



Full wwPDB EM Validation Report ⓘ

Mar 24, 2026 – 02:21 PM UTC

PDB ID : 6GXN / pdb_00006gxn
EMDB ID : EMD-0081
Title : Cryo-EM structure of an E. coli 70S ribosome in complex with RF3-GDPCP, RF1(GAQ) and Pint-tRNA (State III)
Authors : Graf, M.; Huter, P.; Maracci, C.; Peterek, M.; Rodnina, M.V.; Wilson, D.N.
Deposited on : 2018-06-27
Resolution : 3.90 Å(reported)

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

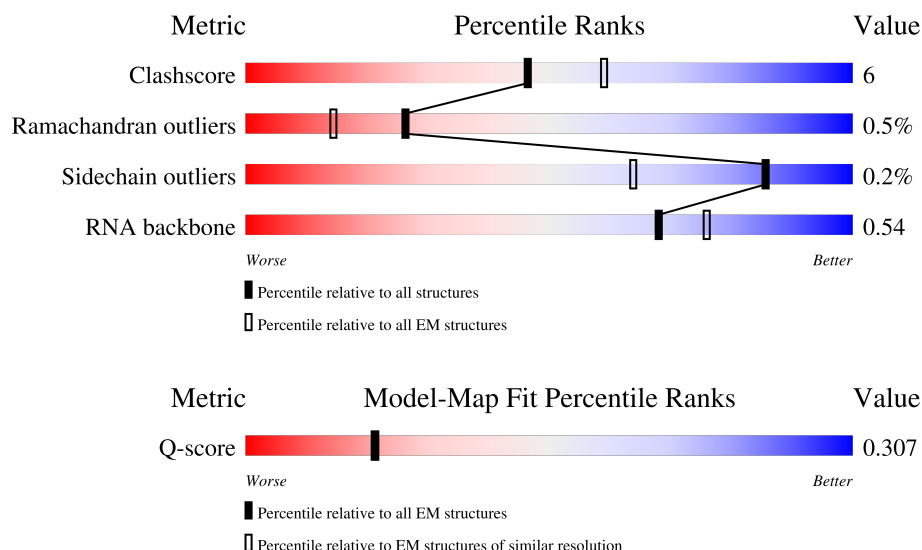
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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 3.90 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	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	8855 (3.40 - 4.40)

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	
2	B	120	
3	C	271	

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Mol	Chain	Length	Quality of chain
4	D	209	
5	E	201	
6	F	177	
7	G	176	
8	H	149	
9	I	141	
10	J	142	
11	K	122	
12	L	143	
13	M	136	
14	N	120	
15	O	116	
16	P	114	
17	Q	117	
18	R	103	
19	S	110	
20	T	93	
21	U	102	
22	V	94	
23	W	75	
24	X	77	
25	Y	63	
26	Z	58	
27	0	56	
28	1	50	

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Mol	Chain	Length	Quality of chain
29	2	46	
30	3	64	
31	4	38	
32	5	131	
33	7	7	
34	a	1539	
35	b	218	
36	c	206	
37	d	205	
38	e	157	
39	f	100	
40	g	151	
41	h	129	
42	i	127	
43	j	98	
44	k	116	
45	l	123	
46	m	114	
47	n	101	
48	o	88	
49	p	82	
50	q	80	
51	r	65	
52	s	79	
53	t	85	

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Mol	Chain	Length	Quality of chain
54	u	65	
55	v	350	
56	w	529	
57	x	77	
58	z	14	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
59	GCP	w	601	-	-	X	-

2 Entry composition

There are 59 unique types of molecules in this entry. The entry contains 151860 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	2895	Total	C	N	O	P	0	0
			62153	27726	11439	20093	2895		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	747	C	U	conflict	GB 1036415628
A	1847	G	A	conflict	GB 1036415628

- 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	-	expression tag	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	S	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 mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	7	7	Total	C	N	O	P	0	0
			151	68	29	47	7		

- Molecule 34 is a RNA chain called 16S ribosomal RNA.

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

- Molecule 35 is a protein called 30S ribosomal protein S2.

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

- Molecule 36 is a protein called 30S ribosomal protein S3.

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

- Molecule 37 is a protein called 30S ribosomal protein S4.

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

- Molecule 38 is a protein called 30S ribosomal protein S5.

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

- Molecule 39 is a protein called 30S ribosomal protein S6.

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

- Molecule 40 is a protein called 30S ribosomal protein S7.

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

- Molecule 41 is a protein called 30S ribosomal protein S8.

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

- Molecule 42 is a protein called 30S ribosomal protein S9.

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

- Molecule 43 is a protein called 30S ribosomal protein S10.

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

- Molecule 44 is a protein called 30S ribosomal protein S11.

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

- Molecule 45 is a protein called 30S ribosomal protein S12.

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

- Molecule 46 is a protein called 30S ribosomal protein S13.

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

- Molecule 47 is a protein called 30S ribosomal protein S14.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	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 48 is a protein called 30S ribosomal protein S15.

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

- Molecule 49 is a protein called 30S ribosomal protein S16.

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

- Molecule 50 is a protein called 30S ribosomal protein S17.

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

- Molecule 51 is a protein called 30S ribosomal protein S18.

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

- Molecule 52 is a protein called 30S ribosomal protein S19.

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

- Molecule 53 is a protein called 30S ribosomal protein S20.

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

- Molecule 54 is a protein called 30S ribosomal protein S21.

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

- Molecule 55 is a protein called Peptide chain release factor RF1.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	v	348	Total	C	N	O	S	0	0
			2436	1483	469	475	9		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
v	167	CYS	SER	conflict	UNP P0A7I0

- Molecule 56 is a protein called Peptide chain release factor RF3.

Mol	Chain	Residues	Atoms					AltConf	Trace
56	w	496	Total	C	N	O	S	0	0
			3923	2487	674	742	20		

- Molecule 57 is a RNA chain called fMet-tRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
57	x	77	Total	C	N	O	P	0	0
			1640	732	297	535	76		

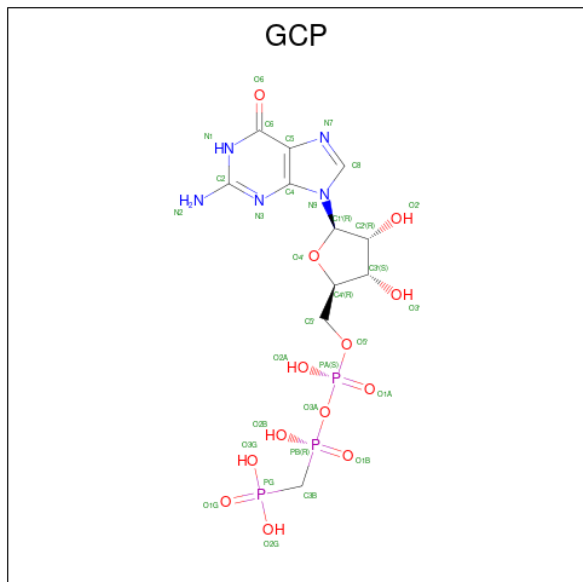
- Molecule 58 is a protein called Apidaecin.

Mol	Chain	Residues	Atoms				AltConf	Trace
58	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 59 is PHOSPHOMETHYLPHOSPHONIC ACID GUANYLATE ESTER (CCD ID: GCP) (formula: $C_{11}H_{18}N_5O_{13}P_3$).

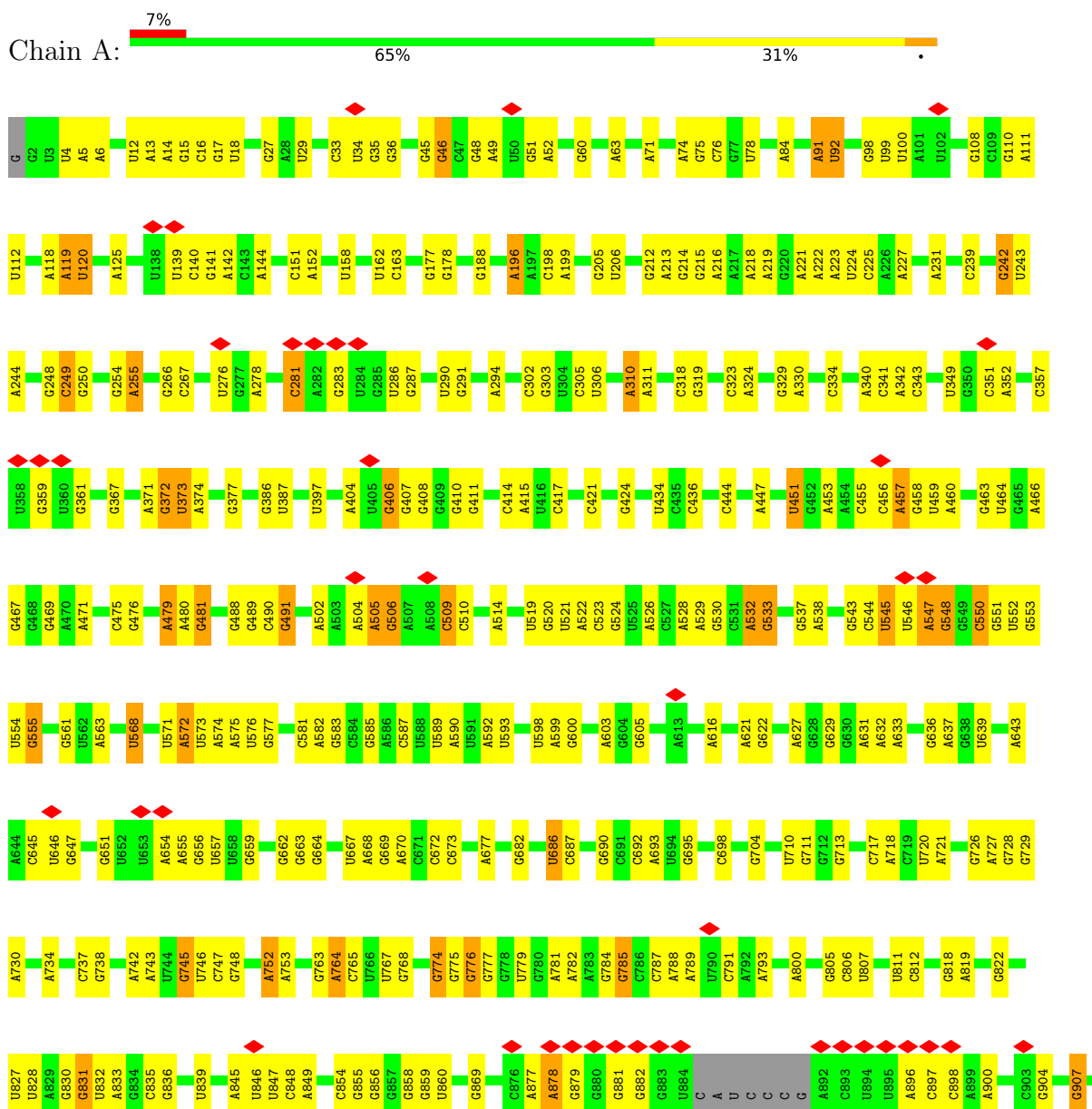


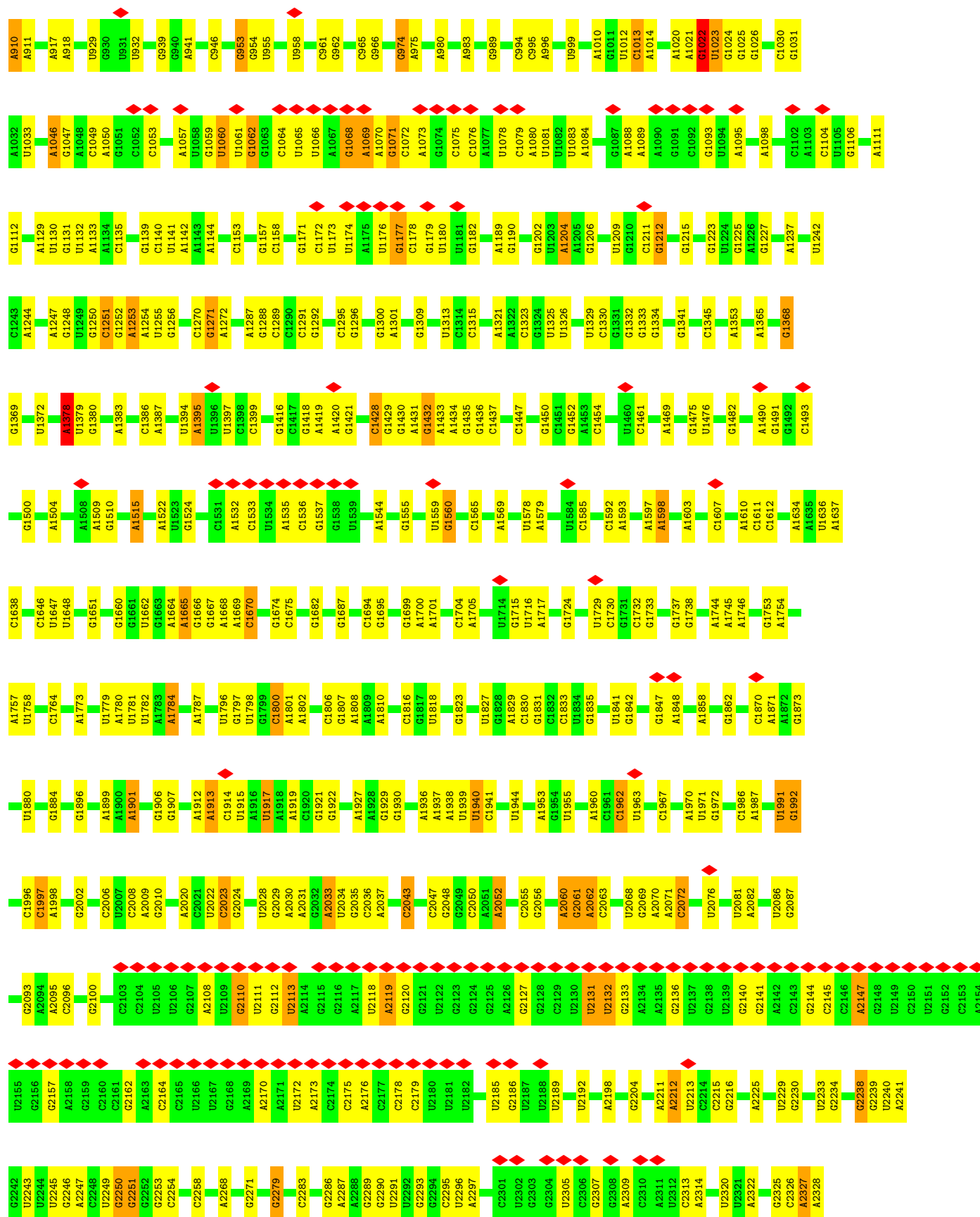
Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
59	w	1	32	11	5	13	3	0

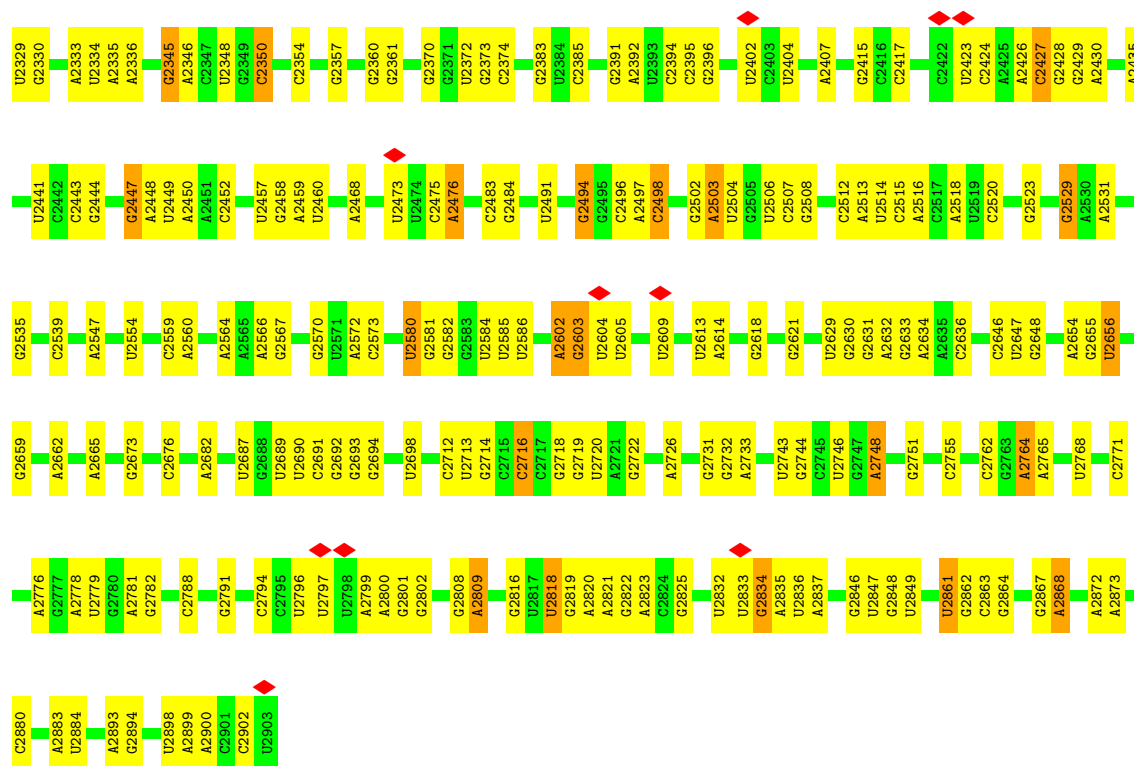
3 Residue-property plots

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

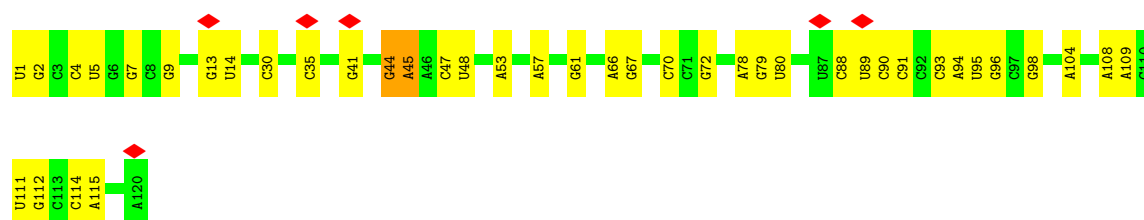
• Molecule 1: 23S ribosomal RNA



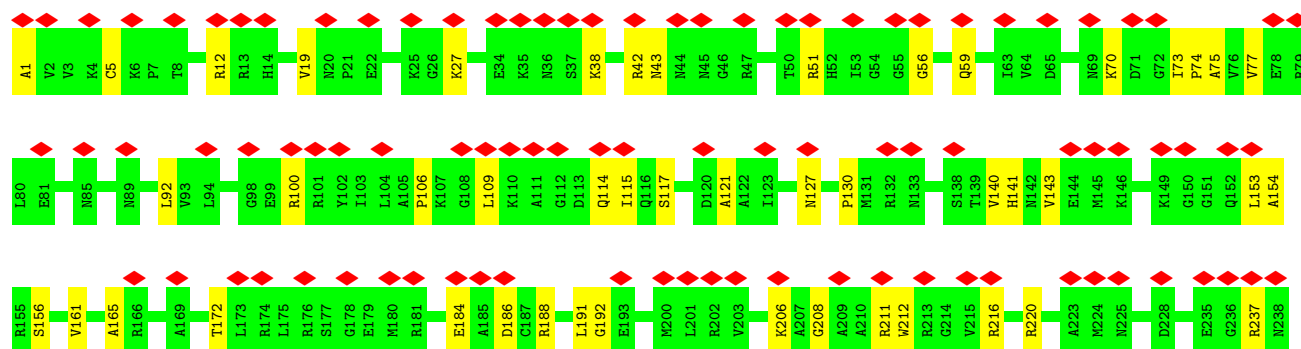
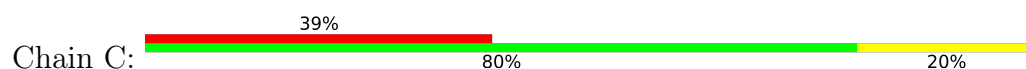




• Molecule 2: 5S ribosomal RNA

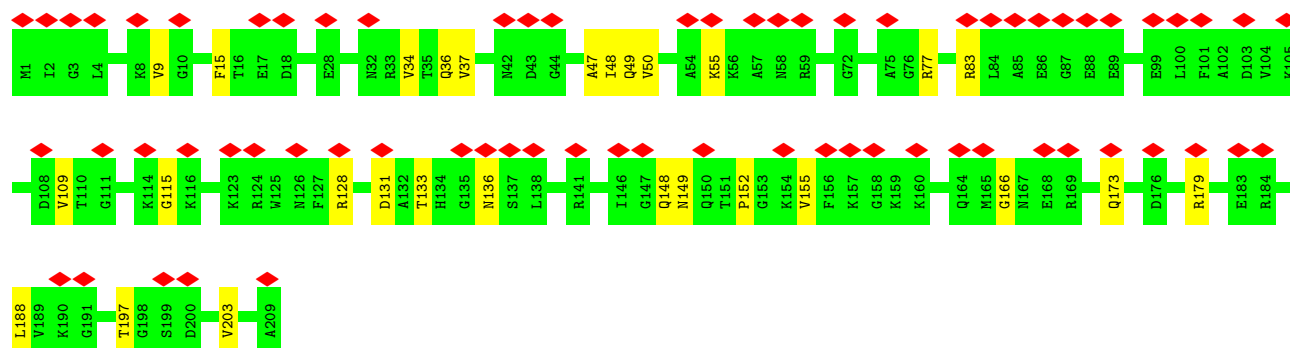
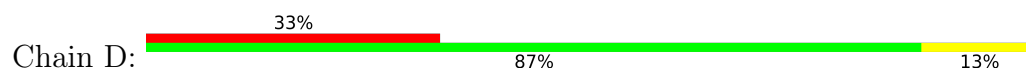


• Molecule 3: 50S ribosomal protein L2

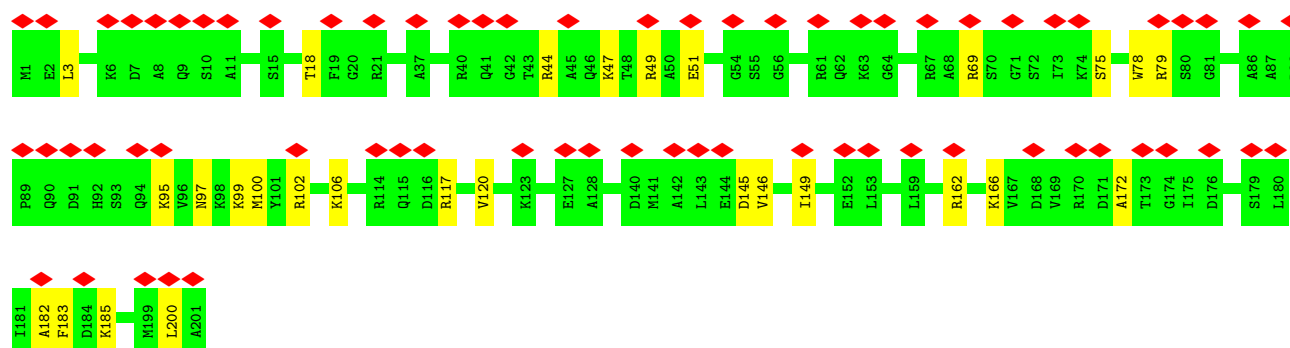
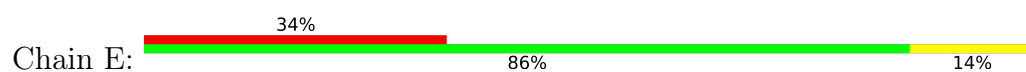




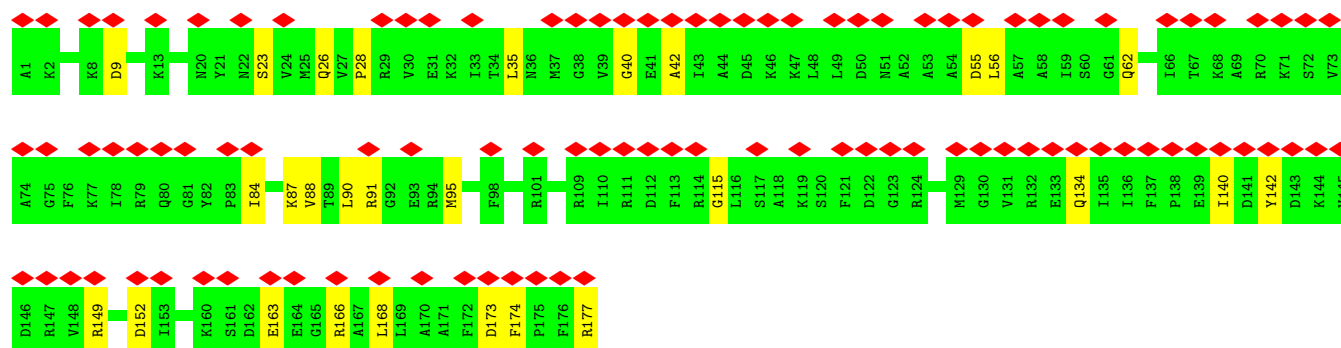
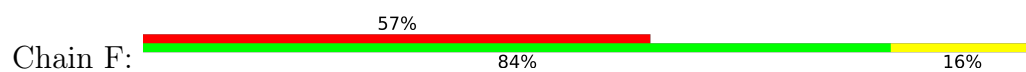
• Molecule 4: 50S ribosomal protein L3



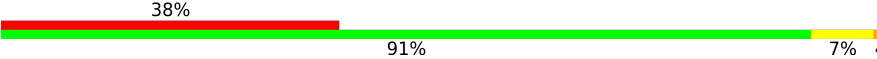
• Molecule 5: 50S ribosomal protein L4

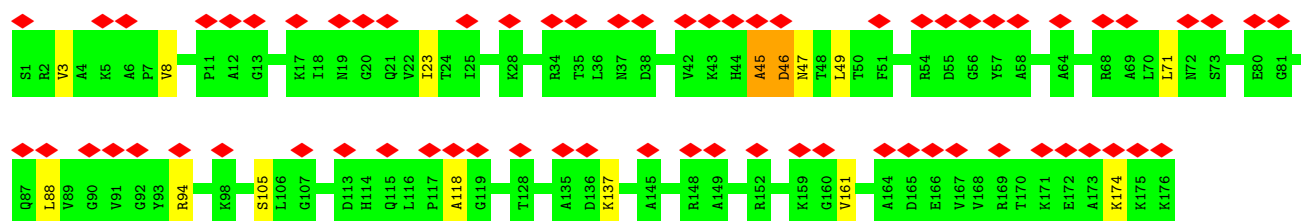


• Molecule 6: 50S ribosomal protein L5



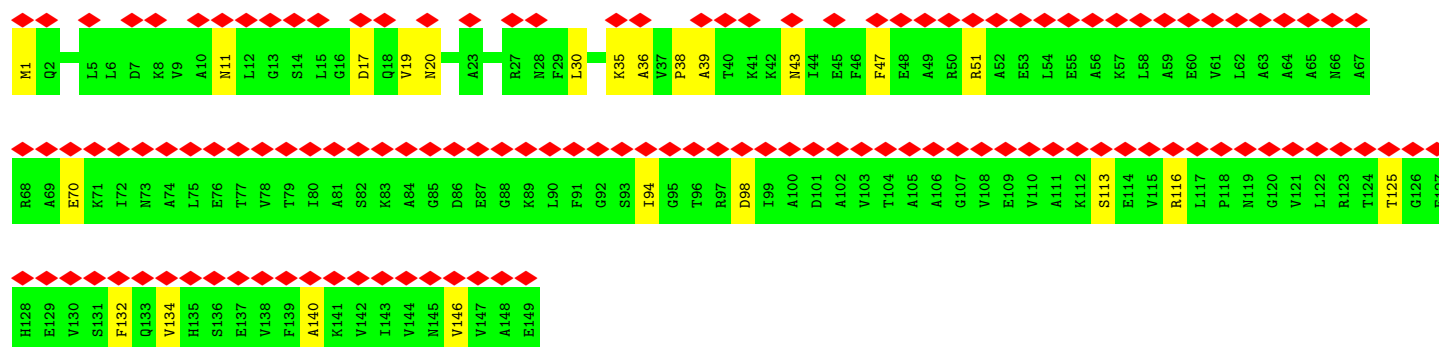
• Molecule 7: 50S ribosomal protein L6

Chain G: 



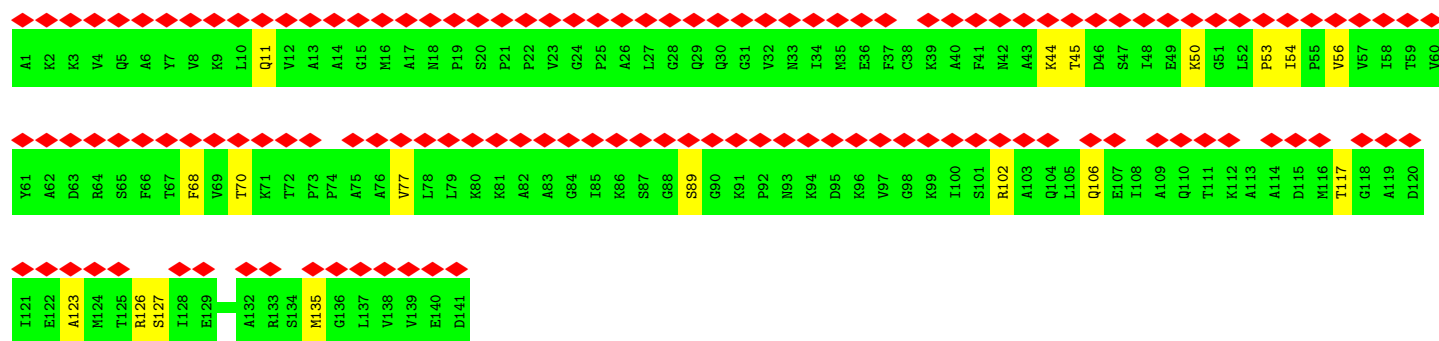
• Molecule 8: 50S ribosomal protein L9

Chain H: 



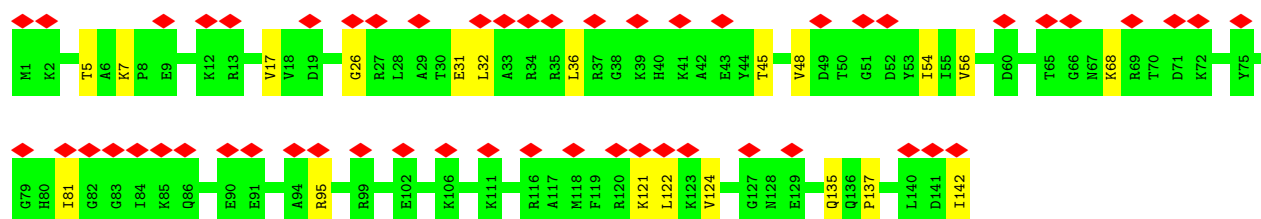
• Molecule 9: 50S ribosomal protein L11

Chain I: 

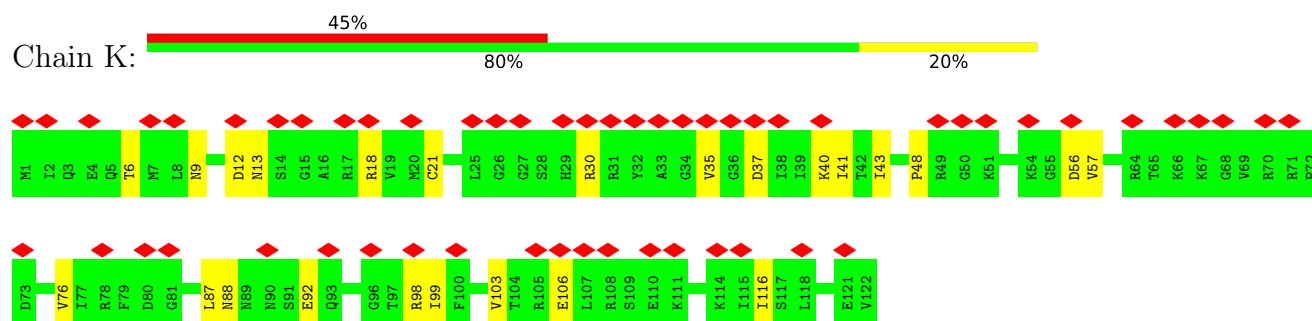


• Molecule 10: 50S ribosomal protein L13

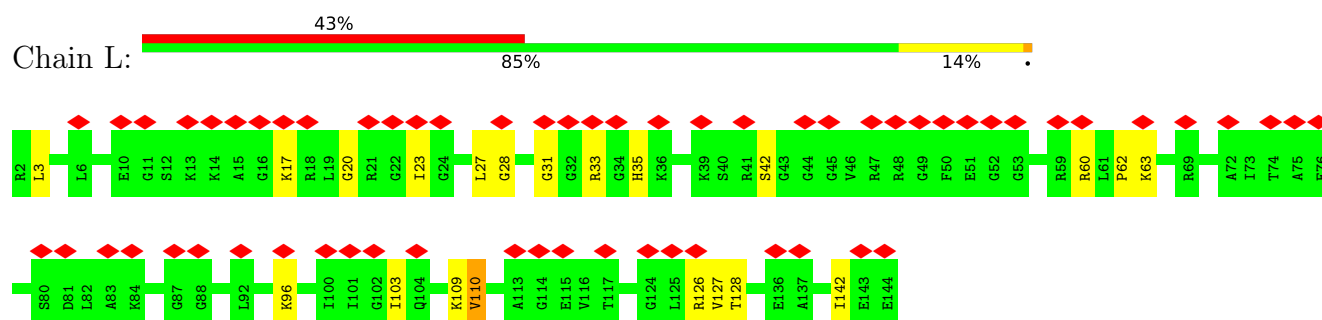
Chain J: 



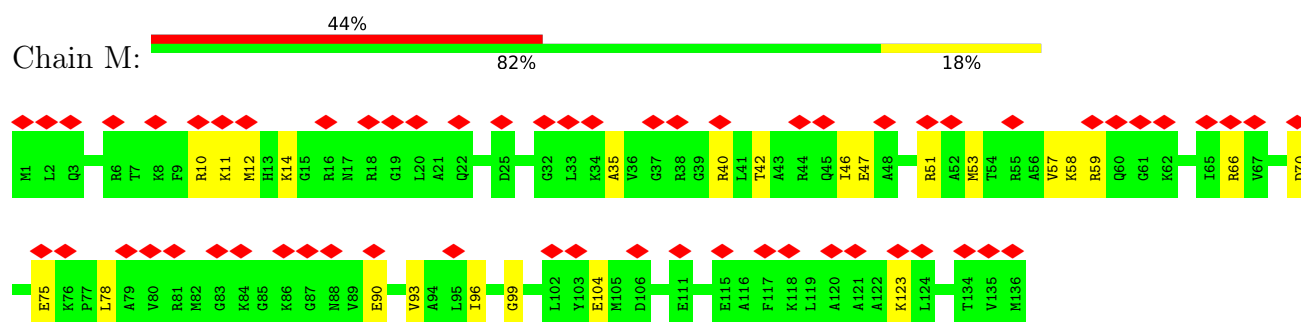
- Molecule 11: 50S ribosomal protein L14



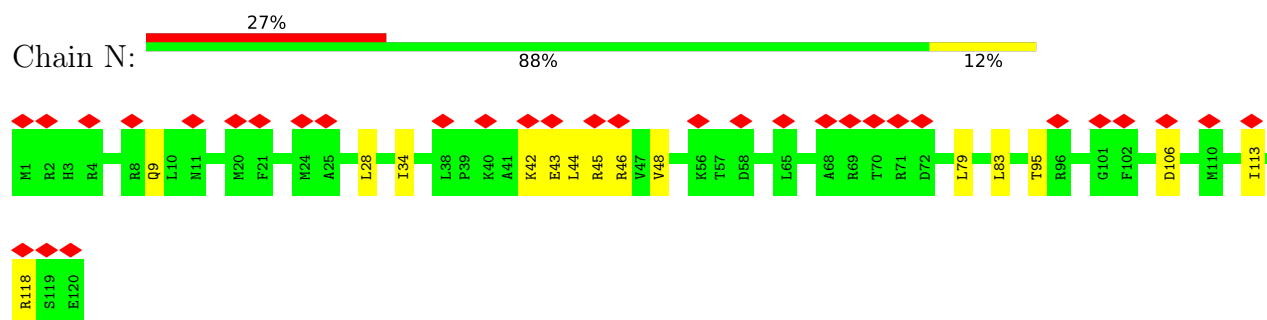
- Molecule 12: 50S ribosomal protein L15



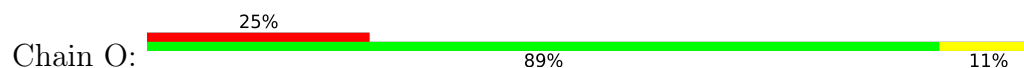
- Molecule 13: 50S ribosomal protein L16

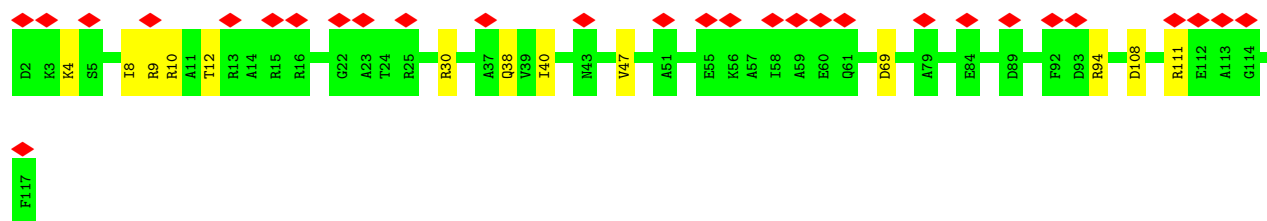


- Molecule 14: 50S ribosomal protein L17

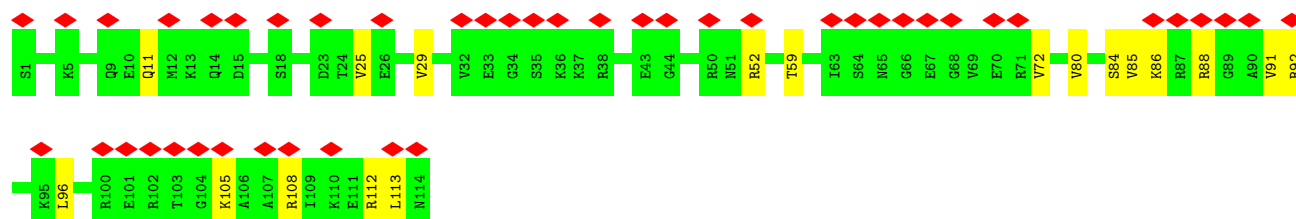
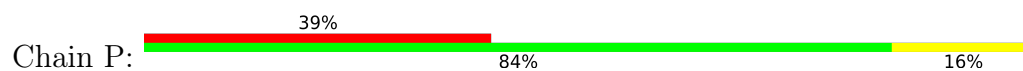


- Molecule 15: 50S ribosomal protein L18

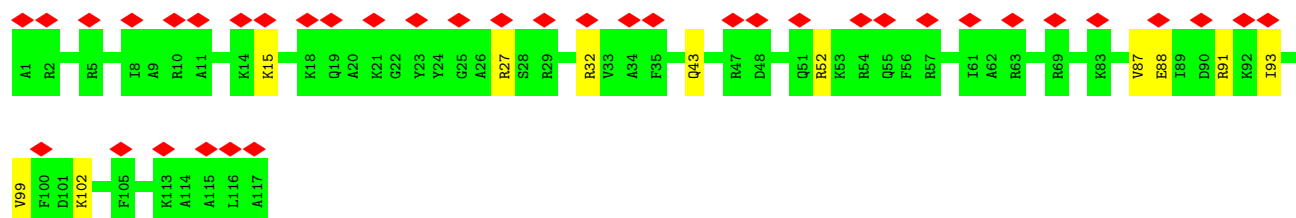
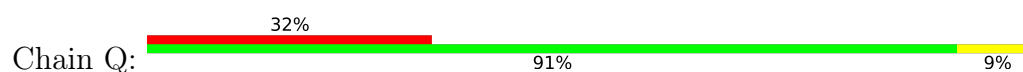




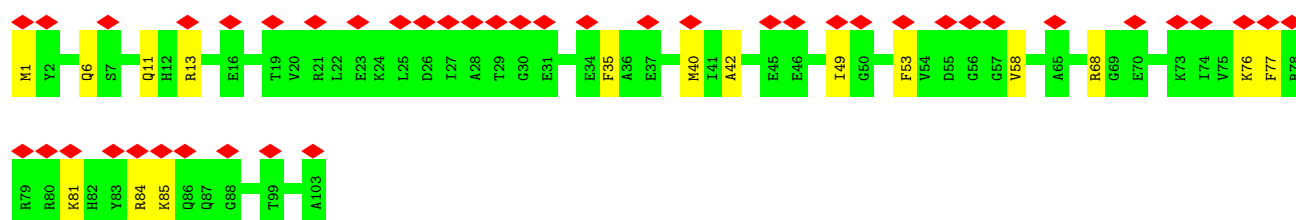
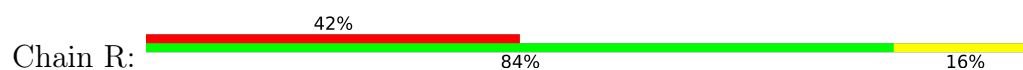
• Molecule 16: 50S ribosomal protein L19



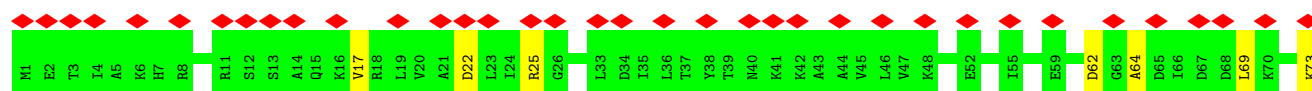
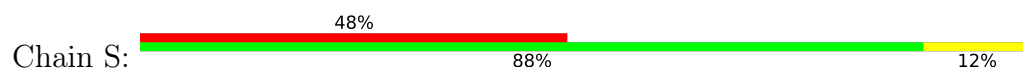
• Molecule 17: 50S ribosomal protein L20

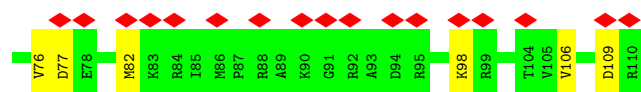


• Molecule 18: 50S ribosomal protein L21

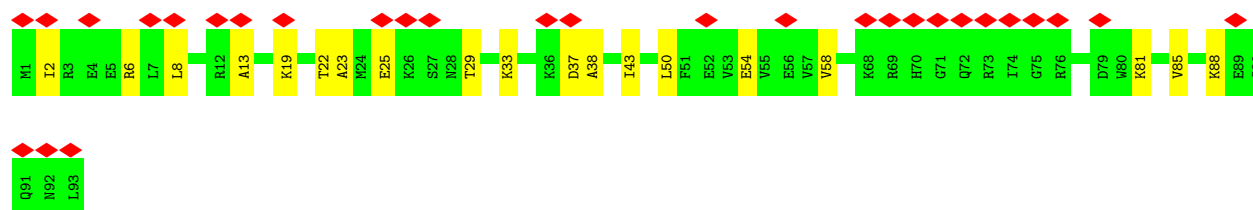
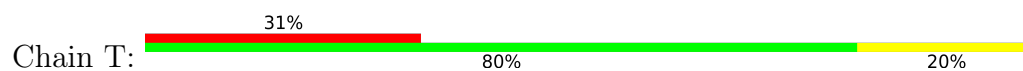


• Molecule 19: 50S ribosomal protein L22

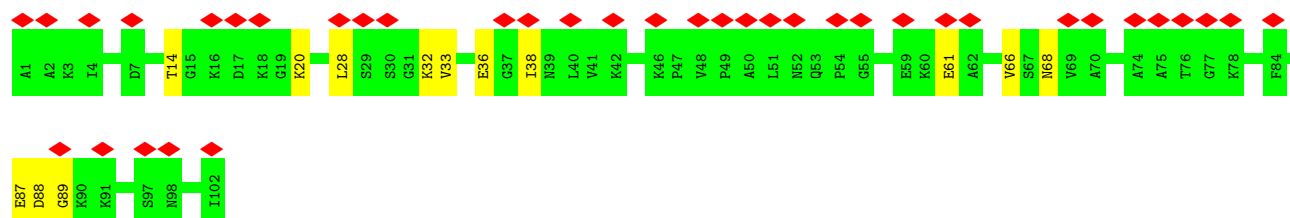
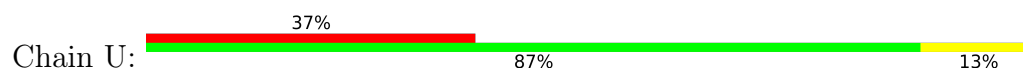




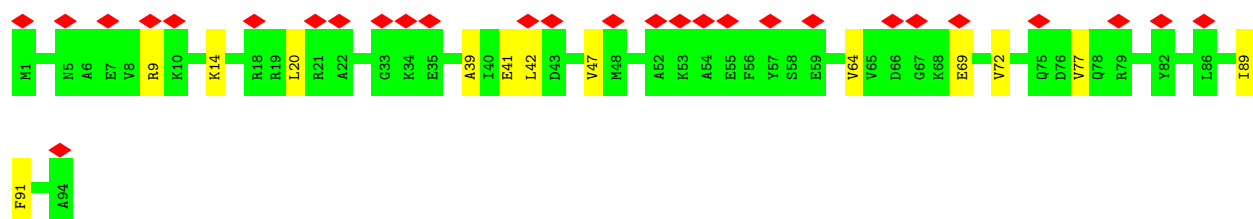
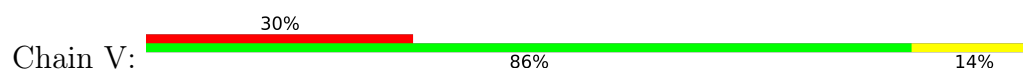
- Molecule 20: 50S ribosomal protein L23



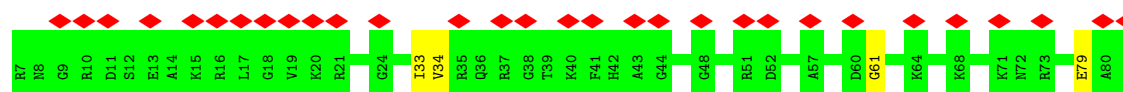
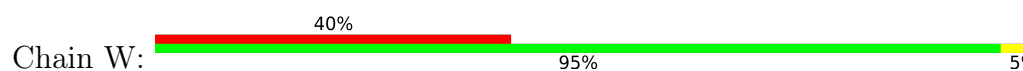
- Molecule 21: 50S ribosomal protein L24



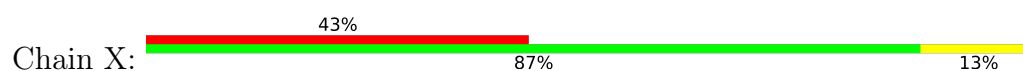
- Molecule 22: 50S ribosomal protein L25

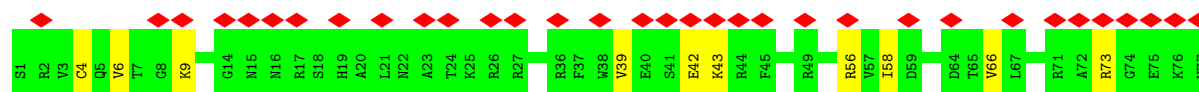


- Molecule 23: 50S ribosomal protein L27

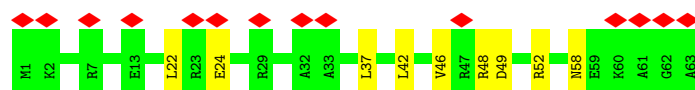
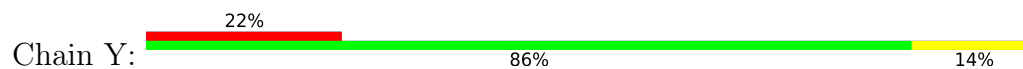


- Molecule 24: 50S ribosomal protein L28

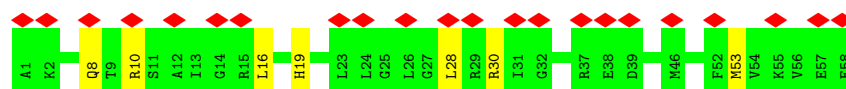
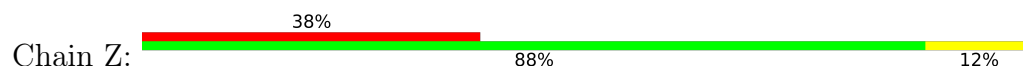




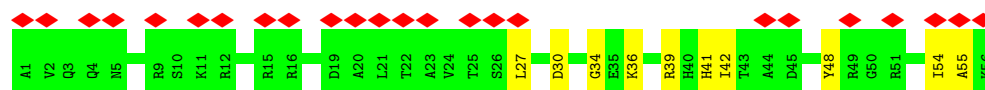
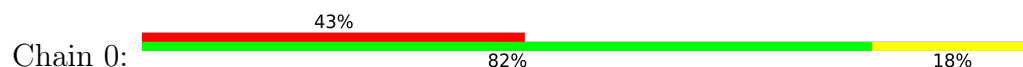
- Molecule 25: 50S ribosomal protein L29



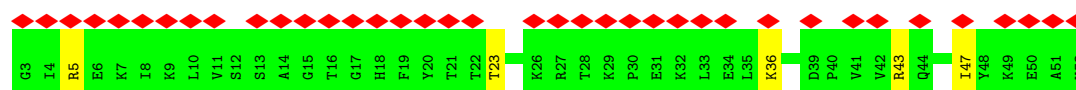
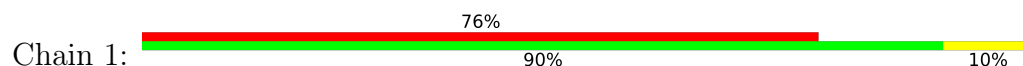
- Molecule 26: 50S ribosomal protein L30



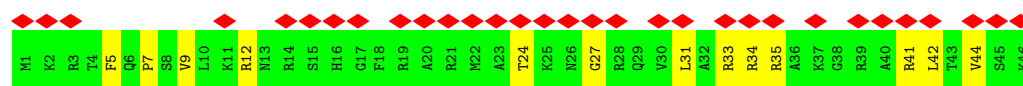
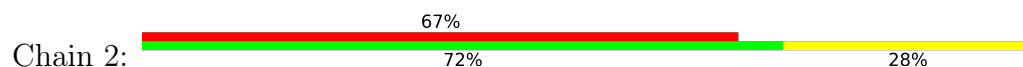
- Molecule 27: 50S ribosomal protein L32



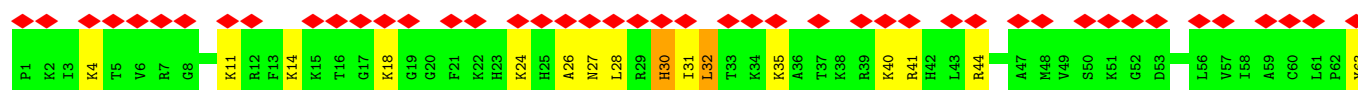
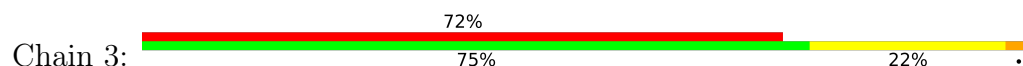
- Molecule 28: 50S ribosomal protein L33



- Molecule 29: 50S ribosomal protein L34

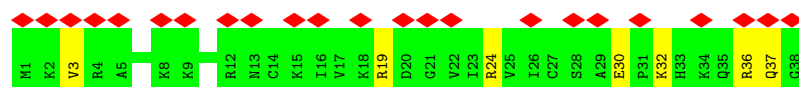
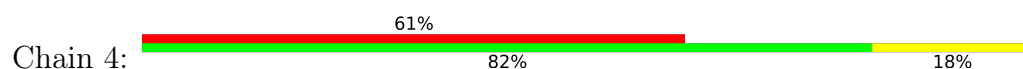


- Molecule 30: 50S ribosomal protein L35

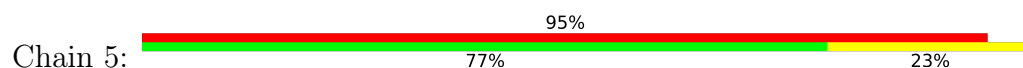




- Molecule 31: 50S ribosomal protein L36



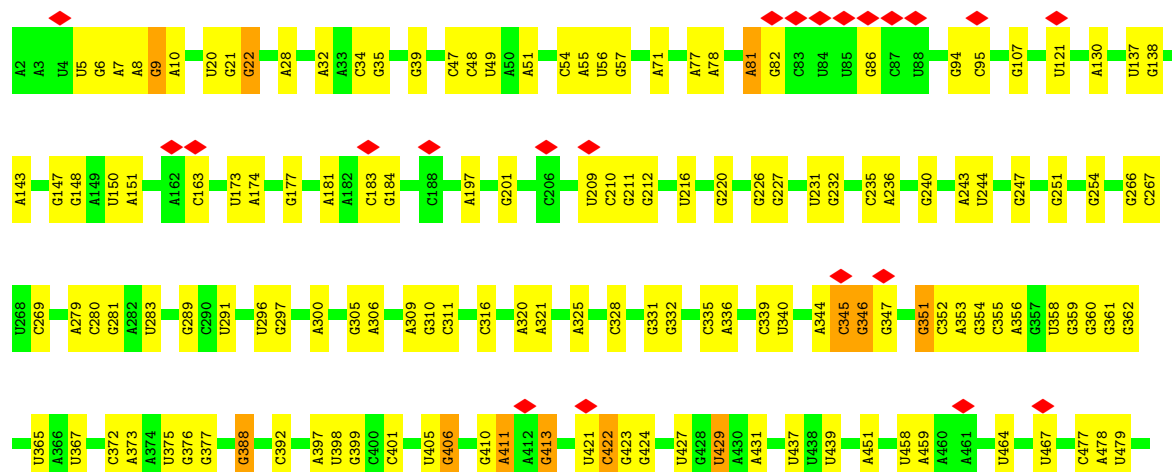
- Molecule 32: 50S ribosomal protein L10

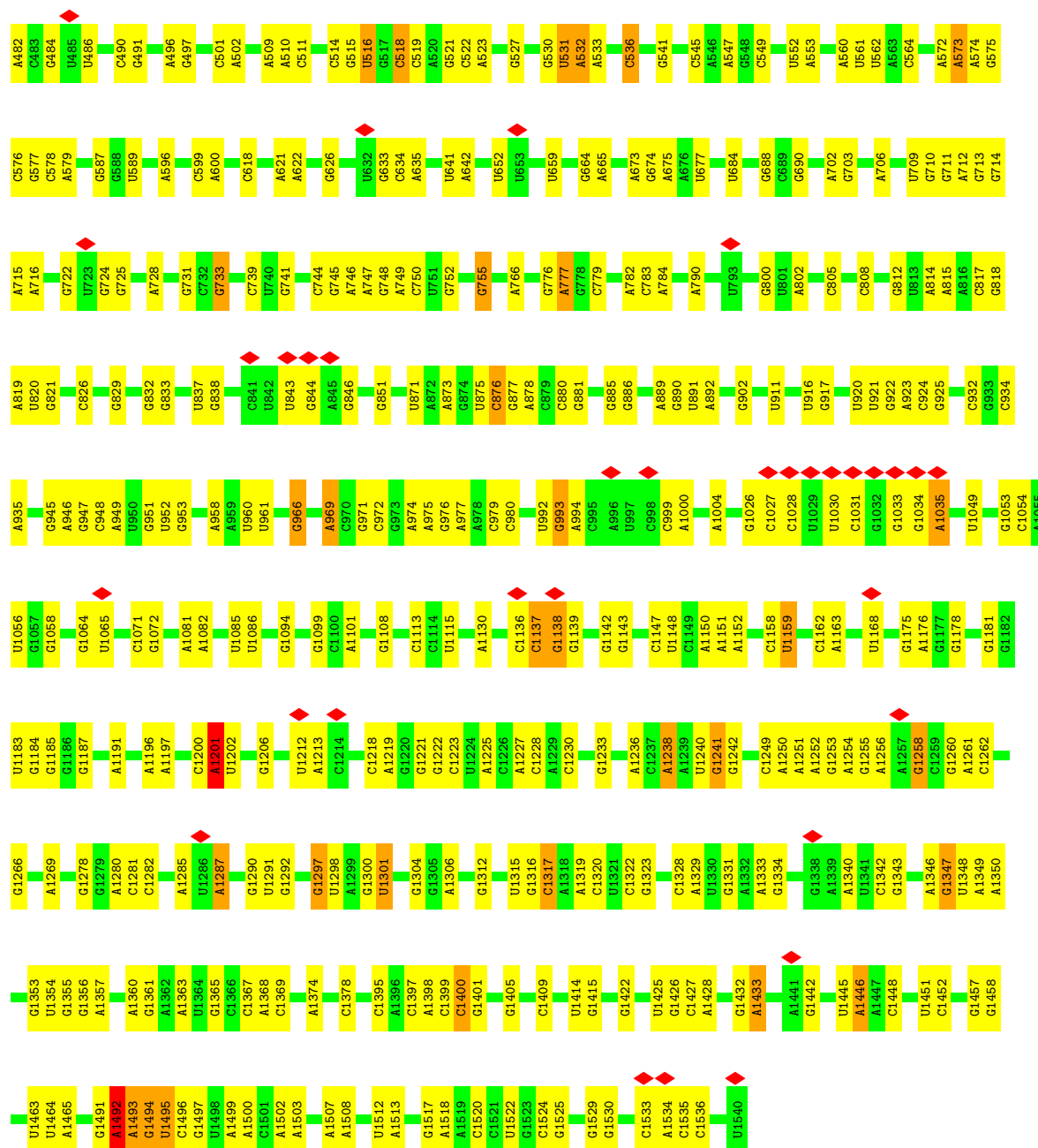


- Molecule 33: mRNA

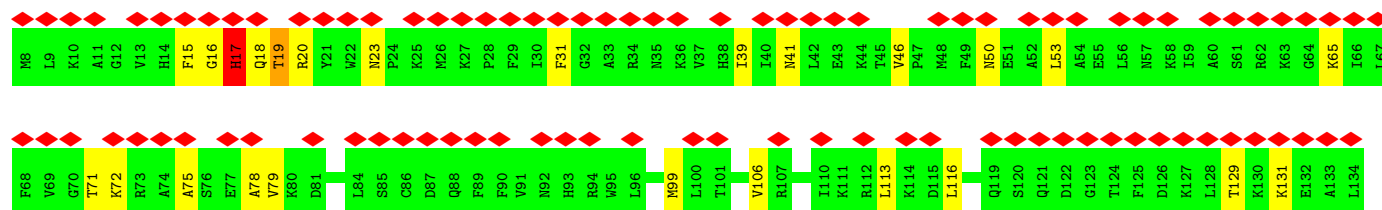
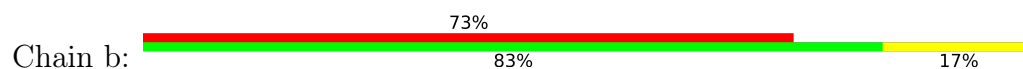


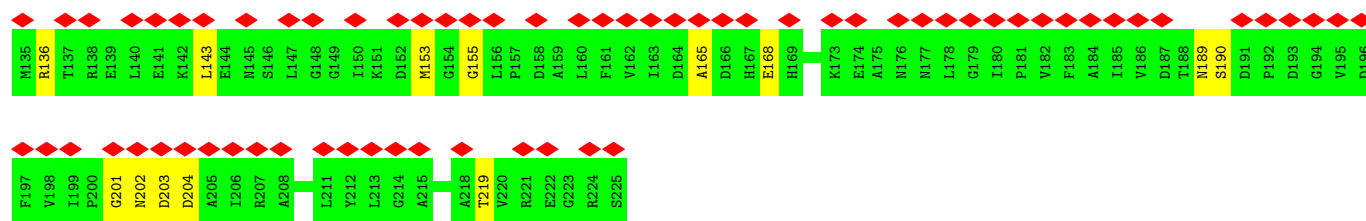
- Molecule 34: 16S ribosomal RNA



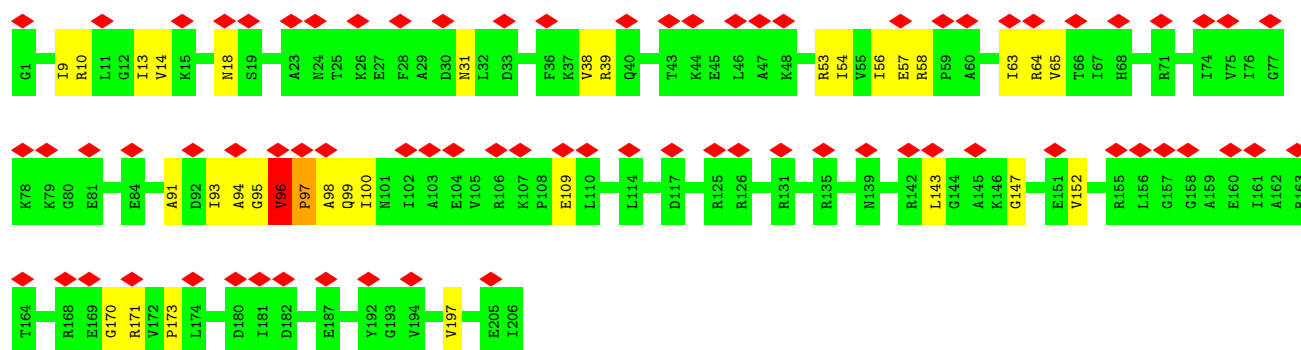
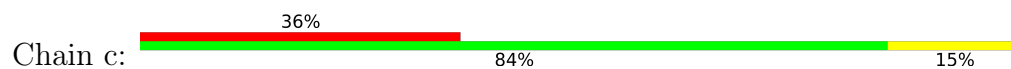


• Molecule 35: 30S ribosomal protein S2

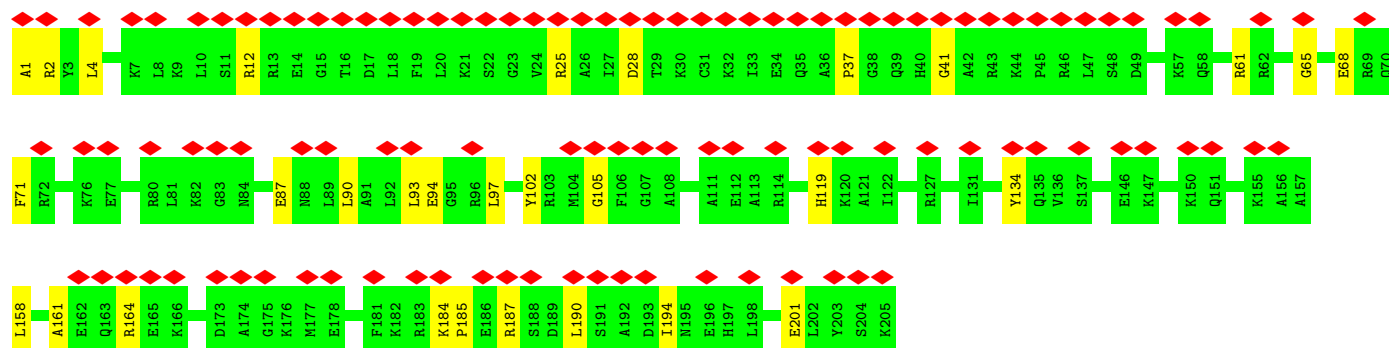
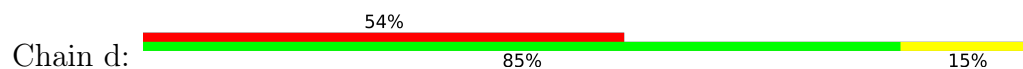




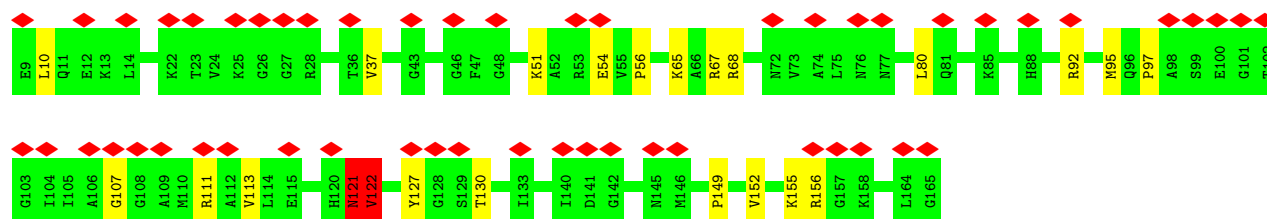
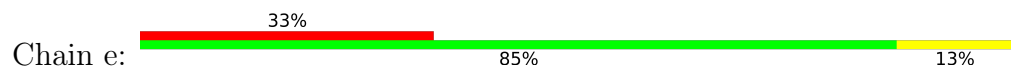
• Molecule 36: 30S ribosomal protein S3



• Molecule 37: 30S ribosomal protein S4

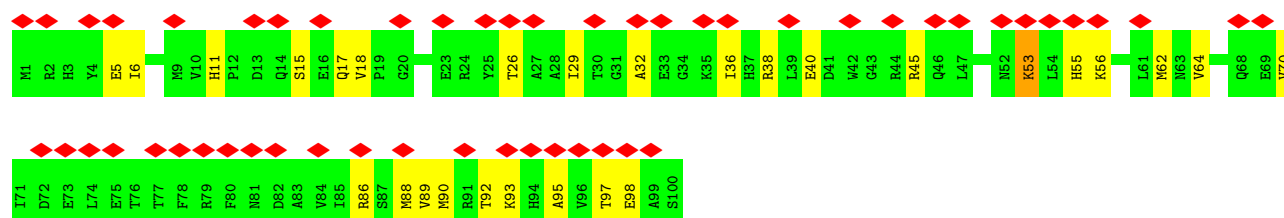


• Molecule 38: 30S ribosomal protein S5



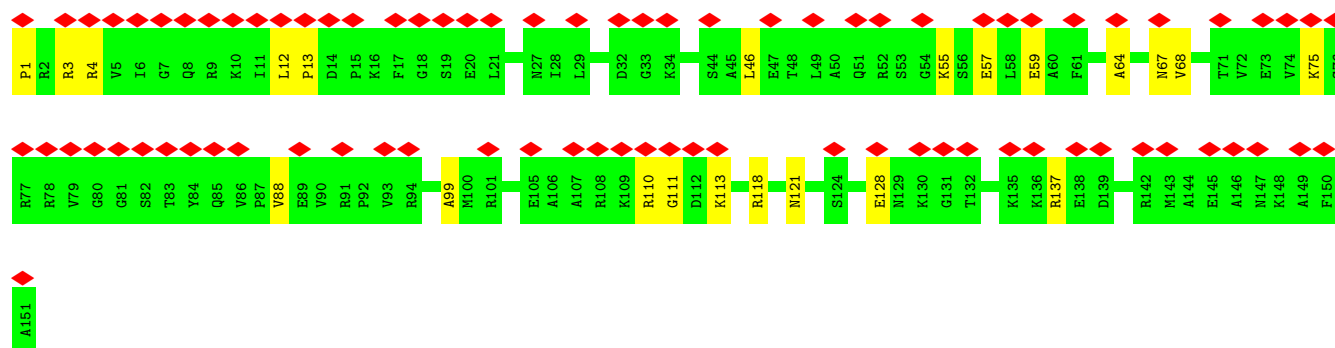
• Molecule 39: 30S ribosomal protein S6

Chain f: 



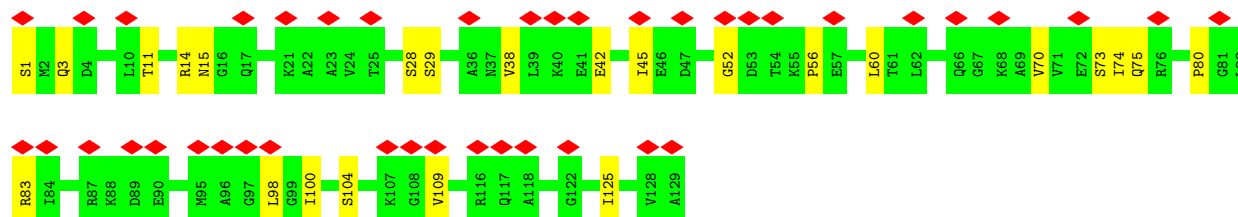
• Molecule 40: 30S ribosomal protein S7

Chain g: 



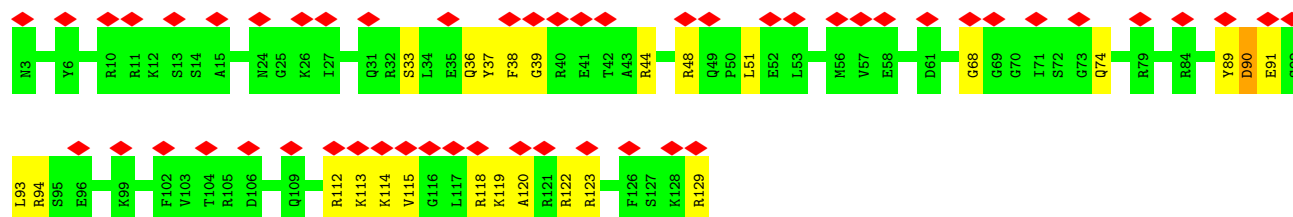
• Molecule 41: 30S ribosomal protein S8

Chain h: 



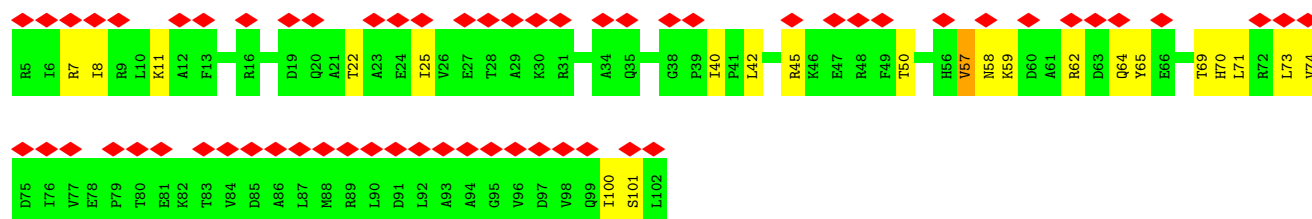
• Molecule 42: 30S ribosomal protein S9

Chain i: 

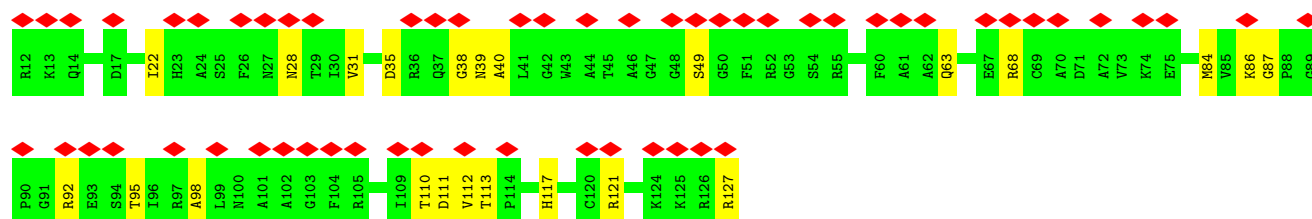
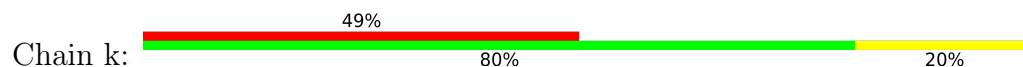


• Molecule 43: 30S ribosomal protein S10

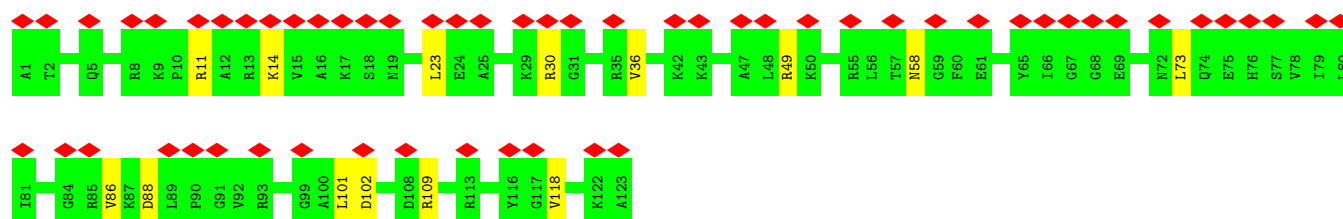
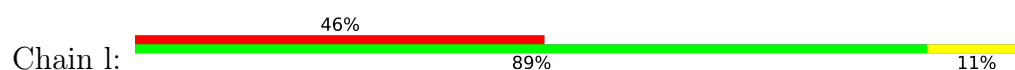
Chain j: 



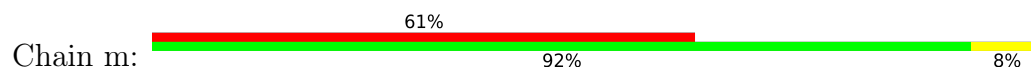
• Molecule 44: 30S ribosomal protein S11



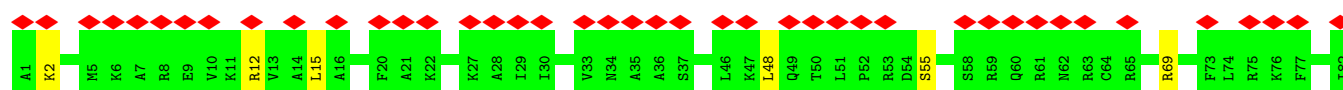
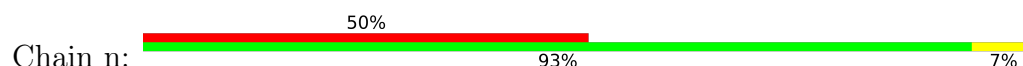
• Molecule 45: 30S ribosomal protein S12

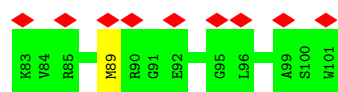


• Molecule 46: 30S ribosomal protein S13

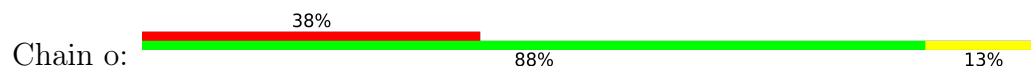


• Molecule 47: 30S ribosomal protein S14

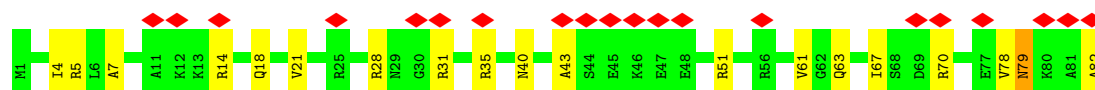
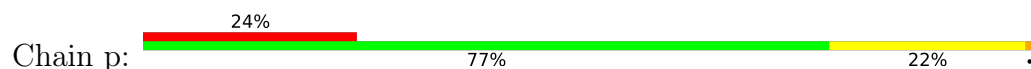




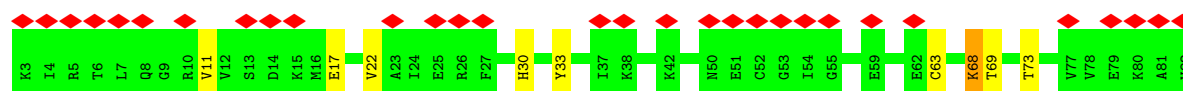
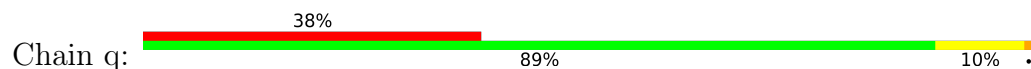
- Molecule 48: 30S ribosomal protein S15



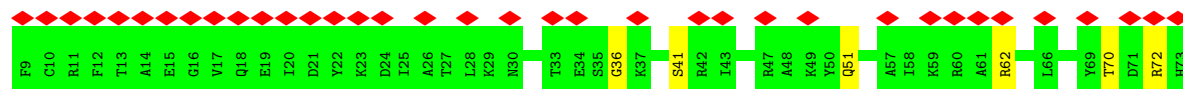
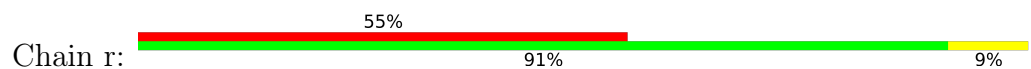
- Molecule 49: 30S ribosomal protein S16



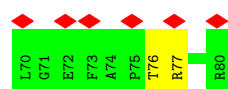
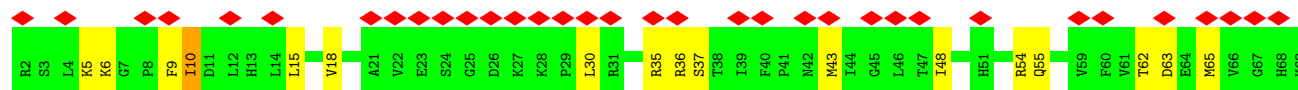
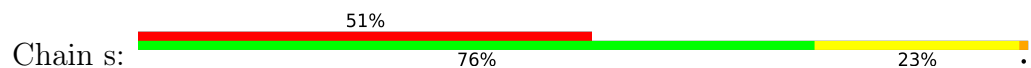
- Molecule 50: 30S ribosomal protein S17



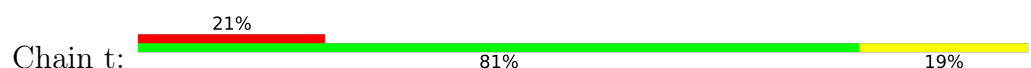
- Molecule 51: 30S ribosomal protein S18

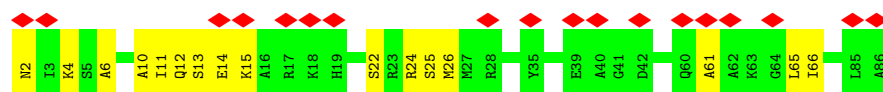


- Molecule 52: 30S ribosomal protein S19

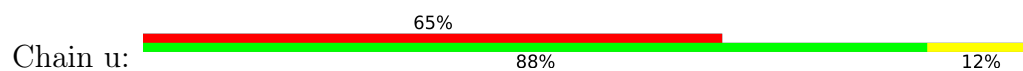


- Molecule 53: 30S ribosomal protein S20

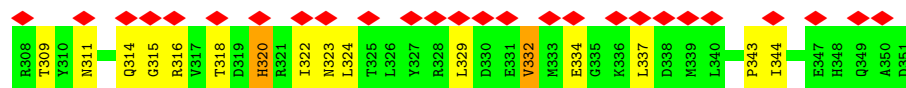
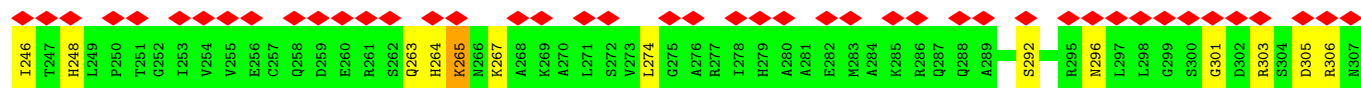
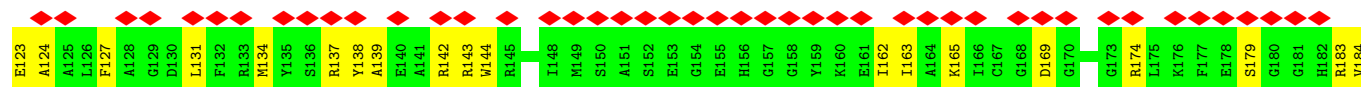
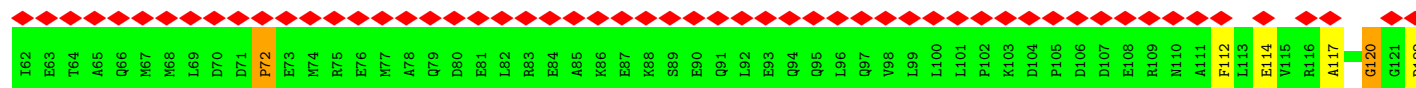
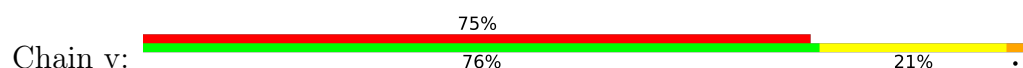




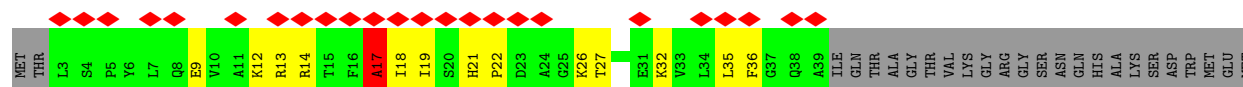
• Molecule 54: 30S ribosomal protein S21

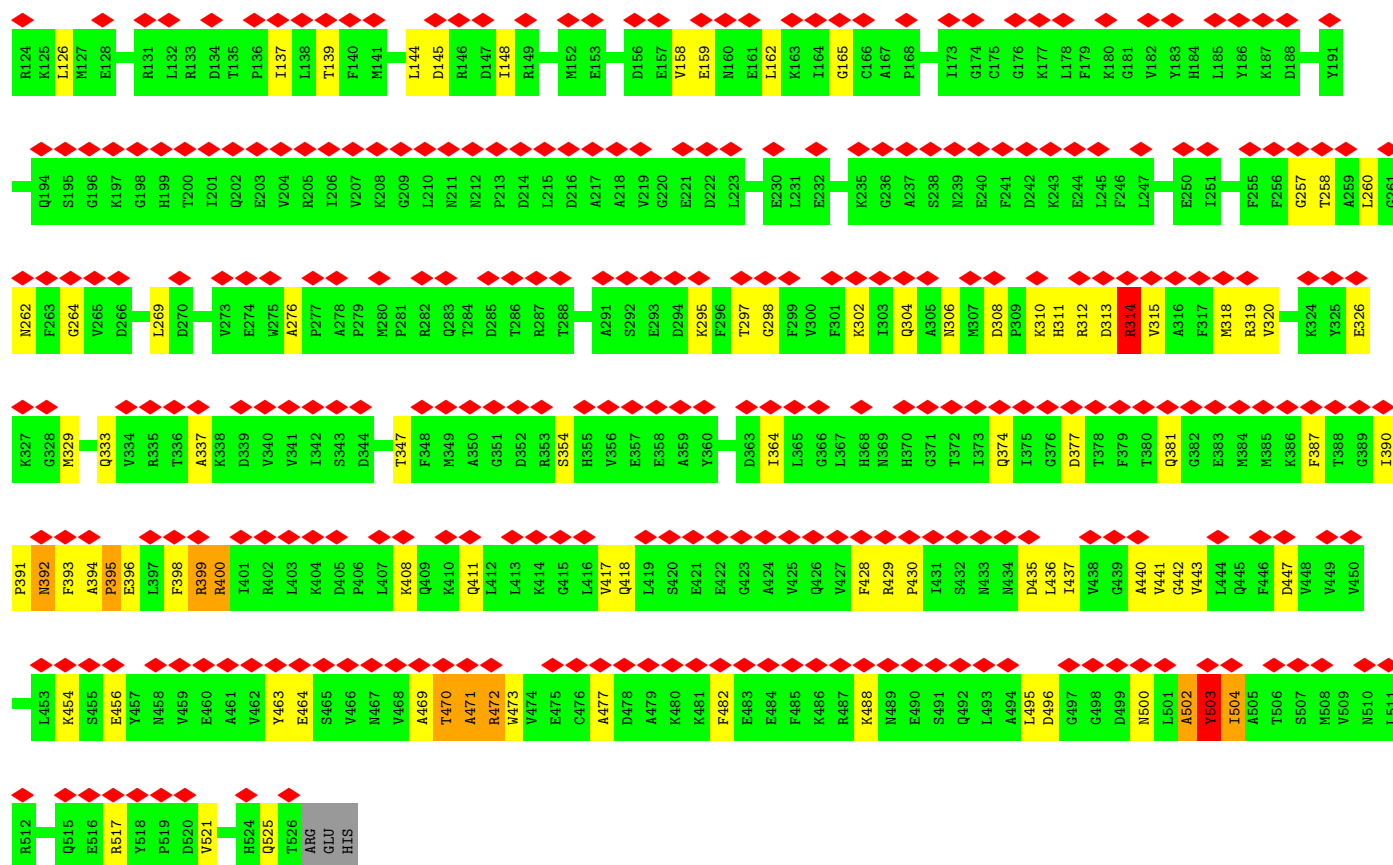


• Molecule 55: Peptide chain release factor RF1

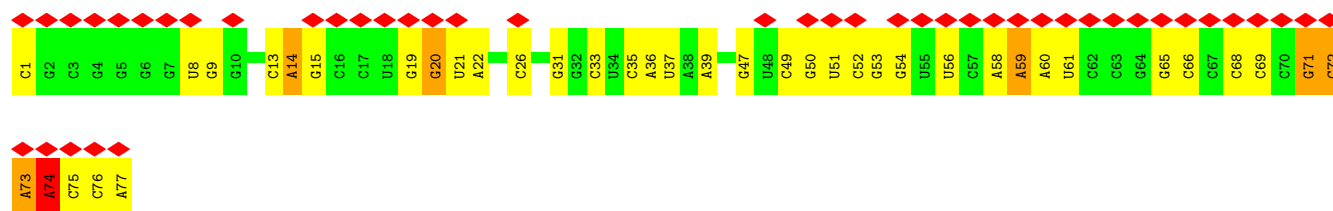


• Molecule 56: Peptide chain release factor RF3

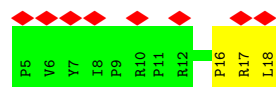
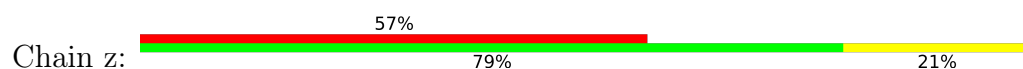




• Molecule 57: fMet-tRNA



• Molecule 58: Apidaecin



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	54142	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	0.119	Depositor
Minimum map value	-0.051	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.009	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	0/69612	0.33	3/108599 (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	0.51	0/2134
5	E	0.19	0/1571	0.51	0/2113
6	F	0.25	0/1434	0.63	0/1926
7	G	0.21	0/1343	0.58	2/1816 (0.1%)
8	H	0.19	0/1122	0.50	0/1515
9	I	0.25	0/1046	0.60	0/1410
10	J	0.18	0/1152	0.46	0/1551
11	K	0.22	0/947	0.60	0/1268
12	L	0.24	0/1054	0.70	4/1403 (0.3%)
13	M	0.24	0/1093	0.69	3/1460 (0.2%)
14	N	0.24	0/973	0.67	0/1301
15	O	0.21	0/902	0.50	0/1209
16	P	0.20	0/929	0.53	0/1242
17	Q	0.19	0/960	0.51	0/1278
18	R	0.20	0/829	0.52	0/1107
19	S	0.21	0/864	0.58	0/1156
20	T	0.20	0/744	0.56	0/994
21	U	0.26	0/787	0.74	2/1051 (0.2%)
22	V	0.19	0/766	0.50	0/1025
23	W	0.16	0/582	0.46	0/769
24	X	0.17	0/635	0.46	0/848
25	Y	0.16	0/510	0.50	0/677
26	Z	0.18	0/453	0.42	0/605
27	0	0.18	0/450	0.50	0/599
28	1	0.20	0/416	0.55	0/554
29	2	0.19	0/380	0.54	0/498
30	3	0.23	0/513	0.71	2/676 (0.3%)
31	4	0.22	0/303	0.68	0/397
32	5	0.35	1/1001 (0.1%)	0.81	2/1350 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	7	0.42	0/169	0.78	0/261
34	a	0.15	0/36967	0.32	3/57666 (0.0%)
35	b	0.24	0/1735	0.69	4/2338 (0.2%)
36	c	0.21	0/1651	0.58	3/2225 (0.1%)
37	d	0.22	0/1665	0.65	0/2227
38	e	0.24	0/1154	0.72	3/1554 (0.2%)
39	f	0.35	0/835	0.82	2/1128 (0.2%)
40	g	0.23	0/1195	0.64	3/1602 (0.2%)
41	h	0.21	0/989	0.60	0/1326
42	i	0.24	0/1034	0.75	0/1375
43	j	0.28	0/796	0.74	0/1077
44	k	0.22	0/885	0.57	0/1195
45	l	0.26	0/969	0.72	0/1300
46	m	0.25	0/892	0.63	0/1193
47	n	0.20	0/811	0.57	0/1081
48	o	0.21	0/722	0.66	3/964 (0.3%)
49	p	0.21	0/659	0.61	3/884 (0.3%)
50	q	0.27	0/657	0.73	2/881 (0.2%)
51	r	0.21	0/511	0.66	0/689
52	s	0.20	0/652	0.56	0/877
53	t	0.25	0/671	0.64	0/888
54	u	0.35	0/500	1.00	5/668 (0.7%)
55	v	0.27	0/2468	0.72	5/3351 (0.1%)
56	w	0.27	0/3996	0.81	14/5402 (0.3%)
57	x	0.20	0/1832	0.52	2/2855 (0.1%)
58	z	0.20	0/127	0.62	0/175
All	All	0.18	1/164496 (0.0%)	0.44	70/245048 (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	2
32	5	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
35	b	0	3
38	e	0	1
39	f	0	2
42	i	0	1
43	j	0	1
45	l	0	1
46	m	0	1
50	q	0	1
55	v	0	1
56	w	0	3
All	All	0	27

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	5	118	ILE	C-N	6.75	1.39	1.33

All (70) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
56	w	399	ARG	N-CA-C	20.83	133.99	111.28
57	x	74	A	C1'-C2'-O2'	10.42	127.42	111.80
56	w	470	THR	N-CA-C	8.60	122.34	108.76
55	v	265	LYS	N-CA-C	-8.19	102.44	111.36
40	g	64	ALA	N-CA-C	-7.71	105.03	114.75
56	w	313	ASP	CA-C-N	7.62	136.10	121.54
56	w	313	ASP	C-N-CA	7.62	136.10	121.54
35	b	17	HIS	CA-C-N	7.12	130.69	120.79
35	b	17	HIS	C-N-CA	7.12	130.69	120.79
35	b	19	THR	N-CA-C	6.55	116.70	108.45
34	a	1492	A	C4'-C3'-O3'	-6.52	99.62	109.40
55	v	72	PRO	N-CA-CB	6.46	110.04	103.25
56	w	314	ARG	CA-C-N	6.46	133.59	121.97
56	w	314	ARG	C-N-CA	6.46	133.59	121.97
7	G	45	ALA	CA-C-N	6.42	133.79	121.54
7	G	45	ALA	C-N-CA	6.42	133.79	121.54
56	w	17	ALA	CA-C-N	6.23	133.18	121.97
56	w	17	ALA	C-N-CA	6.23	133.18	121.97
21	U	87	GLU	CA-C-N	6.22	130.58	121.31
21	U	87	GLU	C-N-CA	6.22	130.58	121.31
56	w	502	ALA	CA-C-N	6.19	133.37	121.54
56	w	502	ALA	C-N-CA	6.19	133.37	121.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
56	w	471	ALA	N-CA-C	6.18	120.15	112.24
54	u	23	GLU	CA-C-N	6.08	129.25	120.79
54	u	23	GLU	C-N-CA	6.08	129.25	120.79
35	b	201	GLY	N-CA-C	6.00	118.69	110.58
54	u	34	ARG	N-CA-C	5.93	117.84	110.91
55	v	193	GLN	N-CA-C	5.92	117.74	111.28
36	c	96	VAL	N-CA-C	5.92	121.66	108.88
13	M	96	ILE	CA-C-N	5.91	133.54	121.48
13	M	96	ILE	C-N-CA	5.91	133.54	121.48
56	w	503	TYR	N-CA-C	-5.89	98.26	110.80
56	w	471	ALA	CA-C-N	-5.85	110.37	121.54
56	w	471	ALA	C-N-CA	-5.85	110.37	121.54
38	e	121	ASN	CA-C-N	5.84	132.49	121.97
38	e	121	ASN	C-N-CA	5.84	132.49	121.97
54	u	35	GLU	CA-C-N	5.81	132.64	121.54
54	u	35	GLU	C-N-CA	5.81	132.64	121.54
12	L	110	VAL	CA-C-N	5.76	128.43	120.49
12	L	110	VAL	C-N-CA	5.76	128.43	120.49
30	3	30	HIS	CA-C-N	5.75	132.32	121.97
30	3	30	HIS	C-N-CA	5.75	132.32	121.97
13	M	53	MET	N-CA-C	-5.68	108.14	114.62
50	q	68	LYS	CA-C-N	5.62	132.28	121.54
50	q	68	LYS	C-N-CA	5.62	132.28	121.54
12	L	35	HIS	CA-C-N	5.50	128.90	120.82
12	L	35	HIS	C-N-CA	5.50	128.90	120.82
48	o	13	GLU	N-CA-C	-5.46	108.39	114.62
55	v	332	VAL	N-CA-C	-5.45	107.54	112.12
55	v	239	THR	N-CA-C	5.39	117.24	111.36
39	f	17	GLN	CA-C-N	5.38	124.63	120.33
39	f	17	GLN	C-N-CA	5.38	124.63	120.33
1	A	752	A	P-O3'-C3'	5.33	128.19	120.20
1	A	1378	A	P-O3'-C3'	5.29	128.13	120.20
40	g	128	GLU	CA-C-N	5.22	129.82	122.46
40	g	128	GLU	C-N-CA	5.22	129.82	122.46
48	o	44	GLU	CA-C-N	5.21	131.50	121.54
48	o	44	GLU	C-N-CA	5.21	131.50	121.54
49	p	78	VAL	CA-C-N	5.17	129.01	121.31
49	p	78	VAL	C-N-CA	5.17	129.01	121.31
57	x	74	A	N9-C1'-C2'	-5.14	106.30	114.00
34	a	1201	A	P-O3'-C3'	5.08	127.81	120.20
32	5	50	VAL	CA-C-N	5.07	127.78	120.38
32	5	50	VAL	C-N-CA	5.07	127.78	120.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1022	G	P-O3'-C3'	5.05	127.78	120.20
34	a	1297	G	P-O3'-C3'	5.04	127.75	120.20
38	e	122	VAL	N-CA-C	5.03	119.81	109.34
49	p	79	ASN	N-CA-C	5.03	117.39	110.35
36	c	95	GLY	CA-C-N	5.02	131.42	122.13
36	c	95	GLY	C-N-CA	5.02	131.42	122.13

There are no chirality outliers.

All (27) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
30	3	27	ASN	Peptide
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
35	b	15	PHE	Peptide
35	b	16	GLY	Peptide
35	b	18	GLN	Peptide
38	e	121	ASN	Peptide
39	f	53	LYS	Peptide
39	f	95	ALA	Peptide
42	i	90	ASP	Peptide
43	j	57	VAL	Peptide
45	l	101	LEU	Peptide
46	m	4	ALA	Peptide
50	q	68	LYS	Peptide
55	v	320	HIS	Mainchain
56	w	17	ALA	Peptide
56	w	314	ARG	Peptide
56	w	76	GLN	Peptide

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	62153	0	31259	464	0
2	B	2572	0	1302	19	0
3	C	2082	0	2157	37	0
4	D	1565	0	1616	18	0
5	E	1552	0	1619	20	0
6	F	1410	0	1447	17	0
7	G	1323	0	1374	6	0
8	H	1111	0	1148	13	0
9	I	1032	0	1088	11	0
10	J	1129	0	1162	14	0
11	K	938	0	1012	15	0
12	L	1045	0	1117	15	0
13	M	1074	0	1157	14	0
14	N	960	0	1000	11	0
15	O	892	0	923	10	0
16	P	917	0	965	16	0
17	Q	947	0	1022	10	0
18	R	816	0	839	12	0
19	S	857	0	922	8	0
20	T	738	0	807	13	0
21	U	779	0	834	5	0
22	V	753	0	780	7	0
23	W	575	0	592	3	0
24	X	625	0	655	9	0
25	Y	509	0	543	7	0
26	Z	449	0	491	4	0
27	0	444	0	461	6	0
28	1	409	0	440	3	0
29	2	377	0	418	12	0
30	3	504	0	574	13	0
31	4	302	0	343	5	0
32	5	988	0	1025	15	0
33	7	151	0	76	28	0
34	a	33016	0	16616	288	0
35	b	1704	0	1732	20	0
36	c	1624	0	1699	29	0
37	d	1643	0	1710	24	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
38	e	1141	0	1170	14	0
39	f	817	0	808	14	0
40	g	1181	0	1240	11	0
41	h	979	0	1034	18	0
42	i	1022	0	1070	17	0
43	j	786	0	828	19	0
44	k	869	0	878	18	0
45	l	955	0	1019	12	0
46	m	883	0	944	6	0
47	n	799	0	841	6	0
48	o	714	0	737	8	0
49	p	649	0	666	14	0
50	q	648	0	691	5	0
51	r	504	0	502	4	0
52	s	637	0	665	13	0
53	t	665	0	714	9	0
54	u	495	0	486	3	0
55	v	2436	0	2125	144	0
56	w	3923	0	3916	180	0
57	x	1640	0	837	47	0
58	z	120	0	128	10	0
59	w	32	0	14	18	0
All	All	151860	0	104238	1497	0

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

All (1497) 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)
56:w:393:PHE:CD2	56:w:525:GLN:HG3	1.45	1.49
56:w:395:PRO:HB3	56:w:441:VAL:CG2	1.45	1.43
55:v:191:GLU:OE1	55:v:197:HIS:CD2	1.75	1.37
55:v:134:MET:HE1	55:v:332:VAL:O	1.27	1.31
33:7:26:U:N3	57:x:36:A:N1	1.75	1.31
56:w:260:LEU:HD22	59:w:601:GCP:C2	1.66	1.25
56:w:393:PHE:CE2	56:w:525:GLN:HG3	1.53	1.25
1:A:1913:A:OP1	34:a:1494:G:O2'	1.55	1.25
56:w:395:PRO:CB	56:w:441:VAL:HG22	1.66	1.23
56:w:97:GLU:O	56:w:392:ASN:ND2	1.70	1.23
55:v:122:ASP:OD1	55:v:190:THR:HG21	1.06	1.22

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
56:w:471:ALA:O	56:w:473:TRP:N	1.73	1.21
36:c:91:ALA:HA	36:c:94:ALA:HB3	1.20	1.19
56:w:260:LEU:CD2	59:w:601:GCP:N2	2.05	1.19
11:K:98:ARG:NH2	34:a:340:U:O4	1.75	1.17
33:7:25:A:N1	57:x:37:U:N3	1.92	1.16
56:w:399:ARG:O	56:w:400:ARG:HG2	1.39	1.16
55:v:112:PHE:CE1	55:v:165:LYS:HG2	1.81	1.15
56:w:260:LEU:HB2	59:w:601:GCP:C6	1.79	1.12
56:w:393:PHE:HE2	56:w:525:GLN:O	1.27	1.12
33:7:25:A:N6	57:x:37:U:O4	1.83	1.11
55:v:122:ASP:OD1	55:v:190:THR:CG2	1.98	1.10
36:c:91:ALA:HB1	36:c:96:VAL:O	1.50	1.09
1:A:2253:G:O6	57:x:75:C:N4	1.86	1.08
55:v:184:VAL:HB	55:v:199:SER:OG	1.51	1.08
56:w:393:PHE:CD2	56:w:525:GLN:CG	2.35	1.08
1:A:2452:C:H4'	55:v:239:THR:CG2	1.84	1.08
1:A:2452:C:C4'	55:v:239:THR:HG21	1.84	1.07
1:A:2602:A:N1	55:v:236:HIS:CD2	2.21	1.07
56:w:395:PRO:HB2	56:w:440:ALA:O	1.54	1.07
33:7:26:U:O2	57:x:36:A:H2	1.38	1.07
56:w:260:LEU:HD23	59:w:601:GCP:N2	1.68	1.06
56:w:393:PHE:CE2	56:w:525:GLN:O	2.09	1.05
1:A:745:G:N7	1:A:746:U:C5	2.25	1.04
56:w:260:LEU:CD2	59:w:601:GCP:C2	2.36	1.03
56:w:393:PHE:CE2	56:w:525:GLN:CG	2.40	1.03
55:v:225:ASP:HB2	55:v:245:ARG:CG	1.90	1.02
55:v:322:ILE:CD1	55:v:344:ILE:HA	1.89	1.01
56:w:395:PRO:HB2	56:w:440:ALA:C	1.86	1.00
56:w:260:LEU:CB	59:w:601:GCP:N1	2.24	1.00
55:v:224:ILE:HD13	55:v:267:LYS:HZ1	1.26	1.00
56:w:260:LEU:HD22	59:w:601:GCP:N2	1.71	0.99
56:w:399:ARG:CD	56:w:464:GLU:H	1.76	0.98
55:v:224:ILE:HD13	55:v:267:LYS:NZ	1.78	0.97
55:v:195:ARG:HE	55:v:197:HIS:CE1	1.83	0.96
1:A:2063:C:H5'	58:z:18:LEU:HD22	1.46	0.96
55:v:134:MET:CE	55:v:332:VAL:O	2.13	0.96
1:A:2602:A:N1	55:v:236:HIS:HD2	1.61	0.96
1:A:1476:U:H3	1:A:1515:A:H62	0.99	0.96
56:w:399:ARG:O	56:w:400:ARG:CG	2.13	0.95
33:7:26:U:O2	57:x:36:A:C2	2.19	0.95
55:v:195:ARG:HE	55:v:197:HIS:HE1	0.99	0.95

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
55:v:134:MET:CE	55:v:337:LEU:HD21	1.96	0.95
55:v:195:ARG:NE	55:v:197:HIS:CE1	2.35	0.95
1:A:2253:G:N1	57:x:75:C:N3	2.14	0.95
34:a:1238:A:H62	34:a:1301:U:H3	0.96	0.95
56:w:260:LEU:HB2	59:w:601:GCP:N1	1.79	0.94
56:w:314:ARG:NH2	56:w:418:GLN:HG2	1.81	0.94
55:v:123:GLU:OE2	55:v:199:SER:HB3	1.67	0.94
56:w:314:ARG:HH22	56:w:418:GLN:HG2	1.30	0.94
55:v:191:GLU:CD	55:v:197:HIS:HE2	1.75	0.94
1:A:545:U:H3	1:A:548:G:H1	1.00	0.93
55:v:195:ARG:NE	55:v:197:HIS:HE1	1.66	0.93
1:A:2475:C:H42	1:A:2529:G:N2	1.66	0.93
33:7:27:G:O6	57:x:35:C:N4	2.01	0.92
56:w:395:PRO:HB3	56:w:441:VAL:HG22	0.94	0.92
34:a:518:C:OP2	55:v:183:ARG:NH1	2.03	0.92
56:w:503:TYR:CD2	56:w:504:ILE:N	2.38	0.92
56:w:503:TYR:HD2	56:w:504:ILE:H	1.07	0.91
55:v:191:GLU:OE1	55:v:197:HIS:HD2	1.20	0.91
1:A:306:U:H3	1:A:310:A:H62	0.95	0.91
56:w:306:ASN:O	56:w:454:LYS:NZ	2.03	0.90
1:A:2028:U:H3	1:A:2033:A:H62	1.12	0.90
55:v:191:GLU:OE2	55:v:195:ARG:HG2	1.72	0.90
56:w:395:PRO:CB	56:w:441:VAL:HA	2.01	0.90
55:v:322:ILE:HD12	55:v:344:ILE:HA	1.54	0.90
56:w:101:ARG:HB3	56:w:391:PRO:HG2	1.54	0.90
56:w:471:ALA:O	56:w:472:ARG:C	2.11	0.89
56:w:395:PRO:HB3	56:w:441:VAL:CB	2.04	0.88
34:a:966:G:N2	57:x:35:C:O4'	2.06	0.88
34:a:1409:C:N3	34:a:1491:G:N1	2.22	0.88
55:v:191:GLU:CD	55:v:197:HIS:NE2	2.32	0.87
1:A:2457:U:H5	1:A:2494:G:H1	0.90	0.87
56:w:469:ALA:O	56:w:470:THR:CG2	2.22	0.87
56:w:395:PRO:CB	56:w:441:VAL:CA	2.54	0.86
56:w:260:LEU:CB	59:w:601:GCP:C6	2.54	0.86
1:A:2475:C:H42	1:A:2529:G:H22	1.20	0.86
55:v:122:ASP:CG	55:v:190:THR:HG21	2.02	0.85
34:a:1445:U:H3	34:a:1457:G:H1	1.26	0.84
55:v:184:VAL:CB	55:v:199:SER:OG	2.26	0.84
56:w:260:LEU:HD23	59:w:601:GCP:HN21	1.40	0.84
1:A:306:U:H3	1:A:310:A:N6	1.75	0.83
56:w:393:PHE:CG	56:w:525:GLN:HG3	2.10	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
55:v:322:ILE:HD11	55:v:344:ILE:HA	1.59	0.83
56:w:399:ARG:HD2	56:w:464:GLU:O	1.78	0.83
55:v:127:PHE:HE2	55:v:131:LEU:HD11	1.44	0.83
56:w:260:LEU:HB3	59:w:601:GCP:N1	1.93	0.83
55:v:179:SER:HA	55:v:203:VAL:O	1.77	0.82
56:w:101:ARG:NH1	56:w:392:ASN:HD22	1.78	0.82
55:v:127:PHE:CE1	55:v:184:VAL:HG22	2.15	0.82
56:w:393:PHE:CG	56:w:525:GLN:CG	2.63	0.81
55:v:191:GLU:OE2	55:v:197:HIS:NE2	2.13	0.81
56:w:395:PRO:HB3	56:w:441:VAL:CA	2.11	0.81
55:v:117:ALA:HB1	55:v:124:ALA:CB	2.10	0.80
42:i:129:ARG:NH1	57:x:33:C:OP2	2.14	0.80
1:A:244:A:H62	1:A:254:G:H21	1.28	0.80
1:A:745:G:C5	1:A:746:U:C6	2.69	0.80
1:A:593:U:H3	1:A:664:G:H1	1.29	0.80
55:v:134:MET:HE3	55:v:337:LEU:HD21	1.64	0.80
55:v:191:GLU:CD	55:v:197:HIS:CD2	2.59	0.79
1:A:2475:C:N4	1:A:2529:G:H22	1.80	0.79
1:A:2457:U:H5	1:A:2494:G:N1	1.75	0.79
55:v:142:ARG:NH1	55:v:174:ARG:HD3	1.98	0.78
55:v:322:ILE:HD12	55:v:344:ILE:CA	2.12	0.78
55:v:225:ASP:HB2	55:v:245:ARG:HG2	1.63	0.78
36:c:91:ALA:HA	36:c:94:ALA:CB	2.09	0.78
55:v:127:PHE:CD1	55:v:184:VAL:HG22	2.19	0.78
33:7:29:A:H1'	55:v:303:ARG:HH22	1.49	0.78
34:a:1493:A:OP2	34:a:1493:A:H2'	1.84	0.78
36:c:38:VAL:HG12	36:c:93:ILE:CD1	2.12	0.78
55:v:127:PHE:CE2	55:v:131:LEU:HD11	2.18	0.77
34:a:518:C:OP1	55:v:183:ARG:NH2	2.18	0.77
55:v:191:GLU:OE1	55:v:197:HIS:NE2	2.16	0.77
1:A:2508:G:N1	1:A:2580:U:O4	2.16	0.77
1:A:2602:A:C2	55:v:237:VAL:HG22	2.20	0.77
56:w:260:LEU:N	59:w:601:GCP:O6	2.17	0.77
56:w:101:ARG:HH11	56:w:392:ASN:HD22	1.28	0.77
1:A:2602:A:C2	55:v:237:VAL:CG2	2.68	0.76
55:v:227:PHE:CE1	55:v:245:ARG:HD2	2.21	0.76
33:7:26:U:C2	57:x:36:A:C2	2.73	0.76
56:w:260:LEU:HB3	59:w:601:GCP:HN1	1.50	0.76
55:v:309:THR:HG23	55:v:320:HIS:NE2	2.00	0.75
55:v:309:THR:OG1	55:v:318:THR:O	2.04	0.75
56:w:101:ARG:HH11	56:w:392:ASN:ND2	1.84	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
56:w:469:ALA:O	56:w:470:THR:HG23	1.85	0.74
1:A:2254:C:O2	57:x:74:A:N1	2.20	0.74
1:A:2514:U:H3	1:A:2570:G:H1	1.35	0.74
55:v:127:PHE:CD1	55:v:184:VAL:CG2	2.70	0.74
34:a:362:G:OP2	56:w:408:LYS:NZ	2.21	0.74
55:v:117:ALA:HB1	55:v:124:ALA:HB1	1.68	0.73
55:v:301:GLY:H	55:v:306:ARG:HH12	1.36	0.73
1:A:745:G:N7	1:A:746:U:C6	2.57	0.73
23:W:61:GLY:HA3	23:W:79:GLU:O	1.89	0.73
33:7:25:A:N1	57:x:37:U:C2	2.56	0.73
33:7:26:U:C2	57:x:36:A:N1	2.55	0.73
55:v:112:PHE:HE1	55:v:165:LYS:HE2	1.52	0.73
55:v:112:PHE:CE1	55:v:165:LYS:CG	2.66	0.72
55:v:225:ASP:HB2	55:v:245:ARG:HG3	1.71	0.72
56:w:399:ARG:HD2	56:w:464:GLU:C	2.13	0.72
34:a:1409:C:N4	34:a:1491:G:O6	2.14	0.72
55:v:112:PHE:CE1	55:v:165:LYS:HE2	2.24	0.72
16:P:108:ARG:HD2	34:a:1463:U:OP1	1.89	0.72
36:c:38:VAL:HG12	36:c:93:ILE:HG13	1.71	0.72
34:a:1491:G:H3'	34:a:1492:A:H5''	1.72	0.71
56:w:503:TYR:HD2	56:w:504:ILE:O	1.73	0.71
55:v:322:ILE:CD1	55:v:344:ILE:CA	2.66	0.71
56:w:395:PRO:CA	56:w:441:VAL:HA	2.21	0.71
34:a:321:A:H61	34:a:332:G:H1	1.39	0.71
34:a:1409:C:O2	34:a:1491:G:N2	2.15	0.70
33:7:29:A:O2'	34:a:1492:A:C2	2.40	0.70
1:A:600:G:H1	1:A:657:U:H3	1.38	0.69
36:c:91:ALA:CB	36:c:96:VAL:O	2.37	0.69
1:A:1476:U:H3	1:A:1515:A:N6	1.84	0.69
55:v:117:ALA:CB	55:v:124:ALA:HB1	2.23	0.69
1:A:955:U:C5	1:A:962:G:N1	2.58	0.69
36:c:99:GLN:OE1	36:c:99:GLN:N	2.19	0.69
55:v:112:PHE:CD1	55:v:165:LYS:HG2	2.28	0.69
34:a:522:C:H41	45:l:49:ARG:HH22	1.38	0.68
55:v:322:ILE:HD12	55:v:344:ILE:CG1	2.23	0.68
56:w:399:ARG:O	56:w:400:ARG:CB	2.41	0.68
56:w:308:ASP:OD2	56:w:454:LYS:HB3	1.93	0.68
55:v:137:ARG:NH1	55:v:334:GLU:HG2	2.09	0.68
34:a:1357:A:H61	34:a:1365:G:H1	1.42	0.68
56:w:17:ALA:HB2	56:w:106:VAL:HG21	1.74	0.68
56:w:395:PRO:HA	56:w:441:VAL:HG13	1.75	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2457:U:O4	1:A:2494:G:O6	2.13	0.67
1:A:1912:A:N7	1:A:1917:U:O4	2.27	0.67
11:K:13:ASN:ND2	34:a:339:C:OP2	2.27	0.67
2:B:78:A:H62	2:B:98:G:H21	1.40	0.67
55:v:311:ASN:O	55:v:329:LEU:HD11	1.94	0.67
56:w:302:LYS:HE2	56:w:304:GLN:HA	1.77	0.67
16:P:59:THR:HG22	16:P:72:VAL:HG12	1.77	0.67
56:w:70:ILE:HD13	56:w:447:ASP:OD1	1.93	0.67
56:w:398:PHE:CE2	56:w:442:GLY:O	2.48	0.67
56:w:399:ARG:HE	56:w:464:GLU:HB2	1.59	0.66
34:a:1054:C:N4	55:v:195:ARG:HA	2.11	0.66
56:w:295:LYS:HG2	56:w:381:GLN:HB2	1.78	0.66
56:w:395:PRO:CB	56:w:441:VAL:CG2	2.39	0.66
40:g:111:GLY:HA2	40:g:118:ARG:HD3	1.77	0.66
56:w:312:ARG:NH1	56:w:418:GLN:HE21	1.93	0.66
55:v:309:THR:CG2	55:v:320:HIS:NE2	2.58	0.66
56:w:393:PHE:CE2	56:w:525:GLN:C	2.73	0.66
39:f:6:ILE:HG12	39:f:89:VAL:HG22	1.78	0.66
34:a:886:G:H1	34:a:911:U:H3	1.44	0.66
1:A:78:U:H3	1:A:108:G:H1	1.43	0.65
57:x:72:C:C6	57:x:72:C:H3'	2.31	0.65
56:w:469:ALA:C	56:w:470:THR:HG23	2.21	0.65
36:c:38:VAL:HG12	36:c:93:ILE:CG1	2.26	0.65
34:a:673:A:H4'	39:f:86:ARG:HH21	1.60	0.65
1:A:2508:G:C6	1:A:2580:U:O4	2.49	0.65
34:a:55:A:C6	56:w:311:HIS:CE1	2.85	0.64
33:7:25:A:C2	57:x:37:U:O2	2.51	0.64
1:A:1418:G:N2	1:A:1579:A:N7	2.46	0.64
34:a:966:G:C2	57:x:35:C:O4'	2.50	0.64
1:A:955:U:H5	1:A:962:G:H1	1.43	0.64
1:A:1666:G:H4'	11:K:6:THR:HG23	1.78	0.64
55:v:235:GLN:HE21	58:z:18:LEU:C	2.04	0.64
34:a:1054:C:H42	55:v:195:ARG:HA	1.63	0.64
39:f:45:ARG:O	39:f:56:LYS:HA	1.98	0.64
55:v:238:ASN:OD1	55:v:238:ASN:N	2.29	0.64
44:k:87:GLY:H	44:k:113:THR:HG22	1.63	0.64
1:A:745:G:C5	1:A:746:U:C5	2.86	0.63
14:N:28:LEU:HD23	14:N:48:VAL:HG21	1.81	0.63
56:w:394:ALA:O	56:w:441:VAL:HG13	1.97	0.63
56:w:469:ALA:O	56:w:470:THR:HG22	1.96	0.63
56:w:21:HIS:HA	56:w:122:ARG:HG2	1.81	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
56:w:399:ARG:HD3	56:w:464:GLU:H	1.58	0.63
34:a:516:U:O4	34:a:533:A:N7	2.32	0.63
1:A:955:U:H5	1:A:962:G:N1	1.96	0.63
49:p:4:ILE:HG12	49:p:21:VAL:HG22	1.79	0.63
1:A:1687:G:H21	1:A:1701:A:H62	1.46	0.63
33:7:28:U:O4	55:v:123:GLU:HG3	1.99	0.63
56:w:395:PRO:CG	56:w:441:VAL:HG22	2.29	0.63
34:a:958:A:N6	52:s:76:THR:O	2.32	0.63
1:A:1433:A:H61	1:A:1560:G:H1	1.44	0.62
35:b:31:PHE:HB2	35:b:39:ILE:HB	1.81	0.62
1:A:244:A:H62	1:A:254:G:N2	1.97	0.62
1:A:2254:C:O2	57:x:74:A:C2	2.52	0.62
34:a:675:A:H1'	44:k:117:HIS:HD2	1.64	0.62
1:A:2508:G:O6	1:A:2580:U:O4	2.18	0.62
33:7:27:G:N7	34:a:1400:C:H5'	2.14	0.62
34:a:530:G:N2	55:v:198:THR:OG1	2.33	0.61
34:a:659:U:H3	34:a:747:A:H61	1.47	0.61
52:s:54:ARG:HG3	52:s:55:GLN:HG2	1.82	0.61
34:a:790:A:OP1	57:x:39:A:O2'	2.18	0.61
16:P:108:ARG:NH1	34:a:1464:U:OP1	2.34	0.61
34:a:1086:U:H3	34:a:1099:G:H22	1.48	0.61
34:a:1304:G:H21	34:a:1333:A:H62	1.49	0.61
1:A:1046:A:H62	32:5:4:ASN:HD21	1.48	0.61
34:a:1238:A:N6	34:a:1301:U:H3	1.82	0.61
1:A:2028:U:H3	1:A:2033:A:N6	1.92	0.61
1:A:306:U:O4	1:A:310:A:N7	2.34	0.61
55:v:242:SER:H	55:v:263:GLN:HE21	1.47	0.61
56:w:308:ASP:CG	56:w:454:LYS:HB3	2.26	0.61
1:A:745:G:C6	1:A:746:U:C6	2.89	0.61
43:j:8:ILE:HG12	43:j:100:ILE:HG22	1.83	0.61
57:x:74:A:H4'	57:x:74:A:OP1	1.99	0.61
1:A:2514:U:H5''	10:J:81:ILE:HD11	1.83	0.60
22:V:64:VAL:HG22	22:V:69:GLU:HG2	1.83	0.60
55:v:265:LYS:HD2	57:x:75:C:O5'	2.00	0.60
2:B:78:A:H62	2:B:98:G:N2	1.98	0.60
4:D:34:VAL:HA	4:D:50:VAL:HG12	1.83	0.60
1:A:955:U:O4	1:A:962:G:O6	2.20	0.60
19:S:82:MET:HB2	19:S:98:LYS:HB2	1.83	0.60
1:A:1081:U:H4'	9:I:123:ALA:HB1	1.84	0.60
1:A:1252:G:N2	17:Q:32:ARG:O	2.35	0.60
35:b:165:ALA:HB3	35:b:190:SER:HB3	1.84	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
55:v:137:ARG:HH12	55:v:334:GLU:HG2	1.65	0.60
55:v:322:ILE:HD12	55:v:344:ILE:HG12	1.84	0.60
1:A:818:G:H21	1:A:1189:A:H62	1.47	0.60
20:T:8:LEU:HA	20:T:50:LEU:HD21	1.84	0.60
37:d:94:GLU:HG2	37:d:185:PRO:HG2	1.83	0.60
6:F:62:GLN:HE22	6:F:90:LEU:HB3	1.66	0.60
39:f:32:ALA:HB2	39:f:70:VAL:HG11	1.84	0.60
1:A:2656:U:O2	1:A:2665:A:N7	2.35	0.60
34:a:1493:A:C4'	55:v:120:GLY:H	2.14	0.60
56:w:298:GLY:HA2	56:w:319:ARG:H	1.67	0.60
56:w:398:PHE:CZ	56:w:443:VAL:HA	2.37	0.60
1:A:488:G:H22	1:A:491:G:H5''	1.66	0.59
8:H:39:ALA:HA	8:H:43:ASN:HB2	1.84	0.59
34:a:359:G:H5''	56:w:456:GLU:HB3	1.83	0.59
55:v:112:PHE:HE1	55:v:165:LYS:CE	2.15	0.59
1:A:1093:G:H21	1:A:1098:A:H62	1.48	0.59
1:A:1940:U:OP1	1:A:2603:G:N2	2.34	0.59
1:A:2296:U:OP2	15:O:9:ARG:NH2	2.35	0.59
29:2:24:THR:HG23	29:2:27:GLY:H	1.67	0.59
32:5:58:THR:HG21	32:5:82:ILE:H	1.68	0.59
36:c:91:ALA:HB1	36:c:96:VAL:C	2.26	0.59
56:w:308:ASP:OD1	56:w:454:LYS:HD3	2.02	0.59
1:A:1798:U:H5''	3:C:257:ARG:HB2	1.84	0.59
5:E:146:VAL:HG12	5:E:185:LYS:HB2	1.83	0.59
44:k:84:MET:SD	44:k:110:THR:OG1	2.60	0.59
56:w:308:ASP:CG	56:w:454:LYS:HD3	2.27	0.59
1:A:629:G:N3	1:A:639:U:O2'	2.34	0.59
33:7:26:U:N3	57:x:36:A:C2	2.60	0.59
43:j:7:ARG:HB3	43:j:101:SER:HB2	1.85	0.59
56:w:312:ARG:NH1	56:w:418:GLN:NE2	2.50	0.59
1:A:2748:A:H5'	7:G:3:VAL:HG21	1.85	0.59
1:A:281:C:H42	1:A:359:G:H1	1.50	0.59
1:A:538:A:H4'	10:J:7:LYS:HG2	1.85	0.59
1:A:2452:C:O2	58:z:17:ARG:NH2	2.36	0.59
34:a:1306:A:N6	34:a:1331:G:O2'	2.35	0.59
2:B:72:G:H21	2:B:104:A:H62	1.51	0.59
1:A:463:G:N2	1:A:466:A:OP2	2.35	0.59
1:A:1153:C:OP1	17:Q:91:ARG:NH2	2.35	0.58
57:x:72:C:C6	57:x:72:C:C3'	2.85	0.58
15:O:40:ILE:HG12	15:O:47:VAL:HG12	1.85	0.58
43:j:42:LEU:HD11	43:j:73:LEU:HG	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
50:q:30:HIS:HD2	50:q:33:TYR:H	1.49	0.58
1:A:1060:U:H5'	1:A:1062:G:H5'	1.84	0.58
1:A:2063:C:C5'	58:z:18:LEU:HD22	2.27	0.58
34:a:674:G:O6	34:a:716:A:N1	2.37	0.58
56:w:503:TYR:HD2	56:w:504:ILE:N	1.89	0.58
1:A:839:U:H3	1:A:939:G:H1	1.51	0.58
34:a:664:G:H22	34:a:741:G:H1	1.52	0.58
42:i:48:ARG:HA	42:i:51:LEU:HD12	1.86	0.58
56:w:488:LYS:HE2	56:w:517:ARG:HH21	1.68	0.58
56:w:393:PHE:CG	56:w:525:GLN:HG2	2.39	0.58
1:A:1862:G:H1	1:A:1880:U:H3	1.50	0.58
2:B:30:C:H1'	2:B:57:A:H61	1.69	0.58
45:l:30:ARG:HH22	56:w:408:LYS:NZ	2.02	0.58
55:v:142:ARG:HH12	55:v:174:ARG:HD3	1.69	0.58
37:d:201:GLU:OE2	38:e:111:ARG:NH2	2.37	0.58
57:x:75:C:H2'	57:x:75:C:O2	2.02	0.58
2:B:79:G:N7	22:V:14:LYS:NZ	2.52	0.57
34:a:1238:A:N7	34:a:1301:U:O4	2.37	0.57
56:w:399:ARG:NE	56:w:464:GLU:H	2.01	0.57
1:A:585:G:H21	1:A:1254:A:H62	1.52	0.57
1:A:2743:U:OP2	1:A:2755:C:N4	2.38	0.57
42:i:33:SER:H	42:i:36:GLN:HE21	1.52	0.57
56:w:101:ARG:NH1	56:w:392:ASN:ND2	2.48	0.57
1:A:1309:G:H5''	29:2:9:VAL:HG23	1.87	0.57
55:v:227:PHE:HE1	55:v:245:ARG:HD2	1.69	0.57
9:I:11:GLN:NE2	9:I:54:ILE:O	2.38	0.57
34:a:20:U:O2'	34:a:573:A:N6	2.37	0.57
56:w:390:ILE:HG22	56:w:390:ILE:O	2.02	0.57
1:A:2185:U:H2'	1:A:2186:G:H8	1.69	0.57
1:A:1450:G:H21	1:A:1452:G:H1	1.53	0.57
26:Z:8:GLN:HB2	26:Z:28:LEU:HD13	1.87	0.57
30:3:32:LEU:HD23	30:3:35:LYS:HD2	1.86	0.57
56:w:14:ARG:HB2	56:w:84:VAL:HG22	1.87	0.57
56:w:32:LYS:HD2	56:w:262:ASN:HA	1.87	0.57
1:A:1986:C:H2'	1:A:1987:A:H8	1.70	0.57
1:A:1992:G:N2	1:A:1996:C:O2'	2.37	0.57
1:A:962:G:O2'	1:A:2250:G:N2	2.38	0.57
1:A:587:C:O2	12:L:33:ARG:NH1	2.38	0.57
5:E:117:ARG:NH2	5:E:183:PHE:O	2.38	0.57
24:X:6:VAL:HG21	24:X:58:ILE:HD11	1.86	0.57
40:g:46:LEU:HD23	40:g:57:GLU:HB3	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
56:w:395:PRO:HB3	56:w:441:VAL:HG23	1.72	0.57
56:w:503:TYR:CD2	56:w:504:ILE:O	2.56	0.57
1:A:698:C:O2'	1:A:734:A:N6	2.35	0.57
4:D:179:ARG:HB3	4:D:188:LEU:HD12	1.86	0.57
40:g:75:LYS:HE3	40:g:88:VAL:HG11	1.85	0.57
1:A:2515:C:H2'	1:A:2516:A:H8	1.70	0.56
1:A:2692:G:H1'	1:A:2847:U:H1'	1.87	0.56
1:A:605:G:H1'	1:A:657:U:H1'	1.87	0.56
36:c:39:ARG:HG3	36:c:54:ILE:HD11	1.87	0.56
56:w:306:ASN:ND2	56:w:312:ARG:O	2.38	0.56
1:A:2028:U:O4	1:A:2033:A:N7	2.38	0.56
6:F:23:SER:HB3	6:F:26:GLN:HG3	1.86	0.56
11:K:48:PRO:HG3	34:a:1422:G:H5'	1.87	0.56
13:M:10:ARG:NH2	57:x:1:C:O2'	2.39	0.56
20:T:23:ALA:HB1	20:T:29:THR:HB	1.87	0.56
34:a:837:U:H2'	34:a:838:G:H8	1.71	0.56
34:a:951:G:OP2	46:m:100:ARG:NH2	2.36	0.56
48:o:38:LEU:HD23	48:o:42:PHE:HE2	1.71	0.56
56:w:326:GLU:HB2	56:w:329:MET:HB2	1.87	0.56
1:A:605:G:OP1	5:E:99:LYS:NZ	2.38	0.56
1:A:2291:U:H1'	1:A:2374:C:H1'	1.88	0.56
23:W:33:ILE:HG22	23:W:34:VAL:HG23	1.88	0.56
41:h:42:GLU:HG2	41:h:100:ILE:HG12	1.87	0.56
55:v:134:MET:HE3	55:v:337:LEU:CD2	2.35	0.56
1:A:1476:U:O4	1:A:1515:A:N7	2.39	0.56
6:F:134:GLN:NE2	6:F:149:ARG:O	2.38	0.56
56:w:314:ARG:HH22	56:w:418:GLN:CG	2.10	0.56
56:w:395:PRO:HB2	56:w:441:VAL:N	2.20	0.56
3:C:92:LEU:HD11	3:C:100:ARG:HB3	1.86	0.56
37:d:97:LEU:HB2	37:d:134:TYR:HB3	1.88	0.56
57:x:50:G:H1	57:x:66:C:H42	1.54	0.56
1:A:605:G:N3	1:A:657:U:O2'	2.38	0.56
17:Q:43:GLN:HE21	18:R:77:PHE:HB3	1.71	0.56
21:U:33:VAL:HG13	21:U:66:VAL:HG22	1.87	0.56
34:a:362:G:N2	34:a:365:U:OP2	2.39	0.56
34:a:1367:C:H4'	43:j:50:THR:HG21	1.87	0.56
56:w:395:PRO:CB	56:w:440:ALA:C	2.71	0.56
1:A:1500:G:H4'	3:C:100:ARG:HH12	1.71	0.56
1:A:2062:A:H62	1:A:2503:A:H62	1.53	0.56
34:a:56:U:H2'	34:a:57:G:H8	1.71	0.56
41:h:14:ARG:NH2	41:h:74:ILE:O	2.39	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
55:v:134:MET:HE3	55:v:337:LEU:HD11	1.87	0.56
55:v:235:GLN:NE2	58:z:18:LEU:C	2.63	0.56
56:w:394:ALA:O	56:w:441:VAL:CG1	2.53	0.56
7:G:88:LEU:HG	7:G:161:VAL:HG22	1.87	0.55
22:V:42:LEU:HD13	22:V:47:VAL:HG21	1.86	0.55
33:7:25:A:N6	57:x:37:U:C4	2.53	0.55
1:A:318:C:H2'	1:A:319:G:H8	1.72	0.55
3:C:51:ARG:HH22	3:C:246:PRO:HG2	1.70	0.55
27:0:30:ASP:HB3	27:0:34:GLY:H	1.71	0.55
51:r:36:GLY:O	51:r:62:ARG:NH2	2.40	0.55
1:A:2095:A:OP1	8:H:11:ASN:ND2	2.40	0.55
24:X:39:VAL:HG12	24:X:42:GLU:H	1.70	0.55
34:a:8:A:N6	37:d:201:GLU:O	2.37	0.55
34:a:684:U:H1'	44:k:39:ASN:HB2	1.87	0.55
34:a:1159:U:OP1	35:b:131:LYS:NZ	2.40	0.55
56:w:399:ARG:NH2	56:w:463:TYR:HA	2.22	0.55
3:C:143:VAL:HB	3:C:153:LEU:HB2	1.87	0.55
34:a:335:C:H2'	34:a:336:A:H8	1.72	0.55
40:g:68:VAL:HG23	40:g:99:ALA:HB1	1.89	0.55
42:i:39:GLY:HA2	42:i:44:ARG:HB2	1.88	0.55
1:A:682:G:O2'	29:2:33:ARG:NH1	2.40	0.55
1:A:2314:A:OP1	6:F:87:LYS:NZ	2.39	0.55
34:a:722:G:H1	34:a:733:G:H1	1.55	0.55
34:a:1222:G:OP2	34:a:1322:C:N4	2.40	0.55
56:w:399:ARG:NE	56:w:464:GLU:HB2	2.21	0.55
1:A:1668:A:N3	1:A:1670:C:N4	2.55	0.55
1:A:2893:A:H5''	1:A:2894:G:H5'	1.89	0.55
7:G:94:ARG:HB2	7:G:105:SER:HB2	1.88	0.55
34:a:406:G:H5'	37:d:4:LEU:HD22	1.89	0.55
1:A:686:U:O4	29:2:12:ARG:NH2	2.39	0.55
1:A:911:A:N6	13:M:11:LYS:O	2.37	0.55
39:f:38:ARG:NH2	39:f:40:GLU:OE1	2.39	0.55
42:i:89:TYR:HB3	42:i:93:LEU:HD12	1.89	0.55
52:s:5:LYS:HG3	52:s:6:LYS:HG2	1.89	0.55
56:w:92:HIS:HB2	56:w:95:PHE:HB2	1.88	0.55
56:w:393:PHE:CD1	56:w:525:GLN:CG	2.90	0.55
1:A:144:A:H4'	20:T:2:ILE:HD11	1.89	0.55
1:A:514:A:N3	1:A:581:C:O2'	2.37	0.55
34:a:514:C:H2'	34:a:515:G:H8	1.71	0.55
57:x:20:G:OP1	57:x:60:A:N6	2.40	0.55
1:A:647:G:N2	1:A:2350:C:O2'	2.40	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:X:58:ILE:HG12	24:X:66:VAL:HG21	1.88	0.54
34:a:725:G:OP1	34:a:833:G:N2	2.40	0.54
45:l:109:ARG:HB2	45:l:118:VAL:HG21	1.89	0.54
56:w:101:ARG:CB	56:w:391:PRO:HG2	2.33	0.54
56:w:145:ASP:OD2	59:w:601:GCP:N2	2.40	0.54
1:A:13:A:O2'	1:A:15:G:N7	2.39	0.54
1:A:45:G:H5''	1:A:46:G:H5'	1.88	0.54
34:a:518:C:P	55:v:183:ARG:HH22	2.29	0.54
34:a:1414:U:H2'	34:a:1415:G:H8	1.71	0.54
1:A:2720:U:OP1	16:P:52:ARG:NH2	2.40	0.54
1:A:2523:G:HO2'	1:A:2764:A:HO2'	1.53	0.54
34:a:358:U:H2'	34:a:359:G:H8	1.72	0.54
36:c:57:GLU:OE1	36:c:64:ARG:NH2	2.36	0.54
50:q:63:CYS:SG	50:q:73:THR:OG1	2.59	0.54
55:v:114:GLU:HG2	55:v:163:ILE:HG12	1.88	0.54
1:A:1798:U:OP2	3:C:270:ARG:NH2	2.41	0.54
3:C:70:LYS:HB3	3:C:73:ILE:HD12	1.90	0.54
24:X:39:VAL:O	24:X:43:LYS:N	2.41	0.54
56:w:260:LEU:HD22	59:w:601:GCP:N3	2.17	0.54
1:A:1204:A:N6	1:A:1242:U:O4	2.41	0.54
1:A:585:G:H21	1:A:1254:A:N6	2.06	0.54
1:A:1309:G:H4'	29:2:7:PRO:HB2	1.90	0.54
1:A:2229:U:H2'	1:A:2230:G:H8	1.72	0.54
34:a:1297:G:N2	40:g:113:LYS:O	2.40	0.54
34:a:1458:G:H5'	53:t:26:MET:HB3	1.89	0.54
42:i:112:ARG:NH2	43:j:64:GLN:OE1	2.41	0.54
44:k:49:SER:HA	44:k:68:ARG:HH11	1.73	0.54
56:w:14:ARG:NH1	56:w:82:CYS:SG	2.80	0.54
56:w:314:ARG:HH12	56:w:418:GLN:HB3	1.73	0.54
1:A:550:C:H2'	1:A:551:G:H8	1.73	0.54
1:A:713:G:H21	1:A:718:A:H62	1.55	0.54
3:C:106:PRO:HD2	3:C:109:LEU:HD22	1.90	0.54
32:5:3:LEU:HD12	32:5:5:LEU:H	1.73	0.54
56:w:395:PRO:CB	56:w:441:VAL:N	2.70	0.54
1:A:538:A:N6	1:A:555:G:O2'	2.41	0.54
2:B:48:U:OP2	15:O:30:ARG:NH2	2.41	0.54
11:K:40:LYS:HE3	11:K:57:VAL:HG12	1.90	0.54
34:a:216:U:H4'	34:a:464:U:H4'	1.90	0.54
34:a:1200:C:H5''	34:a:1201:A:H3'	1.89	0.54
34:a:1329:A:H5''	46:m:24:VAL:HA	1.89	0.54
1:A:1913:A:C8	34:a:1494:G:H1'	2.42	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:165:ALA:HB3	3:C:172:THR:HB	1.90	0.53
34:a:545:C:OP1	37:d:61:ARG:NH1	2.36	0.53
41:h:28:SER:HB3	41:h:56:PRO:HB2	1.90	0.53
1:A:1800:C:N4	1:A:1818:U:O2'	2.42	0.53
20:T:6:ARG:NH2	20:T:37:ASP:OD2	2.42	0.53
34:a:311:C:OP1	49:p:31:ARG:NH1	2.41	0.53
34:a:1027:C:N4	34:a:1035:A:N1	2.56	0.53
38:e:80:LEU:HD13	38:e:122:VAL:HG21	1.89	0.53
55:v:225:ASP:HB2	55:v:245:ARG:CD	2.39	0.53
56:w:391:PRO:O	56:w:392:ASN:HB2	2.08	0.53
1:A:589:U:H2'	1:A:590:A:H8	1.74	0.53
56:w:469:ALA:C	56:w:470:THR:CG2	2.79	0.53
1:A:1223:G:OP1	18:R:68:ARG:NH2	2.42	0.53
1:A:1288:G:OP2	1:A:1288:G:N2	2.40	0.53
1:A:2320:U:O2'	1:A:2322:A:N6	2.40	0.53
1:A:2452:C:H4'	55:v:239:THR:HG21	0.88	0.53
36:c:38:VAL:HG12	36:c:93:ILE:HD11	1.86	0.53
4:D:148:GLN:HB2	4:D:152:PRO:HG2	1.90	0.53
7:G:8:VAL:HB	7:G:49:LEU:HB2	1.90	0.53
11:K:43:ILE:HD12	11:K:56:ASP:HB2	1.91	0.53
32:5:22:ALA:HB3	32:5:87:GLU:HB2	1.89	0.53
1:A:2602:A:N1	55:v:236:HIS:NE2	2.57	0.53
4:D:15:PHE:H	16:P:11:GLN:HE22	1.56	0.53
34:a:1347:G:N2	34:a:1374:A:OP2	2.37	0.53
49:p:7:ALA:HB3	49:p:18:GLN:HB2	1.91	0.53
1:A:745:G:C6	1:A:746:U:H6	2.26	0.53
1:A:958:U:OP2	13:M:14:LYS:NZ	2.41	0.53
1:A:1818:U:H5'	3:C:156:SER:HB2	1.91	0.53
1:A:2861:U:H2'	1:A:2862:G:H8	1.73	0.53
1:A:537:G:H4'	10:J:5:THR:HG21	1.90	0.53
1:A:1270:C:H5''	1:A:1271:G:H5'	1.91	0.53
14:N:44:LEU:HD23	14:N:113:ILE:HD13	1.90	0.53
29:2:12:ARG:HE	29:2:44:VAL:HG21	1.74	0.53
34:a:231:U:H2'	34:a:232:G:H8	1.74	0.53
34:a:969:A:OP2	43:j:58:ASN:ND2	2.41	0.53
38:e:54:GLU:HG2	38:e:56:PRO:HD2	1.90	0.53
47:n:15:LEU:HD23	47:n:55:SER:HB3	1.89	0.53
12:L:62:PRO:HD3	30:3:26:ALA:HB2	1.91	0.53
1:A:523:C:O2	1:A:554:U:O2'	2.27	0.53
13:M:75:GLU:HB3	13:M:90:GLU:HG3	1.90	0.53
37:d:102:TYR:O	37:d:164:ARG:NH1	2.40	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:632:A:OP1	30:3:14:LYS:NZ	2.42	0.52
1:A:1953:A:O2'	1:A:2559:C:O2	2.25	0.52
1:A:2394:C:H5''	12:L:63:LYS:HE3	1.91	0.52
11:K:30:ARG:NH2	11:K:37:ASP:OD2	2.41	0.52
20:T:38:ALA:HB1	20:T:43:ILE:HD11	1.91	0.52
34:a:331:G:O2'	53:t:2:ASN:ND2	2.42	0.52
34:a:1323:G:N2	34:a:1361:G:O2'	2.41	0.52
51:r:70:THR:HG23	51:r:72:ARG:H	1.73	0.52
1:A:119:A:H4'	1:A:120:U:H5'	1.90	0.52
1:A:2251:G:H1	57:x:77:A:H61	1.54	0.52
26:Z:10:ARG:HB2	26:Z:53:MET:HB2	1.90	0.52
29:2:31:LEU:HG	29:2:42:LEU:HD21	1.90	0.52
34:a:291:U:H3'	34:a:305:G:H22	1.74	0.52
55:v:127:PHE:CD1	55:v:184:VAL:HG21	2.43	0.52
1:A:576:U:H2'	1:A:577:G:C8	2.45	0.52
1:A:918:A:N3	2:B:80:U:O2'	2.42	0.52
1:A:1796:U:H3	1:A:1823:G:H1	1.57	0.52
1:A:2507:C:O3'	55:v:228:ARG:NH1	2.42	0.52
12:L:109:LYS:HD2	12:L:126:ARG:HH11	1.74	0.52
34:a:1113:C:H4'	36:c:13:ILE:HG12	1.90	0.52
38:e:10:LEU:HD22	38:e:67:ARG:HH22	1.74	0.52
55:v:112:PHE:HE1	55:v:165:LYS:HG2	1.61	0.52
56:w:27:THR:HB	59:w:601:GCP:O2A	2.08	0.52
1:A:475:C:H4'	1:A:510:C:H5'	1.90	0.52
1:A:2659:G:N2	1:A:2662:A:OP2	2.42	0.52
11:K:9:ASN:OD1	11:K:18:ARG:NH1	2.43	0.52
18:R:1:MET:N	18:R:42:ALA:O	2.36	0.52
35:b:19:THR:OG1	35:b:20:ARG:N	2.40	0.52
44:k:92:ARG:NH2	44:k:111:ASP:OD1	2.42	0.52
46:m:76:ILE:HG22	46:m:80:MET:HE2	1.91	0.52
56:w:13:ARG:NH1	56:w:76:GLN:OE1	2.43	0.52
1:A:177:G:H3'	1:A:178:G:H8	1.73	0.52
1:A:444:C:OP2	5:E:44:ARG:NH2	2.42	0.52
1:A:835:C:H2'	1:A:836:G:H8	1.73	0.52
33:7:30:A:O2'	55:v:195:ARG:HD2	2.09	0.52
36:c:152:VAL:HG12	36:c:197:VAL:HG22	1.90	0.52
55:v:191:GLU:OE2	55:v:195:ARG:CG	2.52	0.52
56:w:308:ASP:OD1	56:w:454:LYS:HB3	2.09	0.52
1:A:877:A:O2'	1:A:900:A:N6	2.42	0.52
1:A:2693:G:H2'	1:A:2694:G:H8	1.75	0.52
10:J:17:VAL:HG23	10:J:137:PRO:HB2	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:X:4:CYS:HB3	24:X:9:LYS:H	1.74	0.52
34:a:1137:C:O2'	34:a:1138:G:N2	2.43	0.52
34:a:1323:G:H1'	34:a:1361:G:H21	1.74	0.52
55:v:137:ARG:HG2	55:v:334:GLU:HA	1.92	0.52
1:A:1724:G:O6	1:A:1737:G:N2	2.43	0.52
1:A:1753:G:H5''	16:P:92:ARG:HD3	1.90	0.52
6:F:35:LEU:HB2	6:F:88:VAL:HB	1.91	0.52
56:w:399:ARG:NE	56:w:464:GLU:N	2.57	0.52
1:A:2307:G:H1	6:F:40:GLY:HA3	1.74	0.52
10:J:56:VAL:HB	10:J:124:VAL:HG12	1.91	0.52
34:a:54:C:OP1	34:a:351:G:N2	2.42	0.52
34:a:766:A:OP2	34:a:812:G:N2	2.43	0.52
36:c:38:VAL:CG1	36:c:93:ILE:HG13	2.38	0.52
44:k:22:ILE:HG12	44:k:31:VAL:HG22	1.92	0.52
56:w:395:PRO:HB2	56:w:441:VAL:HA	1.86	0.52
1:A:854:C:H2'	1:A:855:G:H8	1.75	0.52
8:H:30:LEU:HB3	8:H:36:ALA:HB3	1.91	0.52
8:H:47:PHE:HA	8:H:51:ARG:HB2	1.90	0.52
34:a:254:G:N2	50:q:17:GLU:OE1	2.42	0.52
34:a:359:G:C5'	56:w:456:GLU:HB3	2.39	0.52
56:w:398:PHE:HE2	56:w:442:GLY:O	1.92	0.52
1:A:727:A:OP2	1:A:1431:A:O2'	2.28	0.52
1:A:2692:G:N3	1:A:2847:U:O2'	2.40	0.52
4:D:131:ASP:O	4:D:136:ASN:ND2	2.41	0.52
8:H:38:PRO:O	8:H:43:ASN:ND2	2.41	0.52
18:R:35:PHE:O	18:R:58:VAL:HA	2.10	0.52
55:v:117:ALA:HB1	55:v:124:ALA:HB3	1.91	0.52
1:A:1013:C:H2'	1:A:1014:A:H8	1.74	0.51
1:A:1428:C:OP2	3:C:27:LYS:NZ	2.43	0.51
3:C:184:GLU:HG3	3:C:186:ASP:H	1.75	0.51
29:2:34:ARG:NH2	29:2:41:ARG:O	2.43	0.51
33:7:28:U:H3	55:v:120:GLY:HA2	1.75	0.51
34:a:755:G:H21	41:h:3:GLN:HE22	1.58	0.51
34:a:1222:G:H5''	52:s:77:ARG:HH11	1.74	0.51
35:b:153:MET:HG2	35:b:155:GLY:H	1.74	0.51
52:s:10:ILE:HD13	52:s:15:LEU:HB2	1.91	0.51
1:A:227:A:H61	1:A:410:G:H21	1.58	0.51
1:A:1779:U:OP2	1:A:1784:A:N6	2.43	0.51
1:A:2081:U:H2'	1:A:2082:A:H8	1.75	0.51
52:s:30:LEU:HB2	52:s:48:ILE:HG22	1.92	0.51
1:A:407:G:H2'	1:A:408:G:H8	1.75	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2023:C:H2'	1:A:2024:G:H8	1.75	0.51
34:a:1464:U:H2'	34:a:1465:A:H8	1.74	0.51
53:t:4:LYS:HG3	53:t:6:ALA:H	1.74	0.51
1:A:1394:U:O2	20:T:19:LYS:NZ	2.41	0.51
53:t:11:ILE:O	53:t:14:GLU:HB2	2.09	0.51
56:w:395:PRO:HA	56:w:441:VAL:HA	1.92	0.51
3:C:77:VAL:HG21	3:C:109:LEU:HD11	1.91	0.51
13:M:35:ALA:O	13:M:99:GLY:N	2.42	0.51
34:a:684:U:H3	34:a:706:A:H61	1.59	0.51
34:a:744:C:H2'	34:a:745:G:H8	1.75	0.51
38:e:37:VAL:HG11	38:e:113:VAL:HG23	1.92	0.51
56:w:14:ARG:HD3	56:w:276:ALA:HB3	1.91	0.51
57:x:72:C:H6	57:x:72:C:C5'	2.23	0.51
1:A:767:U:H2'	1:A:768:G:H8	1.76	0.51
1:A:787:C:H5''	1:A:788:A:H5'	1.92	0.51
34:a:532:A:N6	34:a:1206:G:O2'	2.43	0.51
34:a:674:G:H2'	34:a:675:A:H8	1.76	0.51
34:a:916:U:H2'	34:a:917:G:H8	1.74	0.51
36:c:96:VAL:HB	36:c:97:PRO:HD3	1.93	0.51
1:A:878:A:H3'	1:A:879:G:H8	1.75	0.51
55:v:134:MET:HE2	55:v:337:LEU:HD21	1.91	0.51
56:w:399:ARG:CD	56:w:464:GLU:N	2.59	0.51
8:H:1:MET:N	8:H:20:ASN:OD1	2.43	0.51
8:H:132:PHE:H	8:H:140:ALA:HB3	1.74	0.51
15:O:108:ASP:OD1	15:O:111:ARG:NH1	2.43	0.51
53:t:22:SER:O	53:t:25:SER:HB3	2.10	0.51
1:A:631:A:N3	1:A:2415:G:O2'	2.40	0.51
9:I:45:THR:HG22	9:I:50:LYS:HG2	1.93	0.51
12:L:17:LYS:HE3	12:L:27:LEU:HD22	1.93	0.51
34:a:618:C:H1'	49:p:14:ARG:HH12	1.75	0.51
37:d:61:ARG:NH1	37:d:68:GLU:OE1	2.43	0.51
1:A:2279:G:HO2'	1:A:2327:A:HO2'	1.52	0.51
31:4:19:ARG:HD2	31:4:24:ARG:HD2	1.92	0.51
32:5:26:VAL:HG21	32:5:114:GLU:HG2	1.93	0.51
34:a:297:G:N2	34:a:300:A:OP2	2.39	0.51
34:a:749:A:O2'	48:o:19:ASN:OD1	2.29	0.51
34:a:1137:C:H5'	34:a:1138:G:H5'	1.92	0.51
36:c:9:ILE:HG23	36:c:10:ARG:HG3	1.94	0.51
1:A:99:U:H5''	1:A:100:U:H5'	1.91	0.50
1:A:774:G:N2	1:A:787:C:O2'	2.44	0.50
32:5:56:ARG:HE	32:5:83:ALA:HB2	1.74	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:5:68:PRO:HA	32:5:72:LEU:HG	1.93	0.50
44:k:87:GLY:O	44:k:92:ARG:NH1	2.43	0.50
27:0:27:LEU:HD23	27:0:36:LYS:HB3	1.94	0.50
33:7:25:A:N6	57:x:37:U:H3	2.08	0.50
34:a:401:C:O2'	34:a:621:A:N3	2.43	0.50
35:b:53:LEU:HB3	35:b:219:THR:HG21	1.92	0.50
1:A:2110:G:N2	1:A:2179:C:N3	2.59	0.50
11:K:12:ASP:HB3	11:K:99:ILE:HG12	1.94	0.50
22:V:9:ARG:HD3	22:V:39:ALA:HB1	1.92	0.50
1:A:283:G:H1	1:A:357:C:H42	1.58	0.50
1:A:481:G:O2'	1:A:506:G:N2	2.44	0.50
1:A:672:C:OP2	12:L:42:SER:OG	2.29	0.50
1:A:907:G:N2	13:M:70:ASP:OD2	2.44	0.50
1:A:1378:A:O2'	1:A:1380:G:OP2	2.30	0.50
1:A:2008:C:H2'	1:A:2009:A:H8	1.75	0.50
1:A:2539:C:H4'	31:4:36:ARG:HH12	1.77	0.50
56:w:9:GLU:HG2	56:w:12:LYS:HD2	1.93	0.50
56:w:398:PHE:CD2	56:w:440:ALA:HB3	2.46	0.50
1:A:779:U:O2	1:A:785:G:O6	2.30	0.50
4:D:55:LYS:HE2	4:D:77:ARG:HA	1.94	0.50
34:a:673:A:H2'	34:a:674:G:C8	2.46	0.50
10:J:36:LEU:HD22	10:J:121:LYS:HB2	1.92	0.50
21:U:36:GLU:HA	21:U:61:GLU:HG2	1.93	0.50
34:a:235:C:H2'	34:a:236:A:H8	1.77	0.50
34:a:1222:G:OP1	52:s:77:ARG:NH1	2.44	0.50
53:t:10:ALA:O	53:t:13:SER:OG	2.28	0.50
55:v:224:ILE:HG12	55:v:246:ILE:HG12	1.93	0.50
56:w:97:GLU:HA	56:w:100:TYR:HD2	1.76	0.50
57:x:14:A:H3'	57:x:15:G:H8	1.75	0.50
1:A:848:C:H2'	1:A:849:A:H8	1.77	0.50
1:A:1326:U:H5'	1:A:2010:G:H21	1.77	0.50
1:A:2360:G:H1'	12:L:60:ARG:HH22	1.77	0.50
34:a:946:A:O2'	34:a:1333:A:N3	2.40	0.50
55:v:184:VAL:O	55:v:198:THR:HA	2.11	0.50
1:A:340:A:O2'	5:E:162:ARG:NH1	2.45	0.50
34:a:673:A:H2'	34:a:674:G:H8	1.77	0.50
56:w:36:PHE:HB3	56:w:269:LEU:HD11	1.92	0.50
56:w:430:PRO:HD2	56:w:436:LEU:HD23	1.93	0.50
1:A:1806:C:H1'	3:C:43:ASN:HD21	1.76	0.50
1:A:2295:C:OP1	15:O:10:ARG:NH1	2.44	0.50
1:A:2746:U:H5''	7:G:137:LYS:HE2	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:163:GLU:OE1	6:F:166:ARG:NH1	2.45	0.50
34:a:626:G:O2'	49:p:51:ARG:NH1	2.45	0.50
34:a:972:C:H1'	43:j:57:VAL:HG23	1.93	0.50
50:q:63:CYS:HG	50:q:73:THR:HG1	1.50	0.50
52:s:10:ILE:HG22	52:s:37:SER:HB2	1.94	0.50
55:v:112:PHE:HE1	55:v:165:LYS:CG	2.19	0.50
56:w:100:TYR:HB2	56:w:392:ASN:OD1	2.12	0.50
56:w:399:ARG:HD2	56:w:464:GLU:H	1.69	0.50
1:A:48:G:N2	1:A:177:G:OP2	2.44	0.49
1:A:242:G:N2	1:A:255:A:OP2	2.42	0.49
1:A:537:G:H22	1:A:555:G:H2'	1.77	0.49
1:A:1068:G:N2	1:A:1095:A:O2'	2.36	0.49
14:N:28:LEU:HD13	14:N:34:ILE:HG12	1.94	0.49
34:a:1425:U:H2'	34:a:1426:G:H8	1.76	0.49
39:f:36:ILE:HA	39:f:64:VAL:HG23	1.93	0.49
42:i:122:ARG:NH1	42:i:123:ARG:O	2.45	0.49
56:w:395:PRO:HB2	56:w:441:VAL:CA	2.35	0.49
1:A:464:U:H4'	29:2:12:ARG:HH22	1.76	0.49
16:P:105:LYS:O	16:P:108:ARG:NH2	2.45	0.49
25:Y:49:ASP:OD1	25:Y:52:ARG:NH2	2.45	0.49
34:a:993:G:O2'	34:a:994:A:N7	2.45	0.49
44:k:63:GLN:HG3	44:k:98:ALA:HB2	1.94	0.49
56:w:26:LYS:N	59:w:601:GCP:O2B	2.43	0.49
1:A:76:C:OP1	25:Y:48:ARG:NH1	2.46	0.49
1:A:1754:A:N1	1:A:2716:C:O2'	2.44	0.49
1:A:1899:A:H4'	1:A:1901:A:H5''	1.93	0.49
36:c:65:VAL:HB	36:c:100:ILE:HG22	1.94	0.49
56:w:312:ARG:HH11	56:w:418:GLN:NE2	2.09	0.49
1:A:574:A:N6	1:A:2034:U:OP1	2.43	0.49
1:A:966:G:H4'	1:A:2271:G:H22	1.78	0.49
1:A:1080:A:H1'	9:I:127:SER:HA	1.94	0.49
1:A:1807:G:N2	1:A:1810:A:OP2	2.44	0.49
1:A:2788:C:O2'	1:A:2809:A:N3	2.41	0.49
11:K:87:LEU:HD13	11:K:92:GLU:HB3	1.94	0.49
34:a:1081:A:OP2	38:e:51:LYS:NZ	2.45	0.49
1:A:1682:G:OP2	1:A:1699:G:N2	2.44	0.49
33:7:25:A:N6	57:x:37:U:N3	2.60	0.49
45:l:30:ARG:NH2	56:w:408:LYS:HZ1	2.10	0.49
1:A:2291:U:O2'	1:A:2374:C:O2	2.31	0.49
31:4:36:ARG:HD3	31:4:37:GLN:H	1.78	0.49
55:v:183:ARG:NH2	55:v:305:ASP:OD1	2.45	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:746:U:H1'	1:A:748:G:N2	2.28	0.49
1:A:2002:G:OP2	14:N:9:GLN:NE2	2.46	0.49
1:A:2483:C:N3	13:M:123:LYS:NZ	2.58	0.49
34:a:405:U:O4	37:d:1:ALA:N	2.44	0.49
34:a:618:C:O2	34:a:622:A:N6	2.46	0.49
43:j:45:ARG:HB2	43:j:69:THR:HB	1.95	0.49
56:w:390:ILE:N	56:w:391:PRO:CD	2.76	0.49
1:A:1022:G:N2	1:A:1023:U:O4	2.45	0.49
43:j:11:LYS:HB3	43:j:71:LEU:HG	1.95	0.49
54:u:16:ARG:HB2	54:u:19:LYS:HD3	1.93	0.49
1:A:598:U:H2'	1:A:599:A:H8	1.78	0.49
1:A:1049:C:H2'	1:A:1050:A:H8	1.78	0.49
1:A:1447:C:O2'	1:A:1544:A:N3	2.39	0.49
1:A:2060:A:H62	5:E:69:ARG:HH22	1.60	0.49
1:A:2258:C:O2'	1:A:2427:C:OP2	2.31	0.49
3:C:1:ALA:N	3:C:19:VAL:O	2.43	0.49
13:M:78:LEU:HD22	55:v:264:HIS:CE1	2.48	0.49
19:S:73:LYS:HB2	19:S:106:VAL:HB	1.94	0.49
21:U:14:THR:OG1	21:U:68:ASN:ND2	2.44	0.49
34:a:55:A:C5	56:w:311:HIS:CE1	3.01	0.49
52:s:9:PHE:HE2	52:s:36:ARG:HE	1.61	0.49
55:v:114:GLU:HB2	55:v:204:ALA:HB3	1.93	0.49
57:x:72:C:H2'	57:x:73:A:H5'	1.94	0.49
1:A:1024:G:O2'	1:A:1144:A:O2'	2.31	0.49
12:L:20:GLY:H	12:L:28:GLY:HA2	1.77	0.49
30:3:32:LEU:HB3	30:3:40:LYS:HD3	1.95	0.49
33:7:25:A:C5	33:7:26:U:C5	3.01	0.49
36:c:63:ILE:HG23	36:c:98:ALA:CB	2.42	0.49
1:A:629:G:H1'	1:A:639:U:H1'	1.95	0.48
1:A:737:C:N4	1:A:738:G:O6	2.46	0.48
1:A:793:A:OP2	1:A:2071:A:O2'	2.28	0.48
1:A:1173:U:O2'	1:A:1177:G:N2	2.40	0.48
1:A:2113:U:O4	1:A:2119:A:N6	2.45	0.48
2:B:5:U:OP1	2:B:61:G:O2'	2.29	0.48
3:C:243:PRO:O	3:C:250:GLN:NE2	2.46	0.48
34:a:28:A:O2'	34:a:296:U:OP1	2.30	0.48
39:f:6:ILE:HA	39:f:88:MET:O	2.12	0.48
1:A:526:A:O2'	1:A:2043:C:O2	2.28	0.48
2:B:95:U:H2'	2:B:96:G:H8	1.79	0.48
3:C:140:VAL:HG12	3:C:191:LEU:HD23	1.93	0.48
34:a:148:G:H21	34:a:1446:A:H2	1.60	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:a:360:G:P	56:w:411:GLN:HE21	2.36	0.48
34:a:1187:G:H5'	42:i:114:LYS:HE3	1.95	0.48
36:c:171:ARG:HG2	36:c:173:PRO:HD3	1.95	0.48
8:H:94:ILE:HG23	8:H:98:ASP:HB2	1.95	0.48
31:4:3:VAL:HA	31:4:36:ARG:HB3	1.94	0.48
34:a:316:C:O3'	34:a:353:A:N6	2.46	0.48
34:a:522:C:H1'	34:a:536:C:H5''	1.94	0.48
1:A:466:A:OP1	29:2:34:ARG:NH1	2.46	0.48
1:A:2647:U:H2'	1:A:2648:G:H8	1.78	0.48
5:E:75:SER:HB3	5:E:78:TRP:HD1	1.77	0.48
9:I:44:LYS:HG2	9:I:70:THR:HG21	1.95	0.48
34:a:243:A:H4'	34:a:244:U:H3'	1.96	0.48
40:g:67:ASN:O	40:g:137:ARG:NE	2.46	0.48
43:j:40:ILE:HB	43:j:73:LEU:HB2	1.94	0.48
54:u:40:PRO:HA	54:u:43:GLU:HG2	1.94	0.48
56:w:158:VAL:HG13	56:w:162:LEU:HD12	1.94	0.48
1:A:177:G:OP2	1:A:177:G:N2	2.36	0.48
1:A:1323:C:OP1	19:S:98:LYS:NZ	2.45	0.48
1:A:1469:A:OP2	1:A:1522:A:N6	2.47	0.48
1:A:2345:G:H4'	1:A:2346:A:H3'	1.95	0.48
5:E:97:ASN:ND2	5:E:100:MET:SD	2.86	0.48
34:a:826:C:O2	41:h:15:ASN:ND2	2.47	0.48
34:a:1071:C:H2'	34:a:1072:G:H8	1.79	0.48
1:A:2233:U:H2'	1:A:2234:G:H8	1.77	0.48
1:A:2602:A:C2	55:v:236:HIS:CD2	3.00	0.48
1:A:2822:G:O2'	1:A:2825:G:N1	2.40	0.48
34:a:137:U:H2'	34:a:138:G:H8	1.79	0.48
34:a:201:G:H1	34:a:216:U:H3	1.61	0.48
35:b:75:ALA:O	35:b:79:VAL:N	2.46	0.48
2:B:1:U:H2'	2:B:2:G:H8	1.78	0.48
8:H:17:ASP:HB3	8:H:19:VAL:HG23	1.96	0.48
34:a:1142:G:H3'	34:a:1143:G:H8	1.79	0.48
56:w:503:TYR:CG	56:w:504:ILE:N	2.71	0.48
1:A:673:C:OP1	5:E:49:ARG:NH2	2.45	0.48
4:D:36:GLN:OE1	4:D:49:GLN:NE2	2.46	0.48
57:x:51:U:H3	57:x:65:G:H1	1.61	0.48
1:A:1912:A:N3	34:a:1495:U:H1'	2.29	0.48
6:F:152:ASP:N	6:F:152:ASP:OD1	2.42	0.48
1:A:451:U:O2	1:A:453:A:N6	2.47	0.48
1:A:807:U:O2'	1:A:2060:A:N1	2.42	0.48
1:A:2076:U:OP2	1:A:2238:G:N2	2.45	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2618:G:H21	4:D:155:VAL:HG21	1.78	0.48
33:7:25:A:H2	57:x:37:U:O2	1.93	0.48
34:a:335:C:O2'	34:a:1433:A:N3	2.40	0.48
56:w:488:LYS:HB2	56:w:517:ARG:HH21	1.79	0.48
1:A:291:G:H1	1:A:349:U:H3	1.61	0.47
1:A:1129:A:O2'	1:A:2515:C:O2	2.29	0.47
1:A:2602:A:H2	55:v:237:VAL:HG22	1.75	0.47
9:I:102:ARG:NH1	9:I:106:GLN:OE1	2.47	0.47
34:a:589:U:H5''	41:h:29:SER:HB2	1.96	0.47
34:a:783:C:H2'	34:a:784:A:H8	1.79	0.47
39:f:15:SER:HA	39:f:18:VAL:HG23	1.96	0.47
1:A:776:G:H22	1:A:2072:C:H5'	1.80	0.47
1:A:1830:C:H2'	1:A:1831:G:H8	1.79	0.47
1:A:2602:A:C2	55:v:237:VAL:HG23	2.47	0.47
1:A:2848:G:O2'	1:A:2868:A:N6	2.46	0.47
5:E:182:ALA:HB2	12:L:3:LEU:HD22	1.96	0.47
17:Q:87:VAL:HG13	18:R:49:ILE:HD11	1.96	0.47
34:a:776:G:N2	34:a:802:A:OP2	2.47	0.47
34:a:1178:G:N2	34:a:1181:G:OP2	2.45	0.47
34:a:1357:A:N6	34:a:1365:G:H1	2.09	0.47
1:A:659:G:O2'	5:E:95:LYS:O	2.30	0.47
1:A:1638:C:O2	1:A:2698:U:O2'	2.32	0.47
12:L:28:GLY:H	12:L:31:GLY:HA2	1.78	0.47
16:P:25:VAL:HG22	16:P:85:VAL:HG22	1.96	0.47
1:A:213:A:H2'	1:A:214:G:C8	2.50	0.47
1:A:1069:A:N7	1:A:1073:A:N6	2.62	0.47
1:A:1936:A:OP2	1:A:1962:C:N4	2.41	0.47
1:A:2063:C:O4'	58:z:18:LEU:HA	2.14	0.47
6:F:9:ASP:OD1	6:F:9:ASP:N	2.45	0.47
21:U:20:LYS:HB3	21:U:38:ILE:HD12	1.96	0.47
33:7:25:A:N1	57:x:37:U:O2	2.48	0.47
34:a:979:C:OP1	34:a:1223:C:N4	2.47	0.47
1:A:91:A:O2'	1:A:92:U:O4'	2.32	0.47
1:A:720:U:H2'	1:A:721:A:H8	1.80	0.47
34:a:150:U:H2'	34:a:151:A:H8	1.79	0.47
34:a:429:U:H3	34:a:431:A:H62	1.61	0.47
34:a:1081:A:H2'	34:a:1082:A:H8	1.80	0.47
34:a:1228:C:OP1	46:m:106:ARG:NH1	2.43	0.47
34:a:1317:C:H4'	47:n:48:LEU:HD21	1.97	0.47
1:A:302:C:H2'	1:A:303:G:H8	1.79	0.47
1:A:505:A:HO2'	1:A:509:C:HO2'	1.63	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1429:G:H2'	1:A:1430:G:H8	1.79	0.47
2:B:7:G:O2'	15:O:38:GLN:NE2	2.47	0.47
20:T:13:ALA:HB3	20:T:33:LYS:HD3	1.96	0.47
35:b:116:LEU:HG	35:b:136:ARG:HH21	1.79	0.47
42:i:91:GLU:OE2	42:i:94:ARG:NH1	2.47	0.47
1:A:239:C:HO2'	1:A:622:G:HO2'	1.61	0.47
1:A:290:U:H2'	1:A:291:G:H8	1.80	0.47
1:A:806:C:O2	1:A:2444:G:O2'	2.33	0.47
1:A:917:A:H5''	1:A:2268:A:H61	1.80	0.47
1:A:1046:A:H4'	32:5:61:ARG:HB3	1.95	0.47
1:A:1071:G:N2	1:A:1089:A:O2'	2.45	0.47
11:K:35:VAL:HG11	11:K:106:GLU:HB2	1.97	0.47
14:N:43:GLU:OE2	14:N:46:ARG:NH2	2.47	0.47
14:N:118:ARG:NH1	27:0:55:ALA:O	2.48	0.47
16:P:105:LYS:HG2	34:a:1432:G:O5'	2.15	0.47
22:V:77:VAL:HG23	22:V:89:ILE:HG12	1.95	0.47
26:Z:16:LEU:HB2	26:Z:19:HIS:HD2	1.79	0.47
31:4:30:GLU:HG3	31:4:32:LYS:H	1.80	0.47
34:a:309:A:H2'	34:a:310:G:H8	1.79	0.47
34:a:531:U:OP2	55:v:314:GLN:NE2	2.47	0.47
34:a:690:G:OP2	44:k:28:ASN:ND2	2.40	0.47
34:a:1368:A:OP1	43:j:64:GLN:NE2	2.45	0.47
34:a:1445:U:O2	34:a:1457:G:N2	2.39	0.47
36:c:18:ASN:OD1	36:c:53:ARG:NH2	2.48	0.47
37:d:71:PHE:HE1	37:d:93:LEU:HD11	1.78	0.47
1:A:1597:A:H4'	1:A:1598:A:H8	1.80	0.47
1:A:2512:C:OP2	4:D:128:ARG:NH2	2.48	0.47
34:a:361:G:OP2	56:w:408:LYS:HE2	2.15	0.47
34:a:376:G:H2'	34:a:377:G:H8	1.80	0.47
34:a:921:U:H2'	34:a:922:G:H8	1.80	0.47
34:a:1304:G:N2	34:a:1333:A:H62	2.13	0.47
56:w:394:ALA:HA	56:w:395:PRO:HD3	1.67	0.47
1:A:590:A:H61	1:A:667:U:H3	1.62	0.47
1:A:2458:G:O2'	1:A:2460:U:O4	2.32	0.47
1:A:2768:U:O2'	10:J:95:ARG:NH2	2.48	0.47
6:F:55:ASP:OD2	6:F:149:ARG:NH2	2.47	0.47
13:M:40:ARG:HH11	13:M:93:VAL:HG11	1.79	0.47
20:T:37:ASP:OD1	20:T:37:ASP:N	2.47	0.47
33:7:26:U:H2'	33:7:27:G:C1'	2.45	0.47
34:a:1049:U:H2'	47:n:2:LYS:HD3	1.95	0.47
55:v:127:PHE:CE1	55:v:184:VAL:CG2	2.93	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1912:A:O2'	34:a:1495:U:H5'	2.15	0.47
55:v:217:ILE:HG22	55:v:222:LEU:HD11	1.97	0.47
1:A:651:G:H5'	30:3:18:LYS:HG3	1.98	0.46
2:B:114:C:H2'	2:B:115:A:H8	1.79	0.46
3:C:267:VAL:HG12	3:C:268:ARG:HG2	1.97	0.46
12:L:62:PRO:HG2	30:3:24:LYS:HB3	1.96	0.46
1:A:577:G:O2'	1:A:1254:A:OP1	2.32	0.46
1:A:582:A:H2'	1:A:583:G:H8	1.81	0.46
1:A:690:G:H4'	3:C:216:ARG:HH22	1.80	0.46
1:A:1209:U:H4'	1:A:1212:G:H4'	1.97	0.46
1:A:1333:G:H2'	1:A:1334:G:H8	1.81	0.46
22:V:20:LEU:HD11	22:V:41:GLU:HG3	1.97	0.46
34:a:107:G:OP1	34:a:325:A:N6	2.49	0.46
34:a:745:G:H2'	34:a:746:A:H8	1.80	0.46
56:w:496:ASP:HB2	56:w:500:ASN:HB2	1.97	0.46
1:A:377:G:H1	1:A:397:U:H3	1.63	0.46
1:A:633:A:O2'	1:A:2404:U:OP1	2.33	0.46
19:S:69:LEU:HA	19:S:109:ASP:HA	1.97	0.46
29:2:31:LEU:HD23	29:2:35:ARG:HH12	1.80	0.46
32:5:24:SER:HB2	32:5:116:GLU:HG3	1.97	0.46
34:a:143:A:H2	34:a:220:G:H1	1.62	0.46
42:i:113:LYS:HA	42:i:120:ALA:HB2	1.98	0.46
45:l:30:ARG:NH2	56:w:408:LYS:NZ	2.62	0.46
55:v:139:ALA:HA	55:v:144:TRP:HD1	1.80	0.46
55:v:224:ILE:HD13	55:v:267:LYS:HZ2	1.74	0.46
1:A:519:U:H2'	1:A:520:G:H8	1.80	0.46
1:A:2602:A:N3	55:v:237:VAL:CG2	2.78	0.46
3:C:141:HIS:ND1	3:C:192:GLY:O	2.43	0.46
5:E:3:LEU:HD13	5:E:120:VAL:HG21	1.97	0.46
34:a:321:A:N6	34:a:332:G:H1	2.08	0.46
34:a:885:G:OP1	45:l:14:LYS:NZ	2.47	0.46
34:a:1349:A:OP2	42:i:119:LYS:NZ	2.46	0.46
45:l:30:ARG:HH22	56:w:408:LYS:HZ2	1.62	0.46
56:w:257:GLY:HA3	56:w:264:GLY:HA3	1.97	0.46
56:w:333:GLN:O	56:w:337:ALA:N	2.49	0.46
1:A:1432:G:H2'	1:A:1433:A:H8	1.81	0.46
18:R:40:MET:HE3	18:R:42:ALA:HB2	1.97	0.46
34:a:946:A:H2'	34:a:947:G:C8	2.51	0.46
34:a:1491:G:C3'	34:a:1492:A:H5''	2.40	0.46
39:f:6:ILE:HB	39:f:62:MET:HB2	1.95	0.46
57:x:52:C:H2'	57:x:53:G:H8	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:476:G:O2'	1:A:502:A:N6	2.45	0.46
1:A:1291:C:H2'	1:A:1292:G:H8	1.81	0.46
1:A:2816:G:N3	1:A:2883:A:O2'	2.47	0.46
10:J:36:LEU:HD11	10:J:122:LEU:HD13	1.97	0.46
56:w:97:GLU:O	56:w:101:ARG:NH1	2.49	0.46
56:w:144:LEU:HB2	56:w:258:THR:HB	1.97	0.46
56:w:159:GLU:HG2	56:w:165:GLY:HA2	1.98	0.46
56:w:395:PRO:CB	56:w:441:VAL:CB	2.85	0.46
1:A:254:G:OP2	30:3:4:LYS:NZ	2.45	0.46
1:A:1921:G:H2'	1:A:1922:G:H8	1.80	0.46
1:A:2245:U:H5''	1:A:2246:G:H5'	1.96	0.46
32:5:33:VAL:HG12	32:5:35:VAL:H	1.80	0.46
34:a:1221:G:OP1	52:s:35:ARG:NH1	2.48	0.46
36:c:99:GLN:H	36:c:99:GLN:CD	2.16	0.46
55:v:322:ILE:O	55:v:324:LEU:N	2.48	0.46
1:A:249:C:O2	30:3:11:LYS:NZ	2.47	0.46
1:A:720:U:H2'	1:A:721:A:C8	2.51	0.46
6:F:115:GLY:HA3	6:F:177:ARG:HB2	1.97	0.46
12:L:127:VAL:HG21	12:L:142:ILE:HD13	1.97	0.46
34:a:923:A:O2'	34:a:1399:C:OP2	2.33	0.46
37:d:187:ARG:NH2	37:d:194:ILE:O	2.49	0.46
43:j:59:LYS:HE2	43:j:62:ARG:HH21	1.80	0.46
1:A:196:A:H61	1:A:831:G:H21	1.64	0.46
1:A:568:U:O4	18:R:81:LYS:NZ	2.42	0.46
1:A:1368:G:H2'	1:A:1369:G:H8	1.81	0.46
1:A:1387:A:H5'	1:A:1469:A:H1'	1.97	0.46
1:A:1432:G:H2'	1:A:1433:A:C8	2.51	0.46
34:a:427:U:O2'	34:a:541:G:OP1	2.34	0.46
34:a:1343:G:H4'	42:i:123:ARG:HB2	1.97	0.46
1:A:581:C:H2'	1:A:582:A:C8	2.51	0.46
1:A:1386:C:H2'	1:A:1387:A:C8	2.51	0.46
2:B:111:U:H2'	2:B:112:G:H8	1.81	0.46
3:C:154:ALA:HB2	3:C:161:VAL:HG23	1.98	0.46
28:1:5:ARG:HG2	28:1:23:THR:HB	1.98	0.46
33:7:25:A:C6	33:7:26:U:C4	3.03	0.46
34:a:355:C:H1'	34:a:388:G:H1'	1.98	0.46
34:a:1493:A:OP2	34:a:1493:A:H8	1.99	0.46
39:f:11:HIS:O	39:f:15:SER:N	2.49	0.46
1:A:212:G:H2'	1:A:213:A:C8	2.50	0.45
1:A:372:G:O6	24:X:56:ARG:NH2	2.49	0.45
1:A:1913:A:H8	34:a:1494:G:H1'	1.79	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2052:A:O2'	4:D:149:ASN:O	2.35	0.45
1:A:2063:C:C1'	58:z:18:LEU:HA	2.45	0.45
1:A:2417:C:H5''	30:3:44:ARG:HG3	1.97	0.45
24:X:6:VAL:HA	24:X:73:ARG:HH22	1.79	0.45
1:A:33:C:O2	1:A:447:A:N6	2.49	0.45
1:A:224:U:OP2	1:A:408:G:N2	2.41	0.45
1:A:351:C:H2'	1:A:352:A:H8	1.81	0.45
1:A:373:U:H2'	1:A:374:A:H8	1.81	0.45
1:A:2313:C:H2'	1:A:2314:A:H8	1.79	0.45
8:H:70:GLU:HB2	8:H:134:VAL:HG21	1.98	0.45
30:3:28:LEU:HA	30:3:32:LEU:HD11	1.98	0.45
34:a:552:U:H2'	34:a:553:A:H8	1.81	0.45
34:a:677:U:O2	34:a:777:A:O2'	2.31	0.45
34:a:876:C:H2'	34:a:877:G:H8	1.80	0.45
34:a:1316:G:N1	34:a:1319:A:OP2	2.50	0.45
37:d:90:LEU:HD23	37:d:93:LEU:HD12	1.97	0.45
40:g:12:LEU:HD12	40:g:13:PRO:HD2	1.99	0.45
44:k:86:LYS:NZ	44:k:112:VAL:O	2.46	0.45
55:v:138:TYR:OH	55:v:142:ARG:CZ	2.64	0.45
55:v:184:VAL:CG1	55:v:199:SER:OG	2.64	0.45
6:F:140:ILE:HG22	6:F:142:TYR:H	1.82	0.45
36:c:13:ILE:HG22	36:c:14:VAL:HG23	1.99	0.45
53:t:12:GLN:O	53:t:15:LYS:HB3	2.16	0.45
55:v:114:GLU:HA	55:v:162:ILE:O	2.16	0.45
5:E:102:ARG:NH1	5:E:200:LEU:O	2.49	0.45
11:K:98:ARG:NH2	34:a:340:U:C4	2.71	0.45
34:a:501:C:H2'	34:a:502:A:C8	2.52	0.45
36:c:147:GLY:HA2	36:c:170:GLY:HA3	1.97	0.45
43:j:8:ILE:HB	43:j:74:VAL:HB	1.97	0.45
1:A:1254:A:H5''	1:A:1255:U:H5''	1.99	0.45
1:A:2047:C:H2'	1:A:2048:G:H8	1.82	0.45
1:A:2086:U:H2'	1:A:2087:G:C8	2.52	0.45
1:A:2348:U:OP2	30:3:41:ARG:NH1	2.50	0.45
1:A:2468:A:OP2	1:A:2476:A:N6	2.50	0.45
10:J:32:LEU:HD22	10:J:54:ILE:HG21	1.99	0.45
34:a:429:U:OP1	37:d:12:ARG:NH2	2.50	0.45
34:a:477:C:H2'	34:a:478:A:C8	2.51	0.45
34:a:684:U:O2'	44:k:40:ALA:O	2.35	0.45
34:a:714:G:H2'	34:a:715:A:C8	2.51	0.45
56:w:477:ALA:HB3	56:w:482:PHE:HB3	1.97	0.45
1:A:111:A:O2'	25:Y:58:ASN:ND2	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:662:G:H2'	1:A:663:G:H8	1.80	0.45
1:A:1997:C:H2'	1:A:1998:A:H8	1.82	0.45
4:D:115:GLY:HA2	4:D:166:GLY:HA3	1.98	0.45
44:k:86:LYS:HB2	44:k:112:VAL:HG23	1.96	0.45
56:w:318:MET:H	56:w:364:ILE:HG23	1.81	0.45
56:w:391:PRO:O	56:w:392:ASN:CB	2.64	0.45
1:A:585:G:N2	1:A:1254:A:H62	2.14	0.45
1:A:1395:A:O2'	1:A:1397:U:OP2	2.35	0.45
1:A:2293:G:OP1	15:O:94:ARG:NH1	2.50	0.45
4:D:109:VAL:HG22	4:D:203:VAL:HG22	1.99	0.45
10:J:31:GLU:HG2	10:J:142:ILE:HG12	1.98	0.45
16:P:91:VAL:HG21	16:P:96:LEU:HD11	1.99	0.45
33:7:27:G:N7	34:a:1400:C:C5'	2.78	0.45
34:a:808:C:H5''	48:o:46:LYS:HD2	1.99	0.45
34:a:1150:A:H2'	34:a:1151:A:C8	2.52	0.45
34:a:1250:A:H4'	42:i:68:GLY:HA2	1.98	0.45
1:A:460:A:H62	1:A:469:G:H21	1.64	0.45
1:A:1171:G:N2	1:A:1179:G:N7	2.65	0.45
1:A:1636:U:H2'	1:A:1637:A:H8	1.82	0.45
17:Q:99:VAL:O	17:Q:102:LYS:NZ	2.49	0.45
18:R:76:LYS:HB2	18:R:85:LYS:HB3	1.99	0.45
34:a:335:C:H2'	34:a:336:A:C8	2.51	0.45
34:a:1356:G:H2'	34:a:1357:A:C8	2.52	0.45
34:a:1493:A:H4'	55:v:120:GLY:H	1.82	0.45
1:A:29:U:O2	1:A:1215:G:O2'	2.34	0.45
1:A:302:C:H2'	1:A:303:G:C8	2.52	0.45
1:A:589:U:H2'	1:A:590:A:C8	2.51	0.45
1:A:1509:A:H2'	1:A:1510:G:C8	2.52	0.45
1:A:1612:C:O2'	29:2:5:PHE:O	2.35	0.45
4:D:37:VAL:HG22	4:D:48:ILE:HG22	1.99	0.45
34:a:715:A:OP1	34:a:805:C:O2'	2.33	0.45
34:a:880:C:H2'	34:a:881:G:H8	1.82	0.45
35:b:113:LEU:HD13	35:b:143:LEU:HB3	1.99	0.45
38:e:149:PRO:HA	38:e:152:VAL:HG22	1.98	0.45
56:w:27:THR:OG1	59:w:601:GCP:O1B	2.25	0.45
1:A:286:U:H2'	1:A:287:G:H8	1.82	0.45
32:5:30:SER:HB3	32:5:109:LYS:HD2	1.98	0.45
34:a:562:U:H1'	45:l:11:ARG:HD2	1.98	0.45
34:a:599:C:H2'	34:a:600:A:H8	1.82	0.45
34:a:891:U:H2'	34:a:892:A:H8	1.82	0.45
34:a:1230:C:H5'	57:x:31:G:H5''	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:a:1255:G:O2'	34:a:1258:G:N3	2.42	0.45
34:a:1496:C:H2'	34:a:1497:G:C8	2.51	0.45
1:A:581:C:H2'	1:A:582:A:H8	1.81	0.44
1:A:692:C:H5''	3:C:38:LYS:HB3	1.99	0.44
1:A:1081:U:H5'	9:I:126:ARG:HH21	1.82	0.44
1:A:2086:U:H2'	1:A:2087:G:H8	1.81	0.44
1:A:2719:G:H4'	1:A:2846:G:H4'	1.98	0.44
1:A:2818:U:H2'	1:A:2819:G:C8	2.52	0.44
14:N:118:ARG:NH2	27:O:54:ILE:O	2.50	0.44
34:a:652:U:O4	34:a:752:G:O2'	2.29	0.44
35:b:75:ALA:O	35:b:78:ALA:HB3	2.17	0.44
35:b:202:ASN:HD22	35:b:203:ASP:H	1.65	0.44
36:c:54:ILE:HD12	36:c:56:ILE:HD11	1.99	0.44
48:o:35:ILE:HG13	48:o:58:MET:HE2	1.99	0.44
1:A:764:A:N3	3:C:211:ARG:NH1	2.65	0.44
1:A:2070:A:H2'	1:A:2071:A:H8	1.81	0.44
1:A:2370:G:O2'	28:1:43:ARG:NH1	2.51	0.44
3:C:130:PRO:HA	3:C:188:ARG:HA	2.00	0.44
15:O:8:ILE:O	15:O:12:THR:OG1	2.29	0.44
20:T:54:GLU:HB3	20:T:88:LYS:HD2	1.98	0.44
25:Y:37:LEU:HD11	25:Y:42:LEU:HD12	1.98	0.44
34:a:1493:A:OP2	34:a:1493:A:C8	2.70	0.44
34:a:1500:A:H5''	34:a:1508:A:H5''	1.99	0.44
35:b:129:THR:HG22	35:b:131:LYS:H	1.82	0.44
1:A:16:C:H2'	1:A:17:G:H8	1.81	0.44
1:A:2144:G:H1'	1:A:2147:A:H61	1.82	0.44
1:A:2656:U:C2	1:A:2665:A:N7	2.85	0.44
1:A:2771:C:O2'	4:D:173:GLN:NE2	2.47	0.44
3:C:5:CYS:SG	3:C:12:ARG:NH2	2.91	0.44
17:Q:93:ILE:HG23	18:R:13:ARG:HB2	1.99	0.44
34:a:360:G:OP2	56:w:411:GLN:NE2	2.48	0.44
34:a:373:A:O2'	34:a:451:A:N7	2.50	0.44
38:e:92:ARG:HB2	38:e:127:TYR:HB2	1.98	0.44
55:v:144:TRP:HZ3	55:v:169:ASP:H	1.65	0.44
1:A:592:A:O2'	30:3:63:TYR:OH	2.35	0.44
2:B:93:C:H2'	2:B:94:A:H8	1.82	0.44
34:a:360:G:P	56:w:411:GLN:NE2	2.90	0.44
34:a:422:C:O2'	34:a:423:G:N2	2.50	0.44
34:a:946:A:H2'	34:a:947:G:H8	1.83	0.44
36:c:109:GLU:HB2	36:c:143:LEU:HD13	1.99	0.44
49:p:18:GLN:HE22	49:p:35:ARG:HH21	1.65	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
55:v:263:GLN:O	55:v:267:LYS:N	2.50	0.44
1:A:2443:C:H2'	1:A:2444:G:C8	2.52	0.44
1:A:2676:C:O2	1:A:2732:G:N2	2.47	0.44
32:5:48:ALA:HB3	32:5:51:TYR:HE1	1.82	0.44
34:a:745:G:OP1	34:a:851:G:O2'	2.32	0.44
34:a:924:C:H2'	34:a:925:G:H8	1.82	0.44
34:a:1218:C:H2'	34:a:1219:A:C8	2.52	0.44
55:v:311:ASN:O	55:v:329:LEU:CD1	2.65	0.44
56:w:73:SER:OG	56:w:88:ASP:OD2	2.36	0.44
1:A:6:A:N3	10:J:135:GLN:NE2	2.65	0.44
1:A:552:U:H2'	1:A:553:G:H8	1.82	0.44
1:A:2559:C:H2'	1:A:2560:A:H8	1.82	0.44
16:P:105:LYS:HG2	34:a:1432:G:P	2.58	0.44
19:S:17:VAL:HG12	19:S:76:VAL:HG21	2.00	0.44
27:0:42:ILE:HG22	27:0:48:TYR:HB2	1.99	0.44
34:a:361:G:P	56:w:408:LYS:HE2	2.58	0.44
34:a:1254:A:OP2	43:j:45:ARG:NH2	2.51	0.44
34:a:1350:A:OP1	42:i:118:ARG:NH2	2.50	0.44
36:c:63:ILE:HG21	36:c:94:ALA:HB1	2.00	0.44
37:d:158:LEU:O	37:d:161:ALA:HB3	2.17	0.44
45:l:86:VAL:HG23	45:l:88:ASP:H	1.82	0.44
55:v:315:GLY:HA2	55:v:329:LEU:HD12	1.99	0.44
1:A:18:U:O2'	1:A:554:U:OP1	2.35	0.44
6:F:28:PRO:HB2	6:F:168:LEU:HD22	2.00	0.44
24:X:39:VAL:O	24:X:43:LYS:CA	2.65	0.44
34:a:34:C:H2'	34:a:35:G:H8	1.82	0.44
34:a:1233:G:O2'	34:a:1365:G:OP1	2.32	0.44
34:a:1287:A:H2	34:a:1353:G:H1'	1.82	0.44
40:g:55:LYS:HB3	40:g:59:GLU:HG3	2.00	0.44
51:r:41:SER:HB3	51:r:51:GLN:HE21	1.83	0.44
1:A:1141:U:OP2	10:J:68:LYS:NZ	2.45	0.44
1:A:2776:A:O2'	1:A:2782:G:N7	2.46	0.44
35:b:99:MET:HA	35:b:106:VAL:HG21	1.99	0.44
55:v:134:MET:HE3	55:v:337:LEU:CG	2.48	0.44
56:w:473:TRP:O	56:w:502:ALA:HB1	2.18	0.44
1:A:1796:U:H2'	1:A:1797:G:C8	2.53	0.44
1:A:2899:A:H2'	1:A:2900:A:C8	2.53	0.44
3:C:56:GLY:HA2	3:C:212:TRP:HA	2.00	0.44
4:D:9:VAL:HA	4:D:197:THR:HG23	2.00	0.44
6:F:56:LEU:HD13	6:F:88:VAL:HG23	2.00	0.44
34:a:5:U:H4'	34:a:6:G:C4	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:a:398:U:H2'	34:a:399:G:H8	1.82	0.44
38:e:65:LYS:HA	38:e:68:ARG:HG2	2.00	0.44
49:p:61:VAL:HG22	49:p:67:ILE:HD11	2.00	0.44
1:A:198:C:H4'	1:A:2243:U:H4'	2.00	0.43
1:A:2291:U:O2	1:A:2374:C:O2'	2.32	0.43
34:a:9:G:H5'	38:e:107:GLY:HA3	2.00	0.43
36:c:31:ASN:OD1	36:c:58:ARG:NH2	2.51	0.43
56:w:308:ASP:OD2	56:w:454:LYS:CB	2.64	0.43
1:A:1841:U:H2'	1:A:1842:G:H8	1.83	0.43
1:A:2459:A:H2	13:M:78:LEU:HD21	1.83	0.43
3:C:74:PRO:HB3	3:C:114:GLN:HE21	1.83	0.43
6:F:42:ALA:HB3	6:F:84:ILE:HD12	2.00	0.43
8:H:125:THR:HG23	8:H:146:VAL:HG12	1.99	0.43
19:S:62:ASP:N	19:S:62:ASP:OD1	2.49	0.43
34:a:235:C:H2'	34:a:236:A:C8	2.53	0.43
34:a:920:U:O2'	34:a:1081:A:O2'	2.30	0.43
43:j:22:THR:HA	43:j:25:ILE:HG22	2.00	0.43
50:q:11:VAL:HG22	50:q:22:VAL:HG22	1.99	0.43
1:A:605:G:O2'	1:A:657:U:O2	2.33	0.43
1:A:2035:G:H5''	1:A:2036:C:H5	1.83	0.43
1:A:2691:C:H2'	1:A:2692:G:H8	1.82	0.43
1:A:2898:U:H2'	1:A:2899:A:C8	2.54	0.43
15:O:4:LYS:HE2	15:O:8:ILE:HD11	2.00	0.43
34:a:410:G:OP1	37:d:25:ARG:NH1	2.51	0.43
34:a:1266:G:N2	34:a:1269:A:OP2	2.40	0.43
1:A:854:C:H2'	1:A:855:G:C8	2.53	0.43
1:A:2457:U:C5	1:A:2494:G:N1	2.62	0.43
34:a:587:G:OP1	41:h:83:ARG:NH2	2.49	0.43
34:a:674:G:H2'	34:a:675:A:C8	2.53	0.43
34:a:779:C:H1'	44:k:121:ARG:HD2	2.00	0.43
39:f:5:GLU:HB2	39:f:90:MET:HB2	2.00	0.43
1:A:2246:G:H2'	1:A:2247:A:H8	1.84	0.43
16:P:84:SER:OG	16:P:86:LYS:NZ	2.51	0.43
16:P:88:ARG:HB3	16:P:112:ARG:HD3	2.01	0.43
32:5:119:PRO:HG2	32:5:121:SER:HB2	2.01	0.43
34:a:376:G:H5''	49:p:5:ARG:HB2	2.01	0.43
34:a:1261:A:H5''	34:a:1262:C:H5	1.83	0.43
55:v:322:ILE:O	55:v:324:LEU:HG	2.18	0.43
56:w:314:ARG:HH12	56:w:418:GLN:CB	2.32	0.43
56:w:374:GLN:N	56:w:377:ASP:OD2	2.51	0.43
56:w:395:PRO:CA	56:w:441:VAL:HG22	2.41	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1093:G:N2	1:A:1098:A:H62	2.15	0.43
1:A:1287:A:H62	14:N:106:ASP:HB3	1.83	0.43
24:X:39:VAL:O	24:X:43:LYS:HA	2.19	0.43
25:Y:24:GLU:HB3	25:Y:46:VAL:HG21	1.99	0.43
39:f:92:THR:OG1	39:f:93:LYS:N	2.50	0.43
42:i:37:TYR:HD2	42:i:38:PHE:HD1	1.65	0.43
55:v:227:PHE:CD2	55:v:228:ARG:O	2.72	0.43
56:w:308:ASP:OD1	56:w:308:ASP:N	2.50	0.43
56:w:417:VAL:HG21	56:w:429:ARG:HH21	1.84	0.43
1:A:2452:C:H5''	55:v:239:THR:OG1	2.17	0.43
8:H:30:LEU:HA	8:H:35:LYS:HB2	2.00	0.43
11:K:76:VAL:H	16:P:72:VAL:HG22	1.83	0.43
54:u:16:ARG:HH21	54:u:19:LYS:HG2	1.84	0.43
55:v:244:ILE:HD11	55:v:263:GLN:HB3	2.01	0.43
1:A:1431:A:H2'	1:A:1432:G:H8	1.82	0.43
1:A:1919:A:N1	34:a:1495:U:O2'	2.44	0.43
5:E:18:THR:HA	5:E:106:LYS:HE3	2.01	0.43
19:S:77:ASP:OD1	19:S:77:ASP:N	2.52	0.43
34:a:1457:G:H2'	34:a:1458:G:H8	1.83	0.43
41:h:38:VAL:HG21	41:h:109:VAL:HG12	2.01	0.43
41:h:45:ILE:HG21	41:h:60:LEU:HD22	1.99	0.43
43:j:40:ILE:HG21	43:j:73:LEU:HD12	2.01	0.43
1:A:655:A:H4'	1:A:656:G:H5'	2.00	0.43
5:E:75:SER:HB3	5:E:78:TRP:CD1	2.54	0.43
5:E:145:ASP:HA	5:E:166:LYS:HB3	2.01	0.43
34:a:739:C:HO2'	48:o:41:HIS:HD1	1.66	0.43
34:a:945:G:N2	34:a:1334:G:O2'	2.52	0.43
34:a:1315:U:O2'	34:a:1360:A:N3	2.46	0.43
53:t:24:ARG:HB2	53:t:65:LEU:HD21	2.01	0.43
56:w:477:ALA:HA	56:w:521:VAL:HG23	2.00	0.43
1:A:2372:U:H2'	1:A:2373:G:H8	1.84	0.43
19:S:22:ASP:OD1	19:S:25:ARG:NH2	2.51	0.43
34:a:634:C:H2'	34:a:635:A:H8	1.84	0.43
35:b:23:ASN:HB2	35:b:189:ASN:HA	2.00	0.43
35:b:71:THR:OG1	35:b:168:GLU:OE2	2.26	0.43
56:w:111:MET:HB2	56:w:139:THR:HG22	2.01	0.43
57:x:56:U:N3	57:x:59:A:OP2	2.45	0.43
57:x:72:C:C6	57:x:72:C:C4'	3.01	0.43
1:A:546:U:H2'	1:A:547:A:H4'	1.99	0.42
1:A:1295:C:H2'	1:A:1296:G:H8	1.84	0.42
1:A:1667:G:O2'	1:A:1991:U:O4	2.37	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2175:C:H2'	1:A:2176:A:H8	1.84	0.42
34:a:711:G:H2'	34:a:712:A:H8	1.84	0.42
34:a:1115:U:H3	34:a:1185:G:H1	1.66	0.42
34:a:1291:U:H2'	34:a:1292:G:C8	2.54	0.42
34:a:1291:U:H2'	34:a:1292:G:H8	1.84	0.42
34:a:1427:C:H2'	34:a:1428:A:H8	1.84	0.42
34:a:1524:C:H2'	34:a:1525:G:H8	1.84	0.42
36:c:99:GLN:N	36:c:99:GLN:CD	2.77	0.42
39:f:97:THR:OG1	39:f:98:GLU:N	2.50	0.42
55:v:248:HIS:CD2	55:v:274:LEU:HD22	2.54	0.42
1:A:239:C:O2'	1:A:622:G:O2'	2.33	0.42
1:A:2395:C:H2'	1:A:2396:G:H8	1.84	0.42
34:a:1522:U:OP1	44:k:127:ARG:NH2	2.52	0.42
40:g:1:PRO:HD2	40:g:4:ARG:HB2	2.00	0.42
41:h:45:ILE:HD13	41:h:60:LEU:HD22	1.99	0.42
45:l:23:LEU:HD22	45:l:58:ASN:HD22	1.83	0.42
56:w:21:HIS:NE2	56:w:120:GLU:OE1	2.44	0.42
56:w:395:PRO:HB3	56:w:441:VAL:N	2.33	0.42
56:w:400:ARG:HE	56:w:435:ASP:HB3	1.84	0.42
1:A:1024:G:HO2'	1:A:1144:A:HO2'	1.61	0.42
1:A:1687:G:N2	1:A:1701:A:H62	2.16	0.42
13:M:42:THR:HG22	13:M:93:VAL:HG12	2.01	0.42
14:N:79:LEU:HD23	14:N:83:LEU:HD12	2.02	0.42
34:a:490:C:H2'	34:a:491:G:H8	1.83	0.42
34:a:739:C:O2'	48:o:41:HIS:ND1	2.52	0.42
34:a:878:A:H5'	41:h:80:PRO:HG2	2.02	0.42
56:w:396:GLU:O	56:w:440:ALA:O	2.36	0.42
1:A:2832:U:H1'	1:A:2834:G:C2	2.54	0.42
3:C:121:ALA:HB1	3:C:127:ASN:HB3	2.02	0.42
3:C:206:LYS:HE2	3:C:208:GLY:HA3	2.01	0.42
34:a:1252:A:H61	34:a:1285:A:H61	1.66	0.42
38:e:156:ARG:NH1	41:h:98:LEU:O	2.53	0.42
56:w:109:CYS:HB3	56:w:137:ILE:HG12	2.00	0.42
56:w:312:ARG:C	56:w:314:ARG:H	2.28	0.42
56:w:429:ARG:O	56:w:495:LEU:N	2.52	0.42
1:A:636:G:N7	12:L:109:LYS:NZ	2.56	0.42
1:A:2691:C:H2'	1:A:2692:G:C8	2.54	0.42
9:I:56:VAL:HG22	9:I:68:PHE:HB2	2.00	0.42
16:P:113:LEU:HD22	34:a:1442:G:O4'	2.19	0.42
34:a:999:C:H2'	34:a:1000:A:H8	1.84	0.42
37:d:37:PRO:HD2	37:d:41:GLY:HA3	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:d:105:GLY:HA3	37:d:161:ALA:HB2	2.01	0.42
52:s:62:THR:H	52:s:65:MET:HE3	1.85	0.42
1:A:4:U:H2'	1:A:5:A:H8	1.85	0.42
1:A:818:G:N2	1:A:1189:A:H62	2.14	0.42
1:A:1700:A:H3'	1:A:1701:A:H8	1.85	0.42
1:A:2630:G:H2'	1:A:2631:G:C8	2.55	0.42
9:I:89:SER:HB3	9:I:135:MET:HA	2.00	0.42
12:L:23:ILE:HD13	18:R:84:ARG:HH22	1.83	0.42
30:3:32:LEU:HD22	30:3:40:LYS:HG2	2.00	0.42
37:d:61:ARG:O	37:d:65:GLY:N	2.52	0.42
43:j:11:LYS:HA	43:j:70:HIS:O	2.19	0.42
56:w:428:PHE:HB2	56:w:437:ILE:HB	2.02	0.42
57:x:75:C:O2	57:x:75:C:C2'	2.68	0.42
1:A:244:A:N6	1:A:254:G:H21	2.05	0.42
1:A:414:C:H2'	1:A:415:A:H8	1.84	0.42
1:A:568:U:N3	1:A:571:U:OP2	2.46	0.42
1:A:788:A:OP1	1:A:791:C:N4	2.42	0.42
1:A:1665:A:H2'	1:A:1666:G:H8	1.84	0.42
1:A:2006:C:O2'	1:A:2823:A:N3	2.51	0.42
1:A:2061:G:H22	58:z:17:ARG:CB	2.32	0.42
1:A:2253:G:N2	57:x:75:C:O2	2.28	0.42
3:C:70:LYS:O	3:C:117:SER:OG	2.31	0.42
5:E:47:LYS:HB2	5:E:51:GLU:HB2	2.01	0.42
18:R:6:GLN:HE21	18:R:11:GLN:NE2	2.16	0.42
21:U:28:LEU:HD12	21:U:32:LYS:HB2	2.00	0.42
33:7:25:A:C6	57:x:37:U:N3	2.63	0.42
34:a:227:G:O2'	49:p:63:GLN:NE2	2.37	0.42
34:a:1405:G:O2'	34:a:1518:A:O2'	2.26	0.42
49:p:79:ASN:HB2	49:p:82:ALA:HB3	2.01	0.42
52:s:18:VAL:HG11	52:s:43:MET:HG2	2.01	0.42
55:v:211:ASP:N	55:v:211:ASP:OD1	2.47	0.42
1:A:849:A:H61	1:A:929:U:H3	1.68	0.42
1:A:2313:C:H2'	1:A:2314:A:C8	2.54	0.42
1:A:2836:U:H2'	1:A:2837:A:H8	1.85	0.42
34:a:358:U:O2'	56:w:310:LYS:O	2.23	0.42
34:a:458:U:H2'	34:a:459:A:C8	2.55	0.42
34:a:579:A:O2'	48:o:53:ARG:NH2	2.50	0.42
34:a:750:C:O2'	48:o:20:ASP:OD1	2.33	0.42
34:a:1236:A:H4'	34:a:1304:G:H4'	2.01	0.42
34:a:1507:A:H2'	34:a:1508:A:C8	2.54	0.42
49:p:40:ASN:HB3	49:p:43:ALA:HB2	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
56:w:314:ARG:NH1	56:w:418:GLN:HB3	2.35	0.42
1:A:2447:G:N2	1:A:2450:A:N7	2.67	0.42
1:A:2497:A:H1'	1:A:2498:C:H5	1.85	0.42
17:Q:88:GLU:O	18:R:11:GLN:NE2	2.53	0.42
34:a:1162:C:H2'	34:a:1163:A:H8	1.84	0.42
34:a:1241:G:H2'	34:a:1242:G:H8	1.84	0.42
34:a:1251:A:N3	34:a:1369:C:O2'	2.46	0.42
53:t:61:ALA:HA	53:t:66:ILE:HB	2.01	0.42
1:A:1251:C:O2'	1:A:1253:A:OP2	2.38	0.42
1:A:2131:U:H5'	1:A:2132:U:H5''	2.01	0.42
1:A:2240:U:H2'	1:A:2241:A:H8	1.84	0.42
1:A:2584:U:H4'	55:v:232:ALA:HA	2.01	0.42
2:B:114:C:H2'	2:B:115:A:C8	2.54	0.42
3:C:75:ALA:HB3	3:C:115:ILE:HG13	2.01	0.42
34:a:523:A:H61	45:l:88:ASP:HB2	1.85	0.42
34:a:948:C:H2'	34:a:949:A:H8	1.85	0.42
37:d:90:LEU:HD13	37:d:190:LEU:HD11	2.02	0.42
38:e:80:LEU:HD21	38:e:95:MET:HE2	2.02	0.42
40:g:110:ARG:HH12	40:g:121:ASN:HB3	1.84	0.42
45:l:36:VAL:HG21	45:l:73:LEU:HB3	2.02	0.42
56:w:144:LEU:HD13	56:w:148:ILE:HD12	2.01	0.42
1:A:1716:U:H2'	1:A:1717:A:H8	1.85	0.41
1:A:2801:G:H2'	1:A:2802:G:H8	1.85	0.41
2:B:44:G:H1'	2:B:47:C:H42	1.85	0.41
13:M:66:ARG:NH1	13:M:104:GLU:OE2	2.52	0.41
34:a:501:C:H1'	34:a:549:C:H1'	2.01	0.41
34:a:1175:G:H2'	34:a:1176:A:H8	1.85	0.41
34:a:1249:C:O2'	42:i:74:GLN:NE2	2.53	0.41
34:a:1354:U:H2'	34:a:1355:G:H8	1.85	0.41
35:b:71:THR:HG22	35:b:72:LYS:H	1.85	0.41
37:d:28:ASP:OD1	37:d:28:ASP:N	2.52	0.41
55:v:127:PHE:CE2	55:v:131:LEU:CD1	2.96	0.41
1:A:4:U:H2'	1:A:5:A:C8	2.55	0.41
1:A:406:G:H2'	1:A:407:G:H8	1.84	0.41
1:A:781:A:OP1	3:C:216:ARG:NH2	2.51	0.41
1:A:1431:A:H2'	1:A:1432:G:C8	2.55	0.41
1:A:2327:A:H2'	1:A:2328:A:C8	2.55	0.41
3:C:38:LYS:HE3	3:C:59:GLN:HG2	2.02	0.41
9:I:117:THR:HG22	32:5:42:ARG:HH21	1.85	0.41
14:N:45:ARG:HG2	14:N:95:THR:HG21	2.02	0.41
20:T:22:THR:HA	20:T:25:GLU:HG2	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:a:501:C:H2'	34:a:502:A:H8	1.84	0.41
34:a:578:C:O2'	34:a:728:A:N3	2.45	0.41
35:b:46:VAL:O	35:b:50:ASN:HB2	2.20	0.41
35:b:65:LYS:HD2	35:b:153:MET:HG3	2.02	0.41
46:m:49:GLU:HA	46:m:52:ILE:HB	2.02	0.41
55:v:127:PHE:HB3	55:v:201:CYS:HG	1.85	0.41
55:v:235:GLN:NE2	58:z:17:ARG:C	2.78	0.41
1:A:151:C:H2'	1:A:152:A:H8	1.86	0.41
1:A:476:G:N1	1:A:479:A:OP2	2.40	0.41
1:A:532:A:OP1	1:A:561:G:N2	2.43	0.41
1:A:533:G:O5'	17:Q:27:ARG:NH1	2.54	0.41
1:A:746:U:H1'	1:A:748:G:H21	1.85	0.41
1:A:1435:G:H2'	1:A:1436:G:C8	2.56	0.41
1:A:2821:A:OP2	4:D:115:GLY:N	2.51	0.41
34:a:77:A:H2'	34:a:78:A:C8	2.56	0.41
34:a:81:A:H2'	34:a:82:G:C8	2.55	0.41
34:a:1053:G:N2	34:a:1058:G:O6	2.53	0.41
55:v:229:SER:HB3	55:v:243:ALA:HB2	2.02	0.41
56:w:314:ARG:HH12	56:w:418:GLN:CA	2.33	0.41
56:w:347:THR:OG1	56:w:354:SER:OG	2.36	0.41
1:A:5:A:H2'	1:A:6:A:C8	2.55	0.41
1:A:693:A:O2'	1:A:1353:A:N3	2.53	0.41
1:A:1140:C:H5'	10:J:26:GLY:HA3	2.03	0.41
1:A:2023:C:H2'	1:A:2024:G:C8	2.55	0.41
1:A:2581:G:OP2	1:A:2581:G:N2	2.37	0.41
1:A:2781:A:H5''	1:A:2782:G:H5'	2.02	0.41
20:T:8:LEU:HD11	25:Y:22:LEU:HD12	2.01	0.41
38:e:155:LYS:HB3	41:h:70:VAL:HG13	2.01	0.41
1:A:742:A:H2'	1:A:743:A:C8	2.55	0.41
1:A:1024:G:OP2	1:A:1025:G:O2'	2.36	0.41
1:A:2863:C:H2'	1:A:2864:G:H8	1.86	0.41
6:F:91:ARG:HA	6:F:95:MET:HB3	2.03	0.41
34:a:10:A:OP2	38:e:130:THR:OG1	2.35	0.41
34:a:320:A:H2'	34:a:321:A:C8	2.55	0.41
34:a:411:A:O2'	34:a:413:G:OP2	2.34	0.41
55:v:311:ASN:HB2	55:v:316:ARG:HB2	2.02	0.41
1:A:453:A:N3	1:A:457:A:O2'	2.51	0.41
1:A:545:U:N3	1:A:548:G:N1	2.45	0.41
1:A:2140:G:H2'	1:A:2141:G:H8	1.85	0.41
1:A:2215:C:H2'	1:A:2216:G:C8	2.56	0.41
1:A:2329:U:H2'	1:A:2330:G:C8	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:a:782:A:H62	34:a:800:G:H21	1.68	0.41
56:w:297:THR:HB	56:w:387:PHE:HZ	1.86	0.41
1:A:572:A:H61	1:A:2029:G:H21	1.69	0.41
1:A:1433:A:H2'	1:A:1434:A:C8	2.55	0.41
1:A:1592:C:H2'	1:A:1593:A:H8	1.85	0.41
1:A:1858:A:N6	1:A:1884:G:O2'	2.48	0.41
20:T:58:VAL:HG22	20:T:85:VAL:HG13	2.02	0.41
22:V:72:VAL:HB	22:V:91:PHE:HB3	2.01	0.41
23:W:61:GLY:CA	23:W:79:GLU:O	2.66	0.41
33:7:27:G:C5	34:a:1400:C:H5'	2.56	0.41
34:a:405:U:OP2	37:d:2:ARG:NH1	2.52	0.41
34:a:974:A:OP1	47:n:69:ARG:NH2	2.54	0.41
1:A:1433:A:H2'	1:A:1434:A:H8	1.86	0.41
1:A:1744:A:H3'	1:A:1745:A:H8	1.86	0.41
1:A:2036:C:H2'	1:A:2037:A:C8	2.56	0.41
9:I:53:PRO:HG2	9:I:77:VAL:HG11	2.02	0.41
13:M:47:GLU:OE2	13:M:51:ARG:NE	2.54	0.41
34:a:345:C:O2'	34:a:346:G:N2	2.53	0.41
34:a:437:U:HO2'	37:d:119:HIS:HD1	1.67	0.41
42:i:115:VAL:HG21	43:j:62:ARG:HB2	2.01	0.41
55:v:134:MET:SD	55:v:332:VAL:O	2.79	0.41
55:v:224:ILE:CD1	55:v:267:LYS:NZ	2.67	0.41
56:w:19:ILE:HD12	56:w:126:LEU:HB3	2.03	0.41
56:w:32:LYS:HG3	56:w:35:LEU:HD12	2.02	0.41
1:A:112:U:H5'	25:Y:58:ASN:HD21	1.85	0.41
1:A:414:C:H2'	1:A:415:A:C8	2.56	0.41
1:A:521:U:H2'	1:A:522:A:H8	1.85	0.41
1:A:728:G:H4'	3:C:12:ARG:HD3	2.02	0.41
1:A:832:U:H2'	1:A:833:A:C8	2.55	0.41
1:A:974:G:H1'	1:A:975:A:C8	2.56	0.41
1:A:1227:G:OP2	17:Q:15:LYS:NZ	2.50	0.41
1:A:1372:U:O2'	1:A:2212:A:N3	2.48	0.41
1:A:1939:U:H5''	1:A:2604:U:C5	2.56	0.41
1:A:2110:G:N1	1:A:2120:G:N7	2.69	0.41
1:A:2692:G:H2'	1:A:2693:G:C8	2.56	0.41
2:B:45:A:O4'	6:F:91:ARG:NH2	2.54	0.41
5:E:149:ILE:HD11	5:E:172:ALA:HA	2.03	0.41
7:G:23:ILE:HG21	7:G:71:LEU:HD21	2.03	0.41
14:N:42:LYS:HA	14:N:45:ARG:HE	1.86	0.41
16:P:29:VAL:HG22	16:P:80:VAL:HG12	2.01	0.41
20:T:37:ASP:O	20:T:81:LYS:NZ	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:0:39:ARG:O	27:0:41:HIS:ND1	2.54	0.41
28:1:36:LYS:HG3	28:1:47:ILE:HG13	2.02	0.41
32:5:18:VAL:HA	32:5:86:MET:HE2	2.01	0.41
34:a:746:A:H2'	34:a:747:A:C8	2.56	0.41
34:a:875:U:O2	41:h:11:THR:OG1	2.39	0.41
34:a:1355:G:H2'	34:a:1356:G:H8	1.85	0.41
34:a:1491:G:H3'	34:a:1492:A:C5'	2.48	0.41
35:b:17:HIS:HE2	35:b:204:ASP:CG	2.26	0.41
55:v:142:ARG:HH11	55:v:174:ARG:HD3	1.79	0.41
55:v:235:GLN:HE22	58:z:17:ARG:C	2.29	0.41
55:v:329:LEU:HD23	55:v:329:LEU:HA	1.92	0.41
57:x:53:G:H2'	57:x:54:G:H8	1.86	0.41
1:A:318:C:H2'	1:A:319:G:C8	2.54	0.41
1:A:690:G:H21	3:C:42:ARG:HH12	1.69	0.41
1:A:953:G:H2'	1:A:954:G:H8	1.86	0.41
1:A:994:C:OP1	17:Q:52:ARG:NH2	2.54	0.41
1:A:1030:C:H2'	1:A:1031:G:C8	2.56	0.41
1:A:1158:C:H5''	26:Z:30:ARG:HD2	2.03	0.41
1:A:1827:U:OP2	3:C:220:ARG:NH1	2.53	0.41
2:B:14:U:OP2	2:B:70:C:O2'	2.38	0.41
5:E:106:LYS:HG3	5:E:200:LEU:HD23	2.03	0.41
11:K:103:VAL:HG21	11:K:116:ILE:HG22	2.03	0.41
34:a:375:U:H5''	49:p:70:ARG:HG3	2.02	0.41
34:a:952:U:H2'	34:a:953:G:H8	1.86	0.41
34:a:980:C:O3'	47:n:12:ARG:NH2	2.53	0.41
34:a:1355:G:H2'	34:a:1356:G:C8	2.56	0.41
37:d:87:GLU:HG3	37:d:187:ARG:HB2	2.01	0.41
41:h:104:SER:HB2	41:h:125:ILE:HD11	2.02	0.41
44:k:95:THR:O	44:k:98:ALA:HB3	2.21	0.41
55:v:322:ILE:HD13	55:v:343:PRO:C	2.46	0.41
57:x:71:G:H2'	57:x:72:C:H5''	2.01	0.41
57:x:72:C:C2'	57:x:73:A:H5'	2.51	0.41
1:A:225:C:N3	1:A:231:A:N6	2.69	0.40
1:A:1202:G:O6	1:A:1244:A:N6	2.53	0.40
1:A:1313:U:H4'	1:A:1332:G:H4'	2.03	0.40
1:A:1662:U:O2'	1:A:2687:U:OP1	2.39	0.40
1:A:2632:A:H2'	1:A:2633:G:C8	2.56	0.40
34:a:227:G:N2	49:p:63:GLN:O	2.50	0.40
34:a:375:U:O2	49:p:28:ARG:NH2	2.50	0.40
34:a:1071:C:H2'	34:a:1072:G:C8	2.56	0.40
34:a:1328:C:OP1	46:m:27:THR:OG1	2.37	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:a:1342:C:H2'	34:a:1343:G:C8	2.55	0.40
39:f:26:THR:HA	39:f:29:ILE:HB	2.03	0.40
55:v:292:SER:O	55:v:296:ASN:ND2	2.54	0.40
1:A:471:A:OP1	5:E:79:ARG:NH1	2.49	0.40
1:A:523:C:H2'	1:A:524:G:C8	2.56	0.40
1:A:576:U:H2'	1:A:577:G:H8	1.87	0.40
1:A:1745:A:H2'	1:A:1746:A:H8	1.86	0.40
1:A:2863:C:H2'	1:A:2864:G:C8	2.56	0.40
2:B:78:A:N6	2:B:98:G:H21	2.14	0.40
15:O:69:ASP:OD1	15:O:69:ASP:N	2.50	0.40
37:d:184:LYS:HA	37:d:185:PRO:HD3	1.95	0.40
41:h:52:GLY:HA3	41:h:56:PRO:HA	2.03	0.40
41:h:73:SER:OG	41:h:75:GLN:NE2	2.54	0.40
43:j:65:TYR:OH	47:n:89:MET:SD	2.71	0.40
55:v:322:ILE:CD1	55:v:344:ILE:N	2.84	0.40
56:w:94:ASP:HB3	56:w:442:GLY:HA3	2.03	0.40
1:A:434:U:O2'	1:A:436:C:N4	2.55	0.40
1:A:598:U:H2'	1:A:599:A:C8	2.56	0.40
1:A:1787:A:OP1	3:C:237:ARG:NH2	2.55	0.40
10:J:45:THR:HB	10:J:48:VAL:HB	2.03	0.40
34:a:458:U:H2'	34:a:459:A:H8	1.85	0.40
34:a:709:U:H2'	34:a:710:G:C8	2.55	0.40
34:a:999:C:H2'	34:a:1000:A:C8	2.57	0.40
55:v:138:TYR:CD1	55:v:337:LEU:HB2	2.56	0.40
55:v:142:ARG:HB2	55:v:144:TRP:NE1	2.36	0.40
55:v:142:ARG:O	55:v:143:ARG:HB2	2.20	0.40
1:A:341:C:H2'	1:A:342:A:C8	2.57	0.40
1:A:910:A:H62	13:M:12:MET:HA	1.86	0.40
1:A:1675:C:O2	4:D:133:THR:OG1	2.37	0.40
1:A:2250:G:O2'	1:A:2496:C:OP1	2.26	0.40
8:H:113:SER:O	8:H:116:ARG:NH1	2.48	0.40
11:K:21:CYS:HA	11:K:41:ILE:HG22	2.02	0.40
12:L:96:LYS:HE3	12:L:103:ILE:HA	2.04	0.40
34:a:147:G:H2'	34:a:148:G:C8	2.55	0.40
34:a:932:C:OP1	40:g:3:ARG:NE	2.53	0.40
34:a:1147:C:H2'	34:a:1148:U:H6	1.86	0.40
34:a:1512:U:H2'	34:a:1513:A:C8	2.56	0.40
35:b:31:PHE:HE2	35:b:41:ASN:HB2	1.86	0.40
41:h:1:SER:H2	41:h:3:GLN:HG2	1.86	0.40
44:k:35:ASP:OD1	44:k:38:GLY:N	2.55	0.40
56:w:21:HIS:ND1	56:w:22:PRO:O	2.55	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:305:C:H2'	1:A:306:U:C6	2.57	0.40
1:A:881:G:H2'	1:A:882:G:C8	2.56	0.40
1:A:1704:C:H2'	1:A:1705:A:C8	2.57	0.40
1:A:2289:G:H2'	1:A:2290:G:H8	1.86	0.40
1:A:2508:G:P	55:v:228:ARG:HH12	2.44	0.40
4:D:47:ALA:HB2	4:D:83:ARG:HD2	2.02	0.40
34:a:21:G:H2'	34:a:22:G:C8	2.56	0.40
34:a:641:U:H4'	34:a:642:A:H8	1.86	0.40
44:k:111:ASP:O	51:r:72:ARG:NH2	2.54	0.40
52:s:62:THR:HG22	52:s:63:ASP:H	1.87	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%)	261 (97%)	8 (3%)	0	100	100
4	D	207/209 (99%)	194 (94%)	13 (6%)	0	100	100
5	E	199/201 (99%)	188 (94%)	11 (6%)	0	100	100
6	F	175/177 (99%)	161 (92%)	14 (8%)	0	100	100
7	G	174/176 (99%)	161 (92%)	10 (6%)	3 (2%)	7	35
8	H	147/149 (99%)	138 (94%)	9 (6%)	0	100	100
9	I	139/141 (99%)	121 (87%)	18 (13%)	0	100	100
10	J	140/142 (99%)	137 (98%)	3 (2%)	0	100	100
11	K	120/122 (98%)	107 (89%)	13 (11%)	0	100	100
12	L	141/143 (99%)	124 (88%)	16 (11%)	1 (1%)	18	53
13	M	134/136 (98%)	124 (92%)	8 (6%)	2 (2%)	8	37
14	N	118/120 (98%)	110 (93%)	8 (7%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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%)	100 (93%)	7 (6%)	1 (1%)	14	47
20	T	91/93 (98%)	82 (90%)	9 (10%)	0	100	100
21	U	100/102 (98%)	89 (89%)	10 (10%)	1 (1%)	12	45
22	V	92/94 (98%)	91 (99%)	1 (1%)	0	100	100
23	W	73/75 (97%)	69 (94%)	4 (6%)	0	100	100
24	X	75/77 (97%)	72 (96%)	3 (4%)	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%)	56 (90%)	4 (6%)	2 (3%)	3	25
31	4	36/38 (95%)	31 (86%)	5 (14%)	0	100	100
32	5	129/131 (98%)	102 (79%)	27 (21%)	0	100	100
35	b	216/218 (99%)	196 (91%)	19 (9%)	1 (0%)	24	59
36	c	204/206 (99%)	196 (96%)	6 (3%)	2 (1%)	12	45
37	d	203/205 (99%)	183 (90%)	20 (10%)	0	100	100
38	e	155/157 (99%)	137 (88%)	15 (10%)	3 (2%)	6	33
39	f	98/100 (98%)	81 (83%)	15 (15%)	2 (2%)	6	32
40	g	149/151 (99%)	136 (91%)	13 (9%)	0	100	100
41	h	127/129 (98%)	122 (96%)	5 (4%)	0	100	100
42	i	125/127 (98%)	109 (87%)	15 (12%)	1 (1%)	16	50
43	j	96/98 (98%)	81 (84%)	15 (16%)	0	100	100
44	k	114/116 (98%)	103 (90%)	11 (10%)	0	100	100
45	l	121/123 (98%)	97 (80%)	23 (19%)	1 (1%)	16	50
46	m	112/114 (98%)	99 (88%)	13 (12%)	0	100	100
47	n	99/101 (98%)	89 (90%)	10 (10%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
48	o	86/88 (98%)	77 (90%)	9 (10%)	0	100	100
49	p	80/82 (98%)	73 (91%)	7 (9%)	0	100	100
50	q	78/80 (98%)	66 (85%)	11 (14%)	1 (1%)	9	40
51	r	63/65 (97%)	59 (94%)	4 (6%)	0	100	100
52	s	77/79 (98%)	74 (96%)	3 (4%)	0	100	100
53	t	83/85 (98%)	79 (95%)	4 (5%)	0	100	100
54	u	63/65 (97%)	51 (81%)	11 (18%)	1 (2%)	7	36
55	v	346/350 (99%)	322 (93%)	21 (6%)	3 (1%)	14	47
56	w	492/529 (93%)	429 (87%)	55 (11%)	8 (2%)	7	36
58	z	12/14 (86%)	11 (92%)	0	1 (8%)	0	10
All	All	6633/6776 (98%)	6065 (91%)	534 (8%)	34 (0%)	26	59

All (34) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
7	G	46	ASP
13	M	58	LYS
30	3	31	ILE
36	c	96	VAL
50	q	69	THR
56	w	315	VAL
56	w	395	PRO
56	w	400	ARG
56	w	472	ARG
56	w	503	TYR
7	G	47	ASN
30	3	32	LEU
38	e	122	VAL
39	f	53	LYS
45	l	102	ASP
55	v	120	GLY
55	v	323	ASN
56	w	392	ASN
21	U	89	GLY
39	f	55	HIS
54	u	37	TYR
56	w	18	ILE
55	v	72	PRO

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Mol	Chain	Res	Type
12	L	128	THR
13	M	59	ARG
19	S	64	ALA
36	c	97	PRO
38	e	121	ASN
56	w	77	PHE
7	G	174	LYS
35	b	17	HIS
42	i	90	ASP
58	z	16	PRO
38	e	97	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	75
13	M	109/109 (100%)	108 (99%)	1 (1%)	70	75
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
17	Q	89/89 (100%)	89 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
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
35	b	180/180 (100%)	180 (100%)	0	100	100
36	c	170/170 (100%)	170 (100%)	0	100	100
37	d	172/172 (100%)	172 (100%)	0	100	100
38	e	114/119 (96%)	114 (100%)	0	100	100
39	f	87/87 (100%)	87 (100%)	0	100	100
40	g	124/124 (100%)	124 (100%)	0	100	100
41	h	104/104 (100%)	104 (100%)	0	100	100
42	i	105/105 (100%)	105 (100%)	0	100	100
43	j	86/86 (100%)	86 (100%)	0	100	100
44	k	89/89 (100%)	89 (100%)	0	100	100
45	l	103/103 (100%)	103 (100%)	0	100	100
46	m	92/92 (100%)	92 (100%)	0	100	100
47	n	79/83 (95%)	79 (100%)	0	100	100
48	o	76/76 (100%)	76 (100%)	0	100	100
49	p	65/65 (100%)	65 (100%)	0	100	100
50	q	74/74 (100%)	74 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
51	r	48/56 (86%)	48 (100%)	0	100	100
52	s	70/70 (100%)	69 (99%)	1 (1%)	59	71
53	t	65/65 (100%)	65 (100%)	0	100	100
54	u	44/55 (80%)	44 (100%)	0	100	100
55	v	203/292 (70%)	200 (98%)	3 (2%)	57	70
56	w	426/453 (94%)	423 (99%)	3 (1%)	76	78
58	z	14/14 (100%)	14 (100%)	0	100	100
All	All	5407/5551 (97%)	5398 (100%)	9 (0%)	85	87

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

Mol	Chain	Res	Type
12	L	110	VAL
13	M	46	ILE
52	s	10	ILE
55	v	214	LEU
55	v	236	HIS
55	v	238	ASN
56	w	71	THR
56	w	320	VAL
56	w	504	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (91) such sidechains are listed below:

Mol	Chain	Res	Type
3	C	36	ASN
3	C	43	ASN
3	C	45	ASN
3	C	52	HIS
3	C	85	ASN
3	C	114	GLN
3	C	199	HIS
3	C	250	GLN
4	D	164	GLN
5	E	136	GLN
7	G	63	GLN
7	G	103	ASN
7	G	127	GLN

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Mol	Chain	Res	Type
7	G	138	GLN
8	H	33	GLN
10	J	58	ASN
10	J	135	GLN
11	K	5	GLN
12	L	38	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	71	ASN
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	9	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
32	5	4	ASN
35	b	23	ASN
35	b	35	ASN
35	b	169	HIS
37	d	35	GLN
37	d	39	GLN
37	d	115	GLN
38	e	69	ASN
38	e	120	HIS
39	f	11	HIS
39	f	58	HIS
41	h	3	GLN
41	h	66	GLN
41	h	75	GLN
42	i	4	GLN

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Mol	Chain	Res	Type
42	i	30	ASN
42	i	36	GLN
42	i	74	GLN
43	j	58	ASN
43	j	70	HIS
44	k	100	ASN
44	k	117	HIS
45	l	45	ASN
47	n	49	GLN
48	o	45	HIS
49	p	9	HIS
49	p	18	GLN
49	p	29	ASN
50	q	8	GLN
50	q	30	HIS
50	q	44	HIS
51	r	51	GLN
52	s	55	GLN
53	t	2	ASN
53	t	47	GLN
55	v	156	HIS
55	v	197	HIS
55	v	235	GLN
55	v	236	HIS
55	v	263	GLN
55	v	296	ASN
56	w	184	HIS
56	w	202	GLN
56	w	311	HIS
56	w	418	GLN
56	w	434	ASN
56	w	445	GLN
56	w	492	GLN
56	w	510	ASN
56	w	524	HIS
58	z	15	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	2893/2903 (99%)	533 (18%)	30 (1%)

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	B	119/120 (99%)	14 (11%)	2 (1%)
33	7	6/7 (85%)	5 (83%)	0
34	a	1538/1539 (99%)	219 (14%)	0
57	x	76/77 (98%)	21 (27%)	0
All	All	4632/4646 (99%)	792 (17%)	32 (0%)

All (792) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	12	U
1	A	14	A
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	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	188	G
1	A	196	A

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Mol	Chain	Res	Type
1	A	199	A
1	A	205	G
1	A	206	U
1	A	215	G
1	A	216	A
1	A	218	A
1	A	219	A
1	A	221	A
1	A	222	A
1	A	223	A
1	A	242	G
1	A	243	U
1	A	248	G
1	A	249	C
1	A	250	G
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	367	G
1	A	371	A
1	A	372	G
1	A	373	U
1	A	386	G
1	A	387	U
1	A	404	A
1	A	406	G
1	A	411	G
1	A	417	C
1	A	421	C

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Mol	Chain	Res	Type
1	A	424	G
1	A	451	U
1	A	455	C
1	A	456	C
1	A	457	A
1	A	458	G
1	A	459	U
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	528	A
1	A	529	A
1	A	530	G
1	A	532	A
1	A	533	G
1	A	543	G
1	A	544	C
1	A	545	U
1	A	547	A
1	A	548	G
1	A	550	C
1	A	555	G
1	A	563	A
1	A	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

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Mol	Chain	Res	Type
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	704	G
1	A	711	G
1	A	717	C
1	A	726	G
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	800	A
1	A	805	G
1	A	811	U
1	A	812	C
1	A	819	A
1	A	822	G
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

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Mol	Chain	Res	Type
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	898	C
1	A	904	G
1	A	907	G
1	A	910	A
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	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	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

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Mol	Chain	Res	Type
1	A	1066	U
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
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	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

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Mol	Chain	Res	Type
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	1315	C
1	A	1321	A
1	A	1325	U
1	A	1329	U
1	A	1330	C
1	A	1341	G
1	A	1345	C
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

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Mol	Chain	Res	Type
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
1	A	1610	A
1	A	1611	C
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	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

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Mol	Chain	Res	Type
1	A	1829	A
1	A	1833	C
1	A	1835	G
1	A	1847	G
1	A	1848	A
1	A	1870	C
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	1915	U
1	A	1917	U
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	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

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Mol	Chain	Res	Type
1	A	2050	C
1	A	2052	A
1	A	2055	C
1	A	2056	G
1	A	2060	A
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	2096	C
1	A	2100	G
1	A	2108	A
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	2178	C
1	A	2189	U
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

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Mol	Chain	Res	Type
1	A	2238	G
1	A	2239	G
1	A	2249	U
1	A	2250	G
1	A	2251	G
1	A	2279	G
1	A	2283	C
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	2427	C
1	A	2428	G
1	A	2429	G
1	A	2430	A
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	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	2506	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	2605	U
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	2673	G
1	A	2682	A
1	A	2689	U
1	A	2690	U
1	A	2712	C

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Mol	Chain	Res	Type
1	A	2713	U
1	A	2714	G
1	A	2716	C
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	2751	G
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

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Mol	Chain	Res	Type
2	B	41	G
2	B	44	G
2	B	45	A
2	B	53	A
2	B	67	G
2	B	89	U
2	B	90	C
2	B	91	C
2	B	108	A
2	B	109	A
33	7	27	G
33	7	28	U
33	7	29	A
33	7	30	A
33	7	31	A
34	a	7	A
34	a	9	G
34	a	22	G
34	a	32	A
34	a	39	G
34	a	47	C
34	a	48	C
34	a	49	U
34	a	51	A
34	a	71	A
34	a	81	A
34	a	86	G
34	a	94	G
34	a	95	C
34	a	121	U
34	a	130	A
34	a	163	C
34	a	173	U
34	a	174	A
34	a	177	G
34	a	181	A
34	a	183	C
34	a	184	G
34	a	197	A
34	a	209	U
34	a	210	C
34	a	211	G

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Mol	Chain	Res	Type
34	a	212	G
34	a	226	G
34	a	240	G
34	a	247	G
34	a	251	G
34	a	266	G
34	a	267	C
34	a	269	C
34	a	279	A
34	a	280	C
34	a	281	G
34	a	283	U
34	a	289	G
34	a	306	A
34	a	328	C
34	a	344	A
34	a	345	C
34	a	346	G
34	a	347	G
34	a	351	G
34	a	352	C
34	a	354	G
34	a	356	A
34	a	367	U
34	a	372	C
34	a	388	G
34	a	392	C
34	a	397	A
34	a	406	G
34	a	411	A
34	a	413	G
34	a	421	U
34	a	422	C
34	a	424	G
34	a	429	U
34	a	439	U
34	a	467	U
34	a	479	U
34	a	482	A
34	a	484	G
34	a	486	U
34	a	496	A

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Mol	Chain	Res	Type
34	a	497	G
34	a	509	A
34	a	510	A
34	a	511	C
34	a	516	U
34	a	518	C
34	a	519	C
34	a	521	G
34	a	527	G
34	a	531	U
34	a	532	A
34	a	536	C
34	a	547	A
34	a	560	A
34	a	561	U
34	a	564	C
34	a	572	A
34	a	573	A
34	a	574	A
34	a	575	G
34	a	576	C
34	a	577	G
34	a	596	A
34	a	633	G
34	a	665	A
34	a	688	G
34	a	702	A
34	a	703	G
34	a	713	G
34	a	724	G
34	a	731	G
34	a	733	G
34	a	748	G
34	a	755	G
34	a	777	A
34	a	814	A
34	a	815	A
34	a	817	C
34	a	818	G
34	a	819	A
34	a	820	U
34	a	821	G

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Mol	Chain	Res	Type
34	a	829	G
34	a	832	G
34	a	843	U
34	a	844	G
34	a	846	G
34	a	871	U
34	a	873	A
34	a	876	C
34	a	889	A
34	a	890	G
34	a	902	G
34	a	934	C
34	a	935	A
34	a	960	U
34	a	961	U
34	a	966	G
34	a	969	A
34	a	971	G
34	a	975	A
34	a	976	G
34	a	977	A
34	a	992	U
34	a	993	G
34	a	1004	A
34	a	1026	G
34	a	1028	C
34	a	1030	U
34	a	1031	C
34	a	1033	G
34	a	1034	G
34	a	1035	A
34	a	1056	U
34	a	1064	G
34	a	1065	U
34	a	1085	U
34	a	1094	G
34	a	1101	A
34	a	1108	G
34	a	1130	A
34	a	1136	C
34	a	1137	C
34	a	1138	G

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Mol	Chain	Res	Type
34	a	1139	G
34	a	1152	A
34	a	1158	C
34	a	1159	U
34	a	1168	U
34	a	1183	U
34	a	1184	G
34	a	1191	A
34	a	1196	A
34	a	1197	A
34	a	1201	A
34	a	1202	U
34	a	1212	U
34	a	1213	A
34	a	1225	A
34	a	1227	A
34	a	1238	A
34	a	1240	U
34	a	1241	G
34	a	1253	G
34	a	1256	A
34	a	1258	G
34	a	1260	G
34	a	1278	G
34	a	1280	A
34	a	1281	C
34	a	1282	C
34	a	1287	A
34	a	1290	G
34	a	1298	U
34	a	1300	G
34	a	1301	U
34	a	1312	G
34	a	1317	C
34	a	1320	C
34	a	1340	A
34	a	1346	A
34	a	1347	G
34	a	1348	U
34	a	1363	A
34	a	1378	C
34	a	1395	C

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Mol	Chain	Res	Type
34	a	1397	C
34	a	1398	A
34	a	1400	C
34	a	1401	G
34	a	1433	A
34	a	1446	A
34	a	1448	C
34	a	1451	U
34	a	1452	C
34	a	1492	A
34	a	1493	A
34	a	1494	G
34	a	1495	U
34	a	1499	A
34	a	1502	A
34	a	1503	A
34	a	1517	G
34	a	1520	C
34	a	1529	G
34	a	1530	G
34	a	1533	C
34	a	1534	A
34	a	1535	C
34	a	1536	C
57	x	8	U
57	x	9	G
57	x	13	C
57	x	14	A
57	x	19	G
57	x	20	G
57	x	21	U
57	x	22	A
57	x	26	C
57	x	47	G
57	x	49	C
57	x	58	A
57	x	59	A
57	x	61	U
57	x	68	C
57	x	69	C
57	x	71	G
57	x	72	C

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Mol	Chain	Res	Type
57	x	73	A
57	x	74	A
57	x	76	C

All (32) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	51	G
1	A	242	G
1	A	372	G
1	A	479	A
1	A	490	C
1	A	710	U
1	A	752	A
1	A	858	G
1	A	859	G
1	A	897	C
1	A	1020	A
1	A	1022	G
1	A	1070	A
1	A	1111	A
1	A	1130	U
1	A	1182	G
1	A	1190	G
1	A	1300	G
1	A	1378	A
1	A	1399	C
1	A	1432	G
1	A	1491	G
1	A	1940	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	$\# Z > 2$
59	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
59	GCP	w	601	-	-	6/19/38/38	0/3/3/3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
59	w	601	GCP	PB-O3A	5.61	1.64	1.58
59	w	601	GCP	PB-O2B	-2.14	1.51	1.56

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
59	w	601	GCP	PB-O3A-PA	-2.46	124.35	132.37

There are no chirality outliers.

All (6) torsion outliers are listed below:

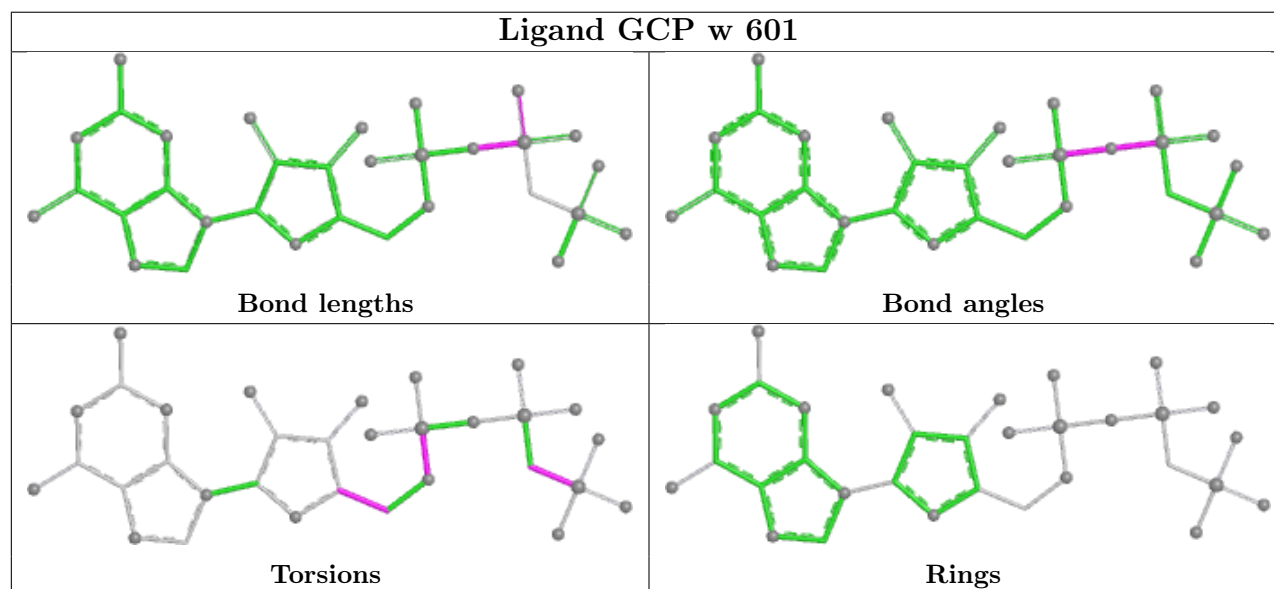
Mol	Chain	Res	Type	Atoms
59	w	601	GCP	C5'-O5'-PA-O3A
59	w	601	GCP	C5'-O5'-PA-O2A
59	w	601	GCP	O4'-C4'-C5'-O5'
59	w	601	GCP	C3'-C4'-C5'-O5'
59	w	601	GCP	C5'-O5'-PA-O1A
59	w	601	GCP	PB-C3B-PG-O1G

There are no ring outliers.

1 monomer is involved in 18 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
59	w	601	GCP	18	0

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



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

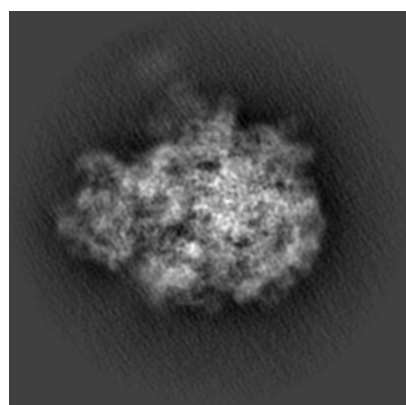
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-0081. These allow visual inspection of the internal detail of the map and identification of artifacts.

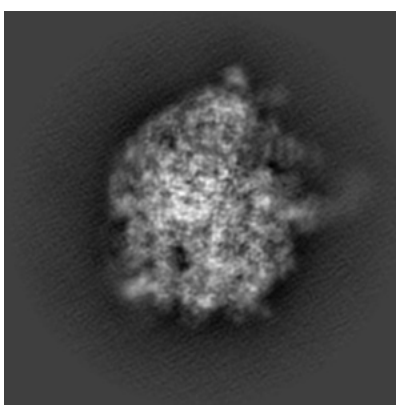
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

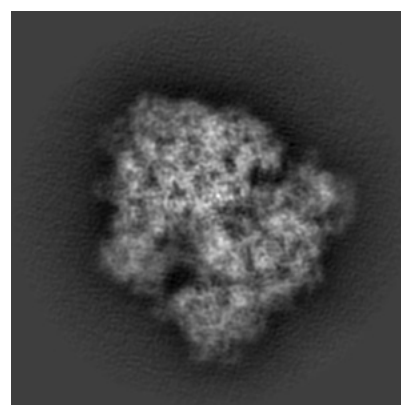
6.1.1 Primary map



X



Y

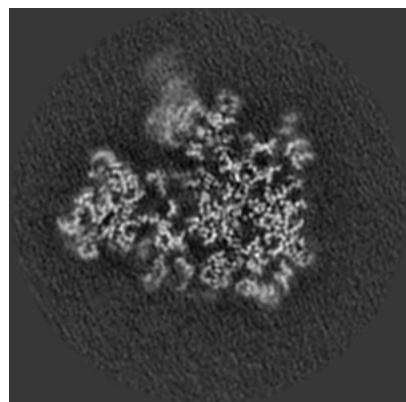


Z

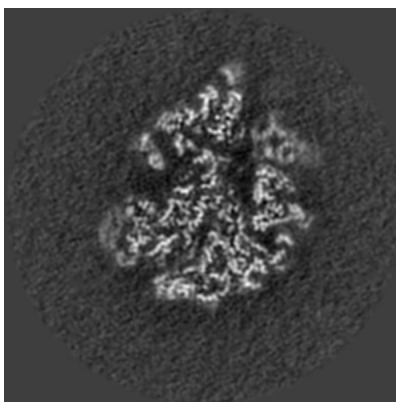
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

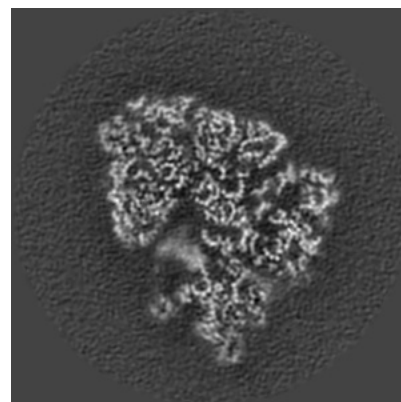
6.2.1 Primary map



X Index: 180



Y Index: 180

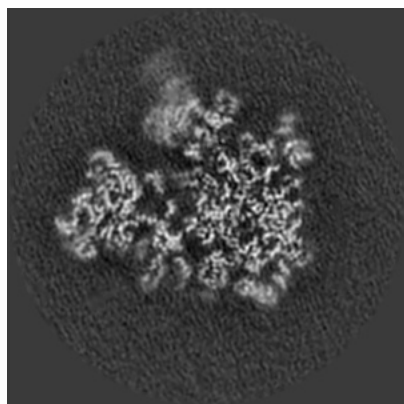


Z Index: 180

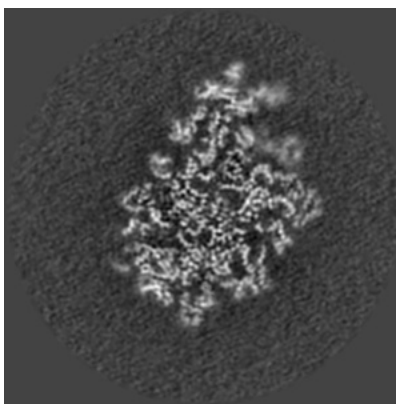
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

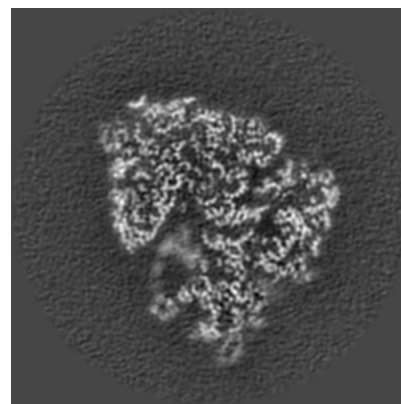
6.3.1 Primary map



X Index: 179



Y Index: 195

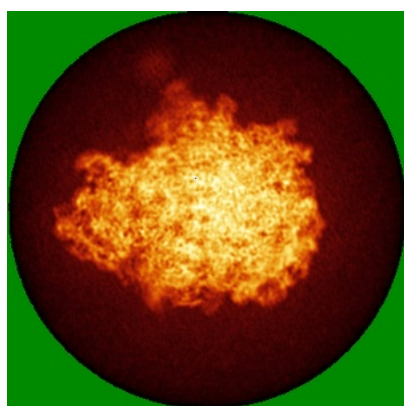


Z Index: 183

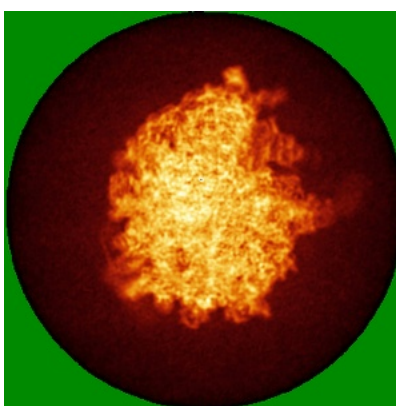
The images above show the largest variance slices of the map in three orthogonal directions.

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

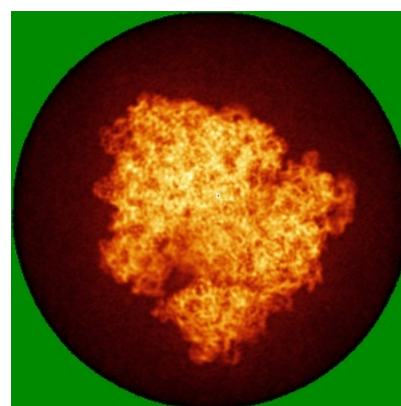
6.4.1 Primary map



X



Y

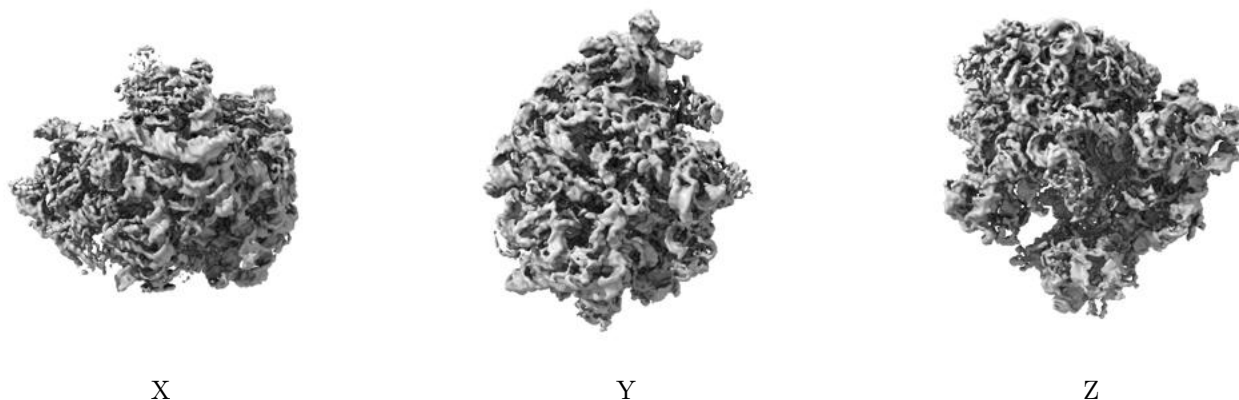


Z

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.

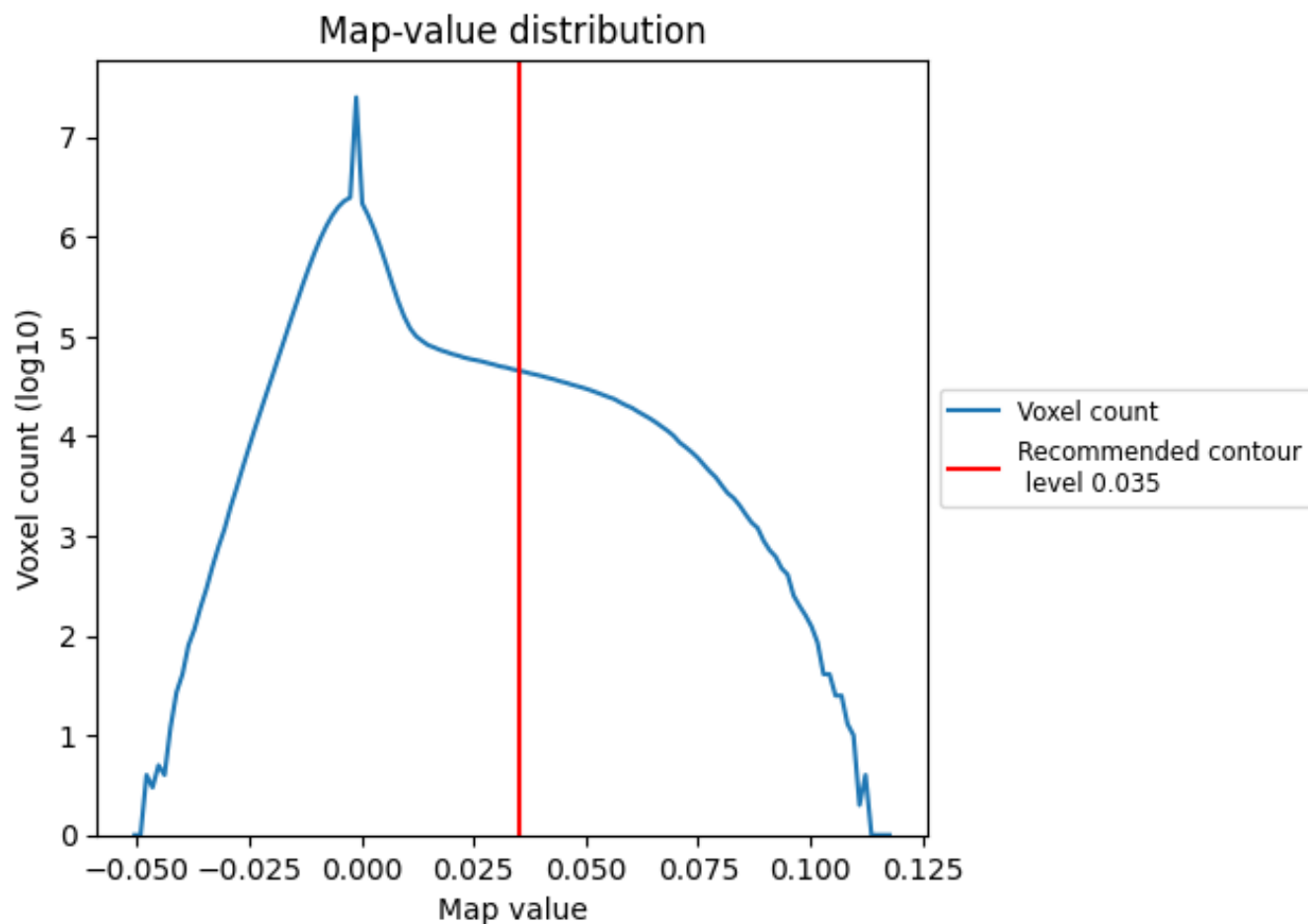
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

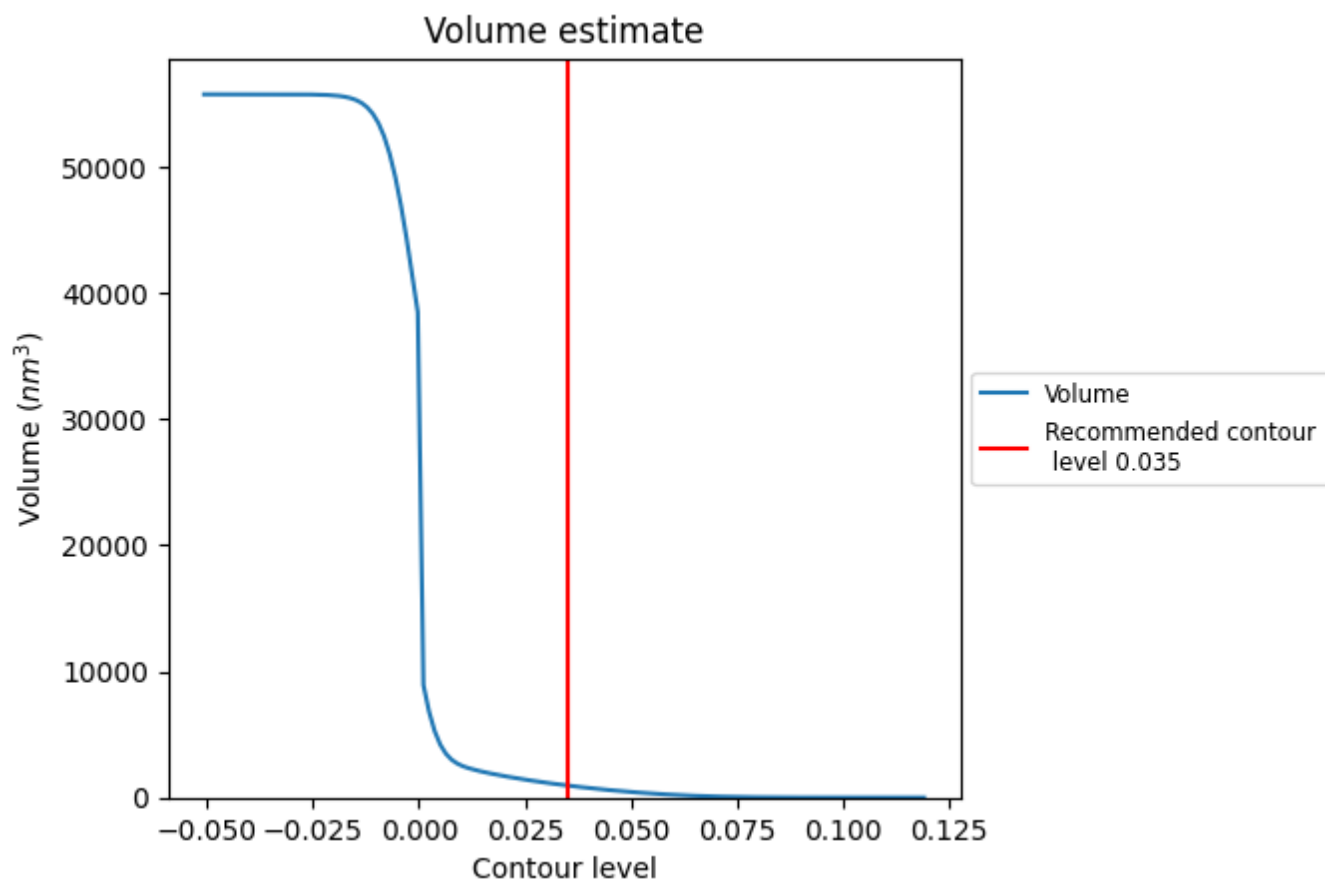
This section contains the results of statistical analysis of the map.

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.

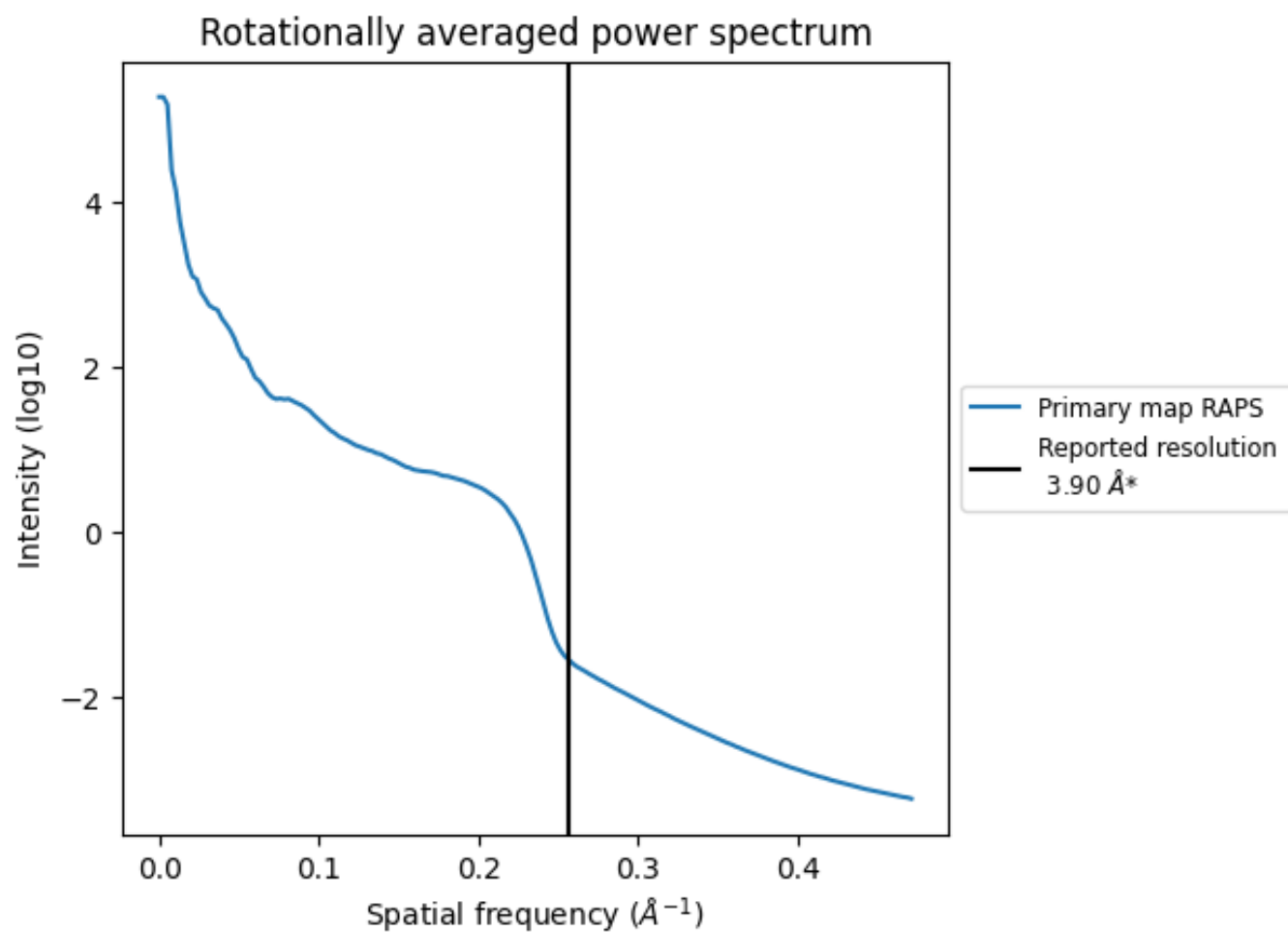
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 954 nm³; this corresponds to an approximate mass of 862 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ



*Reported resolution corresponds to spatial frequency of 0.256 Å⁻¹

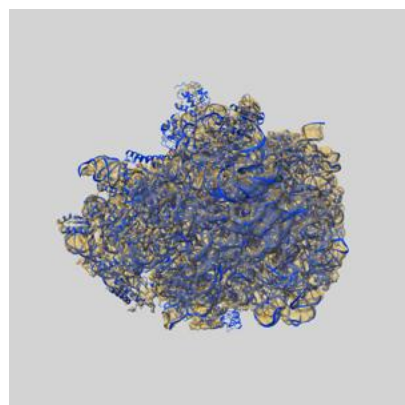
8 Fourier-Shell correlation

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

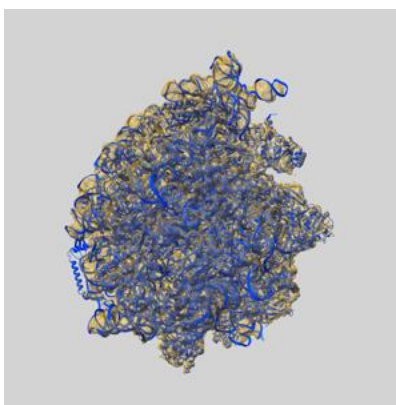
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-0081 and PDB model 6GXN. Per-residue inclusion information can be found in [section 3](#) on [page 16](#).

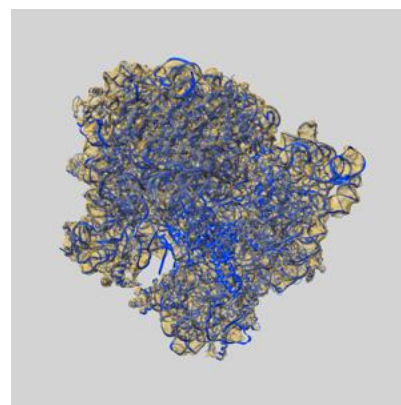
9.1 Map-model overlay [i](#)



X



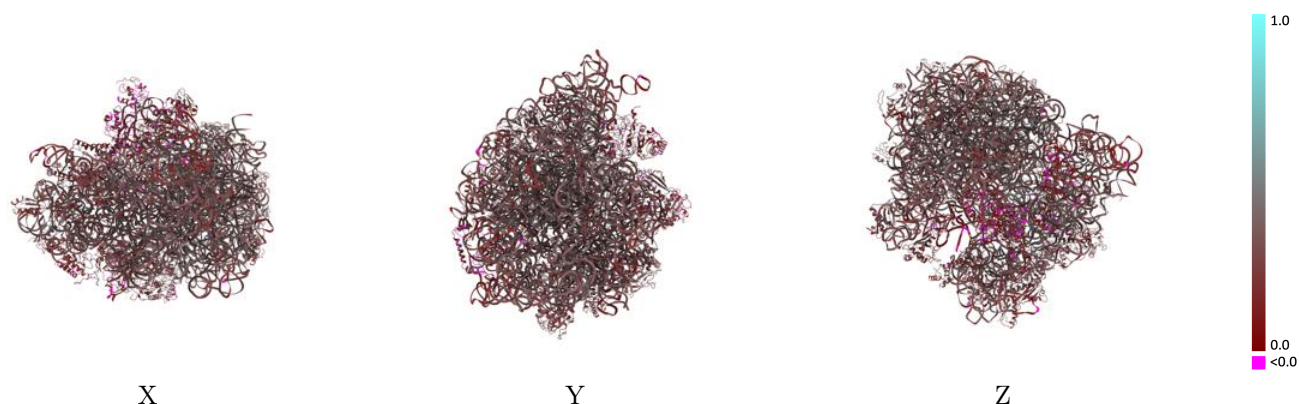
Y



Z

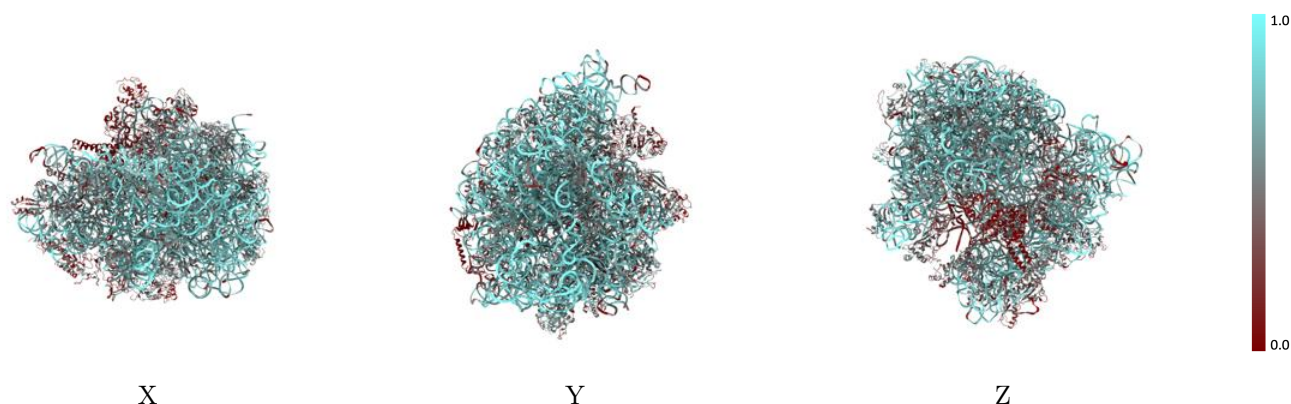
The images above show the 3D surface view of the map at the recommended contour level 0.035 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



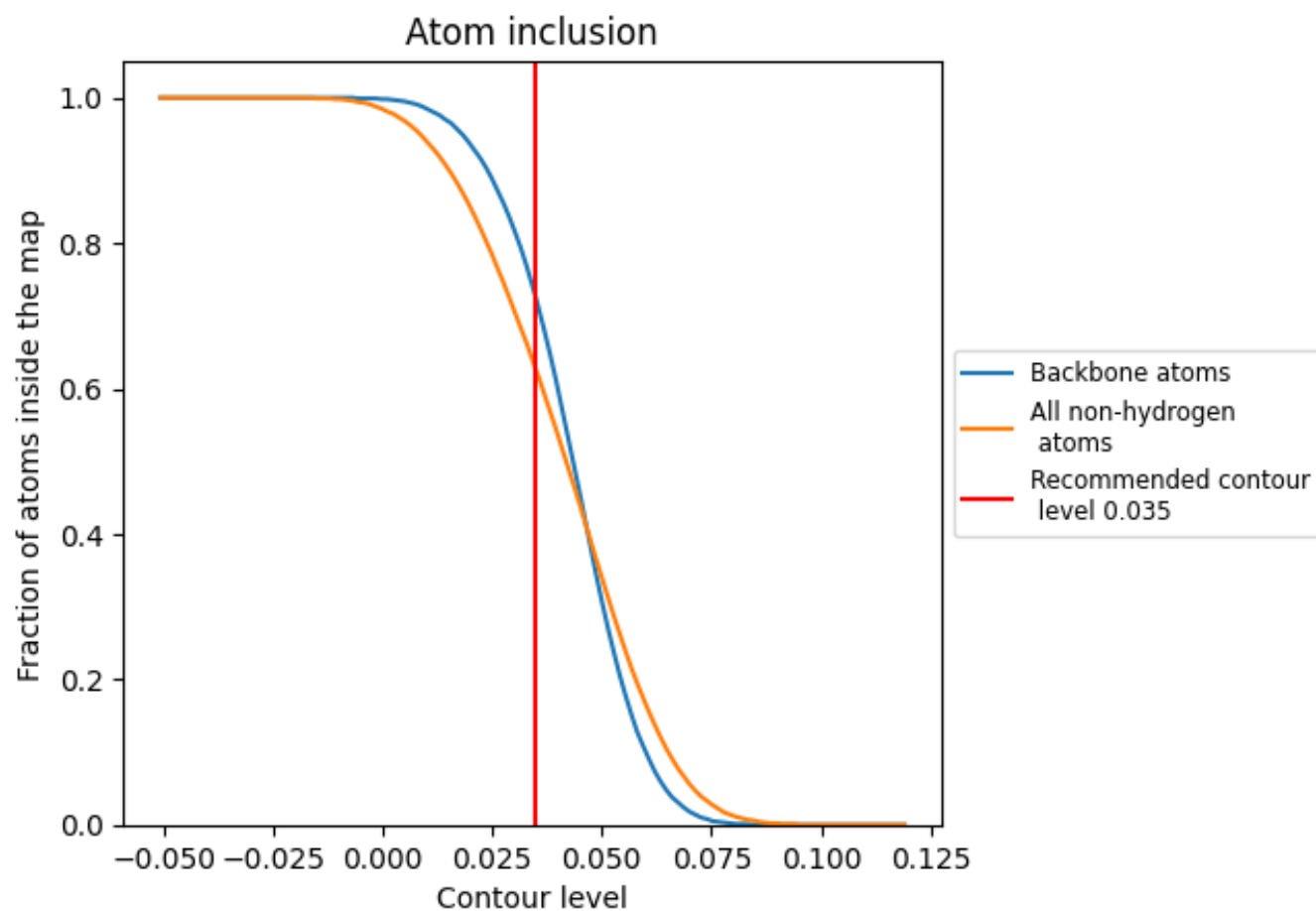
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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, 72% of all backbone atoms, 62% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.035) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6250	 0.3070
0	 0.4560	 0.3020
1	 0.2690	 0.1740
2	 0.3040	 0.1430
3	 0.3120	 0.2060
4	 0.3600	 0.2210
5	 0.0640	 0.1060
7	 0.7680	 0.3630
A	 0.7430	 0.3320
B	 0.7990	 0.3180
C	 0.4570	 0.3510
D	 0.4690	 0.3620
E	 0.4610	 0.3020
F	 0.3750	 0.2170
G	 0.4460	 0.2980
H	 0.1360	 0.1970
I	 0.0700	 0.0790
J	 0.4690	 0.3210
K	 0.4210	 0.3490
L	 0.4430	 0.3250
M	 0.4230	 0.3440
N	 0.5220	 0.3250
O	 0.5230	 0.2800
P	 0.4430	 0.3350
Q	 0.4930	 0.2980
R	 0.4440	 0.3140
S	 0.4310	 0.3200
T	 0.4570	 0.3250
U	 0.4680	 0.3060
V	 0.4860	 0.3170
W	 0.4510	 0.3370
X	 0.4510	 0.3130
Y	 0.5110	 0.2510
Z	 0.4530	 0.3200
a	 0.7650	 0.3230



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Chain	Atom inclusion	Q-score
b	 0.2750	 0.2310
c	 0.4680	 0.3030
d	 0.3650	 0.2620
e	 0.4860	 0.2960
f	 0.4260	 0.2390
g	 0.3610	 0.2390
h	 0.5000	 0.3080
i	 0.4470	 0.2710
j	 0.3220	 0.2590
k	 0.4350	 0.2800
l	 0.4220	 0.3330
m	 0.3520	 0.2350
n	 0.4060	 0.2690
o	 0.4590	 0.2540
p	 0.5140	 0.3080
q	 0.4490	 0.3130
r	 0.3750	 0.2530
s	 0.3880	 0.2620
t	 0.5290	 0.2820
u	 0.3110	 0.1940
v	 0.2810	 0.2700
w	 0.2710	 0.1630
x	 0.3600	 0.2110
z	 0.3980	 0.3660