



Full wwPDB EM Validation Report ⓘ

Mar 9, 2026 – 04:30 AM UTC

PDB ID : 6R6P / pdb_00006r6p
EMDB ID : EMD-4737
Title : Structure of XBP1u-paused ribosome nascent chain complex (rotated state)
Authors : Shanmuganathan, V.; Cheng, J.; Berninghausen, O.; Beckmann, R.
Deposited on : 2019-03-27
Resolution : 3.10 Å(reported)

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

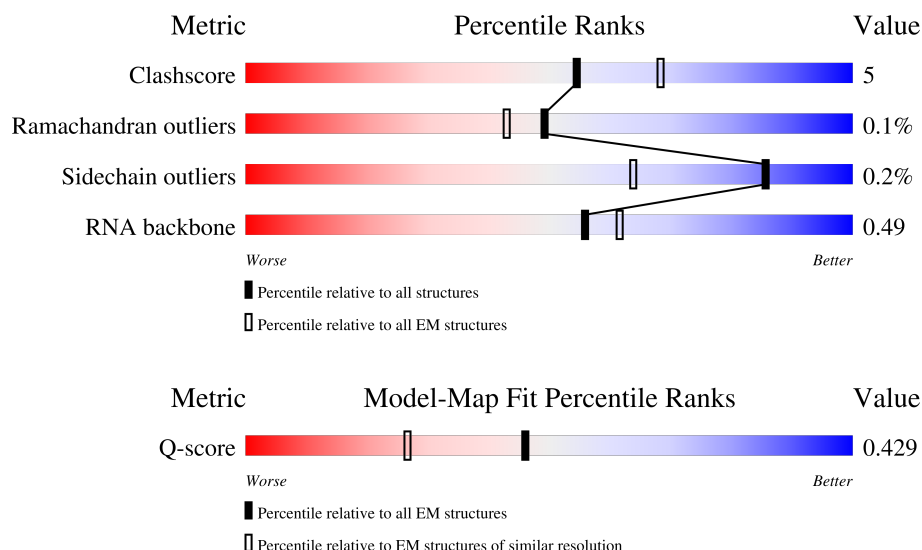
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.10 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.



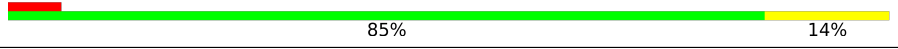
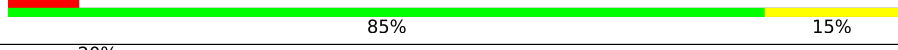
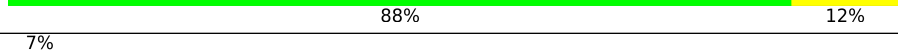
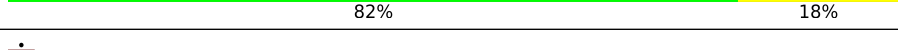
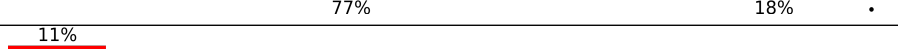
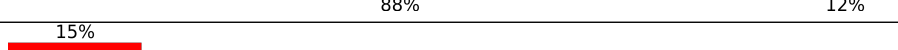
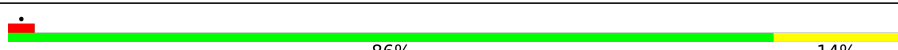
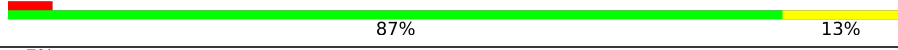
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	14724 (2.60 - 3.60)

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	5	3662	16% 60% 35% 5%
2	7	120	72% 23% 5%
3	8	156	12% 59% 33% 8%

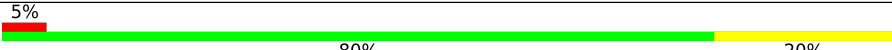
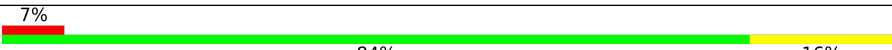
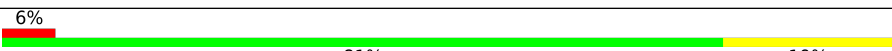
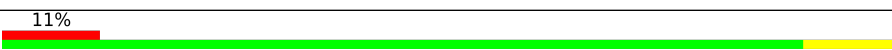
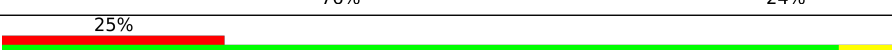
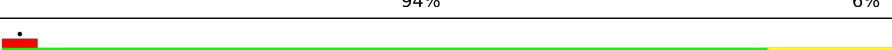
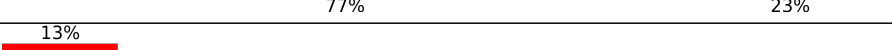
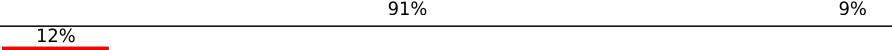
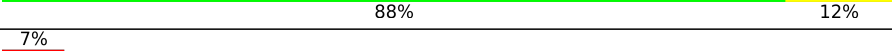
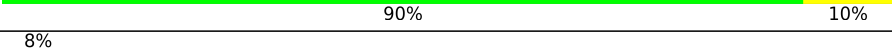
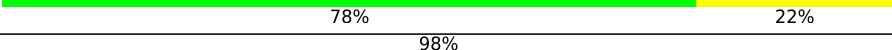
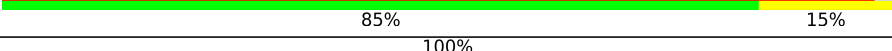
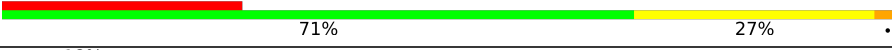
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Mol	Chain	Length	Quality of chain
4	A	244	
5	B	394	
6	C	362	
7	D	292	
8	E	248	
9	F	225	
10	G	241	
11	H	190	
12	I	213	
13	J	169	
14	L	210	
15	M	138	
16	N	203	
17	O	199	
18	P	153	
19	Q	187	
20	R	180	
21	S	175	
22	T	159	
23	U	99	
24	V	131	
25	W	63	
26	X	119	
27	Y	134	
28	Z	135	

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Mol	Chain	Length	Quality of chain
29	a	147	
30	b	75	
31	c	94	
32	d	107	
33	e	128	
34	f	109	
35	g	114	
36	h	122	
37	i	102	
38	j	86	
39	k	69	
40	l	50	
41	m	52	
42	n	23	
43	o	104	
44	p	91	
45	r	125	
46	s	198	
47	t	163	
48	1	24	
49	2	76	
50	3	75	
51	K	1698	
52	q	217	
53	u	213	

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Mol	Chain	Length	Quality of chain
54	v	221	34% 85% 15%
55	x	262	56% 85% 15%
56	z	237	54% 85% 15%
57	y	189	60% 86% 12%
58	CC	206	39% 87% 13%
59	XX	185	53% 88% 12%
60	EE	151	27% 79% 16% 5%
61	QQ	149	28% 93% 7%
62	MM	136	20% 85% 15%
63	UU	142	54% 86% 14%
64	YY	132	70% 86% 14%
65	HH	83	45% 82% 18%
66	TT	129	24% 83% 17%
67	VV	141	8% 85% 13%
68	NN	124	63% 81% 19%
69	ZZ	101	23% 83% 17%
70	JJ	83	41% 81% 19%
71	AA	55	67% 87% 13%
72	DD	228	62% 86% 14%
73	BB	191	44% 82% 15%
74	SS	96	73% 79% 20%
75	RR	117	94% 87% 13%
76	9	120	39% 85% 15%
77	II	144	39% 76% 24%
78	PP	141	50% 84% 16%

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Mol	Chain	Length	Quality of chain
79	GG	100	
80	OO	75	
81	FF	62	
82	w	55	
83	0	68	
84	6	313	
85	4	10	

2 Entry composition

There are 87 unique types of molecules in this entry. The entry contains 218067 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 28S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	5	3662	Total	C	N	O	P	0	0
			78486	34947	14363	25515	3661		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	7	120	Total	C	N	O	P	0	0
			2558	1141	456	842	119		

- Molecule 3 is a RNA chain called 5.8S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	8	156	Total	C	N	O	P	0	0
			3314	1480	585	1094	155		

- Molecule 4 is a protein called uL2.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	A	244	Total	C	N	O	S	0	0
			1868	1171	382	309	6		

- Molecule 5 is a protein called uL3.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	B	394	Total	C	N	O	S	0	0
			3148	2007	591	537	13		

- Molecule 6 is a protein called uL4.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	C	362	Total	C	N	O	S	0	0
			2883	1812	577	480	14		

- Molecule 7 is a protein called 60S ribosomal protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	D	292	Total	C	N	O	S	0	0
			2386	1509	437	426	14		

- Molecule 8 is a protein called 60S ribosomal protein L6.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	E	236	Total	C	N	O	S	0	0
			1898	1215	362	318	3		

- Molecule 9 is a protein called uL30.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	F	225	Total	C	N	O	S	0	0
			1870	1202	358	301	9		

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	175	ALA	THR	conflict	UNP G1SV32
F	185	GLY	ASN	conflict	UNP G1SV32
F	202	ARG	HIS	conflict	UNP G1SV32
F	233	GLU	GLY	conflict	UNP G1SV32

- Molecule 10 is a protein called eL8.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	G	241	Total	C	N	O	S	0	0
			1934	1233	371	326	4		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	191	GLY	CYS	conflict	UNP G1STW0

- Molecule 11 is a protein called uL6.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	H	190	Total	C	N	O	S	0	0
			1516	954	284	272	6		

- Molecule 12 is a protein called Ribosomal protein L10 (Predicted).

Mol	Chain	Residues	Atoms					AltConf	Trace
12	I	204	Total	C	N	O	S	0	0
			1655	1051	319	272	13		

- Molecule 13 is a protein called uL5.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	J	169	Total	C	N	O	S	0	0
			1353	855	252	240	6		

- Molecule 14 is a protein called 60S ribosomal protein L13.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	L	210	Total	C	N	O	S	0	0
			1703	1065	354	280	4		

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
L	47	ALA	-	insertion	UNP G1TPV0
L	48	PRO	-	insertion	UNP G1TPV0
L	49	ARG	-	insertion	UNP G1TPV0
L	50	PRO	-	insertion	UNP G1TPV0
L	51	ALA	-	insertion	UNP G1TPV0
L	52	SER	-	insertion	UNP G1TPV0
L	53	GLY	-	insertion	UNP G1TPV0
L	54	PRO	-	insertion	UNP G1TPV0
L	55	LEU	-	insertion	UNP G1TPV0

- Molecule 15 is a protein called Ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	M	138	Total	C	N	O	S	0	0
			1137	727	221	182	7		

- Molecule 16 is a protein called Ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	N	203	Total	C	N	O	S	0	0
			1701	1072	359	266	4		

- Molecule 17 is a protein called uL13.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	O	199	Total	C	N	O	S	0	0
			1638	1056	321	256	5		

- Molecule 18 is a protein called uL22.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	P	153	Total	C	N	O	S	0	0
			1242	777	241	215	9		

- Molecule 19 is a protein called eL18.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	Q	187	Total	C	N	O	S	0	0
			1506	941	311	249	5		

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Q	6	ARG	LEU	conflict	UNP G1TX70
Q	14	ARG	TRP	conflict	UNP G1TX70
Q	23	ILE	MET	conflict	UNP G1TX70
Q	24	TYR	CYS	conflict	UNP G1TX70
Q	38	ARG	HIS	conflict	UNP G1TX70
Q	57	ASN	LYS	conflict	UNP G1TX70
Q	66	MET	VAL	conflict	UNP G1TX70
Q	74	GLY	ASP	conflict	UNP G1TX70
Q	75	ARG	PRO	conflict	UNP G1TX70
Q	77	GLY	ASN	conflict	UNP G1TX70
Q	106	SER	THR	conflict	UNP G1TX70
Q	110	ARG	HIS	conflict	UNP G1TX70
Q	117	GLY	GLU	conflict	UNP G1TX70
Q	124	ASP	HIS	conflict	UNP G1TX70
Q	134	CYS	ARG	conflict	UNP G1TX70
Q	150	ARG	GLN	conflict	UNP G1TX70
Q	172	ARG	GLY	conflict	UNP G1TX70
Q	184	ARG	TRP	conflict	UNP G1TX70

- Molecule 20 is a protein called eL19.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	R	180	Total	C	N	O	S	0	0
			1508	933	328	238	9		

- Molecule 21 is a protein called eL20.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	S	175	Total	C	N	O	S	0	0
			1454	925	284	235	10		

- Molecule 22 is a protein called eL21.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	T	159	Total	C	N	O	S	0	0
			1298	823	252	217	6		

- Molecule 23 is a protein called Ribosomal protein L22.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	U	99	Total	C	N	O	S	0	0
			808	518	141	147	2		

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
U	32	GLY	ARG	conflict	UNP G1TSG1
U	36	ALA	GLU	conflict	UNP G1TSG1
U	39	PHE	SER	conflict	UNP G1TSG1
U	54	GLY	ARG	conflict	UNP G1TSG1
U	60	VAL	ALA	conflict	UNP G1TSG1
U	97	ARG	HIS	conflict	UNP G1TSG1

- Molecule 24 is a protein called uL14.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	V	131	Total	C	N	O	S	0	0
			979	618	184	172	5		

- Molecule 25 is a protein called Ribosomal protein L24.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	W	63	Total	C	N	O	S	0	0
			528	337	103	85	3		

- Molecule 26 is a protein called uL23.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	X	119	Total	C	N	O	S	0	0
			976	624	183	168	1		

- Molecule 27 is a protein called Ribosomal protein L26.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	Y	134	Total	C	N	O	S	0	0
			1115	700	226	186	3		

- Molecule 28 is a protein called 60S ribosomal protein L27.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	Z	135	Total	C	N	O	S	0	0
			1107	714	208	182	3		

- Molecule 29 is a protein called uL15.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	a	147	Total	C	N	O	S	0	0
			1162	734	239	185	4		

- Molecule 30 is a protein called 60S ribosomal protein L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	b	75	Total	C	N	O	S	0	0
			609	378	130	98	3		

- Molecule 31 is a protein called eL30.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	c	94	Total	C	N	O	S	0	0
			732	465	130	131	6		

- Molecule 32 is a protein called eL31.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	d	107	Total	C	N	O	S	0	0
			888	560	171	155	2		

- Molecule 33 is a protein called eL32.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	e	128	Total	C	N	O	S	0	0
			1053	667	216	165	5		

- Molecule 34 is a protein called eL33.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	f	109	Total	C	N	O	S	0	0
			876	555	174	143	4		

- Molecule 35 is a protein called eL34.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	g	114	Total	C	N	O	S	0	0
			906	566	187	147	6		

- Molecule 36 is a protein called uL29.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	h	122	Total	C	N	O	S	0	0
			1013	640	204	168	1		

- Molecule 37 is a protein called 60S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	i	102	Total	C	N	O	S	0	0
			830	520	176	129	5		

- Molecule 38 is a protein called Ribosomal protein L37.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	j	86	Total	C	N	O	S	0	0
			705	434	155	111	5		

- Molecule 39 is a protein called eL38.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	k	69	Total	C	N	O	S	0	0
			569	366	103	99	1		

- Molecule 40 is a protein called ribosomal protein eL39.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	l	50	Total	C	N	O	S	0	0
			444	281	98	64	1		

- Molecule 41 is a protein called eL40.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	m	52	Total	C	N	O	S	0	0
			429	266	90	67	6		

- Molecule 42 is a protein called 60s ribosomal protein l41.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	n	23	Total	C	N	O	S	0	0
			222	134	61	25	2		

- Molecule 43 is a protein called eL42.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	o	104	Total	C	N	O	S	0	0
			851	533	174	138	6		

- Molecule 44 is a protein called ribosomal protein eL43.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	p	91	Total	C	N	O	S	0	0
			708	445	136	120	7		

- Molecule 45 is a protein called eL28.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	r	125	Total	C	N	O	S	0	0
			1001	621	206	168	6		

- Molecule 46 is a protein called 60S acidic ribosomal protein P0.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	s	198	Total	C	N	O	S	0	0
			1523	969	265	280	9		

- Molecule 47 is a protein called Ribosomal protein L12.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	t	163	Total	C	N	O	S	0	0
			1238	773	230	230	5		

- Molecule 48 is a protein called X-box-binding protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	1	24	Total	C	N	O	S	0	0
			204	137	35	30	2		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
1	255	ALA	SER	conflict	UNP P17861

- Molecule 49 is a RNA chain called A/P-tRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	2	76	Total	C	N	O	P	0	0
			1614	722	287	530	75		

- Molecule 50 is a RNA chain called P/E-tRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	3	75	Total	C	N	O	P	0	0
			1597	714	287	522	74		

- Molecule 51 is a RNA chain called 18S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	K	1698	Total	C	N	O	P	0	0
			36248	16180	6508	11863	1697		

- Molecule 52 is a protein called uS2.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	q	217	Total	C	N	O	S	0	0
			1710	1086	300	316	8		

- Molecule 53 is a protein called 40S ribosomal protein S3a.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	u	213	Total	C	N	O	S	0	0
			1729	1098	309	308	14		

- Molecule 54 is a protein called uS5.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	v	221	Total	C	N	O	S	0	0
			1716	1111	295	301	9		

- Molecule 55 is a protein called 40S ribosomal protein S4.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	x	262	Total	C	N	O	S	0	0
			2076	1324	386	358	8		

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
x	25	GLY	SER	conflict	UNP G1TK17
x	51	ARG	LYS	conflict	UNP G1TK17
x	78	THR	ALA	conflict	UNP G1TK17
x	156	VAL	MET	conflict	UNP G1TK17

- Molecule 56 is a protein called 40S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
56	z	237	Total	C	N	O	S	0	0
			1923	1200	387	329	7		

- Molecule 57 is a protein called 40S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
57	y	185	Total	C	N	O	S	0	0
			1488	952	271	264	1		

- Molecule 58 is a protein called 40S ribosomal protein S8.

Mol	Chain	Residues	Atoms					AltConf	Trace
58	CC	206	Total	C	N	O	S	0	0
			1686	1058	332	291	5		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
CC	47	ARG	GLY	conflict	UNP G1TJW1

- Molecule 59 is a protein called Ribosomal protein S9 (Predicted).

Mol	Chain	Residues	Atoms					AltConf	Trace
59	XX	185	Total	C	N	O	S	0	0
			1525	969	306	248	2		

- Molecule 60 is a protein called Ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
60	EE	143	Total	C	N	O	S	0	0
			1175	749	222	198	6		

- Molecule 61 is a protein called ribosomal protein uS15.

Mol	Chain	Residues	Atoms					AltConf	Trace
61	QQ	149	Total	C	N	O	S	0	0
			1202	770	228	203	1		

- Molecule 62 is a protein called uS11.

Mol	Chain	Residues	Atoms					AltConf	Trace
62	MM	136	Total	C	N	O	S	0	0
			1016	621	199	190	6		

- Molecule 63 is a protein called Ribosomal protein S16.

Mol	Chain	Residues	Atoms					AltConf	Trace
63	UU	142	Total	C	N	O	S	0	0
			1128	717	213	195	3		

- Molecule 64 is a protein called eS17.

Mol	Chain	Residues	Atoms					AltConf	Trace
64	YY	132	Total	C	N	O	S	0	0
			1068	670	199	195	4		

- Molecule 65 is a protein called eS21.

Mol	Chain	Residues	Atoms					AltConf	Trace
65	HH	83	Total	C	N	O	S	0	0
			636	393	117	121	5		

- Molecule 66 is a protein called Ribosomal protein S15a.

Mol	Chain	Residues	Atoms					AltConf	Trace
66	TT	129	Total	C	N	O	S	0	0
			1034	659	193	176	6		

- Molecule 67 is a protein called Ribosomal protein S23.

Mol	Chain	Residues	Atoms					AltConf	Trace
67	VV	141	Total	C	N	O	S	0	0
			1098	693	219	183	3		

- Molecule 68 is a protein called eS24.

Mol	Chain	Residues	Atoms					AltConf	Trace
68	NN	124	Total	C	N	O	S	0	0
			1011	640	198	168	5		

- Molecule 69 is a protein called eS26.

Mol	Chain	Residues	Atoms					AltConf	Trace
69	ZZ	101	Total	C	N	O	S	0	0
			814	507	170	132	5		

- Molecule 70 is a protein called 40S ribosomal protein S27.

Mol	Chain	Residues	Atoms					AltConf	Trace
70	JJ	83	Total	C	N	O	S	0	0
			651	408	121	115	7		

- Molecule 71 is a protein called 40S ribosomal protein S30.

Mol	Chain	Residues	Atoms					AltConf	Trace
71	AA	55	Total	C	N	O	S	0	0
			443	274	97	71	1		

- Molecule 72 is a protein called Ribosomal protein S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
72	DD	228	Total	C	N	O	S	0	0
			1768	1126	318	316	8		

- Molecule 73 is a protein called Ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
73	BB	185	Total	C	N	O	S	0	0
			1471	921	277	266	7		

- Molecule 74 is a protein called eS10.

Mol	Chain	Residues	Atoms					AltConf	Trace
74	SS	96	Total	C	N	O	S	0	0
			810	530	143	131	6		

- Molecule 75 is a protein called 40S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
75	RR	117	Total	C	N	O	S	0	0
			908	570	161	169	8		

- Molecule 76 is a protein called uS14.

Mol	Chain	Residues	Atoms					AltConf	Trace
76	9	120	Total	C	N	O	S	0	0
			997	635	187	168	7		

- Molecule 77 is a protein called uS13.

Mol	Chain	Residues	Atoms					AltConf	Trace
77	II	144	Total	C	N	O	S	0	0
			1190	746	241	202	1		

- Molecule 78 is a protein called eS19.

Mol	Chain	Residues	Atoms					AltConf	Trace
78	PP	141	Total	C	N	O	S	0	0
			1097	688	211	195	3		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
PP	119	GLY	TRP	conflict	UNP G1TN62

- Molecule 79 is a protein called uS10.

Mol	Chain	Residues	Atoms					AltConf	Trace
79	GG	100	Total	C	N	O	S	0	0
			795	498	152	141	4		

- Molecule 80 is a protein called ribosomal protein eS25.

Mol	Chain	Residues	Atoms					AltConf	Trace
80	OO	75	Total	C	N	O	S	0	0
			598	382	111	104	1		

- Molecule 81 is a protein called Ribosomal protein S28.

Mol	Chain	Residues	Atoms					AltConf	Trace
81	FF	62	Total	C	N	O	S	0	0
			488	297	97	92	2		

- Molecule 82 is a protein called S29.

Mol	Chain	Residues	Atoms					AltConf	Trace
82	w	55	Total	C	N	O	S	0	0
			459	286	94	74	5		

- Molecule 83 is a protein called eS31.

Mol	Chain	Residues	Atoms					AltConf	Trace
83	0	68	Total	C	N	O	S	0	0
			555	351	103	94	7		

- Molecule 84 is a protein called ribosomal protein RACK1.

Mol	Chain	Residues	Atoms					AltConf	Trace
84	6	313	Total	C	N	O	S	0	0
			2436	1535	424	465	12		

- Molecule 85 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
85	4	10	Total	C	N	O	P	0	0
			211	95	37	69	10		

- Molecule 86 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
86	5	148	Total	Mg	0
			148	148	
86	7	4	Total	Mg	0
			4	4	
86	8	1	Total	Mg	0
			1	1	
86	I	1	Total	Mg	0
			1	1	
86	P	1	Total	Mg	0
			1	1	
86	Q	1	Total	Mg	0
			1	1	
86	V	1	Total	Mg	0
			1	1	
86	e	1	Total	Mg	0
			1	1	
86	g	1	Total	Mg	0
			1	1	

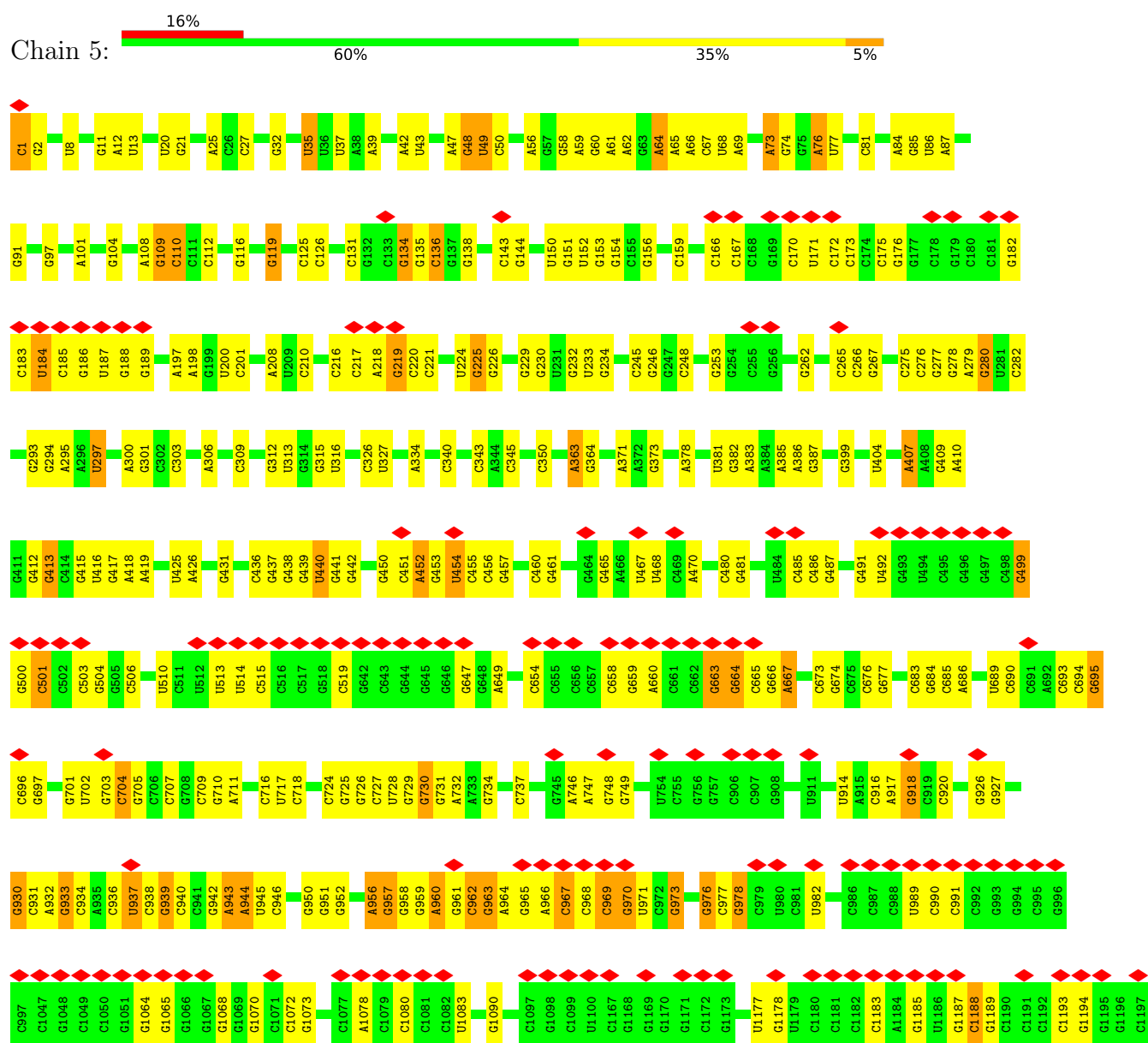
- Molecule 87 is ZINC ION (CCD ID: ZN) (formula: Zn).

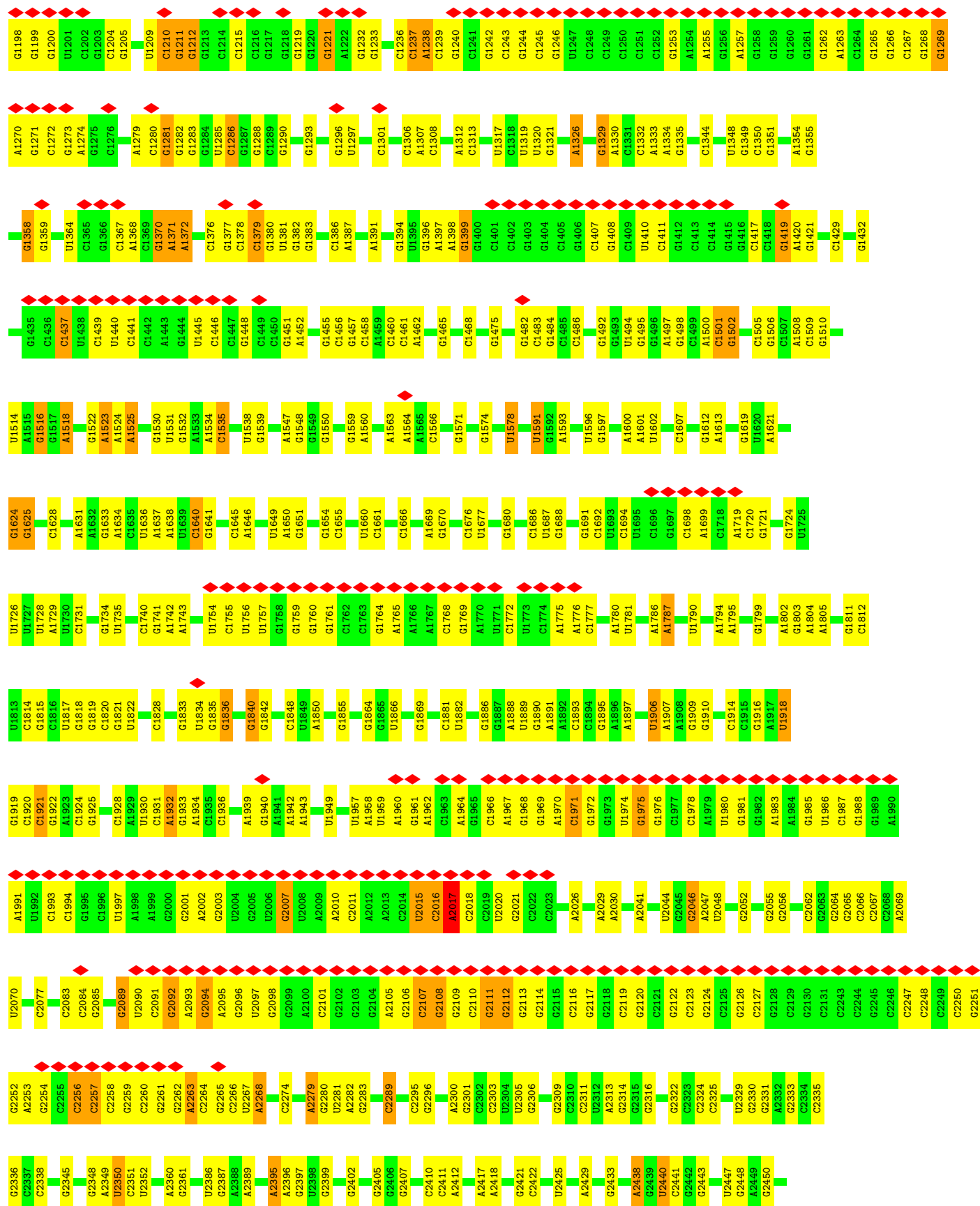
Mol	Chain	Residues	Atoms		AltConf
87	g	1	Total	Zn	0
			1	1	
87	j	1	Total	Zn	0
			1	1	
87	m	1	Total	Zn	0
			1	1	
87	o	1	Total	Zn	0
			1	1	
87	p	1	Total	Zn	0
			1	1	

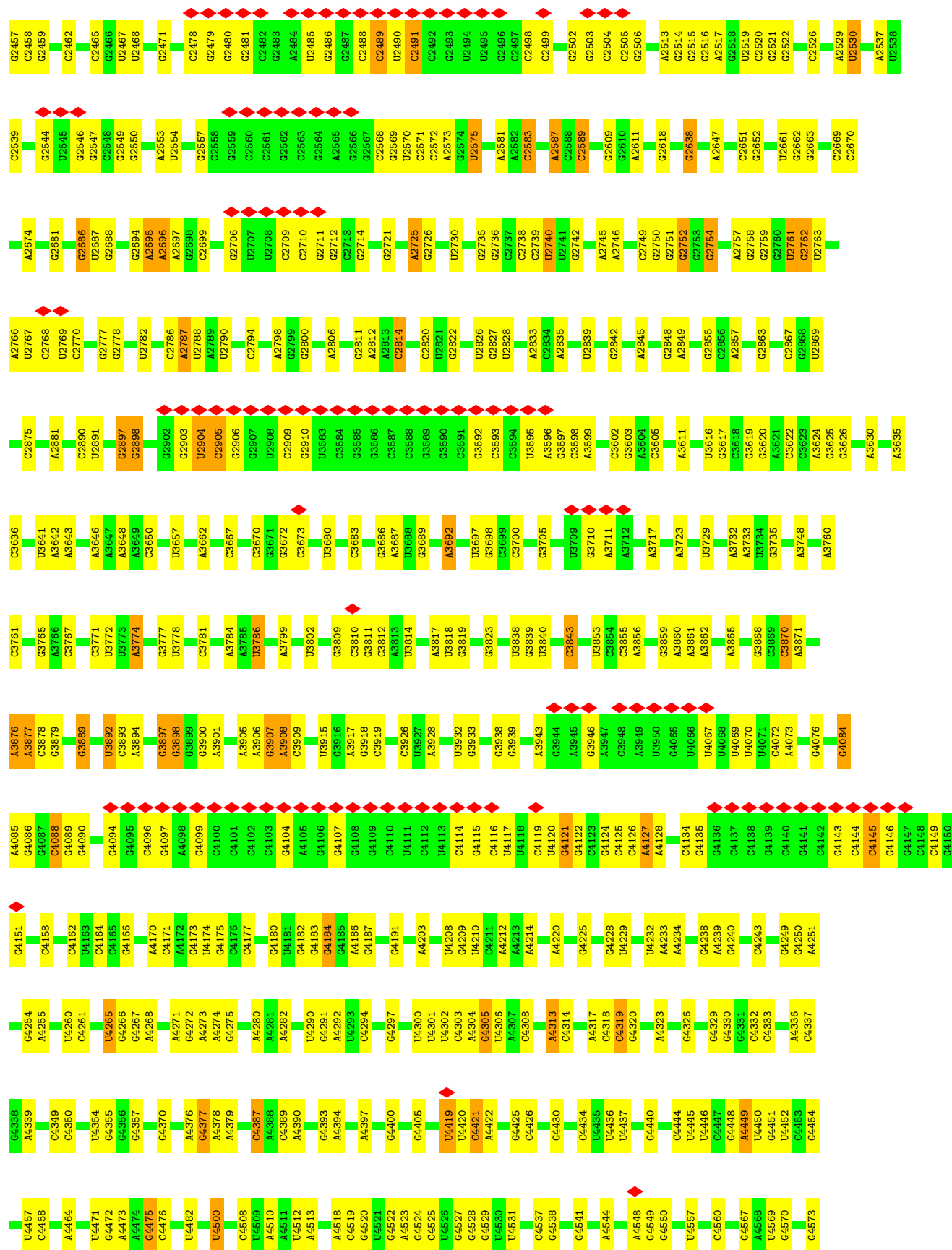
3 Residue-property plots

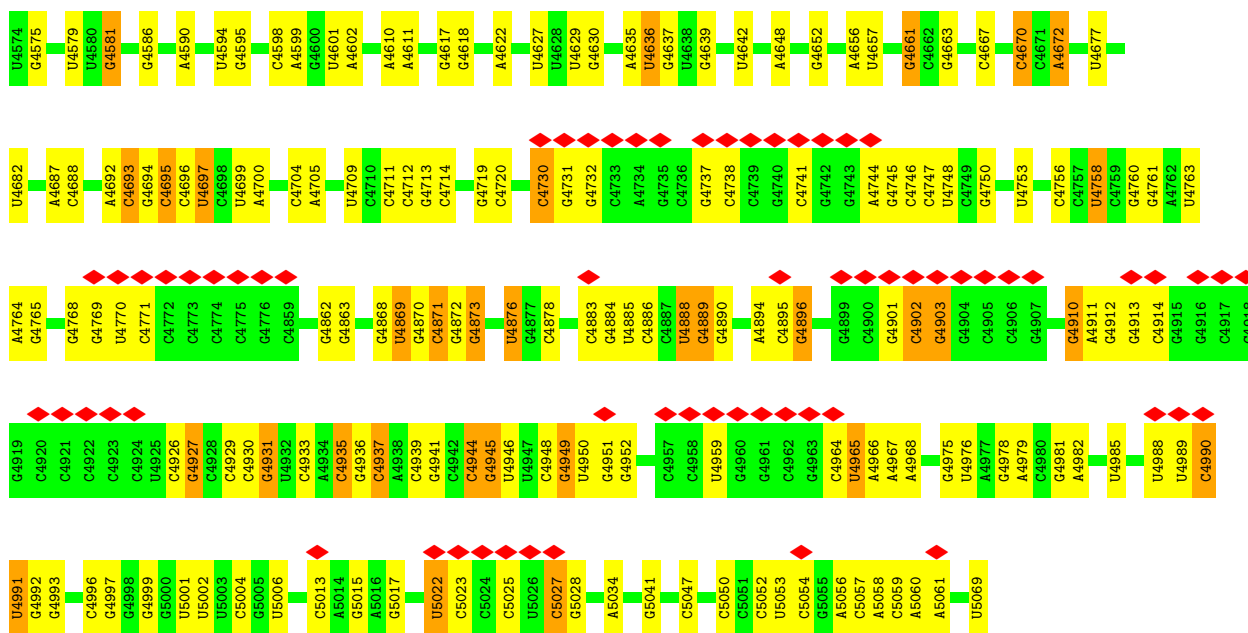
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

• Molecule 1: 28S ribosomal RNA





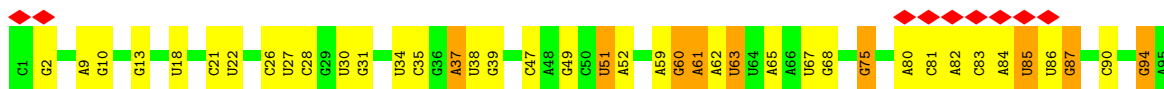




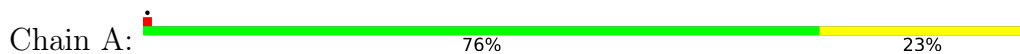
- Molecule 2: 5S ribosomal RNA



- Molecule 3: 5.8S ribosomal RNA

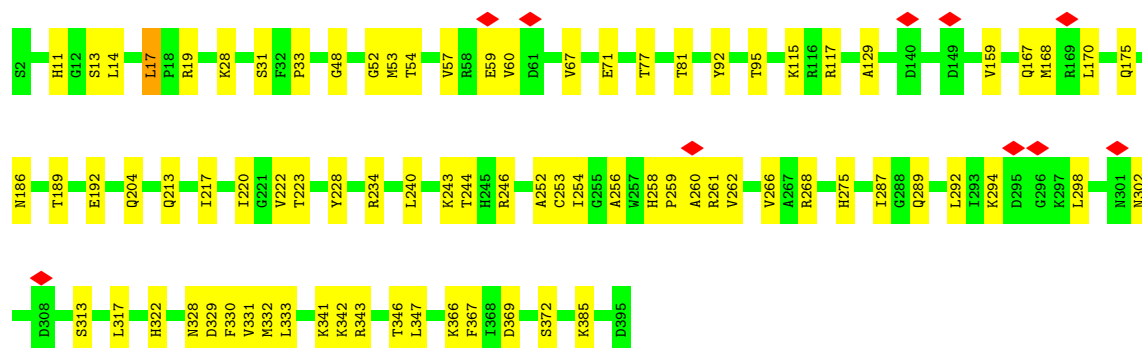


- Molecule 4: uL2



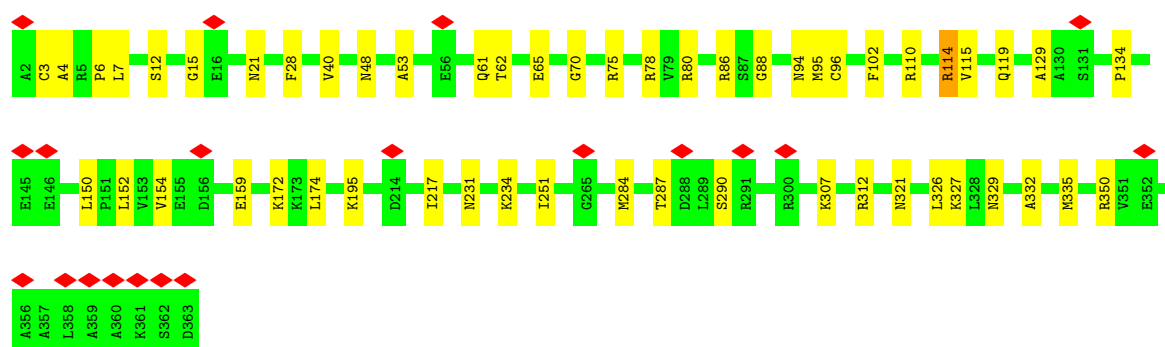
- Molecule 5: uL3

Chain B:  79% 20%



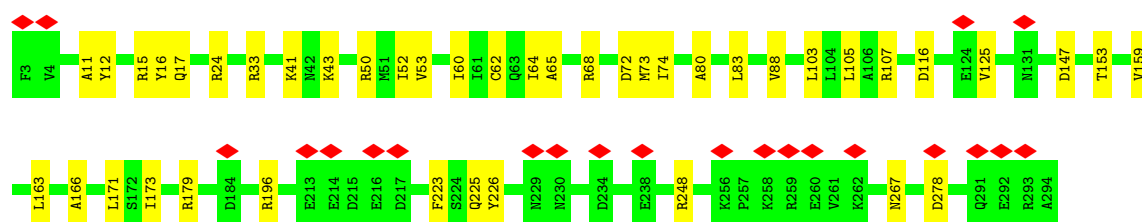
• Molecule 6: uL4

Chain C:  6% 85% 14%



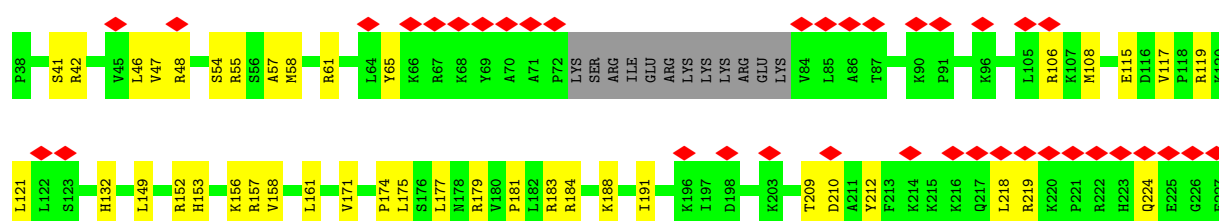
• Molecule 7: 60S ribosomal protein L5

Chain D:  8% 85% 15%



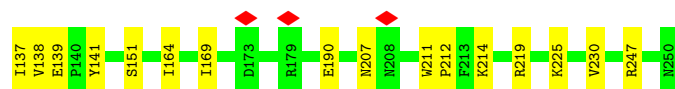
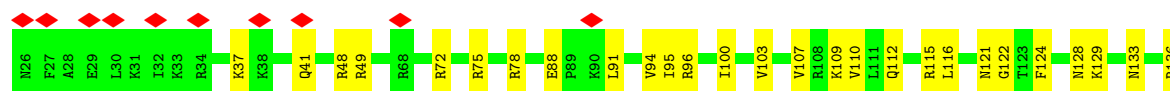
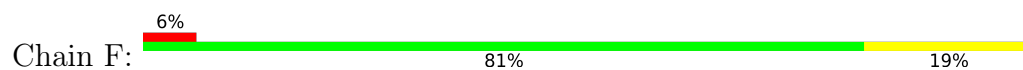
• Molecule 8: 60S ribosomal protein L6

Chain E:  20% 75% 20% 5%

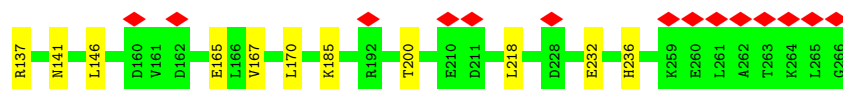
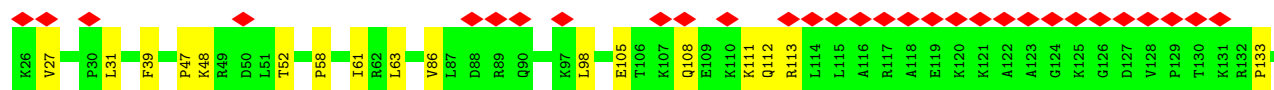
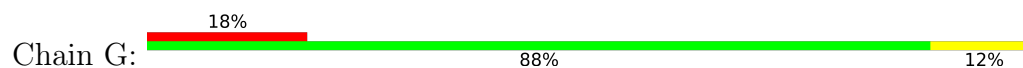




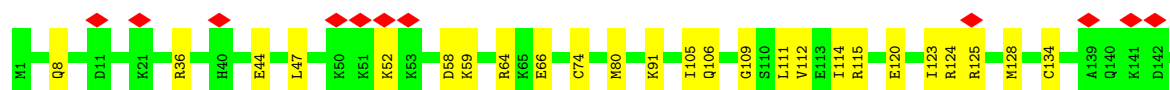
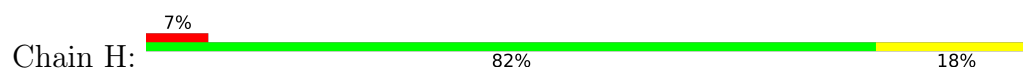
• Molecule 9: uL30



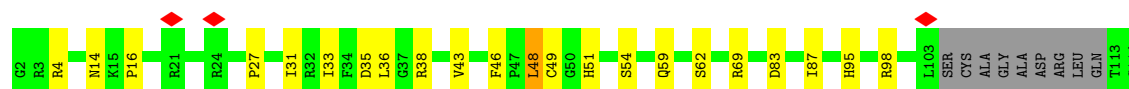
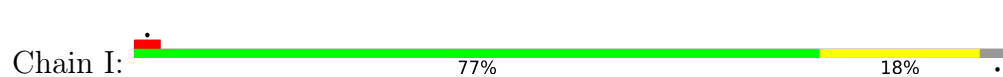
• Molecule 10: eL8



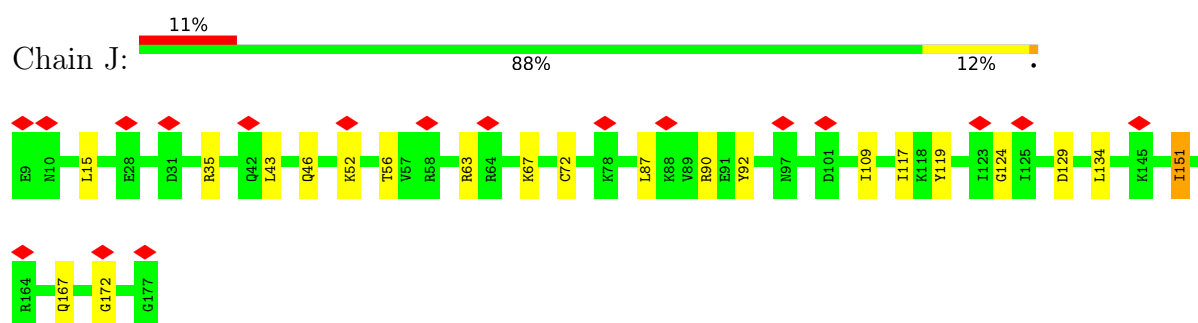
• Molecule 11: uL6



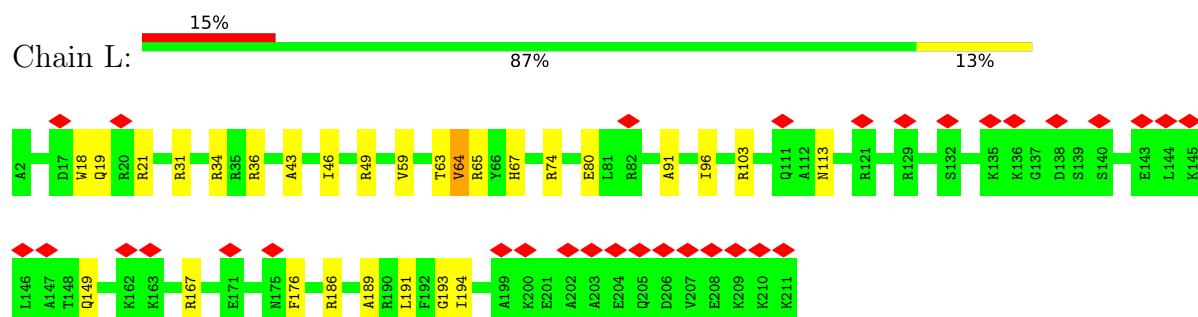
• Molecule 12: Ribosomal protein L10 (Predicted)



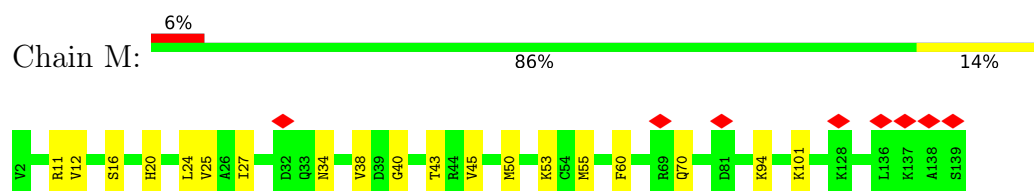
• Molecule 13: uL5



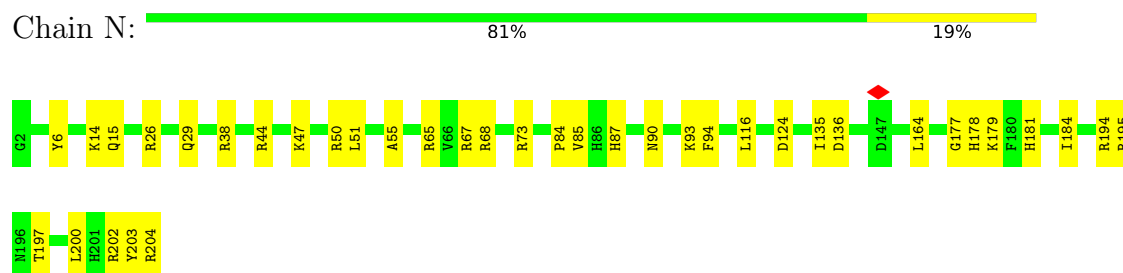
- Molecule 14: 60S ribosomal protein L13



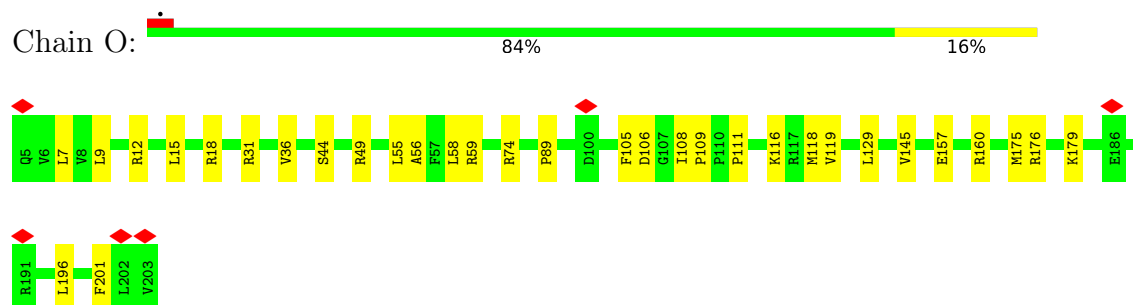
- Molecule 15: Ribosomal protein L14



- Molecule 16: Ribosomal protein L15

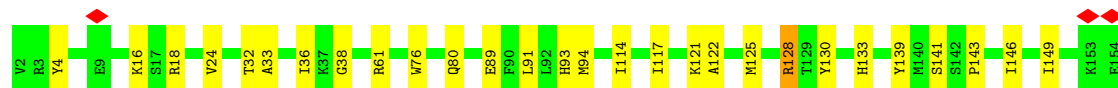


- Molecule 17: uL13



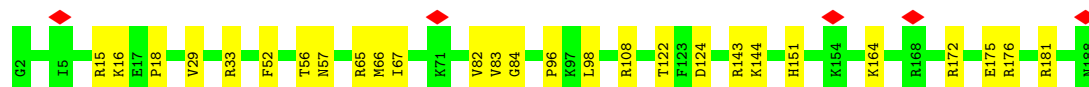
- Molecule 18: uL22

Chain P: 

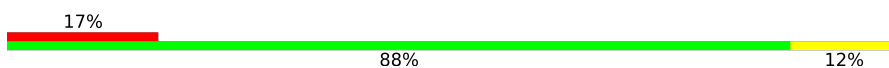


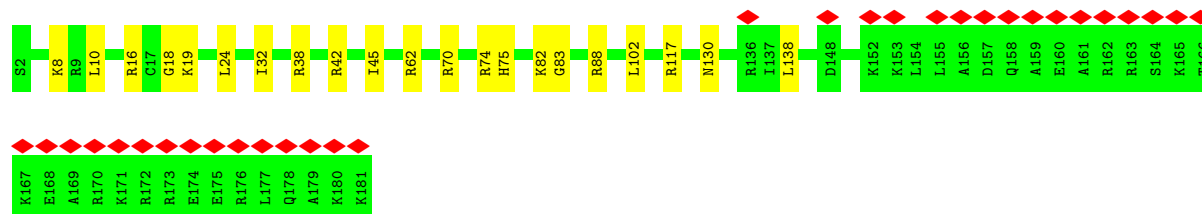
- Molecule 19: eL18

Chain Q: 



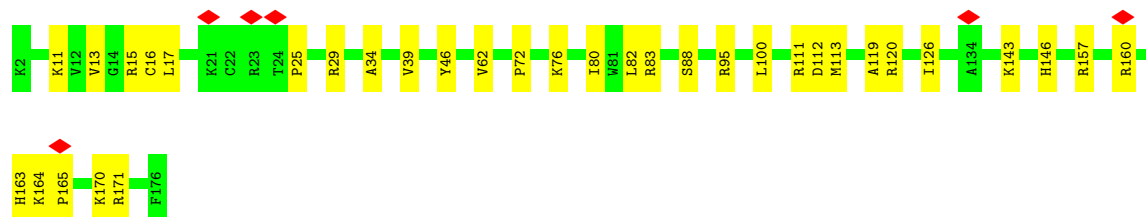
- Molecule 20: eL19

Chain R: 



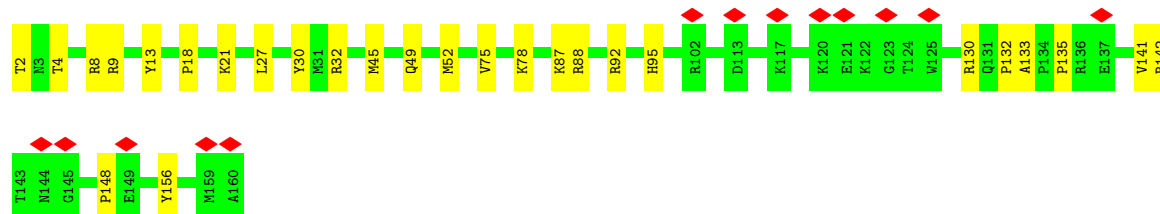
- Molecule 21: eL20

Chain S: 

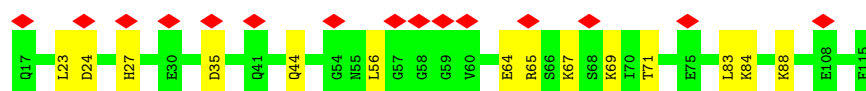
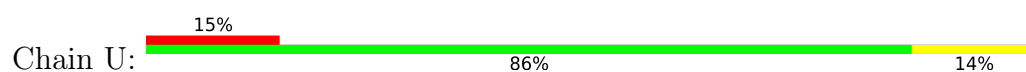


- Molecule 22: eL21

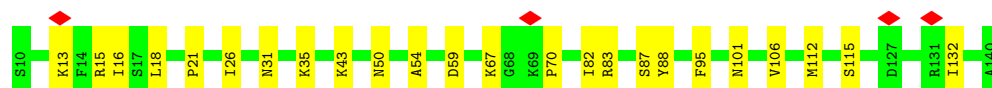
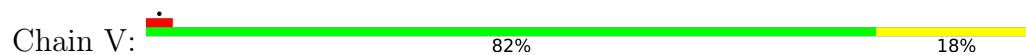
Chain T: 



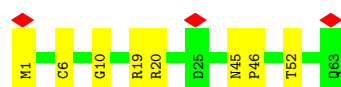
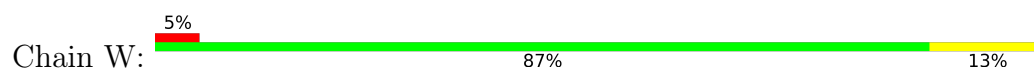
- Molecule 23: Ribosomal protein L22



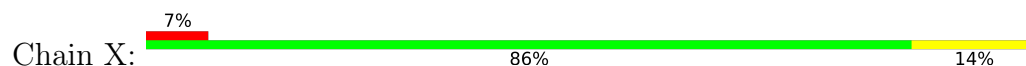
- Molecule 24: uL14



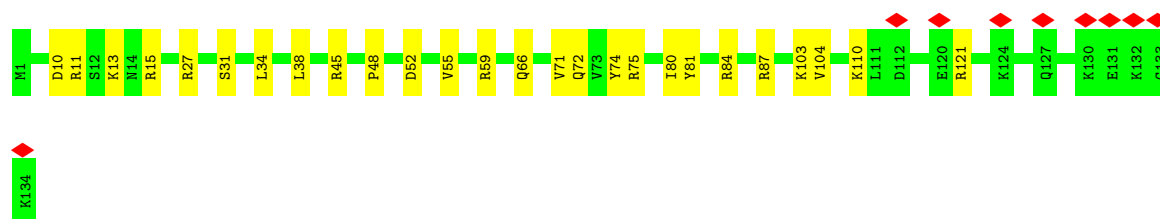
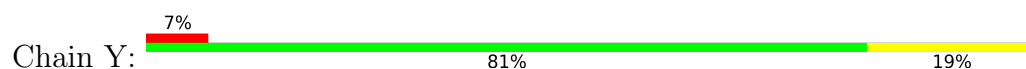
- Molecule 25: Ribosomal protein L24



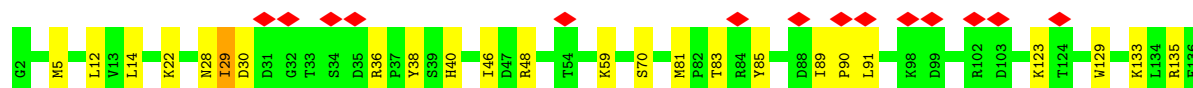
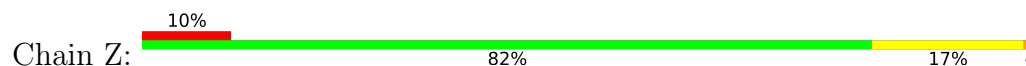
- Molecule 26: uL23



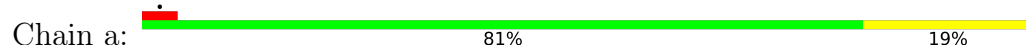
- Molecule 27: Ribosomal protein L26

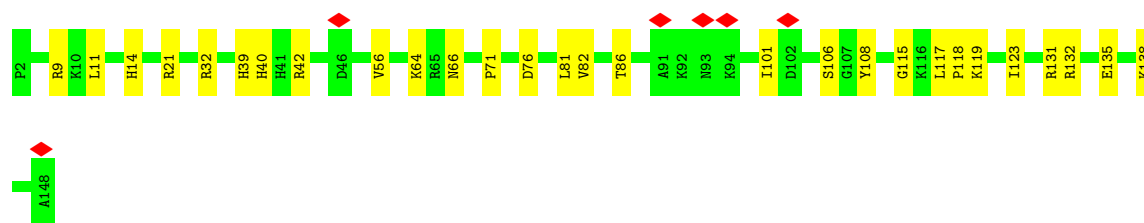


- Molecule 28: 60S ribosomal protein L27

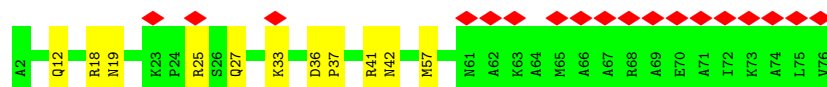
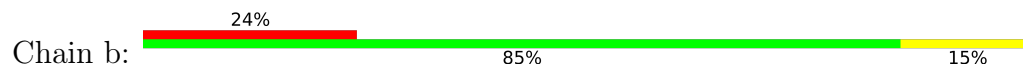


- Molecule 29: uL15

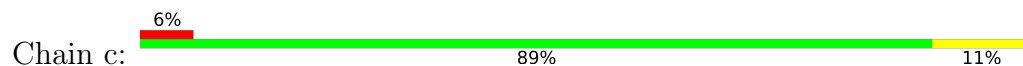




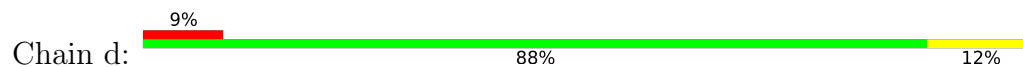
- Molecule 30: 60S ribosomal protein L29



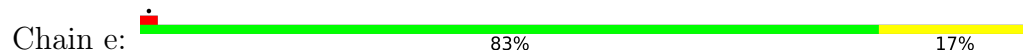
- Molecule 31: eL30



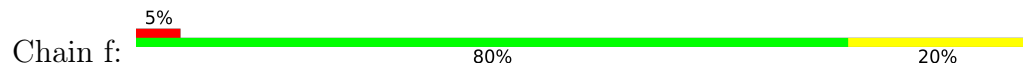
- Molecule 32: eL31



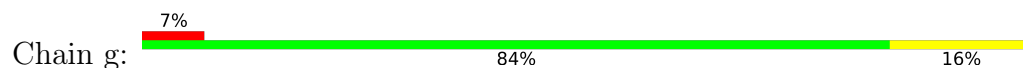
- Molecule 33: eL32

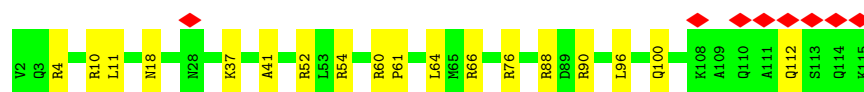


- Molecule 34: eL33

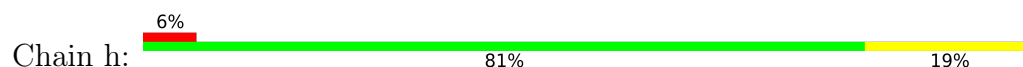


- Molecule 35: eL34

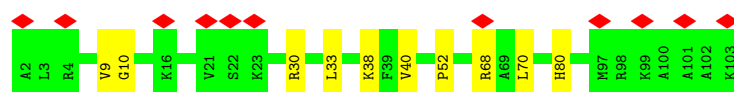




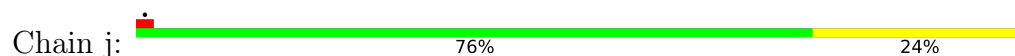
• Molecule 36: uL29



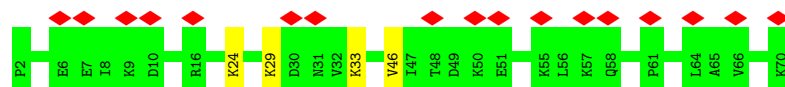
• Molecule 37: 60S ribosomal protein L36



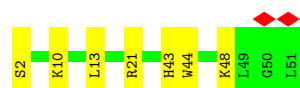
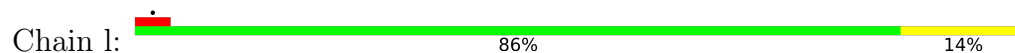
• Molecule 38: Ribosomal protein L37



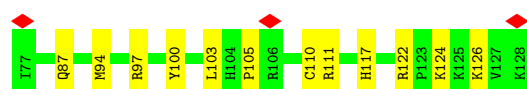
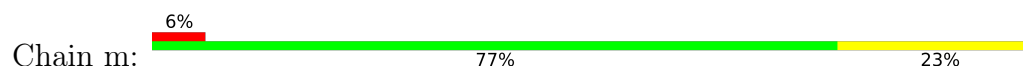
• Molecule 39: eL38



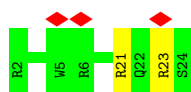
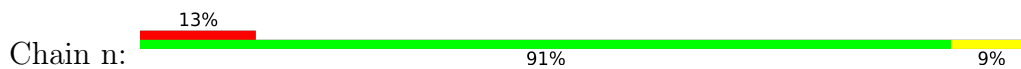
• Molecule 40: ribosomal protein eL39



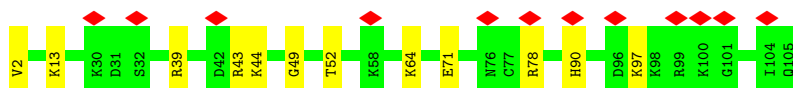
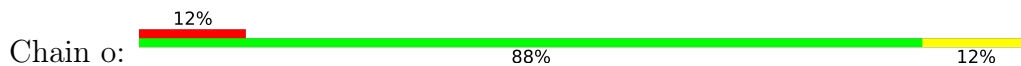
• Molecule 41: eL40



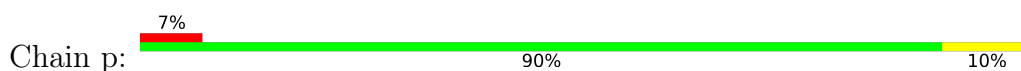
• Molecule 42: 60s ribosomal protein l41



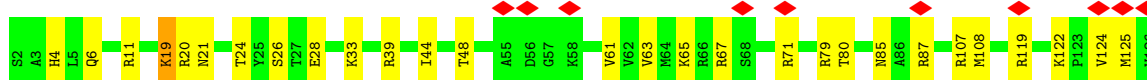
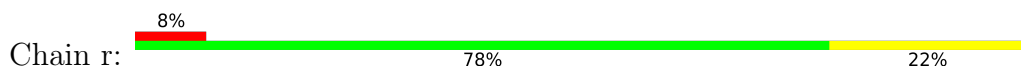
• Molecule 43: eL42



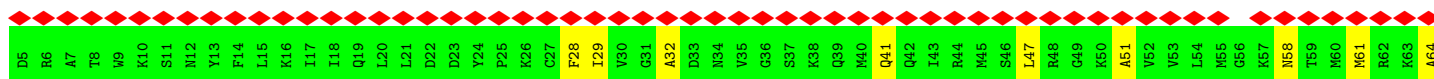
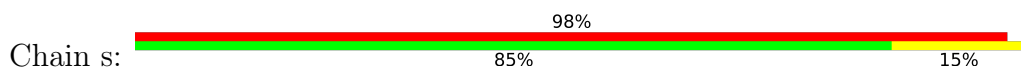
• Molecule 44: ribosomal protein eL43



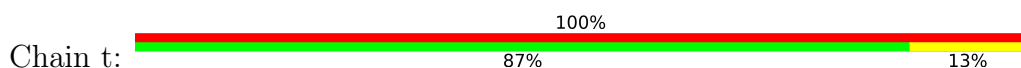
• Molecule 45: eL28

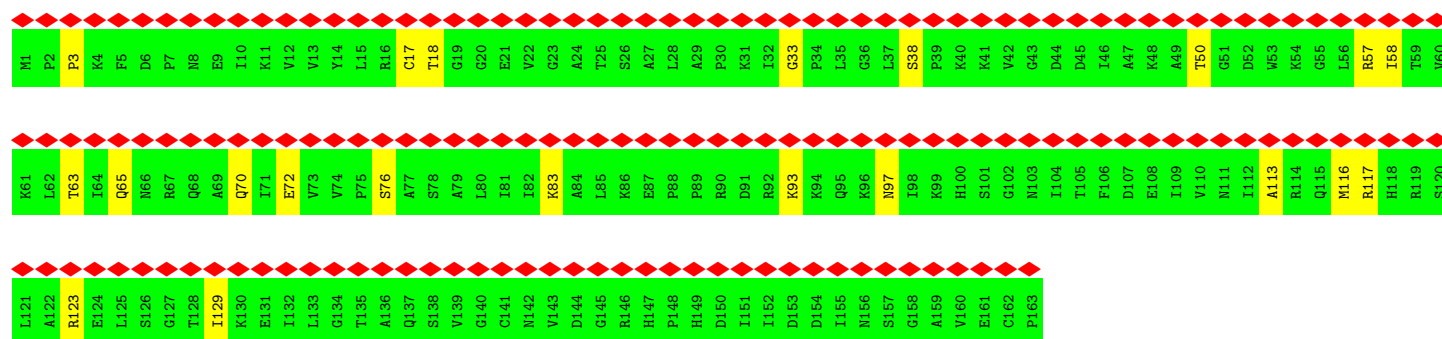


• Molecule 46: 60S acidic ribosomal protein P0

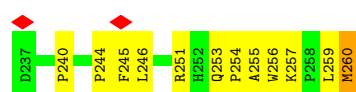


• Molecule 47: Ribosomal protein L12





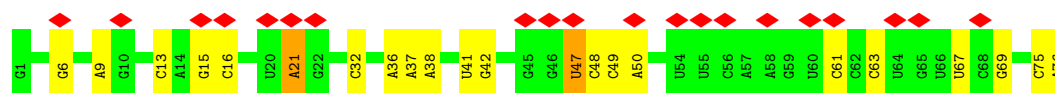
• Molecule 48: X-box-binding protein 1



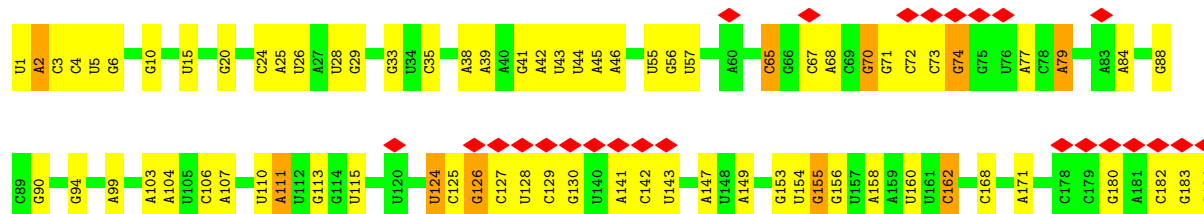
• Molecule 49: A/P-tRNA

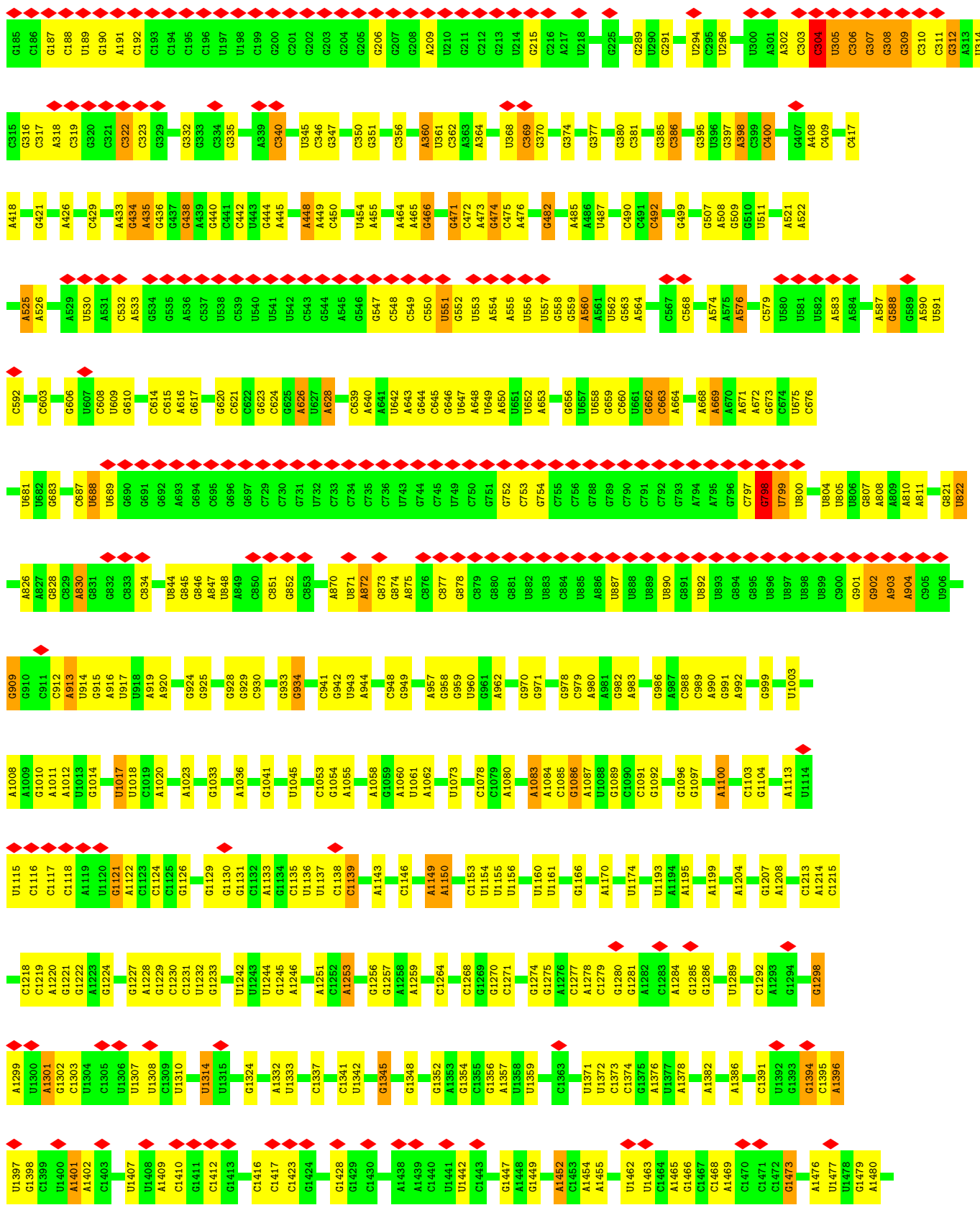


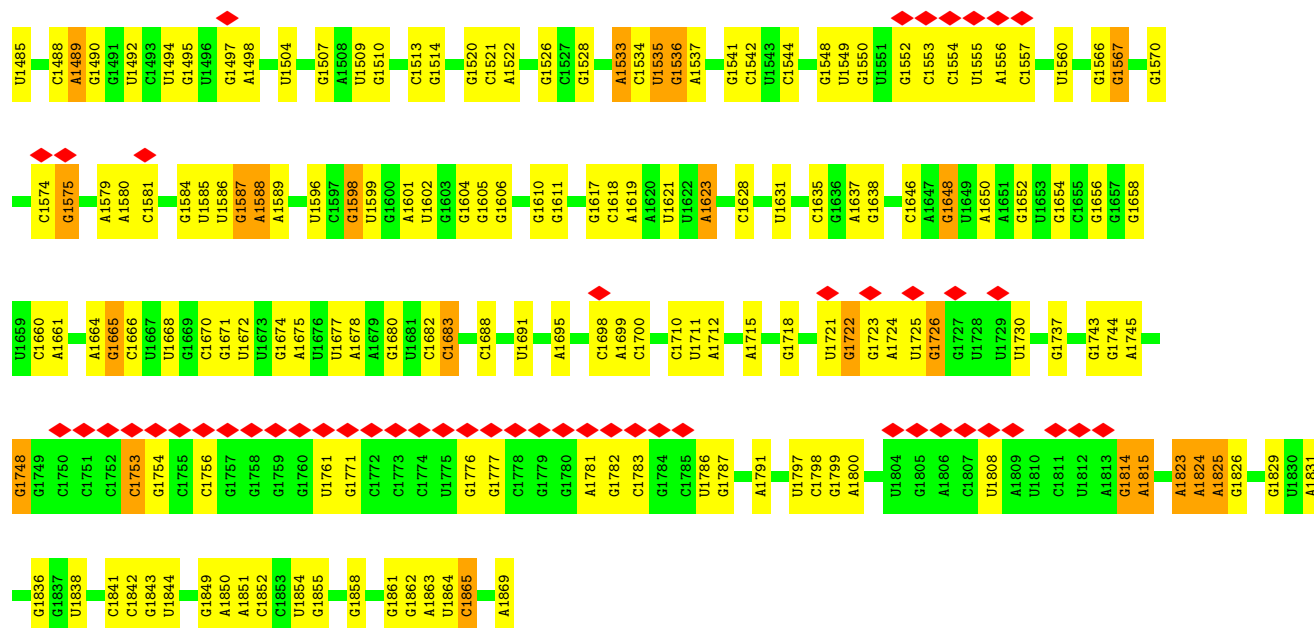
• Molecule 50: P/E-tRNA



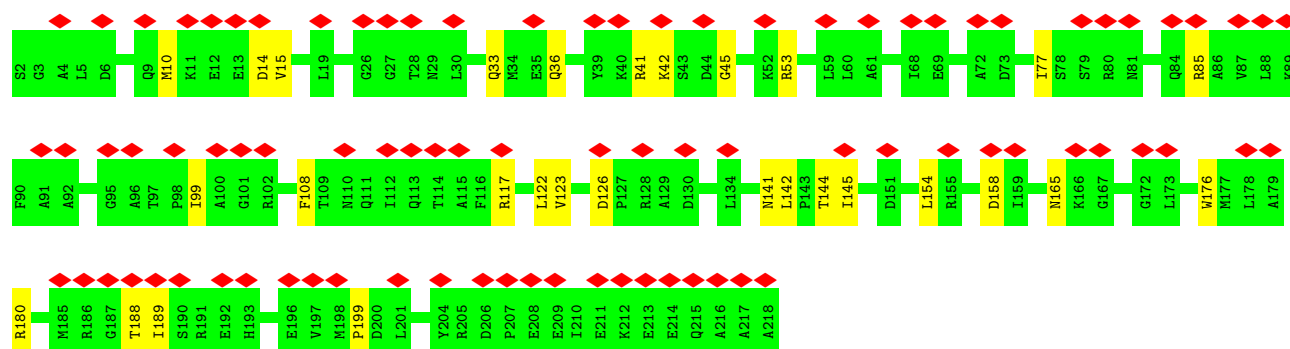
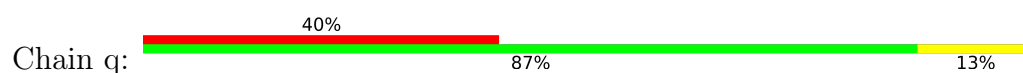
• Molecule 51: 18S rRNA



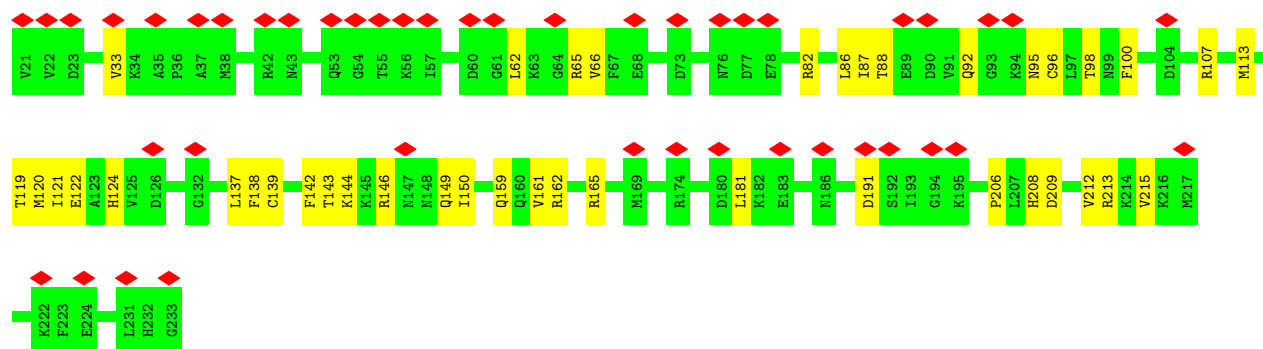
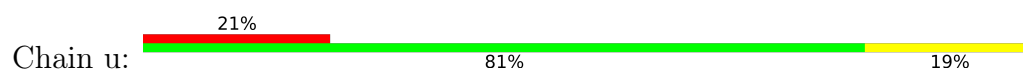




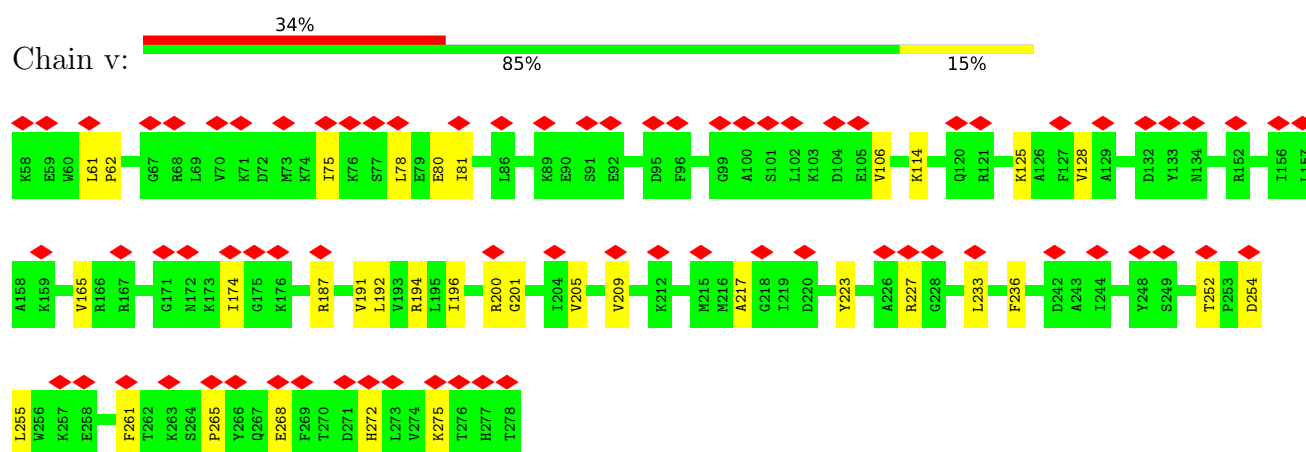
- Molecule 52: uS2



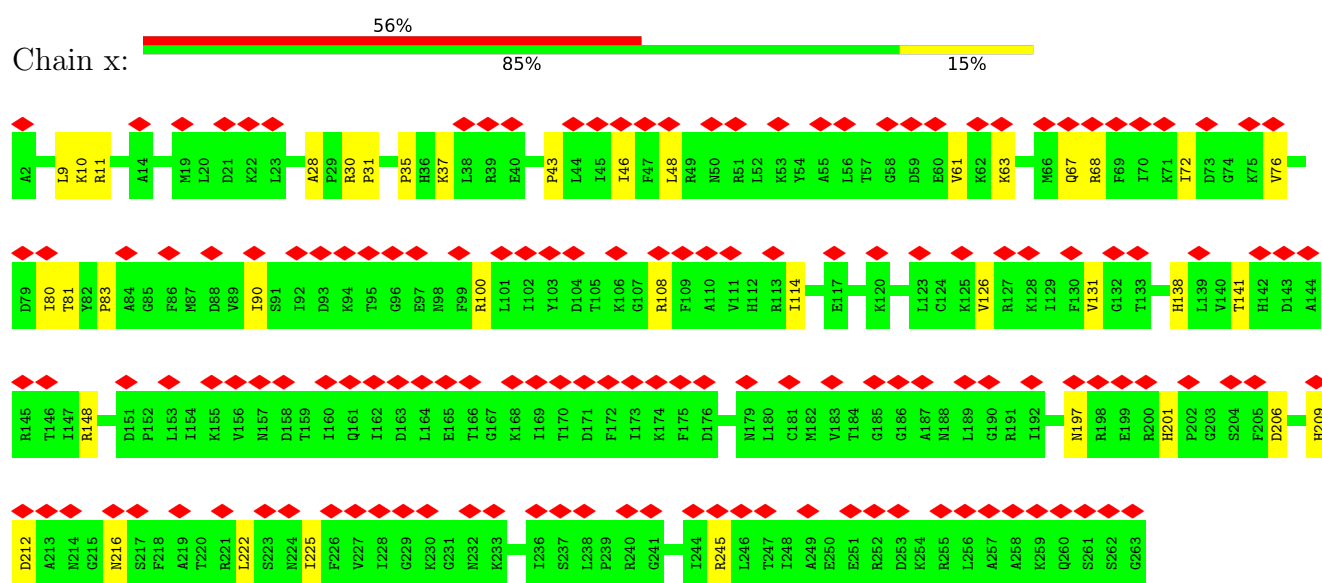
- Molecule 53: 40S ribosomal protein S3a



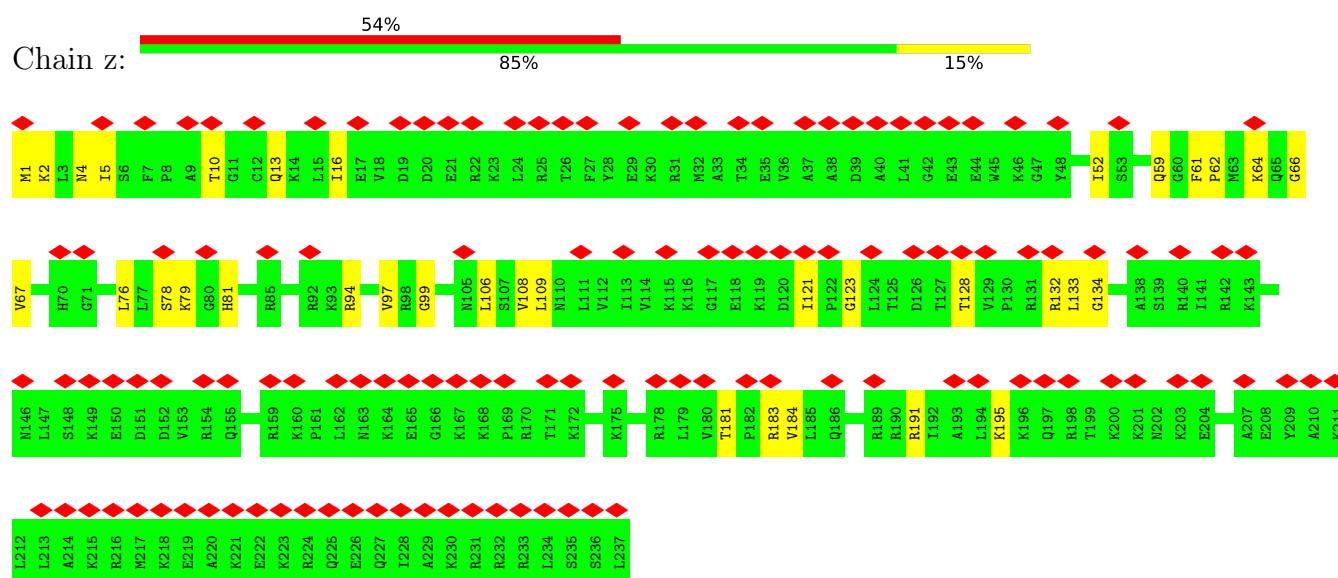
- Molecule 54: uS5



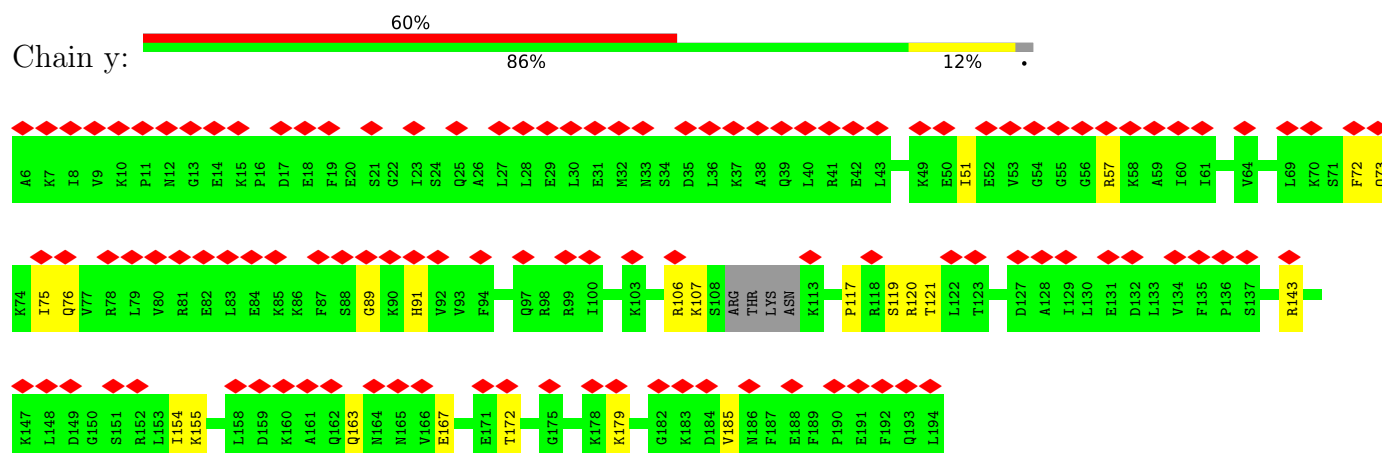
• Molecule 55: 40S ribosomal protein S4



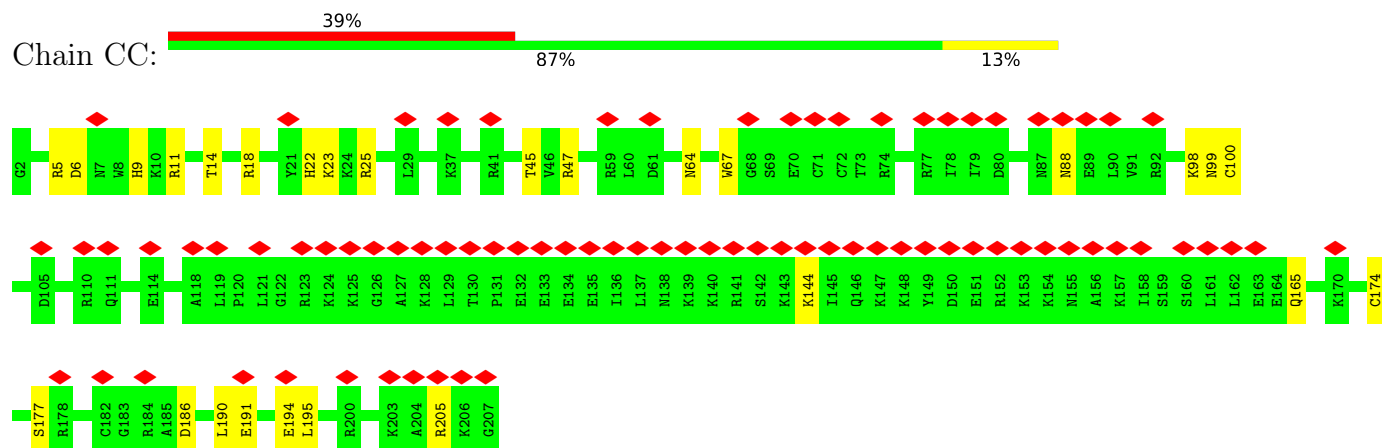
• Molecule 56: 40S ribosomal protein S6



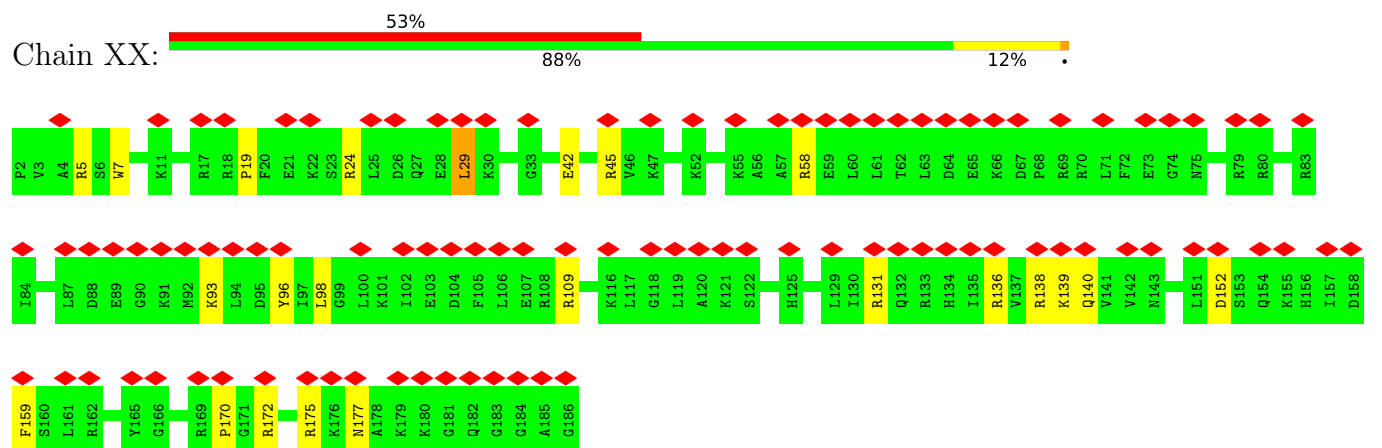
- Molecule 57: 40S ribosomal protein S7



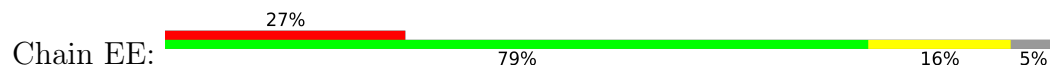
- Molecule 58: 40S ribosomal protein S8

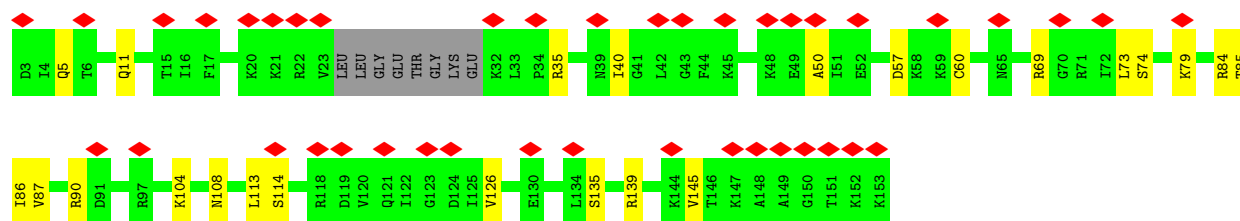


- Molecule 59: Ribosomal protein S9 (Predicted)

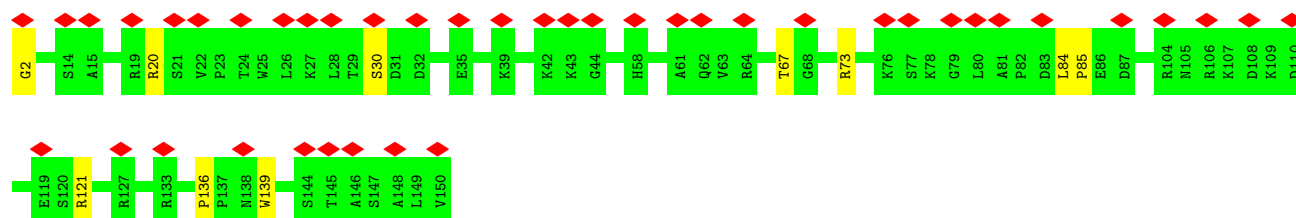


- Molecule 60: Ribosomal protein S11

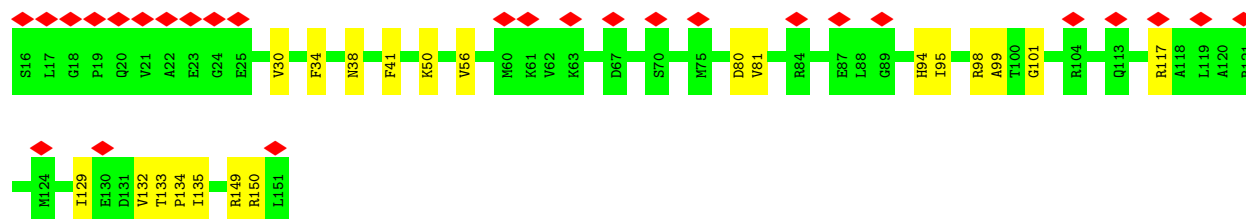
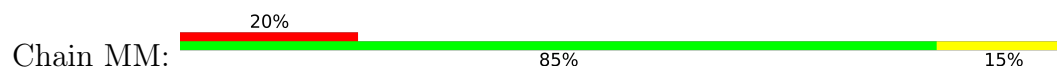




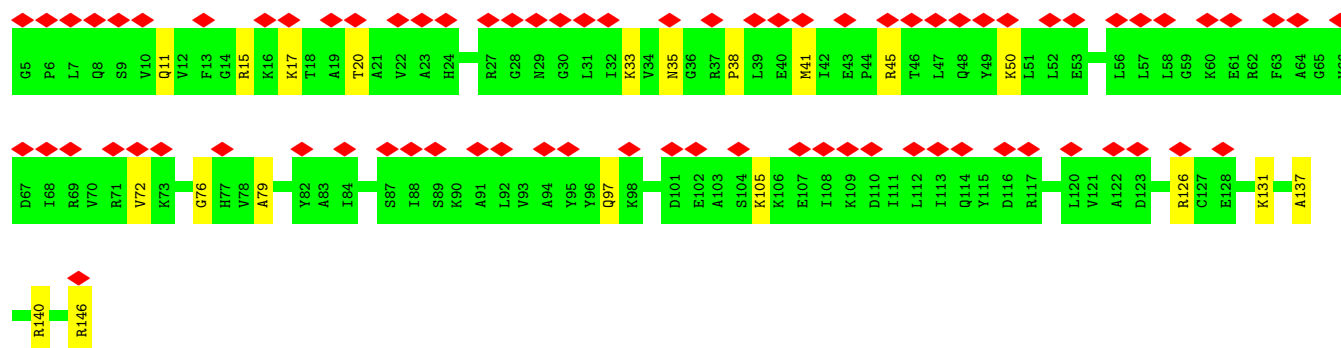
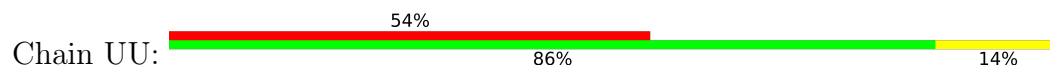
- Molecule 61: ribosomal protein uS15



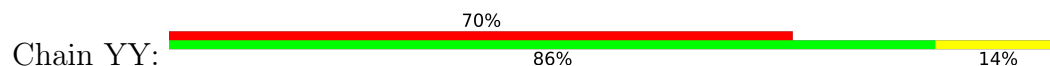
- Molecule 62: uS11

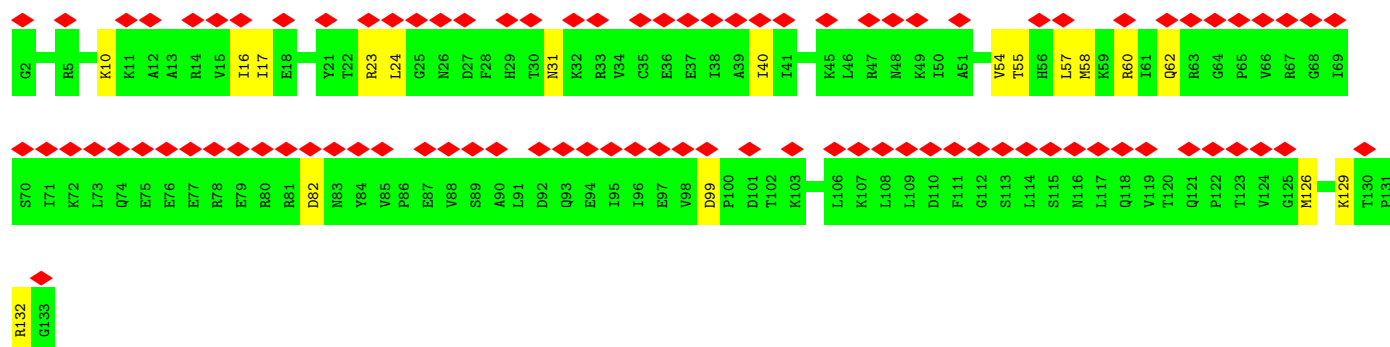


- Molecule 63: Ribosomal protein S16

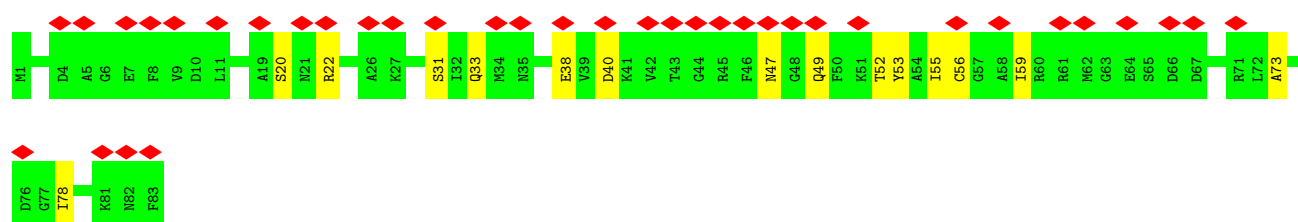
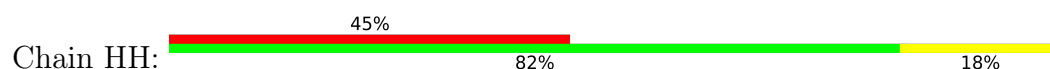


- Molecule 64: eS17

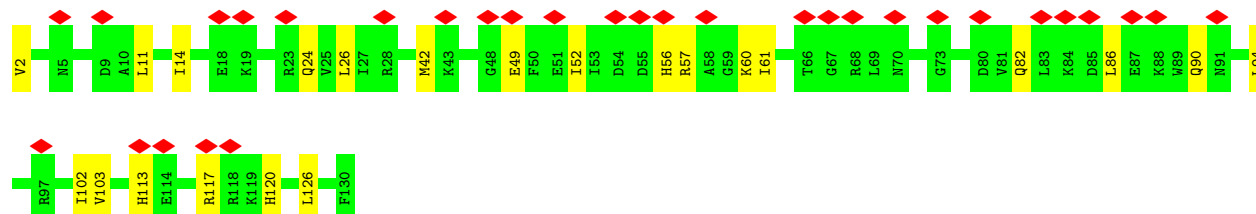
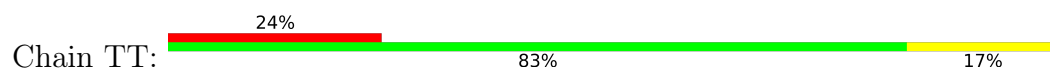




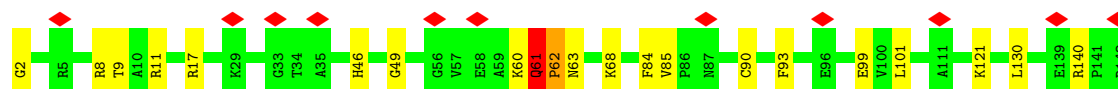
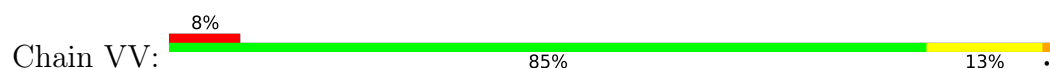
- Molecule 65: eS21



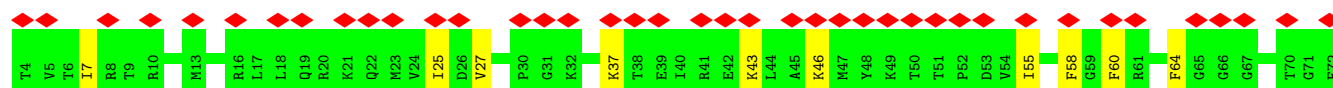
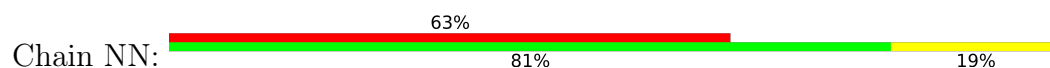
- Molecule 66: Ribosomal protein S15a

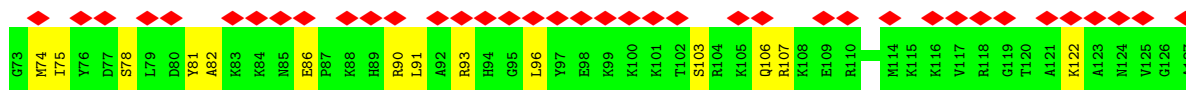


- Molecule 67: Ribosomal protein S23

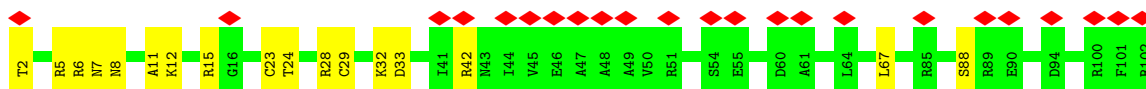
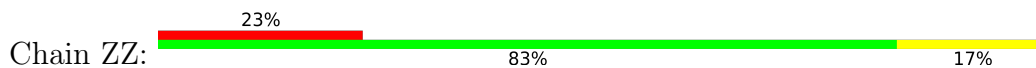


- Molecule 68: eS24

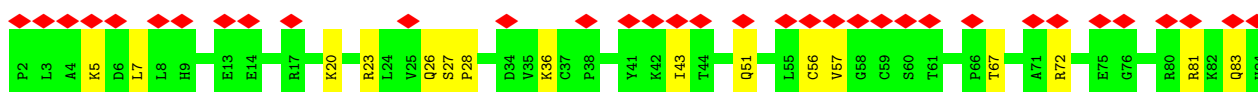
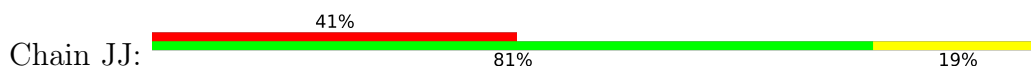




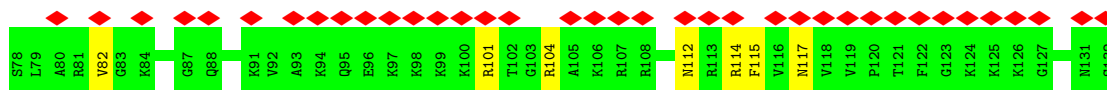
- Molecule 69: eS26



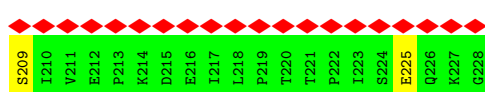
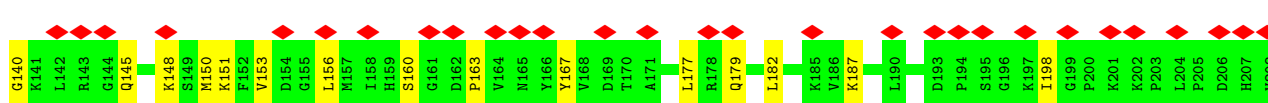
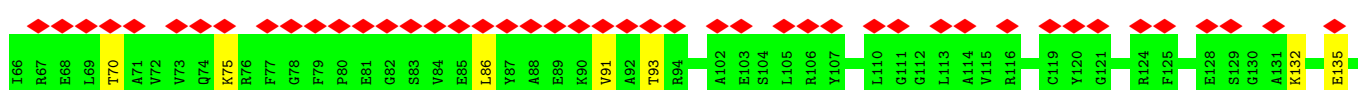
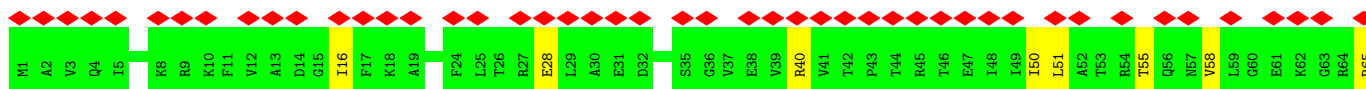
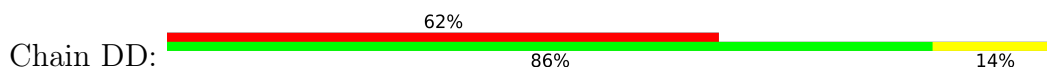
- Molecule 70: 40S ribosomal protein S27



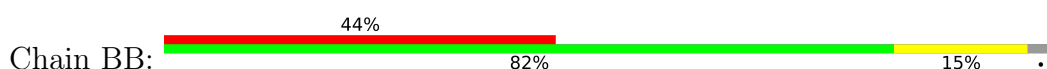
- Molecule 71: 40S ribosomal protein S30

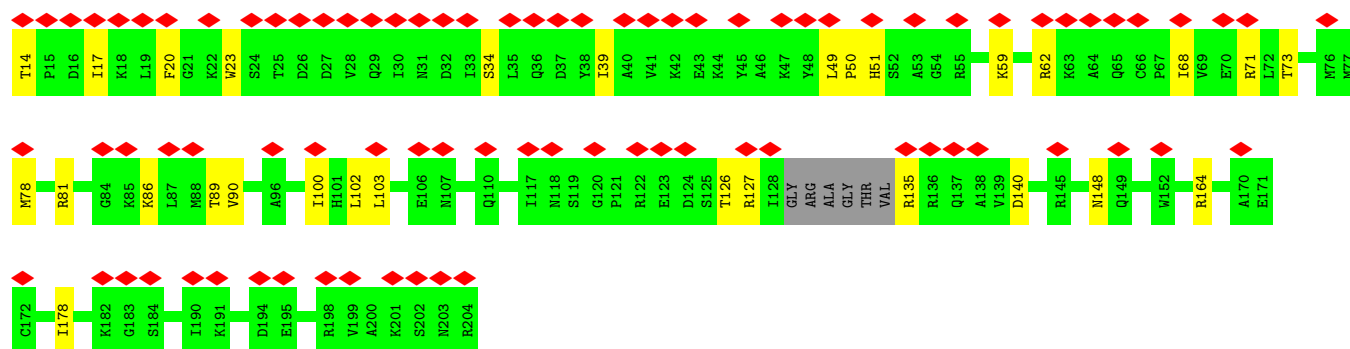


- Molecule 72: Ribosomal protein S3

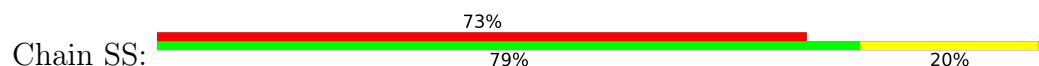


- Molecule 73: Ribosomal protein S5

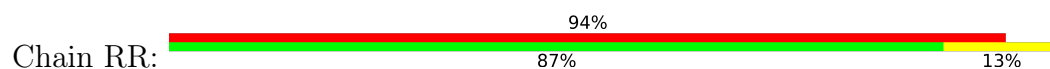




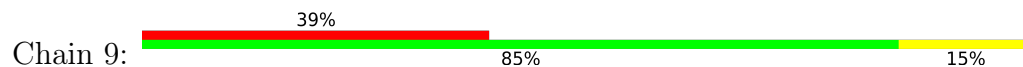
• Molecule 74: eS10



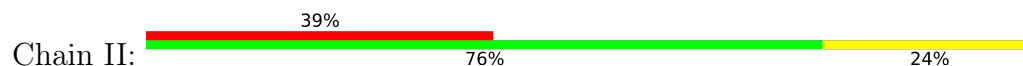
• Molecule 75: 40S ribosomal protein S12

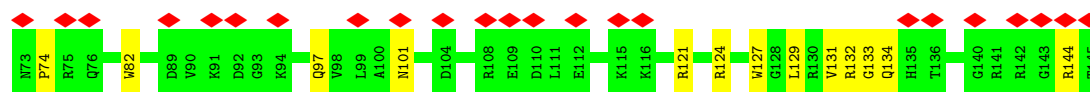


• Molecule 76: uS14

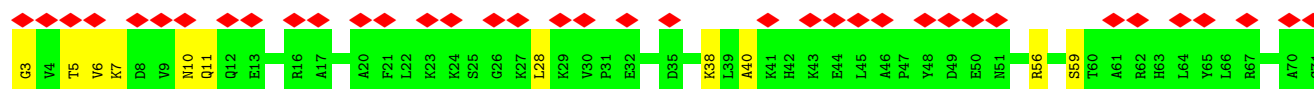
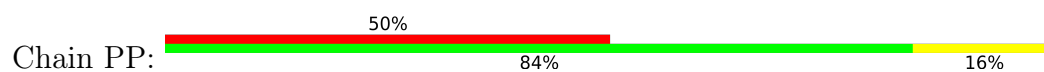


• Molecule 77: uS13

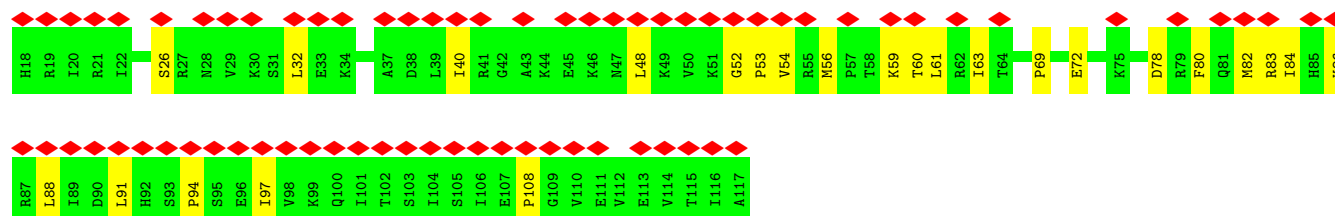
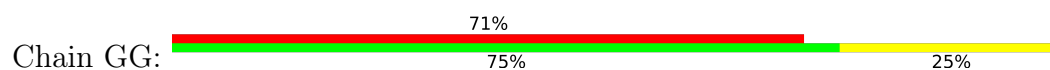




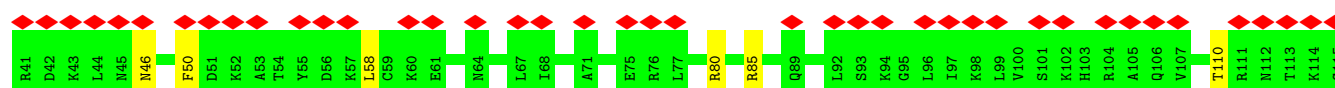
• Molecule 78: eS19



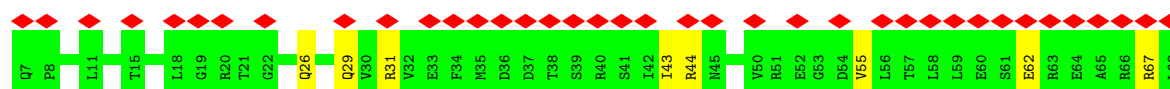
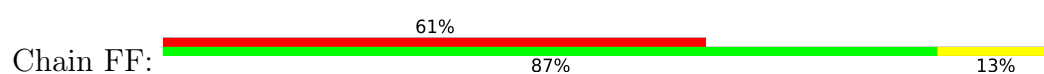
• Molecule 79: uS10



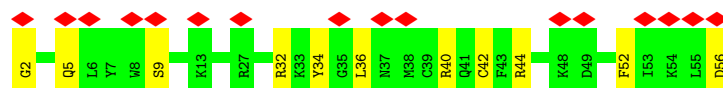
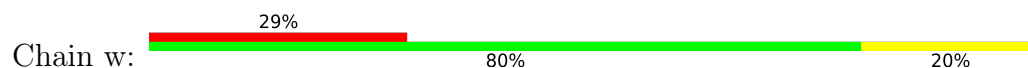
• Molecule 80: ribosomal protein eS25



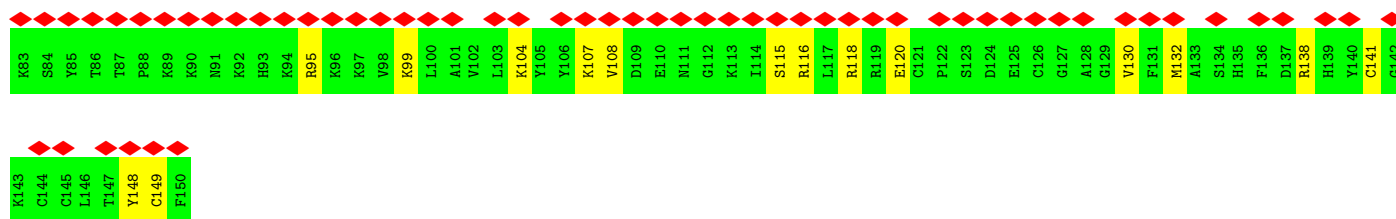
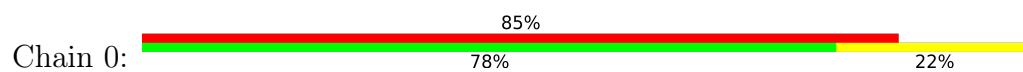
• Molecule 81: Ribosomal protein S28



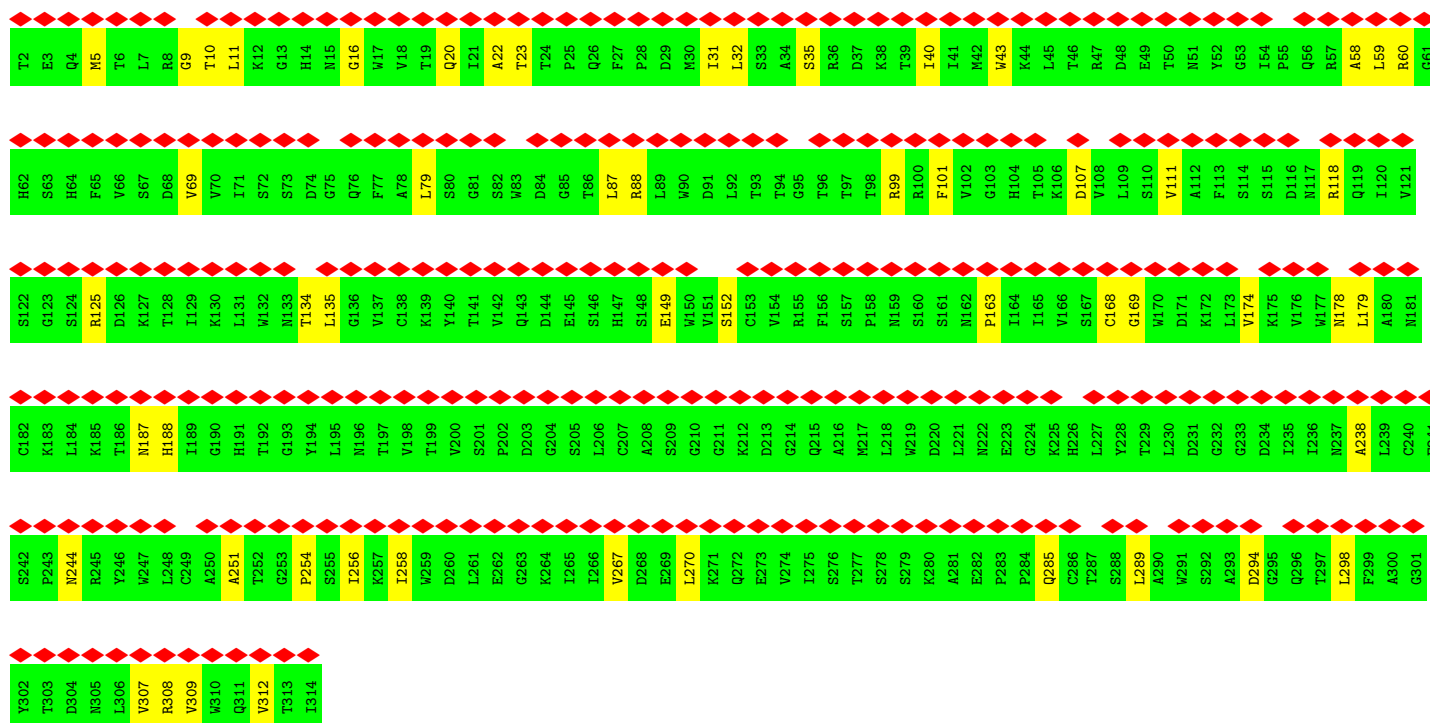
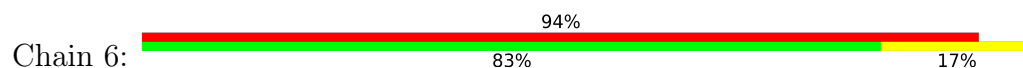
• Molecule 82: S29



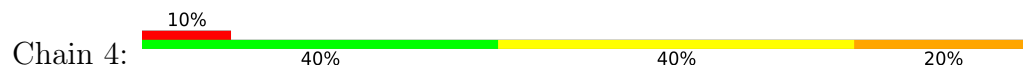
• Molecule 83: eS31



• Molecule 84: ribosomal protein RACK1



• Molecule 85: mRNA



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	94923	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	28	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	FEI FALCON II (4k x 4k)	Depositor
Maximum map value	0.741	Depositor
Minimum map value	-0.435	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.024	Depositor
Recommended contour level	0.08	Depositor
Map size ($\text{\AA}$)	429.264, 429.264, 429.264	wwPDB
Map dimensions	396, 396, 396	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.084, 1.084, 1.084	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	5	0.17	0/87794	0.36	11/136953 (0.0%)
2	7	0.15	0/2858	0.30	0/4455
3	8	0.16	0/3701	0.34	0/5766
4	A	0.21	0/1906	0.54	0/2556
5	B	0.18	0/3216	0.50	2/4311 (0.0%)
6	C	0.19	0/2937	0.49	0/3946
7	D	0.17	0/2432	0.49	0/3257
8	E	0.21	0/1936	0.62	2/2600 (0.1%)
9	F	0.21	0/1905	0.52	0/2539
10	G	0.21	0/1967	0.57	1/2647 (0.0%)
11	H	0.19	0/1535	0.53	0/2063
12	I	0.17	0/1693	0.43	0/2260
13	J	0.19	0/1376	0.52	0/1841
14	L	0.22	0/1734	0.58	0/2317
15	M	0.20	0/1158	0.51	0/1547
16	N	0.20	0/1746	0.55	1/2338 (0.0%)
17	O	0.21	0/1671	0.49	0/2234
18	P	0.30	0/1268	0.54	0/1700
19	Q	0.19	0/1530	0.53	0/2041
20	R	0.22	0/1524	0.59	2/2013 (0.1%)
21	S	0.19	0/1493	0.47	0/2002
22	T	0.18	0/1326	0.50	0/1770
23	U	0.17	0/822	0.50	0/1103
24	V	0.19	0/993	0.54	0/1332
25	W	0.17	0/541	0.49	0/720
26	X	0.18	0/993	0.46	0/1334
27	Y	0.18	0/1132	0.49	0/1504
28	Z	0.20	0/1130	0.54	2/1507 (0.1%)
29	a	0.19	0/1191	0.50	0/1590
30	b	0.18	0/619	0.47	0/818
31	c	0.18	0/742	0.44	0/996
32	d	0.21	0/903	0.50	0/1216

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	e	0.18	0/1071	0.50	0/1429
34	f	0.18	0/895	0.53	0/1198
35	g	0.19	0/916	0.53	0/1220
36	h	0.21	0/1021	0.52	0/1348
37	i	0.18	0/841	0.51	0/1112
38	j	0.19	0/720	0.49	0/952
39	k	0.25	0/575	0.67	2/761 (0.3%)
40	l	0.19	0/454	0.45	0/599
41	m	0.23	0/435	0.60	0/575
42	n	0.21	0/223	0.50	0/284
43	o	0.19	0/864	0.55	0/1140
44	p	0.17	0/718	0.47	0/953
45	r	0.27	0/1017	0.73	1/1364 (0.1%)
46	s	0.18	0/1547	0.47	0/2088
47	t	0.30	0/1257	0.77	4/1697 (0.2%)
48	1	0.42	0/216	0.57	0/298
49	2	0.19	0/1802	0.39	0/2804
50	3	0.14	0/1783	0.32	0/2773
51	K	0.16	0/40530	0.35	4/63160 (0.0%)
52	q	0.17	0/1747	0.45	0/2374
53	u	0.17	0/1756	0.46	0/2350
54	v	0.17	0/1753	0.44	0/2369
55	x	0.15	0/2118	0.44	0/2849
56	z	0.16	0/1946	0.42	0/2590
57	y	0.17	0/1510	0.45	0/2022
58	CC	0.17	0/1715	0.46	0/2287
59	XX	0.17	0/1550	0.45	0/2069
60	EE	0.16	0/1195	0.44	0/1597
61	QQ	0.17	0/1226	0.40	0/1649
62	MM	0.15	0/1029	0.43	0/1380
63	UU	0.19	0/1146	0.48	0/1534
64	YY	0.16	0/1082	0.41	0/1452
65	HH	0.15	0/643	0.41	0/860
66	TT	0.18	0/1051	0.47	0/1406
67	VV	0.20	0/1116	0.50	0/1490
68	NN	0.15	0/1028	0.43	0/1366
69	ZZ	0.18	0/828	0.49	0/1109
70	JJ	0.15	0/665	0.41	0/891
71	AA	0.15	0/447	0.45	0/587
72	DD	0.20	0/1796	0.50	0/2417
73	BB	0.19	0/1492	0.48	0/2005
74	SS	0.20	0/834	0.54	0/1125
75	RR	0.21	0/918	0.51	0/1233

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
76	9	0.19	0/1017	0.51	0/1358
77	II	0.20	0/1208	0.53	0/1618
78	PP	0.18	0/1115	0.46	0/1493
79	GG	0.16	0/805	0.44	0/1081
80	OO	0.16	0/604	0.41	0/810
81	FF	0.13	0/490	0.39	0/656
82	w	0.15	0/470	0.45	0/623
83	0	0.13	0/567	0.38	0/753
84	6	0.15	0/2493	0.43	0/3394
85	4	0.32	0/235	0.53	0/363
All	All	0.18	0/234252	0.42	32/344191 (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
5	B	0	2
20	R	0	1
21	S	0	1
23	U	0	1
34	f	0	1
67	VV	0	2
76	9	0	2
All	All	0	10

There are no bond length outliers.

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	5	2015	U	C2'-C3'-O3'	8.14	125.91	113.70
10	G	27	VAL	N-CA-C	-6.26	106.61	113.43
1	5	2017	A	C2'-C3'-O3'	-6.11	104.54	113.70
51	K	798	G	C2'-C3'-O3'	5.65	117.98	109.50
47	t	93	LYS	CA-C-N	5.51	130.47	122.36
47	t	93	LYS	C-N-CA	5.51	130.47	122.36
1	5	2017	A	C3'-C2'-O2'	5.46	118.89	110.70
8	E	65	TYR	CA-C-N	5.43	131.91	121.54
8	E	65	TYR	C-N-CA	5.43	131.91	121.54
1	5	2256	C	P-O3'-C3'	5.41	128.31	120.20
1	5	956	A	P-O3'-C3'	5.37	128.25	120.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	5	2046	G	P-O3'-C3'	5.34	128.21	120.20
1	5	2107	C	P-O3'-C3'	5.33	128.20	120.20
1	5	5027	C	P-O3'-C3'	5.33	128.19	120.20
45	r	20	ARG	CA-CB-CG	5.33	124.75	114.10
51	K	304	C	C2'-C3'-O3'	5.33	117.49	109.50
1	5	4889	G	P-O3'-C3'	5.28	128.12	120.20
51	K	798	G	C4'-C3'-O3'	5.27	117.31	109.40
16	N	177	GLY	N-CA-C	5.25	118.39	111.52
1	5	2695	A	P-O3'-C3'	5.23	128.05	120.20
20	R	38	ARG	CA-C-N	5.23	131.52	121.54
20	R	38	ARG	C-N-CA	5.23	131.52	121.54
39	k	29	LYS	CA-C-N	5.21	131.96	123.93
39	k	29	LYS	C-N-CA	5.21	131.96	123.93
47	t	97	ASN	CA-C-N	5.20	131.05	121.70
47	t	97	ASN	C-N-CA	5.20	131.05	121.70
28	Z	29	ILE	CA-C-N	5.13	131.35	121.54
28	Z	29	ILE	C-N-CA	5.13	131.35	121.54
51	K	688	U	P-O3'-C3'	5.13	127.89	120.20
1	5	2257	C	P-O3'-C3'	5.08	127.82	120.20
5	B	213	GLN	CA-C-N	5.01	129.52	122.46
5	B	213	GLN	C-N-CA	5.01	129.52	122.46

There are no chirality outliers.

All (10) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
76	9	17	TYR	Peptide
76	9	37	TYR	Peptide
5	B	17	LEU	Peptide
5	B	258	HIS	Peptide
20	R	18	GLY	Peptide
21	S	164	LYS	Peptide
23	U	27	HIS	Peptide
67	VV	61	GLN	Peptide,Mainchain
34	f	106	TYR	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	5	78486	0	39654	633	0
2	7	2558	0	1296	20	0
3	8	3314	0	1683	33	0
4	A	1868	0	1959	44	0
5	B	3148	0	3267	53	0
6	C	2883	0	3053	39	0
7	D	2386	0	2419	32	0
8	E	1898	0	2035	35	0
9	F	1870	0	1994	34	0
10	G	1934	0	2087	20	0
11	H	1516	0	1597	20	0
12	I	1655	0	1704	26	0
13	J	1353	0	1386	12	0
14	L	1703	0	1820	23	0
15	M	1137	0	1211	16	0
16	N	1701	0	1749	33	0
17	O	1638	0	1777	25	0
18	P	1242	0	1274	18	0
19	Q	1506	0	1623	18	0
20	R	1508	0	1664	15	0
21	S	1454	0	1496	26	0
22	T	1298	0	1366	24	0
23	U	808	0	831	7	0
24	V	979	0	1039	16	0
25	W	528	0	541	6	0
26	X	976	0	1053	10	0
27	Y	1115	0	1205	19	0
28	Z	1107	0	1182	14	0
29	a	1162	0	1209	21	0
30	b	609	0	650	10	0
31	c	732	0	769	8	0
32	d	888	0	930	10	0
33	e	1053	0	1147	20	0
34	f	876	0	912	19	0
35	g	906	0	998	16	0
36	h	1013	0	1147	22	0
37	i	830	0	916	8	0
38	j	705	0	737	18	0
39	k	569	0	637	2	0
40	l	444	0	483	8	0
41	m	429	0	465	11	0
42	n	222	0	264	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
43	o	851	0	921	8	0
44	p	708	0	757	7	0
45	r	1001	0	1060	20	0
46	s	1523	0	1577	16	0
47	t	1238	0	1295	12	0
48	1	204	0	193	24	0
49	2	1614	0	821	25	0
50	3	1597	0	813	6	0
51	K	36248	0	18309	340	0
52	q	1710	0	1708	17	0
53	u	1729	0	1803	26	0
54	v	1716	0	1806	21	0
55	x	2076	0	2177	24	0
56	z	1923	0	2089	23	0
57	y	1488	0	1582	13	0
58	CC	1686	0	1772	22	0
59	XX	1525	0	1640	19	0
60	EE	1175	0	1249	16	0
61	QQ	1202	0	1289	7	0
62	MM	1016	0	1039	15	0
63	UU	1128	0	1195	16	0
64	YY	1068	0	1121	13	0
65	HH	636	0	637	9	0
66	TT	1034	0	1080	16	0
67	VV	1098	0	1167	20	0
68	NN	1011	0	1083	15	0
69	ZZ	814	0	867	14	0
70	JJ	651	0	672	11	0
71	AA	443	0	492	6	0
72	DD	1768	0	1866	22	0
73	BB	1471	0	1522	21	0
74	SS	810	0	836	12	0
75	RR	908	0	939	9	0
76	9	997	0	1045	13	0
77	II	1190	0	1249	24	0
78	PP	1097	0	1132	16	0
79	GG	795	0	862	17	0
80	OO	598	0	656	7	0
81	FF	488	0	514	8	0
82	w	459	0	452	11	0
83	0	555	0	567	11	0
84	6	2436	0	2393	35	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
85	4	211	0	108	7	0
86	5	148	0	0	0	0
86	7	4	0	0	0	0
86	8	1	0	0	0	0
86	I	1	0	0	0	0
86	P	1	0	0	0	0
86	Q	1	0	0	0	0
86	V	1	0	0	0	0
86	e	1	0	0	0	0
86	g	1	0	0	0	0
87	g	1	0	0	0	0
87	j	1	0	0	0	0
87	m	1	0	0	0	0
87	o	1	0	0	0	0
87	p	1	0	0	0	0
All	All	218067	0	161584	1872	0

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

All (1872) 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)
51:K:1096:G:H1	51:K:1136:U:H3	1.07	1.02
51:K:1452:A:H61	51:K:1473:G:H21	1.02	0.98
1:5:2017:A:H5'	1:5:2017:A:C8	1.99	0.97
51:K:1726:G:H1	51:K:1808:U:H3	0.99	0.96
1:5:2017:A:H5'	1:5:2017:A:H8	1.30	0.94
1:5:4451:G:O4'	48:1:256:TRP:NE1	2.02	0.92
51:K:1232:U:H3	51:K:1526:G:H1	1.15	0.91
1:5:4397:A:C2	48:1:259:LEU:HD22	2.07	0.90
51:K:1718:G:H21	51:K:1815:A:H62	1.16	0.89
49:2:1:G:O6	49:2:73:A:N6	2.05	0.88
51:K:305:U:OP2	51:K:309:G:OP1	1.92	0.88
51:K:925:G:H1	51:K:1017:U:H3	1.21	0.87
1:5:184:U:H3	1:5:253:G:H1	1.23	0.87
51:K:1652:G:H1	51:K:1672:U:H3	1.17	0.87
51:K:1452:A:H61	51:K:1473:G:N2	1.74	0.86
51:K:1452:A:N6	51:K:1473:G:H21	1.72	0.85
1:5:2573:A:H62	1:5:2761:U:H3	1.23	0.85
51:K:1352:G:H1	51:K:1359:U:H3	1.20	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:5:3907:G:HO2'	1:5:3909:C:H5	1.26	0.84
51:K:1656:G:H1	51:K:1668:U:H3	1.24	0.83
1:5:3946:G:H1	1:5:4067:U:H3	1.25	0.83
49:2:35:A:O2'	51:K:626:A:C8	2.31	0.82
49:2:34:C:N4	85:4:51:G:H1	1.78	0.82
1:5:2557:G:H1	1:5:2570:U:H3	1.27	0.82
67:VV:61:GLN:OE1	67:VV:61:GLN:HA	1.79	0.81
1:5:2845:A:H61	1:5:3843:C:H42	1.28	0.81
51:K:924:G:H1	51:K:1018:U:H3	1.27	0.80
51:K:944:A:H61	51:K:982:G:H1	1.26	0.79
50:3:6:G:H1	50:3:67:U:H3	1.28	0.79
1:5:81:C:H1'	1:5:1359:G:H21	1.48	0.78
49:2:34:C:H42	85:4:51:G:H1	1.29	0.78
51:K:442:C:H42	51:K:449:A:H62	1.31	0.78
51:K:305:U:OP2	51:K:309:G:P	2.42	0.78
1:5:3909:C:O2'	49:2:76:A:O2'	1.85	0.76
51:K:1718:G:N2	51:K:1815:A:H62	1.82	0.75
51:K:322:C:C6	51:K:322:C:H5''	2.22	0.74
51:K:797:C:O2'	51:K:798:G:H5'	1.87	0.74
1:5:4451:G:N9	48:1:256:TRP:CD1	2.56	0.74
1:5:4451:G:C8	48:1:256:TRP:CD1	2.75	0.74
51:K:799:U:OP1	57:y:107:LYS:O	2.05	0.74
51:K:1718:G:H21	51:K:1815:A:N6	1.86	0.73
8:E:171:VAL:HB	8:E:183:ARG:O	1.89	0.72
49:2:1:G:C6	49:2:73:A:N1	2.56	0.72
51:K:1166:G:H1	51:K:1193:U:H3	1.35	0.72
51:K:1533:A:H62	51:K:1602:U:H3	1.34	0.72
32:d:70:LYS:O	32:d:74:ALA:HB2	1.89	0.72
1:5:4451:G:C8	48:1:256:TRP:HD1	2.08	0.71
1:5:4945:G:H21	34:f:71:TRP:HE1	1.38	0.71
12:I:48:LEU:HB2	12:I:140:THR:O	1.91	0.70
12:I:87:ILE:HG12	12:I:138:ILE:HG12	1.74	0.70
51:K:303:C:C2'	51:K:304:C:H5'	2.22	0.70
60:EE:85:THR:HA	60:EE:113:LEU:H	1.57	0.69
1:5:4397:A:N3	48:1:259:LEU:HD22	2.08	0.69
51:K:1533:A:N6	51:K:1602:U:H3	1.89	0.69
49:2:1:G:C6	49:2:73:A:C6	2.80	0.69
8:E:158:VAL:HG11	8:E:171:VAL:HG13	1.72	0.69
1:5:3692:A:H62	1:5:3823:G:H21	1.41	0.69
62:MM:34:PHE:HB3	62:MM:41:PHE:HB2	1.75	0.69
68:NN:82:ALA:O	68:NN:86:GLU:HB3	1.93	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:E:54:SER:HG	8:E:57:ALA:H	1.41	0.68
51:K:322:C:H5''	51:K:322:C:H6	1.58	0.68
51:K:934:G:H1	51:K:1008:A:H2	1.40	0.68
51:K:1033:G:H1	51:K:1080:A:HO2'	1.41	0.68
1:5:4926:C:H2'	1:5:4927:G:H21	1.58	0.68
51:K:1533:A:N6	51:K:1602:U:N3	2.43	0.67
51:K:1743:G:H21	51:K:1791:A:H62	1.41	0.67
52:q:77:ILE:HG12	52:q:99:ILE:HD12	1.76	0.67
84:6:87:LEU:HB2	84:6:101:PHE:HB2	1.76	0.67
35:g:60:ARG:HD3	35:g:61:PRO:HD2	1.77	0.67
1:5:2845:A:H61	1:5:3843:C:N4	1.92	0.66
15:M:40:GLY:HA3	15:M:45:VAL:HB	1.77	0.66
1:5:5022:U:H3	1:5:5025:C:N4	1.92	0.66
4:A:180:LEU:HD21	44:p:26:VAL:HG21	1.76	0.66
1:5:3642:A:HO2'	38:j:2:THR:N	1.94	0.65
51:K:798:G:OP2	51:K:798:G:H8	1.78	0.65
51:K:851:C:H5''	51:K:852:G:H5'	1.78	0.65
67:VV:49:GLY:O	67:VV:99:GLU:HA	1.95	0.65
51:K:38:A:H5''	59:XX:5:ARG:HD3	1.79	0.65
51:K:1844:U:H3	51:K:1855:G:H1	1.42	0.65
51:K:1737:G:H1	51:K:1797:U:H3	1.43	0.65
21:S:82:LEU:HG	21:S:113:MET:HE3	1.79	0.64
1:5:978:G:H5''	8:E:41:SER:HA	1.79	0.64
1:5:2845:A:N6	1:5:3843:C:H42	1.96	0.64
3:8:96:C:H5''	36:h:66:LYS:HD2	1.78	0.64
51:K:380:G:N3	58:CC:5:ARG:NH1	2.45	0.64
1:5:1740:C:O2	1:5:1786:A:N6	2.31	0.64
7:D:103:LEU:HD11	7:D:248:ARG:HE	1.63	0.64
36:h:70:ARG:O	36:h:74:LYS:HB2	1.98	0.64
84:6:107:ASP:HB2	84:6:125:ARG:HD2	1.80	0.63
14:L:31:ARG:HG2	14:L:34:ARG:HH21	1.63	0.63
65:HH:40:ASP:HB2	65:HH:47:ASN:HD21	1.63	0.63
1:5:4397:A:C2	48:1:259:LEU:CD2	2.80	0.63
10:G:58:PRO:HD2	10:G:61:ILE:HD12	1.79	0.63
64:YY:23:ARG:HH12	84:6:149:GLU:HG2	1.64	0.63
2:7:49:A:H3'	7:D:225:GLN:HE22	1.63	0.62
57:y:154:ILE:HB	57:y:185:VAL:HG22	1.80	0.62
51:K:1396:A:O2'	51:K:1398:G:N7	2.33	0.62
74:SS:3:MET:HG2	74:SS:44:HIS:HD2	1.65	0.62
1:5:1743:A:H1'	7:D:15:ARG:HH21	1.64	0.62
9:F:94:VAL:O	9:F:122:GLY:HA2	2.00	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:5:3868:G:H22	1:5:3900:G:H1'	1.64	0.62
1:5:962:C:H1'	45:r:108:MET:HG2	1.81	0.62
1:5:1398:A:H61	1:5:1419:G:H2'	1.64	0.62
15:M:24:LEU:HB2	15:M:43:THR:HG21	1.82	0.62
1:5:1972:G:H1	1:5:1994:C:H42	1.47	0.62
84:6:22:ALA:HB3	84:6:32:LEU:HB3	1.82	0.62
84:6:152:SER:H	84:6:169:GLY:HA2	1.63	0.61
1:5:2891:U:OP2	20:R:74:ARG:NH2	2.33	0.61
22:T:75:VAL:HG22	22:T:88:ARG:HG2	1.82	0.61
1:5:3907:G:O2'	1:5:3909:C:H5	1.84	0.61
18:P:125:MET:HB2	18:P:141:SER:HB3	1.82	0.61
45:r:63:VAL:HG22	45:r:79:ARG:HG2	1.83	0.61
1:5:4688:C:HO2'	11:H:155:SER:HG	1.49	0.61
2:7:28:C:H1'	2:7:54:A:H61	1.65	0.61
6:C:134:PRO:HD3	45:r:71:ARG:HE	1.64	0.61
13:J:167:GLN:HA	13:J:172:GLY:H	1.65	0.61
49:2:34:C:N3	85:4:51:G:N2	2.47	0.61
1:5:959:G:H21	8:E:121:LEU:H	1.48	0.61
1:5:1726:U:H3	1:5:1836:G:H1	1.48	0.61
72:DD:40:ARG:HG2	79:GG:108:PRO:HG3	1.83	0.61
1:5:1358:G:N2	1:5:1359:G:O6	2.34	0.61
76:9:98:ASN:ND2	76:9:103:ASN:OD1	2.34	0.61
1:5:4871:C:H42	21:S:157:ARG:HE	1.49	0.61
1:5:4910:G:H4'	5:B:95:THR:HG22	1.83	0.61
51:K:639:C:H2'	51:K:640:A:H8	1.66	0.61
58:CC:165:GLN:HE22	58:CC:195:LEU:HD11	1.64	0.61
72:DD:163:PRO:O	72:DD:167:TYR:HB2	1.99	0.61
51:K:302:A:N3	58:CC:64:ASN:ND2	2.49	0.60
1:5:5022:U:N3	1:5:5025:C:N4	2.49	0.60
1:5:1185:G:N2	7:D:278:ASP:OD2	2.35	0.60
1:5:4747:C:H5''	34:f:54:LYS:HE3	1.82	0.60
22:T:4:THR:O	22:T:9:ARG:NH1	2.35	0.60
51:K:944:A:N6	51:K:982:G:H1	1.99	0.60
65:HH:31:SER:HA	65:HH:55:ILE:O	2.02	0.60
1:5:3697:U:H5''	1:5:3698:G:H5'	1.83	0.60
49:2:30:G:H1	49:2:40:C:H42	1.49	0.60
1:5:295:A:OP2	43:o:39:ARG:NH1	2.35	0.60
1:5:944:A:N6	9:F:190:GLU:OE1	2.35	0.60
1:5:2089:G:N3	6:C:307:LYS:NZ	2.50	0.60
51:K:957:A:H3'	51:K:958:G:H21	1.67	0.60
51:K:1091:C:HO2'	66:TT:2:VAL:N	2.00	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
51:K:1533:A:N6	51:K:1602:U:C2	2.70	0.60
4:A:30:ARG:O	4:A:163:ARG:NH2	2.35	0.59
7:D:83:LEU:HB3	7:D:88:VAL:HB	1.83	0.59
51:K:305:U:OP2	51:K:308:G:O3'	2.19	0.59
54:v:192:LEU:HB3	54:v:227:ARG:HB3	1.83	0.59
78:PP:124:THR:HG23	78:PP:127:GLY:H	1.67	0.59
24:V:70:PRO:HG2	51:K:1724:A:H5''	1.82	0.59
48:1:253:GLN:HE21	48:1:255:ALA:HB2	1.66	0.59
84:6:118:ARG:HH21	84:6:134:THR:H	1.50	0.59
1:5:2638:G:H1	1:5:2697:A:H61	1.48	0.59
1:5:3650:C:OP1	4:A:200:ARG:NH2	2.36	0.59
51:K:1611:G:OP2	77:II:121:ARG:NH1	2.35	0.59
1:5:2489:C:O2'	1:5:2491:C:N4	2.35	0.59
2:7:6:C:O2'	7:D:50:ARG:NH1	2.36	0.59
20:R:102:LEU:HD22	20:R:138:LEU:HD13	1.84	0.59
51:K:1854:U:OP1	62:MM:150:ARG:NH1	2.36	0.59
54:v:272:HIS:HA	54:v:275:LYS:HG2	1.85	0.59
84:6:10:THR:HG22	84:6:308:ARG:HG2	1.84	0.59
1:5:1320:U:O2'	1:5:1891:A:N1	2.34	0.59
1:5:1524:A:H61	1:5:1651:G:H22	1.50	0.59
1:5:2335:C:H2'	1:5:2336:G:H8	1.67	0.59
83:0:107:LYS:HB2	83:0:115:SER:HB3	1.84	0.59
1:5:2777:G:H5''	1:5:2778:G:H5'	1.84	0.59
1:5:3892:U:O2'	18:P:80:GLN:NE2	2.36	0.59
60:EE:60:CYS:HG	60:EE:114:SER:HG	1.51	0.59
11:H:44:GLU:HB3	11:H:58:ASP:HB2	1.85	0.59
1:5:4397:A:N3	48:1:259:LEU:CD2	2.66	0.58
3:8:21:C:OP1	6:C:195:LYS:NZ	2.36	0.58
5:B:220:ILE:HB	5:B:346:THR:HB	1.85	0.58
1:5:3907:G:N2	48:1:259:LEU:O	2.36	0.58
4:A:234:LYS:HG2	4:A:238:ILE:HD12	1.85	0.58
18:P:133:HIS:CG	48:1:246:LEU:HD21	2.38	0.58
51:K:1398:G:O2'	84:6:88:ARG:NH2	2.36	0.58
73:BB:71:ARG:NH1	73:BB:148:ASN:OD1	2.36	0.58
1:5:734:G:N2	1:5:930:G:O2'	2.36	0.58
2:7:59:G:H4'	7:D:267:ASN:HD21	1.69	0.58
51:K:1623:A:N7	77:II:132:ARG:NH1	2.49	0.58
84:6:256:ILE:HB	84:6:270:LEU:HB2	1.85	0.58
1:5:454:U:OP1	8:E:224:GLN:NE2	2.36	0.58
1:5:977:C:H2'	1:5:978:G:H8	1.67	0.58
12:I:33:ILE:O	12:I:69:ARG:NH2	2.36	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:d:64:ILE:HG23	32:d:68:LEU:HD23	1.84	0.58
55:x:80:ILE:HG13	55:x:81:THR:HG23	1.86	0.58
68:NN:7:ILE:HG12	68:NN:27:VAL:HG22	1.85	0.58
1:5:119:G:H1	10:G:133:PRO:HD2	1.68	0.58
1:5:3898:G:H1'	5:B:261:ARG:HA	1.84	0.58
1:5:280:G:OP2	16:N:44:ARG:NH1	2.36	0.58
5:B:14:LEU:HD23	5:B:17:LEU:HD21	1.86	0.58
51:K:1014:G:N2	70:JJ:51:GLN:OE1	2.36	0.58
79:GG:60:THR:HG22	79:GG:83:ARG:HG2	1.84	0.58
1:5:4949:G:N2	1:5:4950:U:O2'	2.36	0.58
51:K:1748:G:H1	51:K:1786:U:H3	1.51	0.58
1:5:404:U:O3'	27:Y:87:ARG:NH1	2.37	0.58
1:5:2458:C:H5''	16:N:67:ARG:HD2	1.86	0.58
51:K:1298:G:N7	76:9:79:HIS:ND1	2.51	0.58
62:MM:99:ALA:H	62:MM:133:THR:HG22	1.68	0.58
1:5:2303:C:H5''	33:e:104:SER:HB2	1.86	0.58
51:K:925:G:OP1	61:QQ:121:ARG:NH2	2.37	0.58
51:K:1854:U:H2'	51:K:1855:G:H8	1.67	0.58
54:v:191:VAL:HG11	54:v:236:PHE:HA	1.86	0.58
11:H:36:ARG:HB2	11:H:80:MET:HE1	1.85	0.57
51:K:1598:G:H3'	80:OO:80:ARG:HH21	1.68	0.57
63:UU:97:GLN:HE22	84:6:60:ARG:HE	1.52	0.57
1:5:2699:C:H5''	20:R:16:ARG:HH22	1.68	0.57
9:F:95:ILE:HA	9:F:121:ASN:O	2.03	0.57
36:h:80:PRO:HD2	36:h:83:LEU:HD12	1.86	0.57
77:II:14:ARG:HE	77:II:17:ASN:HA	1.68	0.57
84:6:11:LEU:HB2	84:6:307:VAL:HB	1.85	0.57
21:S:95:ARG:NH1	21:S:112:ASP:OD2	2.37	0.57
51:K:804:U:OP1	66:TT:82:GLN:NE2	2.37	0.57
76:9:81:ARG:NH1	76:9:98:ASN:OD1	2.35	0.57
1:5:35:U:O2'	1:5:1525:A:N1	2.38	0.57
1:5:1492:G:O2'	30:b:41:ARG:NH1	2.37	0.57
5:B:262:VAL:HG11	5:B:268:ARG:HH11	1.69	0.57
8:E:46:LEU:HD13	8:E:47:VAL:HG23	1.86	0.57
8:E:108:MET:O	45:r:87:ARG:NH1	2.38	0.57
84:6:152:SER:HG	84:6:168:CYS:HG	1.48	0.57
1:5:4761:G:OP2	17:O:12:ARG:NH2	2.38	0.57
3:8:52:A:OP1	40:l:21:ARG:NH1	2.38	0.57
9:F:151:SER:OG	9:F:247:ARG:NH2	2.38	0.57
47:t:57:ARG:HH11	47:t:83:LYS:HB3	1.69	0.57
1:5:933:G:H2'	1:5:940:C:H41	1.69	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:V:31:ASN:HD21	24:V:115:SER:HB2	1.69	0.57
1:5:279:A:OP2	16:N:50:ARG:NH2	2.38	0.57
1:5:1468:C:OP1	29:a:132:ARG:NH2	2.37	0.57
21:S:80:ILE:HD11	21:S:126:ILE:HD12	1.84	0.57
53:u:137:LEU:HG	53:u:215:VAL:HG22	1.86	0.57
1:5:2786:C:H5''	1:5:2787:A:H5'	1.85	0.57
1:5:4635:A:H2	1:5:4663:G:H21	1.53	0.57
18:P:130:TYR:CD2	18:P:130:TYR:N	2.73	0.57
51:K:1495:G:N2	82:w:42:CYS:SG	2.76	0.57
35:g:61:PRO:HA	35:g:64:LEU:HD13	1.86	0.57
1:5:3641:U:OP2	1:5:3646:A:N6	2.38	0.56
1:5:4712:C:H2'	1:5:4713:G:H8	1.69	0.56
4:A:54:ARG:HG2	4:A:56:ALA:H	1.70	0.56
7:D:41:LYS:NZ	22:T:32:ARG:O	2.38	0.56
9:F:129:LYS:HE2	9:F:133:ASN:HD21	1.70	0.56
51:K:444:G:OP2	58:CC:47:ARG:NH2	2.38	0.56
51:K:1222:G:H5''	73:BB:78:MET:HE3	1.86	0.56
68:NN:55:ILE:HG12	68:NN:75:ILE:HG12	1.87	0.56
1:5:658:C:H2'	1:5:659:G:H8	1.70	0.56
1:5:973:G:H21	6:C:327:LYS:HD2	1.70	0.56
1:5:1312:A:O2'	33:e:52:GLN:NE2	2.38	0.56
1:5:2457:G:OP1	16:N:65:ARG:NH1	2.38	0.56
1:5:1432:G:O2'	1:5:1452:A:N6	2.38	0.56
1:5:1802:A:N3	22:T:130:ARG:NH1	2.53	0.56
1:5:2345:G:N7	29:a:9:ARG:NH1	2.54	0.56
3:8:22:U:OP1	27:Y:11:ARG:NH2	2.39	0.56
20:R:42:ARG:HA	20:R:45:ILE:HD12	1.88	0.56
31:c:51:ASN:ND2	31:c:77:ASN:OD1	2.38	0.56
51:K:84:A:H5''	68:NN:122:LYS:HD2	1.88	0.56
51:K:986:G:OP2	51:K:988:C:N4	2.38	0.56
64:YY:40:ILE:HB	72:DD:209:SER:HB3	1.87	0.56
77:II:132:ARG:HB2	77:II:134:GLN:HE22	1.70	0.56
1:5:416:U:O2'	1:5:2309:G:N2	2.38	0.56
1:5:1571:G:O2'	20:R:130:ASN:ND2	2.39	0.56
1:5:4648:A:OP1	20:R:62:ARG:NH2	2.39	0.56
6:C:326:LEU:O	9:F:49:ARG:NH2	2.34	0.56
9:F:136:ARG:HA	9:F:139:GLU:HG3	1.88	0.56
51:K:482:G:N1	51:K:485:A:OP2	2.34	0.56
1:5:343:C:O2'	38:j:75:ARG:NH2	2.38	0.56
1:5:1332:C:H2'	1:5:1333:A:H8	1.71	0.56
1:5:2017:A:C8	1:5:2017:A:C5'	2.84	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:Q:16:LYS:O	19:Q:33:ARG:NH2	2.39	0.56
51:K:1373:C:O2'	64:YY:10:LYS:NZ	2.38	0.56
53:u:150:ILE:HD13	64:YY:129:LYS:HB2	1.86	0.56
1:5:74:G:O6	14:L:103:ARG:NH2	2.39	0.56
1:5:230:G:OP1	27:Y:15:ARG:NH1	2.38	0.56
1:5:303:C:OP2	16:N:68:ARG:NH2	2.39	0.56
1:5:4072:C:H2'	1:5:4073:A:H8	1.69	0.56
46:s:102:LEU:HB3	46:s:187:LEU:HD11	1.86	0.56
79:GG:78:ASP:OD2	82:w:44:ARG:NH1	2.39	0.56
51:K:913:A:N6	57:y:119:SER:O	2.38	0.56
60:EE:79:LYS:HB2	60:EE:87:VAL:HB	1.88	0.56
79:GG:40:ILE:HD11	79:GG:53:PRO:HG3	1.87	0.56
1:5:491:G:H1'	1:5:665:C:H42	1.71	0.56
1:5:1621:A:HO2'	4:A:14:SER:HG	1.53	0.56
1:5:2274:C:H5'	6:C:312:ARG:HB2	1.87	0.56
1:5:3657:U:OP1	4:A:245:ARG:NH1	2.39	0.56
1:5:4944:C:O2	1:5:4945:G:N2	2.39	0.56
12:I:16:PRO:HA	12:I:95:HIS:HD2	1.71	0.56
51:K:800:U:O4	57:y:106:ARG:NH1	2.39	0.56
66:TT:102:ILE:H	66:TT:113:HIS:HD2	1.54	0.56
1:5:1204:C:H2'	1:5:1205:G:H8	1.71	0.56
1:5:1269:G:N7	1:5:2111:G:N2	2.50	0.56
51:K:442:C:N4	51:K:449:A:H62	2.02	0.56
59:XX:136:ARG:NH1	59:XX:159:PHE:O	2.39	0.56
60:EE:74:SER:O	60:EE:90:ARG:NH1	2.39	0.56
67:VV:84:PHE:H	67:VV:121:LYS:HA	1.71	0.56
74:SS:20:VAL:HA	74:SS:69:TRP:O	2.05	0.56
47:t:123:ARG:HG3	47:t:129:ILE:HD11	1.86	0.56
51:K:492:C:OP2	68:NN:107:ARG:NH2	2.38	0.56
52:q:33:GLN:HB3	52:q:154:LEU:HD12	1.88	0.56
55:x:126:VAL:HA	55:x:141:THR:HA	1.88	0.56
76:9:44:ARG:NH1	76:9:48:GLY:O	2.39	0.56
1:5:248:C:O2	27:Y:121:ARG:NH2	2.39	0.55
1:5:1866:U:OP1	12:I:4:ARG:NH2	2.38	0.55
37:i:70:LEU:HD21	37:i:80:HIS:HE2	1.70	0.55
51:K:1036:A:N3	51:K:1844:U:O2'	2.40	0.55
55:x:72:ILE:HG12	55:x:90:ILE:HG12	1.88	0.55
79:GG:94:PRO:HD2	79:GG:97:ILE:HD12	1.87	0.55
51:K:1156:U:O4	54:v:194:ARG:NH1	2.39	0.55
1:5:1850:A:N3	1:5:2283:G:O2'	2.40	0.55
1:5:2447:U:H2'	1:5:2448:G:H8	1.70	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:48:GLY:HA3	5:B:81:THR:HG22	1.88	0.55
41:m:94:MET:HG2	41:m:105:PRO:HA	1.88	0.55
51:K:1617:G:O6	76:9:43:ARG:NH1	2.39	0.55
1:5:959:G:O2'	8:E:119:ARG:O	2.25	0.55
1:5:4768:G:H5'	17:O:176:ARG:HH12	1.71	0.55
45:r:119:ARG:HA	45:r:122:LYS:HE3	1.89	0.55
48:1:253:GLN:HG3	48:1:255:ALA:H	1.71	0.55
49:2:1:G:C6	49:2:73:A:N6	2.74	0.55
51:K:15:U:O2'	51:K:669:A:N6	2.38	0.55
51:K:877:C:H42	51:K:909:G:H1	1.55	0.55
69:ZZ:11:ALA:HB3	69:ZZ:33:ASP:HB2	1.87	0.55
84:6:244:ASN:ND2	84:6:294:ASP:O	2.39	0.55
1:5:109:G:OP2	14:L:74:ARG:NH2	2.39	0.55
1:5:3781:C:OP1	42:n:23:ARG:NH2	2.39	0.55
3:8:63:U:O2'	36:h:52:LYS:NZ	2.38	0.55
27:Y:59:ARG:HB2	27:Y:103:LYS:HD2	1.89	0.55
51:K:1301:A:OP2	82:w:2:GLY:N	2.39	0.55
53:u:122:GLU:O	53:u:165:ARG:NH2	2.40	0.55
1:5:726:G:OP1	9:F:75:ARG:NH2	2.39	0.55
1:5:969:C:O2'	1:5:970:G:N3	2.36	0.55
1:5:3680:U:OP1	4:A:54:ARG:NH2	2.39	0.55
5:B:170:LEU:O	5:B:328:ASN:ND2	2.39	0.55
68:NN:103:SER:OG	68:NN:106:GLN:OE1	2.25	0.55
1:5:3877:A:O2'	1:5:4400:G:N2	2.40	0.55
1:5:4145:C:H2'	1:5:4146:G:H8	1.71	0.55
51:K:57:U:O2'	51:K:499:G:N3	2.40	0.55
75:RR:56:CYS:SG	75:RR:82:ASN:ND2	2.80	0.55
1:5:67:C:OP2	1:5:312:G:N2	2.40	0.55
1:5:2020:U:OP1	46:s:58:ASN:ND2	2.40	0.55
3:8:75:G:OP2	27:Y:74:TYR:OH	2.24	0.55
48:1:260:MET:O	49:2:76:A:H4'	2.05	0.55
51:K:1533:A:OP2	73:BB:164:ARG:NH2	2.40	0.55
51:K:1824:A:N3	51:K:1824:A:O2'	2.36	0.55
53:u:86:LEU:HB3	53:u:98:THR:HB	1.88	0.55
63:UU:35:ASN:HD21	63:UU:72:VAL:HB	1.72	0.55
1:5:481:G:OP2	45:r:67:ARG:NH2	2.39	0.55
1:5:4419:U:OP1	1:5:4421:C:N4	2.40	0.55
4:A:147:ARG:HE	4:A:155:LYS:HE2	1.72	0.55
7:D:107:ARG:NH2	7:D:116:ASP:OD1	2.40	0.55
14:L:189:ALA:HB2	37:i:10:GLY:HA2	1.87	0.55
31:c:90:ARG:HH21	44:p:44:LYS:HE2	1.71	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
51:K:153:G:N3	56:z:13:GLN:NE2	2.55	0.55
51:K:1479:G:N2	82:w:56:ASP:OD1	2.39	0.55
1:5:436:C:H2'	1:5:437:G:H8	1.72	0.55
1:5:1306:C:H2'	1:5:1307:A:H8	1.72	0.55
1:5:1914:C:H4'	17:O:89:PRO:HD3	1.88	0.55
4:A:137:ILE:HD11	4:A:149:LYS:HB2	1.88	0.55
10:G:108:GLN:HG3	10:G:111:LYS:HD3	1.89	0.55
22:T:88:ARG:NH1	30:b:33:LYS:O	2.39	0.55
51:K:1864:U:H3'	69:ZZ:5:ARG:HH22	1.72	0.55
1:5:136:C:N4	36:h:76:LYS:O	2.40	0.54
1:5:730:G:H22	1:5:939:G:H22	1.55	0.54
1:5:1550:G:H1	1:5:1578:U:H3	1.54	0.54
23:U:65:ARG:HE	23:U:67:LYS:H	1.55	0.54
51:K:308:G:H3'	51:K:309:G:C5'	2.38	0.54
51:K:1599:U:OP2	80:OO:46:ASN:ND2	2.40	0.54
1:5:2280:G:N2	1:5:2281:U:O4	2.40	0.54
6:C:61:GLN:O	38:j:52:LYS:NZ	2.40	0.54
7:D:50:ARG:NH1	7:D:72:ASP:OD2	2.38	0.54
27:Y:10:ASP:HB3	27:Y:13:LYS:HB2	1.90	0.54
46:s:47:LEU:HB3	46:s:51:ALA:HB3	1.90	0.54
51:K:190:G:O2'	51:K:209:A:N6	2.40	0.54
75:RR:58:GLU:HB3	75:RR:61:TYR:HB3	1.89	0.54
1:5:431:G:H1'	1:5:3889:G:H5'	1.88	0.54
45:r:48:THR:HB	45:r:65:LYS:HB2	1.89	0.54
47:t:63:THR:HG22	47:t:72:GLU:HG3	1.88	0.54
59:XX:170:PRO:O	59:XX:175:ARG:NH1	2.40	0.54
1:5:1670:G:OP1	30:b:12:GLN:NE2	2.40	0.54
1:5:3908:A:N7	1:5:4449:A:N6	2.56	0.54
3:8:134:G:H5''	26:X:63:LYS:HD2	1.89	0.54
6:C:62:THR:HG21	6:C:86:ARG:HH21	1.72	0.54
10:G:137:ARG:HG3	10:G:146:LEU:HD21	1.88	0.54
12:I:193:ASP:OD2	12:I:198:LYS:NZ	2.40	0.54
27:Y:66:GLN:HB3	27:Y:84:ARG:HH21	1.73	0.54
28:Z:12:LEU:HB2	28:Z:81:MET:HB3	1.88	0.54
55:x:43:PRO:HD2	55:x:46:ILE:HD12	1.89	0.54
55:x:68:ARG:HG3	55:x:76:VAL:HG11	1.90	0.54
72:DD:148:LYS:NZ	72:DD:150:MET:SD	2.80	0.54
74:SS:59:LYS:HB3	74:SS:70:TYR:HB2	1.88	0.54
1:5:382:G:H4'	1:5:407:A:H61	1.72	0.54
1:5:3723:A:OP2	37:i:68:ARG:NH1	2.40	0.54
17:O:109:PRO:HB2	17:O:111:PRO:HD2	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
51:K:444:G:H3'	58:CC:47:ARG:HH12	1.71	0.54
1:5:4174:U:H2'	1:5:4175:G:H8	1.72	0.54
1:5:4760:G:OP2	17:O:12:ARG:NH1	2.41	0.54
5:B:223:THR:HB	5:B:275:HIS:H	1.72	0.54
7:D:166:ALA:HB1	7:D:171:LEU:HD12	1.88	0.54
55:x:222:LEU:HA	55:x:225:ILE:HD12	1.89	0.54
1:5:1921:C:N4	15:M:16:SER:OG	2.41	0.54
1:5:2106:G:H21	1:5:2108:G:H21	1.55	0.54
1:5:4997:G:OP1	32:d:83:ARG:NH1	2.41	0.54
21:S:143:LYS:HA	21:S:146:HIS:HD1	1.71	0.54
51:K:303:C:H2'	51:K:304:C:H5'	1.89	0.54
51:K:962:A:N1	51:K:1055:A:O2'	2.40	0.54
51:K:1596:U:OP2	80:OO:85:ARG:NH2	2.36	0.54
53:u:146:ARG:HB2	53:u:149:GLN:HB2	1.90	0.54
1:5:1376:C:OP2	1:5:1379:C:N4	2.41	0.54
1:5:1391:A:OP2	19:Q:181:ARG:NH1	2.41	0.54
1:5:4333:C:O2	22:T:8:ARG:NH1	2.40	0.54
53:u:142:PHE:HB2	53:u:209:ASP:HB3	1.90	0.54
55:x:197:ASN:HB3	55:x:209:HIS:HB2	1.90	0.54
6:C:65:GLU:HB3	6:C:80:ARG:HD3	1.90	0.54
19:Q:67:ILE:HD12	19:Q:96:PRO:HD2	1.90	0.54
34:f:36:ARG:HB2	34:f:80:ASN:HA	1.89	0.54
51:K:454:U:H5''	56:z:94:ARG:HG2	1.90	0.54
51:K:1012:A:O2'	51:K:1129:G:N2	2.35	0.54
55:x:100:ARG:HB2	55:x:114:ILE:HD13	1.89	0.54
1:5:419:A:N3	1:5:1332:C:O2'	2.39	0.54
3:8:51:U:OP2	40:l:21:ARG:NH2	2.39	0.54
15:M:11:ARG:HB3	15:M:27:ILE:HD12	1.89	0.54
43:o:2:VAL:N	43:o:90:HIS:O	2.41	0.54
47:t:57:ARG:NH1	47:t:83:LYS:O	2.41	0.54
49:2:1:G:N1	49:2:73:A:C6	2.76	0.54
51:K:1087:A:OP2	69:ZZ:8:ASN:ND2	2.41	0.54
54:v:252:THR:HB	54:v:255:LEU:HD23	1.90	0.54
81:FF:29:GLN:HE22	81:FF:67:ARG:HG3	1.73	0.54
1:5:4377:G:O6	29:a:42:ARG:NH2	2.41	0.53
1:5:4451:G:C1'	48:1:256:TRP:NE1	2.71	0.53
1:5:4670:C:O2'	1:5:4672:A:OP2	2.26	0.53
5:B:71:GLU:OE1	25:W:1:MET:N	2.41	0.53
11:H:59:LYS:HE3	11:H:66:GLU:HB3	1.89	0.53
67:VV:61:GLN:HB3	67:VV:62:PRO:HD3	1.90	0.53
3:8:150:C:N4	10:G:52:THR:O	2.40	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
72:DD:16:ILE:HD11	82:w:36:LEU:HD23	1.89	0.53
1:5:151:G:N7	10:G:141:ASN:ND2	2.57	0.53
1:5:717:U:H3	1:5:951:G:H1	1.56	0.53
1:5:2725:A:N6	20:R:88:ARG:O	2.42	0.53
3:8:27:U:H4'	6:C:53:ALA:HB3	1.90	0.53
3:8:122:G:H21	3:8:128:C:H5	1.56	0.53
34:f:7:CYS:HB2	34:f:103:VAL:HG23	1.89	0.53
34:f:40:GLU:O	34:f:109:ARG:NH2	2.42	0.53
51:K:930:C:O2'	51:K:1104:G:OP1	2.27	0.53
51:K:1661:A:OP2	82:w:32:ARG:NH1	2.42	0.53
78:PP:76:THR:HB	78:PP:94:ARG:HB3	1.91	0.53
83:0:116:ARG:NH1	83:0:120:GLU:OE2	2.42	0.53
1:5:110:C:O3'	36:h:110:LYS:NZ	2.41	0.53
1:5:279:A:O2'	16:N:14:LYS:NZ	2.41	0.53
1:5:2647:A:H62	1:5:2686:G:H8	1.56	0.53
1:5:967:C:H5'	8:E:106:ARG:HH22	1.73	0.53
1:5:2289:C:N4	45:r:24:THR:OG1	2.40	0.53
1:5:2706:G:N2	1:5:2709:C:OP2	2.42	0.53
1:5:4697:U:O3'	41:m:111:ARG:NH1	2.41	0.53
6:C:329:ASN:ND2	9:F:190:GLU:OE2	2.41	0.53
11:H:166:THR:OG1	11:H:168:LYS:NZ	2.41	0.53
23:U:24:ASP:HB3	23:U:69:LYS:HG3	1.91	0.53
66:TT:60:LYS:NZ	70:JJ:23:ARG:O	2.42	0.53
1:5:963:G:OP2	45:r:107:ARG:NH2	2.42	0.53
1:5:1518:A:H61	14:L:19:GLN:HE22	1.57	0.53
51:K:1086:G:OP2	69:ZZ:12:LYS:NZ	2.40	0.53
56:z:5:ILE:HD12	56:z:16:ILE:HD13	1.90	0.53
1:5:68:U:OP1	16:N:178:HIS:ND1	2.34	0.53
1:5:976:G:OP2	8:E:55:ARG:NH1	2.37	0.53
1:5:977:C:H5''	8:E:58:MET:HE2	1.91	0.53
1:5:2875:C:OP2	44:p:7:LYS:NZ	2.41	0.53
4:A:95:GLN:O	4:A:100:ASN:ND2	2.41	0.53
51:K:2:A:H5''	54:v:205:VAL:HG11	1.91	0.53
69:ZZ:11:ALA:O	69:ZZ:15:ARG:NH2	2.40	0.53
72:DD:70:THR:HG22	72:DD:86:LEU:HD13	1.90	0.53
72:DD:140:GLY:HA3	72:DD:182:LEU:HG	1.90	0.53
1:5:1210:C:O2	9:F:72:ARG:NH2	2.42	0.53
1:5:4661:G:N2	1:5:5004:C:O3'	2.41	0.53
3:8:141:C:O2'	16:N:136:ASP:OD2	2.26	0.53
8:E:184:ARG:NH2	8:E:210:ASP:OD1	2.41	0.53
9:F:164:ILE:HB	9:F:169:ILE:HD12	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
51:K:70:G:O2'	51:K:79:A:N6	2.42	0.53
54:v:196:ILE:HB	54:v:223:TYR:HB2	1.90	0.53
69:ZZ:42:ARG:HH21	69:ZZ:67:LEU:HD13	1.73	0.53
1:5:1350:C:O2	6:C:119:GLN:NE2	2.41	0.53
1:5:4177:C:OP1	16:N:93:LYS:NZ	2.38	0.53
5:B:287:ILE:HG12	5:B:331:VAL:HG12	1.91	0.53
46:s:29:ILE:HD12	46:s:191:GLN:HB3	1.90	0.53
51:K:934:G:O6	51:K:1008:A:N1	2.42	0.53
53:u:62:LEU:HD12	53:u:65:ARG:HD2	1.90	0.53
70:JJ:56:CYS:SG	70:JJ:57:VAL:N	2.81	0.53
1:5:2611:A:H5'	1:5:2688:G:H4'	1.90	0.53
1:5:5001:U:H4'	5:B:317:LEU:HB3	1.90	0.53
9:F:124:PHE:O	9:F:207:ASN:ND2	2.41	0.53
51:K:943:U:H2'	51:K:944:A:H8	1.74	0.53
51:K:1596:U:O2'	77:II:25:LYS:NZ	2.42	0.53
62:MM:56:VAL:HG12	62:MM:81:VAL:HG23	1.91	0.53
1:5:3839:G:N2	1:5:3843:C:O2'	2.42	0.52
1:5:4601:U:H2'	1:5:4602:A:H8	1.73	0.52
2:7:97:G:O5'	9:F:136:ARG:NH1	2.42	0.52
6:C:159:GLU:HA	6:C:217:ILE:HB	1.91	0.52
6:C:332:ALA:HA	6:C:335:MET:HB2	1.90	0.52
19:Q:82:VAL:HG12	19:Q:84:GLY:H	1.74	0.52
24:V:95:PHE:O	25:W:20:ARG:HB3	2.10	0.52
29:a:131:ARG:NH1	29:a:135:GLU:OE2	2.42	0.52
51:K:1227:G:N2	51:K:1635:C:O2'	2.42	0.52
72:DD:75:LYS:NZ	74:SS:34:GLU:OE2	2.39	0.52
1:5:499:G:OP2	1:5:501:C:N4	2.37	0.52
1:5:2459:G:N2	1:5:2462:C:OP2	2.42	0.52
15:M:55:MET:O	21:S:157:ARG:NH2	2.43	0.52
50:3:32:C:OP2	63:UU:146:ARG:NH2	2.42	0.52
84:6:23:THR:HG22	84:6:31:ILE:HD11	1.92	0.52
1:5:689:U:H4'	45:r:85:ASN:HB2	1.91	0.52
1:5:1795:A:N3	2:7:79:U:O2'	2.42	0.52
1:5:2800:G:H1'	38:j:9:GLY:HA3	1.91	0.52
1:5:4618:G:H5'	24:V:15:ARG:HB2	1.91	0.52
1:5:4939:C:OP1	8:E:152:ARG:NH1	2.42	0.52
10:G:86:VAL:HG11	10:G:185:LYS:HG2	1.91	0.52
13:J:46:GLN:NE2	13:J:72:CYS:SG	2.83	0.52
26:X:110:LYS:NZ	26:X:121:VAL:O	2.42	0.52
51:K:55:U:H6	51:K:90:G:H21	1.57	0.52
51:K:106:C:H2'	51:K:107:A:H8	1.74	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
51:K:1231:C:O2'	51:K:1253:A:N6	2.41	0.52
84:6:79:LEU:HD21	84:6:87:LEU:HB3	1.90	0.52
1:5:4523:A:O3'	5:B:246:ARG:NH1	2.42	0.52
6:C:94:ASN:HD22	6:C:102:PHE:HB2	1.75	0.52
9:F:110:VAL:HG21	9:F:137:ILE:HD11	1.90	0.52
18:P:122:ALA:HB3	18:P:143:PRO:HG2	1.92	0.52
24:V:82:ILE:HG22	24:V:83:ARG:HG3	1.92	0.52
28:Z:5:MET:O	28:Z:28:ASN:ND2	2.37	0.52
79:GG:26:SER:HB3	79:GG:32:LEU:HD22	1.90	0.52
84:6:31:ILE:HG22	84:6:43:TRP:HB2	1.92	0.52
7:D:153:THR:O	7:D:179:ARG:NH2	2.42	0.52
10:G:108:GLN:O	10:G:112:GLN:NE2	2.43	0.52
28:Z:36:ARG:NH1	28:Z:38:TYR:OH	2.39	0.52
51:K:99:A:H61	51:K:433:A:H1'	1.74	0.52
51:K:1610:G:N7	77:I:132:ARG:NH2	2.58	0.52
51:K:1658:G:OP2	51:K:1660:C:N4	2.40	0.52
1:5:1321:G:H21	1:5:3876:A:H5'	1.74	0.52
1:5:1372:A:OP1	16:N:202:ARG:NH2	2.42	0.52
1:5:2526:C:H5''	20:R:10:LEU:HD11	1.91	0.52
1:5:4711:C:O2'	17:O:145:VAL:O	2.26	0.52
5:B:289:GLN:O	5:B:302:ASN:ND2	2.43	0.52
6:C:3:CYS:SG	6:C:4:ALA:N	2.82	0.52
9:F:133:ASN:HA	9:F:136:ARG:HG2	1.91	0.52
72:DD:51:LEU:HG	72:DD:91:VAL:HG22	1.92	0.52
75:RR:63:LYS:HG2	83:O:108:VAL:HG21	1.91	0.52
1:5:1080:C:N4	1:5:1221:G:O6	2.42	0.52
1:5:1090:G:OP1	22:T:142:ARG:NH1	2.43	0.52
6:C:231:ASN:HB3	6:C:234:LYS:HB2	1.92	0.52
44:p:89:LEU:HA	44:p:92:GLN:HE21	1.73	0.52
49:2:18:G:O2'	49:2:57:G:N2	2.39	0.52
51:K:1618:C:H4'	76:9:50:ARG:HH21	1.73	0.52
67:VV:61:GLN:HB3	67:VV:62:PRO:CD	2.39	0.52
72:DD:225:GLU:HB3	84:6:187:ASN:HB2	1.91	0.52
1:5:1523:A:N3	1:5:4389:C:O2'	2.41	0.52
1:5:2062:C:O2'	21:S:111:ARG:NH1	2.43	0.52
1:5:2066:C:H4'	34:f:79:GLY:HA2	1.92	0.52
1:5:4272:G:OP2	1:5:4272:G:N2	2.37	0.52
18:P:89:GLU:O	18:P:93:HIS:ND1	2.40	0.52
51:K:1314:U:O2'	74:SS:8:ARG:NH2	2.43	0.52
51:K:1536:G:H2'	51:K:1537:A:H8	1.73	0.52
64:YY:58:MET:O	64:YY:62:GLN:NE2	2.43	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:5:4765:G:H22	1:5:4869:U:H3	1.56	0.52
5:B:240:LEU:HB3	5:B:244:THR:HG21	1.92	0.52
7:D:125:VAL:O	7:D:196:ARG:NH1	2.43	0.52
17:O:55:LEU:HD23	17:O:58:LEU:HD12	1.91	0.52
46:s:180:ILE:HG22	46:s:182:PRO:HD3	1.92	0.52
52:q:85:ARG:NH2	64:YY:82:ASP:O	2.43	0.52
54:v:252:THR:HG22	54:v:254:ASP:H	1.75	0.52
73:BB:100:ILE:HA	73:BB:178:ILE:HD11	1.91	0.52
1:5:510:U:H5'	29:a:86:THR:HG22	1.91	0.52
1:5:1646:A:O2'	38:j:49:TRP:O	2.27	0.52
1:5:2754:G:OP2	28:Z:133:LYS:NZ	2.42	0.52
1:5:2759:G:O2'	1:5:2762:G:N2	2.43	0.52
15:M:12:VAL:HA	15:M:25:VAL:O	2.10	0.52
24:V:106:VAL:HG21	24:V:132:ILE:HD11	1.90	0.52
83:0:132:MET:HG2	83:0:141:CYS:HB2	1.91	0.52
1:5:386:A:O2'	27:Y:87:ARG:NH2	2.44	0.51
1:5:1371:A:N6	3:8:28:C:O2'	2.43	0.51
1:5:1974:U:H4'	1:5:1975:G:H5'	1.92	0.51
4:A:14:SER:H	4:A:17:ARG:HG3	1.74	0.51
9:F:230:VAL:HA	21:S:39:VAL:HG12	1.92	0.51
10:G:31:LEU:HD21	28:Z:123:LYS:HA	1.93	0.51
46:s:192:VAL:HG23	46:s:201:PRO:HG3	1.92	0.51
73:BB:126:THR:OG1	81:FF:26:GLN:NE2	2.43	0.51
1:5:219:G:OP2	6:C:172:LYS:NZ	2.35	0.51
1:5:1636:U:H5''	1:5:1637:A:H5'	1.92	0.51
1:5:1787:A:N3	1:5:4210:U:O2'	2.43	0.51
1:5:4929:C:H5'	8:E:262:GLN:HG2	1.92	0.51
4:A:23:ARG:HA	4:A:52:PRO:HD2	1.92	0.51
21:S:29:ARG:HB2	22:T:148:PRO:HB2	1.92	0.51
24:V:26:ILE:HG22	24:V:101:ASN:HB3	1.92	0.51
51:K:448:A:OP1	58:CC:25:ARG:NH2	2.43	0.51
51:K:1100:A:O5'	64:YY:132:ARG:NH2	2.43	0.51
51:K:1130:G:N2	51:K:1130:G:OP2	2.40	0.51
53:u:138:PHE:O	53:u:213:ARG:N	2.41	0.51
1:5:2325:C:O2'	33:e:124:ASN:ND2	2.44	0.51
21:S:15:ARG:HH21	22:T:141:VAL:HG22	1.75	0.51
51:K:508:A:H3'	51:K:509:G:H8	1.75	0.51
53:u:82:ARG:NH1	53:u:191:ASP:OD1	2.43	0.51
56:z:2:LYS:HB2	56:z:108:VAL:HG22	1.92	0.51
1:5:156:G:OP2	36:h:106:LYS:NZ	2.43	0.51
1:5:1073:G:H1	1:5:1238:A:H2	1.58	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:5:4937:C:H1'	8:E:181:PRO:HB3	1.93	0.51
5:B:54:THR:OG1	5:B:369:ASP:O	2.24	0.51
24:V:13:LYS:NZ	24:V:59:ASP:OD1	2.43	0.51
51:K:948:C:H2'	51:K:949:G:H8	1.75	0.51
51:K:1092:G:OP1	61:QQ:2:GLY:N	2.43	0.51
51:K:1698:C:O2	85:4:52:A:N6	2.44	0.51
51:K:1829:G:H1'	51:K:1850:A:H2	1.75	0.51
1:5:1817:U:H4'	7:D:43:LYS:HE2	1.91	0.51
1:5:2589:C:HO2'	1:5:2766:A:HO2'	1.56	0.51
1:5:4088:C:H2'	1:5:4089:G:H8	1.75	0.51
1:5:4301:U:OP1	22:T:78:LYS:NZ	2.41	0.51
35:g:96:LEU:O	35:g:100:GLN:NE2	2.43	0.51
51:K:1213:C:H2'	51:K:1214:A:H8	1.76	0.51
70:JJ:81:ARG:HH12	70:JJ:83:GLN:HB3	1.76	0.51
73:BB:140:ASP:H	81:FF:44:ARG:HH12	1.58	0.51
1:5:1188:C:H2'	1:5:1189:G:H8	1.76	0.51
1:5:1743:A:H5'	7:D:11:ALA:HB1	1.92	0.51
1:5:3598:C:H2'	1:5:3599:A:H8	1.75	0.51
3:8:153:C:H4'	10:G:185:LYS:HB3	1.93	0.51
51:K:1219:C:O2'	81:FF:26:GLN:OE1	2.29	0.51
59:XX:140:GLN:NE2	68:NN:64:PHE:O	2.44	0.51
62:MM:101:GLY:HA3	62:MM:134:PRO:HG2	1.92	0.51
67:VV:62:PRO:HB3	85:4:51:G:H4'	1.92	0.51
1:5:727:C:OP1	9:F:78:ARG:NH2	2.43	0.51
1:5:2739:C:O2	4:A:174:ARG:NH1	2.43	0.51
1:5:3700:C:O2'	1:5:3774:A:N3	2.41	0.51
4:A:116:LEU:HB3	4:A:126:LEU:HB2	1.92	0.51
5:B:59:GLU:HB2	5:B:366:LYS:HD2	1.92	0.51
9:F:91:LEU:HD21	9:F:124:PHE:HB3	1.92	0.51
9:F:129:LYS:HB2	22:T:133:ALA:HB3	1.93	0.51
18:P:114:ILE:HD11	18:P:117:ILE:HB	1.92	0.51
51:K:10:G:H21	54:v:114:LYS:HA	1.74	0.51
51:K:526:A:OP1	71:AA:101:ARG:NH1	2.44	0.51
51:K:1354:G:N2	51:K:1357:A:OP2	2.37	0.51
57:y:117:PRO:HG2	57:y:120:ARG:HD3	1.91	0.51
68:NN:91:LEU:HD22	68:NN:96:LEU:HD11	1.92	0.51
1:5:1364:U:OP2	14:L:36:ARG:NH2	2.44	0.51
1:5:2016:C:H2'	1:5:2016:C:O2	2.08	0.51
1:5:4910:G:N2	17:O:106:ASP:O	2.43	0.51
3:8:13:G:O2'	18:P:121:LYS:O	2.28	0.51
8:E:209:THR:H	8:E:212:TYR:HB3	1.75	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:T:27:LEU:HA	22:T:30:TYR:HD2	1.76	0.51
28:Z:83:THR:HG23	28:Z:85:TYR:H	1.75	0.51
51:K:822:U:H3	51:K:826:A:H62	1.58	0.51
68:NN:82:ALA:O	68:NN:86:GLU:CB	2.58	0.51
1:5:957:G:N2	1:5:1286:C:OP2	2.44	0.51
5:B:254:ILE:HG23	5:B:266:VAL:HG11	1.92	0.51
14:L:65:ARG:HB2	29:a:66:ASN:HA	1.91	0.51
17:O:7:LEU:HG	17:O:31:ARG:HE	1.76	0.51
17:O:157:GLU:HA	17:O:160:ARG:HG2	1.92	0.51
25:W:45:ASN:HD22	25:W:46:PRO:HD2	1.76	0.51
51:K:345:U:H5'	55:x:37:LYS:HG2	1.93	0.51
81:FF:31:ARG:HH11	81:FF:43:ILE:HG13	1.76	0.51
1:5:937:U:OP1	15:M:20:HIS:NE2	2.43	0.51
1:5:1530:G:O2'	38:j:45:ARG:NH1	2.39	0.51
1:5:2745:A:H2'	1:5:2746:A:H8	1.76	0.51
1:5:4301:U:OP2	1:5:4303:C:N4	2.44	0.51
1:5:4451:G:C4	48:1:256:TRP:CD1	2.99	0.51
1:5:4537:C:H2'	1:5:4538:G:H8	1.76	0.51
3:8:65:A:O2'	36:h:10:ARG:NH2	2.44	0.51
6:C:284:MET:HE2	6:C:287:THR:HA	1.93	0.51
33:e:90:MET:HG3	45:r:33:LYS:HA	1.93	0.51
35:g:11:LEU:O	35:g:18:ASN:ND2	2.43	0.51
51:K:872:A:O2'	51:K:874:G:OP2	2.29	0.51
51:K:1122:A:N3	53:u:146:ARG:NH1	2.58	0.51
60:EE:73:LEU:HB3	60:EE:90:ARG:HH12	1.76	0.51
66:TT:24:GLN:NE2	70:JJ:5:LYS:O	2.42	0.51
1:5:1522:G:N3	6:C:75:ARG:NH2	2.59	0.50
1:5:3809:G:OP2	1:5:3809:G:N2	2.38	0.50
3:8:38:U:H5'	36:h:81:LEU:HD13	1.93	0.50
46:s:132:PRO:HG3	46:s:150:GLY:HA2	1.93	0.50
51:K:1584:G:OP1	78:PP:77:LYS:NZ	2.43	0.50
63:UU:76:GLY:H	63:UU:79:ALA:HB3	1.75	0.50
1:5:1313:C:H2'	33:e:44:ARG:HH22	1.76	0.50
1:5:1692:C:H5'	19:Q:57:ASN:HD21	1.76	0.50
1:5:1886:G:HO2'	1:5:1909:G:HO2'	1.58	0.50
2:7:7:G:O3'	7:D:33:ARG:NH2	2.44	0.50
65:HH:33:GLN:HA	65:HH:53:TYR:O	2.12	0.50
67:VV:46:HIS:HB3	67:VV:101:LEU:HD11	1.93	0.50
84:6:163:PRO:O	84:6:178:ASN:ND2	2.44	0.50
1:5:2869:U:O2'	1:5:2881:A:N7	2.42	0.50
1:5:4594:U:H2'	1:5:4595:G:H8	1.75	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:8:94:G:OP2	38:j:72:ARG:NH2	2.44	0.50
15:M:38:VAL:HG21	15:M:50:MET:HE2	1.93	0.50
51:K:1654:G:OP1	78:PP:90:SER:OG	2.29	0.50
84:6:16:GLY:O	84:6:35:SER:OG	2.29	0.50
84:6:163:PRO:HB2	84:6:179:LEU:HB2	1.91	0.50
1:5:1266:G:H21	1:5:2111:G:H1'	1.77	0.50
27:Y:71:VAL:N	27:Y:81:TYR:O	2.43	0.50
47:t:33:GLY:O	47:t:38:SER:OG	2.30	0.50
51:K:797:C:C2'	51:K:798:G:H5'	2.42	0.50
51:K:846:G:OP2	55:x:108:ARG:NH2	2.44	0.50
72:DD:50:ILE:HD11	72:DD:86:LEU:HD23	1.93	0.50
78:PP:28:LEU:HD23	78:PP:110:LEU:HD21	1.93	0.50
1:5:37:U:H4'	29:a:32:ARG:HD2	1.92	0.50
1:5:1460:C:H5''	19:Q:144:LYS:HG2	1.93	0.50
1:5:5002:U:OP2	5:B:385:LYS:NZ	2.36	0.50
19:Q:151:HIS:ND1	19:Q:164:LYS:O	2.43	0.50
38:j:19:CYS:SG	38:j:20:ARG:N	2.84	0.50
51:K:291:G:N2	60:EE:40:ILE:O	2.41	0.50
51:K:562:U:O4	59:XX:172:ARG:NH2	2.45	0.50
65:HH:73:ALA:HB1	65:HH:78:ILE:HB	1.94	0.50
77:II:35:GLY:O	77:II:97:GLN:NE2	2.44	0.50
84:6:79:LEU:HD22	84:6:111:VAL:HG21	1.93	0.50
3:8:60:G:O6	36:h:62:ASN:ND2	2.44	0.50
5:B:217:ILE:HD11	5:B:333:LEU:HD21	1.93	0.50
21:S:113:MET:HB3	21:S:119:ALA:HB3	1.93	0.50
47:t:17:CYS:SG	47:t:18:THR:N	2.83	0.50
51:K:1533:A:O2'	73:BB:81:ARG:NH2	2.42	0.50
59:XX:19:PRO:O	59:XX:24:ARG:NH2	2.45	0.50
61:QQ:20:ARG:HH22	66:TT:56:HIS:CG	2.30	0.50
64:YY:17:ILE:HD11	64:YY:54:VAL:HA	1.94	0.50
83:0:99:LYS:O	83:0:104:LYS:NZ	2.44	0.50
1:5:1326:A:OP2	1:5:4445:U:O2'	2.29	0.50
1:5:2486:G:N2	3:8:126:C:OP2	2.42	0.50
1:5:4622:A:H4'	5:B:13:SER:HB2	1.94	0.50
1:5:4888:U:H3	1:5:4931:G:H1	1.58	0.50
5:B:167:GLN:NE2	5:B:204:GLN:OE1	2.44	0.50
5:B:240:LEU:HD21	5:B:252:ALA:HB2	1.93	0.50
14:L:21:ARG:HB3	16:N:197:THR:HG22	1.93	0.50
51:K:560:A:OP2	59:XX:177:ASN:ND2	2.45	0.50
51:K:959:G:OP2	62:MM:38:ASN:ND2	2.40	0.50
56:z:67:VAL:HG13	56:z:99:GLY:HA2	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:5:294:G:OP2	43:o:43:ARG:NH2	2.45	0.50
1:5:1332:C:H2'	1:5:1333:A:C8	2.46	0.50
1:5:1502:G:OP1	19:Q:65:ARG:NH2	2.45	0.50
1:5:4122:G:H4'	35:g:90:ARG:HG3	1.94	0.50
47:t:18:THR:HA	47:t:58:ILE:HG23	1.94	0.50
49:2:33:U:H6	49:2:36:U:H5	1.60	0.50
51:K:1244:U:H2'	51:K:1245:G:H8	1.76	0.50
51:K:1488:C:H3'	51:K:1489:A:H4'	1.94	0.50
51:K:1579:A:O2'	51:K:1581:C:OP2	2.29	0.50
70:JJ:36:LYS:HB3	70:JJ:43:ILE:HG12	1.94	0.50
77:II:127:TRP:O	77:II:144:ARG:NH2	2.44	0.50
1:5:1508:A:OP1	6:C:110:ARG:NH1	2.44	0.50
1:5:1538:U:H2'	1:5:1539:G:H8	1.77	0.50
1:5:1790:U:OP2	22:T:13:TYR:OH	2.27	0.50
1:5:2520:C:H2'	1:5:2521:G:H8	1.75	0.50
1:5:4873:G:OP2	15:M:94:LYS:NZ	2.45	0.50
11:H:47:LEU:HG	11:H:52:LYS:HD2	1.93	0.50
26:X:107:HIS:O	26:X:111:GLN:NE2	2.45	0.50
51:K:830:A:OP2	51:K:846:G:N2	2.45	0.50
58:CC:88:ASN:HD22	58:CC:205:ARG:HH12	1.59	0.50
59:XX:138:ARG:NH1	59:XX:152:ASP:OD2	2.45	0.50
1:5:2848:G:O2'	1:5:3838:U:O4	2.30	0.49
1:5:4134:C:H2'	1:5:4135:G:H8	1.77	0.49
1:5:4149:C:OP1	28:Z:59:LYS:N	2.40	0.49
2:7:6:C:H4'	7:D:52:ILE:HD13	1.93	0.49
4:A:101:VAL:HB	4:A:165:VAL:HG12	1.93	0.49
14:L:43:ALA:O	14:L:149:GLN:NE2	2.38	0.49
33:e:98:GLU:OE1	33:e:123:THR:OG1	2.30	0.49
51:K:154:U:O2	56:z:4:ASN:ND2	2.45	0.49
51:K:311:C:H5''	51:K:312:G:H5''	1.93	0.49
52:q:126:ASP:OD1	52:q:165:ASN:ND2	2.45	0.49
68:NN:90:ARG:HG3	68:NN:93:ARG:HD2	1.93	0.49
1:5:492:U:O2	1:5:663:G:O6	2.29	0.49
1:5:2485:U:H2'	1:5:2486:G:H8	1.77	0.49
2:7:13:A:O2'	7:D:24:ARG:NH2	2.45	0.49
14:L:46:ILE:HB	14:L:49:ARG:HB2	1.94	0.49
14:L:167:ARG:HH21	29:a:123:ILE:HG21	1.77	0.49
51:K:551:U:H2'	51:K:552:G:H8	1.77	0.49
51:K:1146:C:O2'	51:K:1150:A:N1	2.42	0.49
51:K:1199:A:H5''	69:ZZ:2:THR:HB	1.94	0.49
53:u:121:ILE:HG12	53:u:161:VAL:HG13	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:5:4458:C:OP1	5:B:11:HIS:NE2	2.45	0.49
38:j:35:GLY:O	38:j:45:ARG:NH2	2.45	0.49
51:K:628:A:N7	72:DD:179:GLN:NE2	2.56	0.49
51:K:1391:C:O2'	79:GG:83:ARG:NH2	2.41	0.49
56:z:52:ILE:HD11	56:z:109:LEU:HD22	1.94	0.49
1:5:442:G:OP1	34:f:68:ARG:NH1	2.43	0.49
1:5:1281:G:OP1	8:E:48:ARG:NE	2.43	0.49
1:5:1484:G:O2'	1:5:1486:C:OP2	2.30	0.49
1:5:1548:G:O2'	1:5:2812:A:N3	2.43	0.49
1:5:2395:A:N6	1:5:2820:C:O2	2.44	0.49
1:5:2568:C:H2'	1:5:2569:G:H8	1.78	0.49
1:5:3683:C:OP1	4:A:132:ASN:ND2	2.45	0.49
4:A:181:LYS:HE3	4:A:184:ARG:HG3	1.95	0.49
54:v:201:GLY:HA3	59:XX:98:LEU:HD22	1.94	0.49
66:TT:52:ILE:HG22	66:TT:61:ILE:HG12	1.94	0.49
1:5:300:A:O2'	16:N:94:PHE:O	2.29	0.49
1:5:1348:U:H2'	1:5:1349:G:H8	1.77	0.49
1:5:3853:U:O2'	1:5:4979:A:N3	2.45	0.49
1:5:4220:A:OP2	22:T:2:THR:N	2.45	0.49
4:A:104:VAL:HA	4:A:107:MET:HG2	1.93	0.49
7:D:65:ALA:HB2	7:D:74:ILE:HD13	1.94	0.49
34:f:50:VAL:HG22	34:f:69:VAL:HG12	1.95	0.49
1:5:2550:G:O2'	1:5:2587:A:N1	2.43	0.49
1:5:2652:G:N2	44:p:59:SER:O	2.46	0.49
15:M:101:LYS:HE2	17:O:201:PHE:HE1	1.78	0.49
51:K:94:G:O2'	51:K:508:A:O2'	2.29	0.49
51:K:475:C:O2'	51:K:507:G:N3	2.40	0.49
51:K:1204:A:O2'	51:K:1700:C:OP2	2.31	0.49
53:u:139:CYS:HA	53:u:212:VAL:HA	1.93	0.49
1:5:460:C:H2'	1:5:461:G:H8	1.78	0.49
1:5:1535:C:H5''	38:j:10:LYS:HG3	1.93	0.49
1:5:2465:C:H1'	1:5:3672:G:H1	1.77	0.49
1:5:4758:U:OP1	17:O:116:LYS:NZ	2.46	0.49
6:C:152:LEU:HD23	6:C:251:ILE:HG12	1.94	0.49
30:b:36:ASP:N	30:b:36:ASP:OD1	2.46	0.49
51:K:1096:G:O6	51:K:1136:U:O4	2.30	0.49
51:K:1277:C:H2'	51:K:1278:A:H8	1.78	0.49
52:q:36:GLN:O	52:q:53:ARG:NH1	2.45	0.49
66:TT:24:GLN:HG3	70:JJ:7:LEU:HD12	1.94	0.49
82:w:5:GLN:O	82:w:9:SER:OG	2.30	0.49
1:5:1814:C:O2'	30:b:42:ASN:OD1	2.31	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:Z:22:LYS:NZ	28:Z:129:TRP:O	2.46	0.49
51:K:658:U:O2	67:VV:17:ARG:NH2	2.46	0.49
51:K:1652:G:O6	51:K:1672:U:O4	2.31	0.49
51:K:1743:G:N2	51:K:1791:A:H62	2.08	0.49
75:RR:62:VAL:HA	75:RR:65:VAL:HG12	1.95	0.49
1:5:1211:G:H2'	1:5:1212:G:H8	1.78	0.49
1:5:1699:A:N6	1:5:2094:G:O2'	2.45	0.49
1:5:2583:C:OP2	35:g:76:ARG:NH1	2.46	0.49
1:5:3765:G:O2'	1:5:3767:C:N4	2.46	0.49
1:5:4126:C:H5''	1:5:4127:A:H5''	1.95	0.49
1:5:4182:G:O2'	1:5:4184:G:N7	2.46	0.49
1:5:4541:G:N2	1:5:4544:A:OP2	2.41	0.49
1:5:5015:G:O2'	1:5:5034:A:N6	2.45	0.49
12:I:43:VAL:O	12:I:171:TRP:NE1	2.42	0.49
21:S:15:ARG:HD2	21:S:25:PRO:HG2	1.94	0.49
26:X:104:ALA:O	26:X:134:LYS:NZ	2.45	0.49
26:X:119:ILE:HG13	26:X:144:TYR:HD2	1.77	0.49
51:K:1:U:H5'	59:XX:58:ARG:HH22	1.77	0.49
1:5:66:A:O2'	1:5:326:C:O2	2.29	0.49
1:5:371:A:N3	1:5:1531:U:O2'	2.45	0.49
1:5:381:U:H4'	1:5:415:G:H5'	1.94	0.49
1:5:1975:G:N2	1:5:1983:A:OP1	2.46	0.49
1:5:2411:C:O2'	1:5:2526:C:O2	2.31	0.49
1:5:4265:U:N3	7:D:17:GLN:O	2.46	0.49
1:5:4421:C:H42	1:5:4475:G:N2	2.10	0.49
4:A:178:PRO:HB2	4:A:180:LEU:HD22	1.95	0.49
21:S:34:ALA:HB1	21:S:39:VAL:HG23	1.94	0.49
51:K:155:G:H2'	51:K:156:G:H8	1.78	0.49
51:K:308:G:H3'	51:K:309:G:H5''	1.94	0.49
51:K:395:G:N2	58:CC:14:THR:O	2.43	0.49
51:K:645:C:H2'	51:K:646:G:H8	1.78	0.49
51:K:989:C:O2	69:ZZ:32:LYS:NZ	2.46	0.49
51:K:1599:U:OP1	80:OO:80:ARG:NH2	2.46	0.49
51:K:1718:G:N2	51:K:1814:G:O2'	2.40	0.49
1:5:2573:A:N7	1:5:2761:U:O4	2.45	0.48
1:5:2663:G:O2'	20:R:117:ARG:NH1	2.46	0.48
1:5:3870:C:H2'	1:5:3871:A:H8	1.78	0.48
4:A:59:ALA:HB2	4:A:78:ALA:HB2	1.95	0.48
5:B:60:VAL:HG11	5:B:67:VAL:HG13	1.94	0.48
7:D:223:PHE:HB3	7:D:226:TYR:HB2	1.95	0.48
9:F:128:ASN:HB2	22:T:132:PRO:HB2	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:G:165:GLU:OE2	16:N:26:ARG:NH1	2.41	0.48
62:MM:95:ILE:HB	62:MM:129:ILE:HG12	1.94	0.48
65:HH:22:ARG:NH2	65:HH:56:CYS:SG	2.86	0.48
5:B:115:LYS:NZ	5:B:129:ALA:O	2.46	0.48
15:M:25:VAL:HG21	15:M:50:MET:HE1	1.95	0.48
33:e:79:VAL:HG13	33:e:84:GLU:HB3	1.95	0.48
51:K:1416:C:O2	78:PP:3:GLY:N	2.46	0.48
67:VV:85:VAL:HG13	67:VV:130:LEU:HD11	1.95	0.48
1:5:664:G:N2	1:5:667:A:N1	2.62	0.48
19:Q:122:THR:OG1	19:Q:124:ASP:OD1	2.29	0.48
51:K:1270:G:O2'	51:K:1301:A:N7	2.47	0.48
58:CC:99:ASN:ND2	58:CC:174:CYS:SG	2.87	0.48
59:XX:136:ARG:HD2	59:XX:139:LYS:HA	1.94	0.48
72:DD:28:GLU:OE2	72:DD:65:ARG:NH2	2.47	0.48
1:5:1516:G:O2'	14:L:18:TRP:NE1	2.42	0.48
1:5:2411:C:H2'	1:5:2412:A:H8	1.79	0.48
1:5:2778:G:N1	3:8:113:C:OP1	2.46	0.48
1:5:4387:C:H5'	48:1:251:ARG:HH12	1.78	0.48
58:CC:22:HIS:ND1	58:CC:23:LYS:O	2.46	0.48
84:6:254:PRO:HA	84:6:285:GLN:HA	1.95	0.48
1:5:1317:U:OP1	29:a:21:ARG:NH2	2.46	0.48
1:5:2429:A:OP1	40:l:43:HIS:NE2	2.45	0.48
7:D:68:ARG:HG3	7:D:73:MET:HE2	1.94	0.48
12:I:14:ASN:O	12:I:128:ARG:NH2	2.42	0.48
48:1:254:PRO:HA	48:1:257:LYS:HE2	1.94	0.48
49:2:74:C:H2'	49:2:74:C:O2	2.13	0.48
51:K:398:A:H5''	51:K:400:C:H5'	1.95	0.48
55:x:63:LYS:O	55:x:67:GLN:NE2	2.46	0.48
1:5:2041:A:H62	1:5:4434:C:H1'	1.79	0.48
1:5:2738:C:O2'	1:5:2740:U:O2	2.30	0.48
1:5:2835:A:O2'	5:B:228:TYR:O	2.27	0.48
1:5:3917:A:H2'	1:5:3918:G:H8	1.79	0.48
21:S:76:LYS:NZ	21:S:100:LEU:O	2.45	0.48
33:e:85:LEU:HD11	33:e:111:ILE:HG23	1.95	0.48
47:t:76:SER:O	47:t:117:ARG:NH2	2.42	0.48
51:K:1373:C:O2	51:K:1465:A:O2'	2.31	0.48
51:K:1722:G:H2'	51:K:1723:G:H8	1.78	0.48
1:5:74:G:H5'	14:L:59:VAL:HG13	1.96	0.48
1:5:1924:C:OP1	15:M:34:ASN:ND2	2.46	0.48
1:5:3928:A:OP1	16:N:90:ASN:ND2	2.46	0.48
9:F:37:LYS:O	9:F:41:GLN:NE2	2.47	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:I:49:CYS:SG	12:I:51:HIS:NE2	2.77	0.48
13:J:52:LYS:HA	13:J:67:LYS:HA	1.96	0.48
21:S:13:VAL:HG23	21:S:62:VAL:HB	1.95	0.48
51:K:1292:C:N3	83:O:138:ARG:NH1	2.61	0.48
60:EE:86:ILE:HG12	60:EE:113:LEU:HB2	1.94	0.48
84:6:118:ARG:NH2	84:6:134:THR:OG1	2.46	0.48
1:5:438:G:OP1	33:e:16:ARG:NH2	2.46	0.48
1:5:701:G:H5'	8:E:117:VAL:HG21	1.95	0.48
1:5:950:G:H2'	1:5:951:G:H8	1.79	0.48
1:5:1494:U:H2'	1:5:1495:G:C8	2.49	0.48
1:5:1601:A:OP2	1:5:3643:A:N6	2.47	0.48
1:5:4420:U:H5''	1:5:4421:C:H5	1.78	0.48
16:N:47:LYS:HE3	16:N:51:LEU:HD11	1.95	0.48
47:t:65:GLN:HG3	47:t:70:GLN:HG3	1.95	0.48
51:K:360:A:H4'	51:K:361:U:H3'	1.96	0.48
51:K:1550:G:H3'	51:K:1579:A:H61	1.79	0.48
77:II:28:PHE:HE1	77:II:38:ARG:HE	1.62	0.48
1:5:152:U:OP1	16:N:55:ALA:N	2.46	0.48
1:5:4096:C:H1'	35:g:112:GLN:HE22	1.78	0.48
11:H:91:LYS:HB2	11:H:183:GLU:HB3	1.95	0.48
51:K:206:G:O6	58:CC:144:LYS:NZ	2.47	0.48
51:K:305:U:H3'	51:K:306:C:C5'	2.42	0.48
51:K:1670:C:H2'	51:K:1671:G:H8	1.79	0.48
8:E:42:ARG:HD3	8:E:61:ARG:HG2	1.96	0.48
51:K:24:C:H42	51:K:650:A:H61	1.61	0.48
51:K:1220:A:N3	51:K:1677:U:O2'	2.42	0.48
52:q:122:LEU:HD13	52:q:142:LEU:HB3	1.95	0.48
52:q:144:THR:H	52:q:158:ASP:HB2	1.79	0.48
63:UU:45:ARG:NH2	78:PP:10:ASN:OD1	2.47	0.48
1:5:1308:C:O2'	34:f:94:ALA:O	2.31	0.47
1:5:1500:A:H5''	1:5:1501:C:H5''	1.94	0.47
1:5:2279:A:O2'	33:e:48:ARG:NH2	2.45	0.47
1:5:2309:G:O2'	3:8:18:U:O2	2.31	0.47
1:5:2407:G:H2'	40:l:13:LEU:HD22	1.97	0.47
51:K:1605:G:H5''	78:PP:84:ARG:HH11	1.79	0.47
51:K:1677:U:H2'	51:K:1678:A:H8	1.78	0.47
1:5:69:A:H5'	29:a:64:LYS:HE2	1.96	0.47
1:5:119:G:H22	10:G:133:PRO:HG2	1.79	0.47
1:5:731:G:H21	21:S:72:PRO:HG2	1.80	0.47
1:5:1253:G:O2'	1:5:1257:A:N6	2.46	0.47
1:5:1591:U:OP2	5:B:243:LYS:NZ	2.41	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:5:2305:U:HO2'	33:e:104:SER:HG	1.58	0.47
1:5:2589:C:O2'	1:5:2766:A:O2'	2.28	0.47
1:5:4451:G:C4	48:1:256:TRP:HD1	2.32	0.47
5:B:57:VAL:HB	5:B:367:PHE:HB3	1.95	0.47
12:I:31:ILE:HG22	12:I:62:SER:HB2	1.96	0.47
17:O:15:LEU:HB2	17:O:18:ARG:HB2	1.95	0.47
26:X:83:THR:HG22	26:X:85:SER:H	1.79	0.47
27:Y:34:LEU:HD23	27:Y:38:LEU:HB3	1.96	0.47
46:s:64:ALA:O	46:s:68:HIS:ND1	2.37	0.47
54:v:75:ILE:HD11	54:v:80:GLU:HB2	1.95	0.47
61:QQ:30:SER:HB2	61:QQ:67:THR:HG22	1.96	0.47
84:6:99:ARG:NH2	84:6:135:LEU:O	2.47	0.47
1:5:709:C:H2'	1:5:710:G:H8	1.78	0.47
1:5:2324:C:O2	33:e:76:LYS:NZ	2.47	0.47
9:F:211:TRP:HE1	9:F:214:LYS:HE2	1.79	0.47
46:s:32:ALA:O	46:s:85:ASN:ND2	2.46	0.47
46:s:145:THR:HG22	46:s:154:ILE:HG13	1.94	0.47
51:K:377:G:H5'	58:CC:98:LYS:HB3	1.95	0.47
51:K:1279:C:H2'	51:K:1280:G:H8	1.80	0.47
51:K:1628:C:O2'	77:II:82:TRP:O	2.32	0.47
51:K:1710:C:H42	51:K:1823:A:H61	1.62	0.47
62:MM:98:ARG:HB2	62:MM:132:VAL:HG23	1.95	0.47
67:VV:61:GLN:O	67:VV:63:ASN:N	2.47	0.47
1:5:1637:A:OP1	1:5:1640:C:N4	2.40	0.47
3:8:47:C:H1'	3:8:61:A:H2'	1.95	0.47
5:B:92:TYR:HB2	5:B:159:VAL:HB	1.96	0.47
10:G:48:LYS:HB3	26:X:42:THR:HG23	1.95	0.47
65:HH:38:GLU:HG3	65:HH:49:GLN:HG3	1.96	0.47
84:6:5:MET:HE1	84:6:312:VAL:HG22	1.97	0.47
1:5:1:C:N4	3:8:156:U:O2	2.47	0.47
1:5:417:G:OP1	1:5:2329:U:O2'	2.33	0.47
1:5:724:C:H2'	1:5:725:G:H8	1.78	0.47
1:5:4357:G:H4'	14:L:193:GLY:HA3	1.96	0.47
1:5:4635:A:OP1	1:5:4636:U:O2'	2.31	0.47
2:7:15:C:H2'	2:7:16:A:H8	1.79	0.47
10:G:98:LEU:HD13	10:G:218:LEU:HD12	1.95	0.47
16:N:116:LEU:HD22	16:N:135:ILE:HD11	1.96	0.47
17:O:175:MET:HE3	17:O:179:LYS:HE3	1.95	0.47
23:U:64:GLU:HB2	23:U:71:THR:HB	1.95	0.47
49:2:3:U:H3	49:2:70:G:H1	1.63	0.47
53:u:144:LYS:HD3	53:u:208:HIS:HB3	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
58:CC:6:ASP:OD1	58:CC:9:HIS:ND1	2.47	0.47
1:5:734:G:H5''	15:M:70:GLN:HG2	1.96	0.47
2:7:13:A:HO2'	7:D:24:ARG:HH22	1.63	0.47
12:I:46:PHE:HB2	12:I:139:ARG:HH11	1.80	0.47
18:P:61:ARG:HH21	18:P:76:TRP:HB3	1.79	0.47
22:T:45:MET:H	22:T:95:HIS:CD2	2.33	0.47
22:T:49:GLN:HA	22:T:52:MET:HE3	1.96	0.47
39:k:33:LYS:HG2	39:k:46:VAL:HG22	1.96	0.47
51:K:490:C:O2'	51:K:574:A:N1	2.45	0.47
51:K:681:U:O2'	51:K:1160:U:OP1	2.32	0.47
56:z:64:LYS:HE2	56:z:97:VAL:HG11	1.95	0.47
1:5:960:A:N6	1:5:1283:G:O6	2.47	0.47
1:5:1380:G:N2	1:5:1381:U:O4	2.40	0.47
1:5:1949:U:OP1	11:H:64:ARG:NH1	2.47	0.47
1:5:2407:G:OP2	1:5:2407:G:N2	2.40	0.47
1:5:2897:G:H2'	1:5:2898:G:H8	1.80	0.47
1:5:4313:A:OP1	22:T:92:ARG:NH2	2.41	0.47
1:5:4996:C:H4'	32:d:26:THR:HG23	1.96	0.47
2:7:92:C:H2'	2:7:93:G:H8	1.79	0.47
5:B:322:HIS:O	5:B:342:LYS:NZ	2.47	0.47
9:F:115:ARG:HH11	9:F:212:PRO:HD3	1.80	0.47
16:N:200:LEU:HB3	16:N:204:ARG:HH21	1.80	0.47
18:P:16:LYS:HG2	18:P:149:ILE:HG12	1.95	0.47
29:a:82:VAL:HG21	29:a:101:ILE:HG12	1.96	0.47
32:d:23:ARG:HB2	32:d:121:ASN:HA	1.97	0.47
36:h:67:GLU:HA	36:h:70:ARG:HG2	1.96	0.47
51:K:43:U:OP2	51:K:485:A:N6	2.47	0.47
51:K:111:A:O2'	60:EE:69:ARG:NH1	2.47	0.47
51:K:124:U:H3	51:K:340:C:H42	1.62	0.47
51:K:551:U:H2'	51:K:552:G:C8	2.49	0.47
51:K:1587:G:H5''	78:PP:77:LYS:HD3	1.96	0.47
54:v:165:VAL:HG21	54:v:217:ALA:HB1	1.96	0.47
55:x:35:PRO:HD2	55:x:83:PRO:HG2	1.95	0.47
60:EE:5:GLN:HG2	60:EE:11:GLN:HB2	1.96	0.47
70:JJ:23:ARG:NH1	70:JJ:27:SER:O	2.48	0.47
72:DD:135:GLU:HB3	72:DD:187:LYS:HB3	1.95	0.47
79:GG:80:PHE:HB3	82:w:52:PHE:HB3	1.96	0.47
1:5:313:U:H5''	16:N:179:LYS:HE3	1.97	0.47
1:5:2352:U:OP1	6:C:78:ARG:NH2	2.46	0.47
1:5:4451:G:N2	1:5:4452:U:O4	2.46	0.47
11:H:111:LEU:HD21	11:H:125:ARG:HB2	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:I:38:ARG:HD3	12:I:83:ASP:HB2	1.96	0.47
25:W:6:CYS:HB3	25:W:10:GLY:H	1.79	0.47
26:X:89:LYS:HD3	26:X:93:ASN:HD22	1.78	0.47
36:h:12:LYS:NZ	36:h:20:GLN:OE1	2.47	0.47
46:s:122:THR:HG22	46:s:159:GLN:HG2	1.97	0.47
47:t:50:THR:HG21	47:t:72:GLU:HB2	1.97	0.47
51:K:35:C:H5''	51:K:579:C:H5''	1.97	0.47
63:UU:15:ARG:HG2	63:UU:20:THR:HG22	1.97	0.47
67:VV:60:LYS:HB3	67:VV:61:GLN:H	1.50	0.47
74:SS:60:GLU:OE1	74:SS:69:TRP:NE1	2.48	0.47
1:5:916:C:N4	1:5:918:G:O6	2.48	0.47
1:5:2740:U:O2'	1:5:2742:G:N2	2.48	0.47
7:D:53:VAL:HG11	7:D:159:VAL:HA	1.96	0.47
38:j:55:ARG:HA	38:j:58:THR:HG23	1.97	0.47
49:2:29:A:H3'	49:2:30:G:H8	1.79	0.47
51:K:149:A:OP2	51:K:168:C:N4	2.46	0.47
51:K:903:A:H2'	51:K:904:A:H8	1.80	0.47
51:K:979:C:H2'	51:K:980:A:C8	2.50	0.47
51:K:1218:C:H1'	51:K:1683:C:H42	1.80	0.47
73:BB:102:LEU:HD22	80:OO:110:THR:HG21	1.97	0.47
1:5:364:G:O6	38:j:55:ARG:NH1	2.47	0.47
1:5:1355:G:OP1	19:Q:108:ARG:NH1	2.47	0.47
1:5:1933:G:H2'	1:5:1934:A:C8	2.50	0.47
1:5:2077:C:O2	33:e:15:LYS:NZ	2.42	0.47
1:5:3919:C:H4'	4:A:207:VAL:HG12	1.97	0.47
13:J:35:ARG:HD3	13:J:124:GLY:H	1.80	0.47
51:K:828:G:N2	51:K:830:A:O2'	2.46	0.47
51:K:1010:G:H2'	51:K:1011:A:H8	1.79	0.47
51:K:1560:U:O2	51:K:1575:G:O6	2.33	0.47
51:K:1631:U:O3'	77:II:34:LYS:NZ	2.48	0.47
55:x:9:LEU:HB2	55:x:30:ARG:HD3	1.96	0.47
55:x:201:HIS:N	55:x:206:ASP:OD1	2.48	0.47
55:x:212:ASP:HB3	55:x:216:ASN:H	1.80	0.47
56:z:10:THR:HB	56:z:128:THR:HA	1.97	0.47
57:y:72:PHE:HA	57:y:75:ILE:HG22	1.95	0.47
72:DD:177:LEU:HD13	72:DD:182:LEU:HD13	1.97	0.47
1:5:327:U:O2'	37:i:30:ARG:NH1	2.40	0.46
1:5:3861:A:H2'	1:5:3862:A:H8	1.80	0.46
1:5:5022:U:O2	1:5:5025:C:N3	2.48	0.46
4:A:117:GLU:HG2	4:A:124:GLY:H	1.80	0.46
5:B:17:LEU:HA	5:B:19:ARG:HG3	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:Z:46:ILE:HA	28:Z:70:SER:HA	1.97	0.46
29:a:76:ASP:HB2	29:a:115:GLY:HA3	1.97	0.46
51:K:88:G:N2	51:K:499:G:O3'	2.48	0.46
51:K:525:A:O2'	71:AA:104:ARG:NH1	2.48	0.46
51:K:1228:A:H2'	51:K:1229:G:H8	1.80	0.46
51:K:1246:A:O2'	79:GG:72:GLU:OE2	2.33	0.46
53:u:66:VAL:HG22	53:u:87:ILE:HG22	1.96	0.46
1:5:1494:U:H2'	1:5:1495:G:H8	1.80	0.46
1:5:1666:C:O2'	1:5:1688:G:OP1	2.32	0.46
1:5:2407:G:O6	40:l:2:SER:N	2.49	0.46
2:7:57:C:H2'	2:7:58:A:H8	1.79	0.46
11:H:115:ARG:HG3	11:H:123:ILE:HG22	1.97	0.46
49:2:30:G:H2'	49:2:31:G:H8	1.80	0.46
51:K:1337:C:OP1	82:w:44:ARG:NH2	2.45	0.46
51:K:1726:G:O6	51:K:1808:U:O4	2.33	0.46
52:q:10:MET:HE2	52:q:15:VAL:HG22	1.97	0.46
66:TT:26:LEU:HD11	66:TT:60:LYS:HB3	1.98	0.46
77:II:22:GLY:HA2	77:II:56:ALA:HB3	1.96	0.46
1:5:4122:G:O3'	35:g:90:ARG:NH1	2.49	0.46
5:B:262:VAL:HG21	5:B:268:ARG:HE	1.80	0.46
5:B:317:LEU:HB2	5:B:372:SER:HB2	1.96	0.46
17:O:9:LEU:HD23	17:O:118:MET:HB2	1.98	0.46
31:c:28:VAL:HG21	31:c:37:MET:HG3	1.97	0.46
49:2:10:G:O6	49:2:45:G:N2	2.48	0.46
52:q:141:ASN:ND2	65:HH:31:SER:O	2.48	0.46
62:MM:30:VAL:HG23	62:MM:94:HIS:HB2	1.97	0.46
1:5:48:G:N2	1:5:49:U:O4	2.36	0.46
1:5:62:A:N3	1:5:77:U:O2'	2.44	0.46
1:5:197:A:N1	1:5:225:G:O2'	2.43	0.46
1:5:3667:C:H4'	4:A:8:GLN:HA	1.98	0.46
1:5:3897:G:N2	1:5:3898:G:O6	2.45	0.46
4:A:27:ALA:O	4:A:128:ARG:NH2	2.39	0.46
7:D:163:LEU:HD11	7:D:173:ILE:HG21	1.96	0.46
19:Q:33:ARG:HE	19:Q:52:PHE:HZ	1.63	0.46
31:c:47:ILE:HD12	31:c:94:LEU:HD11	1.96	0.46
51:K:522:A:H4'	59:XX:131:ARG:HH22	1.81	0.46
77:II:4:VAL:HA	80:OO:50:PHE:HB2	1.96	0.46
79:GG:54:VAL:HB	79:GG:88:LEU:HG	1.97	0.46
1:5:86:U:H2'	1:5:87:A:H8	1.81	0.46
1:5:4457:U:OP1	24:V:50:ASN:ND2	2.36	0.46
49:2:34:C:H2'	49:2:35:A:C8	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
51:K:647:U:H2'	51:K:648:A:H8	1.80	0.46
63:UU:131:LYS:HB2	63:UU:140:ARG:HH12	1.81	0.46
74:SS:24:LYS:O	74:SS:42:ASN:ND2	2.46	0.46
1:5:32:G:OP1	16:N:73:ARG:NH1	2.49	0.46
1:5:85:G:O2'	1:5:97:G:O6	2.30	0.46
1:5:1864:G:O2'	12:I:118:ALA:O	2.34	0.46
1:5:4305:G:H1	22:T:87:LYS:HZ2	1.63	0.46
1:5:4910:G:H1	17:O:108:ILE:H	1.63	0.46
12:I:98:ARG:HB3	12:I:120:GLY:HA3	1.98	0.46
51:K:1549:U:OP1	82:w:34:TYR:OH	2.33	0.46
53:u:113:MET:HB3	53:u:142:PHE:HE2	1.78	0.46
71:AA:112:ASN:O	71:AA:117:ASN:ND2	2.49	0.46
1:5:101:A:O2'	14:L:63:THR:OG1	2.34	0.46
8:E:157:ARG:NH2	8:E:269:SER:OG	2.48	0.46
8:E:188:LYS:HG2	34:f:107:PRO:HA	1.98	0.46
51:K:511:U:O2'	51:K:576:A:N6	2.48	0.46
51:K:1394:G:H4'	63:UU:126:ARG:HH11	1.81	0.46
51:K:1528:G:O2'	51:K:1666:C:OP1	2.34	0.46
51:K:1648:G:N2	51:K:1675:A:OP2	2.47	0.46
53:u:100:PHE:HB3	53:u:181:LEU:HD11	1.97	0.46
58:CC:177:SER:OG	58:CC:186:ASP:N	2.49	0.46
63:UU:17:LYS:HG3	63:UU:126:ARG:HG3	1.98	0.46
1:5:717:U:OP1	9:F:219:ARG:NH1	2.45	0.46
1:5:730:G:H1	1:5:939:G:H1	1.62	0.46
1:5:1396:G:HO2'	1:5:1468:C:HO2'	1.58	0.46
1:5:2751:G:H2'	1:5:2752:G:H8	1.80	0.46
1:5:4274:A:H2'	1:5:4275:G:C8	2.51	0.46
3:8:65:A:OP1	36:h:56:ARG:NE	2.45	0.46
6:C:28:PHE:HA	6:C:129:ALA:HA	1.97	0.46
7:D:62:CYS:HB3	7:D:105:LEU:HD22	1.98	0.46
9:F:109:LYS:HD2	9:F:112:GLN:HE21	1.81	0.46
17:O:196:LEU:HB3	17:O:201:PHE:HB2	1.97	0.46
31:c:47:ILE:HB	31:c:94:LEU:HG	1.98	0.46
51:K:434:G:H2'	51:K:435:A:C8	2.51	0.46
66:TT:57:ARG:NH1	70:JJ:26:GLN:OE1	2.49	0.46
1:5:4454:G:O2'	1:5:4500:U:O2'	2.34	0.46
18:P:32:THR:HG23	18:P:91:LEU:HD21	1.97	0.46
45:r:61:VAL:HG21	45:r:79:ARG:HH21	1.80	0.46
51:K:5:U:H2'	51:K:6:G:H8	1.81	0.46
51:K:316:G:H3'	56:z:183:ARG:HH22	1.80	0.46
51:K:943:U:H2'	51:K:944:A:C8	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
54:v:174:ILE:O	54:v:200:ARG:NH1	2.49	0.46
60:EE:126:VAL:HG23	60:EE:145:VAL:HG22	1.98	0.46
1:5:297:U:O2'	16:N:179:LYS:O	2.22	0.46
1:5:701:G:O2'	33:e:7:LEU:O	2.29	0.46
1:5:2070:U:OP1	34:f:22:ARG:NH2	2.39	0.46
12:I:162:ARG:NH2	21:S:88:SER:OG	2.48	0.46
14:L:91:ALA:HB1	14:L:96:ILE:HB	1.98	0.46
29:a:71:PRO:HG2	29:a:108:TYR:HA	1.98	0.46
66:TT:86:LEU:HD23	66:TT:117:ARG:HE	1.79	0.46
68:NN:58:PHE:HE1	68:NN:74:MET:HE1	1.81	0.46
77:II:124:ARG:HE	77:II:129:LEU:HB2	1.81	0.46
79:GG:59:LYS:HB2	79:GG:84:ILE:HG22	1.97	0.46
80:OO:50:PHE:HE1	80:OO:58:LEU:HD13	1.81	0.46
1:5:198:A:OP2	27:Y:45:ARG:NH1	2.46	0.45
16:N:184:ILE:HG23	16:N:194:ARG:HH12	1.80	0.45
17:O:119:VAL:HG11	21:S:171:ARG:HG2	1.98	0.45
19:Q:172:ARG:NH2	29:a:56:VAL:O	2.49	0.45
36:h:81:LEU:HD23	36:h:84:ARG:HD2	1.98	0.45
55:x:11:ARG:HA	55:x:28:ALA:HB2	1.98	0.45
72:DD:55:THR:HA	72:DD:58:VAL:HG22	1.99	0.45
84:6:22:ALA:HB2	84:6:69:VAL:HG13	1.98	0.45
1:5:1794:A:H5''	1:5:4214:A:H61	1.81	0.45
1:5:4451:G:C1'	48:1:256:TRP:CD1	3.00	0.45
1:5:4870:G:H4'	1:5:4872:G:H4'	1.99	0.45
13:J:90:ARG:HD3	13:J:109:ILE:HG22	1.98	0.45
14:L:191:LEU:HD23	14:L:194:ILE:HD13	1.99	0.45
51:K:72:C:O2'	51:K:74:G:OP2	2.30	0.45
51:K:307:G:H1'	58:CC:45:THR:HG22	1.97	0.45
51:K:346:C:O2'	55:x:30:ARG:NH2	2.49	0.45
51:K:609:U:H2'	51:K:610:G:H8	1.81	0.45
51:K:991:G:N7	69:ZZ:7:ASN:ND2	2.64	0.45
51:K:1650:A:OP1	63:UU:137:ALA:N	2.49	0.45
51:K:1745:A:H1'	56:z:66:GLY:HA2	1.98	0.45
52:q:99:ILE:HD11	52:q:117:ARG:HH22	1.81	0.45
77:II:74:PRO:HG3	77:II:97:GLN:H	1.81	0.45
1:5:61:A:H5''	16:N:164:LEU:HD21	1.98	0.45
1:5:382:G:N1	1:5:385:A:OP2	2.43	0.45
1:5:2429:A:H5''	40:l:43:HIS:HE2	1.80	0.45
1:5:2749:C:H2'	1:5:2750:G:C8	2.51	0.45
9:F:88:GLU:HB2	22:T:135:PRO:HB3	1.97	0.45
31:c:45:LEU:HD23	31:c:96:ILE:HD12	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
51:K:1281:G:OP2	75:RR:102:LYS:NZ	2.47	0.45
51:K:1485:U:OP1	72:DD:151:LYS:NZ	2.49	0.45
51:K:1492:U:O2'	51:K:1495:G:OP1	2.31	0.45
51:K:1619:A:O2'	76:9:82:ASP:OD2	2.29	0.45
58:CC:11:ARG:O	58:CC:18:ARG:NH1	2.50	0.45
66:TT:103:VAL:HG13	66:TT:126:LEU:HB2	1.98	0.45
1:5:2478:C:N4	1:5:2479:G:O6	2.50	0.45
1:5:2735:G:H2'	1:5:2736:G:H8	1.82	0.45
13:J:151:ILE:H	13:J:151:ILE:HG13	1.55	0.45
43:o:71:GLU:OE2	43:o:78:ARG:NH1	2.50	0.45
49:2:36:U:O2'	51:K:1825:A:N1	2.44	0.45
51:K:1207:G:N1	85:4:45:A:O2'	2.49	0.45
1:5:20:U:H3'	1:5:21:G:H8	1.82	0.45
1:5:27:C:O2'	1:5:60:G:N3	2.44	0.45
1:5:673:C:H2'	1:5:674:G:H8	1.82	0.45
1:5:1281:G:O3'	6:C:321:ASN:ND2	2.47	0.45
1:5:1370:G:OP1	6:C:48:ASN:ND2	2.49	0.45
1:5:1619:G:OP2	38:j:13:ASN:ND2	2.49	0.45
1:5:1628:C:H5''	4:A:15:VAL:HG21	1.98	0.45
51:K:1143:A:OP2	54:v:187:ARG:NH2	2.49	0.45
51:K:1289:U:OP2	83:0:95:ARG:NH1	2.49	0.45
1:5:1624:G:H4'	1:5:1625:G:H5'	1.98	0.45
1:5:4581:G:OP2	5:B:28:LYS:NZ	2.50	0.45
31:c:81:LEU:HD11	31:c:94:LEU:HD23	1.99	0.45
51:K:903:A:H2'	51:K:904:A:C8	2.51	0.45
51:K:1674:G:OP1	73:BB:51:HIS:NE2	2.49	0.45
55:x:31:PRO:HG3	55:x:43:PRO:HG3	1.98	0.45
62:MM:117:ARG:NH2	81:FF:62:GLU:O	2.50	0.45
77:II:13:LEU:HB2	77:II:20:ILE:HB	1.97	0.45
1:5:440:U:O2'	34:f:91:ASN:O	2.32	0.45
1:5:1932:A:OP2	17:O:49:ARG:NH1	2.49	0.45
1:5:2352:U:H1'	6:C:96:CYS:HA	1.98	0.45
1:5:4544:A:H5''	4:A:213:GLY:HA3	1.99	0.45
4:A:117:GLU:HB2	4:A:162:ASN:HB2	1.98	0.45
6:C:40:VAL:HG22	6:C:115:VAL:HG11	1.99	0.45
11:H:173:ARG:HD3	41:m:124:LYS:HE2	1.99	0.45
18:P:94:MET:HE1	18:P:146:ILE:HB	1.99	0.45
25:W:46:PRO:O	25:W:52:THR:OG1	2.32	0.45
51:K:296:U:O2'	55:x:131:VAL:O	2.31	0.45
51:K:436:G:OP1	51:K:471:G:O2'	2.35	0.45
51:K:587:A:H5''	51:K:592:C:H41	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:5:2017:A:C8	1:5:2017:A:OP2	2.70	0.45
1:5:2539:C:H5''	35:g:66:ARG:HD2	1.98	0.45
1:5:4180:G:N2	4:A:228:ASP:OD2	2.50	0.45
7:D:53:VAL:HB	7:D:159:VAL:HG13	1.98	0.45
9:F:96:ARG:HH12	9:F:100:ILE:HD12	1.82	0.45
10:G:63:LEU:HD21	16:N:29:GLN:HG3	1.98	0.45
26:X:61:PRO:HG2	36:h:80:PRO:HG3	1.99	0.45
51:K:65:C:N4	56:z:134:GLY:O	2.41	0.45
72:DD:135:GLU:HA	72:DD:153:VAL:HG22	1.98	0.45
73:BB:140:ASP:HB2	81:FF:44:ARG:HH22	1.81	0.45
79:GG:56:MET:HG3	79:GG:86:LYS:HE3	1.97	0.45
1:5:439:G:O3'	34:f:91:ASN:ND2	2.49	0.45
1:5:4300:U:H5''	22:T:87:LYS:HE2	1.99	0.45
5:B:294:LYS:HE3	5:B:298:LEU:HD11	1.99	0.45
8:E:174:PRO:HG2	8:E:177:LEU:HD12	1.99	0.45
24:V:35:LYS:HB2	24:V:67:LYS:HG3	1.98	0.45
45:r:61:VAL:HA	45:r:80:THR:O	2.16	0.45
51:K:305:U:H3'	51:K:306:C:H5'	1.99	0.45
51:K:429:C:OP2	55:x:10:LYS:NZ	2.50	0.45
51:K:929:G:H21	51:K:1104:G:H4'	1.82	0.45
51:K:983:A:OP1	51:K:1073:U:O2'	2.32	0.45
51:K:1324:G:H1	51:K:1504:U:H3	1.65	0.45
66:TT:11:LEU:HA	66:TT:14:ILE:HG12	1.98	0.45
74:SS:15:LEU:HD22	74:SS:49:MET:HE1	1.98	0.45
1:5:32:G:H21	1:5:50:C:H5	1.65	0.45
1:5:1600:A:C5	48:1:244:PRO:HG2	2.51	0.45
1:5:2498:C:H2'	1:5:2499:C:H6	1.82	0.45
1:5:3687:A:H3'	4:A:198:ARG:HH22	1.82	0.45
1:5:4239:A:H2'	1:5:4240:G:C8	2.52	0.45
1:5:4303:C:H2'	1:5:4305:G:H8	1.82	0.45
1:5:4693:C:H1'	1:5:4695:C:H41	1.81	0.45
1:5:4992:G:H2'	1:5:4993:G:C8	2.52	0.45
8:E:273:LEU:HD11	34:f:105:LEU:HD11	1.99	0.45
29:a:117:LEU:HD12	29:a:118:PRO:HD2	1.98	0.45
51:K:304:C:OP2	51:K:304:C:C6	2.70	0.45
51:K:1534:C:H4'	51:K:1535:U:H5''	1.98	0.45
51:K:1536:G:H2'	51:K:1537:A:C8	2.51	0.45
1:5:134:G:OP2	36:h:79:LYS:NZ	2.48	0.44
1:5:1237:C:H41	9:F:49:ARG:HG3	1.82	0.44
1:5:1398:A:N6	1:5:1419:G:C2	2.85	0.44
1:5:1628:C:H42	4:A:3:ARG:HD3	1.81	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:5:1728:U:O4	1:5:1729:A:N6	2.51	0.44
3:8:85:U:O2'	3:8:87:G:OP1	2.33	0.44
5:B:19:ARG:HB2	5:B:234:ARG:HH21	1.82	0.44
10:G:167:VAL:HG13	10:G:170:LEU:HB3	1.98	0.44
12:I:135:ILE:HG22	12:I:136:MET:HG3	1.98	0.44
37:i:33:LEU:HD11	37:i:38:LYS:HD2	1.99	0.44
50:3:38:A:O2'	51:K:1058:A:OP1	2.29	0.44
51:K:805:U:O3'	66:TT:120:HIS:NE2	2.50	0.44
58:CC:100:CYS:O	58:CC:174:CYS:HA	2.17	0.44
83:0:138:ARG:HB2	83:0:149:CYS:HA	1.99	0.44
1:5:293:G:N2	16:N:178:HIS:O	2.40	0.44
1:5:2904:U:H5''	1:5:2905:C:H5	1.81	0.44
4:A:92:LYS:HG3	4:A:106:THR:HG21	2.00	0.44
4:A:210:PRO:O	4:A:221:LYS:NZ	2.49	0.44
6:C:7:LEU:HG	6:C:21:ASN:HB3	1.98	0.44
51:K:1513:C:H2'	51:K:1514:G:H8	1.82	0.44
51:K:1814:G:H5''	51:K:1815:A:H5'	1.99	0.44
67:VV:68:LYS:HE2	71:AA:82:VAL:HG22	1.99	0.44
84:6:20:GLN:HG2	84:6:69:VAL:H	1.82	0.44
84:6:174:VAL:HB	84:6:188:HIS:HB2	1.98	0.44
1:5:1655:C:O2	1:5:4390:A:O2'	2.34	0.44
1:5:4472:G:O2'	41:m:100:TYR:O	2.29	0.44
7:D:52:ILE:HA	7:D:147:ASP:HB3	1.98	0.44
14:L:186:ARG:HE	37:i:9:VAL:HG11	1.83	0.44
51:K:681:U:H5''	67:VV:8:ARG:HG3	1.98	0.44
51:K:941:C:H2'	51:K:942:G:C8	2.53	0.44
51:K:1139:C:H41	51:K:1149:A:H62	1.64	0.44
73:BB:20:PHE:N	73:BB:23:TRP:O	2.51	0.44
79:GG:63:ILE:HB	79:GG:80:PHE:HB2	2.00	0.44
1:5:4430:G:H1'	12:I:158:LYS:HD2	2.00	0.44
1:5:4586:G:OP2	17:O:74:ARG:NH1	2.51	0.44
29:a:39:HIS:O	29:a:40:HIS:ND1	2.50	0.44
41:m:87:GLN:OE1	41:m:126:LYS:NZ	2.42	0.44
51:K:1228:A:H2'	51:K:1229:G:C8	2.53	0.44
51:K:1776:G:H2'	51:K:1777:G:H8	1.82	0.44
63:UU:33:LYS:HA	63:UU:38:PRO:HA	1.99	0.44
83:0:104:LYS:O	83:0:118:ARG:NH1	2.44	0.44
1:5:418:A:H4'	1:5:2311:C:H5'	2.00	0.44
1:5:1335:G:N2	6:C:95:MET:O	2.46	0.44
1:5:2438:A:O2'	1:5:2440:U:OP1	2.32	0.44
1:5:2515:G:OP1	35:g:37:LYS:NZ	2.50	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:5:4527:G:OP2	1:5:4527:G:N2	2.42	0.44
1:5:4902:C:N4	1:5:4903:G:O6	2.51	0.44
4:A:3:ARG:N	4:A:207:VAL:O	2.45	0.44
18:P:4:TYR:HE1	18:P:18:ARG:HD2	1.83	0.44
51:K:659:G:HO2'	51:K:662:G:HO2'	1.60	0.44
53:u:107:ARG:HD3	62:MM:135:ILE:HD12	1.99	0.44
1:5:673:C:H2'	1:5:674:G:C8	2.53	0.44
1:5:1621:A:O2'	4:A:14:SER:OG	2.27	0.44
1:5:1691:G:H5'	19:Q:15:ARG:HG3	2.00	0.44
1:5:1840:G:O2'	1:5:1842:G:O3'	2.32	0.44
1:5:2263:A:H5''	45:r:39:ARG:HH12	1.83	0.44
1:5:2782:U:OP2	40:l:10:LYS:NZ	2.46	0.44
11:H:8:GLN:NE2	11:H:74:CYS:SG	2.91	0.44
22:T:18:PRO:HG2	22:T:21:LYS:HB2	1.98	0.44
22:T:45:MET:H	22:T:95:HIS:HD2	1.64	0.44
51:K:912:C:H3'	51:K:913:A:H3'	1.99	0.44
51:K:1036:A:H4'	51:K:1855:G:H21	1.82	0.44
51:K:1135:C:OP2	69:ZZ:6:ARG:NH1	2.51	0.44
54:v:61:LEU:HD12	54:v:62:PRO:HD2	1.99	0.44
54:v:78:LEU:HA	54:v:81:ILE:HD12	2.00	0.44
1:5:136:C:H4'	36:h:96:ASN:HD21	1.83	0.44
1:5:153:G:H2'	1:5:154:G:H8	1.83	0.44
1:5:659:G:H2'	1:5:660:A:H8	1.82	0.44
1:5:4748:U:O4	1:5:4952:G:O6	2.35	0.44
3:8:67:U:H2'	3:8:68:G:H8	1.82	0.44
17:O:36:VAL:HG23	17:O:105:PHE:HB2	2.00	0.44
51:K:5:U:H2'	51:K:6:G:C8	2.52	0.44
52:q:42:LYS:NZ	64:YY:99:ASP:OD2	2.45	0.44
75:RR:48:HIS:HD2	75:RR:112:LYS:HG2	1.83	0.44
1:5:951:G:H2'	1:5:952:G:H8	1.83	0.44
1:5:1265:G:N2	1:5:2112:G:OP2	2.49	0.44
1:5:2386:U:H5''	20:R:24:LEU:HD12	1.98	0.44
1:5:4473:A:O2'	41:m:122:ARG:NH2	2.50	0.44
1:5:4760:G:H3'	17:O:12:ARG:HH22	1.81	0.44
5:B:331:VAL:HG21	5:B:347:LEU:HD21	1.99	0.44
8:E:115:GLU:HB3	33:e:7:LEU:HD22	1.99	0.44
11:H:167:VAL:HB	11:H:172:ILE:HG22	2.00	0.44
43:o:44:LYS:HE2	43:o:52:THR:HB	2.00	0.44
51:K:1003:U:H1'	53:u:124:HIS:HE1	1.83	0.44
51:K:1865:C:OP2	69:ZZ:5:ARG:NH2	2.49	0.44
64:YY:31:ASN:HD21	64:YY:55:THR:HG22	1.83	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
76:9:60:LEU:HD13	76:9:89:MET:HG3	1.99	0.44
1:5:1864:G:H21	12:I:115:MET:HE2	1.81	0.44
1:5:2897:G:H2'	1:5:2898:G:C8	2.52	0.44
1:5:4692:A:H62	1:5:4696:C:H42	1.66	0.44
1:5:4991:U:H2'	1:5:4992:G:C8	2.53	0.44
17:O:44:SER:HB3	17:O:129:LEU:HD11	1.99	0.44
36:h:91:MET:HA	36:h:94:ARG:HG3	1.99	0.44
51:K:305:U:O5'	51:K:305:U:H6	2.01	0.44
51:K:960:U:H5''	62:MM:149:ARG:HH21	1.83	0.44
51:K:1623:A:H5''	77:II:133:GLY:HA3	2.00	0.44
54:v:106:VAL:HG22	54:v:128:VAL:HG22	2.00	0.44
74:SS:93:THR:HG23	74:SS:94:LEU:HD12	1.99	0.44
1:5:86:U:H2'	1:5:87:A:C8	2.53	0.43
1:5:416:U:H4'	1:5:2330:G:H4'	2.00	0.43
1:5:4522:G:O2'	1:5:4525:C:OP2	2.36	0.43
1:5:4714:C:OP1	5:B:31:SER:OG	2.32	0.43
1:5:4894:A:O2'	1:5:4896:G:OP1	2.30	0.43
8:E:153:HIS:HB3	8:E:156:LYS:HD2	1.99	0.43
12:I:27:PRO:HA	49:2:64:U:H4'	2.00	0.43
23:U:84:LYS:HG2	23:U:88:LYS:HE2	1.99	0.43
54:v:265:PRO:HA	54:v:268:GLU:HB2	2.00	0.43
57:y:57:ARG:NE	57:y:89:GLY:O	2.50	0.43
59:XX:29:LEU:HD12	71:AA:115:PHE:HE2	1.83	0.43
60:EE:135:SER:O	60:EE:139:ARG:NH1	2.49	0.43
63:UU:41:MET:N	63:UU:41:MET:SD	2.91	0.43
1:5:198:A:O2'	1:5:221:C:O2	2.33	0.43
1:5:3689:G:O2'	1:5:3818:U:OP2	2.31	0.43
12:I:54:SER:HB2	12:I:135:ILE:HD11	2.00	0.43
27:Y:31:SER:HA	27:Y:48:PRO:HA	1.99	0.43
41:m:97:ARG:HE	41:m:122:ARG:HB3	1.83	0.43
1:5:1593:A:H5''	1:5:2839:U:H5''	1.99	0.43
1:5:2402:G:O2'	35:g:10:ARG:O	2.35	0.43
1:5:2405:G:H5''	38:j:14:LYS:HE3	2.01	0.43
1:5:2674:A:N6	31:c:51:ASN:O	2.50	0.43
1:5:2903:G:H5'	1:5:3592:G:H1	1.84	0.43
5:B:222:VAL:O	5:B:343:ARG:NH1	2.52	0.43
7:D:64:ILE:HG13	7:D:105:LEU:HD21	2.01	0.43
10:G:105:GLU:OE2	10:G:113:ARG:NH1	2.50	0.43
24:V:18:LEU:HD13	24:V:54:ALA:HB3	2.00	0.43
51:K:1084:A:OP1	51:K:1858:G:O2'	2.35	0.43
51:K:1691:U:H4'	69:ZZ:88:SER:HB3	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
53:u:65:ARG:HE	62:MM:50:LYS:HD3	1.83	0.43
73:BB:50:PRO:HG2	73:BB:90:VAL:HG22	2.00	0.43
76:9:108:LYS:HG2	76:9:111:MET:HE2	2.00	0.43
84:6:258:ILE:HG13	84:6:267:VAL:HB	2.00	0.43
1:5:2361:G:O2'	1:5:3859:G:O6	2.35	0.43
1:5:2386:U:H2'	1:5:2387:G:H8	1.83	0.43
1:5:2519:U:O2'	1:5:2530:U:O2	2.30	0.43
1:5:4274:A:H2'	1:5:4275:G:H8	1.83	0.43
1:5:4451:G:N9	48:1:256:TRP:HD1	2.06	0.43
6:C:290:SER:OG	45:r:4:HIS:NE2	2.40	0.43
8:E:161:LEU:HD21	8:E:253:ILE:HD11	2.00	0.43
16:N:6:TYR:CZ	37:i:40:VAL:HG22	2.53	0.43
17:O:56:ALA:HA	17:O:59:ARG:HE	1.83	0.43
18:P:38:GLY:H	18:P:114:ILE:HG23	1.83	0.43
34:f:71:TRP:HB2	34:f:89:ARG:HH11	1.83	0.43
51:K:90:G:OP1	51:K:445:A:N6	2.41	0.43
51:K:521:A:OP1	59:XX:45:ARG:NH1	2.49	0.43
51:K:1722:G:H2'	51:K:1723:G:C8	2.53	0.43
68:NN:78:SER:HB3	68:NN:81:TYR:HD2	1.83	0.43
1:5:1188:C:H2'	1:5:1189:G:C8	2.53	0.43
1:5:1329:G:H2'	1:5:3865:A:H5'	2.00	0.43
1:5:1906:U:H2'	1:5:1907:A:H8	1.83	0.43
1:5:1986:U:O2	1:5:2007:G:N2	2.51	0.43
1:5:2521:G:H2'	1:5:2522:G:C8	2.54	0.43
1:5:4537:C:H2'	1:5:4538:G:C8	2.53	0.43
13:J:43:LEU:HD13	13:J:117:ILE:HD11	2.00	0.43
51:K:1786:U:H2'	51:K:1787:G:H8	1.83	0.43
52:q:188:THR:HG22	52:q:189:ILE:HG13	1.99	0.43
1:5:2399:G:O2'	1:5:2822:G:O2'	2.34	0.43
1:5:3620:G:OP1	1:5:3622:C:N4	2.51	0.43
1:5:4737:G:H5''	1:5:5069:U:H2'	1.99	0.43
1:5:4748:U:H3	1:5:4952:G:H1	1.66	0.43
2:7:94:C:OP1	21:S:46:TYR:OH	2.32	0.43
5:B:256:ALA:H	5:B:260:ALA:HB3	1.83	0.43
28:Z:89:ILE:HG12	28:Z:91:LEU:HG	1.99	0.43
51:K:104:A:H62	51:K:356:C:H5	1.65	0.43
51:K:126:G:H5''	56:z:195:LYS:HB3	2.00	0.43
51:K:603:C:N4	51:K:620:G:O6	2.52	0.43
52:q:14:ASP:OD1	52:q:180:ARG:NH2	2.49	0.43
72:DD:93:THR:HG21	72:DD:198:ILE:HG13	1.99	0.43
1:5:695:G:OP1	8:E:219:ARG:NH2	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:5:2520:C:H2'	1:5:2521:G:C8	2.52	0.43
2:7:63:C:H5'	2:7:64:G:H5''	2.01	0.43
13:J:56:THR:HG23	13:J:63:ARG:HA	2.01	0.43
14:L:176:PHE:O	29:a:138:LYS:NZ	2.52	0.43
15:M:53:LYS:HE3	21:S:160:ARG:HG3	1.99	0.43
16:N:181:HIS:O	16:N:195:ARG:NH2	2.44	0.43
46:s:28:PHE:HB2	46:s:89:VAL:HB	2.00	0.43
51:K:919:A:O2'	51:K:1020:A:N1	2.41	0.43
51:K:1083:A:N7	51:K:1841:C:O2'	2.47	0.43
52:q:41:ARG:HE	52:q:45:GLY:HA2	1.83	0.43
54:v:261:PHE:HB2	65:HH:52:THR:HG21	2.00	0.43
62:MM:56:VAL:HG11	62:MM:80:ASP:HB3	2.01	0.43
68:NN:43:LYS:HA	68:NN:46:LYS:HG2	1.99	0.43
73:BB:86:LYS:HA	73:BB:89:THR:HG22	2.01	0.43
1:5:4421:C:H42	1:5:4475:G:H22	1.65	0.43
5:B:168:MET:HE2	5:B:175:GLN:HG3	2.00	0.43
12:I:48:LEU:HD21	12:I:145:LYS:HG2	2.00	0.43
15:M:38:VAL:HG21	15:M:50:MET:HB3	2.01	0.43
51:K:807:G:H2'	51:K:808:A:C8	2.53	0.43
51:K:1401:A:H4'	79:GG:52:GLY:HA3	2.01	0.43
51:K:1417:C:N3	51:K:1423:C:N4	2.61	0.43
53:u:92:GLN:HB3	53:u:95:ASN:HB2	1.99	0.43
63:UU:97:GLN:HE21	84:6:58:ALA:HB3	1.83	0.43
69:ZZ:23:CYS:SG	69:ZZ:24:THR:N	2.91	0.43
79:GG:48:LEU:HD11	79:GG:91:LEU:HD22	2.00	0.43
1:5:2812:A:OP1	20:R:83:GLY:N	2.44	0.43
1:5:4991:U:H2'	1:5:4992:G:H8	1.84	0.43
2:7:105:C:OP2	12:I:203:ARG:NH2	2.46	0.43
5:B:33:PRO:O	5:B:186:ASN:ND2	2.52	0.43
11:H:105:ILE:HG22	11:H:112:VAL:HG22	2.01	0.43
27:Y:27:ARG:HB2	27:Y:75:ARG:HH11	1.84	0.43
32:d:23:ARG:HA	32:d:122:VAL:HG22	2.00	0.43
47:t:57:ARG:HD3	47:t:83:LYS:HZ2	1.84	0.43
51:K:1253:A:N6	51:K:1665:G:O2'	2.52	0.43
63:UU:97:GLN:HB2	63:UU:105:LYS:HE3	2.00	0.43
1:5:1240:G:OP2	1:5:1271:G:O2'	2.35	0.43
1:5:1417:C:OP2	29:a:119:LYS:NZ	2.52	0.43
1:5:3598:C:H2'	1:5:3599:A:C8	2.52	0.43
1:5:4319:C:H2'	1:5:4320:G:H8	1.84	0.43
2:7:11:A:N1	2:7:66:G:O2'	2.44	0.43
4:A:117:GLU:O	4:A:162:ASN:ND2	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:L:80:GLU:OE2	14:L:113:ASN:ND2	2.51	0.43
51:K:160:U:O2'	51:K:162:C:O5'	2.36	0.43
60:EE:35:ARG:NE	60:EE:50:ALA:O	2.43	0.43
1:5:724:C:OP2	6:C:350:ARG:NH2	2.49	0.42
1:5:2096:G:O6	9:F:48:ARG:NH1	2.52	0.42
1:5:2338:C:OP1	45:r:19:LYS:NZ	2.43	0.42
1:5:4508:C:H4'	24:V:43:LYS:HA	2.01	0.42
1:5:4945:G:H5'	1:5:4946:U:H5'	2.00	0.42
4:A:147:ARG:HH21	4:A:155:LYS:HE2	1.84	0.42
8:E:175:LEU:HD22	8:E:179:ARG:HA	2.01	0.42
16:N:15:GLN:HG3	37:i:52:PRO:HD2	2.01	0.42
19:Q:18:PRO:HG3	19:Q:29:VAL:HG21	2.00	0.42
19:Q:66:MET:HE3	19:Q:98:LEU:HD13	2.01	0.42
29:a:81:LEU:HD22	29:a:106:SER:HB2	2.00	0.42
44:p:56:HIS:NE2	44:p:61:MET:SD	2.91	0.42
50:3:47:U:O2'	50:3:50:A:OP1	2.25	0.42
56:z:1:MET:HE3	56:z:106:LEU:HB2	2.00	0.42
57:y:73:GLN:HA	57:y:76:GLN:HB2	2.00	0.42
1:5:150:U:OP2	10:G:200:THR:OG1	2.37	0.42
1:5:1461:C:H2'	1:5:1462:A:C8	2.55	0.42
1:5:2091:C:H1'	1:5:2092:G:H2'	2.01	0.42
1:5:4627:U:H5'	5:B:53:MET:HB2	2.01	0.42
9:F:103:VAL:HG23	9:F:141:TYR:HE2	1.84	0.42
12:I:36:LEU:HD21	12:I:69:ARG:HD3	1.99	0.42
13:J:119:TYR:O	77:II:101:ASN:ND2	2.42	0.42
27:Y:72:GLN:HE22	27:Y:74:TYR:HB2	1.84	0.42
29:a:11:LEU:HA	29:a:14:HIS:HD2	1.84	0.42
34:f:8:LYS:HB3	34:f:100:ARG:HH11	1.85	0.42
57:y:143:ARG:HB2	57:y:155:LYS:HB2	2.01	0.42
1:5:363:A:N7	1:5:378:A:N6	2.67	0.42
1:5:1348:U:OP2	19:Q:56:THR:OG1	2.34	0.42
1:5:1940:G:N2	1:5:4434:C:OP1	2.42	0.42
1:5:2411:C:H2'	1:5:2412:A:C8	2.54	0.42
1:5:2467:U:H4'	1:5:2468:U:H5'	2.02	0.42
1:5:2749:C:H2'	1:5:2750:G:H8	1.83	0.42
1:5:4520:G:N2	5:B:253:CYS:SG	2.92	0.42
1:5:4870:G:OP2	1:5:4870:G:N2	2.41	0.42
3:8:26:C:O2'	6:C:53:ALA:O	2.31	0.42
11:H:109:GLY:HA3	11:H:134:CYS:H	1.84	0.42
12:I:35:ASP:HA	12:I:87:ILE:O	2.19	0.42
14:L:64:VAL:HA	14:L:67:HIS:HB2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
41:m:110:CYS:O	41:m:117:HIS:ND1	2.42	0.42
51:K:374:G:H4'	60:EE:84:ARG:HD2	2.01	0.42
51:K:1407:U:O2'	63:UU:11:GLN:NE2	2.52	0.42
53:u:33:VAL:HA	53:u:96:CYS:HB2	2.02	0.42
62:MM:150:ARG:HD3	62:MM:150:ARG:H	1.84	0.42
1:5:1199:G:H2'	1:5:1200:G:H8	1.84	0.42
1:5:1669:A:H62	1:5:1881:C:H5	1.66	0.42
1:5:1918:U:O2	1:5:2064:G:O6	2.37	0.42
1:5:2020:U:H2'	1:5:2021:G:H8	1.84	0.42
1:5:2863:G:O2'	20:R:82:LYS:O	2.35	0.42
1:5:3619:G:H22	1:5:3624:A:H1'	1.83	0.42
1:5:4238:G:H2'	1:5:4239:A:H8	1.84	0.42
1:5:4993:G:H22	1:5:5058:A:H2	1.66	0.42
5:B:302:ASN:HB2	5:B:313:SER:HA	2.00	0.42
6:C:12:SER:OG	6:C:15:GLY:O	2.30	0.42
6:C:152:LEU:HD11	6:C:174:LEU:HD22	2.01	0.42
23:U:44:GLN:HA	23:U:56:LEU:HD21	2.01	0.42
51:K:438:G:H8	51:K:1800:A:H4'	1.84	0.42
51:K:557:U:H2'	51:K:558:G:C8	2.55	0.42
51:K:1268:C:O2	76:9:97:TYR:OH	2.37	0.42
58:CC:190:LEU:HD12	58:CC:194:GLU:HB3	2.02	0.42
69:ZZ:28:ARG:NH1	69:ZZ:29:CYS:O	2.52	0.42
70:JJ:20:LYS:HE3	70:JJ:28:PRO:HA	2.01	0.42
73:BB:73:THR:HG23	73:BB:89:THR:HG23	2.00	0.42
77:II:20:ILE:HD11	77:II:33:ILE:HD11	2.01	0.42
1:5:229:G:H5''	27:Y:11:ARG:HD2	2.01	0.42
1:5:704:C:H2'	1:5:705:G:H8	1.84	0.42
1:5:1811:G:H21	30:b:57:MET:HE2	1.85	0.42
1:5:2268:A:OP1	45:r:11:ARG:NH2	2.43	0.42
1:5:4862:G:H2'	1:5:4863:G:H8	1.84	0.42
4:A:33:ASP:H	4:A:36:GLU:HB2	1.84	0.42
16:N:68:ARG:NH1	16:N:124:ASP:O	2.46	0.42
24:V:87:SER:HB2	25:W:19:ARG:HH11	1.84	0.42
40:l:44:TRP:O	40:l:48:LYS:NZ	2.42	0.42
51:K:915:G:OP2	51:K:915:G:N2	2.40	0.42
51:K:916:A:C5	61:QQ:73:ARG:HD3	2.55	0.42
51:K:1542:C:OP1	78:PP:59:SER:OG	2.33	0.42
55:x:126:VAL:HG12	55:x:141:THR:HG22	2.01	0.42
73:BB:14:THR:OG1	73:BB:17:ILE:O	2.32	0.42
78:PP:5:THR:HG23	78:PP:7:LYS:H	1.84	0.42
1:5:667:A:H4'	6:C:6:PRO:HB3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:5:943:A:OP1	9:F:247:ARG:NH1	2.53	0.42
1:5:1460:C:H5'	19:Q:143:ARG:HB3	2.02	0.42
1:5:1939:A:H5'	1:5:1940:G:H4'	2.01	0.42
1:5:2282:A:H4'	29:a:21:ARG:HB2	2.00	0.42
1:5:2890:C:H42	1:5:3611:A:H61	1.68	0.42
1:5:4124:G:H5'	28:Z:135:ARG:HH21	1.84	0.42
8:E:254:LEU:HA	8:E:257:ILE:HG12	2.01	0.42
20:R:70:ARG:HE	20:R:75:HIS:HB2	1.85	0.42
23:U:23:LEU:HD12	23:U:83:LEU:HD23	2.02	0.42
33:e:77:PHE:HB3	33:e:88:LEU:HD11	2.02	0.42
51:K:928:G:H2'	51:K:929:G:C8	2.54	0.42
51:K:1373:C:H2'	51:K:1374:C:H6	1.84	0.42
51:K:1468:C:H2'	51:K:1469:A:C8	2.54	0.42
51:K:1479:G:H2'	51:K:1480:A:H8	1.85	0.42
68:NN:7:ILE:HG23	68:NN:25:ILE:HG23	2.01	0.42
84:6:289:LEU:HD12	84:6:298:LEU:HD21	2.00	0.42
1:5:373:G:O2'	1:5:1645:C:O2'	2.36	0.42
1:5:1386:C:O2'	1:5:1502:G:N2	2.52	0.42
1:5:3732:A:H2'	1:5:3733:A:C8	2.55	0.42
51:K:448:A:H3'	58:CC:23:LYS:HD2	2.02	0.42
51:K:848:U:OP1	55:x:245:ARG:NH2	2.51	0.42
51:K:1541:G:H5''	78:PP:59:SER:HB2	2.00	0.42
61:QQ:84:LEU:HA	61:QQ:85:PRO:HD3	1.94	0.42
77:II:6:PRO:HG2	77:II:58:GLU:HG2	2.01	0.42
1:5:1364:U:H5''	14:L:36:ARG:HH22	1.85	0.42
1:5:2465:C:H1'	1:5:3672:G:H22	1.84	0.42
1:5:2575:U:H3'	28:Z:48:ARG:HH22	1.85	0.42
1:5:4336:A:H5''	1:5:4337:C:H5'	2.01	0.42
6:C:78:ARG:HB3	6:C:88:GLY:HA2	2.01	0.42
11:H:120:GLU:OE1	11:H:124:ARG:NH2	2.51	0.42
30:b:25:ARG:NE	30:b:27:GLN:OE1	2.53	0.42
36:h:70:ARG:HB3	36:h:83:LEU:HD22	2.01	0.42
36:h:87:LYS:O	38:j:73:ARG:NH2	2.48	0.42
45:r:124:VAL:HG13	45:r:125:MET:HG2	2.01	0.42
46:s:28:PHE:HZ	46:s:95:LEU:HA	1.84	0.42
51:K:397:G:OP2	60:EE:108:ASN:ND2	2.52	0.42
51:K:440:G:OP1	51:K:1798:C:O2'	2.37	0.42
51:K:681:U:H4'	67:VV:9:THR:HG22	2.00	0.42
60:EE:57:ASP:HB3	60:EE:60:CYS:HB2	2.01	0.42
64:YY:57:LEU:HD23	64:YY:60:ARG:HD3	2.02	0.42
76:9:44:ARG:HG2	76:9:84:ILE:HD11	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
78:PP:56:ARG:HH22	78:PP:99:VAL:HB	1.85	0.42
1:5:1245:C:H2'	1:5:1246:G:C8	2.54	0.42
1:5:1919:G:N2	21:S:163:HIS:O	2.41	0.42
1:5:4186:A:H2'	1:5:4187:G:C8	2.55	0.42
1:5:4730:C:O2	1:5:4965:U:N3	2.53	0.42
5:B:77:THR:O	5:B:332:MET:HA	2.20	0.42
7:D:12:TYR:O	7:D:16:TYR:HB2	2.19	0.42
7:D:60:ILE:HB	7:D:80:ALA:HB2	2.02	0.42
51:K:454:U:H4'	56:z:76:LEU:HD21	2.02	0.42
52:q:123:VAL:HG22	52:q:145:ILE:HD12	2.01	0.42
1:5:1333:A:H2'	1:5:1334:A:H8	1.85	0.42
1:5:1907:A:H4'	9:F:225:LYS:HE3	2.00	0.42
1:5:2389:A:H5'	32:d:70:LYS:HE2	2.02	0.42
1:5:2480:G:H2'	1:5:2481:G:H8	1.84	0.42
1:5:4598:C:H2'	1:5:4611:A:H61	1.83	0.42
1:5:4967:A:H2'	1:5:4968:A:H8	1.84	0.42
1:5:4990:C:H3'	1:5:4991:U:H4'	2.01	0.42
1:5:5057:C:H2'	1:5:5058:A:C8	2.54	0.42
18:P:4:TYR:HE2	18:P:16:LYS:HB3	1.85	0.42
20:R:24:LEU:HD22	20:R:32:ILE:HG21	2.02	0.42
38:j:64:MET:HE3	38:j:67:LEU:HD23	2.02	0.42
51:K:369:C:H41	51:K:1730:U:H5''	1.84	0.42
51:K:522:A:O3'	59:XX:131:ARG:NH2	2.53	0.42
51:K:639:C:H5''	71:AA:114:ARG:HH21	1.85	0.42
51:K:1588:A:H2'	51:K:1589:A:H8	1.85	0.42
51:K:1648:G:O2'	51:K:1674:G:O6	2.37	0.42
73:BB:34:SER:HA	81:FF:55:VAL:HB	2.02	0.42
73:BB:103:LEU:HD23	73:BB:178:ILE:HD13	2.02	0.42
1:5:208:A:N3	1:5:232:G:O2'	2.47	0.41
1:5:440:U:H4'	34:f:91:ASN:HB2	2.01	0.41
1:5:2609:G:H1	1:5:2730:U:H3	1.67	0.41
1:5:3909:C:O2'	48:1:260:MET:O	2.37	0.41
1:5:4594:U:H2'	1:5:4595:G:C8	2.54	0.41
1:5:4978:G:HO2'	1:5:4981:G:H1	1.66	0.41
24:V:16:ILE:HB	24:V:88:TYR:HB2	2.01	0.41
33:e:7:LEU:HB2	33:e:93:LYS:HB3	2.01	0.41
38:j:34:CYS:HB3	38:j:38:GLY:H	1.84	0.41
41:m:103:LEU:HD22	41:m:111:ARG:HD3	2.02	0.41
50:3:41:U:H2'	50:3:42:G:H8	1.84	0.41
51:K:28:U:H2'	51:K:29:G:H8	1.85	0.41
51:K:652:U:H2'	51:K:653:A:C8	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
51:K:687:C:O3'	57:y:121:THR:OG1	2.38	0.41
51:K:1588:A:H2'	51:K:1589:A:C8	2.55	0.41
51:K:1753:C:H2'	51:K:1754:G:H8	1.85	0.41
53:u:159:GLN:OE1	53:u:162:ARG:NH1	2.53	0.41
56:z:78:SER:H	56:z:81:HIS:CD2	2.37	0.41
78:PP:38:LYS:NZ	78:PP:40:ALA:O	2.40	0.41
84:6:238:ALA:H	84:6:251:ALA:HB3	1.85	0.41
1:5:1350:C:H2'	1:5:1351:G:C8	2.55	0.41
1:5:3717:A:OP2	1:5:3735:G:N2	2.45	0.41
1:5:4266:G:O2'	1:5:4267:G:N2	2.53	0.41
1:5:4876:U:H5'	21:S:170:LYS:HE2	2.02	0.41
1:5:4935:C:OP2	8:E:179:ARG:NH1	2.52	0.41
5:B:329:ASP:OD1	5:B:329:ASP:N	2.53	0.41
11:H:114:ILE:HB	11:H:124:ARG:HB2	2.00	0.41
27:Y:52:ASP:OD2	27:Y:110:LYS:NZ	2.41	0.41
27:Y:80:ILE:HD11	27:Y:104:VAL:HG21	2.02	0.41
49:2:4:U:H3	49:2:69:G:H22	1.67	0.41
55:x:48:LEU:HD23	55:x:61:VAL:HG13	2.01	0.41
56:z:132:ARG:HG3	56:z:133:LEU:HD12	2.02	0.41
75:RR:40:LYS:HE2	83:0:130:VAL:HG22	2.02	0.41
1:5:1064:G:H2'	1:5:1065:G:H8	1.85	0.41
1:5:1437:C:O2'	1:5:2098:G:OP2	2.32	0.41
1:5:1971:C:O2	46:s:41:GLN:NE2	2.54	0.41
1:5:2418:A:N1	1:5:2429:A:O2'	2.48	0.41
1:5:2421:G:H1'	18:P:139:TYR:CE2	2.56	0.41
1:5:3686:G:OP2	4:A:193:ARG:NH2	2.48	0.41
2:7:48:G:OP1	7:D:226:TYR:OH	2.38	0.41
5:B:302:ASN:HD22	5:B:330:PHE:HE1	1.68	0.41
16:N:85:VAL:HA	43:o:49:GLY:HA2	2.01	0.41
33:e:44:ARG:HG2	33:e:52:GLN:HG3	2.01	0.41
67:VV:93:PHE:O	67:VV:140:ARG:NH1	2.53	0.41
76:9:98:ASN:HB3	76:9:122:THR:HA	2.02	0.41
78:PP:6:VAL:O	78:PP:11:GLN:NE2	2.53	0.41
83:0:132:MET:HE1	83:0:148:TYR:HD2	1.84	0.41
1:5:709:C:H2'	1:5:710:G:C8	2.54	0.41
1:5:1262:G:H2'	1:5:1263:A:H8	1.85	0.41
1:5:1399:G:O6	1:5:1419:G:N2	2.53	0.41
1:5:1509:C:H2'	1:5:1510:G:H8	1.85	0.41
1:5:1645:C:H2'	1:5:1646:A:C8	2.55	0.41
1:5:4084:G:O6	4:A:72:ARG:NH2	2.54	0.41
1:5:4425:G:OP1	41:m:100:TYR:OH	2.30	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:P:128:ARG:HH12	48:1:240:PRO:HD3	1.83	0.41
21:S:11:LYS:HD2	21:S:29:ARG:HD2	2.03	0.41
24:V:21:PRO:HA	24:V:54:ALA:HA	2.02	0.41
28:Z:29:ILE:HD13	28:Z:40:HIS:CD2	2.56	0.41
33:e:122:VAL:HG12	33:e:124:ASN:H	1.85	0.41
51:K:125:C:OP1	51:K:127:C:N4	2.54	0.41
51:K:656:G:H21	51:K:663:C:H5''	1.84	0.41
57:y:91:HIS:HB2	57:y:172:THR:HG21	2.03	0.41
59:XX:42:GLU:OE2	59:XX:109:ARG:NH1	2.53	0.41
66:TT:42:MET:HE2	66:TT:49:GLU:HA	2.01	0.41
77:II:36:VAL:HG23	77:II:40:TYR:HD2	1.84	0.41
1:5:441:G:H2'	1:5:442:G:H8	1.85	0.41
1:5:4208:U:H2'	1:5:4209:G:H8	1.85	0.41
18:P:33:ALA:HA	18:P:36:ILE:HG22	2.03	0.41
35:g:41:ALA:O	35:g:52:ARG:NH1	2.47	0.41
45:r:26:SER:OG	45:r:28:GLU:OE1	2.26	0.41
51:K:902:G:C8	51:K:902:G:H5''	2.56	0.41
51:K:1124:C:O2'	64:YY:126:MET:O	2.37	0.41
51:K:1230:C:O2'	51:K:1665:G:N1	2.47	0.41
51:K:1711:U:H2'	51:K:1712:A:C8	2.56	0.41
56:z:78:SER:OG	56:z:79:LYS:N	2.53	0.41
77:II:61:GLU:HA	77:II:64:VAL:HG22	2.03	0.41
77:II:124:ARG:HB2	77:II:131:VAL:HG23	2.03	0.41
1:5:131:C:N4	1:5:138:G:O6	2.54	0.41
1:5:425:U:H2'	1:5:426:A:H8	1.86	0.41
1:5:710:G:H2'	1:5:711:A:C8	2.55	0.41
1:5:1686:C:O2'	30:b:18:ARG:NH2	2.53	0.41
1:5:2651:C:H1'	35:g:54:ARG:HH22	1.84	0.41
1:5:2696:A:N1	39:k:24:LYS:NZ	2.63	0.41
1:5:2757:A:H2'	1:5:2758:G:C8	2.56	0.41
3:8:9:A:H2'	3:8:10:G:H8	1.86	0.41
5:B:292:LEU:HG	5:B:298:LEU:HD12	2.03	0.41
6:C:70:GLY:O	48:1:245:PHE:HE1	2.03	0.41
16:N:84:PRO:HA	16:N:87:HIS:ND1	2.36	0.41
52:q:108:PHE:HE2	52:q:122:LEU:HD21	1.86	0.41
53:u:120:MET:HG3	53:u:142:PHE:HE1	1.86	0.41
72:DD:132:LYS:HG3	72:DD:156:LEU:HB3	2.03	0.41
77:II:28:PHE:O	77:II:31:THR:OG1	2.34	0.41
84:6:9:GLY:H	84:6:309:VAL:HG22	1.85	0.41
1:5:3855:C:H2'	1:5:3856:A:H8	1.85	0.41
9:F:107:VAL:HG13	9:F:138:VAL:HG12	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:G:232:GLU:O	10:G:236:HIS:HB2	2.19	0.41
11:H:106:GLN:HG3	11:H:111:LEU:HD12	2.02	0.41
21:S:16:CYS:SG	21:S:17:LEU:N	2.94	0.41
24:V:106:VAL:HG22	24:V:112:MET:HG2	2.03	0.41
35:g:11:LEU:HD22	35:g:18:ASN:HB2	2.01	0.41
51:K:1345:G:OP1	51:K:1688:C:O2'	2.39	0.41
70:JJ:67:THR:HG21	70:JJ:72:ARG:HG3	2.03	0.41
1:5:49:U:H2'	1:5:50:C:H6	1.85	0.41
1:5:66:A:H61	1:5:282:C:HO2'	1.64	0.41
1:5:73:A:N7	14:L:103:ARG:NH1	2.69	0.41
1:5:659:G:H2'	1:5:660:A:C8	2.56	0.41
1:5:2349:A:H5''	1:5:2350:U:H5''	2.02	0.41
1:5:4569:U:OP1	1:5:4982:A:O2'	2.35	0.41
1:5:5001:U:O2'	5:B:372:SER:OG	2.30	0.41
3:8:142:U:OP1	16:N:38:ARG:NH2	2.45	0.41
8:E:278:TYR:HA	8:E:279:PRO:HD3	1.93	0.41
12:I:35:ASP:N	12:I:35:ASP:OD1	2.54	0.41
12:I:59:GLN:HG2	12:I:128:ARG:HD3	2.03	0.41
28:Z:14:LEU:HG	35:g:88:ARG:HB2	2.03	0.41
32:d:29:ILE:O	32:d:33:ILE:HB	2.20	0.41
33:e:41:ILE:O	33:e:46:ARG:NH2	2.54	0.41
51:K:466:G:H1'	56:z:59:GLN:HG2	2.03	0.41
51:K:649:U:H2'	51:K:650:A:H8	1.85	0.41
51:K:1711:U:H2'	51:K:1712:A:H8	1.85	0.41
55:x:138:HIS:CD2	55:x:148:ARG:HB3	2.56	0.41
1:5:456:C:H2'	1:5:457:G:H8	1.85	0.41
1:5:1265:G:O3'	1:5:2112:G:N2	2.54	0.41
1:5:1350:C:H2'	1:5:1351:G:H8	1.86	0.41
1:5:1382:G:H2'	1:5:1383:G:H8	1.85	0.41
1:5:1942:A:H2'	1:5:1943:A:C8	2.56	0.41
1:5:2065:G:O2'	34:f:80:ASN:OD1	2.37	0.41
1:5:2443:G:OP2	1:5:2516:G:N2	2.48	0.41
1:5:2811:G:N1	1:5:2814:C:OP2	2.38	0.41
1:5:2909:C:H2'	1:5:2910:G:C8	2.56	0.41
1:5:3932:U:H2'	1:5:3933:G:H8	1.85	0.41
1:5:4088:C:H2'	1:5:4089:G:C8	2.55	0.41
1:5:4446:U:O2'	1:5:4450:U:OP1	2.39	0.41
1:5:4579:U:H4'	5:B:117:ARG:HG3	2.02	0.41
1:5:4629:U:H2'	1:5:4630:G:H8	1.85	0.41
1:5:4967:A:H2'	1:5:4968:A:C8	2.56	0.41
2:7:52:C:O2'	2:7:54:A:N7	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:C:114:ARG:HG2	16:N:203:TYR:HB3	2.02	0.41
9:F:96:ARG:HB2	9:F:116:LEU:HB3	2.03	0.41
20:R:8:LYS:HG2	20:R:19:LYS:HB2	2.01	0.41
26:X:150:ALA:HA	26:X:153:ILE:HG12	2.03	0.41
45:r:6:GLN:HE21	45:r:44:ILE:HG23	1.86	0.41
50:3:15:G:H21	50:3:21:A:H1'	1.86	0.41
51:K:588:G:OP2	51:K:588:G:N2	2.50	0.41
51:K:1103:C:N4	51:K:1104:G:O6	2.54	0.41
53:u:119:THR:H	53:u:143:THR:HG1	1.67	0.41
56:z:121:ILE:HG13	56:z:123:GLY:H	1.86	0.41
58:CC:67:TRP:NE1	58:CC:191:GLU:OE2	2.54	0.41
73:BB:127:ARG:NE	73:BB:135:ARG:O	2.54	0.41
79:GG:69:PRO:O	82:w:40:ARG:NH2	2.54	0.41
1:5:1461:C:H2'	1:5:1462:A:H8	1.86	0.41
1:5:2397:G:O6	35:g:4:ARG:NH2	2.52	0.41
1:5:3786:U:OP1	1:5:4550:G:O2'	2.33	0.41
1:5:3893:C:H2'	1:5:3894:A:H8	1.86	0.41
1:5:4250:G:O2'	13:J:129:ASP:OD1	2.37	0.41
1:5:4370:G:H5''	43:o:64:LYS:HG3	2.03	0.41
2:7:86:G:H5'	21:S:120:ARG:HH12	1.86	0.41
11:H:128:MET:SD	11:H:157:SER:HB2	2.61	0.41
19:Q:175:GLU:HB3	19:Q:176:ARG:H	1.71	0.41
51:K:675:U:H2'	51:K:676:C:H6	1.85	0.41
51:K:1232:U:H2'	51:K:1233:G:H8	1.86	0.41
51:K:1356:G:O3'	54:v:125:LYS:NZ	2.54	0.41
56:z:61:PHE:HA	56:z:62:PRO:HD3	1.95	0.41
56:z:78:SER:H	56:z:81:HIS:HD2	1.68	0.41
56:z:181:THR:HG23	56:z:184:VAL:H	1.86	0.41
59:XX:42:GLU:OE2	59:XX:45:ARG:NH2	2.54	0.41
66:TT:90:GLN:HB2	66:TT:94:LEU:HD12	2.02	0.41
84:6:40:ILE:HB	84:6:59:LEU:HB2	2.02	0.41
1:5:175:C:H2'	1:5:176:G:H8	1.85	0.40
1:5:710:G:H21	8:E:132:HIS:HE1	1.68	0.40
1:5:1193:C:H2'	1:5:1194:G:H8	1.86	0.40
1:5:1380:G:O2'	1:5:1382:G:O6	2.30	0.40
1:5:1687:U:OP2	30:b:19:ASN:ND2	2.52	0.40
1:5:1893:C:O2'	1:5:1936:C:N3	2.46	0.40
1:5:2295:C:H2'	1:5:2296:G:H8	1.86	0.40
1:5:4238:G:H2'	1:5:4239:A:C8	2.56	0.40
1:5:4260:U:H2'	1:5:4261:C:C6	2.56	0.40
3:8:141:C:H2'	3:8:142:U:C6	2.57	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:H:176:LEU:HD11	41:m:87:GLN:HE21	1.85	0.40
46:s:61:MET:HE1	46:s:79:LEU:HB3	2.02	0.40
51:K:562:U:H2'	51:K:563:G:C8	2.56	0.40
51:K:616:A:OP1	67:VV:68:LYS:NZ	2.53	0.40
51:K:1230:C:HO2'	51:K:1665:G:H1	1.61	0.40
51:K:1566:G:O3'	51:K:1567:G:N2	2.51	0.40
57:y:163:GLN:O	57:y:167:GLU:HB2	2.21	0.40
60:EE:104:LYS:O	67:VV:11:ARG:NH2	2.54	0.40
63:UU:50:LYS:HE2	73:BB:49:LEU:HB2	2.02	0.40
65:HH:20:SER:HB3	65:HH:59:ILE:HD11	2.03	0.40
73:BB:59:LYS:HB3	73:BB:62:ARG:HB2	2.03	0.40
75:RR:54:SER:OG	75:RR:55:ASN:N	2.54	0.40
1:5:1505:C:H2'	1:5:1506:G:H8	1.86	0.40
1:5:1559:G:H2'	1:5:1560:A:H8	1.86	0.40
1:5:4302:U:O4	1:5:4308:C:N4	2.55	0.40
1:5:4704:C:H2'	1:5:4705:A:H8	1.86	0.40
3:8:37:A:OP1	36:h:86:LYS:NZ	2.54	0.40
4:A:82:ILE:HD11	4:A:99:GLY:HA3	2.03	0.40
13:J:15:LEU:HD21	13:J:134:LEU:HD13	2.03	0.40
15:M:12:VAL:HB	15:M:60:PHE:HB2	2.02	0.40
23:U:35:ASP:OD1	23:U:35:ASP:N	2.53	0.40
32:d:33:ILE:HD11	32:d:41:ARG:HB3	2.03	0.40
32:d:83:ARG:HH11	32:d:114:PHE:HE2	1.68	0.40
51:K:656:G:H1	51:K:1156:U:H3	1.69	0.40
51:K:1781:A:H2'	51:K:1782:G:C8	2.56	0.40
52:q:176:TRP:CD2	52:q:199:PRO:HB3	2.56	0.40
53:u:62:LEU:O	53:u:88:THR:OG1	2.34	0.40
57:y:51:ILE:HG21	57:y:179:LYS:HG2	2.02	0.40
59:XX:93:LYS:HB3	59:XX:96:TYR:HD2	1.87	0.40
68:NN:37:LYS:HG2	68:NN:60:PHE:HE2	1.86	0.40
75:RR:86:GLY:HA2	75:RR:89:VAL:HG12	2.03	0.40
76:9:79:HIS:HA	76:9:97:TYR:HB3	2.03	0.40
84:6:79:LEU:HA	84:6:88:ARG:O	2.21	0.40
1:5:1245:C:H2'	1:5:1246:G:H8	1.87	0.40
1:5:1532:G:N2	1:5:1637:A:OP2	2.40	0.40
1:5:1734:G:N2	1:5:1735:U:O4	2.42	0.40
1:5:1895:G:O2'	1:5:1907:A:N3	2.40	0.40
1:5:2029:A:H2'	1:5:2030:A:C8	2.56	0.40
1:5:2897:G:N3	1:5:3603:G:N2	2.70	0.40
1:5:3870:C:H2'	1:5:3871:A:C8	2.57	0.40
1:5:4601:U:O2	1:5:4610:A:N7	2.54	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:5:4769:G:OP1	17:O:176:ARG:NH1	2.54	0.40
3:8:30:U:H2'	3:8:31:G:C8	2.56	0.40
13:J:87:LEU:HB3	13:J:92:TYR:HD1	1.86	0.40
27:Y:55:VAL:HG13	27:Y:104:VAL:HG13	2.04	0.40
46:s:66:ARG:HH12	46:s:71:ASN:HB3	1.86	0.40
49:2:74:C:O2	49:2:74:C:C2'	2.70	0.40
51:K:386:C:H4'	58:CC:9:HIS:HE1	1.86	0.40
51:K:623:G:N7	67:VV:63:ASN:ND2	2.69	0.40
51:K:663:C:OP2	67:VV:2:GLY:N	2.54	0.40
51:K:1121:G:H21	53:u:206:PRO:HD3	1.86	0.40
54:v:209:VAL:HG11	54:v:233:LEU:HD11	2.04	0.40
73:BB:39:ILE:HG23	73:BB:68:ILE:HD13	2.03	0.40
74:SS:58:VAL:HG23	74:SS:71:LEU:HA	2.03	0.40
79:GG:61:LEU:HB2	79:GG:82:MET:HB3	2.03	0.40
1:5:64:A:H1'	1:5:76:A:H1'	2.03	0.40
1:5:378:A:O2'	1:5:413:G:N2	2.47	0.40
1:5:452:A:H62	8:E:218:LEU:HD21	1.86	0.40
1:5:676:C:H2'	1:5:677:G:H8	1.87	0.40
1:5:1198:G:H2'	1:5:1199:G:C8	2.57	0.40
1:5:2067:C:H5''	34:f:78:HIS:CD2	2.56	0.40
1:5:4294:C:O3'	43:o:13:LYS:NZ	2.55	0.40
5:B:52:GLY:HA2	5:B:341:LYS:HE3	2.04	0.40
30:b:36:ASP:HA	30:b:37:PRO:HD3	1.90	0.40
36:h:87:LYS:NZ	38:j:78:PHE:O	2.48	0.40
42:n:21:ARG:NH1	51:K:1174:U:OP1	2.55	0.40
49:2:9:A:H62	49:2:23:C:H41	1.68	0.40
51:K:433:A:OP1	58:CC:25:ARG:NH1	2.55	0.40
51:K:1761:U:O2	51:K:1771:G:N2	2.54	0.40
51:K:1842:C:H2'	51:K:1843:G:H8	1.86	0.40
61:QQ:136:PRO:HG2	61:QQ:139:TRP:HB2	2.03	0.40
64:YY:16:ILE:HG22	64:YY:24:LEU:HD11	2.04	0.40
74:SS:5:LYS:HE3	74:SS:9:ILE:HD11	2.04	0.40
74:SS:89:ILE:H	74:SS:89:ILE:HG13	1.66	0.40
85:4:49:A:H8	85:4:49:A:O5'	2.04	0.40
1:5:2905:C:H2'	1:5:2906:G:C8	2.56	0.40
1:5:4121:G:N2	4:A:46:LYS:O	2.55	0.40
4:A:31:ALA:HB2	4:A:123:ARG:HH11	1.87	0.40
4:A:112:ILE:HG13	44:p:79:VAL:HG22	2.03	0.40
5:B:189:THR:HG23	5:B:192:GLU:H	1.86	0.40
8:E:149:LEU:HD11	8:E:191:ILE:HG13	2.04	0.40
10:G:39:PHE:CD1	10:G:47:PRO:HD3	2.57	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:S:83:ARG:HE	22:T:156:TYR:HB2	1.87	0.40
47:t:113:ALA:HA	47:t:116:MET:HG2	2.04	0.40
51:K:39:A:H5'	59:XX:7:TRP:HE1	1.87	0.40
51:K:474:G:N2	51:K:507:G:O2'	2.38	0.40
51:K:1053:C:H2'	51:K:1054:G:H8	1.86	0.40
51:K:1332:A:O2'	72:DD:145:GLN:O	2.34	0.40
51:K:1386:A:OP2	72:DD:160:SER:OG	2.38	0.40
67:VV:90:CYS:HA	67:VV:93:PHE:HD2	1.86	0.40
78:PP:104:LEU:HD22	78:PP:121:ARG:HG3	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	A	242/244 (99%)	222 (92%)	20 (8%)	0	100	100
5	B	392/394 (100%)	370 (94%)	21 (5%)	1 (0%)	36	67
6	C	360/362 (99%)	338 (94%)	22 (6%)	0	100	100
7	D	290/292 (99%)	273 (94%)	17 (6%)	0	100	100
8	E	232/248 (94%)	195 (84%)	37 (16%)	0	100	100
9	F	223/225 (99%)	216 (97%)	7 (3%)	0	100	100
10	G	239/241 (99%)	213 (89%)	26 (11%)	0	100	100
11	H	188/190 (99%)	174 (93%)	14 (7%)	0	100	100
12	I	200/213 (94%)	192 (96%)	8 (4%)	0	100	100
13	J	167/169 (99%)	155 (93%)	12 (7%)	0	100	100
14	L	208/210 (99%)	190 (91%)	17 (8%)	1 (0%)	24	57
15	M	136/138 (99%)	128 (94%)	8 (6%)	0	100	100
16	N	201/203 (99%)	190 (94%)	11 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
17	O	197/199 (99%)	191 (97%)	6 (3%)	0	100	100
18	P	151/153 (99%)	145 (96%)	6 (4%)	0	100	100
19	Q	185/187 (99%)	176 (95%)	9 (5%)	0	100	100
20	R	178/180 (99%)	170 (96%)	8 (4%)	0	100	100
21	S	173/175 (99%)	164 (95%)	8 (5%)	1 (1%)	21	52
22	T	157/159 (99%)	147 (94%)	10 (6%)	0	100	100
23	U	97/99 (98%)	90 (93%)	7 (7%)	0	100	100
24	V	129/131 (98%)	120 (93%)	9 (7%)	0	100	100
25	W	61/63 (97%)	58 (95%)	3 (5%)	0	100	100
26	X	117/119 (98%)	113 (97%)	4 (3%)	0	100	100
27	Y	132/134 (98%)	126 (96%)	6 (4%)	0	100	100
28	Z	133/135 (98%)	122 (92%)	9 (7%)	2 (2%)	8	32
29	a	145/147 (99%)	136 (94%)	9 (6%)	0	100	100
30	b	73/75 (97%)	68 (93%)	5 (7%)	0	100	100
31	c	92/94 (98%)	89 (97%)	3 (3%)	0	100	100
32	d	105/107 (98%)	101 (96%)	4 (4%)	0	100	100
33	e	126/128 (98%)	122 (97%)	4 (3%)	0	100	100
34	f	107/109 (98%)	99 (92%)	8 (8%)	0	100	100
35	g	112/114 (98%)	110 (98%)	2 (2%)	0	100	100
36	h	120/122 (98%)	113 (94%)	7 (6%)	0	100	100
37	i	100/102 (98%)	92 (92%)	8 (8%)	0	100	100
38	j	84/86 (98%)	79 (94%)	5 (6%)	0	100	100
39	k	67/69 (97%)	59 (88%)	8 (12%)	0	100	100
40	l	48/50 (96%)	44 (92%)	4 (8%)	0	100	100
41	m	50/52 (96%)	50 (100%)	0	0	100	100
42	n	21/23 (91%)	21 (100%)	0	0	100	100
43	o	102/104 (98%)	94 (92%)	7 (7%)	1 (1%)	12	41
44	p	89/91 (98%)	84 (94%)	5 (6%)	0	100	100
45	r	123/125 (98%)	110 (89%)	11 (9%)	2 (2%)	7	30
46	s	196/198 (99%)	178 (91%)	18 (9%)	0	100	100
47	t	161/163 (99%)	124 (77%)	36 (22%)	1 (1%)	21	52

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
48	1	22/24 (92%)	21 (96%)	1 (4%)	0	100	100
52	q	215/217 (99%)	204 (95%)	11 (5%)	0	100	100
53	u	211/213 (99%)	199 (94%)	12 (6%)	0	100	100
54	v	219/221 (99%)	213 (97%)	6 (3%)	0	100	100
55	x	260/262 (99%)	247 (95%)	13 (5%)	0	100	100
56	z	235/237 (99%)	232 (99%)	3 (1%)	0	100	100
57	y	181/189 (96%)	172 (95%)	9 (5%)	0	100	100
58	CC	204/206 (99%)	189 (93%)	15 (7%)	0	100	100
59	XX	183/185 (99%)	178 (97%)	5 (3%)	0	100	100
60	EE	139/151 (92%)	131 (94%)	8 (6%)	0	100	100
61	QQ	147/149 (99%)	146 (99%)	1 (1%)	0	100	100
62	MM	134/136 (98%)	127 (95%)	7 (5%)	0	100	100
63	UU	140/142 (99%)	135 (96%)	5 (4%)	0	100	100
64	YY	130/132 (98%)	124 (95%)	6 (5%)	0	100	100
65	HH	81/83 (98%)	78 (96%)	3 (4%)	0	100	100
66	TT	127/129 (98%)	122 (96%)	5 (4%)	0	100	100
67	VV	139/141 (99%)	134 (96%)	4 (3%)	1 (1%)	18	49
68	NN	122/124 (98%)	121 (99%)	1 (1%)	0	100	100
69	ZZ	99/101 (98%)	90 (91%)	9 (9%)	0	100	100
70	JJ	81/83 (98%)	79 (98%)	2 (2%)	0	100	100
71	AA	53/55 (96%)	52 (98%)	1 (2%)	0	100	100
72	DD	226/228 (99%)	221 (98%)	5 (2%)	0	100	100
73	BB	181/191 (95%)	170 (94%)	11 (6%)	0	100	100
74	SS	94/96 (98%)	88 (94%)	6 (6%)	0	100	100
75	RR	115/117 (98%)	106 (92%)	9 (8%)	0	100	100
76	9	118/120 (98%)	110 (93%)	8 (7%)	0	100	100
77	II	142/144 (99%)	129 (91%)	13 (9%)	0	100	100
78	PP	139/141 (99%)	133 (96%)	6 (4%)	0	100	100
79	GG	98/100 (98%)	96 (98%)	2 (2%)	0	100	100
80	OO	73/75 (97%)	70 (96%)	3 (4%)	0	100	100
81	FF	60/62 (97%)	60 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
82	w	53/55 (96%)	53 (100%)	0	0	100	100
83	0	66/68 (97%)	61 (92%)	5 (8%)	0	100	100
84	6	311/313 (99%)	289 (93%)	22 (7%)	0	100	100
All	All	11507/11712 (98%)	10831 (94%)	666 (6%)	10 (0%)	49	78

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
14	L	64	VAL
67	VV	62	PRO
43	o	97	LYS
45	r	19	LYS
45	r	21	ASN
28	Z	30	ASP
47	t	3	PRO
21	S	165	PRO
28	Z	90	PRO
5	B	259	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	
4	A	187/187 (100%)	185 (99%)	2 (1%)	65	78
5	B	336/342 (98%)	336 (100%)	0	100	100
6	C	302/302 (100%)	299 (99%)	3 (1%)	68	79
7	D	247/247 (100%)	247 (100%)	0	100	100
8	E	208/221 (94%)	208 (100%)	0	100	100
9	F	194/195 (100%)	194 (100%)	0	100	100
10	G	206/206 (100%)	206 (100%)	0	100	100
11	H	169/169 (100%)	169 (100%)	0	100	100
12	I	174/180 (97%)	172 (99%)	2 (1%)	65	78

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
13	J	142/142 (100%)	141 (99%)	1 (1%)	76	82
14	L	176/176 (100%)	176 (100%)	0	100	100
15	M	117/117 (100%)	117 (100%)	0	100	100
16	N	171/171 (100%)	171 (100%)	0	100	100
17	O	171/171 (100%)	171 (100%)	0	100	100
18	P	134/134 (100%)	132 (98%)	2 (2%)	57	75
19	Q	163/163 (100%)	162 (99%)	1 (1%)	78	83
20	R	159/159 (100%)	159 (100%)	0	100	100
21	S	156/156 (100%)	156 (100%)	0	100	100
22	T	139/139 (100%)	139 (100%)	0	100	100
23	U	89/89 (100%)	89 (100%)	0	100	100
24	V	101/101 (100%)	101 (100%)	0	100	100
25	W	55/55 (100%)	55 (100%)	0	100	100
26	X	107/107 (100%)	107 (100%)	0	100	100
27	Y	124/124 (100%)	124 (100%)	0	100	100
28	Z	117/117 (100%)	117 (100%)	0	100	100
29	a	119/119 (100%)	119 (100%)	0	100	100
30	b	62/62 (100%)	62 (100%)	0	100	100
31	c	79/79 (100%)	79 (100%)	0	100	100
32	d	98/98 (100%)	98 (100%)	0	100	100
33	e	114/114 (100%)	114 (100%)	0	100	100
34	f	88/88 (100%)	88 (100%)	0	100	100
35	g	98/98 (100%)	98 (100%)	0	100	100
36	h	109/109 (100%)	109 (100%)	0	100	100
37	i	86/86 (100%)	86 (100%)	0	100	100
38	j	73/73 (100%)	73 (100%)	0	100	100
39	k	64/64 (100%)	64 (100%)	0	100	100
40	l	47/47 (100%)	47 (100%)	0	100	100
41	m	48/48 (100%)	48 (100%)	0	100	100
42	n	22/22 (100%)	22 (100%)	0	100	100
43	o	92/92 (100%)	92 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
44	p	74/74 (100%)	74 (100%)	0	100	100
45	r	109/109 (100%)	109 (100%)	0	100	100
46	s	166/166 (100%)	166 (100%)	0	100	100
47	t	136/136 (100%)	136 (100%)	0	100	100
48	l	22/22 (100%)	21 (96%)	1 (4%)	24	56
52	q	180/181 (99%)	180 (100%)	0	100	100
53	u	194/194 (100%)	194 (100%)	0	100	100
54	v	187/187 (100%)	187 (100%)	0	100	100
55	x	224/224 (100%)	224 (100%)	0	100	100
56	z	207/207 (100%)	206 (100%)	1 (0%)	81	85
57	y	165/169 (98%)	165 (100%)	0	100	100
58	CC	178/178 (100%)	178 (100%)	0	100	100
59	XX	161/161 (100%)	160 (99%)	1 (1%)	78	83
60	EE	130/136 (96%)	130 (100%)	0	100	100
61	QQ	130/130 (100%)	130 (100%)	0	100	100
62	MM	106/106 (100%)	106 (100%)	0	100	100
63	UU	117/117 (100%)	117 (100%)	0	100	100
64	YY	119/119 (100%)	119 (100%)	0	100	100
65	HH	67/67 (100%)	67 (100%)	0	100	100
66	TT	112/112 (100%)	112 (100%)	0	100	100
67	VV	113/113 (100%)	112 (99%)	1 (1%)	70	80
68	NN	107/107 (100%)	107 (100%)	0	100	100
69	ZZ	88/88 (100%)	88 (100%)	0	100	100
70	JJ	75/75 (100%)	75 (100%)	0	100	100
71	AA	46/46 (100%)	46 (100%)	0	100	100
72	DD	190/190 (100%)	190 (100%)	0	100	100
73	BB	158/161 (98%)	158 (100%)	0	100	100
74	SS	87/87 (100%)	86 (99%)	1 (1%)	65	78
75	RR	99/99 (100%)	99 (100%)	0	100	100
76	9	109/109 (100%)	109 (100%)	0	100	100
77	II	125/125 (100%)	124 (99%)	1 (1%)	73	81

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
78	PP	111/111 (100%)	111 (100%)	0	100	100
79	GG	92/92 (100%)	92 (100%)	0	100	100
80	OO	66/66 (100%)	66 (100%)	0	100	100
81	FF	55/55 (100%)	55 (100%)	0	100	100
82	w	48/48 (100%)	48 (100%)	0	100	100
83	0	61/61 (100%)	61 (100%)	0	100	100
84	6	272/272 (100%)	272 (100%)	0	100	100
All	All	10029/10069 (100%)	10012 (100%)	17 (0%)	85	89

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	A	163	ARG
4	A	207	VAL
6	C	114	ARG
6	C	150	LEU
6	C	154	VAL
12	I	48	LEU
12	I	144	ASN
13	J	151	ILE
18	P	24	VAL
18	P	128	ARG
19	Q	83	VAL
48	1	260	MET
56	z	191	ARG
59	XX	29	LEU
67	VV	61	GLN
74	SS	89	ILE
77	II	8	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (180) such sidechains are listed below:

Mol	Chain	Res	Type
4	A	50	HIS
4	A	216	HIS
5	B	25	HIS
5	B	167	GLN
5	B	184	GLN

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Mol	Chain	Res	Type
5	B	186	ASN
5	B	203	GLN
5	B	204	GLN
5	B	302	ASN
5	B	354	GLN
6	C	50	GLN
6	C	61	GLN
6	C	85	HIS
6	C	321	ASN
6	C	329	ASN
7	D	9	ASN
7	D	191	ASN
7	D	225	GLN
8	E	178	ASN
8	E	187	GLN
8	E	246	GLN
8	E	275	ASN
8	E	280	HIS
9	F	41	GLN
9	F	112	GLN
9	F	133	ASN
10	G	38	ASN
10	G	46	GLN
10	G	81	ASN
10	G	90	GLN
10	G	112	GLN
10	G	153	GLN
10	G	206	GLN
10	G	240	ASN
11	H	8	GLN
11	H	39	ASN
12	I	95	HIS
12	I	144	ASN
12	I	163	GLN
13	J	71	HIS
13	J	168	GLN
14	L	19	GLN
14	L	27	ASN
14	L	104	ASN
14	L	205	GLN
15	M	66	HIS
15	M	70	GLN

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Mol	Chain	Res	Type
16	N	196	ASN
16	N	199	GLN
16	N	201	HIS
17	O	50	ASN
17	O	65	ASN
18	P	75	GLN
18	P	137	ASN
19	Q	8	ASN
19	Q	125	GLN
20	R	40	GLN
20	R	58	HIS
20	R	130	ASN
20	R	141	HIS
21	S	50	GLN
21	S	77	ASN
21	S	163	HIS
22	T	3	ASN
22	T	22	HIS
22	T	95	HIS
22	T	127	GLN
22	T	131	GLN
23	U	17	GLN
24	V	77	HIS
25	W	17	HIS
25	W	45	ASN
25	W	48	GLN
25	W	59	HIS
26	X	57	GLN
26	X	93	ASN
26	X	94	ASN
26	X	105	ASN
26	X	107	HIS
26	X	108	GLN
26	X	111	GLN
26	X	125	ASN
28	Z	97	ASN
29	a	14	HIS
29	a	120	GLN
30	b	12	GLN
31	c	51	ASN
32	d	18	ASN
32	d	30	HIS

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Mol	Chain	Res	Type
33	e	43	ASN
33	e	52	GLN
33	e	124	ASN
34	f	65	ASN
34	f	99	HIS
35	g	112	GLN
36	h	63	GLN
36	h	96	ASN
38	j	76	HIS
40	l	33	ASN
41	m	84	GLN
41	m	104	HIS
43	o	21	HIS
44	p	92	GLN
45	r	12	ASN
45	r	31	ASN
45	r	83	ASN
46	s	190	GLN
46	s	191	GLN
48	l	253	GLN
52	q	50	ASN
52	q	111	GLN
52	q	113	GLN
52	q	131	HIS
53	u	75	GLN
53	u	118	GLN
53	u	124	HIS
53	u	147	ASN
53	u	202	GLN
54	v	136	HIS
55	x	36	HIS
55	x	67	GLN
55	x	112	HIS
55	x	142	HIS
55	x	224	ASN
55	x	232	ASN
56	z	81	HIS
56	z	202	ASN
57	y	97	GLN
57	y	157	HIS
57	y	193	GLN
58	CC	7	ASN

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Mol	Chain	Res	Type
58	CC	84	ASN
58	CC	87	ASN
58	CC	88	ASN
58	CC	99	ASN
58	CC	138	ASN
58	CC	146	GLN
58	CC	165	GLN
59	XX	111	GLN
59	XX	143	ASN
59	XX	156	HIS
60	EE	11	GLN
60	EE	19	ASN
60	EE	83	GLN
60	EE	121	GLN
62	MM	94	HIS
63	UU	11	GLN
63	UU	35	ASN
63	UU	48	GLN
63	UU	77	HIS
63	UU	80	GLN
63	UU	97	GLN
65	HH	2	GLN
65	HH	29	HIS
65	HH	47	ASN
66	TT	113	HIS
68	NN	15	ASN
68	NN	63	HIS
68	NN	112	ASN
70	JJ	65	GLN
70	JJ	84	HIS
72	DD	22	ASN
73	BB	65	GLN
73	BB	79	HIS
73	BB	114	ASN
74	SS	44	HIS
74	SS	61	GLN
74	SS	84	HIS
75	RR	48	HIS
75	RR	72	HIS
75	RR	73	GLN
75	RR	82	ASN
76	9	128	HIS

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Mol	Chain	Res	Type
77	II	72	GLN
78	PP	85	ASN
79	GG	47	ASN
81	FF	29	GLN
84	6	159	ASN
84	6	178	ASN
84	6	305	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	5	3649/3662 (99%)	842 (23%)	72 (1%)
2	7	119/120 (99%)	16 (13%)	0
3	8	155/156 (99%)	40 (25%)	1 (0%)
49	2	74/76 (97%)	23 (31%)	1 (1%)
50	3	72/75 (96%)	13 (18%)	1 (1%)
51	K	1686/1698 (99%)	353 (20%)	22 (1%)
85	4	9/10 (90%)	4 (44%)	0
All	All	5764/5797 (99%)	1291 (22%)	97 (1%)

All (1291) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	5	2	G
1	5	8	U
1	5	11	G
1	5	12	A
1	5	13	U
1	5	25	A
1	5	35	U
1	5	39	A
1	5	42	A
1	5	43	U
1	5	47	A
1	5	48	G
1	5	49	U
1	5	56	A
1	5	58	G
1	5	59	A
1	5	64	A
1	5	65	A

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Mol	Chain	Res	Type
1	5	73	A
1	5	76	A
1	5	84	A
1	5	91	G
1	5	104	G
1	5	108	A
1	5	109	G
1	5	110	C
1	5	112	C
1	5	116	G
1	5	119	G
1	5	126	C
1	5	134	G
1	5	135	G
1	5	136	C
1	5	143	C
1	5	144	G
1	5	159	C
1	5	166	C
1	5	167	C
1	5	171	U
1	5	172	C
1	5	173	C
1	5	182	G
1	5	183	C
1	5	184	U
1	5	185	C
1	5	186	G
1	5	187	U
1	5	188	G
1	5	189	G
1	5	200	U
1	5	201	C
1	5	210	C
1	5	216	C
1	5	217	C
1	5	218	A
1	5	219	G
1	5	220	C
1	5	224	U
1	5	225	G
1	5	226	G

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Mol	Chain	Res	Type
1	5	233	U
1	5	234	G
1	5	246	G
1	5	262	G
1	5	265	C
1	5	266	C
1	5	267	G
1	5	276	C
1	5	277	G
1	5	278	G
1	5	280	G
1	5	297	U
1	5	301	G
1	5	306	A
1	5	309	C
1	5	315	G
1	5	316	U
1	5	334	A
1	5	340	C
1	5	345	C
1	5	350	C
1	5	363	A
1	5	383	A
1	5	387	G
1	5	399	G
1	5	407	A
1	5	409	G
1	5	410	A
1	5	412	G
1	5	413	G
1	5	440	U
1	5	450	G
1	5	451	C
1	5	452	A
1	5	453	G
1	5	454	U
1	5	455	C
1	5	465	G
1	5	467	U
1	5	468	U
1	5	470	A
1	5	480	C

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Mol	Chain	Res	Type
1	5	485	C
1	5	486	C
1	5	487	G
1	5	499	G
1	5	500	G
1	5	501	C
1	5	503	C
1	5	504	G
1	5	506	C
1	5	513	U
1	5	514	U
1	5	515	C
1	5	519	C
1	5	647	G
1	5	649	A
1	5	654	C
1	5	663	G
1	5	664	G
1	5	666	G
1	5	667	A
1	5	683	C
1	5	684	G
1	5	685	C
1	5	686	A
1	5	690	C
1	5	694	C
1	5	695	G
1	5	696	C
1	5	697	G
1	5	702	U
1	5	703	G
1	5	704	C
1	5	707	C
1	5	716	C
1	5	718	C
1	5	728	U
1	5	729	G
1	5	730	G
1	5	732	A
1	5	737	C
1	5	746	A
1	5	747	A

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Mol	Chain	Res	Type
1	5	748	G
1	5	749	G
1	5	914	U
1	5	917	A
1	5	918	G
1	5	920	C
1	5	926	G
1	5	927	G
1	5	930	G
1	5	931	C
1	5	932	A
1	5	933	G
1	5	934	C
1	5	936	C
1	5	937	U
1	5	938	C
1	5	939	G
1	5	942	G
1	5	944	A
1	5	945	U
1	5	946	C
1	5	957	G
1	5	958	G
1	5	960	A
1	5	961	G
1	5	962	C
1	5	963	G
1	5	964	A
1	5	965	G
1	5	966	A
1	5	967	C
1	5	968	C
1	5	969	C
1	5	970	G
1	5	971	U
1	5	973	G
1	5	976	G
1	5	978	G
1	5	982	U
1	5	989	U
1	5	990	C
1	5	991	C

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Mol	Chain	Res	Type
1	5	1068	G
1	5	1070	G
1	5	1072	C
1	5	1078	A
1	5	1083	U
1	5	1177	U
1	5	1178	G
1	5	1183	C
1	5	1187	G
1	5	1188	C
1	5	1209	U
1	5	1210	C
1	5	1211	G
1	5	1212	G
1	5	1215	C
1	5	1219	G
1	5	1221	G
1	5	1233	G
1	5	1237	C
1	5	1238	A
1	5	1239	C
1	5	1242	G
1	5	1243	C
1	5	1244	G
1	5	1255	A
1	5	1267	C
1	5	1268	G
1	5	1269	G
1	5	1270	A
1	5	1272	C
1	5	1273	G
1	5	1274	A
1	5	1279	A
1	5	1280	C
1	5	1281	G
1	5	1282	G
1	5	1285	U
1	5	1286	C
1	5	1288	G
1	5	1290	G
1	5	1293	G
1	5	1297	U

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Mol	Chain	Res	Type
1	5	1301	C
1	5	1319	U
1	5	1326	A
1	5	1330	A
1	5	1344	C
1	5	1354	A
1	5	1358	G
1	5	1367	C
1	5	1368	A
1	5	1370	G
1	5	1371	A
1	5	1372	A
1	5	1377	G
1	5	1378	C
1	5	1379	C
1	5	1387	A
1	5	1394	G
1	5	1397	A
1	5	1399	G
1	5	1408	G
1	5	1410	U
1	5	1411	C
1	5	1419	G
1	5	1420	A
1	5	1421	G
1	5	1429	C
1	5	1437	C
1	5	1439	C
1	5	1440	U
1	5	1441	C
1	5	1445	U
1	5	1446	C
1	5	1448	G
1	5	1451	G
1	5	1456	C
1	5	1457	G
1	5	1458	C
1	5	1465	G
1	5	1475	G
1	5	1482	G
1	5	1483	C
1	5	1497	A

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Mol	Chain	Res	Type
1	5	1498	G
1	5	1501	C
1	5	1502	G
1	5	1514	U
1	5	1516	G
1	5	1518	A
1	5	1523	A
1	5	1525	A
1	5	1534	A
1	5	1535	C
1	5	1547	A
1	5	1563	A
1	5	1564	A
1	5	1566	C
1	5	1574	G
1	5	1578	U
1	5	1591	U
1	5	1596	U
1	5	1597	G
1	5	1602	U
1	5	1607	C
1	5	1612	G
1	5	1613	A
1	5	1624	G
1	5	1625	G
1	5	1631	A
1	5	1633	G
1	5	1634	A
1	5	1638	A
1	5	1640	C
1	5	1641	G
1	5	1649	U
1	5	1650	A
1	5	1654	G
1	5	1660	U
1	5	1661	C
1	5	1676	C
1	5	1677	U
1	5	1680	G
1	5	1694	C
1	5	1698	C
1	5	1719	A

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Mol	Chain	Res	Type
1	5	1720	C
1	5	1721	G
1	5	1724	G
1	5	1731	C
1	5	1741	G
1	5	1742	A
1	5	1754	U
1	5	1755	C
1	5	1756	U
1	5	1757	U
1	5	1759	G
1	5	1760	G
1	5	1761	G
1	5	1764	G
1	5	1765	A
1	5	1768	C
1	5	1769	G
1	5	1772	C
1	5	1775	A
1	5	1776	A
1	5	1777	C
1	5	1780	A
1	5	1781	U
1	5	1787	A
1	5	1799	G
1	5	1803	G
1	5	1804	A
1	5	1805	A
1	5	1812	C
1	5	1815	G
1	5	1819	G
1	5	1820	C
1	5	1821	G
1	5	1822	U
1	5	1828	C
1	5	1833	G
1	5	1834	U
1	5	1835	G
1	5	1836	G
1	5	1840	G
1	5	1848	C
1	5	1855	G

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Mol	Chain	Res	Type
1	5	1869	G
1	5	1882	U
1	5	1888	A
1	5	1889	U
1	5	1890	G
1	5	1897	A
1	5	1906	U
1	5	1910	G
1	5	1916	G
1	5	1918	U
1	5	1920	C
1	5	1921	C
1	5	1922	G
1	5	1925	G
1	5	1928	C
1	5	1930	U
1	5	1931	C
1	5	1932	A
1	5	1957	U
1	5	1958	A
1	5	1959	U
1	5	1960	A
1	5	1961	G
1	5	1962	A
1	5	1964	A
1	5	1966	C
1	5	1967	A
1	5	1968	G
1	5	1969	G
1	5	1970	A
1	5	1971	C
1	5	1975	G
1	5	1976	G
1	5	1978	C
1	5	1980	U
1	5	1981	G
1	5	1985	G
1	5	1987	C
1	5	1988	G
1	5	1991	A
1	5	1993	C
1	5	1997	U

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Mol	Chain	Res	Type
1	5	2001	G
1	5	2002	A
1	5	2003	G
1	5	2007	G
1	5	2010	A
1	5	2011	C
1	5	2016	C
1	5	2017	A
1	5	2018	C
1	5	2026	A
1	5	2044	U
1	5	2047	A
1	5	2048	U
1	5	2052	G
1	5	2055	G
1	5	2056	G
1	5	2069	A
1	5	2084	C
1	5	2085	G
1	5	2089	G
1	5	2090	U
1	5	2092	G
1	5	2093	A
1	5	2094	G
1	5	2095	A
1	5	2097	U
1	5	2101	C
1	5	2105	A
1	5	2107	C
1	5	2108	G
1	5	2109	G
1	5	2110	C
1	5	2111	G
1	5	2112	G
1	5	2113	G
1	5	2114	G
1	5	2116	C
1	5	2117	G
1	5	2119	C
1	5	2120	G
1	5	2122	G
1	5	2123	C

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Mol	Chain	Res	Type
1	5	2124	G
1	5	2126	G
1	5	2127	C
1	5	2247	C
1	5	2248	C
1	5	2250	C
1	5	2251	G
1	5	2252	G
1	5	2253	A
1	5	2254	G
1	5	2257	C
1	5	2258	C
1	5	2259	G
1	5	2260	C
1	5	2261	G
1	5	2263	A
1	5	2264	C
1	5	2265	G
1	5	2266	C
1	5	2267	U
1	5	2268	A
1	5	2279	A
1	5	2289	C
1	5	2300	A
1	5	2301	G
1	5	2306	G
1	5	2313	A
1	5	2314	G
1	5	2316	G
1	5	2322	G
1	5	2331	G
1	5	2333	G
1	5	2348	G
1	5	2350	U
1	5	2351	C
1	5	2360	A
1	5	2395	A
1	5	2396	A
1	5	2410	C
1	5	2417	A
1	5	2422	C
1	5	2425	U

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Mol	Chain	Res	Type
1	5	2433	G
1	5	2438	A
1	5	2440	U
1	5	2441	C
1	5	2450	G
1	5	2471	G
1	5	2488	C
1	5	2489	C
1	5	2490	U
1	5	2491	C
1	5	2503	G
1	5	2504	C
1	5	2505	C
1	5	2506	G
1	5	2513	A
1	5	2514	G
1	5	2517	A
1	5	2529	A
1	5	2530	U
1	5	2537	A
1	5	2544	G
1	5	2546	G
1	5	2547	G
1	5	2549	G
1	5	2553	A
1	5	2554	U
1	5	2571	C
1	5	2572	C
1	5	2575	U
1	5	2581	A
1	5	2583	C
1	5	2587	A
1	5	2589	C
1	5	2618	G
1	5	2638	G
1	5	2661	U
1	5	2662	G
1	5	2669	C
1	5	2670	C
1	5	2681	G
1	5	2686	G
1	5	2687	U

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Mol	Chain	Res	Type
1	5	2694	G
1	5	2695	A
1	5	2696	A
1	5	2710	C
1	5	2711	G
1	5	2712	G
1	5	2714	G
1	5	2721	G
1	5	2725	A
1	5	2726	G
1	5	2740	U
1	5	2752	G
1	5	2754	G
1	5	2761	U
1	5	2762	G
1	5	2763	U
1	5	2767	U
1	5	2768	C
1	5	2769	U
1	5	2770	C
1	5	2787	A
1	5	2788	U
1	5	2790	U
1	5	2794	C
1	5	2798	A
1	5	2806	A
1	5	2814	C
1	5	2826	U
1	5	2827	G
1	5	2828	U
1	5	2833	A
1	5	2842	G
1	5	2849	A
1	5	2855	G
1	5	2857	A
1	5	2867	C
1	5	2897	G
1	5	2898	G
1	5	2904	U
1	5	2905	C
1	5	3593	C
1	5	3595	U

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Mol	Chain	Res	Type
1	5	3596	A
1	5	3597	G
1	5	3602	C
1	5	3605	C
1	5	3616	U
1	5	3617	G
1	5	3625	G
1	5	3626	G
1	5	3630	A
1	5	3635	A
1	5	3636	C
1	5	3648	A
1	5	3662	A
1	5	3670	C
1	5	3673	C
1	5	3692	A
1	5	3705	G
1	5	3710	G
1	5	3711	A
1	5	3729	U
1	5	3748	A
1	5	3760	A
1	5	3761	C
1	5	3772	U
1	5	3774	A
1	5	3777	G
1	5	3778	U
1	5	3784	A
1	5	3786	U
1	5	3799	A
1	5	3802	U
1	5	3810	C
1	5	3811	G
1	5	3812	C
1	5	3814	U
1	5	3817	A
1	5	3819	G
1	5	3840	U
1	5	3843	C
1	5	3860	A
1	5	3870	C
1	5	3876	A

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Mol	Chain	Res	Type
1	5	3877	A
1	5	3878	C
1	5	3879	G
1	5	3889	G
1	5	3892	U
1	5	3897	G
1	5	3898	G
1	5	3901	A
1	5	3905	A
1	5	3906	A
1	5	3907	G
1	5	3908	A
1	5	3915	U
1	5	3926	C
1	5	3938	G
1	5	3939	G
1	5	3943	A
1	5	4069	U
1	5	4070	U
1	5	4076	G
1	5	4084	G
1	5	4085	A
1	5	4086	G
1	5	4088	C
1	5	4090	G
1	5	4094	G
1	5	4097	G
1	5	4099	G
1	5	4104	G
1	5	4107	G
1	5	4114	C
1	5	4115	G
1	5	4116	C
1	5	4117	U
1	5	4119	C
1	5	4120	U
1	5	4121	G
1	5	4125	C
1	5	4127	A
1	5	4128	A
1	5	4143	G
1	5	4144	C

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Mol	Chain	Res	Type
1	5	4145	C
1	5	4151	G
1	5	4158	C
1	5	4162	C
1	5	4164	C
1	5	4166	G
1	5	4170	A
1	5	4171	C
1	5	4173	G
1	5	4183	G
1	5	4184	G
1	5	4191	G
1	5	4203	A
1	5	4212	A
1	5	4225	G
1	5	4228	G
1	5	4229	U
1	5	4233	A
1	5	4234	A
1	5	4243	C
1	5	4249	G
1	5	4251	A
1	5	4254	G
1	5	4255	A
1	5	4265	U
1	5	4268	A
1	5	4271	A
1	5	4273	A
1	5	4280	A
1	5	4282	A
1	5	4290	U
1	5	4291	G
1	5	4292	A
1	5	4297	G
1	5	4304	A
1	5	4305	G
1	5	4306	U
1	5	4313	A
1	5	4314	C
1	5	4317	A
1	5	4318	C
1	5	4319	C

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Mol	Chain	Res	Type
1	5	4323	A
1	5	4326	G
1	5	4329	G
1	5	4330	G
1	5	4332	C
1	5	4339	A
1	5	4349	C
1	5	4350	C
1	5	4354	U
1	5	4355	G
1	5	4376	A
1	5	4377	G
1	5	4378	A
1	5	4379	A
1	5	4387	C
1	5	4393	G
1	5	4394	A
1	5	4405	G
1	5	4419	U
1	5	4421	C
1	5	4422	A
1	5	4426	C
1	5	4436	U
1	5	4437	U
1	5	4440	G
1	5	4444	C
1	5	4448	G
1	5	4449	A
1	5	4464	A
1	5	4471	U
1	5	4475	G
1	5	4476	C
1	5	4482	U
1	5	4500	U
1	5	4510	A
1	5	4512	U
1	5	4513	A
1	5	4518	A
1	5	4519	C
1	5	4524	G
1	5	4528	G
1	5	4529	G

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Mol	Chain	Res	Type
1	5	4531	U
1	5	4548	A
1	5	4549	G
1	5	4557	U
1	5	4560	C
1	5	4567	G
1	5	4570	G
1	5	4573	G
1	5	4575	G
1	5	4581	G
1	5	4590	A
1	5	4599	A
1	5	4617	G
1	5	4636	U
1	5	4637	G
1	5	4639	G
1	5	4642	U
1	5	4652	G
1	5	4656	A
1	5	4657	U
1	5	4661	G
1	5	4667	C
1	5	4670	C
1	5	4672	A
1	5	4677	U
1	5	4682	U
1	5	4687	A
1	5	4693	C
1	5	4694	G
1	5	4695	C
1	5	4697	U
1	5	4700	A
1	5	4709	U
1	5	4719	G
1	5	4720	C
1	5	4730	C
1	5	4731	G
1	5	4732	G
1	5	4738	C
1	5	4741	C
1	5	4744	A
1	5	4745	G

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Mol	Chain	Res	Type
1	5	4746	C
1	5	4750	G
1	5	4753	U
1	5	4756	C
1	5	4758	U
1	5	4763	U
1	5	4764	A
1	5	4770	U
1	5	4771	C
1	5	4868	G
1	5	4869	U
1	5	4871	C
1	5	4873	G
1	5	4876	U
1	5	4878	C
1	5	4883	C
1	5	4884	G
1	5	4886	C
1	5	4889	G
1	5	4890	G
1	5	4895	C
1	5	4896	G
1	5	4901	G
1	5	4902	C
1	5	4903	G
1	5	4910	G
1	5	4911	A
1	5	4912	G
1	5	4913	G
1	5	4914	C
1	5	4927	G
1	5	4930	C
1	5	4931	G
1	5	4933	C
1	5	4936	G
1	5	4937	C
1	5	4941	G
1	5	4944	C
1	5	4945	G
1	5	4949	G
1	5	4951	G
1	5	4959	U

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Mol	Chain	Res	Type
1	5	4964	C
1	5	4965	U
1	5	4966	A
1	5	4975	G
1	5	4976	U
1	5	4985	U
1	5	4988	U
1	5	4989	U
1	5	4990	C
1	5	4991	U
1	5	4999	G
1	5	5006	U
1	5	5013	C
1	5	5017	G
1	5	5023	C
1	5	5027	C
1	5	5028	G
1	5	5041	G
1	5	5047	C
1	5	5050	C
1	5	5052	C
1	5	5053	U
1	5	5054	C
1	5	5056	A
1	5	5060	A
1	5	5061	A
2	7	7	G
2	7	13	A
2	7	22	A
2	7	25	G
2	7	40	U
2	7	53	U
2	7	54	A
2	7	63	C
2	7	64	G
2	7	97	G
2	7	98	G
2	7	100	A
2	7	102	U
2	7	110	G
2	7	111	C
2	7	120	U

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Mol	Chain	Res	Type
3	8	2	G
3	8	34	U
3	8	35	C
3	8	37	A
3	8	39	G
3	8	49	G
3	8	51	U
3	8	59	A
3	8	60	G
3	8	61	A
3	8	62	A
3	8	63	U
3	8	75	G
3	8	80	A
3	8	81	C
3	8	82	A
3	8	83	C
3	8	84	A
3	8	85	U
3	8	86	U
3	8	87	G
3	8	90	C
3	8	94	G
3	8	99	U
3	8	103	A
3	8	105	C
3	8	107	C
3	8	109	C
3	8	110	U
3	8	111	U
3	8	114	G
3	8	123	U
3	8	124	U
3	8	125	C
3	8	126	C
3	8	127	U
3	8	128	C
3	8	147	G
3	8	150	C
3	8	153	C
49	2	4	U
49	2	8	U

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Mol	Chain	Res	Type
49	2	9	A
49	2	13	C
49	2	19	G
49	2	20	C
49	2	21	A
49	2	34	C
49	2	35	A
49	2	39	U
49	2	40	C
49	2	41	U
49	2	44	A
49	2	45	G
49	2	46	G
49	2	47	U
49	2	48	C
49	2	58	A
49	2	59	A
49	2	72	C
49	2	73	A
49	2	74	C
49	2	76	A
50	3	9	A
50	3	13	C
50	3	16	C
50	3	21	A
50	3	37	A
50	3	47	U
50	3	48	C
50	3	49	C
50	3	61	C
50	3	63	C
50	3	69	G
50	3	75	C
50	3	76	A
51	K	2	A
51	K	3	C
51	K	4	C
51	K	20	G
51	K	25	A
51	K	26	U
51	K	33	G
51	K	41	G

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Mol	Chain	Res	Type
51	K	42	A
51	K	44	U
51	K	45	A
51	K	46	A
51	K	56	G
51	K	65	C
51	K	67	C
51	K	68	A
51	K	70	G
51	K	71	G
51	K	73	C
51	K	74	G
51	K	77	A
51	K	79	A
51	K	103	A
51	K	111	A
51	K	113	G
51	K	115	U
51	K	124	U
51	K	126	G
51	K	128	U
51	K	129	C
51	K	130	G
51	K	141	A
51	K	142	C
51	K	143	U
51	K	147	A
51	K	155	G
51	K	158	A
51	K	162	C
51	K	171	A
51	K	180	G
51	K	182	C
51	K	183	G
51	K	184	G
51	K	187	G
51	K	188	C
51	K	189	U
51	K	191	A
51	K	192	C
51	K	215	G
51	K	289	G

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Mol	Chain	Res	Type
51	K	294	U
51	K	304	C
51	K	305	U
51	K	306	C
51	K	307	G
51	K	308	G
51	K	309	G
51	K	310	C
51	K	312	G
51	K	314	U
51	K	317	C
51	K	318	A
51	K	319	C
51	K	322	C
51	K	323	C
51	K	332	G
51	K	335	G
51	K	340	C
51	K	347	G
51	K	350	C
51	K	351	G
51	K	360	A
51	K	362	C
51	K	364	A
51	K	368	U
51	K	369	C
51	K	370	G
51	K	381	C
51	K	385	G
51	K	386	C
51	K	398	A
51	K	400	C
51	K	408	A
51	K	409	C
51	K	417	C
51	K	418	A
51	K	421	G
51	K	426	A
51	K	435	A
51	K	438	G
51	K	448	A
51	K	450	C

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Mol	Chain	Res	Type
51	K	455	A
51	K	464	A
51	K	465	A
51	K	466	G
51	K	471	G
51	K	472	C
51	K	473	A
51	K	474	G
51	K	476	A
51	K	482	G
51	K	487	U
51	K	492	C
51	K	525	A
51	K	530	U
51	K	532	C
51	K	533	A
51	K	547	G
51	K	548	C
51	K	549	C
51	K	550	C
51	K	551	U
51	K	554	A
51	K	555	A
51	K	556	U
51	K	559	G
51	K	560	A
51	K	564	A
51	K	568	C
51	K	576	A
51	K	583	A
51	K	588	G
51	K	590	A
51	K	591	U
51	K	606	G
51	K	608	C
51	K	614	C
51	K	615	C
51	K	617	G
51	K	621	C
51	K	624	C
51	K	626	A
51	K	628	A

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Mol	Chain	Res	Type
51	K	643	A
51	K	644	G
51	K	660	C
51	K	662	G
51	K	663	C
51	K	664	A
51	K	668	A
51	K	669	A
51	K	671	A
51	K	672	A
51	K	673	G
51	K	683	G
51	K	688	U
51	K	689	U
51	K	752	G
51	K	753	C
51	K	754	G
51	K	798	G
51	K	799	U
51	K	810	A
51	K	811	A
51	K	821	G
51	K	822	U
51	K	830	A
51	K	834	C
51	K	844	U
51	K	845	G
51	K	847	A
51	K	870	A
51	K	871	U
51	K	872	A
51	K	873	G
51	K	875	A
51	K	878	G
51	K	887	U
51	K	890	U
51	K	892	U
51	K	901	G
51	K	903	A
51	K	904	A
51	K	909	G
51	K	913	A

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Mol	Chain	Res	Type
51	K	914	U
51	K	917	U
51	K	920	A
51	K	933	G
51	K	934	G
51	K	970	G
51	K	971	G
51	K	978	G
51	K	990	A
51	K	992	A
51	K	999	G
51	K	1017	U
51	K	1023	A
51	K	1041	G
51	K	1045	U
51	K	1060	A
51	K	1061	U
51	K	1062	A
51	K	1078	C
51	K	1083	A
51	K	1085	C
51	K	1086	G
51	K	1089	G
51	K	1097	G
51	K	1100	A
51	K	1113	A
51	K	1115	U
51	K	1116	C
51	K	1117	C
51	K	1118	C
51	K	1121	G
51	K	1126	G
51	K	1131	G
51	K	1133	A
51	K	1138	C
51	K	1139	C
51	K	1149	A
51	K	1150	A
51	K	1153	C
51	K	1154	U
51	K	1155	U
51	K	1161	U

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Mol	Chain	Res	Type
51	K	1170	A
51	K	1195	A
51	K	1208	A
51	K	1215	C
51	K	1221	G
51	K	1224	G
51	K	1242	U
51	K	1251	A
51	K	1253	A
51	K	1256	G
51	K	1257	G
51	K	1259	A
51	K	1264	C
51	K	1271	C
51	K	1274	G
51	K	1275	G
51	K	1284	A
51	K	1285	G
51	K	1286	G
51	K	1298	G
51	K	1299	A
51	K	1301	A
51	K	1302	G
51	K	1303	C
51	K	1307	U
51	K	1308	U
51	K	1310	U
51	K	1314	U
51	K	1333	U
51	K	1341	C
51	K	1342	U
51	K	1345	G
51	K	1348	G
51	K	1371	U
51	K	1372	U
51	K	1376	A
51	K	1378	A
51	K	1382	A
51	K	1394	G
51	K	1395	C
51	K	1396	A
51	K	1397	U

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Mol	Chain	Res	Type
51	K	1401	A
51	K	1402	A
51	K	1409	A
51	K	1410	C
51	K	1412	C
51	K	1428	G
51	K	1442	U
51	K	1447	G
51	K	1449	G
51	K	1452	A
51	K	1454	A
51	K	1455	A
51	K	1462	U
51	K	1463	U
51	K	1466	G
51	K	1473	G
51	K	1476	A
51	K	1477	U
51	K	1489	A
51	K	1490	G
51	K	1494	U
51	K	1497	G
51	K	1498	A
51	K	1507	G
51	K	1509	U
51	K	1510	G
51	K	1521	C
51	K	1522	A
51	K	1533	A
51	K	1535	U
51	K	1536	G
51	K	1544	C
51	K	1548	G
51	K	1552	G
51	K	1553	C
51	K	1554	C
51	K	1555	U
51	K	1556	A
51	K	1557	C
51	K	1567	G
51	K	1570	G
51	K	1574	C

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Mol	Chain	Res	Type
51	K	1575	G
51	K	1580	A
51	K	1585	U
51	K	1586	U
51	K	1587	G
51	K	1588	A
51	K	1598	G
51	K	1601	A
51	K	1604	G
51	K	1606	G
51	K	1621	U
51	K	1623	A
51	K	1637	A
51	K	1638	G
51	K	1646	C
51	K	1648	G
51	K	1664	A
51	K	1665	G
51	K	1680	G
51	K	1682	C
51	K	1683	C
51	K	1695	A
51	K	1699	A
51	K	1715	A
51	K	1721	U
51	K	1722	G
51	K	1725	U
51	K	1726	G
51	K	1744	G
51	K	1748	G
51	K	1753	C
51	K	1756	C
51	K	1783	C
51	K	1799	G
51	K	1814	G
51	K	1815	A
51	K	1823	A
51	K	1824	A
51	K	1825	A
51	K	1826	G
51	K	1831	A
51	K	1836	G

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Mol	Chain	Res	Type
51	K	1838	U
51	K	1849	G
51	K	1851	A
51	K	1852	C
51	K	1861	G
51	K	1862	G
51	K	1863	A
51	K	1865	C
51	K	1869	A
85	4	45	A
85	4	46	U
85	4	49	A
85	4	50	U

All (97) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	5	1	C
1	5	48	G
1	5	125	C
1	5	134	G
1	5	170	C
1	5	187	U
1	5	216	C
1	5	218	A
1	5	245	C
1	5	265	C
1	5	275	C
1	5	451	C
1	5	454	U
1	5	486	C
1	5	684	G
1	5	693	C
1	5	930	G
1	5	943	A
1	5	956	A
1	5	989	U
1	5	1211	G
1	5	1232	G
1	5	1236	C
1	5	1238	A
1	5	1296	G

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Mol	Chain	Res	Type
1	5	1329	G
1	5	1407	C
1	5	1440	U
1	5	1455	G
1	5	1633	G
1	5	1804	A
1	5	1818	G
1	5	1835	G
1	5	2015	U
1	5	2017	A
1	5	2046	G
1	5	2083	C
1	5	2089	G
1	5	2093	A
1	5	2107	C
1	5	2116	C
1	5	2123	C
1	5	2256	C
1	5	2257	C
1	5	2260	C
1	5	2262	G
1	5	2266	C
1	5	2502	G
1	5	2661	U
1	5	2695	A
1	5	3625	G
1	5	3771	C
1	5	3876	A
1	5	4119	C
1	5	4170	A
1	5	4232	U
1	5	4354	U
1	5	4448	G
1	5	4528	G
1	5	4548	A
1	5	4656	A
1	5	4699	U
1	5	4719	G
1	5	4885	U
1	5	4888	U
1	5	4889	G
1	5	4935	C

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Mol	Chain	Res	Type
1	5	4948	C
1	5	5022	U
1	5	5027	C
1	5	5059	C
1	5	5060	A
3	8	124	U
49	2	39	U
50	3	36	A
51	K	110	U
51	K	182	C
51	K	304	C
51	K	305	U
51	K	322	C
51	K	434	G
51	K	465	A
51	K	532	C
51	K	553	U
51	K	614	C
51	K	642	U
51	K	688	U
51	K	752	G
51	K	798	G
51	K	870	A
51	K	902	G
51	K	1061	U
51	K	1137	U
51	K	1395	C
51	K	1520	G
51	K	1637	A
51	K	1664	A

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 164 ligands modelled in this entry, 164 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	5	12
51	K	11
50	3	2
49	2	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	K	697:G	O3'	729:C	P	18.34
1	K	756:C	O3'	788:G	P	17.89
1	K	1761:U	O3'	1771:G	P	17.79
1	5	4776:G	O3'	4859:C	P	17.38
1	5	757:G	O3'	906:C	P	17.23
1	5	2910:G	O3'	3583:U	P	17.01
1	5	519:C	O3'	642:G	P	17.00
1	K	834:C	O3'	841:G	P	16.21
1	K	323:C	O3'	329:G	P	15.96
1	K	1417:C	O3'	1423:C	P	15.13
1	5	3950:U	O3'	4065:G	P	14.95
1	5	997:C	O3'	1047:C	P	14.50
1	5	2131:C	O3'	2243:C	P	14.18

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	K	130:G	O3'	140:U	P	14.04
1	5	1051:G	O3'	1064:G	P	10.03
1	K	745:C	O3'	749:U	P	7.98
1	K	225:G	O3'	287:U	P	7.30
1	K	736:C	O3'	743:U	P	6.33
1	3	19:G	O3'	20:U	P	6.15
1	2	16:C	O3'	18:G	P	5.67
1	5	1699:A	O3'	1718:C	P	5.39
1	3	16:C	O3'	18:U	P	5.26
1	K	1432:U	O3'	1438:A	P	4.82
1	5	1840:G	O3'	1842:G	P	4.76
1	5	1100:U	O3'	1167:C	P	4.13
1	5	1222:A	O3'	1232:G	P	3.81

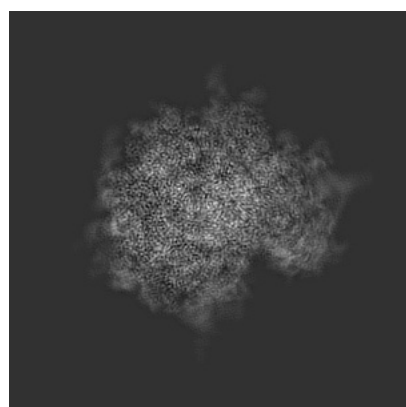
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-4737. These allow visual inspection of the internal detail of the map and identification of artifacts.

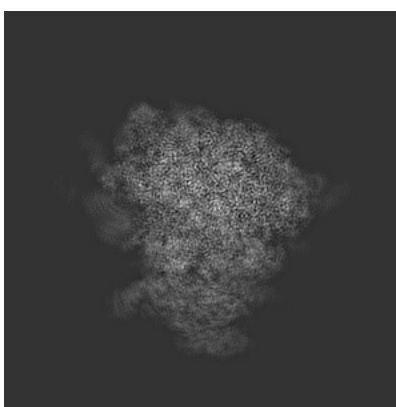
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

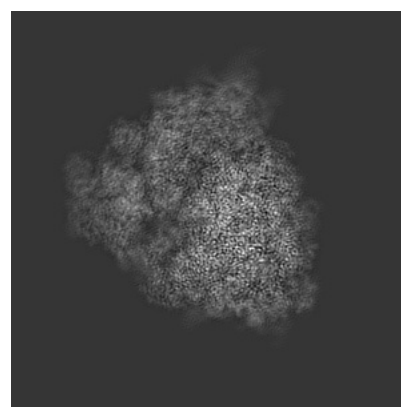
6.1.1 Primary map



X



Y

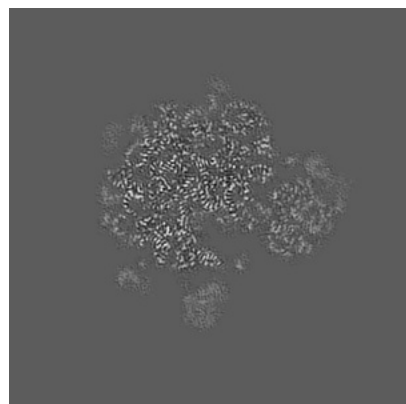


Z

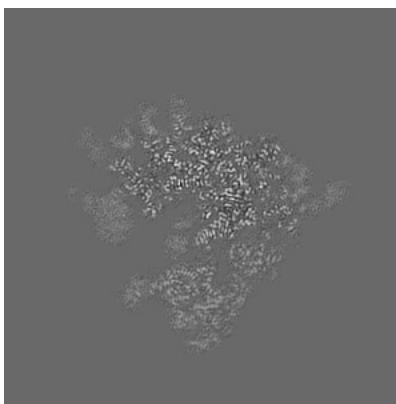
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

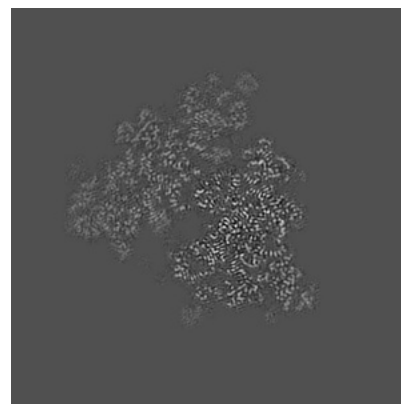
6.2.1 Primary map



X Index: 198



Y Index: 198

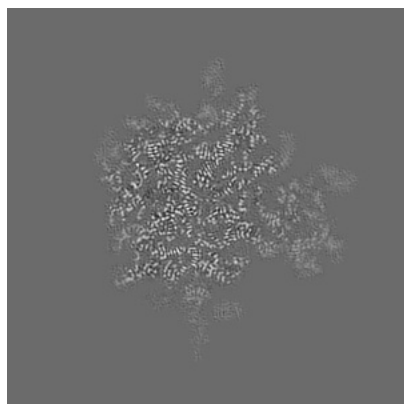


Z Index: 198

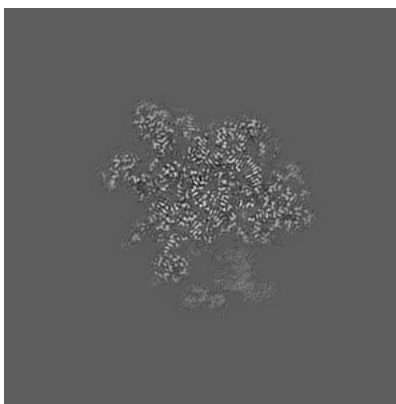
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

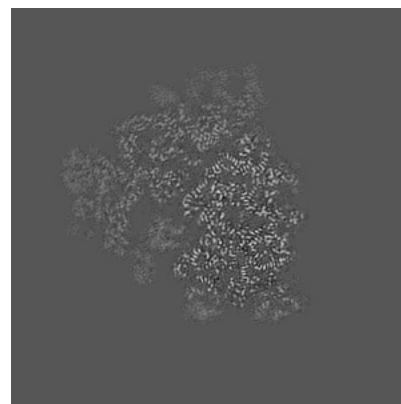
6.3.1 Primary map



X Index: 215



Y Index: 154

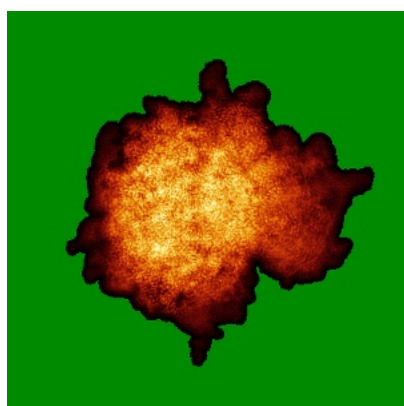


Z Index: 212

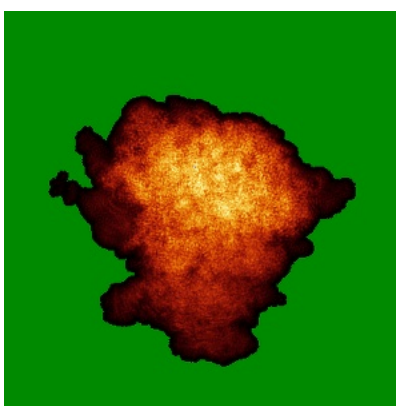
The images above show the largest variance slices of the map in three orthogonal directions.

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

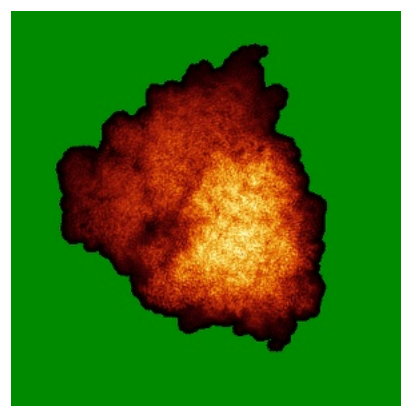
6.4.1 Primary map



X



Y

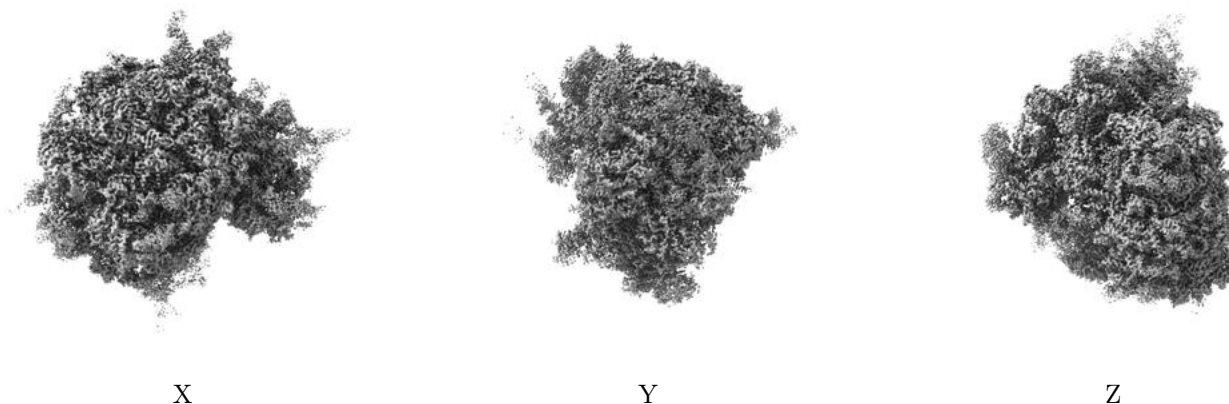


Z

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

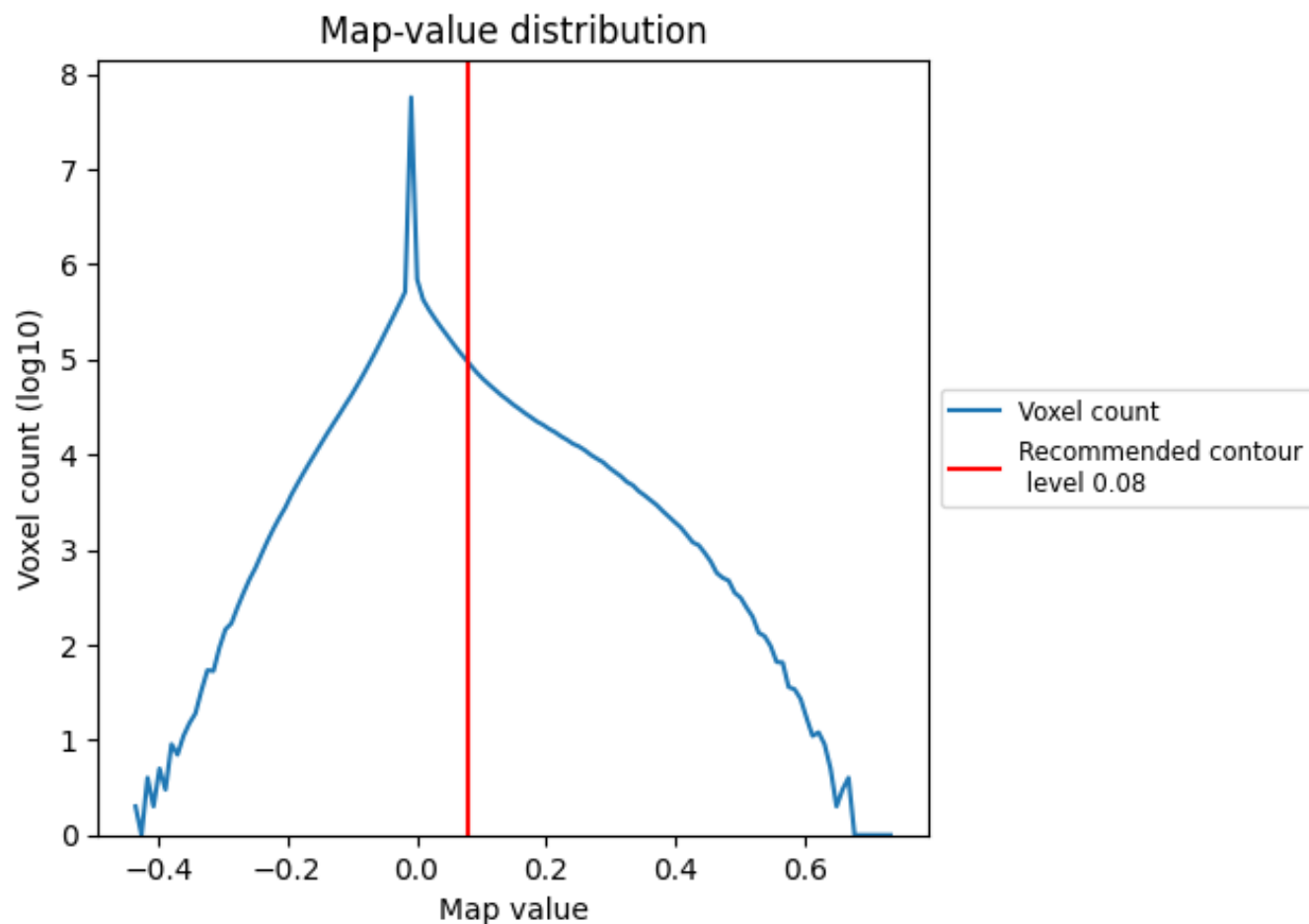
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

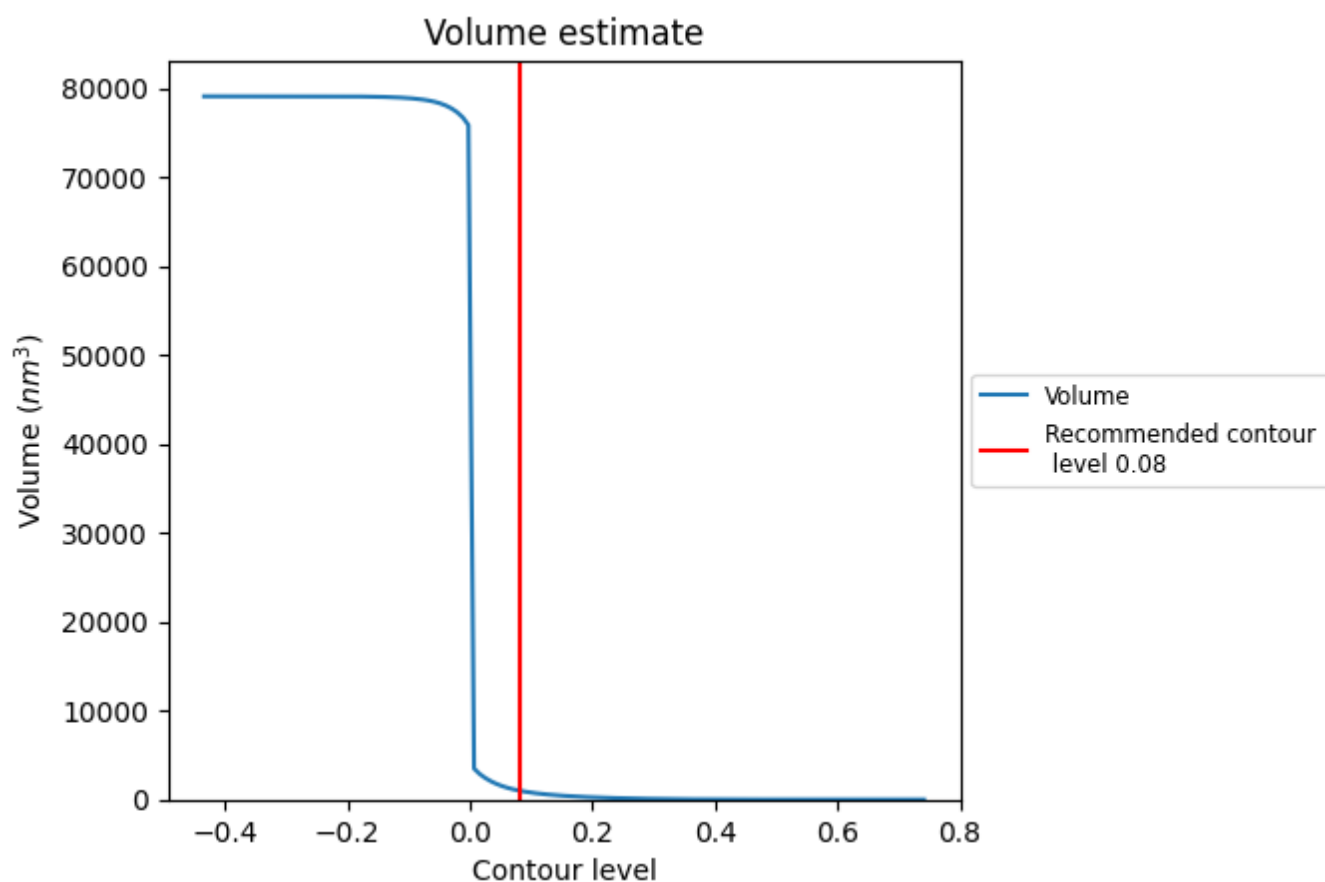
This section contains the results of statistical analysis of the map.

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.

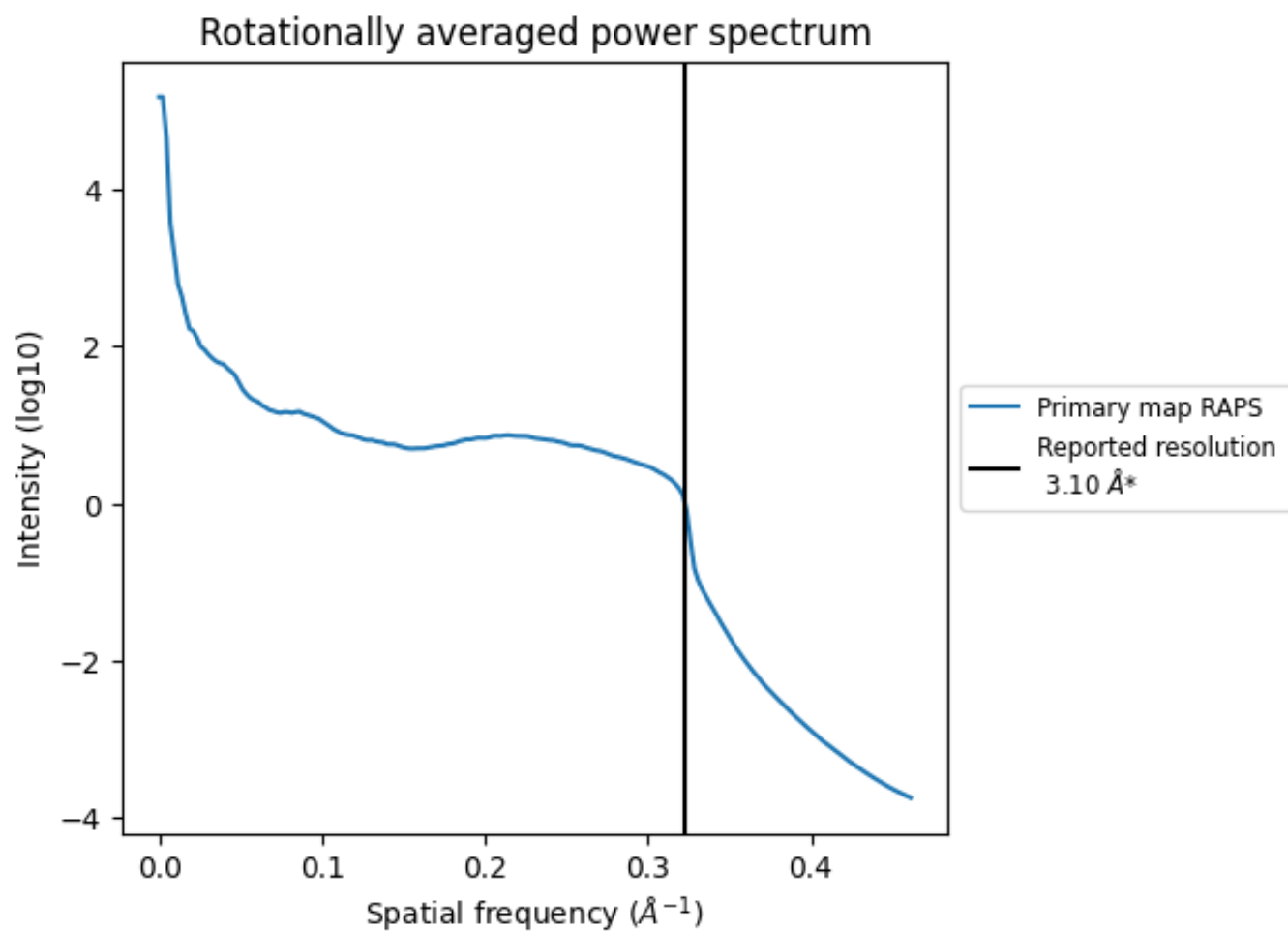
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1009 nm³; this corresponds to an approximate mass of 911 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 ⓘ

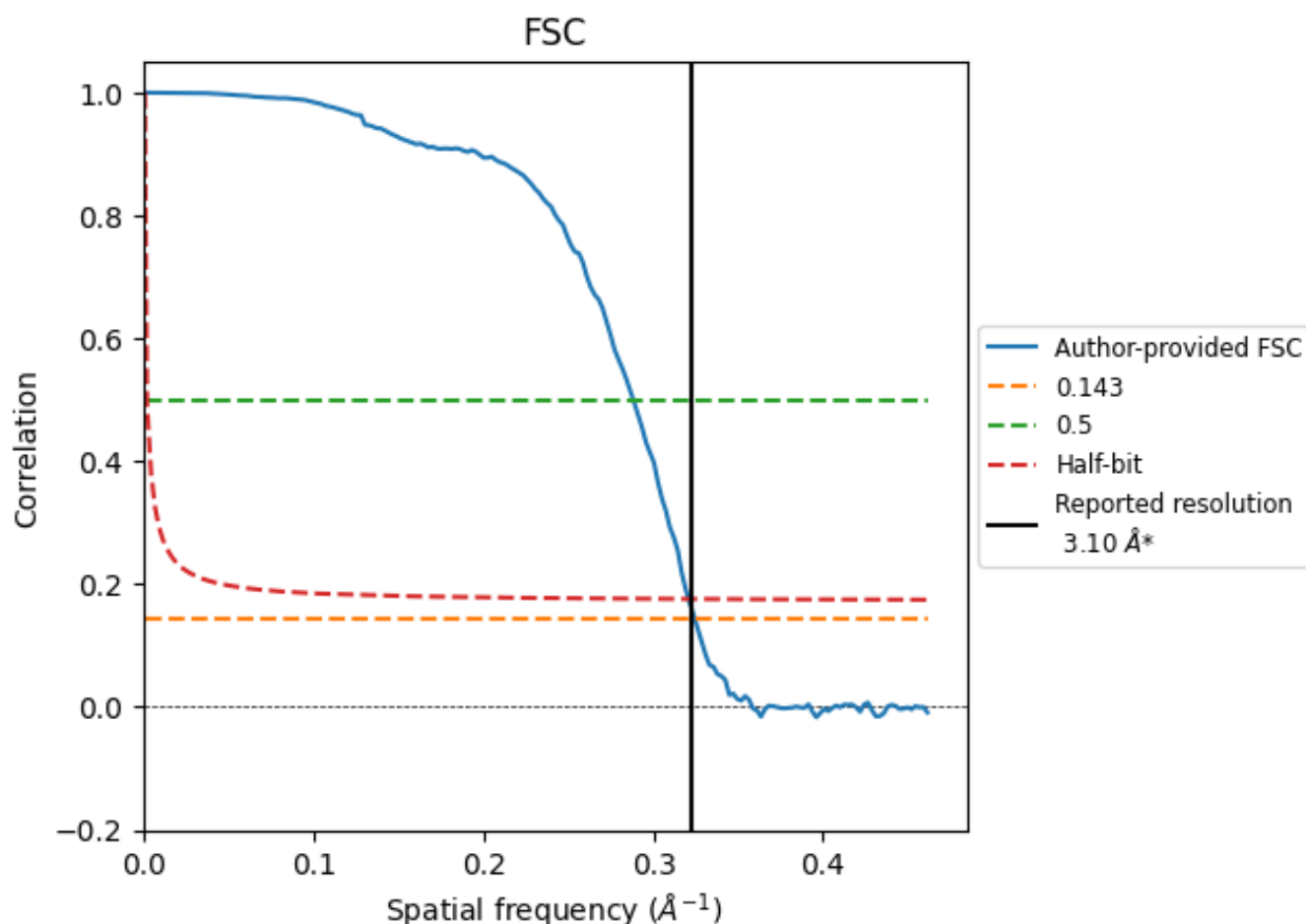


*Reported resolution corresponds to spatial frequency of 0.323 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.323 Å⁻¹

8.2 Resolution estimates [i](#)

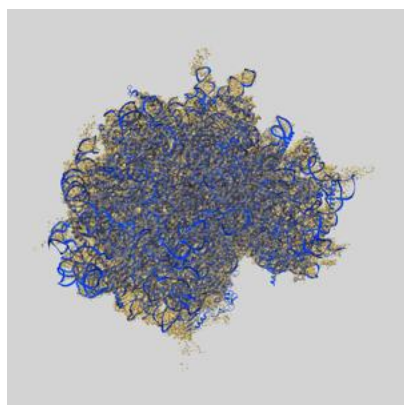
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.10	-	-
Author-provided FSC curve	3.08	3.47	3.12
Unmasked-calculated*	-	-	-

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

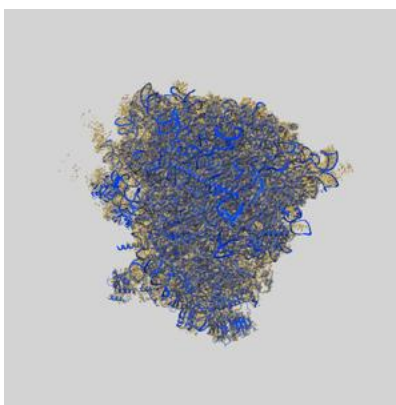
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-4737 and PDB model 6R6P. Per-residue inclusion information can be found in [section 3](#) on [page 22](#).

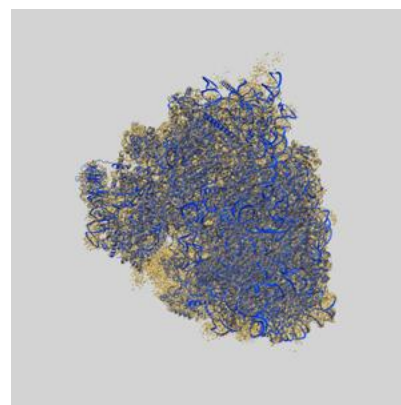
9.1 Map-model overlay [i](#)



X



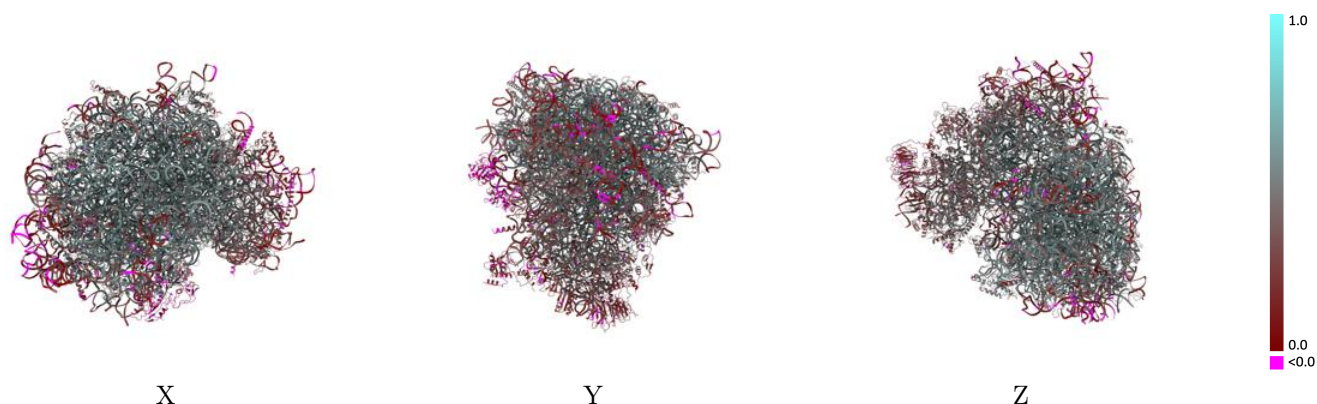
Y



Z

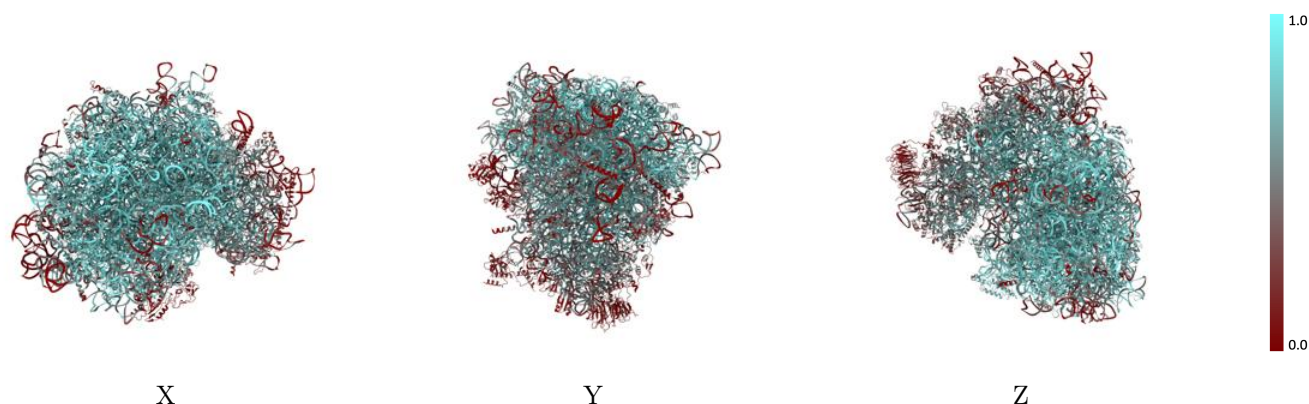
The images above show the 3D surface view of the map at the recommended contour level 0.08 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



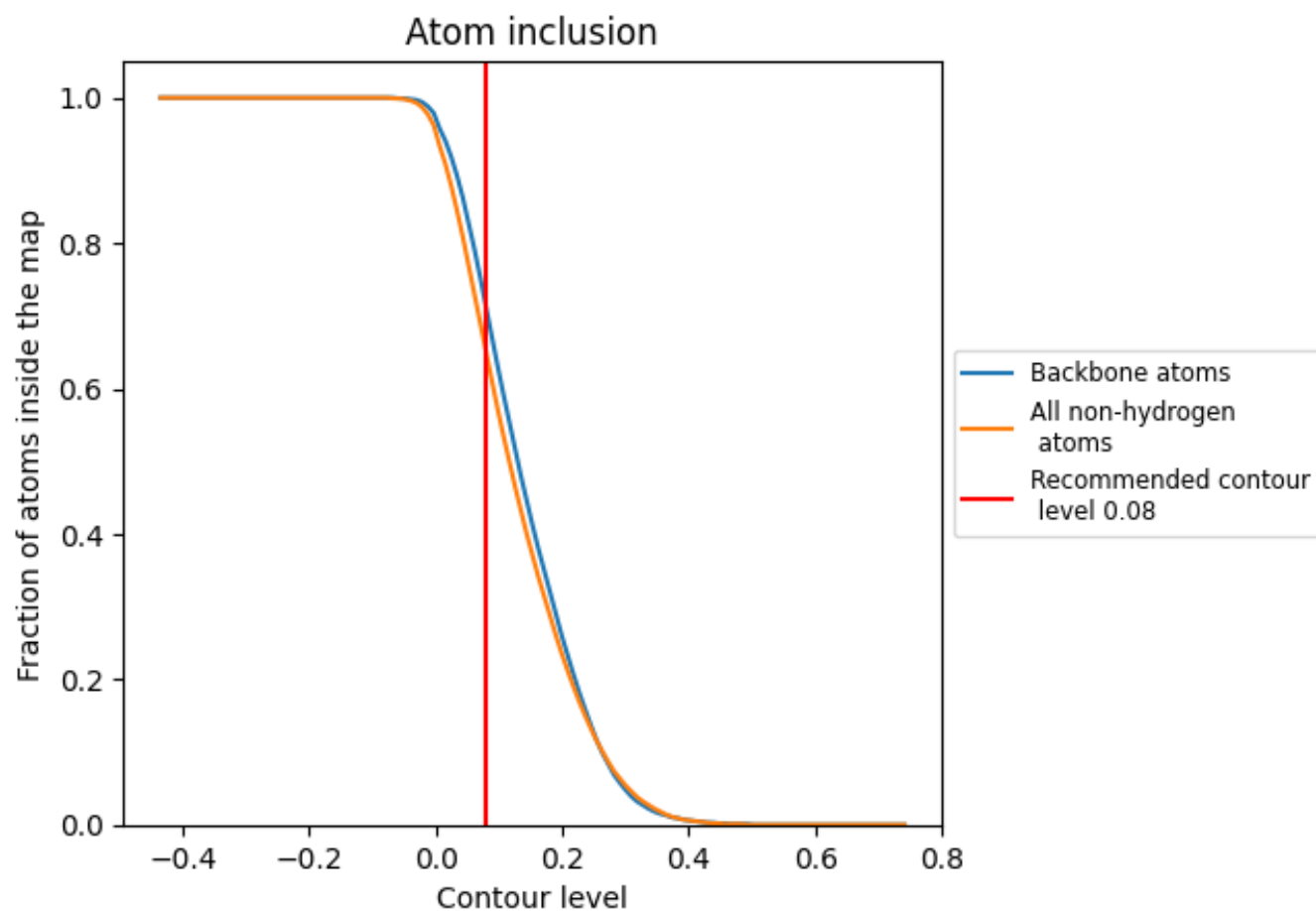
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.08).

9.4 Atom inclusion [i](#)



At the recommended contour level, 71% of all backbone atoms, 65% 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 (0.08) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6500	 0.4290
0	 0.1780	 0.1670
1	 0.7040	 0.5380
2	 0.3430	 0.3240
3	 0.5530	 0.3530
4	 0.7010	 0.4530
5	 0.7440	 0.4610
6	 0.1380	 0.1930
7	 0.8890	 0.5500
8	 0.7930	 0.4960
9	 0.4740	 0.3200
A	 0.7800	 0.5370
AA	 0.3170	 0.2900
B	 0.7660	 0.5170
BB	 0.4130	 0.3620
C	 0.7480	 0.5000
CC	 0.4470	 0.3500
D	 0.7170	 0.4640
DD	 0.3250	 0.2960
E	 0.6050	 0.3850
EE	 0.5460	 0.4230
F	 0.7450	 0.4970
FF	 0.3080	 0.3270
G	 0.6090	 0.4330
GG	 0.2690	 0.2660
H	 0.7120	 0.4930
HH	 0.4470	 0.3600
I	 0.7480	 0.4990
II	 0.4830	 0.3640
J	 0.6650	 0.4450
JJ	 0.4440	 0.3590
K	 0.6400	 0.4080
L	 0.6620	 0.4540
M	 0.7150	 0.4840
MM	 0.5320	 0.4100



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Chain	Atom inclusion	Q-score
N	 0.7990	 0.5320
NN	 0.3690	 0.3220
O	 0.7670	 0.5070
OO	 0.3770	 0.3290
P	 0.7800	 0.5280
PP	 0.4100	 0.3310
Q	 0.7630	 0.5060
QQ	 0.5520	 0.4270
R	 0.6160	 0.4080
RR	 0.1330	 0.1510
S	 0.7710	 0.5060
SS	 0.3080	 0.2490
T	 0.7070	 0.4840
TT	 0.5400	 0.4080
U	 0.5900	 0.4060
UU	 0.3760	 0.3380
V	 0.7500	 0.5240
VV	 0.6160	 0.4600
W	 0.7390	 0.5150
X	 0.6910	 0.4870
XX	 0.4230	 0.3350
Y	 0.7250	 0.4770
YY	 0.3250	 0.2980
Z	 0.6840	 0.4500
ZZ	 0.5450	 0.4200
a	 0.7830	 0.5220
b	 0.6090	 0.3960
c	 0.6900	 0.4770
d	 0.6990	 0.4890
e	 0.7740	 0.5300
f	 0.7800	 0.5240
g	 0.7050	 0.4910
h	 0.7180	 0.4760
i	 0.6630	 0.4640
j	 0.7790	 0.5150
k	 0.5760	 0.4060
l	 0.7380	 0.5060
m	 0.7520	 0.4900
n	 0.6320	 0.4310
o	 0.7030	 0.4880
p	 0.7050	 0.5120
q	 0.4620	 0.3600

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Chain	Atom inclusion	Q-score
r	 0.7310	 0.4760
s	 0.0300	 0.0030
t	 0.0070	 0.0090
u	 0.5460	 0.4130
v	 0.4690	 0.3530
w	 0.5150	 0.3870
x	 0.3910	 0.3360
y	 0.3560	 0.2900
z	 0.3640	 0.2960