1.80	0.46
25:Y:37:LEU:HD11	25:Y:42:LEU:HD12	1.97	0.46
33:a:355:C:H1'	33:a:388:G:H1'	1.98	0.46
33:a:599:C:H2'	33:a:600:A:H8	1.79	0.46
33:a:891:U:H2'	33:a:892:A:H8	1.80	0.46
33:a:979:C:O2	46:n:59:ARG:NH1	2.43	0.46
38:f:6:ILE:HB	38:f:62:MET:HB2	1.97	0.46
2:B:44:G:H1'	2:B:47:C:H42	1.81	0.46
26:Z:16:LEU:HB2	26:Z:19:HIS:HD2	1.80	0.46
33:a:783:C:H2'	33:a:784:A:H8	1.79	0.46
1:A:414:C:H2'	1:A:415:A:H8	1.81	0.46
10:J:36:LEU:HD11	10:J:122:LEU:HD13	1.97	0.46
19:S:69:LEU:HA	19:S:109:ASP:HA	1.98	0.46
32:5:24:SER:HB2	32:5:116:GLU:HG3	1.97	0.46
33:a:143:A:H2	33:a:220:G:H1	1.63	0.46
33:a:477:C:H2'	33:a:478:A:C8	2.51	0.46
33:a:811:C:O2'	33:a:901:A:N1	2.49	0.46
1:A:581:C:H2'	1:A:582:A:H8	1.80	0.46
1:A:2313:C:H2'	1:A:2314:A:H8	1.80	0.46
33:a:876:C:H2'	33:a:877:G:H8	1.80	0.46
33:a:945:G:N2	33:a:1334:G:O2'	2.49	0.46
34:b:91:VAL:HG11	34:b:95:TRP:HD1	1.80	0.46
37:e:98:ALA:HB3	37:e:122:VAL:HA	1.97	0.46
41:i:17:ARG:O	41:i:64:ILE:HA	2.16	0.46
52:t:4:LYS:HG3	52:t:6:ALA:H	1.81	0.46
1:A:581:C:H2'	1:A:582:A:C8	2.51	0.46
1:A:2314:A:OP1	6:F:87:LYS:NZ	2.48	0.46
21:U:20:LYS:HB3	21:U:38:ILE:HD12	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:a:501:C:H2'	33:a:502:A:H8	1.81	0.46
33:a:1162:C:H2'	33:a:1163:A:H8	1.81	0.46
54:w:21:HIS:NE2	54:w:120:GLU:OE1	2.43	0.46
1:A:577:G:O2'	1:A:1254:A:OP1	2.33	0.46
1:A:1209:U:H4'	1:A:1212:G:H4'	1.97	0.46
1:A:1638:C:O2	1:A:2698:U:O2'	2.34	0.46
1:A:1687:G:N2	1:A:1701:A:H62	2.13	0.46
41:i:37:TYR:HD2	41:i:38:PHE:HD1	1.63	0.46
51:s:14:LEU:HD22	51:s:34:SER:HB3	1.98	0.46
1:A:917:A:H5''	1:A:2268:A:H61	1.80	0.45
4:D:37:VAL:HG22	4:D:48:ILE:HG22	1.98	0.45
12:L:20:GLY:H	12:L:28:GLY:HA2	1.80	0.45
33:a:924:C:H2'	33:a:925:G:H8	1.81	0.45
43:k:118:ASN:C	43:k:118:ASN:HD22	2.24	0.45
54:w:144:LEU:HB2	54:w:258:THR:HB	1.98	0.45
1:A:2523:G:O2'	1:A:2764:A:O2'	2.32	0.45
1:A:2719:G:H4'	1:A:2846:G:H4'	1.97	0.45
1:A:212:G:H2'	1:A:213:A:C8	2.50	0.45
1:A:1386:C:H2'	1:A:1387:A:C8	2.51	0.45
1:A:1997:C:H2'	1:A:1998:A:H8	1.82	0.45
20:T:37:ASP:OD1	20:T:37:ASP:N	2.48	0.45
33:a:8:A:N6	36:d:201:GLU:O	2.45	0.45
33:a:620:C:H1'	36:d:131:ILE:HB	1.97	0.45
43:k:111:ASP:H	50:r:72:ARG:NH1	2.13	0.45
1:A:196:A:H61	1:A:831:G:N2	2.11	0.45
1:A:505:A:HO2'	1:A:509:C:HO2'	1.65	0.45
1:A:728:G:H4'	3:C:12:ARG:HD3	1.98	0.45
1:A:994:C:OP1	17:Q:52:ARG:NH2	2.49	0.45
1:A:1827:U:OP2	3:C:220:ARG:NH1	2.49	0.45
33:a:376:G:H2'	33:a:377:G:H8	1.81	0.45
33:a:1233:G:O2'	33:a:1365:G:OP1	2.35	0.45
43:k:115:ILE:HG22	43:k:116:PRO:CD	2.41	0.45
43:k:116:PRO:HB2	43:k:119:GLY:N	2.32	0.45
51:s:49:ALA:HB1	51:s:56:HIS:HB3	1.98	0.45
1:A:1287:A:H62	14:N:106:ASP:HB3	1.81	0.45
1:A:2070:A:H2'	1:A:2071:A:H8	1.80	0.45
1:A:2086:U:H2'	1:A:2087:G:C8	2.52	0.45
1:A:2086:U:H2'	1:A:2087:G:H8	1.81	0.45
2:B:111:U:H2'	2:B:112:G:H8	1.82	0.45
42:j:11:LYS:HB3	42:j:71:LEU:HG	1.97	0.45
43:k:121:ARG:HD3	53:u:31:VAL:O	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1921:G:H2'	1:A:1922:G:H8	1.81	0.45
1:A:2006:C:O2'	1:A:2823:A:N3	2.49	0.45
1:A:2475:C:N4	1:A:2529:G:N2	2.44	0.45
1:A:2818:U:H2'	1:A:2819:G:C8	2.51	0.45
33:a:614:C:OP2	36:d:80:ARG:NH2	2.42	0.45
1:A:2514:U:H5''	10:J:81:ILE:HD11	1.98	0.45
4:D:9:VAL:HA	4:D:197:THR:HG23	1.99	0.45
6:F:91:ARG:HA	6:F:95:MET:HB3	1.99	0.45
9:I:89:SER:HB3	9:I:135:MET:HA	1.98	0.45
24:X:6:VAL:HA	24:X:73:ARG:HH22	1.80	0.45
39:g:12:LEU:HD12	39:g:13:PRO:HD2	1.99	0.45
1:A:1636:U:H2'	1:A:1637:A:H8	1.81	0.45
8:H:70:GLU:HB2	8:H:134:VAL:HG21	1.99	0.45
33:a:427:U:O2'	33:a:541:G:OP1	2.35	0.45
33:a:1457:G:H2'	33:a:1458:G:H8	1.82	0.45
54:w:318:MET:H	54:w:364:ILE:HG23	1.82	0.45
1:A:552:U:H2'	1:A:553:G:H8	1.82	0.45
1:A:2047:C:O2'	1:A:2823:A:N1	2.49	0.45
1:A:2497:A:H1'	1:A:2498:C:H5	1.82	0.45
33:a:1492:A:OP2	44:l:40:THR:OG1	2.28	0.45
33:a:1507:A:H2'	33:a:1508:A:C8	2.52	0.45
35:c:9:ILE:HG23	35:c:10:ARG:HG3	1.97	0.45
36:d:87:GLU:HG3	36:d:187:ARG:HB2	1.97	0.45
54:w:159:GLU:HG2	54:w:165:GLY:HA2	1.99	0.45
54:w:315:VAL:HG22	54:w:316:ALA:N	2.30	0.45
1:A:589:U:H2'	1:A:590:A:C8	2.52	0.45
1:A:1387:A:H5'	1:A:1469:A:H1'	1.98	0.45
1:A:1509:A:H2'	1:A:1510:G:C8	2.52	0.45
1:A:2443:C:H2'	1:A:2444:G:C8	2.52	0.45
4:D:109:VAL:HG22	4:D:203:VAL:HG22	1.99	0.45
33:a:398:U:H2'	33:a:399:G:H8	1.82	0.45
43:k:86:LYS:HZ3	43:k:113:THR:HG23	1.80	0.45
43:k:123:PRO:C	53:u:34:ARG:N	2.75	0.45
54:w:13:ARG:HH21	54:w:360:TYR:HB2	1.82	0.45
54:w:496:ASP:HB2	54:w:500:ASN:HB2	1.98	0.45
1:A:2291:U:O2	1:A:2374:C:O2'	2.32	0.44
2:B:93:C:H2'	2:B:94:A:H8	1.81	0.44
22:V:20:LEU:HD11	22:V:41:GLU:HG3	1.98	0.44
27:0:42:ILE:HG22	27:0:48:TYR:HB2	2.00	0.44
33:a:193:C:H4'	52:t:55:PRO:HB3	1.99	0.44
33:a:720:C:H5'	50:r:40:PRO:HB3	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:a:1368:A:OP2	41:i:113:LYS:NZ	2.42	0.44
34:b:202:ASN:HD22	34:b:203:ASP:H	1.65	0.44
52:t:10:ALA:O	52:t:13:SER:OG	2.27	0.44
1:A:16:C:H2'	1:A:17:G:H8	1.81	0.44
1:A:210:C:OP1	29:2:29:GLN:NE2	2.49	0.44
1:A:1913:A:H5'	33:a:1494:G:H1'	1.98	0.44
6:F:115:GLY:HA3	6:F:177:ARG:HB2	1.99	0.44
33:a:60:A:N1	33:a:107:G:O2'	2.40	0.44
33:a:331:G:O2'	52:t:2:ASN:ND2	2.50	0.44
33:a:345:C:O2'	33:a:346:G:N2	2.49	0.44
33:a:422:C:O2'	33:a:423:G:N2	2.51	0.44
33:a:516:U:H5	33:a:519:C:H42	1.65	0.44
33:a:1500:A:H5''	33:a:1508:A:H5''	1.98	0.44
38:f:10:VAL:HB	38:f:58:HIS:HB3	1.98	0.44
39:g:67:ASN:O	39:g:137:ARG:NE	2.50	0.44
43:k:116:PRO:O	43:k:117:HIS:HB2	2.18	0.44
54:w:97:GLU:HA	54:w:100:TYR:HD2	1.82	0.44
1:A:302:C:H2'	1:A:303:G:C8	2.53	0.44
1:A:464:U:O2	29:2:16:HIS:NE2	2.50	0.44
1:A:476:G:O2'	1:A:502:A:N6	2.46	0.44
33:a:1088:G:H21	33:a:1167:A:H61	1.66	0.44
36:d:60:VAL:HG21	36:d:199:ILE:HD11	1.99	0.44
54:w:347:THR:OG1	54:w:354:SER:OG	2.34	0.44
19:S:17:VAL:HG12	19:S:76:VAL:HG21	2.00	0.44
33:a:1356:G:H2'	33:a:1357:A:C8	2.51	0.44
35:c:13:ILE:HG22	35:c:14:VAL:HG23	1.99	0.44
37:e:65:LYS:HA	37:e:68:ARG:HG2	2.00	0.44
1:A:1801:A:N6	1:A:2201:G:O2'	2.41	0.44
1:A:2781:A:H5''	1:A:2782:G:H5'	1.99	0.44
2:B:45:A:O4'	6:F:91:ARG:NH2	2.51	0.44
37:e:155:LYS:HB3	40:h:70:VAL:HG13	1.99	0.44
38:f:92:THR:OG1	38:f:93:LYS:N	2.51	0.44
45:m:106:ARG:NH2	45:m:112:ARG:HE	2.15	0.44
51:s:52:ASN:O	51:s:54:ARG:NH1	2.50	0.44
54:w:395:PRO:HD2	54:w:527:ARG:HH21	1.83	0.44
1:A:340:A:O2'	5:E:162:ARG:NH1	2.49	0.44
1:A:605:G:O2'	1:A:657:U:O2	2.33	0.44
1:A:636:G:N7	12:L:109:LYS:NZ	2.56	0.44
1:A:818:G:N2	1:A:1189:A:H62	2.12	0.44
1:A:1164:C:H2'	1:A:1165:A:H8	1.82	0.44
1:A:2095:A:O5'	8:H:11:ASN:ND2	2.50	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:115:GLY:HA2	4:D:166:GLY:HA3	1.99	0.44
6:F:28:PRO:HB2	6:F:168:LEU:HD22	2.00	0.44
13:M:42:THR:HG22	13:M:93:VAL:HG12	2.00	0.44
1:A:813:U:OP1	18:R:84:ARG:NH1	2.50	0.44
1:A:2246:G:H2'	1:A:2247:A:H8	1.83	0.44
1:A:2656:U:OP1	54:w:146:ARG:NH2	2.44	0.44
33:a:34:C:H2'	33:a:35:G:H8	1.82	0.44
33:a:501:C:H1'	33:a:549:C:H1'	2.00	0.44
33:a:1310:G:H5''	45:m:78:ARG:HH21	1.83	0.44
33:a:1499:A:H2'	33:a:1500:A:H8	1.82	0.44
39:g:110:ARG:HH12	39:g:121:ASN:HB3	1.83	0.44
43:k:23:HIS:O	43:k:29:THR:HA	2.17	0.44
54:w:431:ILE:HD11	54:w:493:LEU:HB2	2.00	0.44
54:w:525:GLN:HG3	54:w:527:ARG:HB2	2.00	0.44
1:A:224:U:OP2	1:A:408:G:N2	2.41	0.44
1:A:929:U:H2'	1:A:930:G:C8	2.53	0.44
20:T:54:GLU:HB3	20:T:88:LYS:HD2	2.00	0.44
33:a:401:C:O2'	33:a:621:A:N3	2.42	0.44
33:a:1287:A:H2	33:a:1353:G:H1'	1.82	0.44
33:a:1375:A:O2'	39:g:101:ARG:NH2	2.51	0.44
34:b:75:ALA:O	34:b:78:ALA:HB3	2.17	0.44
39:g:70:PRO:O	39:g:95:ARG:NH1	2.48	0.44
42:j:22:THR:HA	42:j:25:ILE:HG22	2.00	0.44
54:w:506:THR:OG1	54:w:510:ASN:ND2	2.51	0.44
1:A:1432:G:H2'	1:A:1433:A:C8	2.53	0.44
1:A:2898:U:H2'	1:A:2899:A:C8	2.53	0.44
32:5:18:VAL:HA	32:5:86:MET:HE2	2.00	0.44
33:a:490:C:H2'	33:a:491:G:H8	1.83	0.44
33:a:1186:G:H2'	33:a:1187:G:C8	2.52	0.44
38:f:97:THR:OG1	38:f:98:GLU:N	2.49	0.44
1:A:248:G:O2'	1:A:2432:A:OP1	2.29	0.43
1:A:1131:G:O2'	1:A:2025:C:O2'	2.35	0.43
1:A:2175:C:H2'	1:A:2176:A:H8	1.82	0.43
1:A:2293:G:OP1	15:O:94:ARG:NH1	2.51	0.43
7:G:25:ILE:HD12	7:G:74:MET:HE2	1.99	0.43
35:c:94:ALA:C	35:c:96:VAL:H	2.22	0.43
37:e:35:LEU:HD22	37:e:133:ILE:HG13	1.99	0.43
1:A:572:A:H61	1:A:2029:G:H21	1.66	0.43
1:A:2468:A:OP2	1:A:2476:A:N6	2.51	0.43
13:M:50:ARG:HD3	13:M:65:ILE:HD11	2.00	0.43
30:3:31:ILE:H	30:3:31:ILE:HG13	1.47	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
43:k:110:THR:HB	50:r:72:ARG:HH12	1.83	0.43
1:A:29:U:O2	1:A:1215:G:O2'	2.34	0.43
1:A:672:C:OP2	12:L:42:SER:OG	2.31	0.43
1:A:1431:A:H2'	1:A:1432:G:H8	1.82	0.43
1:A:2279:G:O2'	1:A:2327:A:O2'	2.30	0.43
3:C:70:LYS:O	3:C:117:SER:OG	2.32	0.43
16:P:91:VAL:HG21	16:P:96:LEU:HD11	2.00	0.43
17:Q:99:VAL:O	17:Q:102:LYS:NZ	2.51	0.43
22:V:77:VAL:HG23	22:V:89:ILE:HG12	2.00	0.43
33:a:880:C:H2'	33:a:881:G:H8	1.83	0.43
34:b:113:LEU:HD13	34:b:143:LEU:HB3	2.00	0.43
35:c:31:ASN:OD1	35:c:58:ARG:NH2	2.51	0.43
41:i:111:GLU:OE1	41:i:114:LYS:NZ	2.52	0.43
43:k:49:SER:HA	43:k:68:ARG:HH11	1.82	0.43
44:l:40:THR:HA	44:l:41:PRO:HD3	1.89	0.43
46:n:61:ARG:HE	46:n:70:PRO:HB2	1.84	0.43
1:A:2298:A:H5''	6:F:71:LYS:HD3	2.00	0.43
8:H:125:THR:HG23	8:H:146:VAL:HG12	2.00	0.43
32:5:56:ARG:HE	32:5:83:ALA:HB2	1.82	0.43
33:a:1099:G:H5''	34:b:94:ARG:HH21	1.84	0.43
42:j:6:ILE:HB	42:j:76:ILE:HB	2.01	0.43
1:A:631:A:N3	1:A:2415:G:O2'	2.42	0.43
1:A:1796:U:H2'	1:A:1797:G:C8	2.54	0.43
1:A:2183:A:H2'	1:A:2184:A:C8	2.54	0.43
2:B:114:C:H2'	2:B:115:A:C8	2.53	0.43
5:E:145:ASP:HA	5:E:166:LYS:HB3	2.00	0.43
6:F:30:VAL:HG13	6:F:95:MET:HE1	1.99	0.43
25:Y:24:GLU:HB3	25:Y:46:VAL:HG21	2.00	0.43
33:a:358:U:O2'	54:w:310:LYS:O	2.19	0.43
33:a:411:A:H62	33:a:413:G:H21	1.67	0.43
36:d:53:GLN:HB3	36:d:202:LEU:HD12	2.00	0.43
1:A:598:U:H2'	1:A:599:A:H8	1.82	0.43
1:A:690:G:H4'	3:C:216:ARG:HH22	1.83	0.43
1:A:751:A:N1	55:z:7:TYR:CE1	2.87	0.43
1:A:787:C:H5''	1:A:788:A:H5'	2.01	0.43
1:A:969:G:H4'	26:Z:14:GLY:HA2	2.01	0.43
6:F:42:ALA:HB3	6:F:84:ILE:HD12	2.01	0.43
10:J:32:LEU:HD22	10:J:54:ILE:HG21	2.01	0.43
13:M:47:GLU:OE2	13:M:51:ARG:NE	2.52	0.43
14:N:42:LYS:HA	14:N:45:ARG:HE	1.83	0.43
20:T:6:ARG:NH1	20:T:42:GLU:OE1	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:a:898:G:N2	33:a:901:A:OP2	2.51	0.43
33:a:1218:C:H2'	33:a:1219:A:C8	2.53	0.43
44:l:33:CYS:HA	44:l:54:VAL:HA	2.00	0.43
47:o:35:ILE:HG13	47:o:58:MET:HE2	2.00	0.43
1:A:1295:C:H2'	1:A:1296:G:H8	1.84	0.43
1:A:2144:G:H1'	1:A:2147:A:H61	1.83	0.43
33:a:832:G:OP1	34:b:20:ARG:NH1	2.46	0.43
33:a:946:A:H2'	33:a:947:G:H8	1.84	0.43
33:a:1392:G:H21	33:a:1502:A:H4'	1.84	0.43
35:c:54:ILE:HD12	35:c:56:ILE:HD11	1.99	0.43
35:c:86:LEU:HA	35:c:89:VAL:CG2	2.48	0.43
41:i:112:ARG:HH22	42:j:64:GLN:HE22	1.65	0.43
54:w:111:MET:HB2	54:w:139:THR:HG22	2.00	0.43
54:w:315:VAL:O	54:w:315:VAL:HG13	2.18	0.43
1:A:261:G:H2'	1:A:262:A:H8	1.83	0.43
1:A:1033:U:O2'	1:A:2750:A:N6	2.52	0.43
1:A:1431:A:H2'	1:A:1432:G:C8	2.53	0.43
1:A:1841:U:H2'	1:A:1842:G:H8	1.83	0.43
3:C:154:ALA:HB2	3:C:161:VAL:HG23	2.01	0.43
33:a:335:C:H2'	33:a:336:A:C8	2.53	0.43
33:a:501:C:OP2	44:l:120:ARG:NH1	2.50	0.43
54:w:297:THR:HB	54:w:387:PHE:HZ	1.84	0.43
1:A:2313:C:H2'	1:A:2314:A:C8	2.53	0.43
11:K:76:VAL:H	16:P:72:VAL:HG22	1.84	0.43
33:a:501:C:H2'	33:a:502:A:C8	2.53	0.43
33:a:634:C:H2'	33:a:635:A:H8	1.84	0.43
1:A:1:G:H2'	1:A:2:G:C8	2.54	0.43
1:A:526:A:O2'	1:A:2043:C:O2	2.29	0.43
1:A:1254:A:H5''	1:A:1255:U:H5''	2.01	0.43
1:A:2307:G:H1	6:F:40:GLY:HA3	1.83	0.43
1:A:2372:U:H2'	1:A:2373:G:H8	1.82	0.43
1:A:2380:C:H2'	1:A:2381:A:C8	2.54	0.43
1:A:2395:C:H2'	1:A:2396:G:H8	1.84	0.43
2:B:8:C:O2'	15:O:25:ARG:NH1	2.51	0.43
2:B:14:U:OP2	2:B:70:C:O2'	2.36	0.43
17:Q:93:ILE:HG23	18:R:13:ARG:HB2	2.00	0.43
33:a:715:A:O5'	33:a:715:A:H8	2.00	0.43
33:a:1427:C:H2'	33:a:1428:A:H8	1.84	0.43
37:e:131:ASN:HB3	37:e:134:ASN:HB2	2.01	0.43
1:A:662:G:H2'	1:A:663:G:H8	1.84	0.42
1:A:2131:U:H5'	1:A:2132:U:H5''	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2836:U:H2'	1:A:2837:A:H8	1.84	0.42
33:a:662:U:H2'	33:a:663:A:C8	2.54	0.42
33:a:1347:G:N2	33:a:1374:A:OP2	2.43	0.42
36:d:86:GLY:HA3	36:d:196:GLU:HG3	2.01	0.42
54:w:428:PHE:HB2	54:w:437:ILE:HB	2.01	0.42
1:A:2240:U:H2'	1:A:2241:A:H8	1.83	0.42
8:H:17:ASP:HB3	8:H:19:VAL:HG23	2.00	0.42
24:X:39:VAL:O	24:X:43:LYS:CA	2.66	0.42
28:1:33:LEU:H	28:1:50:GLU:HB2	1.85	0.42
33:a:1269:A:O2'	33:a:1325:C:O2	2.35	0.42
33:a:1496:C:H2'	33:a:1497:G:C8	2.54	0.42
48:p:79:ASN:HB2	48:p:82:ALA:HB3	2.01	0.42
1:A:18:U:O2'	1:A:554:U:OP1	2.37	0.42
1:A:284:U:H3	1:A:356:G:H1	1.66	0.42
1:A:373:U:H2'	1:A:374:A:H8	1.84	0.42
1:A:2595:G:N2	1:A:2598:A:OP2	2.39	0.42
1:A:2771:C:O2'	4:D:173:GLN:NE2	2.48	0.42
1:A:2899:A:H2'	1:A:2900:A:C8	2.55	0.42
9:I:117:THR:HG22	32:5:42:ARG:HH21	1.84	0.42
28:1:36:LYS:HG3	28:1:47:ILE:HG13	2.02	0.42
32:5:33:VAL:HG12	32:5:35:VAL:H	1.83	0.42
33:a:722:G:OP2	53:u:44:ARG:NH1	2.52	0.42
54:w:109:CYS:HB3	54:w:137:ILE:HG12	2.00	0.42
54:w:477:ALA:HB3	54:w:482:PHE:HB3	2.01	0.42
1:A:1093:G:N2	1:A:1098:A:H62	2.13	0.42
1:A:1675:C:O2	4:D:133:THR:OG1	2.38	0.42
1:A:2691:C:H2'	1:A:2692:G:C8	2.54	0.42
33:a:126:G:OP1	33:a:605:U:O2'	2.29	0.42
33:a:641:U:H4'	33:a:642:A:H8	1.83	0.42
33:a:1342:C:H2'	33:a:1343:G:C8	2.54	0.42
33:a:1512:U:H2'	33:a:1513:A:C8	2.53	0.42
35:c:88:LYS:O	35:c:92:ASP:CG	2.63	0.42
52:t:12:GLN:O	52:t:15:LYS:HB3	2.18	0.42
54:w:429:ARG:O	54:w:495:LEU:N	2.52	0.42
1:A:1597:A:H4'	1:A:1598:A:H8	1.85	0.42
1:A:1665:A:H2'	1:A:1666:G:H8	1.83	0.42
1:A:2035:G:H5''	1:A:2036:C:H5	1.85	0.42
1:A:2251:G:H2'	1:A:2252:G:H8	1.84	0.42
1:A:2361:G:OP1	30:3:25:HIS:ND1	2.38	0.42
1:A:2691:C:H2'	1:A:2692:G:H8	1.83	0.42
1:A:2832:U:H1'	1:A:2834:G:C2	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:40:U:N3	2:B:44:G:OP2	2.41	0.42
15:O:69:ASP:OD1	15:O:69:ASP:N	2.53	0.42
19:S:78:GLU:OE1	19:S:99:ARG:NH2	2.52	0.42
33:a:716:A:C2	43:k:118:ASN:CA	2.95	0.42
53:u:20:ARG:HA	53:u:24:LYS:HB3	2.00	0.42
1:A:546:U:H2'	1:A:547:A:H4'	2.00	0.42
1:A:2630:G:H2'	1:A:2631:G:C8	2.55	0.42
2:B:78:A:N6	2:B:98:G:H21	2.12	0.42
3:C:56:GLY:HA2	3:C:212:TRP:HA	2.01	0.42
11:K:121:GLU:HG2	11:K:122:VAL:HG23	2.01	0.42
16:P:88:ARG:HB3	16:P:112:ARG:HD3	2.01	0.42
1:A:655:A:H4'	1:A:656:G:H5'	2.01	0.42
1:A:1140:C:H5'	10:J:26:GLY:HA3	2.01	0.42
1:A:1395:A:O2'	1:A:1397:U:OP2	2.37	0.42
1:A:1681:G:H21	1:A:1762:A:H3'	1.84	0.42
1:A:1769:U:H2'	1:A:1770:G:H8	1.85	0.42
1:A:2060:A:H62	5:E:69:ARG:HH22	1.68	0.42
1:A:2676:C:O2	1:A:2732:G:N2	2.49	0.42
8:H:30:LEU:HA	8:H:35:LYS:HB2	2.01	0.42
8:H:113:SER:O	8:H:116:ARG:NH1	2.47	0.42
14:N:59:SER:OG	14:N:62:ASN:OD1	2.31	0.42
33:a:107:G:OP1	33:a:325:A:N6	2.51	0.42
45:m:85:TYR:CZ	45:m:89:ARG:HD2	2.55	0.42
49:q:11:VAL:HG22	49:q:22:VAL:HG22	2.02	0.42
1:A:1700:A:H3'	1:A:1701:A:H8	1.85	0.42
6:F:135:ILE:H	6:F:135:ILE:HG13	1.73	0.42
20:T:8:LEU:HD11	25:Y:22:LEU:HD12	2.01	0.42
32:5:48:ALA:HB3	32:5:51:TYR:HE1	1.84	0.42
33:a:925:G:H2'	33:a:927:G:H8	1.85	0.42
33:a:1412:C:OP1	44:l:53:ARG:NH2	2.53	0.42
36:d:71:PHE:HE1	36:d:93:LEU:HD11	1.83	0.42
48:p:52:LEU:HD23	48:p:78:VAL:HG11	2.02	0.42
54:w:488:LYS:HB2	54:w:517:ARG:NH2	2.34	0.42
1:A:414:C:H2'	1:A:415:A:C8	2.55	0.42
1:A:1913:A:C2'	33:a:1408:A:C2	3.03	0.42
1:A:2023:C:H2'	1:A:2024:G:C8	2.55	0.42
1:A:2525:G:H2'	1:A:2526:G:H8	1.84	0.42
1:A:2883:A:OP1	27:O:48:TYR:OH	2.38	0.42
5:E:47:LYS:HB2	5:E:51:GLU:HB2	2.01	0.42
11:K:103:VAL:HG21	11:K:116:ILE:HG22	2.01	0.42
12:L:49:GLY:HA3	12:L:58:TYR:HE1	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:P:105:LYS:O	16:P:108:ARG:NH2	2.52	0.42
26:Z:11:SER:OG	26:Z:12:ALA:N	2.53	0.42
33:a:1015:G:H2'	33:a:1016:A:C8	2.55	0.42
33:a:1320:C:OP2	51:s:2:ARG:NH2	2.53	0.42
44:l:98:ARG:HB2	44:l:116:TYR:HA	2.02	0.42
1:A:5:A:H2'	1:A:6:A:C8	2.55	0.42
1:A:78:U:O4	1:A:108:G:O6	2.38	0.42
3:C:74:PRO:HB3	3:C:114:GLN:HE21	1.85	0.42
3:C:75:ALA:HB3	3:C:115:ILE:HG13	2.01	0.42
19:S:77:ASP:OD1	19:S:77:ASP:N	2.53	0.42
54:w:399:ARG:HG3	54:w:466:VAL:HB	2.02	0.42
1:A:713:G:H21	1:A:718:A:H62	1.68	0.41
1:A:1462:C:O2'	1:A:2702:G:O2'	2.35	0.41
1:A:1592:C:H2'	1:A:1593:A:H8	1.84	0.41
1:A:2329:U:H2'	1:A:2330:G:C8	2.55	0.41
1:A:2581:G:H22	1:A:2610:C:H2'	1.85	0.41
3:C:206:LYS:HE2	3:C:208:GLY:HA3	2.02	0.41
19:S:62:ASP:N	19:S:62:ASP:OD1	2.51	0.41
20:T:22:THR:HA	20:T:25:GLU:HG2	2.01	0.41
22:V:48:MET:SD	22:V:51:GLN:NE2	2.93	0.41
33:a:197:A:N1	33:a:220:G:O2'	2.52	0.41
33:a:808:C:H5''	47:o:46:LYS:HD2	2.02	0.41
33:a:946:A:O2'	33:a:1333:A:N3	2.43	0.41
33:a:1118:U:OP1	41:i:105:ARG:NH2	2.49	0.41
33:a:1247:U:O4	33:a:1290:G:O6	2.37	0.41
33:a:1319:A:H4'	33:a:1320:C:H5'	2.02	0.41
39:g:55:LYS:HB3	39:g:59:GLU:HG3	2.01	0.41
1:A:244:A:H62	1:A:254:G:N2	2.10	0.41
1:A:1716:U:H2'	1:A:1717:A:H8	1.85	0.41
3:C:144:GLU:HB2	3:C:187:CYS:HB3	2.02	0.41
5:E:75:SER:HB3	5:E:78:TRP:CD1	2.53	0.41
18:R:6:GLN:HE21	18:R:11:GLN:NE2	2.18	0.41
33:a:309:A:H2'	33:a:310:G:C8	2.55	0.41
33:a:587:G:OP1	40:h:83:ARG:NH2	2.43	0.41
1:A:225:C:N3	1:A:231:A:N6	2.69	0.41
1:A:406:G:H2'	1:A:407:G:H8	1.84	0.41
7:G:89:VAL:O	7:G:159:LYS:HA	2.21	0.41
33:a:358:U:H2'	33:a:359:G:C8	2.53	0.41
33:a:690:G:OP2	43:k:56:LYS:NZ	2.41	0.41
33:a:746:A:H2'	33:a:747:A:C8	2.55	0.41
43:k:35:ASP:OD1	43:k:38:GLY:N	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:151:C:H2'	1:A:152:A:H8	1.86	0.41
1:A:2487:G:H2'	1:A:2488:G:H8	1.85	0.41
14:N:45:ARG:HG2	14:N:95:THR:HG21	2.02	0.41
33:a:77:A:H2'	33:a:78:A:C8	2.56	0.41
33:a:296:U:O2'	33:a:556:C:O2	2.37	0.41
33:a:320:A:H2'	33:a:321:A:C8	2.55	0.41
33:a:1174:G:H2'	33:a:1175:G:H8	1.86	0.41
33:a:1342:C:O2'	41:i:125:GLN:NE2	2.53	0.41
34:b:71:THR:HG22	34:b:72:LYS:H	1.86	0.41
36:d:131:ILE:HG22	36:d:133:SER:H	1.84	0.41
54:w:315:VAL:HG21	54:w:317:PHE:CZ	2.55	0.41
1:A:65:U:O2'	20:T:73:ARG:NH2	2.53	0.41
1:A:720:U:H2'	1:A:721:A:C8	2.54	0.41
1:A:974:G:H1'	1:A:975:A:C8	2.56	0.41
1:A:1372:U:O2'	1:A:2212:A:N3	2.47	0.41
1:A:1435:G:H2'	1:A:1436:G:C8	2.56	0.41
2:B:24:G:N3	2:B:27:C:N4	2.59	0.41
36:d:197:HIS:NE2	36:d:201:GLU:OE2	2.52	0.41
43:k:115:ILE:CB	43:k:116:PRO:HD3	2.51	0.41
54:w:76:GLN:C	54:w:76:GLN:CD	2.87	0.41
1:A:1515:A:H3'	1:A:1516:G:H8	1.86	0.41
1:A:1653:G:H5''	14:N:2:ARG:HG2	2.02	0.41
1:A:2020:A:N7	27:O:5:ASN:ND2	2.69	0.41
1:A:2189:U:H2'	1:A:2190:G:C8	2.56	0.41
4:D:121:THR:HG21	4:D:143:PRO:HB3	2.02	0.41
30:3:28:LEU:HA	30:3:32:LEU:HD11	2.03	0.41
33:a:715:A:N1	43:k:118:ASN:C	2.79	0.41
33:a:1187:G:N2	46:n:100:SER:OG	2.54	0.41
33:a:1404:C:H2'	33:a:1405:G:C8	2.56	0.41
37:e:80:LEU:HD21	37:e:95:MET:HE2	2.03	0.41
50:r:41:SER:HB3	50:r:51:GLN:HE21	1.85	0.41
1:A:521:U:H2'	1:A:522:A:H8	1.84	0.41
1:A:651:G:H5'	30:3:18:LYS:HG3	2.01	0.41
1:A:1030:C:H2'	1:A:1031:G:C8	2.56	0.41
1:A:2036:C:H2'	1:A:2037:A:C8	2.56	0.41
1:A:2327:A:H2'	1:A:2328:A:C8	2.56	0.41
11:K:21:CYS:HA	11:K:41:ILE:HG22	2.01	0.41
33:a:502:A:OP1	44:l:114:SER:N	2.38	0.41
33:a:1124:G:H1	33:a:1149:C:H42	1.69	0.41
33:a:1346:A:N6	33:a:1375:A:OP2	2.54	0.41
33:a:1354:U:H2'	33:a:1355:G:C8	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:c:38:VAL:HG12	35:c:93:ILE:HG13	2.03	0.41
36:d:84:ASN:O	36:d:88:ASN:ND2	2.54	0.41
51:s:62:THR:HG22	51:s:63:ASP:H	1.86	0.41
54:w:167:ALA:HB2	54:w:251:ILE:HD11	2.02	0.41
1:A:4:U:H2'	1:A:5:A:C8	2.56	0.41
1:A:1024:G:OP2	1:A:1025:G:O2'	2.36	0.41
1:A:1704:C:H2'	1:A:1705:A:C8	2.56	0.41
1:A:2692:G:H2'	1:A:2693:G:C8	2.56	0.41
1:A:2863:C:H2'	1:A:2864:G:H8	1.86	0.41
4:D:47:ALA:HB2	4:D:83:ARG:HD2	2.02	0.41
9:I:56:VAL:HG22	9:I:68:PHE:HB2	2.02	0.41
33:a:458:U:H2'	33:a:459:A:C8	2.55	0.41
33:a:1192:C:OP1	35:c:3:LYS:NZ	2.45	0.41
33:a:1247:U:O2	33:a:1290:G:N2	2.48	0.41
45:m:110:GLY:HA2	45:m:111:PRO:HD3	1.89	0.41
47:o:3:SER:OG	47:o:4:THR:N	2.54	0.41
1:A:466:A:OP1	29:2:34:ARG:NH1	2.54	0.41
1:A:857:G:H4'	23:W:41:PHE:HZ	1.86	0.41
1:A:1501:G:H2'	1:A:1502:A:H8	1.86	0.41
1:A:1744:A:H3'	1:A:1745:A:H8	1.86	0.41
1:A:2087:G:H2'	1:A:2088:A:C8	2.55	0.41
1:A:2215:C:H2'	1:A:2216:G:C8	2.56	0.41
1:A:2304:G:H22	1:A:2312:U:H3	1.69	0.41
6:F:35:LEU:HD23	6:F:151:LEU:HD22	2.03	0.41
9:I:53:PRO:HG2	9:I:77:VAL:HG11	2.03	0.41
10:J:31:GLU:HG2	10:J:142:ILE:HG12	2.01	0.41
20:T:11:LEU:O	25:Y:29:ARG:NH1	2.54	0.41
24:X:39:VAL:O	24:X:43:LYS:HA	2.21	0.41
33:a:81:A:H2'	33:a:82:G:C8	2.55	0.41
33:a:316:C:O3'	33:a:353:A:N6	2.54	0.41
33:a:458:U:H2'	33:a:459:A:H8	1.85	0.41
33:a:1536:C:H5'	33:a:1537:U:H5	1.86	0.41
34:b:17:HIS:HE1	34:b:202:ASN:HA	1.86	0.41
34:b:46:VAL:O	34:b:50:ASN:HB2	2.21	0.41
48:p:2:VAL:HG23	48:p:65:ALA:HA	2.02	0.41
48:p:61:VAL:HG22	48:p:67:ILE:HD11	2.02	0.41
54:w:440:ALA:HB2	54:w:445:GLN:HE21	1.86	0.41
1:A:742:A:H2'	1:A:743:A:C8	2.56	0.41
1:A:1709:U:H2'	1:A:1710:G:H8	1.86	0.41
1:A:1745:A:H2'	1:A:1746:A:H8	1.86	0.41
1:A:2710:C:OP1	14:N:15:SER:OG	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:85:ILE:H	9:I:85:ILE:HG13	1.71	0.41
16:P:38:ARG:CZ	33:a:346:G:H1'	2.51	0.41
33:a:715:A:N1	43:k:119:GLY:HA2	2.36	0.41
34:b:76:SER:HB2	34:b:92:ASN:HB2	2.02	0.41
40:h:45:ILE:HD13	40:h:60:LEU:HD22	2.01	0.41
44:l:23:LEU:HD22	44:l:58:ASN:HD22	1.86	0.41
45:m:49:GLU:HA	45:m:52:ILE:HB	2.03	0.41
50:r:25:ILE:HA	50:r:28:LEU:HB3	2.01	0.41
1:A:568:U:O4	18:R:81:LYS:NZ	2.44	0.40
1:A:1913:A:H8	33:a:1494:G:C4	2.39	0.40
33:a:186:C:H5'	52:t:72:ALA:HB1	2.04	0.40
33:a:599:C:H2'	33:a:600:A:C8	2.56	0.40
33:a:999:C:H2'	33:a:1000:A:C8	2.56	0.40
33:a:1255:G:O2'	33:a:1258:G:N3	2.45	0.40
33:a:1354:U:H2'	33:a:1355:G:H8	1.86	0.40
34:b:77:GLU:O	34:b:80:LYS:HB3	2.21	0.40
36:d:200:VAL:O	36:d:204:SER:OG	2.34	0.40
37:e:83:PRO:HD3	37:e:97:PRO:HG3	2.03	0.40
38:f:50:PRO:HB3	38:f:53:LYS:HG2	2.03	0.40
42:j:11:LYS:HA	42:j:70:HIS:O	2.22	0.40
1:A:576:U:H2'	1:A:577:G:H8	1.86	0.40
1:A:1913:A:C8	33:a:1494:G:C5	3.08	0.40
1:A:1927:A:H2'	1:A:1928:A:C8	2.56	0.40
33:a:41:G:H2'	33:a:42:G:H8	1.86	0.40
33:a:999:C:H2'	33:a:1000:A:H8	1.85	0.40
1:A:75:G:OP1	25:Y:48:ARG:NH2	2.55	0.40
1:A:138:U:O2'	1:A:139:U:OP1	2.38	0.40
1:A:395:U:H2'	1:A:396:G:C8	2.56	0.40
1:A:1709:U:H2'	1:A:1710:G:C8	2.57	0.40
1:A:1858:A:N6	1:A:1884:G:O2'	2.48	0.40
1:A:2070:A:H2'	1:A:2071:A:C8	2.56	0.40
33:a:709:U:H2'	33:a:710:G:C8	2.56	0.40
33:a:1355:G:H2'	33:a:1356:G:C8	2.57	0.40
43:k:88:PRO:HA	53:u:28:LEU:HD11	2.03	0.40
51:s:54:ARG:HG2	51:s:55:GLN:HG2	2.02	0.40
54:w:101:ARG:HB3	54:w:391:PRO:HD2	2.01	0.40
1:A:341:C:H2'	1:A:342:A:C8	2.57	0.40
1:A:523:C:H2'	1:A:524:G:C8	2.56	0.40
1:A:1997:C:H2'	1:A:1998:A:C8	2.57	0.40
1:A:2559:C:H2'	1:A:2560:A:H8	1.86	0.40
5:E:106:LYS:HG3	5:E:200:LEU:HD23	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:a:9:G:N7	33:a:558:G:O2'	2.54	0.40
33:a:147:G:H2'	33:a:148:G:C8	2.55	0.40
35:c:99:GLN:C	35:c:100:ILE:CG2	2.92	0.40
40:h:45:ILE:HG21	40:h:60:LEU:HD22	2.02	0.40
54:w:19:ILE:HD12	54:w:126:LEU:HB3	2.04	0.40
1:A:1826:G:O2'	1:A:1971:U:OP2	2.37	0.40
1:A:2140:G:H2'	1:A:2141:G:H8	1.85	0.40
1:A:2289:G:H2'	1:A:2290:G:H8	1.86	0.40
1:A:2515:C:H2'	1:A:2516:A:C8	2.53	0.40
1:A:2630:G:H2'	1:A:2631:G:H8	1.85	0.40
22:V:30:ILE:HD12	22:V:40:ILE:HG13	2.02	0.40
33:a:936:C:O2'	33:a:1382:C:N3	2.45	0.40
33:a:1530:G:H2'	33:a:1531:A:H8	1.87	0.40
34:b:53:LEU:HD23	34:b:56:LEU:HD12	2.04	0.40
34:b:129:THR:HG22	34:b:131:LYS:H	1.86	0.40
50:r:40:PRO:HB2	50:r:42:ARG:HG2	2.02	0.40
53:u:40:PRO:HA	53:u:43:GLU:HG2	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	C	269/271 (99%)	260 (97%)	9 (3%)	0	100	100
4	D	207/209 (99%)	193 (93%)	14 (7%)	0	100	100
5	E	199/201 (99%)	188 (94%)	11 (6%)	0	100	100
6	F	175/177 (99%)	162 (93%)	13 (7%)	0	100	100
7	G	174/176 (99%)	162 (93%)	9 (5%)	3 (2%)	7	35
8	H	147/149 (99%)	140 (95%)	7 (5%)	0	100	100
9	I	139/141 (99%)	120 (86%)	19 (14%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
10	J	140/142 (99%)	137 (98%)	3 (2%)	0	100	100
11	K	120/122 (98%)	108 (90%)	12 (10%)	0	100	100
12	L	141/143 (99%)	126 (89%)	14 (10%)	1 (1%)	18	55
13	M	134/136 (98%)	123 (92%)	9 (7%)	2 (2%)	8	38
14	N	118/120 (98%)	110 (93%)	8 (7%)	0	100	100
15	O	114/116 (98%)	109 (96%)	5 (4%)	0	100	100
16	P	112/114 (98%)	105 (94%)	7 (6%)	0	100	100
17	Q	115/117 (98%)	113 (98%)	2 (2%)	0	100	100
18	R	101/103 (98%)	94 (93%)	7 (7%)	0	100	100
19	S	108/110 (98%)	99 (92%)	8 (7%)	1 (1%)	14	49
20	T	91/93 (98%)	84 (92%)	7 (8%)	0	100	100
21	U	100/102 (98%)	89 (89%)	10 (10%)	1 (1%)	12	47
22	V	92/94 (98%)	91 (99%)	1 (1%)	0	100	100
23	W	73/75 (97%)	70 (96%)	3 (4%)	0	100	100
24	X	75/77 (97%)	73 (97%)	2 (3%)	0	100	100
25	Y	61/63 (97%)	59 (97%)	2 (3%)	0	100	100
26	Z	56/58 (97%)	55 (98%)	1 (2%)	0	100	100
27	0	54/56 (96%)	53 (98%)	1 (2%)	0	100	100
28	1	48/50 (96%)	46 (96%)	2 (4%)	0	100	100
29	2	44/46 (96%)	43 (98%)	1 (2%)	0	100	100
30	3	62/64 (97%)	55 (89%)	5 (8%)	2 (3%)	3	21
31	4	36/38 (95%)	31 (86%)	5 (14%)	0	100	100
32	5	129/131 (98%)	101 (78%)	27 (21%)	1 (1%)	16	52
34	b	216/218 (99%)	194 (90%)	21 (10%)	1 (0%)	24	62
35	c	204/206 (99%)	196 (96%)	6 (3%)	2 (1%)	12	47
36	d	203/205 (99%)	185 (91%)	18 (9%)	0	100	100
37	e	155/157 (99%)	142 (92%)	11 (7%)	2 (1%)	9	41
38	f	98/100 (98%)	81 (83%)	15 (15%)	2 (2%)	6	31
39	g	149/151 (99%)	136 (91%)	13 (9%)	0	100	100
40	h	127/129 (98%)	118 (93%)	9 (7%)	0	100	100
41	i	125/127 (98%)	109 (87%)	15 (12%)	1 (1%)	16	52

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
42	j	96/98 (98%)	83 (86%)	13 (14%)	0	100	100
43	k	110/112 (98%)	96 (87%)	12 (11%)	2 (2%)	6	33
44	l	121/123 (98%)	96 (79%)	23 (19%)	2 (2%)	7	35
45	m	112/114 (98%)	96 (86%)	15 (13%)	1 (1%)	14	49
46	n	99/101 (98%)	90 (91%)	9 (9%)	0	100	100
47	o	86/88 (98%)	76 (88%)	10 (12%)	0	100	100
48	p	80/82 (98%)	70 (88%)	10 (12%)	0	100	100
49	q	78/80 (98%)	65 (83%)	12 (15%)	1 (1%)	9	41
50	r	63/65 (97%)	56 (89%)	7 (11%)	0	100	100
51	s	77/79 (98%)	73 (95%)	4 (5%)	0	100	100
52	t	83/85 (98%)	78 (94%)	5 (6%)	0	100	100
53	u	63/65 (97%)	49 (78%)	13 (21%)	1 (2%)	7	36
54	w	495/529 (94%)	432 (87%)	59 (12%)	4 (1%)	16	52
55	z	12/14 (86%)	11 (92%)	0	1 (8%)	0	9
All	All	6286/6422 (98%)	5731 (91%)	524 (8%)	31 (0%)	26	62

All (31) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
7	G	46	ASP
13	M	58	LYS
30	3	31	ILE
35	c	96	VAL
38	f	53	LYS
49	q	69	THR
54	w	18	ILE
54	w	315	VAL
7	G	47	ASN
30	3	32	LEU
37	e	122	VAL
13	M	59	ARG
34	b	17	HIS
35	c	97	PRO
38	f	55	HIS
21	U	89	GLY
44	l	102	ASP
54	w	77	PHE

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Mol	Chain	Res	Type
37	e	121	ASN
41	i	90	ASP
44	l	100	ALA
45	m	4	ALA
53	u	37	TYR
54	w	399	ARG
7	G	174	LYS
12	L	128	THR
19	S	64	ALA
43	k	118	ASN
32	5	79	PRO
43	k	115	ILE
55	z	16	PRO

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	H	114/114 (100%)	114 (100%)	0	100	100
9	I	109/109 (100%)	109 (100%)	0	100	100
10	J	116/116 (100%)	116 (100%)	0	100	100
11	K	103/103 (100%)	103 (100%)	0	100	100
12	L	102/102 (100%)	101 (99%)	1 (1%)	68	76
13	M	109/109 (100%)	108 (99%)	1 (1%)	70	76
14	N	100/100 (100%)	100 (100%)	0	100	100
15	O	86/86 (100%)	86 (100%)	0	100	100
16	P	99/99 (100%)	99 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
17	Q	89/89 (100%)	89 (100%)	0	100	100
18	R	84/84 (100%)	84 (100%)	0	100	100
19	S	93/93 (100%)	93 (100%)	0	100	100
20	T	80/80 (100%)	80 (100%)	0	100	100
21	U	83/83 (100%)	83 (100%)	0	100	100
22	V	78/78 (100%)	78 (100%)	0	100	100
23	W	57/57 (100%)	57 (100%)	0	100	100
24	X	67/67 (100%)	67 (100%)	0	100	100
25	Y	55/55 (100%)	55 (100%)	0	100	100
26	Z	48/48 (100%)	48 (100%)	0	100	100
27	0	47/47 (100%)	47 (100%)	0	100	100
28	1	45/45 (100%)	45 (100%)	0	100	100
29	2	38/38 (100%)	38 (100%)	0	100	100
30	3	51/51 (100%)	51 (100%)	0	100	100
31	4	34/34 (100%)	34 (100%)	0	100	100
32	5	100/100 (100%)	100 (100%)	0	100	100
34	b	180/180 (100%)	179 (99%)	1 (1%)	78	80
35	c	170/170 (100%)	168 (99%)	2 (1%)	63	73
36	d	172/172 (100%)	172 (100%)	0	100	100
37	e	114/119 (96%)	113 (99%)	1 (1%)	70	76
38	f	87/87 (100%)	87 (100%)	0	100	100
39	g	124/124 (100%)	123 (99%)	1 (1%)	73	77
40	h	104/104 (100%)	104 (100%)	0	100	100
41	i	105/105 (100%)	105 (100%)	0	100	100
42	j	86/86 (100%)	86 (100%)	0	100	100
43	k	85/85 (100%)	83 (98%)	2 (2%)	43	63
44	l	103/103 (100%)	103 (100%)	0	100	100
45	m	92/92 (100%)	92 (100%)	0	100	100
46	n	79/83 (95%)	79 (100%)	0	100	100
47	o	76/76 (100%)	76 (100%)	0	100	100
48	p	65/65 (100%)	65 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
49	q	74/74 (100%)	74 (100%)	0	100	100
50	r	48/56 (86%)	48 (100%)	0	100	100
51	s	70/70 (100%)	69 (99%)	1 (1%)	59	71
52	t	65/65 (100%)	65 (100%)	0	100	100
53	u	44/55 (80%)	44 (100%)	0	100	100
54	w	427/453 (94%)	423 (99%)	4 (1%)	70	76
55	z	14/14 (100%)	14 (100%)	0	100	100
All	All	5201/5255 (99%)	5187 (100%)	14 (0%)	84	84

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
12	L	110	VAL
13	M	46	ILE
34	b	23	ASN
35	c	89	VAL
35	c	96	VAL
37	e	87	VAL
39	g	47	GLU
43	k	115	ILE
43	k	116	PRO
51	s	10	ILE
54	w	71	THR
54	w	312	ARG
54	w	320	VAL
54	w	504	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (83) such sidechains are listed below:

Mol	Chain	Res	Type
3	C	14	HIS
3	C	36	ASN
3	C	45	ASN
3	C	85	ASN
3	C	114	GLN
3	C	250	GLN
4	D	164	GLN
5	E	62	GLN

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Mol	Chain	Res	Type
5	E	136	GLN
7	G	63	GLN
7	G	103	ASN
7	G	115	GLN
7	G	127	GLN
8	H	33	GLN
8	H	133	GLN
10	J	58	ASN
10	J	86	GLN
10	J	135	GLN
11	K	5	GLN
13	M	45	GLN
14	N	9	GLN
15	O	38	GLN
15	O	98	GLN
16	P	11	GLN
16	P	55	HIS
17	Q	43	GLN
17	Q	55	GLN
18	R	6	GLN
18	R	18	GLN
18	R	43	ASN
18	R	86	GLN
18	R	91	GLN
19	S	7	HIS
19	S	57	ASN
20	T	15	HIS
23	W	8	ASN
23	W	42	HIS
25	Y	58	ASN
28	1	18	HIS
31	4	37	GLN
32	5	4	ASN
34	b	23	ASN
34	b	35	ASN
36	d	35	GLN
36	d	70	GLN
36	d	99	ASN
37	e	69	ASN
37	e	131	ASN
38	f	58	HIS
40	h	15	ASN

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Mol	Chain	Res	Type
40	h	66	GLN
40	h	75	GLN
41	i	49	GLN
41	i	125	GLN
43	k	21	HIS
43	k	28	ASN
43	k	100	ASN
43	k	118	ASN
44	l	28	GLN
45	m	99	GLN
47	o	37	HIS
47	o	49	HIS
48	p	18	GLN
48	p	29	ASN
48	p	63	GLN
49	q	8	GLN
49	q	30	HIS
50	r	51	GLN
50	r	53	GLN
50	r	73	HIS
51	s	55	GLN
52	t	2	ASN
52	t	47	GLN
52	t	69	ASN
54	w	184	HIS
54	w	202	GLN
54	w	311	HIS
54	w	370	HIS
54	w	381	GLN
54	w	445	GLN
54	w	489	ASN
54	w	510	ASN
54	w	524	HIS

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	2893/2903 (99%)	538 (18%)	29 (1%)
2	B	119/120 (99%)	15 (12%)	2 (1%)
33	a	1537/1539 (99%)	251 (16%)	0
All	All	4549/4562 (99%)	804 (17%)	31 (0%)

All (804) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	10	A
1	A	12	U
1	A	27	G
1	A	34	U
1	A	35	G
1	A	36	G
1	A	46	G
1	A	49	A
1	A	51	G
1	A	52	A
1	A	60	G
1	A	63	A
1	A	71	A
1	A	74	A
1	A	75	G
1	A	84	A
1	A	91	A
1	A	92	U
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	137	U
1	A	138	U
1	A	139	U
1	A	140	C
1	A	141	G
1	A	142	A
1	A	158	U
1	A	162	U
1	A	163	C
1	A	181	A
1	A	188	G
1	A	196	A
1	A	199	A
1	A	205	G
1	A	206	U
1	A	215	G
1	A	216	A
1	A	218	A

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Mol	Chain	Res	Type
1	A	219	A
1	A	221	A
1	A	222	A
1	A	223	A
1	A	228	C
1	A	242	G
1	A	243	U
1	A	248	G
1	A	249	C
1	A	255	A
1	A	266	G
1	A	267	C
1	A	276	U
1	A	278	A
1	A	281	C
1	A	294	A
1	A	310	A
1	A	311	A
1	A	323	C
1	A	324	A
1	A	329	G
1	A	330	A
1	A	334	C
1	A	343	C
1	A	361	G
1	A	371	A
1	A	372	G
1	A	373	U
1	A	386	G
1	A	387	U
1	A	401	A
1	A	404	A
1	A	406	G
1	A	411	G
1	A	417	C
1	A	421	C
1	A	424	G
1	A	451	U
1	A	455	C
1	A	456	C
1	A	457	A
1	A	458	G

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Mol	Chain	Res	Type
1	A	467	G
1	A	480	A
1	A	481	G
1	A	489	G
1	A	490	C
1	A	491	G
1	A	504	A
1	A	505	A
1	A	506	G
1	A	509	C
1	A	529	A
1	A	530	G
1	A	532	A
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	568	U
1	A	572	A
1	A	573	U
1	A	575	A
1	A	603	A
1	A	616	A
1	A	621	A
1	A	627	A
1	A	637	A
1	A	643	A
1	A	645	C
1	A	646	U
1	A	654	A
1	A	668	A
1	A	669	G
1	A	670	A
1	A	677	A
1	A	686	U
1	A	687	C
1	A	695	G
1	A	726	G

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Mol	Chain	Res	Type
1	A	729	G
1	A	730	A
1	A	745	G
1	A	747	C
1	A	752	A
1	A	753	A
1	A	763	G
1	A	764	A
1	A	765	C
1	A	774	G
1	A	775	G
1	A	776	G
1	A	777	G
1	A	782	A
1	A	784	G
1	A	785	G
1	A	789	A
1	A	799	G
1	A	800	A
1	A	805	G
1	A	811	U
1	A	812	C
1	A	819	A
1	A	827	U
1	A	828	U
1	A	830	G
1	A	831	G
1	A	845	A
1	A	846	U
1	A	847	U
1	A	856	G
1	A	858	G
1	A	859	G
1	A	860	U
1	A	869	G
1	A	878	A
1	A	896	A
1	A	897	C
1	A	899	A
1	A	901	C
1	A	907	G
1	A	910	A

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Mol	Chain	Res	Type
1	A	932	U
1	A	941	A
1	A	946	C
1	A	953	G
1	A	961	C
1	A	965	C
1	A	974	G
1	A	980	A
1	A	983	A
1	A	989	G
1	A	990	A
1	A	995	C
1	A	996	A
1	A	999	U
1	A	1010	A
1	A	1012	U
1	A	1013	C
1	A	1021	A
1	A	1023	U
1	A	1026	G
1	A	1033	U
1	A	1046	A
1	A	1047	G
1	A	1053	C
1	A	1054	A
1	A	1057	A
1	A	1059	G
1	A	1060	U
1	A	1061	U
1	A	1062	G
1	A	1064	C
1	A	1065	U
1	A	1066	U
1	A	1067	A
1	A	1068	G
1	A	1069	A
1	A	1070	A
1	A	1071	G
1	A	1072	C
1	A	1075	C
1	A	1076	C
1	A	1078	U

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Mol	Chain	Res	Type
1	A	1079	C
1	A	1083	U
1	A	1084	A
1	A	1088	A
1	A	1104	C
1	A	1106	G
1	A	1111	A
1	A	1112	G
1	A	1119	U
1	A	1130	U
1	A	1131	G
1	A	1132	U
1	A	1133	A
1	A	1135	C
1	A	1139	G
1	A	1142	A
1	A	1157	G
1	A	1172	C
1	A	1174	U
1	A	1176	U
1	A	1177	G
1	A	1178	C
1	A	1180	U
1	A	1204	A
1	A	1206	G
1	A	1211	C
1	A	1212	G
1	A	1225	G
1	A	1237	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	1271	G
1	A	1272	A
1	A	1289	C
1	A	1300	G
1	A	1301	A
1	A	1321	A
1	A	1325	U

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Mol	Chain	Res	Type
1	A	1329	U
1	A	1330	C
1	A	1341	G
1	A	1345	C
1	A	1347	A
1	A	1365	A
1	A	1368	G
1	A	1378	A
1	A	1379	U
1	A	1383	A
1	A	1395	A
1	A	1416	G
1	A	1419	A
1	A	1420	A
1	A	1421	G
1	A	1428	C
1	A	1437	C
1	A	1454	C
1	A	1461	C
1	A	1475	G
1	A	1482	G
1	A	1490	A
1	A	1491	G
1	A	1493	C
1	A	1504	A
1	A	1515	A
1	A	1524	G
1	A	1532	A
1	A	1533	C
1	A	1535	A
1	A	1536	C
1	A	1537	G
1	A	1555	G
1	A	1559	U
1	A	1560	G
1	A	1565	C
1	A	1569	A
1	A	1578	U
1	A	1585	C
1	A	1598	A
1	A	1603	A
1	A	1607	C

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Mol	Chain	Res	Type
1	A	1610	A
1	A	1611	C
1	A	1613	G
1	A	1634	A
1	A	1646	C
1	A	1647	U
1	A	1648	U
1	A	1651	G
1	A	1660	G
1	A	1664	A
1	A	1665	A
1	A	1669	A
1	A	1670	C
1	A	1674	G
1	A	1694	C
1	A	1695	G
1	A	1707	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	1757	A
1	A	1758	U
1	A	1764	C
1	A	1773	A
1	A	1780	A
1	A	1781	U
1	A	1782	U
1	A	1784	A
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	1835	G
1	A	1847	G
1	A	1848	A
1	A	1870	C

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Mol	Chain	Res	Type
1	A	1871	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	1917	U
1	A	1918	A
1	A	1927	A
1	A	1929	G
1	A	1930	G
1	A	1937	A
1	A	1938	A
1	A	1940	U
1	A	1941	C
1	A	1944	U
1	A	1955	U
1	A	1960	A
1	A	1962	C
1	A	1963	U
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	2030	A
1	A	2031	A
1	A	2033	A
1	A	2043	C
1	A	2050	C
1	A	2052	A
1	A	2055	C
1	A	2056	G
1	A	2060	A

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Mol	Chain	Res	Type
1	A	2061	G
1	A	2062	A
1	A	2068	U
1	A	2069	G
1	A	2072	C
1	A	2093	G
1	A	2095	A
1	A	2096	C
1	A	2098	U
1	A	2100	G
1	A	2110	G
1	A	2111	U
1	A	2112	G
1	A	2113	U
1	A	2118	U
1	A	2119	A
1	A	2127	G
1	A	2131	U
1	A	2132	U
1	A	2133	G
1	A	2136	G
1	A	2145	C
1	A	2147	A
1	A	2157	G
1	A	2162	G
1	A	2164	C
1	A	2170	A
1	A	2172	U
1	A	2173	A
1	A	2189	U
1	A	2190	G
1	A	2192	U
1	A	2198	A
1	A	2204	G
1	A	2211	A
1	A	2212	A
1	A	2213	U
1	A	2225	A
1	A	2226	C
1	A	2238	G
1	A	2239	G
1	A	2249	U

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Mol	Chain	Res	Type
1	A	2250	G
1	A	2251	G
1	A	2266	A
1	A	2279	G
1	A	2283	C
1	A	2286	G
1	A	2287	A
1	A	2297	A
1	A	2305	U
1	A	2309	A
1	A	2325	G
1	A	2327	A
1	A	2334	U
1	A	2335	A
1	A	2336	A
1	A	2345	G
1	A	2350	C
1	A	2354	C
1	A	2357	G
1	A	2361	G
1	A	2383	G
1	A	2385	C
1	A	2391	G
1	A	2392	A
1	A	2402	U
1	A	2407	A
1	A	2423	U
1	A	2424	C
1	A	2426	A
1	A	2428	G
1	A	2429	G
1	A	2430	A
1	A	2431	U
1	A	2435	A
1	A	2441	U
1	A	2447	G
1	A	2448	A
1	A	2449	U
1	A	2473	U
1	A	2476	A
1	A	2478	A
1	A	2484	G

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Mol	Chain	Res	Type
1	A	2491	U
1	A	2494	G
1	A	2498	C
1	A	2502	G
1	A	2503	A
1	A	2504	U
1	A	2513	A
1	A	2518	A
1	A	2520	C
1	A	2529	G
1	A	2531	A
1	A	2535	G
1	A	2547	A
1	A	2554	U
1	A	2564	A
1	A	2567	G
1	A	2572	A
1	A	2573	C
1	A	2580	U
1	A	2582	G
1	A	2585	U
1	A	2586	U
1	A	2602	A
1	A	2603	G
1	A	2609	U
1	A	2613	U
1	A	2614	A
1	A	2621	G
1	A	2629	U
1	A	2634	A
1	A	2636	C
1	A	2646	C
1	A	2654	A
1	A	2655	G
1	A	2656	U
1	A	2682	A
1	A	2689	U
1	A	2690	U
1	A	2712	C
1	A	2713	U
1	A	2714	G
1	A	2716	C

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Mol	Chain	Res	Type
1	A	2718	G
1	A	2722	G
1	A	2726	A
1	A	2731	G
1	A	2733	A
1	A	2744	G
1	A	2748	A
1	A	2762	C
1	A	2764	A
1	A	2765	A
1	A	2778	A
1	A	2779	U
1	A	2791	G
1	A	2794	C
1	A	2796	U
1	A	2797	U
1	A	2799	A
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	2834	G
1	A	2835	A
1	A	2849	U
1	A	2861	U
1	A	2867	G
1	A	2868	A
1	A	2872	A
1	A	2873	A
1	A	2880	C
1	A	2884	U
1	A	2902	C
2	B	4	C
2	B	9	G
2	B	13	G
2	B	35	C
2	B	41	G
2	B	44	G
2	B	45	A
2	B	53	A

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Mol	Chain	Res	Type
2	B	67	G
2	B	88	C
2	B	89	U
2	B	90	C
2	B	91	C
2	B	108	A
2	B	109	A
33	a	7	A
33	a	9	G
33	a	19	A
33	a	22	G
33	a	32	A
33	a	39	G
33	a	47	C
33	a	48	C
33	a	49	U
33	a	51	A
33	a	71	A
33	a	81	A
33	a	86	G
33	a	94	G
33	a	95	C
33	a	121	U
33	a	130	A
33	a	163	C
33	a	173	U
33	a	174	A
33	a	181	A
33	a	183	C
33	a	184	G
33	a	197	A
33	a	209	U
33	a	210	C
33	a	211	G
33	a	212	G
33	a	226	G
33	a	240	G
33	a	247	G
33	a	251	G
33	a	266	G
33	a	267	C
33	a	269	C

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Mol	Chain	Res	Type
33	a	279	A
33	a	280	C
33	a	281	G
33	a	283	U
33	a	289	G
33	a	306	A
33	a	328	C
33	a	340	U
33	a	344	A
33	a	345	C
33	a	346	G
33	a	347	G
33	a	351	G
33	a	352	C
33	a	354	G
33	a	356	A
33	a	367	U
33	a	372	C
33	a	388	G
33	a	390	U
33	a	392	C
33	a	397	A
33	a	406	G
33	a	411	A
33	a	413	G
33	a	421	U
33	a	422	C
33	a	424	G
33	a	428	G
33	a	429	U
33	a	439	U
33	a	467	U
33	a	479	U
33	a	482	A
33	a	484	G
33	a	486	U
33	a	496	A
33	a	497	G
33	a	510	A
33	a	511	C
33	a	518	C
33	a	519	C

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Mol	Chain	Res	Type
33	a	521	G
33	a	526	C
33	a	527	G
33	a	531	U
33	a	532	A
33	a	547	A
33	a	560	A
33	a	561	U
33	a	564	C
33	a	572	A
33	a	573	A
33	a	574	A
33	a	575	G
33	a	576	C
33	a	577	G
33	a	588	G
33	a	596	A
33	a	633	G
33	a	665	A
33	a	671	G
33	a	674	G
33	a	675	A
33	a	676	A
33	a	688	G
33	a	690	G
33	a	702	A
33	a	703	G
33	a	706	A
33	a	713	G
33	a	714	G
33	a	715	A
33	a	718	A
33	a	720	C
33	a	723	U
33	a	724	G
33	a	731	G
33	a	733	G
33	a	734	G
33	a	748	G
33	a	755	G
33	a	777	A
33	a	793	U

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Mol	Chain	Res	Type
33	a	794	A
33	a	814	A
33	a	815	A
33	a	817	C
33	a	818	G
33	a	819	A
33	a	820	U
33	a	821	G
33	a	829	G
33	a	832	G
33	a	843	U
33	a	844	G
33	a	846	G
33	a	871	U
33	a	873	A
33	a	889	A
33	a	890	G
33	a	902	G
33	a	926	G
33	a	928	G
33	a	934	C
33	a	935	A
33	a	960	U
33	a	961	U
33	a	969	A
33	a	975	A
33	a	976	G
33	a	977	A
33	a	992	U
33	a	993	G
33	a	1004	A
33	a	1014	A
33	a	1022	A
33	a	1026	G
33	a	1028	C
33	a	1030	U
33	a	1031	C
33	a	1033	G
33	a	1034	G
33	a	1035	A
33	a	1053	G
33	a	1056	U

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Mol	Chain	Res	Type
33	a	1065	U
33	a	1085	U
33	a	1094	G
33	a	1101	A
33	a	1108	G
33	a	1118	U
33	a	1130	A
33	a	1136	C
33	a	1137	C
33	a	1138	G
33	a	1139	G
33	a	1140	C
33	a	1157	A
33	a	1158	C
33	a	1159	U
33	a	1168	U
33	a	1183	U
33	a	1184	G
33	a	1191	A
33	a	1196	A
33	a	1197	A
33	a	1201	A
33	a	1202	U
33	a	1208	C
33	a	1212	U
33	a	1213	A
33	a	1220	G
33	a	1224	U
33	a	1225	A
33	a	1226	C
33	a	1227	A
33	a	1233	G
33	a	1236	A
33	a	1238	A
33	a	1240	U
33	a	1241	G
33	a	1253	G
33	a	1256	A
33	a	1258	G
33	a	1260	G
33	a	1278	G
33	a	1280	A

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Mol	Chain	Res	Type
33	a	1281	C
33	a	1282	C
33	a	1286	U
33	a	1287	A
33	a	1298	U
33	a	1300	G
33	a	1301	U
33	a	1305	G
33	a	1306	A
33	a	1318	A
33	a	1319	A
33	a	1321	U
33	a	1322	C
33	a	1323	G
33	a	1331	G
33	a	1335	U
33	a	1346	A
33	a	1347	G
33	a	1348	U
33	a	1353	G
33	a	1363	A
33	a	1364	U
33	a	1378	C
33	a	1400	C
33	a	1401	G
33	a	1433	A
33	a	1446	A
33	a	1448	C
33	a	1451	U
33	a	1452	C
33	a	1491	G
33	a	1492	A
33	a	1493	A
33	a	1494	G
33	a	1499	A
33	a	1502	A
33	a	1503	A
33	a	1506	U
33	a	1517	G
33	a	1520	C
33	a	1523	G
33	a	1529	G

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Mol	Chain	Res	Type
33	a	1530	G
33	a	1533	C
33	a	1534	A
33	a	1535	C
33	a	1536	C
33	a	1537	U

All (31) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	51	G
1	A	138	U
1	A	140	C
1	A	242	G
1	A	372	G
1	A	479	A
1	A	490	C
1	A	752	A
1	A	858	G
1	A	859	G
1	A	898	C
1	A	1020	A
1	A	1022	G
1	A	1070	A
1	A	1130	U
1	A	1182	G
1	A	1190	G
1	A	1378	A
1	A	1399	C
1	A	1432	G
1	A	1940	U
1	A	2189	U
1	A	2286	G
1	A	2326	C
1	A	2333	A
1	A	2391	G
1	A	2566	A
1	A	2655	G
1	A	2808	G
2	B	66	A
2	B	88	C

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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	GCP	w	601	-	32,34,34	1.12	2 (6%)	49,54,54	0.62	1 (2%)

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	GCP	w	601	-	-	5/19/38/38	0/3/3/3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
56	w	601	GCP	PB-O3A	5.61	1.64	1.58
56	w	601	GCP	PB-O2B	-2.15	1.51	1.56

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
56	w	601	GCP	PB-O3A-PA	-2.52	124.14	132.37

There are no chirality outliers.

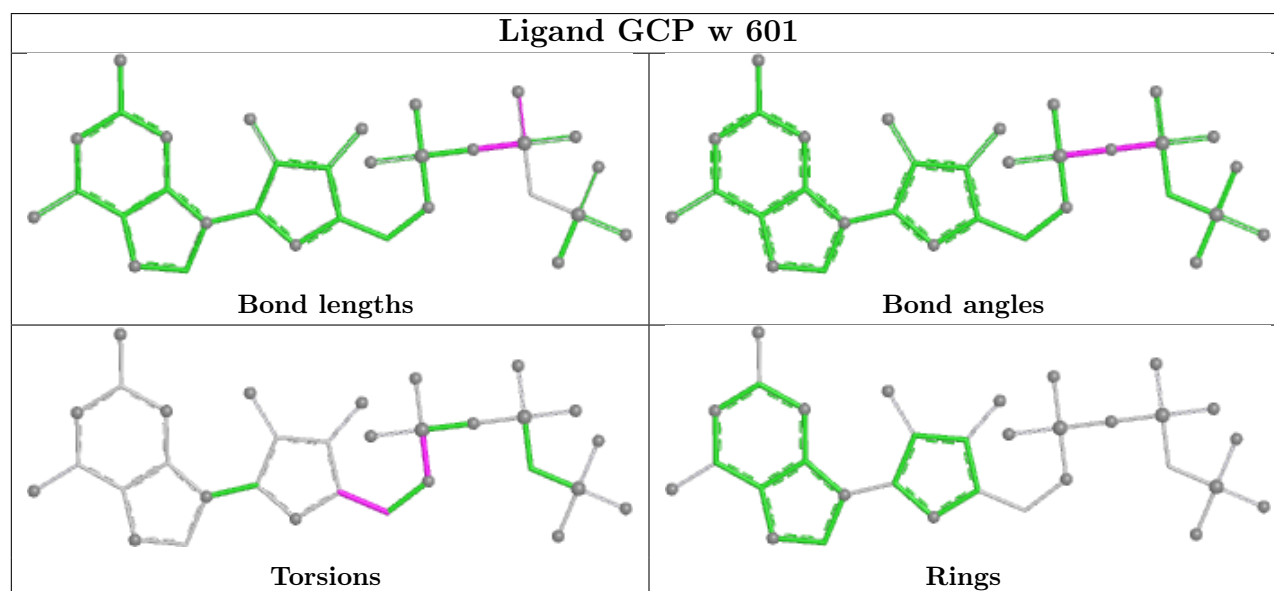
All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
56	w	601	GCP	C5'-O5'-PA-O2A
56	w	601	GCP	O4'-C4'-C5'-O5'
56	w	601	GCP	C3'-C4'-C5'-O5'
56	w	601	GCP	C5'-O5'-PA-O3A
56	w	601	GCP	C5'-O5'-PA-O1A

There are no ring outliers.

No monomer is involved in short contacts.

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



5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

The following chains have linkage breaks:

Mol	Chain	Number of breaks
33	a	2
1	A	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	2179:C	O3'	2180:U	P	3.63
1	a	917:G	O3'	918:A	P	3.57
1	a	1394:A	O3'	1395:C	P	3.30

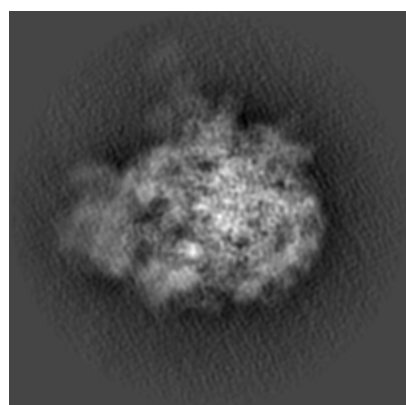
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-0083. These allow visual inspection of the internal detail of the map and identification of artifacts.

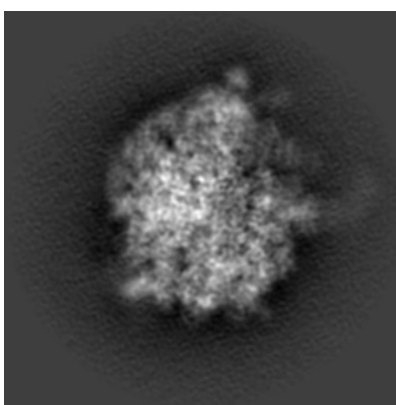
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

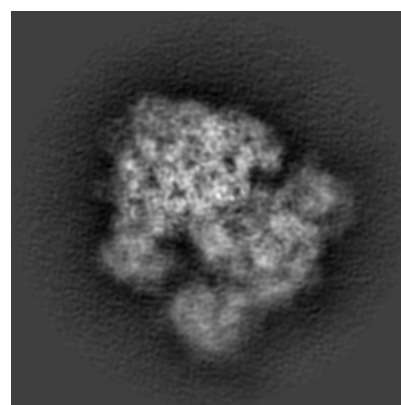
6.1.1 Primary map



X



Y

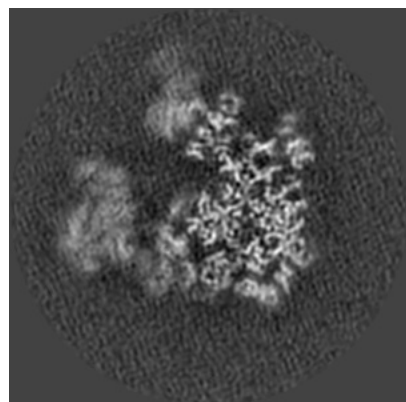


Z

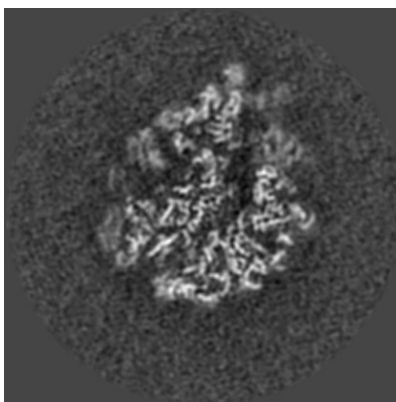
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

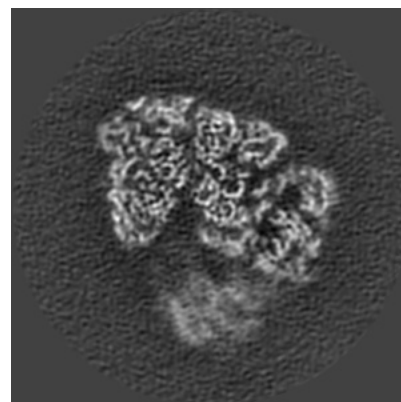
6.2.1 Primary map



X Index: 180



Y Index: 180

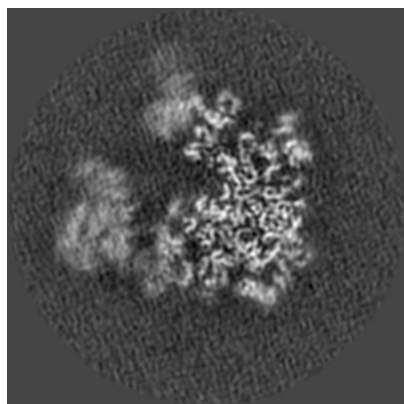


Z Index: 180

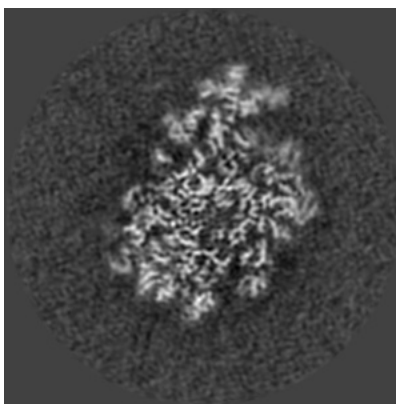
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

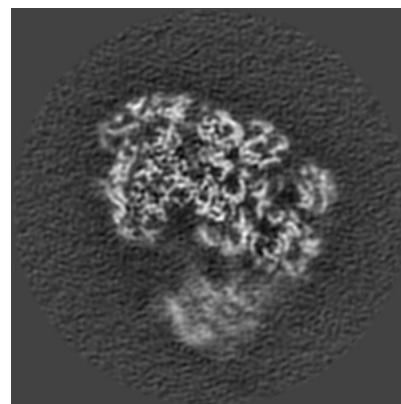
6.3.1 Primary map



X Index: 178



Y Index: 191

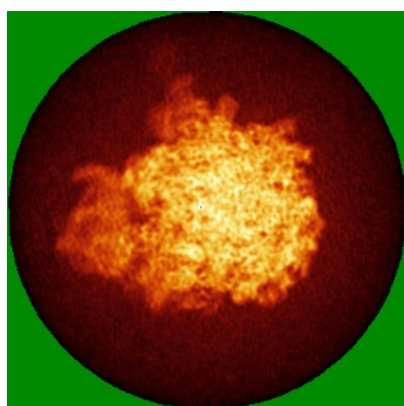


Z Index: 177

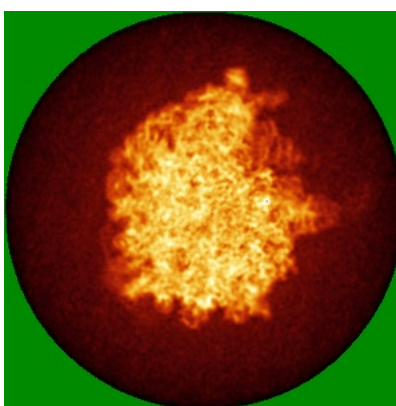
The images above show the largest variance slices of the map in three orthogonal directions.

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

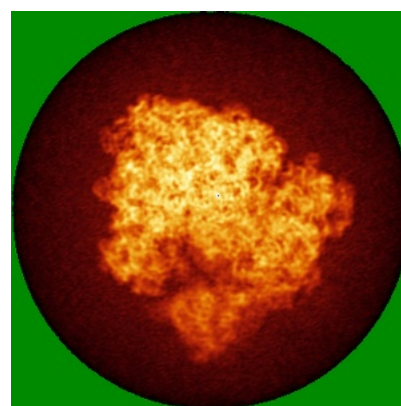
6.4.1 Primary map



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

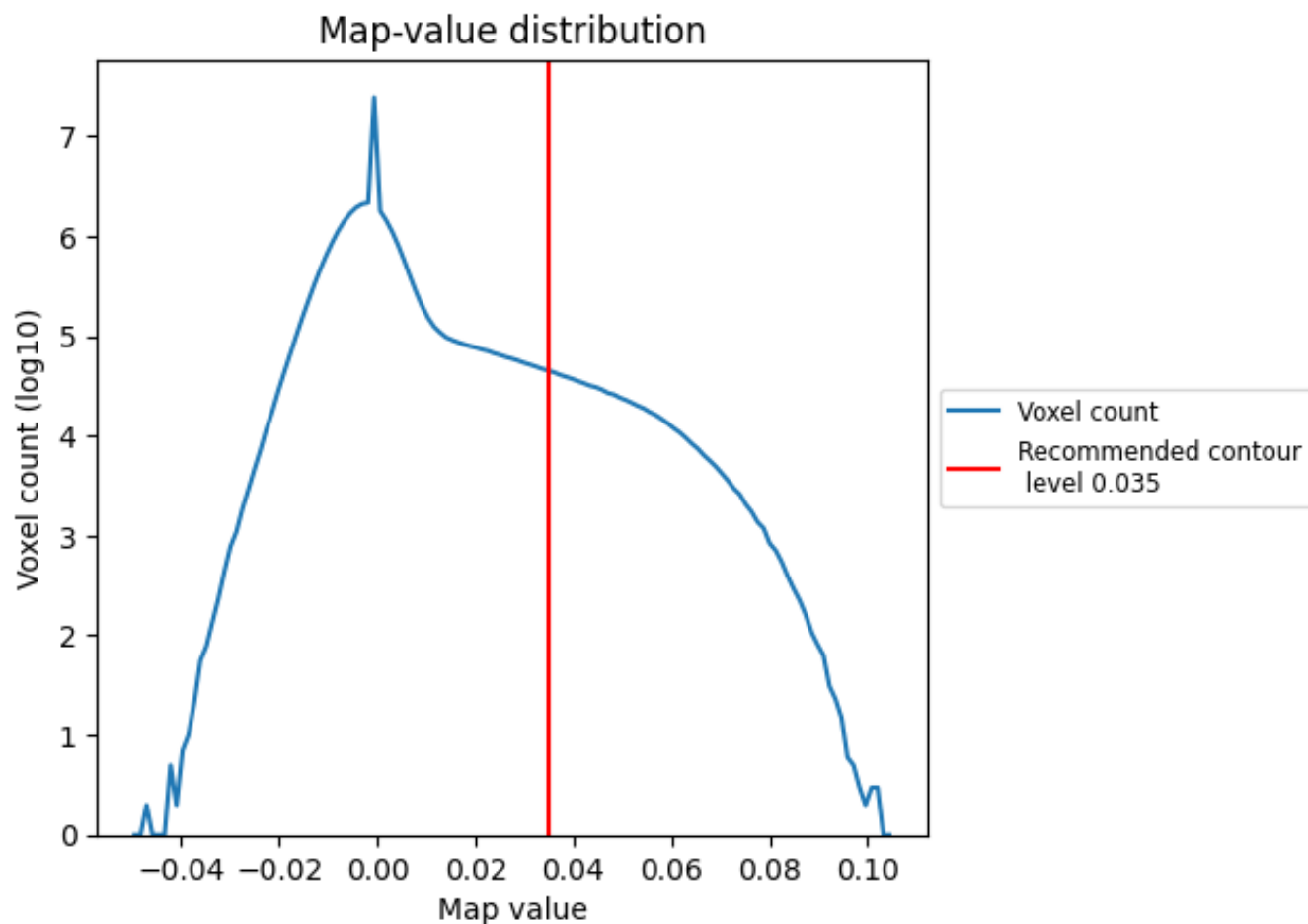
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

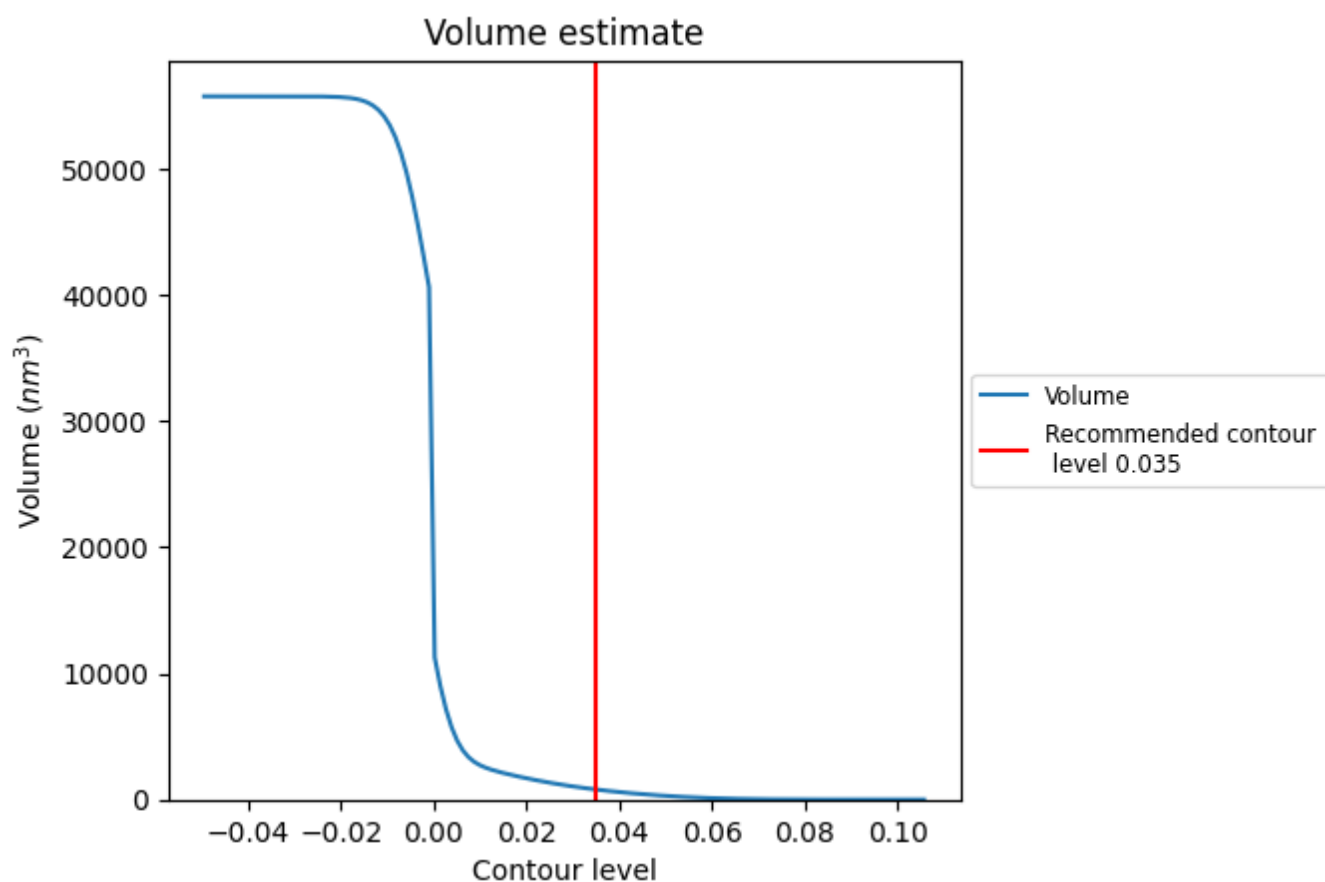
This section contains the results of statistical analysis of the map.

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.

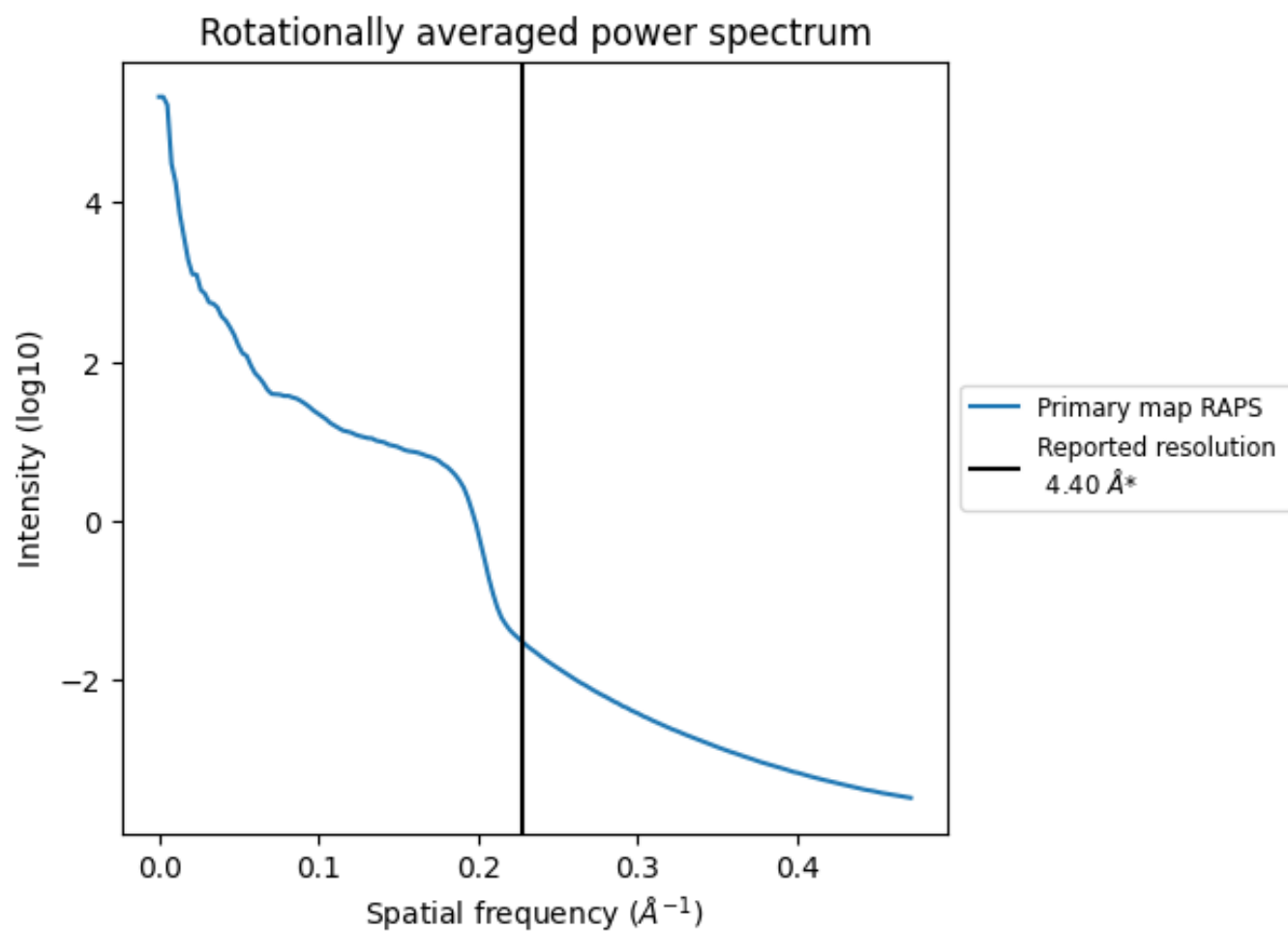
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 796 nm³; this corresponds to an approximate mass of 719 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 0.227 Å⁻¹

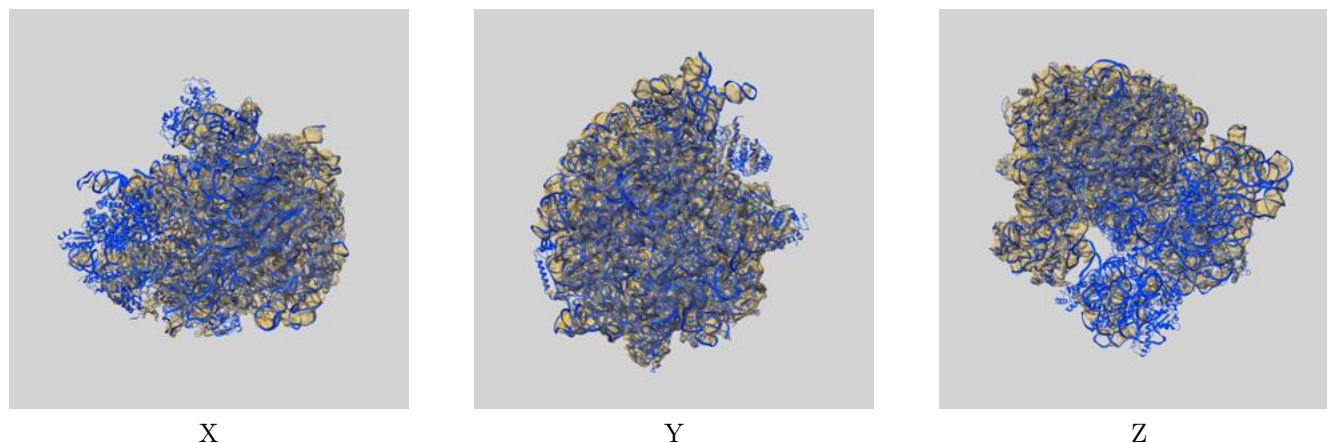
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

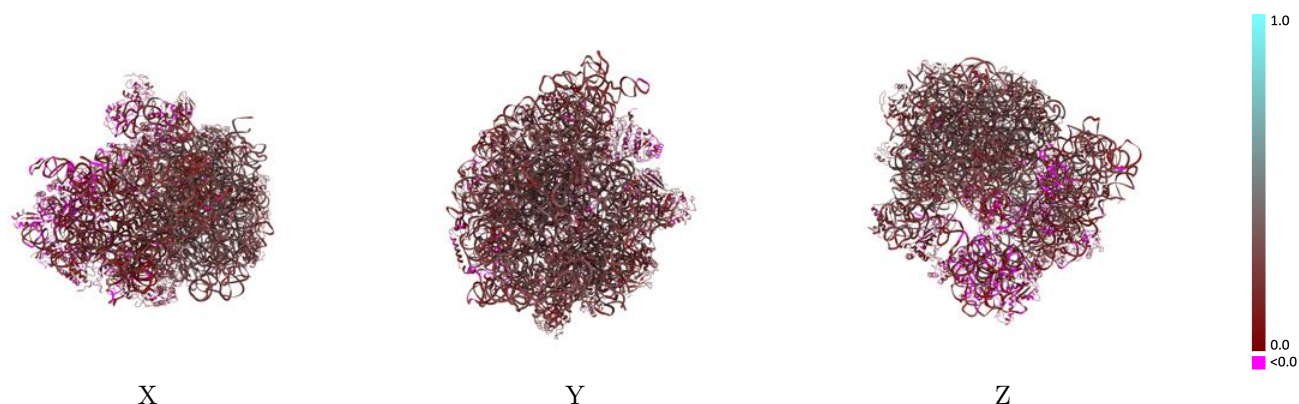
This section contains information regarding the fit between EMDB map EMD-0083 and PDB model 6GXP. Per-residue inclusion information can be found in section [3](#) on page [15](#).

9.1 Map-model overlay [i](#)



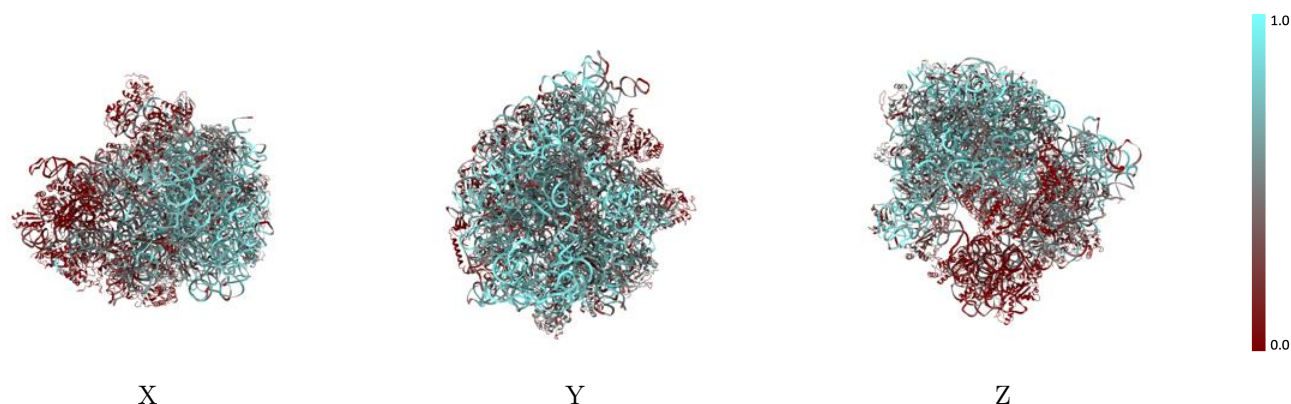
The images above show the 3D surface view of the map at the recommended contour level 0.035 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



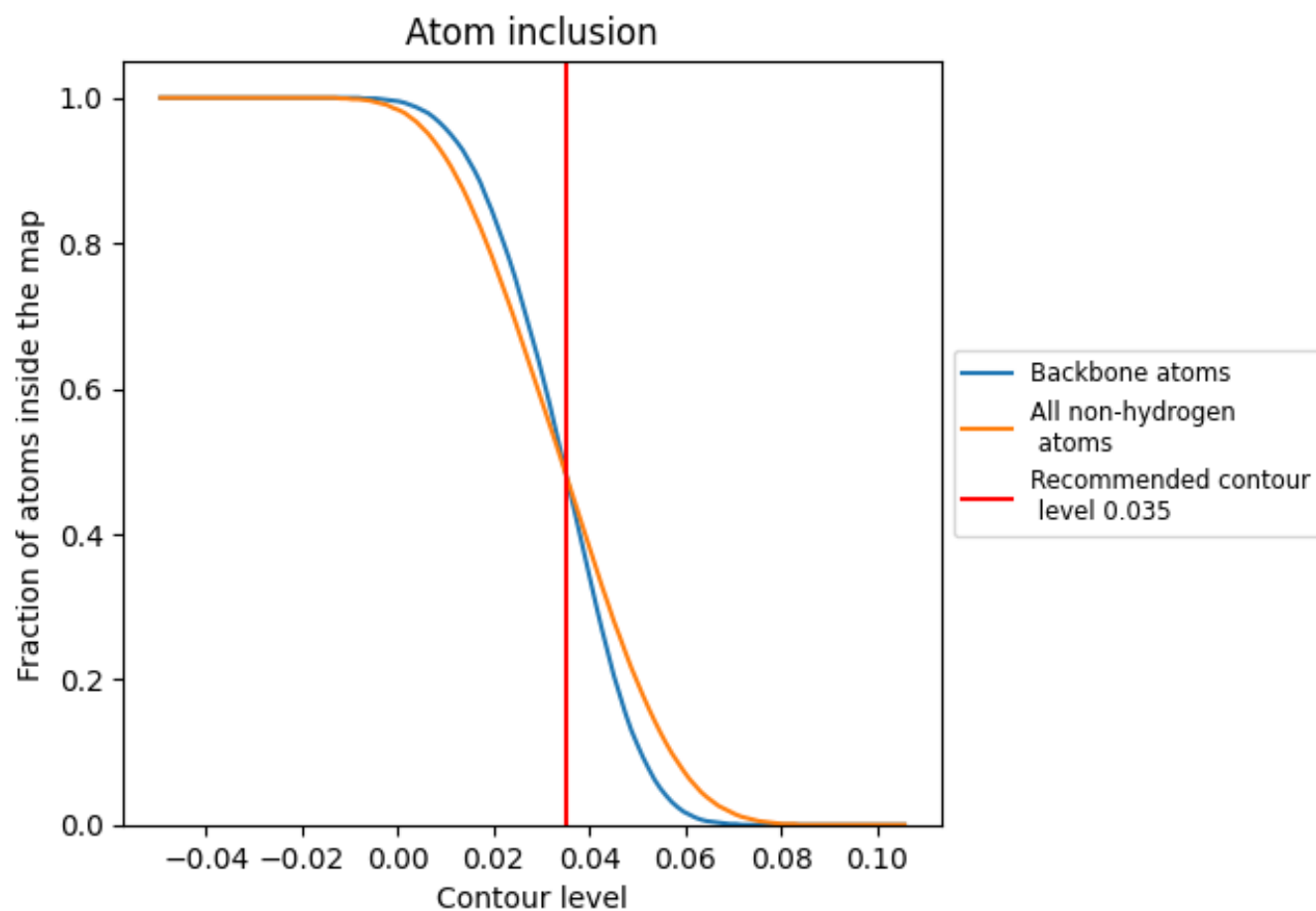
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.035).

9.4 Atom inclusion [i](#)



At the recommended contour level, 48% of all backbone atoms, 48% 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 (0.035) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.4830	 0.2170
0	 0.3410	 0.2290
1	 0.2200	 0.2250
2	 0.3210	 0.2210
3	 0.2830	 0.2480
4	 0.4110	 0.2270
5	 0.0150	 0.0770
A	 0.6990	 0.2770
B	 0.7480	 0.2680
C	 0.3090	 0.2440
D	 0.3600	 0.2550
E	 0.3510	 0.2170
F	 0.2720	 0.1680
G	 0.3450	 0.2280
H	 0.1270	 0.1480
I	 0.0100	 0.0470
J	 0.3900	 0.2540
K	 0.2790	 0.2510
L	 0.3340	 0.2360
M	 0.3020	 0.2480
N	 0.4250	 0.2210
O	 0.4280	 0.1970
P	 0.3450	 0.2430
Q	 0.4100	 0.1970
R	 0.3580	 0.2410
S	 0.2850	 0.2160
T	 0.3850	 0.2220
U	 0.3740	 0.2140
V	 0.3890	 0.2280
W	 0.2950	 0.2390
X	 0.3640	 0.2330
Y	 0.4690	 0.1850
Z	 0.3410	 0.2180
a	 0.4480	 0.1710
b	 0.0970	 0.1530



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Chain	Atom inclusion	Q-score
c	 0.0150	 0.0900
d	 0.1240	 0.1300
e	 0.2490	 0.1620
f	 0.1030	 0.1410
g	 0.0250	 0.0770
h	 0.3010	 0.1970
i	 0.0370	 0.0690
j	 0.0000	 0.0360
k	 0.0990	 0.1440
l	 0.1070	 0.1770
m	 0.0180	 0.0690
n	 0.0080	 0.0340
o	 0.2550	 0.1740
p	 0.3010	 0.2010
q	 0.2230	 0.1840
r	 0.1360	 0.1790
s	 0.0000	 0.0140
t	 0.3690	 0.1720
u	 0.0590	 0.1400
w	 0.0480	 0.0930
z	 0.0710	 0.1890