



Full wwPDB/EMDatabank EM Map/Model Validation Report ⓘ

Jun 29, 2019 – 11:17 PM EDT

PDB ID : 6R6P
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)
Based on PDB ID : ?

This is a Full wwPDB/EMDatabank EM Map/Model Validation Report
for a publicly released PDB/EMDB 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.

MolProbity : 4.02b-467
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : 2.3.2

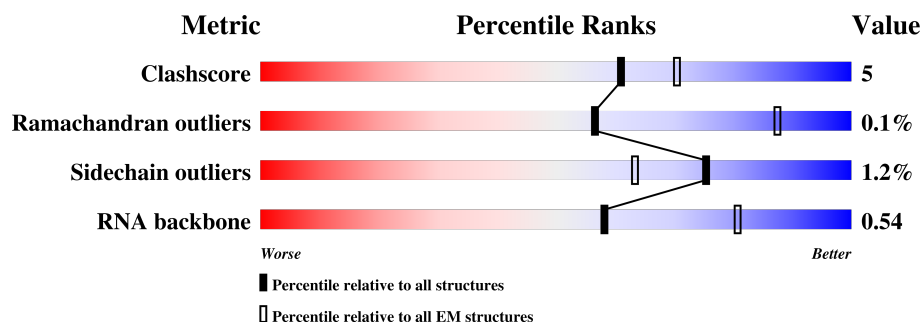
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.10 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.























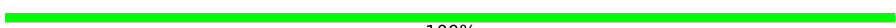

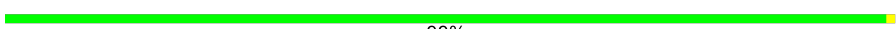


Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	136327	1886
Ramachandran outliers	132723	1663
Sidechain outliers	132532	1531
RNA backbone	3747	458

The table below summarises the geometric issues observed across the polymeric chains. The red, orange, yellow and green segments on the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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 $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	5	3662	
2	7	120	
3	8	156	
4	A	244	
5	B	394	
6	C	362	
7	D	292	
8	E	248	

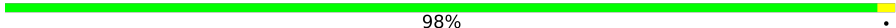
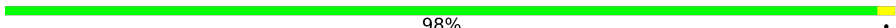
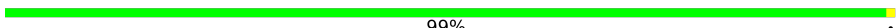
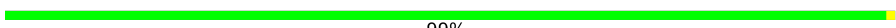
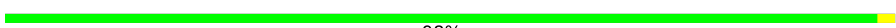








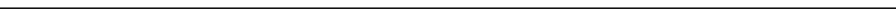





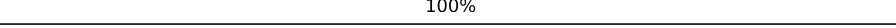
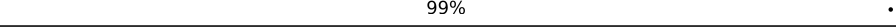
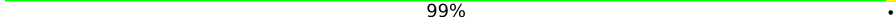
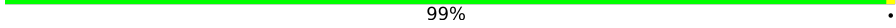
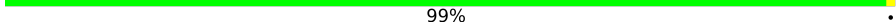
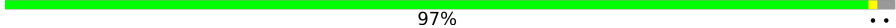
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Mol	Chain	Length	Quality of chain
9	F	225	 80% 20%
10	G	241	 86% 13%
11	H	190	 82% 18%
12	I	213	 77% 19% .
13	J	169	 86% 13% .
14	L	210	 88% 11%
15	M	138	 86% 14%
16	N	203	 83% 16%
17	O	199	 82% 17% .
18	P	153	 84% 15% .
19	Q	187	 89% 11%
20	R	180	 87% 13%
21	S	175	 82% 18%
22	T	159	 84% 16%
23	U	99	 86% 14%
24	V	131	 80% 20%
25	W	63	 86% 13% .
26	X	119	 86% 14%
27	Y	134	 80% 20%
28	Z	135	 82% 17% .
29	a	147	 100%
30	b	75	 99% .
31	c	94	 99% .
32	d	107	 98% .
33	e	128	 99% .



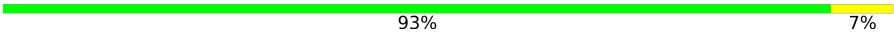




















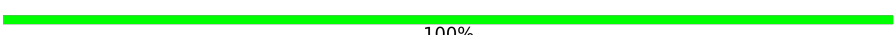

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Mol	Chain	Length	Quality of chain
34	f	109	 98% .
35	g	114	 98% .
36	h	122	 99% .
37	i	102	 99% .
38	j	86	 98% .
39	k	69	 99% .
40	l	50	 94% 6% .
41	m	52	 100% .
42	n	23	 100% .
43	o	104	 96% .
44	p	91	 98% .
45	r	125	 95% . .
46	s	198	 99% .
47	t	163	 98% .
48	1	24	 50% 46% .
49	2	76	 50% 36% 13% .
50	3	75	 68% 28% .
51	K	1698	 60% 33% 7% .
52	q	217	 100% .
53	u	213	 99% .
54	v	221	 99% .
55	x	262	 99% .
56	z	237	 99% .
57	y	189	 97% . .
58	CC	206	 86% 14% .

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Mol	Chain	Length	Quality of chain
59	XX	185	 86% 14%
60	EE	151	 77% 17% • 5%
61	QQ	149	 93% 7%
62	MM	136	 85% 15%
63	UU	142	 85% 13%
64	YY	132	 89% 11%
65	HH	83	 82% 18%
66	TT	129	 84% 16%
67	VV	141	 85% 13%
68	NN	124	 81% 19%
69	ZZ	101	 83% 17%
70	JJ	83	 81% 18%
71	AA	55	 85% 13%
72	DD	228	 85% 15%
73	BB	191	 82% 15%
74	SS	96	 80% 20%
75	RR	117	 87% 13%
76	9	120	 86% 14%
77	II	144	 76% 24%
78	PP	141	 84% 16%
79	GG	100	 75% 25%
80	OO	75	 92% 8%
81	FF	62	 85% 15%
82	w	55	 100%
83	0	68	 79% 19%

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Mol	Chain	Length	Quality of chain
84	6	313	<div><div></div><div>83%</div><div>17%</div></div>
85	4	10	<div><div></div><div>30%</div><div>50%</div><div>20%</div></div>

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 (three-letter code: MG) (formula: Mg).

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

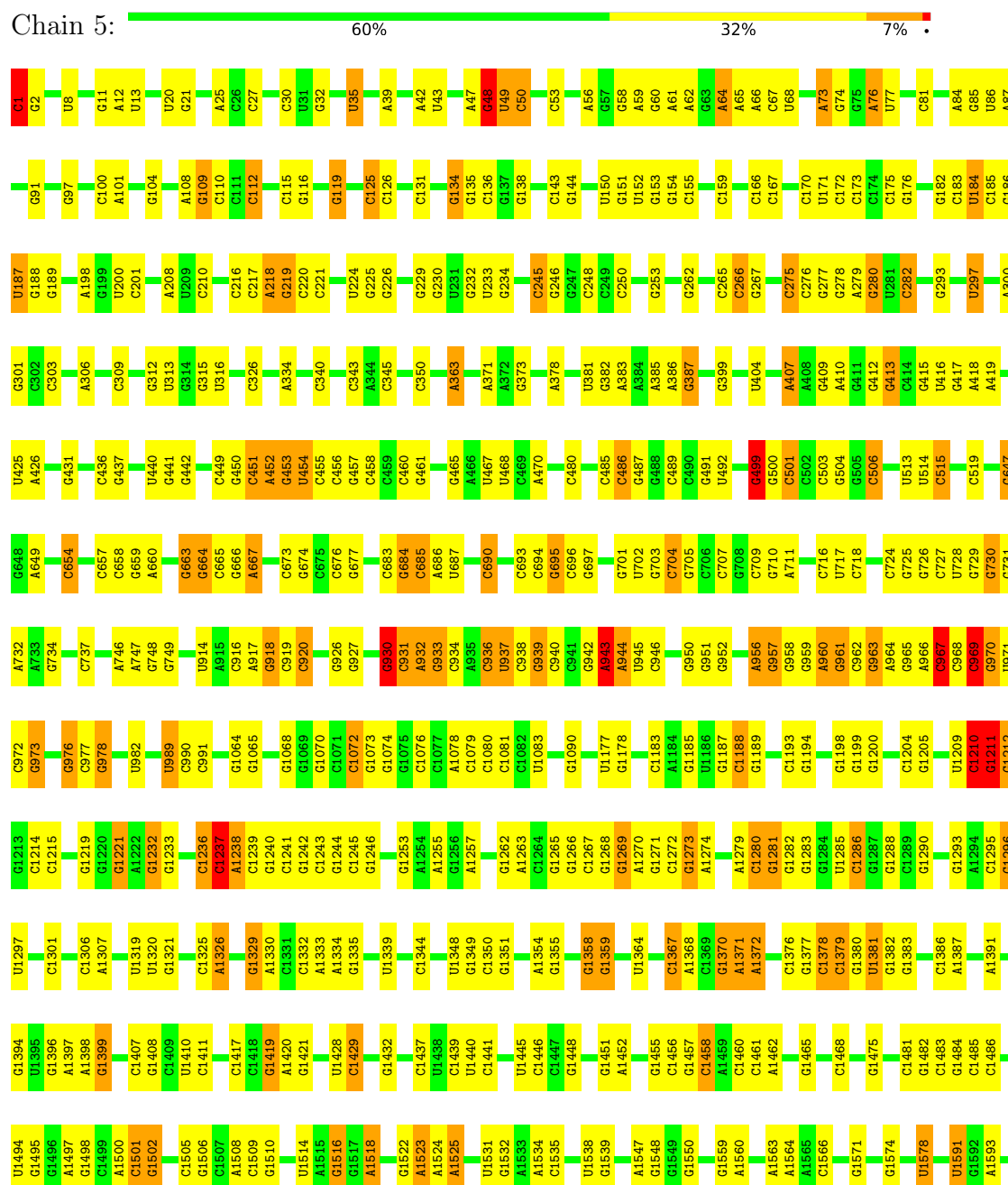
- Molecule 87 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

3 Residue-property plots

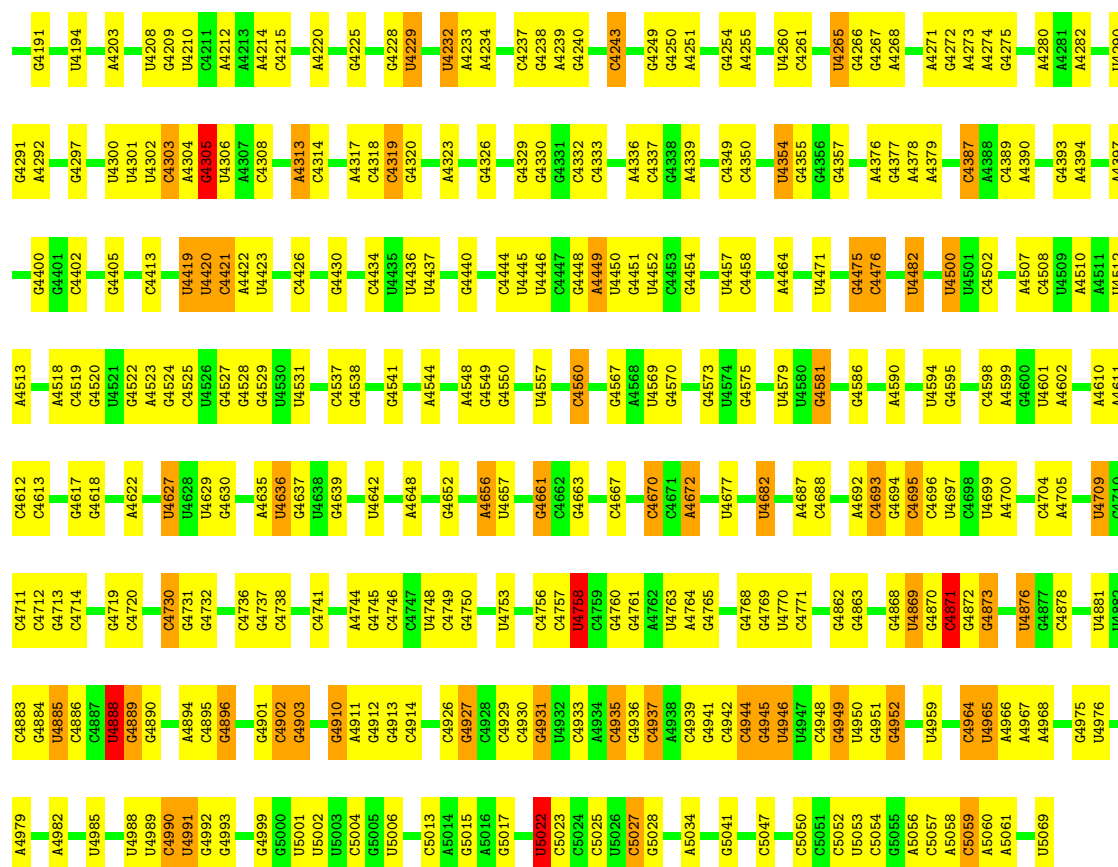
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according 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. 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




WORLDWIDE PDB
 PROTEIN DATA BANK

EMDataBank
 Unified Data Resource for 3DEM



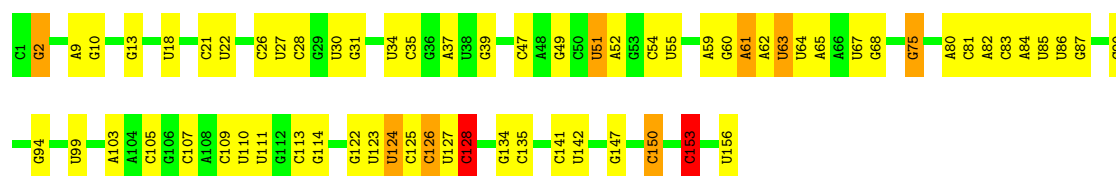
- Molecule 2: 5S ribosomal RNA

Chain 7: 73% 20% 7%



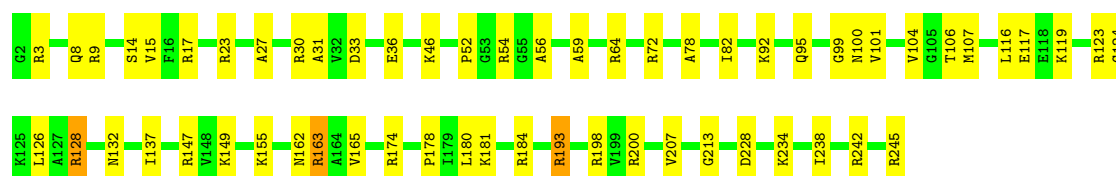
- Molecule 3: 5.8S ribosomal RNA

Chain 8: 58% 36% 5%

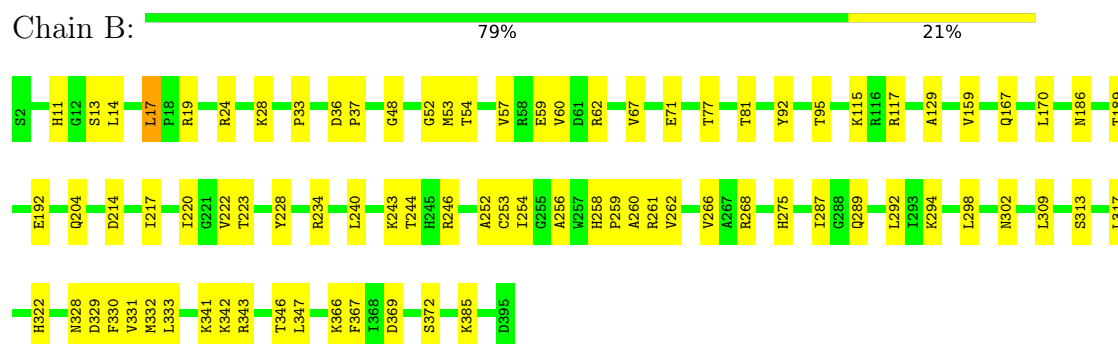


- Molecule 4: uL2

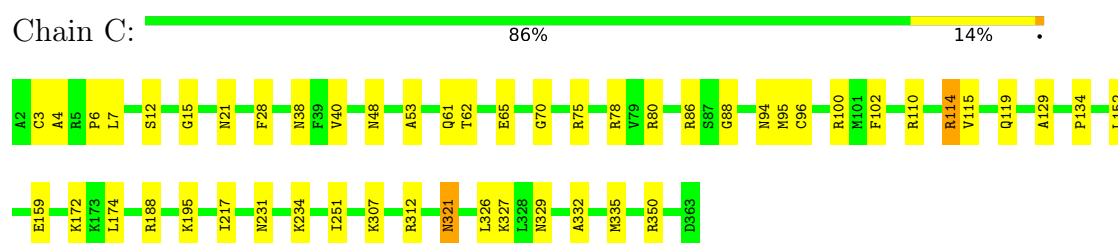
Chain A: 76% 23% 1%



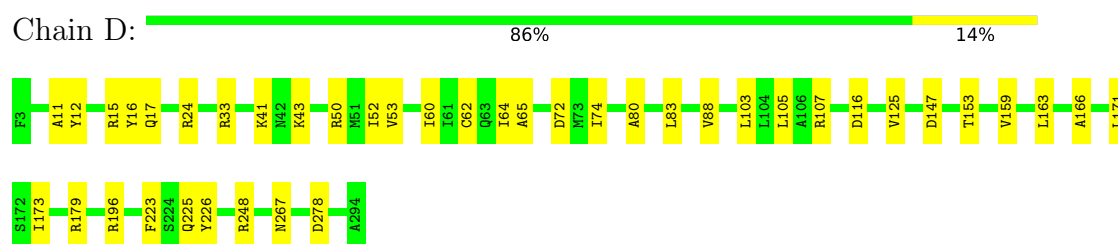
- Molecule 5: uL3



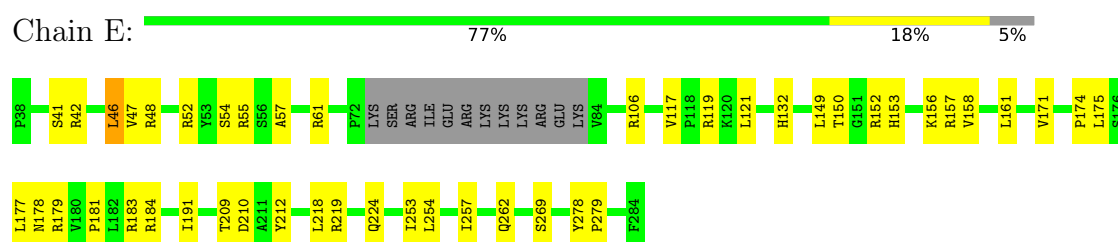
- Molecule 6: uL4



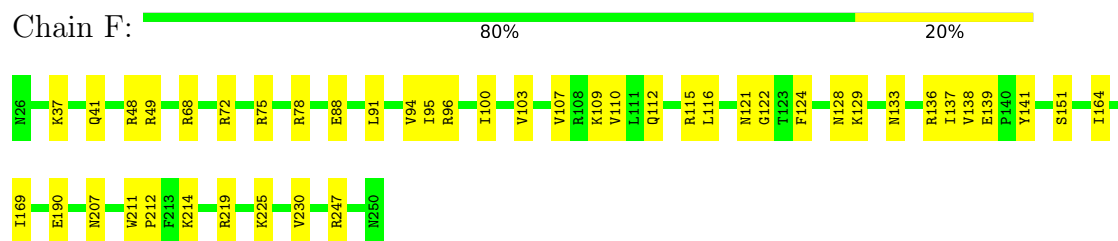
- Molecule 7: 60S ribosomal protein L5



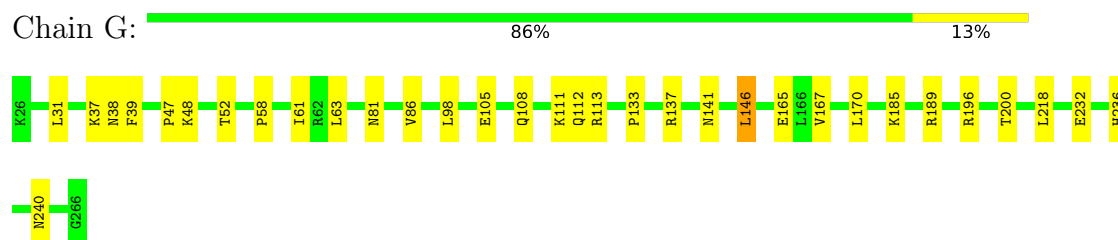
- Molecule 8: 60S ribosomal protein L6



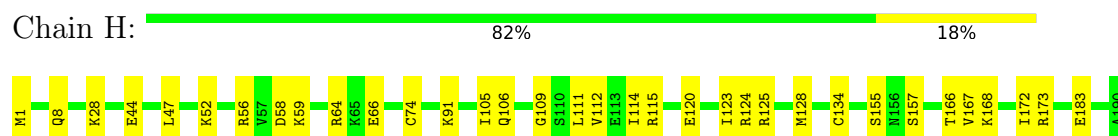
- Molecule 9: uL30



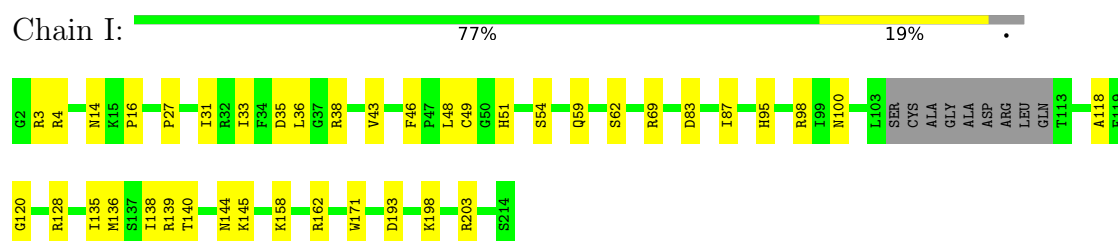
- Molecule 10: eL8



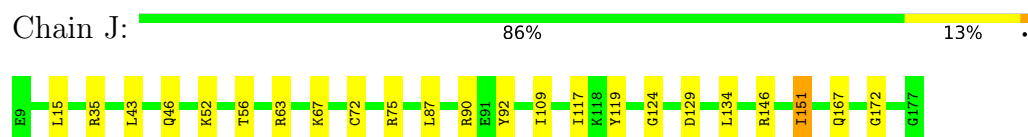
- Molecule 11: uL6



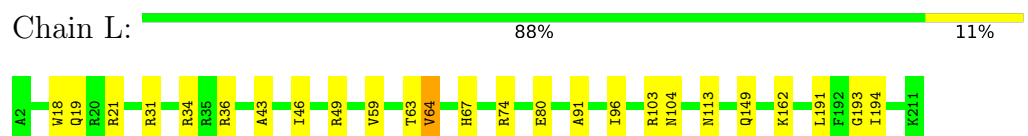
- Molecule 12: Ribosomal protein L10 (Predicted)



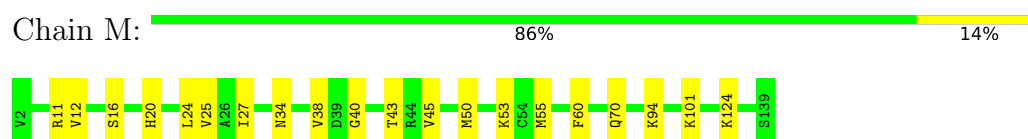
- Molecule 13: uL5



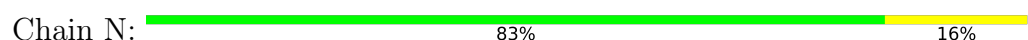
- Molecule 14: 60S ribosomal protein L13

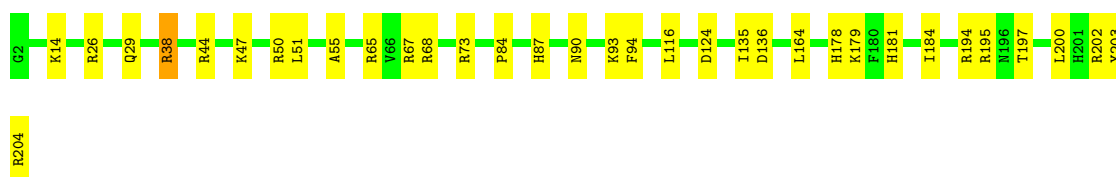


- Molecule 15: Ribosomal protein L14



- Molecule 16: Ribosomal protein L15





- Molecule 17: uL13

Chain O: 82% 17%



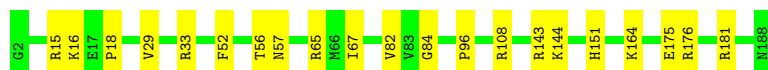
- Molecule 18: uL22

Chain P: 84% 15%



- Molecule 19: eL18

Chain Q: 89% 11%



- Molecule 20: eL19

Chain R: 87% 13%



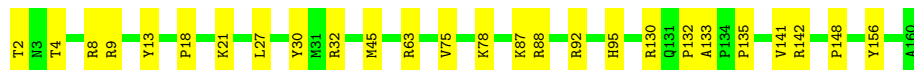
- Molecule 21: eL20

Chain S: 82% 18%




- Molecule 22: eL21

Chain T: 84% 16%




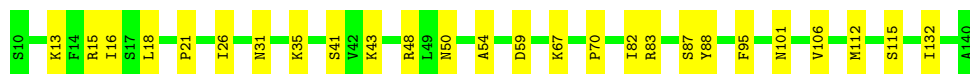
- Molecule 23: Ribosomal protein L22

Chain U:  86% 14%




- Molecule 24: uL14

Chain V:  80% 20%



- Molecule 25: Ribosomal protein L24

Chain W:  86% 13% .




- Molecule 26: uL23

Chain X:  86% 14%




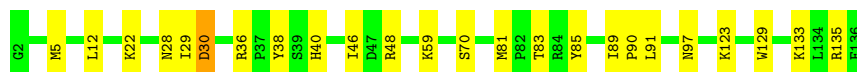
- Molecule 27: Ribosomal protein L26

Chain Y:  80% 20%



- Molecule 28: 60S ribosomal protein L27

Chain Z:  82% 17% .



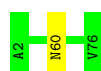
- Molecule 29: uL15

Chain a:  100%

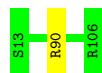
There are no outlier residues recorded for this chain.

- Molecule 30: 60S ribosomal protein L29

Chain b:  99% .



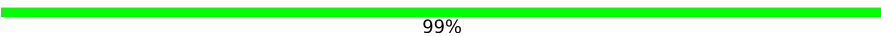
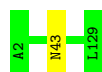
• Molecule 31: eL30

Chain c:  99%

• Molecule 32: eL31

Chain d:  98%

• Molecule 33: eL32

Chain e:  99%

• Molecule 34: eL33

Chain f:  98%

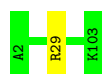
• Molecule 35: eL34

Chain g:  98%

• Molecule 36: uL29

Chain h:  99%

• Molecule 37: 60S ribosomal protein L36

Chain i:  99%

• Molecule 38: Ribosomal protein L37

Chain j:  98%



- Molecule 39: eL38

Chain k: 99%



- Molecule 40: ribosomal protein eL39

Chain l: 94%



- Molecule 41: eL40

Chain m: 100%

There are no outlier residues recorded for this chain.

- Molecule 42: 60s ribosomal protein l41

Chain n: 100%

There are no outlier residues recorded for this chain.

- Molecule 43: eL42

Chain o: 96%



- Molecule 44: ribosomal protein eL43

Chain p: 98%



- Molecule 45: eL28

Chain r: 95%



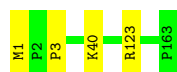
- Molecule 46: 60S acidic ribosomal protein P0

Chain s:  99% .



- Molecule 47: Ribosomal protein L12

Chain t:  98% .



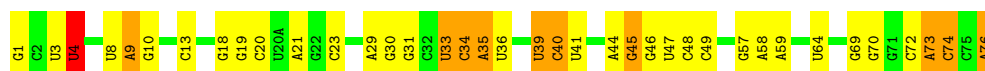
- Molecule 48: X-box-binding protein 1

Chain 1:  50% 46% .



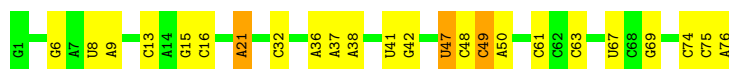
- Molecule 49: A/P-tRNA

Chain 2:  50% 36% 13% .



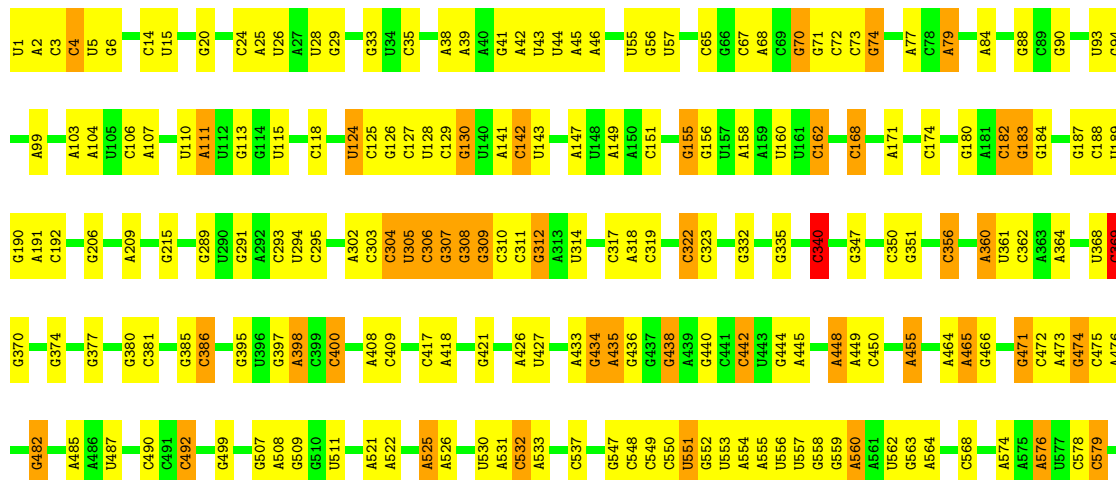
- Molecule 50: P/E-tRNA

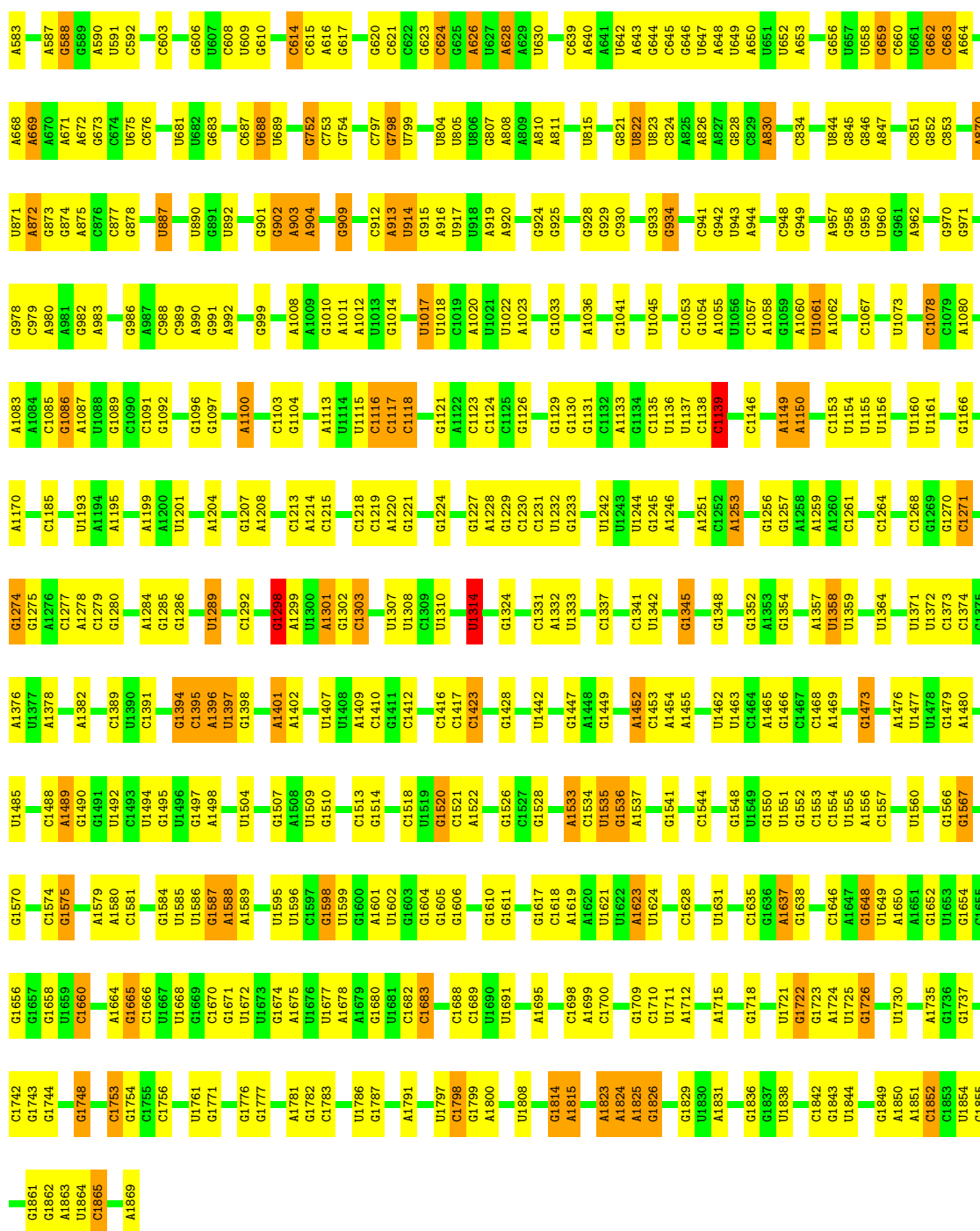
Chain 3:  68% 28% .



- Molecule 51: 18S rRNA

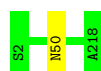
Chain K:  60% 33% 7% .





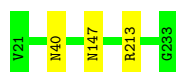
- Molecule 52: uS2

Chain q: 100%



- Molecule 53: 40S ribosomal protein S3a

Chain u: 99%



- Molecule 54: uS5

Chain v: 99%



- Molecule 55: 40S ribosomal protein S4

Chain x: 99%



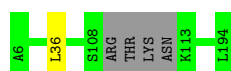
- Molecule 56: 40S ribosomal protein S6

Chain z: 99%



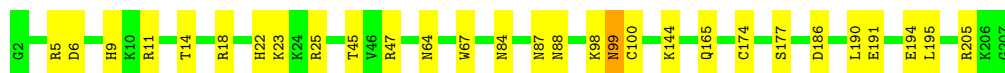
- Molecule 57: 40S ribosomal protein S7

Chain y: 97%



- Molecule 58: 40S ribosomal protein S8

Chain CC: 86%



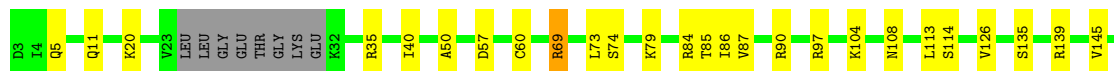
- Molecule 59: Ribosomal protein S9 (Predicted)

Chain XX: 86%



- Molecule 60: Ribosomal protein S11

Chain EE: 77%




K153


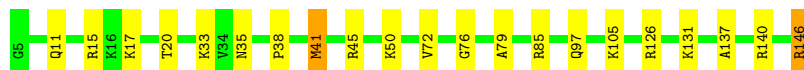
- Molecule 61: ribosomal protein uS15

Chain QQ:  93% 7%

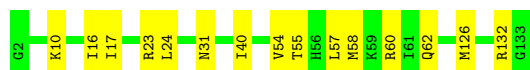

- Molecule 62: uS11

Chain MM:  85% 15%



- Molecule 63: Ribosomal protein S16

Chain UU:  85% 13%


- Molecule 64: eS17

Chain YY:  89% 11%




- Molecule 65: eS21

Chain HH:  82% 18%



- Molecule 66: Ribosomal protein S15a

Chain TT:  84% 16%


- Molecule 67: Ribosomal protein S23


Chain VV:  85% 13%


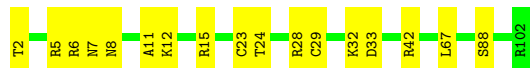
- Molecule 68: eS24

Chain NN:  81% 19%




- Molecule 69: eS26

Chain ZZ:  83% 17%



- Molecule 70: 40S ribosomal protein S27

Chain JJ:  81% 18%




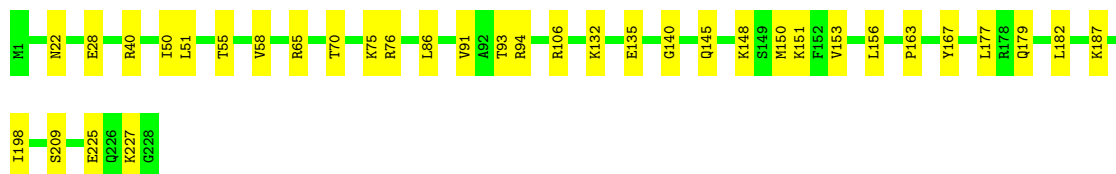
- Molecule 71: 40S ribosomal protein S30

Chain AA:  85% 13%




- Molecule 72: Ribosomal protein S3

Chain DD:  85% 15%




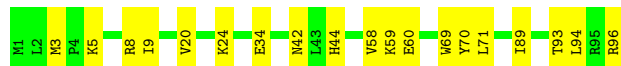
- Molecule 73: Ribosomal protein S5

Chain BB:  82% 15%




- Molecule 74: eS10

Chain SS:  80% 20%




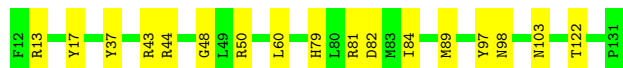
- Molecule 75: 40S ribosomal protein S12

Chain RR:  87% 13%




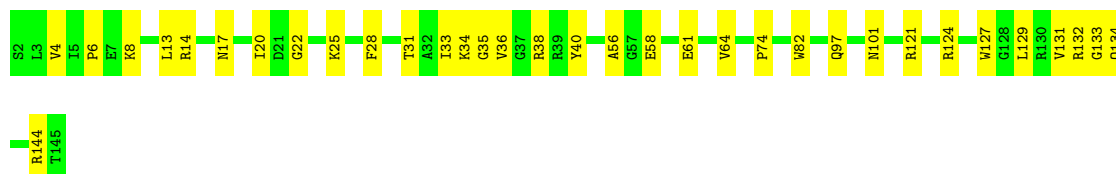
- Molecule 76: uS14

Chain 9:  86% 14%




- Molecule 77: uS13

Chain II:  76% 24%




- Molecule 78: eS19

Chain PP:  84% 16%



- Molecule 79: uS10

Chain GG:  75% 25%



- Molecule 80: ribosomal protein eS25

Chain OO:  92% 8%



- Molecule 81: Ribosomal protein S28

Chain FF:  85% 15%




- Molecule 82: S29

Chain w:  100%


There are no outlier residues recorded for this chain.

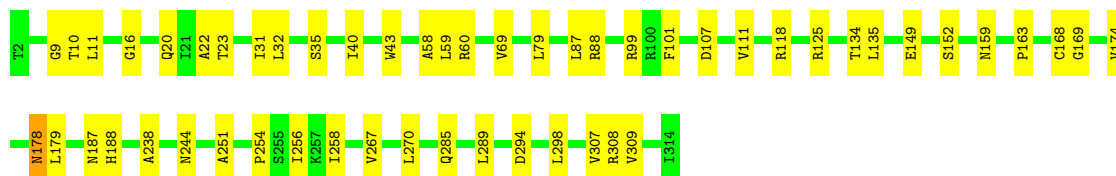
- Molecule 83: eS31

Chain 0:  79% 19%



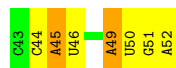
- Molecule 84: ribosomal protein RACK1

Chain 6:  83% 17%



- Molecule 85: mRNA

Chain 4:  30% 50% 20%



4 Experimental information

Property	Value	Source
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	Depositor
Maximum defocus (nm)	Not provided	Depositor
Magnification	Not provided	Depositor
Image detector	FEI FALCON II (4k x 4k)	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 2$	RMSZ	$\# Z > 2$
1	5	0.31	1/87794 (0.0%)	1.05	383/136953 (0.3%)
10	G	0.27	0/1967	0.55	1/2647 (0.0%)
11	H	0.27	0/1535	0.54	0/2063
12	I	0.27	0/1693	0.49	0/2260
13	J	0.27	0/1376	0.56	0/1841
14	L	0.27	0/1734	0.53	0/2317
15	M	0.27	0/1158	0.52	0/1547
16	N	0.27	0/1746	0.51	0/2338
17	O	0.28	0/1671	0.51	0/2234
18	P	0.33	0/1268	0.53	1/1700 (0.1%)
19	Q	0.25	0/1530	0.53	0/2041
2	7	0.28	0/2858	0.99	6/4455 (0.1%)
20	R	0.27	0/1524	0.54	0/2013
21	S	0.27	0/1493	0.51	0/2002
22	T	0.27	0/1326	0.49	0/1770
23	U	0.27	0/822	0.53	0/1103
24	V	0.28	0/993	0.56	0/1332
25	W	0.27	0/541	0.50	0/720
26	X	0.25	0/993	0.51	0/1334
27	Y	0.26	0/1132	0.50	0/1504
28	Z	0.28	0/1130	0.55	1/1507 (0.1%)
29	a	0.29	0/1191	0.51	0/1590
3	8	0.32	0/3701	1.06	10/5766 (0.2%)
30	b	0.25	0/619	0.46	0/818
31	c	0.28	0/742	0.51	0/996
32	d	0.28	0/903	0.51	0/1216
33	e	0.27	0/1071	0.49	0/1429
34	f	0.27	0/895	0.58	0/1198
35	g	0.26	0/916	0.55	0/1220
36	h	0.26	0/1021	0.51	0/1348
37	i	0.26	0/841	0.52	0/1112
38	j	0.26	0/720	0.51	0/952

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >2	RMSZ	# Z >2
39	k	0.30	0/575	0.70	1/761 (0.1%)
4	A	0.29	0/1906	0.55	0/2556
40	l	0.26	0/454	0.47	0/599
41	m	0.28	0/435	0.54	0/575
42	n	0.25	0/223	0.45	0/284
43	o	0.27	0/864	0.59	0/1140
44	p	0.26	0/718	0.54	0/953
45	r	0.29	0/1017	0.67	1/1364 (0.1%)
46	s	0.27	0/1547	0.52	0/2088
47	t	0.32	0/1257	0.65	0/1697
48	1	0.50	0/216	0.56	0/298
49	2	0.28	0/1802	0.95	6/2804 (0.2%)
5	B	0.27	0/3216	0.55	2/4311 (0.0%)
50	3	0.27	0/1783	1.00	3/2773 (0.1%)
51	K	0.29	1/40530 (0.0%)	1.04	165/63160 (0.3%)
52	q	0.26	0/1747	0.50	0/2374
53	u	0.25	0/1756	0.53	0/2350
54	v	0.27	0/1753	0.51	0/2369
55	x	0.25	0/2118	0.51	0/2849
56	z	0.25	0/1946	0.48	0/2590
57	y	0.26	0/1510	0.52	1/2022 (0.0%)
58	CC	0.25	0/1715	0.49	0/2287
59	XX	0.25	0/1550	0.50	0/2069
6	C	0.26	0/2937	0.51	0/3946
60	EE	0.26	0/1195	0.50	0/1597
61	QQ	0.25	0/1226	0.46	0/1649
62	MM	0.26	0/1029	0.51	0/1380
63	UU	0.26	0/1146	0.50	0/1534
64	YY	0.24	0/1082	0.46	0/1452
65	HH	0.27	0/643	0.52	0/860
66	TT	0.27	0/1051	0.51	0/1406
67	VV	0.26	0/1116	0.53	0/1490
68	NN	0.26	0/1028	0.48	0/1366
69	ZZ	0.26	0/828	0.49	0/1109
7	D	0.26	0/2432	0.50	0/3257
70	JJ	0.25	0/665	0.48	0/891
71	AA	0.26	0/447	0.46	0/587
72	DD	0.27	0/1796	0.54	0/2417
73	BB	0.26	0/1492	0.49	0/2005
74	SS	0.27	0/834	0.55	0/1125
75	RR	0.26	0/918	0.56	0/1233
76	9	0.26	0/1017	0.50	0/1358
77	II	0.27	0/1208	0.53	0/1618

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >2	RMSZ	# Z >2
78	PP	0.26	0/1115	0.50	0/1493
79	GG	0.25	0/805	0.50	0/1081
8	E	0.26	0/1936	0.61	1/2600 (0.0%)
80	OO	0.24	0/604	0.51	0/810
81	FF	0.24	0/490	0.48	0/656
82	w	0.26	0/470	0.46	0/623
83	0	0.25	0/567	0.48	0/753
84	6	0.25	0/2493	0.53	0/3394
85	4	0.45	0/235	1.14	1/363 (0.3%)
9	F	0.28	0/1905	0.51	0/2539
All	All	0.29	2/234252 (0.0%)	0.89	583/344191 (0.2%)

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
20	R	0	1
21	S	0	1
23	U	0	1
34	f	0	1
5	B	0	2
67	VV	0	2
76	9	0	2
All	All	0	10

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	5	967	C	N3-C4	-5.24	1.30	1.33
51	K	1520	G	N9-C4	5.10	1.42	1.38

All (583) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	5	961	G	N1-C6-O6	-19.59	108.15	119.90
1	5	967	C	N3-C4-N4	-19.03	104.68	118.00
1	5	967	C	C5-C4-N4	16.73	131.91	120.20
1	5	961	G	C5-C6-O6	13.97	136.98	128.60
1	5	931	C	N1-C2-O2	13.86	127.22	118.90
1	5	931	C	C2-N1-C1'	13.23	133.35	118.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	5	1072	C	N1-C2-O2	12.14	126.19	118.90
1	5	1072	C	C2-N1-C1'	11.32	131.25	118.80
1	5	931	C	N3-C2-O2	-10.89	114.27	121.90
51	K	1520	G	N3-C4-C5	-10.11	123.55	128.60
1	5	4420	U	C2-N1-C1'	10.01	129.72	117.70
1	5	4420	U	N1-C2-O2	10.01	129.80	122.80
51	K	1123	C	N1-C2-O2	9.79	124.77	118.90
1	5	100	C	C2-N1-C1'	9.70	129.47	118.80
51	K	853	C	C2-N1-C1'	9.36	129.09	118.80
51	K	1139	C	N1-C2-O2	9.35	124.51	118.90
1	5	1072	C	N3-C2-O2	-9.25	115.42	121.90
51	K	1261	C	N1-C2-O2	9.16	124.40	118.90
1	5	931	C	C6-N1-C1'	-9.12	109.85	120.80
1	5	4420	U	N3-C2-O2	-9.11	115.82	122.20
51	K	1520	G	C2-N3-C4	9.10	116.45	111.90
51	K	1078	C	N1-C2-O2	8.95	124.27	118.90
1	5	449	C	N1-C2-O2	8.90	124.24	118.90
1	5	4749	C	C2-N1-C1'	8.89	128.58	118.80
1	5	4749	C	N1-C2-O2	8.87	124.22	118.90
51	K	1078	C	C2-N1-C1'	8.85	128.54	118.80
51	K	1123	C	N3-C2-O2	-8.82	115.73	121.90
1	5	4413	C	C2-N1-C1'	8.77	128.45	118.80
1	5	931	C	C6-N1-C2	-8.77	116.79	120.30
51	K	853	C	N1-C2-O2	8.72	124.13	118.90
1	5	100	C	N1-C2-O2	8.54	124.03	118.90
51	K	1453	C	N1-C2-O2	8.44	123.96	118.90
51	K	1453	C	C2-N1-C1'	8.38	128.02	118.80
1	5	4119	C	N1-C2-O2	8.36	123.92	118.90
51	K	174	C	N3-C2-O2	-8.21	116.15	121.90
39	k	30	ASP	CB-CG-OD1	8.19	125.67	118.30
1	5	1381	U	C2-N1-C1'	8.13	127.45	117.70
1	5	1639	U	C2-N1-C1'	8.12	127.45	117.70
1	5	4119	C	C2-N1-C1'	8.11	127.72	118.80
1	5	1822	U	N1-C2-O2	8.04	128.43	122.80
1	5	972	C	N1-C2-O2	8.02	123.71	118.90
51	K	1261	C	C2-N1-C1'	8.00	127.60	118.80
1	5	1072	C	C6-N1-C1'	-7.98	111.22	120.80
1	5	4413	C	N1-C2-O2	7.98	123.69	118.90
51	K	1520	G	N3-C4-N9	7.96	130.78	126.00
51	K	1139	C	C2-N1-C1'	7.93	127.52	118.80
1	5	3594	C	N1-C2-O2	7.87	123.62	118.90
1	5	4413	C	N3-C2-O2	-7.86	116.39	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	5	449	C	C2-N1-C1'	7.85	127.44	118.80
1	5	1822	U	N3-C2-O2	-7.84	116.71	122.20
51	K	1139	C	N3-C2-O2	-7.84	116.41	121.90
51	K	1364	U	N1-C2-O2	7.82	128.27	122.80
51	K	1271	C	N1-C2-O2	7.77	123.56	118.90
1	5	499	G	C4-N9-C1'	7.76	136.59	126.50
1	5	453	G	C4-N9-C1'	7.73	136.55	126.50
1	5	3636	C	N3-C2-O2	-7.73	116.49	121.90
1	5	2023	C	N1-C2-O2	7.71	123.52	118.90
1	5	453	G	N3-C4-C5	-7.63	124.78	128.60
1	5	1236	C	N3-C2-O2	-7.63	116.56	121.90
3	8	128	C	N1-C2-O2	7.62	123.47	118.90
1	5	499	G	N3-C4-N9	7.60	130.56	126.00
51	K	1078	C	C6-N1-C2	-7.58	117.27	120.30
51	K	1261	C	N3-C2-O2	-7.56	116.61	121.90
51	K	1364	U	C2-N1-C1'	7.54	126.75	117.70
1	5	2499	C	N1-C2-O2	7.53	123.42	118.90
1	5	453	G	N3-C4-N9	7.53	130.52	126.00
1	5	687	U	N1-C2-O2	7.52	128.06	122.80
1	5	1639	U	N1-C2-O2	7.50	128.05	122.80
1	5	100	C	N3-C2-O2	-7.47	116.67	121.90
1	5	2015	U	C2'-C3'-O3'	7.46	125.91	109.50
51	K	1298	G	C4-N9-C1'	7.44	136.17	126.50
1	5	931	C	C5-C6-N1	7.38	124.69	121.00
51	K	1078	C	N3-C2-O2	-7.32	116.78	121.90
1	5	4305	G	C4-N9-C1'	7.31	136.00	126.50
51	K	578	C	N1-C2-O2	7.30	123.28	118.90
51	K	1298	G	N3-C4-N9	7.29	130.37	126.00
1	5	2097	U	C2-N1-C1'	7.27	126.42	117.70
1	5	1381	U	N1-C2-O2	7.26	127.88	122.80
1	5	961	G	N9-C4-C5	-7.25	102.50	105.40
51	K	183	G	C4-N9-C1'	7.25	135.92	126.50
1	5	1237	C	N1-C2-O2	7.25	123.25	118.90
51	K	1261	C	C6-N1-C2	-7.25	117.40	120.30
1	5	2097	U	N1-C2-O2	7.23	127.86	122.80
51	K	1303	C	N1-C2-O2	7.22	123.23	118.90
1	5	2819	U	N3-C2-O2	-7.21	117.15	122.20
1	5	2256	C	P-O3'-C3'	7.17	128.31	119.70
51	K	1298	G	N3-C4-C5	-7.17	125.01	128.60
1	5	2499	C	N3-C2-O2	-7.14	116.90	121.90
1	5	956	A	P-O3'-C3'	7.13	128.25	119.70
51	K	1364	U	N3-C2-O2	-7.10	117.23	122.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	5	2046	G	P-O3'-C3'	7.09	128.21	119.70
1	5	1612	G	N3-C4-N9	7.08	130.25	126.00
1	5	2107	C	P-O3'-C3'	7.08	128.20	119.70
1	5	5027	C	P-O3'-C3'	7.08	128.19	119.70
51	K	1303	C	C2-N1-C1'	7.07	126.57	118.80
1	5	1772	C	N3-C2-O2	-7.06	116.96	121.90
51	K	293	C	N1-C2-O2	7.04	123.13	118.90
1	5	1076	C	C2-N1-C1'	7.03	126.54	118.80
51	K	1139	C	C6-N1-C2	-7.03	117.49	120.30
1	5	1072	C	C6-N1-C2	-7.02	117.49	120.30
1	5	4889	G	P-O3'-C3'	7.01	128.12	119.70
51	K	130	G	C4-N9-C1'	7.01	135.62	126.50
1	5	4749	C	N3-C2-O2	-7.00	117.00	121.90
1	5	687	U	N3-C2-O2	-6.98	117.32	122.20
1	5	1822	U	C2-N1-C1'	6.98	126.07	117.70
1	5	4413	C	O4'-C1'-N1	6.97	113.78	108.20
1	5	1772	C	N1-C2-O2	6.96	123.08	118.90
1	5	2695	A	P-O3'-C3'	6.96	128.05	119.70
51	K	1520	G	C4-N9-C1'	6.95	135.54	126.50
51	K	853	C	N3-C2-O2	-6.95	117.03	121.90
1	5	1639	U	N3-C2-O2	-6.92	117.36	122.20
1	5	449	C	N3-C2-O2	-6.89	117.07	121.90
51	K	130	G	N3-C4-N9	6.88	130.13	126.00
51	K	1624	U	C2-N1-C1'	6.88	125.95	117.70
1	5	1612	G	N3-C4-C5	-6.87	125.17	128.60
1	5	4757	C	C2-N1-C1'	6.86	126.34	118.80
1	5	4413	C	C6-N1-C2	-6.85	117.56	120.30
1	5	1481	C	N1-C2-O2	6.84	123.00	118.90
1	5	499	G	N3-C4-C5	-6.84	125.18	128.60
51	K	688	U	P-O3'-C3'	6.83	127.89	119.70
51	K	1274	G	C4-N9-C1'	6.82	135.36	126.50
1	5	4871	C	C2-N1-C1'	6.79	126.27	118.80
1	5	3636	C	N1-C2-O2	6.79	122.97	118.90
51	K	1624	U	N3-C2-O2	-6.78	117.45	122.20
51	K	1057	C	C2-N1-C1'	6.77	126.25	118.80
1	5	2257	C	P-O3'-C3'	6.76	127.82	119.70
51	K	1298	G	C8-N9-C1'	-6.76	118.21	127.00
1	5	499	G	C8-N9-C1'	-6.76	118.21	127.00
1	5	2528	G	C4-N9-C1'	6.76	135.28	126.50
1	5	1236	C	N1-C2-O2	6.74	122.95	118.90
1	5	972	C	N3-C2-O2	-6.74	117.19	121.90
1	5	4709	U	C2-N1-C1'	6.71	125.75	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	5	4757	C	N1-C2-O2	6.71	122.92	118.90
1	5	4871	C	N1-C2-O2	6.69	122.92	118.90
1	5	3594	C	N3-C2-O2	-6.69	117.22	121.90
51	K	1453	C	N3-C2-O2	-6.68	117.22	121.90
1	5	3594	C	C6-N1-C2	-6.68	117.63	120.30
1	5	2528	G	N3-C4-N9	6.67	130.00	126.00
1	5	1612	G	C4-N9-C1'	6.67	135.17	126.50
49	2	4	U	N1-C2-O2	6.67	127.47	122.80
1	5	685	C	N1-C2-O2	6.66	122.89	118.90
1	5	4423	U	C2-N1-C1'	6.66	125.69	117.70
1	5	956	A	OP2-P-O3'	6.65	119.84	105.20
1	5	4714	C	N1-C2-O2	6.65	122.89	118.90
1	5	48	G	P-O3'-C3'	6.63	127.65	119.70
1	5	100	C	C6-N1-C1'	-6.61	112.86	120.80
51	K	1123	C	C2-N1-C1'	6.59	126.04	118.80
51	K	853	C	C6-N1-C1'	-6.58	112.90	120.80
1	5	1686	C	N1-C2-O2	6.58	122.85	118.90
1	5	100	C	C6-N1-C2	-6.58	117.67	120.30
1	5	2097	U	N3-C2-O2	-6.57	117.60	122.20
51	K	130	G	N3-C4-C5	-6.57	125.32	128.60
51	K	183	G	N3-C4-C5	-6.56	125.32	128.60
1	5	3741	C	N3-C2-O2	-6.55	117.32	121.90
1	5	4888	U	P-O3'-C3'	6.54	127.55	119.70
5	B	309	LEU	CA-CB-CG	6.53	130.32	115.30
51	K	1852	C	N1-C2-O2	6.52	122.81	118.90
1	5	4502	C	N1-C2-O2	6.52	122.81	118.90
1	5	2820	C	N1-C2-O2	6.52	122.81	118.90
51	K	1123	C	C6-N1-C2	-6.51	117.69	120.30
1	5	4171	C	N1-C2-O2	6.51	122.81	118.90
1	5	4305	G	N3-C4-N9	6.50	129.90	126.00
51	K	1689	C	C2-N1-C1'	6.50	125.95	118.80
1	5	50	C	N1-C2-O2	6.49	122.79	118.90
1	5	961	G	N3-C4-N9	6.49	129.90	126.00
1	5	2465	C	N1-C2-O2	6.49	122.79	118.90
1	5	1792	U	C2-N1-C1'	6.49	125.48	117.70
1	5	1481	C	C2-N1-C1'	6.48	125.93	118.80
1	5	4420	U	C6-N1-C1'	-6.48	112.13	121.20
1	5	4736	C	N1-C2-O2	6.47	122.78	118.90
1	5	1686	C	N3-C2-O2	-6.46	117.38	121.90
1	5	2011	C	N1-C2-O2	6.46	122.78	118.90
1	5	453	G	C8-N9-C1'	-6.46	118.61	127.00
1	5	4119	C	N3-C2-O2	-6.46	117.38	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
51	K	752	G	P-O3'-C3'	6.45	127.44	119.70
51	K	1274	G	N3-C4-N9	6.45	129.87	126.00
51	K	1274	G	N3-C4-C5	-6.44	125.38	128.60
1	5	4758	U	C2-N1-C1'	6.44	125.43	117.70
51	K	340	C	N1-C2-O2	6.43	122.76	118.90
1	5	489	C	N1-C2-O2	6.41	122.75	118.90
1	5	2023	C	C2-N1-C1'	6.41	125.85	118.80
51	K	1624	U	N1-C2-O2	6.40	127.28	122.80
1	5	1731	C	C2-N1-C1'	6.39	125.83	118.80
1	5	2819	U	N1-C2-O2	6.38	127.27	122.80
1	5	4305	G	N3-C4-C5	-6.37	125.41	128.60
1	5	1072	C	C5-C6-N1	6.37	124.18	121.00
1	5	2661	U	P-O3'-C3'	6.35	127.32	119.70
1	5	4946	U	N1-C2-O2	6.35	127.24	122.80
1	5	4229	U	N3-C2-O2	-6.35	117.76	122.20
51	K	183	G	N3-C4-N9	6.35	129.81	126.00
1	5	969	C	O4'-C1'-N1	6.33	113.27	108.20
51	K	356	C	C2-N1-C1'	6.33	125.77	118.80
1	5	4232	U	P-O3'-C3'	6.32	127.29	119.70
51	K	1689	C	N1-C2-O2	6.32	122.69	118.90
51	K	4	C	C2-N1-C1'	6.32	125.75	118.80
1	5	1812	C	C2-N1-C1'	6.32	125.75	118.80
1	5	2116	C	P-O3'-C3'	6.30	127.26	119.70
1	5	2528	G	N3-C4-C5	-6.30	125.45	128.60
1	5	1632	A	C2-N3-C4	6.29	113.74	110.60
1	5	4758	U	N1-C2-O2	6.27	127.19	122.80
1	5	1378	C	C6-N1-C2	-6.27	117.79	120.30
1	5	4237	C	C2-N1-C1'	6.27	125.69	118.80
1	5	1237	C	N3-C2-O2	-6.26	117.52	121.90
1	5	3594	C	C2-N1-C1'	6.26	125.69	118.80
1	5	4158	C	N3-C2-O2	-6.24	117.53	121.90
1	5	112	C	C2-N1-C1'	6.24	125.66	118.80
1	5	2465	C	N3-C2-O2	-6.22	117.55	121.90
1	5	1847	C	C2-N1-C1'	6.21	125.64	118.80
1	5	4749	C	C6-N1-C1'	-6.19	113.37	120.80
51	K	1271	C	N3-C2-O2	-6.19	117.57	121.90
51	K	1637	A	P-O3'-C3'	6.19	127.13	119.70
51	K	1057	C	N1-C2-O2	6.18	122.61	118.90
3	8	128	C	N3-C2-O2	-6.18	117.58	121.90
1	5	961	G	C4-C5-N7	6.17	113.27	110.80
51	K	1520	G	C8-N9-C4	-6.17	103.93	106.40
1	5	1210	C	C2-N1-C1'	6.17	125.59	118.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	5	2023	C	N3-C2-O2	-6.17	117.58	121.90
49	2	49	C	N1-C2-O2	6.15	122.59	118.90
51	K	118	C	N1-C2-O2	6.13	122.58	118.90
1	5	4305	G	C8-N9-C1'	-6.13	119.04	127.00
51	K	531	A	P-O3'-C3'	6.12	127.04	119.70
1	5	4881	U	C2-N1-C1'	6.11	125.03	117.70
49	2	4	U	N3-C2-O2	-6.09	117.94	122.20
51	K	1078	C	C5-C6-N1	6.09	124.04	121.00
1	5	989	U	N1-C2-O2	6.08	127.05	122.80
51	K	1271	C	C2-N1-C1'	6.07	125.48	118.80
51	K	151	C	N1-C2-O2	6.07	122.54	118.90
1	5	1807	C	C2-N1-C1'	6.07	125.48	118.80
1	5	3636	C	C6-N1-C2	-6.07	117.87	120.30
1	5	685	C	C2-N1-C1'	6.05	125.45	118.80
1	5	687	U	C2-N1-C1'	6.05	124.96	117.70
1	5	1210	C	N1-C2-O2	6.05	122.53	118.90
51	K	293	C	C2-N1-C1'	6.05	125.45	118.80
1	5	1692	C	C2-N1-C1'	6.04	125.44	118.80
1	5	1381	U	N3-C2-O2	-6.03	117.98	122.20
51	K	578	C	N3-C2-O2	-6.03	117.68	121.90
1	5	1485	C	C2-N1-C1'	6.02	125.42	118.80
51	K	1118	C	C2-N1-C1'	6.01	125.41	118.80
2	7	29	C	C2-N1-C1'	6.00	125.40	118.80
18	P	91	LEU	CA-CB-CG	6.00	129.10	115.30
51	K	14	C	C2-N1-C1'	6.00	125.40	118.80
51	K	183	G	C8-N9-C1'	-5.99	119.21	127.00
51	K	1423	C	N1-C2-O2	5.99	122.49	118.90
1	5	2867	C	C2-N1-C1'	5.98	125.38	118.80
1	5	1273	G	C4-N9-C1'	5.98	134.27	126.50
51	K	130	G	C8-N9-C1'	-5.97	119.24	127.00
1	5	972	C	C6-N1-C2	-5.97	117.91	120.30
1	5	684	G	P-O3'-C3'	5.96	126.86	119.70
51	K	1389	C	N1-C2-O2	5.96	122.48	118.90
51	K	624	C	C6-N1-C2	-5.95	117.92	120.30
1	5	1081	C	C2-N1-C1'	5.94	125.33	118.80
1	5	2266	C	P-O3'-C3'	5.94	126.83	119.70
1	5	4177	C	C2-N1-C1'	5.94	125.33	118.80
51	K	824	C	N1-C2-O2	5.94	122.46	118.90
51	K	659	G	C4-N9-C1'	5.94	134.22	126.50
1	5	3741	C	N1-C2-O2	5.93	122.46	118.90
1	5	4215	C	N1-C2-O2	5.93	122.46	118.90
51	K	174	C	N1-C2-O2	5.92	122.45	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	5	1485	C	N1-C2-O2	5.92	122.45	118.90
3	8	153	C	C2-N1-C1'	5.92	125.31	118.80
1	5	3778	U	N1-C2-O2	5.91	126.94	122.80
1	5	4476	C	C2-N1-C1'	5.91	125.31	118.80
1	5	4423	U	N3-C2-O2	-5.91	118.06	122.20
1	5	4656	A	P-O3'-C3'	5.91	126.79	119.70
1	5	4736	C	N3-C2-O2	-5.89	117.78	121.90
1	5	2093	A	P-O3'-C3'	5.89	126.77	119.70
1	5	4354	U	P-O3'-C3'	5.89	126.77	119.70
51	K	1358	U	N3-C2-O2	-5.89	118.08	122.20
51	K	1518	C	C2-N1-C1'	5.89	125.28	118.80
1	5	4423	U	N1-C2-O2	5.89	126.92	122.80
51	K	356	C	N1-C2-O2	5.88	122.43	118.90
1	5	930	G	P-O3'-C3'	5.88	126.75	119.70
1	5	4413	C	C6-N1-C1'	-5.88	113.75	120.80
1	5	4229	U	N1-C2-O2	5.87	126.91	122.80
51	K	1117	C	N1-C2-O2	5.87	122.42	118.90
1	5	4420	U	C5-C6-N1	5.86	125.63	122.70
3	8	124	U	P-O3'-C3'	5.86	126.73	119.70
1	5	2274	C	C2-N1-C1'	5.85	125.23	118.80
51	K	815	U	N3-C2-O2	-5.85	118.11	122.20
1	5	1835	G	P-O3'-C3'	5.84	126.71	119.70
51	K	1303	C	N3-C2-O2	-5.84	117.81	121.90
1	5	1671	U	N3-C2-O2	-5.84	118.11	122.20
1	5	3876	A	P-O3'-C3'	5.84	126.71	119.70
1	5	3739	C	N1-C2-O2	5.83	122.40	118.90
1	5	2117	G	C4-N9-C1'	5.83	134.08	126.50
1	5	2528	G	C8-N9-C1'	-5.83	119.42	127.00
1	5	4749	C	C6-N1-C2	-5.82	117.97	120.30
1	5	506	C	C2-N1-C1'	5.82	125.20	118.80
1	5	134	G	P-O3'-C3'	5.82	126.68	119.70
1	5	4952	G	N3-C4-C5	-5.81	125.69	128.60
51	K	1660	C	C2-N1-C1'	5.81	125.19	118.80
1	5	920	C	C2-N1-C1'	5.81	125.19	118.80
1	5	4758	U	N3-C2-O2	-5.81	118.14	122.20
1	5	115	C	C2-N1-C1'	5.79	125.16	118.80
1	5	4402	C	N1-C2-O2	5.79	122.37	118.90
1	5	2123	C	P-O3'-C3'	5.78	126.64	119.70
1	5	449	C	C6-N1-C2	-5.78	117.99	120.30
51	K	579	C	N1-C2-O2	5.78	122.37	118.90
51	K	1271	C	C6-N1-C2	-5.77	117.99	120.30
1	5	155	C	N3-C2-O2	-5.76	117.86	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	5	4964	C	N1-C2-O2	5.76	122.36	118.90
1	5	1381	U	C6-N1-C1'	-5.76	113.14	121.20
1	5	4303	C	C2-N1-C1'	5.76	125.14	118.80
1	5	245	C	P-O3'-C3'	5.76	126.61	119.70
1	5	1273	G	N3-C4-C5	-5.76	125.72	128.60
1	5	1074	G	N3-C4-N9	5.75	129.45	126.00
51	K	1453	C	C6-N1-C2	-5.75	118.00	120.30
51	K	1709	G	C4-N9-C1'	5.75	133.97	126.50
1	5	1804	A	P-O3'-C3'	5.75	126.60	119.70
1	5	458	C	N1-C2-O2	5.75	122.35	118.90
51	K	1261	C	C5-C6-N1	5.74	123.87	121.00
51	K	853	C	C6-N1-C2	-5.73	118.01	120.30
1	5	1428	U	N1-C2-O2	5.72	126.81	122.80
1	5	1273	G	N3-C4-N9	5.72	129.43	126.00
1	5	1792	U	N3-C2-O2	-5.72	118.19	122.20
1	5	4682	U	N1-C2-O2	5.72	126.80	122.80
49	2	4	U	C2-N1-C1'	5.72	124.56	117.70
1	5	1367	C	C2-N1-C1'	5.71	125.08	118.80
51	K	465	A	P-O3'-C3'	5.71	126.55	119.70
51	K	1358	U	N1-C2-O2	5.71	126.80	122.80
1	5	1792	U	N1-C2-O2	5.70	126.79	122.80
51	K	1274	G	C8-N9-C1'	-5.70	119.59	127.00
2	7	28	C	N1-C2-O2	5.70	122.32	118.90
1	5	451	C	P-O3'-C3'	5.69	126.53	119.70
51	K	614	C	P-O3'-C3'	5.69	126.53	119.70
1	5	4881	U	N1-C2-O2	5.69	126.78	122.80
1	5	1848	C	N1-C2-O2	5.69	122.31	118.90
57	y	36	LEU	CA-CB-CG	5.69	128.38	115.30
1	5	690	C	N1-C2-O2	5.68	122.31	118.90
1	5	943	A	P-O3'-C3'	5.68	126.52	119.70
1	5	4170	A	P-O3'-C3'	5.68	126.52	119.70
51	K	1453	C	C6-N1-C1'	-5.68	113.98	120.80
1	5	967	C	N1-C2-O2	5.67	122.30	118.90
1	5	1612	G	C8-N9-C1'	-5.67	119.63	127.00
1	5	1671	U	N1-C2-O2	5.67	126.77	122.80
1	5	4946	U	N3-C2-O2	-5.66	118.24	122.20
51	K	182	C	P-O3'-C3'	5.66	126.49	119.70
1	5	1429	C	N1-C2-O2	5.66	122.30	118.90
1	5	4612	C	N1-C2-O2	5.66	122.29	118.90
1	5	4482	U	N3-C2-O2	-5.65	118.25	122.20
51	K	531	A	OP1-P-O3'	5.65	117.63	105.20
51	K	4	C	N1-C2-O2	5.65	122.29	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	5	4682	U	N3-C2-O2	-5.64	118.25	122.20
1	5	4119	C	C6-N1-C1'	-5.64	114.03	120.80
1	5	4952	G	N3-C4-N9	5.63	129.38	126.00
1	5	1076	C	N1-C2-O2	5.62	122.28	118.90
51	K	1289	U	N1-C2-O2	5.62	126.74	122.80
51	K	870	A	P-O3'-C3'	5.61	126.43	119.70
1	5	4682	U	C2-N1-C1'	5.61	124.43	117.70
51	K	1742	C	C2-N1-C1'	5.61	124.97	118.80
1	5	4714	C	N3-C2-O2	-5.60	117.98	121.90
1	5	1232	G	P-O3'-C3'	5.60	126.42	119.70
1	5	690	C	C2-N1-C1'	5.60	124.96	118.80
51	K	1057	C	N3-C2-O2	-5.59	117.99	121.90
1	5	218	A	P-O3'-C3'	5.59	126.41	119.70
1	5	2083	C	P-O3'-C3'	5.58	126.40	119.70
1	5	1079	C	N1-C2-O2	5.58	122.25	118.90
51	K	1022	U	C2-N1-C1'	5.58	124.40	117.70
51	K	1116	C	N1-C2-O2	5.58	122.25	118.90
51	K	1078	C	C6-N1-C1'	-5.57	114.12	120.80
1	5	2820	C	N3-C2-O2	-5.56	118.01	121.90
1	5	972	C	C2-N1-C1'	5.55	124.90	118.80
1	5	1598	C	N1-C2-O2	5.54	122.23	118.90
1	5	4964	C	N3-C2-O2	-5.54	118.02	121.90
1	5	2410	C	C2-N1-C1'	5.53	124.89	118.80
1	5	2560	C	C2-N1-C1'	5.53	124.88	118.80
1	5	3657	U	N3-C2-O2	-5.53	118.33	122.20
51	K	1826	G	N3-C4-N9	5.53	129.32	126.00
1	5	1378	C	C5-C6-N1	5.52	123.76	121.00
1	5	2023	C	C6-N1-C2	-5.52	118.09	120.30
51	K	1551	U	C2-N1-C1'	5.52	124.33	117.70
51	K	1826	G	C4-N9-C1'	5.52	133.68	126.50
1	5	221	C	C2-N1-C1'	5.50	124.86	118.80
1	5	453	G	C2-N3-C4	5.50	114.65	111.90
1	5	1893	C	C2-N1-C1'	5.50	124.86	118.80
51	K	1073	U	N3-C2-O2	-5.50	118.35	122.20
1	5	4237	C	C6-N1-C2	-5.50	118.10	120.30
51	K	151	C	C2-N1-C1'	5.49	124.84	118.80
1	5	2704	C	N1-C2-O2	5.47	122.19	118.90
1	5	1359	G	C4-N9-C1'	5.46	133.60	126.50
1	5	1929	A	C4-N9-C1'	5.45	136.12	126.30
1	5	4952	G	C4-N9-C1'	5.45	133.59	126.50
1	5	2787	A	C2-N3-C4	5.45	113.33	110.60
1	5	1359	G	N7-C8-N9	5.45	115.82	113.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	5	2085	G	C4-N9-C1'	5.45	133.58	126.50
1	5	155	C	N1-C2-O2	5.44	122.17	118.90
1	5	685	C	N3-C2-O2	-5.44	118.09	121.90
50	3	49	C	N1-C2-O2	5.44	122.16	118.90
1	5	961	G	C8-N9-C1'	-5.43	119.93	127.00
51	K	151	C	C6-N1-C2	-5.43	118.13	120.30
1	5	4757	C	N3-C2-O2	-5.43	118.10	121.90
51	K	427	U	C2-N1-C1'	5.43	124.21	117.70
1	5	4560	C	N1-C2-O2	5.42	122.16	118.90
1	5	4627	U	N1-C2-O2	5.42	126.60	122.80
1	5	4749	C	O4'-C1'-N1	5.42	112.54	108.20
1	5	4171	C	N3-C2-O2	-5.42	118.11	121.90
1	5	100	C	O4'-C1'-N1	5.41	112.53	108.20
51	K	1709	G	N3-C4-N9	5.41	129.24	126.00
1	5	989	U	N3-C2-O2	-5.41	118.42	122.20
1	5	1458	C	N1-C2-O2	5.41	122.14	118.90
1	5	2117	G	N3-C4-N9	5.41	129.24	126.00
1	5	2117	G	N3-C4-C5	-5.41	125.90	128.60
1	5	2083	C	OP2-P-O3'	5.40	117.08	105.20
1	5	4482	U	N1-C2-O2	5.40	126.58	122.80
85	4	44	C	N1-C2-O2	5.40	122.14	118.90
1	5	4243	C	C6-N1-C2	-5.40	118.14	120.30
51	K	1298	G	O4'-C1'-N9	-5.39	103.89	108.20
1	5	2256	C	N1-C2-O2	5.39	122.14	118.90
1	5	1339	U	N1-C2-O2	5.39	126.57	122.80
1	5	2454	U	N3-C2-O2	-5.38	118.43	122.20
5	B	214	ASP	CB-CG-OD1	5.38	123.14	118.30
2	7	28	C	N3-C2-O2	-5.38	118.14	121.90
3	8	128	C	C2-N1-C1'	5.38	124.71	118.80
1	5	3772	U	C2-N1-C1'	5.37	124.15	117.70
51	K	168	C	N1-C2-O2	5.37	122.12	118.90
51	K	1118	C	N1-C2-O2	5.37	122.12	118.90
1	5	1656	U	N1-C2-O2	5.36	126.55	122.80
1	5	2470	C	N1-C2-O2	5.36	122.12	118.90
1	5	4171	C	C6-N1-C2	-5.36	118.16	120.30
1	5	1929	A	C2-N3-C4	5.36	113.28	110.60
1	5	1	C	P-O3'-C3'	5.35	126.12	119.70
1	5	3778	U	N3-C2-O2	-5.35	118.45	122.20
1	5	5022	U	P-O3'-C3'	5.35	126.12	119.70
51	K	1314	U	C2-N1-C1'	5.35	124.12	117.70
1	5	2072	C	C6-N1-C2	-5.35	118.16	120.30
1	5	4881	U	N3-C2-O2	-5.34	118.46	122.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	5	2257	C	OP1-P-O3'	5.34	116.95	105.20
1	5	245	C	N1-C2-O2	5.34	122.10	118.90
1	5	4502	C	N3-C2-O2	-5.34	118.16	121.90
51	K	624	C	C5-C6-N1	5.33	123.67	121.00
1	5	449	C	C6-N1-C1'	-5.33	114.40	120.80
1	5	48	G	OP2-P-O3'	5.33	116.92	105.20
1	5	1367	C	N1-C2-O2	5.33	122.10	118.90
51	K	1395	C	P-O3'-C3'	5.33	126.09	119.70
1	5	4177	C	C6-N1-C2	-5.32	118.17	120.30
2	7	29	C	N1-C2-O2	5.32	122.09	118.90
1	5	1848	C	C2-N1-C1'	5.32	124.65	118.80
1	5	961	G	N1-C2-N3	-5.32	120.71	123.90
51	K	630	U	C2-N1-C1'	5.31	124.07	117.70
1	5	4171	C	C2-N1-C1'	5.31	124.64	118.80
1	5	1915	C	N1-C2-O2	5.31	122.08	118.90
51	K	537	C	C2-N1-C1'	5.30	124.63	118.80
51	K	1057	C	C6-N1-C2	-5.30	118.18	120.30
1	5	647	G	C4-N9-C1'	5.30	133.39	126.50
51	K	14	C	C6-N1-C2	-5.30	118.18	120.30
51	K	823	U	C2-N1-C1'	5.30	124.06	117.70
51	K	532	C	P-O3'-C3'	5.30	126.06	119.70
1	5	2661	U	OP1-P-O3'	5.29	116.85	105.20
1	5	1639	U	C6-N1-C1'	-5.29	113.79	121.20
1	5	2904	U	C2-N1-C1'	5.29	124.05	117.70
1	5	2726	G	C4-N9-C1'	5.29	133.38	126.50
1	5	489	C	N3-C2-O2	-5.29	118.20	121.90
1	5	3622	C	N1-C2-O2	5.29	122.07	118.90
1	5	2704	C	C2-N1-C1'	5.29	124.61	118.80
51	K	1073	U	N1-C2-O2	5.28	126.49	122.80
1	5	1853	G	C4-N9-C1'	5.27	133.35	126.50
51	K	1139	C	C5-C6-N1	5.27	123.64	121.00
1	5	458	C	C2-N1-C1'	5.27	124.59	118.80
51	K	340	C	N3-C2-O2	-5.27	118.21	121.90
51	K	369	C	N1-C2-O2	5.26	122.06	118.90
1	5	961	G	C5-C6-N1	5.26	114.13	111.50
1	5	1686	C	C6-N1-C2	-5.26	118.20	120.30
1	5	30	C	C2-N1-C1'	5.25	124.58	118.80
1	5	2499	C	C6-N1-C2	-5.25	118.20	120.30
51	K	983	A	N3-C4-N9	5.25	131.60	127.40
1	5	654	C	C6-N1-C2	-5.25	118.20	120.30
1	5	3778	U	C2-N1-C1'	5.25	124.00	117.70
1	5	4162	C	N1-C2-O2	5.25	122.05	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	5	1241	C	OP1-P-O3'	5.24	116.74	105.20
1	5	3772	U	N3-C2-O2	-5.24	118.53	122.20
51	K	1061	U	P-O3'-C3'	5.24	125.98	119.70
1	5	3772	U	N1-C2-O2	5.23	126.46	122.80
1	5	50	C	N3-C2-O2	-5.23	118.24	121.90
1	5	3673	C	N1-C2-O2	5.23	122.04	118.90
1	5	266	C	O5'-P-OP2	-5.23	101.00	105.70
1	5	1211	G	P-O3'-C3'	5.22	125.97	119.70
1	5	1807	C	N1-C2-O2	5.22	122.03	118.90
1	5	4871	C	C6-N1-C1'	-5.22	114.53	120.80
51	K	815	U	N1-C2-O2	5.22	126.45	122.80
1	5	1214	C	N1-C2-O2	5.22	122.03	118.90
51	K	142	C	N1-C2-O2	5.22	122.03	118.90
1	5	3670	C	N1-C2-O2	5.21	122.03	118.90
51	K	1518	C	N1-C2-O2	5.21	122.03	118.90
51	K	1798	C	C6-N1-C2	-5.21	118.21	120.30
1	5	1339	U	N3-C2-O2	-5.21	118.55	122.20
51	K	1364	U	C5-C6-N1	5.21	125.31	122.70
51	K	659	G	C8-N9-C1'	-5.21	120.23	127.00
1	5	2011	C	N3-C2-O2	-5.21	118.25	121.90
8	E	46	LEU	CA-CB-CG	5.21	127.28	115.30
1	5	932	A	C4-N9-C1'	5.20	135.66	126.30
1	5	3926	C	C2-N1-C1'	5.20	124.52	118.80
1	5	2362	U	N3-C2-O2	-5.20	118.56	122.20
1	5	1859	C	N1-C2-O2	5.19	122.02	118.90
1	5	2860	C	N1-C2-O2	5.19	122.02	118.90
51	K	1397	U	N3-C2-O2	-5.19	118.56	122.20
3	8	54	C	N1-C2-O2	5.19	122.01	118.90
1	5	1325	C	N1-C2-O2	5.18	122.01	118.90
1	5	2096	G	C4-N9-C1'	5.18	133.24	126.50
1	5	1633	G	P-O3'-C3'	5.18	125.92	119.70
51	K	1389	C	N3-C2-O2	-5.18	118.27	121.90
1	5	2089	G	N3-C4-N9	5.18	129.11	126.00
28	Z	30	ASP	CB-CG-OD1	5.17	122.96	118.30
1	5	486	C	P-O3'-C3'	5.17	125.91	119.70
1	5	1428	U	N3-C2-O2	-5.17	118.58	122.20
51	K	183	G	C2-N3-C4	5.17	114.49	111.90
51	K	1289	U	N3-C2-O2	-5.17	118.58	122.20
51	K	1624	U	O4'-C1'-N1	5.17	112.34	108.20
1	5	3882	C	C2-N1-C1'	5.17	124.49	118.80
1	5	2502	G	P-O3'-C3'	5.17	125.90	119.70
1	5	4942	C	C2-N1-C1'	5.17	124.48	118.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	5	657	C	N3-C2-O2	-5.16	118.29	121.90
1	5	2096	G	N3-C4-C5	-5.16	126.02	128.60
45	r	20	ARG	CA-CB-CG	5.16	124.75	113.40
50	3	8	U	C2-N1-C1'	5.16	123.89	117.70
1	5	1241	C	P-O3'-C3'	5.16	125.89	119.70
51	K	1331	C	N1-C2-O2	5.16	121.99	118.90
1	5	690	C	C6-N1-C2	-5.15	118.24	120.30
51	K	293	C	N3-C2-O2	-5.15	118.29	121.90
51	K	687	C	N1-C2-O2	5.15	121.99	118.90
1	5	125	C	P-O3'-C3'	5.15	125.88	119.70
51	K	1709	G	N3-C4-C5	-5.14	126.03	128.60
3	8	135	C	C2-N1-C1'	5.14	124.45	118.80
1	5	218	A	OP1-P-O3'	5.13	116.50	105.20
2	7	28	C	C6-N1-C2	-5.13	118.25	120.30
51	K	914	U	C2-N1-C1'	5.13	123.86	117.70
51	K	93	U	N1-C2-O2	5.13	126.39	122.80
1	5	4119	C	C6-N1-C2	-5.13	118.25	120.30
51	K	1397	U	N1-C2-O2	5.13	126.39	122.80
1	5	515	C	C5-C6-N1	5.12	123.56	121.00
1	5	1848	C	C6-N1-C2	-5.12	118.25	120.30
3	8	2	G	C4-N9-C1'	5.11	133.15	126.50
3	8	64	U	N3-C2-O2	-5.11	118.62	122.20
1	5	250	C	C2-N1-C1'	5.11	124.42	118.80
1	5	2532	C	C2-N1-C1'	5.11	124.42	118.80
1	5	2572	C	C2-N1-C1'	5.11	124.42	118.80
1	5	3594	C	C5-C6-N1	5.10	123.55	121.00
51	K	295	C	C2-N1-C1'	5.10	124.41	118.80
1	5	1816	C	C5-C6-N1	5.10	123.55	121.00
1	5	2362	U	N1-C2-O2	5.09	126.37	122.80
1	5	2856	C	N1-C2-O2	5.09	121.96	118.90
1	5	2502	G	OP1-P-O3'	5.09	116.40	105.20
1	5	275	C	P-O3'-C3'	5.09	125.81	119.70
51	K	1595	U	N1-C2-O2	5.09	126.36	122.80
1	5	1296	G	P-O3'-C3'	5.09	125.80	119.70
1	5	1731	C	C5-C6-N1	5.09	123.54	121.00
1	5	4237	C	C5-C6-N1	5.09	123.54	121.00
1	5	489	C	C2-N1-C1'	5.08	124.39	118.80
51	K	442	C	C5-C6-N1	5.08	123.54	121.00
51	K	1389	C	C2-N1-C1'	5.08	124.39	118.80
1	5	5027	C	N1-C2-O2	5.07	121.94	118.90
50	3	74	C	C2-N1-C1'	5.07	124.38	118.80
3	8	55	U	N3-C2-O2	-5.07	118.65	122.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	5	1694	C	C6-N1-C2	-5.07	118.27	120.30
1	5	515	C	C2-N1-C1'	5.06	124.37	118.80
1	5	4627	U	N3-C2-O2	-5.06	118.66	122.20
1	5	187	U	P-O3'-C3'	5.06	125.77	119.70
1	5	2410	C	C6-N1-C2	-5.06	118.28	120.30
49	2	33	U	C2-N1-C1'	5.06	123.77	117.70
51	K	887	U	C2-N1-C1'	5.06	123.77	117.70
1	5	2274	C	C6-N1-C2	-5.06	118.28	120.30
1	5	647	G	N3-C4-N9	5.05	129.03	126.00
1	5	919	C	C2-N1-C1'	5.05	124.36	118.80
1	5	1656	U	N3-C2-O2	-5.05	118.67	122.20
1	5	5059	C	P-O3'-C3'	5.04	125.75	119.70
1	5	1280	C	C6-N1-C2	-5.04	118.28	120.30
1	5	4613	C	N1-C2-O2	5.04	121.92	118.90
1	5	506	C	C5-C6-N1	5.04	123.52	121.00
51	K	578	C	C6-N1-C2	-5.03	118.29	120.30
1	5	4885	U	P-O3'-C3'	5.02	125.72	119.70
1	5	1295	C	C2-N1-C1'	5.02	124.32	118.80
51	K	1798	C	C5-C6-N1	5.02	123.51	121.00
49	2	39	U	P-O3'-C3'	5.02	125.72	119.70
51	K	1067	C	C2-N1-C1'	5.02	124.32	118.80
1	5	936	C	N1-C2-O2	5.01	121.91	118.90
1	5	2008	U	C2-N1-C1'	5.01	123.72	117.70
10	G	146	LEU	CA-CB-CG	5.01	126.83	115.30
2	7	102	U	N1-C2-O2	5.01	126.31	122.80
51	K	1185	C	N1-C2-O2	5.01	121.91	118.90
51	K	1649	U	N1-C2-O2	5.01	126.31	122.80
1	5	2410	C	C5-C6-N1	5.01	123.50	121.00
1	5	282	C	N1-C2-O2	5.01	121.90	118.90
51	K	1271	C	C5-C6-N1	5.01	123.50	121.00
1	5	4194	U	C2-N1-C1'	5.00	123.71	117.70

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

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Mol	Chain	Res	Type	Group
23	U	27	HIS	Peptide
67	VV	61	GLN	Mainchain,Peptide
34	f	106	TYR	Peptide

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	5	78486	0	39654	540	0
2	7	2558	0	1296	17	0
3	8	3314	0	1683	26	0
4	A	1868	0	1959	43	0
5	B	3148	0	3267	53	0
6	C	2883	0	3053	37	0
7	D	2386	0	2419	30	0
8	E	1898	0	2035	32	0
9	F	1870	0	1994	35	0
10	G	1934	0	2087	22	0
11	H	1516	0	1597	20	0
12	I	1655	0	1704	25	0
13	J	1353	0	1386	14	0
14	L	1703	0	1820	21	0
15	M	1137	0	1211	15	0
16	N	1701	0	1749	30	0
17	O	1638	0	1777	24	0
18	P	1242	0	1274	17	0
19	Q	1506	0	1623	15	0
20	R	1508	0	1664	17	0
21	S	1454	0	1496	24	0
22	T	1298	0	1366	21	0
23	U	808	0	831	8	0
24	V	979	0	1039	17	0
25	W	528	0	541	8	0
26	X	976	0	1053	9	0
27	Y	1115	0	1205	19	0
28	Z	1107	0	1182	13	0
29	a	1162	0	1209	0	0
30	b	609	0	650	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
31	c	732	0	769	0	0
32	d	888	0	930	0	0
33	e	1053	0	1147	0	0
34	f	876	0	912	0	0
35	g	906	0	998	0	0
36	h	1013	0	1147	0	0
37	i	830	0	916	0	0
38	j	705	0	737	0	0
39	k	569	0	637	0	0
40	l	444	0	483	0	0
41	m	429	0	465	0	0
42	n	222	0	264	0	0
43	o	851	0	921	0	0
44	p	708	0	757	0	0
45	r	1001	0	1060	0	0
46	s	1523	0	1577	0	0
47	t	1238	0	1295	0	0
48	1	204	0	193	24	0
49	2	1614	0	821	26	0
50	3	1597	0	813	6	0
51	K	36248	0	18309	300	0
52	q	1710	0	1708	0	0
53	u	1729	0	1803	0	0
54	v	1716	0	1806	0	0
55	x	2076	0	2177	0	0
56	z	1923	0	2089	0	0
57	y	1488	0	1582	0	0
58	CC	1686	0	1772	22	0
59	XX	1525	0	1640	18	0
60	EE	1175	0	1249	16	0
61	QQ	1202	0	1289	7	0
62	MM	1016	0	1039	14	0
63	UU	1128	0	1195	16	0
64	YY	1068	0	1121	10	0
65	HH	636	0	637	7	0
66	TT	1034	0	1080	15	0
67	VV	1098	0	1167	20	0
68	NN	1011	0	1083	14	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	20	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
73	BB	1471	0	1522	20	0
74	SS	810	0	836	11	0
75	RR	908	0	939	8	0
76	9	997	0	1045	12	0
77	II	1190	0	1249	24	0
78	PP	1097	0	1132	15	0
79	GG	795	0	862	15	0
80	OO	598	0	656	7	0
81	FF	488	0	514	8	0
82	w	459	0	452	0	0
83	0	555	0	567	10	0
84	6	2436	0	2393	34	0
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	1484	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 (1484) 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:C8	1:5:2017:A:H5'	1.99	0.97
51:K:1726:G:H1	51:K:1808:U:H3	0.99	0.96
1:5:2017:A:H8	1:5:2017:A:H5'	1.30	0.94
1:5:4451:G:O4'	48:1:256:TRP:NE1	2.02	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
1:5:3909:C:HO2'	49:2:76:A:HO2'	0.97	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	0.77
51:K:1718:G:N2	51:K:1815:A:H62	1.82	0.75
51:K:322:C:H5''	51:K:322:C:C6	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
1:5:3907:G:HO2'	1:5:3909:C:H5	1.34	0.73
51:K:1718:G:H21	51:K:1815:A:N6	1.86	0.73
49:2:1:G:C6	49:2:73:A:N1	2.56	0.72
8:E:171:VAL:HB	8:E:183:ARG:O	1.89	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
1:5:4451:G:C8	48:1:256:TRP:HD1	2.08	0.71
12:I:48:LEU:HB2	12:I:140:THR:O	1.91	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
51:K:1033:G:H1	51:K:1080:A:HO2'	1.40	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
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
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
84:6:87:LEU:HB2	84:6:101:PHE:HB2	1.76	0.67
1:5:1516:G:HO2'	14:L:18:TRP:HE1	1.40	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
51:K:1230:C:HO2'	51:K:1665:G:H1	1.43	0.66
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
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
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
84:6:107:ASP:HB2	84:6:125:ARG:HD2	1.80	0.63
65:HH:40:ASP:HB2	65:HH:47:ASN:HD21	1.63	0.63
14:L:31:ARG:HG2	14:L:34:ARG:HH21	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:5:3868:G:H22	1:5:3900:G:H1'	1.64	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
49:2:34:C:N3	85:4:51:G:N2	2.47	0.61
2:7:28:C:H1'	2:7:54:A:H61	1.65	0.61
6:C:134:PRO:HD3	20:R:71:ARG:HE	148.07	0.61
13:J:167:GLN:HA	13:J:172:GLY:H	1.65	0.61
1:5:1726:U:H3	1:5:1836:G:H1	1.48	0.61
1:5:959:G:H21	8:E:121:LEU:H	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
1:5:4910:G:H4'	5:B:95:THR:HG22	1.83	0.61
58:CC:165:GLN:HE22	58:CC:195:LEU:HD11	1.64	0.61
51:K:639:C:H2'	51:K:640:A:H8	1.66	0.61
1:5:4871:C:H42	21:S:157:ARG:HE	1.49	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
22:T:4:THR:O	22:T:9:ARG:NH1	2.35	0.60
65:HH:31:SER:HA	65:HH:55:ILE:O	2.02	0.60
51:K:944:A:N6	51:K:982:G:H1	1.99	0.60
49:2:30:G:H1	49:2:40:C:H42	1.49	0.60
1:5:3697:U:H5''	1:5:3698:G:H5'	1.83	0.60
1:5:4688:C:HO2'	11:H:155:SER:HG	1.50	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:1533:A:N6	51:K:1602:U:C2	2.70	0.60
51:K:957:A:H3'	51:K:958:G:H21	1.67	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
51:K:1091:C:HO2'	66:TT:2:VAL:N	1.98	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
78:PP:124:THR:HG23	78:PP:127:GLY:H	1.67	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
24:V:70:PRO:HG2	51:K:1724:A:H5''	1.82	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
84:6:10:THR:HG22	84:6:308:ARG:HG2	1.84	0.59
2:7:6:C:O2'	7:D:50:ARG:NH1	2.36	0.59
51:K:1854:U:OP1	62:MM:150:ARG:NH1	2.36	0.59
20:R:102:LEU:HD22	20:R:138:LEU:HD13	1.84	0.59
1:5:1524:A:H61	1:5:1651:G:H22	1.50	0.59
83:0:107:LYS:HB2	83:0:115:SER:HB3	1.84	0.59
1:5:2335:C:H2'	1:5:2336:G:H8	1.67	0.59
1:5:2777:G:H5''	1:5:2778:G:H5'	1.84	0.59
60:EE:60:CYS:HG	60:EE:114:SER:HG	1.51	0.59
1:5:3892:U:O2'	18:P:80:GLN:NE2	2.36	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
18:P:133:HIS:CG	48:1:246:LEU:HD21	2.38	0.58
1:5:3907:G:N2	48:1:259:LEU:O	2.36	0.58
51:K:1398:G:O2'	84:6:88:ARG:NH2	2.36	0.58
4:A:234:LYS:HG2	4:A:238:ILE:HD12	1.85	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
84:6:256:ILE:HB	84:6:270:LEU:HB2	1.85	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
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
79:GG:60:THR:HG22	79:GG:83:ARG:HG2	1.84	0.58
51:K:1014:G:N2	70:JJ:51:GLN:OE1	2.36	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
1:5:2458:C:H5''	16:N:67:ARG:HD2	1.86	0.58
1:5:404:U:O3'	27:Y:87:ARG:NH1	2.37	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
51:K:1854:U:H2'	51:K:1855:G:H8	1.67	0.58
51:K:925:G:OP1	61:QQ:121:ARG:NH2	2.37	0.58
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
84:6:11:LEU:HB2	84:6:307:VAL:HB	1.85	0.57
9:F:95:ILE:HA	9:F:121:ASN:O	2.03	0.57
77:II:14:ARG:HE	77:II:17:ASN:HA	1.68	0.57
1:5:2699:C:H5''	20:R:16:ARG:HH22	1.68	0.57
76:9:81:ARG:NH1	76:9:98:ASN:OD1	2.35	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
1:5:35:U:O2'	1:5:1525:A:N1	2.38	0.57
84:6:152:SER:HG	84:6:168:CYS:HG	1.48	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
3:8:52:A:OP1	14:L:21:ARG:NH1	55.54	0.57
9:F:151:SER:OG	9:F:247:ARG:NH2	2.38	0.57
1:5:4761:G:OP2	17:O:12:ARG:NH2	2.38	0.57
1:5:933:G:H2'	1:5:940:C:H41	1.69	0.57
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
21:S:80:ILE:HD11	21:S:126:ILE:HD12	1.84	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
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
51:K:444:G:OP2	58:CC:47:ARG:NH2	2.38	0.56
9:F:129:LYS:HE2	9:F:133:ASN:HD21	1.70	0.56
68:NN:55:ILE:HG12	68:NN:75:ILE:HG12	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:5:2457:G:OP1	16:N:65:ARG:NH1	2.38	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
1:5:2345:G:N7	4:A:9:ARG:NH1	67.42	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
51:K:986:G:OP2	51:K:988:C:N4	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
3:8:22:U:OP1	27:Y:11:ARG:NH2	2.39	0.56
51:K:84:A:H5''	68:NN:122:LYS:HD2	1.88	0.56
20:R:42:ARG:HA	20:R:45:ILE:HD12	1.88	0.56
1:5:416:U:O2'	1:5:2309:G:N2	2.38	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
1:5:1571: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
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
1:5:343:C:O2'	13:J:75:ARG:NH2	139.26	0.56
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
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
1:5:74:G:O6	14:L:103:ARG:NH2	2.39	0.56
25:W:44:ARG:NH1	79:GG:78:ASP:OD2	139.93	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
1:5:4944:C:O2	1:5:4945:G:N2	2.39	0.56
1:5:1621:A:HO2'	4:A:14:SER:HG	1.53	0.56
1:5:3657:U:OP1	4:A:245:ARG:NH1	2.39	0.56
1:5:2274:C:H5'	6:C:312:ARG:HB2	1.87	0.56
12:I:16:PRO:HA	12:I:95:HIS:HD2	1.71	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
60:EE:74:SER:O	60:EE:90:ARG:NH1	2.39	0.56
51:K:442:C:N4	51:K:449:A:H62	2.02	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
74:SS:20:VAL:HA	74:SS:69:TRP:O	2.05	0.56
67:VV:84:PHE:H	67:VV:121:LYS:HA	1.71	0.56
59:XX:136:ARG:NH1	59:XX:159:PHE:O	2.39	0.56
76:9:44:ARG:NH1	76:9:48:GLY:O	2.39	0.56
51:K:492:C:OP2	68:NN:107:ARG:NH2	2.38	0.56
1:5:1866:U:OP1	12:I:4:ARG:NH2	2.38	0.55
1:5:248:C:O2	27:Y:121:ARG:NH2	2.39	0.55
79:GG:94:PRO:HD2	79:GG:97:ILE:HD12	1.87	0.55
51:K:1036:A:N3	51:K:1844:U:O2'	2.40	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
5:B:48:GLY:HA3	5:B:81:THR:HG22	1.88	0.55
51:K:1617:G:O6	76:9:43:ARG:NH1	2.39	0.55
7:D:41:LYS:NZ	22:T:32:ARG:O	2.38	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
1:5:959:G:O2'	8:E:119:ARG:O	2.25	0.55
84:6:244:ASN:ND2	84:6:294:ASP:O	2.39	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
1:5:4768:G:H5'	17:O:176:ARG:HH12	1.71	0.55
69:ZZ:11:ALA:HB3	69:ZZ:33:ASP:HB2	1.87	0.55
1:5:109:G:OP2	14:L:74:ARG:NH2	2.39	0.55
3:8:63:U:O2'	11:H:52:LYS:NZ	161.38	0.55
27:Y:59:ARG:HB2	27:Y:103:LYS:HD2	1.89	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
1:5:726:G:OP1	9:F:75:ARG:NH2	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
48:1:260:MET:O	49:2:76:A:H4'	2.05	0.55
1:5:67:C:OP2	1:5:312:G:N2	2.40	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
63:UU:35:ASN:HD21	63:UU:72:VAL:HB	1.72	0.55
3:8:75:G:OP2	27:Y:74:TYR:OH	2.24	0.55
1:5:4419:U:OP1	1:5:4421:C:N4	2.40	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:5:1306:C:H2'	1:5:1307:A:H8	1.72	0.55
1:5:436:C:H2'	1:5:437:G:H8	1.72	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
1:5:1914:C:H4'	17:O:89:PRO:HD3	1.88	0.55
51:K:1864:U:H3'	69:ZZ:5:ARG:HH22	1.72	0.55
1:5:1550:G:H1	1:5:1578:U:H3	1.54	0.54
1:5:730:G:H22	1:5:939:G:H22	1.55	0.54
51:K:1599:U:OP2	80:OO:46:ASN:ND2	2.40	0.54
51:K:308:G:H3'	51:K:309:G:C5'	2.38	0.54
23:U:65:ARG:HE	23:U:67:LYS:H	1.55	0.54
1:5:2280:G:N2	1:5:2281:U:O4	2.40	0.54
7:D:50:ARG:NH1	7:D:72:ASP:OD2	2.38	0.54
6:C:61:GLN:O	13:J:52:LYS:NZ	103.54	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
27:Y:10:ASP:HB3	27:Y:13:LYS:HB2	1.90	0.54
1:5:431:G:H1'	1:5:3889:G:H5'	1.88	0.54
59:XX:170:PRO:O	59:XX:175:ARG:NH1	2.40	0.54
1:5:3908:A:N7	1:5:4449:A:N6	2.56	0.54
6:C:62:THR:HG21	6:C:86:ARG:HH21	1.72	0.54
72:DD:148:LYS:NZ	72:DD:150:MET:SD	2.80	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
74:SS:59:LYS:HB3	74:SS:70:TYR:HB2	1.88	0.54
3:8:134:G:H5''	26:X:63:LYS:HD2	1.89	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
1:5:382:G:H4'	1:5:407:A:H61	1.72	0.54
51:K:444:G:H3'	58:CC:47:ARG:HH12	1.71	0.54
17:O:109:PRO:HB2	17:O:111:PRO:HD2	1.90	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
1:5:1320:U:O2'	1:5:1891:A:N1	2.34	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
51:K:1596:U:OP2	80:OO:85:ARG:NH2	2.36	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
21:S:143:LYS:HA	21:S:146:HIS:HD1	1.71	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
6:C:65:GLU:HB3	6:C:80:ARG:HD3	1.90	0.54
51:K:1012:A:O2'	51:K:1129:G:N2	2.35	0.54
19:Q:67:ILE:HD12	19:Q:96:PRO:HD2	1.90	0.54
49:2:1:G:N1	49:2:73:A:C6	2.76	0.54
1:5:419:A:N3	1:5:1332:C:O2'	2.39	0.54
3:8:51:U:OP2	14:L:21:ARG:NH2	61.20	0.54
81:FF:29:GLN:HE22	81:FF:67:ARG:HG3	1.73	0.54
51:K:1087:A:OP2	69:ZZ:8:ASN:ND2	2.41	0.54
15:M:11:ARG:HB3	15:M:27:ILE:HD12	1.89	0.54
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
83:0:116:ARG:NH1	83:0:120:GLU:OE2	2.42	0.53
1:5:717:U:H3	1:5:951:G:H1	1.56	0.53
3:8:122:G:H21	3:8:128:C:H5	1.56	0.53
3:8:27:U:H4'	6:C:53:ALA:HB3	1.90	0.53
1:5:151:G:N7	10:G:141:ASN:ND2	2.57	0.53
51:K:930:C:O2'	51:K:1104:G:OP1	2.27	0.53
78:PP:76:THR:HB	78:PP:94:ARG:HB3	1.91	0.53
1:5:2725:A:N6	20:R:88:ARG:O	2.42	0.53
1:5:2647:A:H62	1:5:2686:G:H8	1.56	0.53
1:5:279:A:O2'	16:N:14:LYS:NZ	2.41	0.53
1:5:2706:G:N2	1:5:2709:C:OP2	2.42	0.53
6:C:329:ASN:ND2	9:F:190:GLU:OE2	2.41	0.53
1:5:967:C:H5'	8:E:106:ARG:HH22	1.73	0.53
11:H:166:THR:OG1	11:H:168:LYS:NZ	2.41	0.53
66:TT:60:LYS:NZ	70:JJ:23:ARG:O	2.42	0.53
23:U:24:ASP:HB3	23:U:69:LYS:HG3	1.91	0.53
1:5:1518:A:H61	14:L:19:GLN:HE22	1.57	0.53
1:5:963:G:OP2	20:R:107:ARG:NH2	170.72	0.53
51:K:1086:G:OP2	69:ZZ:12:LYS:NZ	2.40	0.53
1:5:68:U:OP1	16:N:178:HIS:ND1	2.34	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:5:976:G:OP2	8:E:55:ARG:NH1	2.37	0.53
4:A:95:GLN:O	4:A:100:ASN:ND2	2.41	0.53
72:DD:140:GLY:HA3	72:DD:182:LEU:HG	1.90	0.53
72:DD:70:THR:HG22	72:DD:86:LEU:HD13	1.90	0.53
69:ZZ:11:ALA:O	69:ZZ:15:ARG:NH2	2.40	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
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
51:K:70:G:O2'	51:K:79:A:N6	2.42	0.53
3:8:141:C:O2'	16:N:136:ASP:OD2	2.26	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
1:5:373:G:HO2'	1:5:1645:C:HO2'	1.57	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
70:JJ:56:CYS:SG	70:JJ:57:VAL:N	2.81	0.53
51:K:934:G:O6	51:K:1008:A:N1	2.42	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
62:MM:56:VAL:HG12	62:MM:81:VAL:HG23	1.91	0.53
1:5:2589:C:HO2'	1:5:2766:A:HO2'	1.55	0.52
1:5:3709:U:HO2'	1:5:3710:G:H8	1.56	0.52
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
51:K:1227:G:N2	51:K:1635:C:O2'	2.42	0.52
19:Q:82:VAL:HG12	19:Q:84:GLY:H	1.74	0.52
72:DD:75:LYS:NZ	74:SS:34:GLU:OE2	2.39	0.52
24:V:95:PHE:O	25:W:20:ARG:HB3	2.10	0.52
1:5:2459:G:N2	1:5:2462:C:OP2	2.42	0.52
1:5:499:G:OP2	1:5:501:C:N4	2.37	0.52
84:6:23:THR:HG22	84:6:31:ILE:HD11	1.92	0.52
51:K:1201:U:HO2'	51:K:1358:U:HO2'	1.56	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
1:5:1795:A:N3	2:7:79:U:O2'	2.42	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:5:4618:G:H5'	24:V:15:ARG:HB2	1.91	0.52
84:6:79:LEU:HD21	84:6:87:LEU:HB3	1.90	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
51:K:106:C:H2'	51:K:107:A:H8	1.74	0.52
51:K:1231:C:O2'	51:K:1253:A:N6	2.41	0.52
51:K:55:U:H6	51:K:90:G:H21	1.57	0.52
26:X:110:LYS:NZ	26:X:121:VAL:O	2.42	0.52
1:5:4523:A:O3'	5:B:246:ARG:NH1	2.42	0.52
84:6:31:ILE:HG22	84:6:43:TRP:HB2	1.92	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
79:GG:26:SER:HB3	79:GG:32:LEU:HD22	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
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
51:K:1610:G:N7	77:II:132:ARG:NH2	2.58	0.52
51:K:1658:G:OP2	51:K:1660:C:N4	2.40	0.52
51:K:99:A:H61	51:K:433:A:H1'	1.74	0.52
28:Z:36:ARG:NH1	28:Z:38:TYR:OH	2.39	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
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
72:DD:51:LEU:HG	72:DD:91:VAL:HG22	1.92	0.52
9:F:133:ASN:HA	9:F:136:ARG:HG2	1.91	0.52
1:5:4711:C:O2'	17:O:145:VAL:O	2.26	0.52
1:5:2526:C:H5''	20:R:10:LEU:HD11	1.91	0.52
75:RR:63:LYS:HG2	83:O:108:VAL:HG21	1.91	0.52
49:2:18:G:O2'	49:2:57:G:N2	2.39	0.52
1:5:1080:C:N4	1:5:1221:G:O6	2.42	0.52
51:K:1618:C:H4'	76:9:50:ARG:HH21	1.73	0.52
6:C:231:ASN:HB3	6:C:234:LYS:HB2	1.92	0.52
72:DD:225:GLU:HB3	84:6:187:ASN:HB2	1.91	0.52
1:5:1090:G:OP1	22:T:142:ARG:NH1	2.43	0.52
67:VV:61:GLN:HB3	67:VV:62:PRO:CD	2.39	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:5:4272:G:N2	1:5:4272:G:OP2	2.37	0.52
51:K:1536:G:H2'	51:K:1537:A:H8	1.73	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
64:YY:58:MET:O	64:YY:62:GLN:NE2	2.43	0.52
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
73:BB:100:ILE:HA	73:BB:178:ILE:HD11	1.91	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
83:O:132:MET:HG2	83:O:141:CYS:HB2	1.91	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
1:5:2754:G:OP2	28:Z:133:LYS:NZ	2.42	0.52
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
1:5:386:A:O2'	27:Y:87:ARG:NH2	2.44	0.51
4:A:14:SER:H	4:A:17:ARG:HG3	1.74	0.51
73:BB:126:THR:OG1	81:FF:26:GLN:NE2	2.43	0.51
10:G:31:LEU:HD21	28:Z:123:LYS:HA	1.93	0.51
9:F:230:VAL:HA	21:S:39:VAL:HG12	1.92	0.51
1:5:1636:U:H5''	1:5:1637:A:H5'	1.92	0.51
1:5:219:G:OP2	6:C:172:LYS:NZ	2.35	0.51
1:5:1787:A:N3	1:5:4210:U:O2'	2.43	0.51
4:A:23:ARG:HA	4:A:52:PRO:HD2	1.92	0.51
1:5:4929:C:H5'	8:E:262:GLN:HG2	1.92	0.51
51:K:1100:A:O5'	64:YY:132:ARG:NH2	2.43	0.51
51:K:1130:G:OP2	51:K:1130:G:N2	2.40	0.51
51:K:448:A:OP1	58:CC:25:ARG:NH2	2.43	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:508:A:H3'	51:K:509:G:H8	1.75	0.51
21:S:15:ARG:HH21	22:T:141:VAL:HG22	1.75	0.51
1:5:1073:G:H1	1:5:1238:A:H2	1.58	0.51
5:B:54:THR:OG1	5:B:369:ASP:O	2.24	0.51
1:5:4937:C:H1'	8:E:181:PRO:HB3	1.93	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:V:13:LYS:NZ	24:V:59:ASP:OD1	2.43	0.51
1:5:1817:U:H4'	7:D:43:LYS:HE2	1.91	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
73:BB:140:ASP:H	81:FF:44:ARG:HH12	1.58	0.51
70:JJ:81:ARG:HH12	70:JJ:83:GLN:HB3	1.76	0.51
51:K:1213:C:H2'	51:K:1214:A:H8	1.76	0.51
1:5:1188:C:H2'	1:5:1189:G:H8	1.76	0.51
1:5:3598:C:H2'	1:5:3599:A:H8	1.75	0.51
1:5:1743:A:H5'	7:D:11:ALA:HB1	1.92	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
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
59:XX:140:GLN:NE2	68:NN:64:PHE:O	2.44	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
1:5:2739:C:O2	4:A:174:ARG:NH1	2.43	0.51
51:K:526:A:OP1	71:AA:101:ARG:NH1	2.44	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
1:5:727:C:OP1	9:F:78:ARG:NH2	2.43	0.51
51:K:1354:G:N2	51:K:1357:A:OP2	2.37	0.51
68:NN:91:LEU:HD22	68:NN:96:LEU:HD11	1.92	0.51
18:P:114:ILE:HD11	18:P:117:ILE:HB	1.92	0.51
1:5:2016:C:O2	1:5:2016:C:H2'	2.08	0.51
8:E:209:THR:H	8:E:212:TYR:HB3	1.75	0.51
51:K:822:U:H3	51:K:826:A:H62	1.58	0.51
1:5:1364:U:OP2	14:L:36:ARG:NH2	2.44	0.51
68:NN:82:ALA:O	68:NN:86:GLU:CB	2.58	0.51
1:5:4910:G:N2	17:O:106:ASP:O	2.43	0.51
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
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
81:FF:31:ARG:HH11	81:FF:43:ILE:HG13	1.76	0.51
17:O:157:GLU:HA	17:O:160:ARG:HG2	1.92	0.51
17:O:7:LEU:HG	17:O:31:ARG:HE	1.76	0.51
25:W:45:ASN:HD22	25:W:46:PRO:HD2	1.76	0.51
1:5:4451:G:C4	48:1:256:TRP:CD1	2.99	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:5:4537:C:H2'	1:5:4538:G:H8	1.76	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
51:K:872:A:O2'	51:K:874:G:OP2	2.29	0.51
1:5:937:U:OP1	15:M:20:HIS:NE2	2.43	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
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
1:5:1692: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
84:6:163:PRO:O	84:6:178:ASN:ND2	2.44	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
1:5:4594:U:H2'	1:5:4595:G:H8	1.75	0.50
84:6:163:PRO:HB2	84:6:179:LEU:HB2	1.91	0.50
84:6:16:GLY:O	84:6:35:SER:OG	2.29	0.50
51:K:1654:G:OP1	78:PP:90:SER:OG	2.29	0.50
1:5:1266:G:H21	1:5:2111:G:H1'	1.77	0.50
72:DD:50:ILE:HD11	72:DD:86:LEU:HD23	1.93	0.50
51:K:797:C:C2'	51:K:798:G:H5'	2.42	0.50
78:PP:28:LEU:HD23	78:PP:110:LEU:HD21	1.93	0.50
27:Y:71:VAL:N	27:Y:81:TYR:O	2.43	0.50
1:5:5002:U:OP2	5:B:385:LYS:NZ	2.36	0.50
84:6:79:LEU:HD22	84:6:111:VAL:HG21	1.93	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
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
1:5:1460:C:H5''	19:Q:144:LYS:HG2	1.93	0.50
19:Q:151:HIS:ND1	19:Q:164:LYS:O	2.43	0.50
83:0:99:LYS:O	83:0:104:LYS:NZ	2.44	0.50
5:B:217:ILE:HD11	5:B:333:LEU:HD21	1.93	0.50
51:K:1533:A:O2'	73:BB:81:ARG:NH2	2.42	0.50
21:S:113:MET:HB3	21:S:119:ALA:HB3	1.93	0.50
61:QQ:20:ARG:HH22	66:TT:56:HIS:CG	2.30	0.50
59:XX:19:PRO:O	59:XX:24:ARG:NH2	2.45	0.50
64:YY:17:ILE:HD11	64:YY:54:VAL:HA	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:5:2486:G:N2	3:8:126:C:OP2	2.42	0.50
1:5:1326:A:OP2	1:5:4445:U:O2'	2.29	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
51:K:959:G:OP2	62:MM:38:ASN:ND2	2.40	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
49:2:33:U:H6	49:2:36:U:H5	1.60	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
77:II:127:TRP:O	77:II:144:ARG:NH2	2.44	0.50
70:JJ:36:LYS:HB3	70:JJ:43:ILE:HG12	1.94	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
1:5:1538:U:H2'	1:5:1539:G:H8	1.77	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
1:5:1508:A:OP1	6:C:110:ARG:NH1	2.44	0.50
58:CC:88:ASN:HD22	58:CC:205:ARG:HH12	1.59	0.50
11:H:47:LEU:HG	11:H:52:LYS:HD2	1.93	0.50
51:K:830:A:OP2	51:K:846:G:N2	2.45	0.50
3:8:13:G:O2'	18:P:121:LYS:O	2.28	0.50
1:5:1790:U:OP2	22:T:13:TYR:OH	2.27	0.50
26:X:107:HIS:O	26:X:111:GLN:NE2	2.45	0.50
59:XX:138:ARG:NH1	59:XX:152:ASP:OD2	2.45	0.50
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
51:K:311:C:H5''	51:K:312:G:H5''	1.93	0.49
14:L:43:ALA:O	14:L:149:GLN:NE2	2.38	0.49
68:NN:90:ARG:HG3	68:NN:93:ARG:HD2	1.93	0.49
1:5:2485:U:H2'	1:5:2486:G:H8	1.77	0.49
1:5:4507:A:O2'	24:V:41:SER:OG	2.25	0.49
1:5:492:U:O2	1:5:663:G:O6	2.29	0.49
2:7:13:A:O2'	7:D:24:ARG:NH2	2.45	0.49
51:K:551:U:H2'	51:K:552:G:H8	1.77	0.49
14:L:46:ILE:HB	14:L:49:ARG:HB2	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
51:K:1199:A:H5''	69:ZZ:2:THR:HB	1.94	0.49
1:5:4458:C:OP1	5:B:11:HIS:NE2	2.45	0.49
51:K:1391:C:O2'	79:GG:83:ARG:NH2	2.41	0.49
51:K:628:A:N7	72:DD:179:GLN:NE2	2.56	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
1:5:2568:C:H2'	1:5:2569:G:H8	1.78	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
1:5:3683:C:OP1	4:A:132:ASN:ND2	2.45	0.49
1:5:442:G:OP1	9:F:68:ARG:NH1	70.52	0.49
4:A:181:LYS:HE3	4:A:184:ARG:HG3	1.95	0.49
66:TT:52:ILE:HG22	66:TT:61:ILE:HG12	1.94	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
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
1:5:300:A:O2'	16:N:94:PHE:O	2.29	0.49
1:5:4220:A:OP2	22:T:2:THR:N	2.45	0.49
51:K:1204:A:O2'	51:K:1700:C:OP2	2.31	0.49
15:M:101:LYS:HE2	17:O:201:PHE:HE1	1.78	0.49
1:5:2465:C:H1'	1:5:3672:G:H1	1.77	0.49
1:5:460:C:H2'	1:5:461:G:H8	1.78	0.49
1:5:4758:U:OP1	17:O:116:LYS:NZ	2.46	0.49
5:B:36:ASP:OD1	5:B:36:ASP:N	2.56	0.49
6:C:152:LEU:HD23	6:C:251:ILE:HG12	1.94	0.49
66:TT:24:GLN:HG3	70:JJ:7:LEU:HD12	1.94	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
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
51:K:658:U:O2	67:VV:17:ARG:NH2	2.46	0.49
75:RR:62:VAL:HA	75:RR:65:VAL:HG12	1.95	0.49
28:Z:22:LYS:NZ	28:Z:129:TRP:O	2.46	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
1:5:3765: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:119:ILE:HG13	26:X:144:TYR:HD2	1.77	0.49
26:X:104:ALA:O	26:X:134:LYS:NZ	2.45	0.49
51:K:1:U:H5'	59:XX:58:ARG:HH22	1.77	0.49
1:5:1975:G:N2	1:5:1983:A:OP1	2.46	0.49
1:5:66:A:O2'	1:5:326:C:O2	2.29	0.49
1:5:3689:G:O2'	1:5:3818:U:OP2	2.31	0.49
1:5:381:U:H4'	1:5:415:G:H5'	1.94	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
51:K:155:G:H2'	51:K:156:G:H8	1.78	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
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
21:S:34:ALA:HB1	21:S:39:VAL:HG23	1.94	0.49
51:K:989:C:O2	69:ZZ:32:LYS:NZ	2.46	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
10:G:165:GLU:OE2	16:N:26:ARG:NH1	2.41	0.48
65:HH:22:ARG:NH2	65:HH:56:CYS:SG	2.86	0.48
62:MM:95:ILE:HB	62:MM:129:ILE:HG12	1.94	0.48
5:B:115:LYS:NZ	5:B:129:ALA:O	2.46	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
58:CC:99:ASN:ND2	58:CC:174:CYS:SG	2.87	0.48
72:DD:28:GLU:OE2	72:DD:65:ARG:NH2	2.47	0.48
51:K:1270:G:O2'	51:K:1301:A:N7	2.47	0.48
59:XX:136:ARG:HD2	59:XX:139:LYS:HA	1.94	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:5:4387:C:H5'	48:1:251:ARG:HH12	1.78	0.48
84:6:254:PRO:HA	84:6:285:GLN:HA	1.95	0.48
58:CC:22:HIS:ND1	58:CC:23:LYS:O	2.46	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
12:I:14:ASN:O	12:I:128:ARG:NH2	2.42	0.48
51:K:398:A:H5''	51:K:400:C:H5'	1.95	0.48
1:5:3917:A:H2'	1:5:3918:G:H8	1.79	0.48
1:5:2041:A:H62	1:5:4434:C:H1'	1.79	0.48
1:5:2835:A:O2'	5:B:228:TYR:O	2.27	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
21:S:76:LYS:NZ	21:S:100:LEU:O	2.45	0.48
1:5:3928:A:OP1	16:N:90:ASN:ND2	2.46	0.48
1:5:4894:A:O2'	1:5:4896:G:OP1	2.30	0.48
84:6:118:ARG:NH2	84:6:134:THR:OG1	2.46	0.48
60:EE:86:ILE:HG12	60:EE:113:LEU:HB2	1.94	0.48
9:F:37:LYS:O	9:F:41:GLN:NE2	2.47	0.48
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
51:K:1292:C:N3	83:O:138:ARG:NH1	2.61	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
21:S:13:VAL:HG23	21:S:62:VAL:HB	1.95	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
1:5:950:G:H2'	1:5:951:G:H8	1.79	0.48
1:5:701:G:H5'	8:E:117:VAL:HG21	1.95	0.48
77:II:28:PHE:HE1	77:II:38:ARG:HE	1.62	0.48
51:K:1550:G:H3'	51:K:1579:A:H61	1.79	0.48
51:K:360:A:H4'	51:K:361:U:H3'	1.96	0.48
16:N:47:LYS:HE3	16:N:51:LEU:HD11	1.95	0.48
1:5:152:U:OP1	16:N:55:ALA:N	2.46	0.48
1:5:4096:C:H1'	10:G:112:GLN:HE22	80.01	0.48
11:H:91:LYS:HB2	11:H:183:GLU:HB3	1.95	0.48
51:K:1670:C:H2'	51:K:1671:G:H8	1.79	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
63:UU:45:ARG:NH2	78:PP:10:ASN:OD1	2.47	0.48
1:5:1500:A:H5''	1:5:1501:C:H5''	1.94	0.47
1:5:2738:C:O2'	1:5:2740:U:O2	2.30	0.47
1:5:2309:G:O2'	3:8:18:U:O2	2.31	0.47
1:5:2279:A:O2'	8:E:48:ARG:NH2	48.86	0.47
51:K:1596:U:O2'	77:II:25:LYS:NZ	2.42	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
1:5:119:G:H22	10:G:133:PRO:HG2	1.79	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
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
1:5:731:G:H21	21:S:72:PRO:HG2	1.80	0.47
84:6:99:ARG:NH2	84:6:135:LEU:O	2.47	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
61:QQ:30:SER:HB2	61:QQ:67:THR:HG22	1.96	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
1:5:709:C:H2'	1:5:710:G:H8	1.78	0.47
9:F:211:TRP:HE1	9:F:214:LYS:HE2	1.79	0.47
51:K:1628:C:O2'	77:II:82:TRP:O	2.32	0.47
51:K:1279:C:H2'	51:K:1280:G:H8	1.80	0.47
51:K:1710:C:H42	51:K:1823:A:H61	1.62	0.47
51:K:377:G:H5'	58:CC:98:LYS:HB3	1.95	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
65:HH:38:GLU:HG3	65:HH:49:GLN:HG3	1.96	0.47
10:G:48:LYS:HB3	26:X:42:THR:HG23	1.95	0.47
49:2:3:U:H3	49:2:70:G:H1	1.63	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
1:5:4357: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
1:5:724:C:H2'	1:5:725:G:H8	1.78	0.47
2:7:15:C:H2'	2:7:16:A:H8	1.79	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
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
23:U:64:GLU:HB2	23:U:71:THR:HB	1.95	0.47
12:I:46:PHE:HB2	12:I:139:ARG:HH11	1.80	0.47
51:K:681:U:O2'	51:K:1160:U:OP1	2.32	0.47
1:5:734:G:H5''	15:M:70:GLN:HG2	1.96	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
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
70:JJ:23:ARG:NH1	70:JJ:27:SER:O	2.48	0.47
51:K:111:A:O2'	60:EE:69:ARG:NH1	2.47	0.47
18:P:16:LYS:HG2	18:P:149:ILE:HG12	1.95	0.47
51:K:1587:G:H5''	78:PP:77:LYS:HD3	1.96	0.47
1:5:960:A:N6	1:5:1283:G:O6	2.47	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
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
72:DD:135:GLU:HB3	72:DD:187:LYS:HB3	1.95	0.47
60:EE:5:GLN:HG2	60:EE:11:GLN:HB2	1.96	0.47
9:F:115:ARG:HH11	9:F:212:PRO:HD3	1.80	0.47
51:K:124:U:H3	51:K:340:C:H42	1.62	0.47
51:K:43:U:OP2	51:K:485:A:N6	2.47	0.47
51:K:551:U:H2'	51:K:552:G:C8	2.49	0.47
16:N:200:LEU:HB3	16:N:204:ARG:HH21	1.80	0.47
1:5:1396:G:HO2'	1:5:1468:C:HO2'	1.55	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
12:I:38:ARG:HD3	12:I:83:ASP:HB2	1.96	0.47
51:K:35:C:H5''	51:K:579:C:H5''	1.97	0.47
1:5:313:U:H5''	16:N:179:LYS:HE3	1.97	0.47
74:SS:60:GLU:OE1	74:SS:69:TRP:NE1	2.48	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
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
49:2:29:A:H3'	49:2:30:G:H8	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:5:2740:U:O2'	1:5:2742:G:N2	2.48	0.47
1:5:916:C:N4	1:5:918:G:O6	2.48	0.47
73:BB:102:LEU:HD22	80:OO:110:THR:HG21	1.97	0.47
7:D:53:VAL:HG11	7:D:159:VAL:HA	1.96	0.47
51:K:149:A:OP2	51:K:168:C:N4	2.46	0.47
51:K:1218:C:H1'	51:K:1683:C:H42	1.80	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
1:5:1933:G:H2'	1:5:1934:A:C8	2.50	0.47
1:5:3919:C:H4'	4:A:207:VAL:HG12	1.97	0.47
72:DD:177:LEU:HD13	72:DD:182:LEU:HD13	1.97	0.47
51:K:1631:U:O3'	77:II:34:LYS:NZ	2.48	0.47
13:J:35:ARG:HD3	13:J:124:GLY:H	1.80	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:828:G:N2	51:K:830:A:O2'	2.46	0.47
1:5:1355:G:OP1	19:Q:108:ARG:NH1	2.47	0.47
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
51:K:1228:A:H2'	51:K:1229:G:H8	1.80	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
28:Z:46:ILE:HA	28:Z:70:SER:HA	1.97	0.46
49:2:30:G:H2'	49:2:31:G:H8	1.80	0.46
1:5:1494:U:H2'	1:5:1495:G:H8	1.80	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
77:II:22:GLY:HA2	77:II:56:ALA:HB3	1.96	0.46
25:W:44:ARG:NH2	51:K:1337:C:OP1	136.19	0.46
51:K:1726:G:O6	51:K:1808:U:O4	2.33	0.46
66:TT:26:LEU:HD11	66:TT:60:LYS:HB3	1.98	0.46
49:2:10:G:O6	49:2:45:G:N2	2.48	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
62:MM:30:VAL:HG23	62:MM:94:HIS:HB2	1.97	0.46
17:O:9:LEU:HD23	17:O:118:MET:HB2	1.98	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
1:5:48:G:N2	1:5:49:U:O4	2.36	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:5:62:A:N3	1:5:77:U:O2'	2.44	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
79:GG:54:VAL:HB	79:GG:88:LEU:HG	1.97	0.46
77:II:4:VAL:HA	80:OO:50:PHE:HB2	1.96	0.46
19:Q:33:ARG:HE	19:Q:52:PHE:HZ	1.63	0.46
51:K:522:A:H4'	59:XX:131:ARG:HH22	1.81	0.46
49:2:34:C:H2'	49:2:35:A:C8	2.50	0.46
1:5:1895:G:O2'	1:5:1907:A:N3	2.40	0.46
1:5:4457:U:OP1	24:V:50:ASN:ND2	2.36	0.46
1:5:86:U:H2'	1:5:87:A:H8	1.81	0.46
51:K:647:U:H2'	51:K:648:A:H8	1.80	0.46
74:SS:24:LYS:O	74:SS:42:ASN:ND2	2.46	0.46
63:UU:131:LYS:HB2	63:UU:140:ARG:HH12	1.81	0.46
1:5:85:G:O2'	1:5:97:G:O6	2.30	0.46
71:AA:112:ASN:O	71:AA:117:ASN:ND2	2.49	0.46
1:5:1864:G:O2'	12:I:118:ALA:O	2.34	0.46
12:I:98:ARG:HB3	12:I:120:GLY:HA3	1.98	0.46
1:5:32:G:OP1	16:N:73:ARG:NH1	2.49	0.46
1:5:4910:G:H1	17:O:108:ILE:H	1.63	0.46
58:CC:177:SER:OG	58:CC:186:ASP:N	2.49	0.46
8:E:157:ARG:NH2	8:E:269:SER:OG	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
51:K:511:U:O2'	51:K:576:A:N6	2.48	0.46
1:5:101:A:O2'	14:L:63:THR:OG1	2.34	0.46
63:UU:17:LYS:HG3	63:UU:126:ARG:HG3	1.98	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
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
3:8:65:A:OP1	11:H:56:ARG:NE	162.65	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
66:TT:57:ARG:NH1	70:JJ:26:GLN:OE1	2.49	0.46
51:K:434:G:H2'	51:K:435:A:C8	2.51	0.46
17:O:196:LEU:HB3	17:O:201:PHE:HB2	1.97	0.46
1:5:4454:G:O2'	1:5:4500:U:O2'	2.34	0.46
60:EE:126:VAL:HG23	60:EE:145:VAL:HG22	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
51:K:5:U:H2'	51:K:6:G:H8	1.81	0.46
51:K:943:U:H2'	51:K:944:A:C8	2.51	0.46
18:P:32:THR:HG23	18:P:91:LEU:HD21	1.97	0.46
79:GG:59:LYS:HB2	79:GG:84:ILE:HG22	1.97	0.46
77:II:124:ARG:HE	77:II:129:LEU:HB2	1.81	0.46
14:L:91:ALA:HB1	14:L:96:ILE:HB	1.98	0.46
1:5:297:U:O2'	16:N:179:LYS:O	2.22	0.46
80:OO:50:PHE:HE1	80:OO:58:LEU:HD13	1.81	0.46
12:I:162:ARG:NH2	21:S:88:SER:OG	2.48	0.46
66:TT:86:LEU:HD23	66:TT:117:ARG:HE	1.79	0.46
1:5:198:A:OP2	27:Y:45:ARG:NH1	2.46	0.45
84:6:22:ALA:HB2	84:6:69:VAL:HG13	1.98	0.45
72:DD:55:THR:HA	72:DD:58:VAL:HG22	1.99	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
1:5:4451:G:C1'	48:1:256:TRP:CD1	3.00	0.45
1:5:1794:A:H5''	1:5:4214:A:H61	1.81	0.45
1:5:4870:G:H4'	1:5:4872:G:H4'	1.99	0.45
51:K:307:G:H1'	58:CC:45:THR:HG22	1.97	0.45
77:II:74:PRO:HG3	77:II:97:GLN:H	1.81	0.45
13:J:90:ARG:HD3	13:J:109:ILE:HG22	1.98	0.45
51:K:609:U:H2'	51:K:610:G:H8	1.81	0.45
51:K:72:C:O2'	51:K:74:G:OP2	2.30	0.45
51:K:991:G:N7	69:ZZ:7:ASN:ND2	2.64	0.45
14:L:191:LEU:HD23	14:L:194:ILE:HD13	1.99	0.45
51:K:1650:A:OP1	63:UU:137:ALA:N	2.49	0.45
1:5:2749:C:H2'	1:5:2750:G:C8	2.51	0.45
1:5:382:G:N1	1:5:385:A:OP2	2.43	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
51:K:1246:A:O2'	79:GG:72:GLU:OE2	2.33	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
1:5:61:A:H5''	16:N:164:LEU:HD21	1.98	0.45
9:F:88:GLU:HB2	22:T:135:PRO:HB3	1.97	0.45
66:TT:103:VAL:HG13	66:TT:126:LEU:HB2	1.98	0.45
51:K:1207:G:N1	85:4:45:A:O2'	2.49	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
49:2:36:U:O2'	51:K:1825:A:N1	2.44	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:5:20:U:H3'	1:5:21:G:H8	1.82	0.45
1:5:371:A:N3	1:5:1531:U:O2'	2.45	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
1:5:1628:C:H5''	4:A:15:VAL:HG21	1.98	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
77:II:13:LEU:HB2	77:II:20:ILE:HB	1.97	0.45
51:K:903:A:H2'	51:K:904:A:C8	2.51	0.45
62:MM:117:ARG:NH2	81:FF:62:GLU:O	2.50	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
1:5:2352:U:H1'	6:C:96:CYS:HA	1.98	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
11:H:173:ARG:HD3	15:M:124:LYS:HE2	84.10	0.45
1:5:1932:A:OP2	17:O:49:ARG:NH1	2.49	0.45
25:W:46:PRO:O	25:W:52:THR:OG1	2.32	0.45
1:5:2017:A:C8	1:5:2017:A:OP2	2.70	0.45
1:5:4180:G:N2	4:A:228:ASP:OD2	2.50	0.45
73:BB:140:ASP:HB2	81:FF:44:ARG:HH22	1.81	0.45
7:D:53:VAL:HB	7:D:159:VAL:HG13	1.98	0.45
72:DD:135:GLU:HA	72:DD:153:VAL:HG22	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
79:GG:56:MET:HG3	79:GG:86:LYS:HE3	1.97	0.45
1:5:4944:C:OP1	8:E:150:THR:OG1	2.29	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
51:K:929:G:H21	51:K:1104:G:H4'	1.82	0.45
51:K:1324:G:H1	51:K:1504:U:H3	1.65	0.45
51:K:305:U:H3'	51:K:306:C:H5'	1.99	0.45
1:5:4300:U:H5''	22:T:87:LYS:HE2	1.99	0.45
66:TT:11:LEU:HA	66:TT:14:ILE:HG12	1.98	0.45
24:V:35:LYS:HB2	24:V:67:LYS:HG3	1.98	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:5:32:G:H21	1:5:50:C:H5	1.65	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
1:5:3687:A:H3'	4:A:198:ARG:HH22	1.82	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
51:K:304:C:C6	51:K:304:C:OP2	2.70	0.45
83:0:138:ARG:HB2	83:0:149:CYS:HA	1.99	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
1:5:1728:U:O4	1:5:1729:A:N6	2.51	0.44
5:B:19:ARG:HB2	5:B:234:ARG:HH21	1.82	0.44
58:CC:100:CYS:O	58:CC:174:CYS:HA	2.17	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
50:3:38:A:O2'	51:K:1058:A:OP1	2.29	0.44
51:K:94:G:O2'	51:K:508:A:O2'	2.29	0.44
51:K:805:U:O3'	66:TT:120:HIS:NE2	2.50	0.44
1:5:2904:U:H5''	1:5:2905:C:H5	1.81	0.44
84:6:174:VAL:HB	84:6:188:HIS:HB2	1.98	0.44
84:6:20:GLN:HG2	84:6:69:VAL:H	1.82	0.44
4:A:92:LYS:HG3	4:A:106:THR:HG21	2.00	0.44
6:C:7:LEU:HG	6:C:21:ASN:HB3	1.98	0.44
51:K:1220:A:N3	51:K:1677:U:O2'	2.42	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
1:5:293:G:N2	16:N:178:HIS:O	2.40	0.44
67:VV:68:LYS:HE2	71:AA:82:VAL:HG22	1.99	0.44
1:5:1655:C:O2	1:5:4390:A:O2'	2.34	0.44
1:5:385:A:HO2'	1:5:387:G:H8	1.64	0.44
73:BB:20:PHE:N	73:BB:23:TRP:O	2.51	0.44
7:D:52:ILE:HA	7:D:147:ASP:HB3	1.98	0.44
79:GG:63:ILE:HB	79:GG:80:PHE:HB2	2.00	0.44
51:K:1139:C:H41	51:K:1149:A:H62	1.64	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
83:0:104:LYS:O	83:0:118:ARG:NH1	2.44	0.44
1:5:4430:G:H1'	12:I:158:LYS:HD2	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:5:4586:G:OP2	17:O:74:ARG:NH1	2.51	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
1:5:418:A:H4'	1:5:2311:C:H5'	2.00	0.44
1:5:2438:A:O2'	1:5:2440:U:OP1	2.32	0.44
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
1:5:1335:G:N2	6:C:95:MET:O	2.46	0.44
1:5:2515:G:OP1	10:G:37:LYS:NZ	47.17	0.44
51:K:659:G:HO2'	51:K:662:G:HO2'	1.60	0.44
18:P:4:TYR:HE1	18:P:18:ARG:HD2	1.83	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
11:H:8:GLN:NE2	11:H:74:CYS:SG	2.91	0.44
51:K:1135:C:OP2	69:ZZ:6:ARG:NH1	2.51	0.44
51:K:1036:A:H4'	51:K:1855:G:H21	1.82	0.44
51:K:912:C:H3'	51:K:913:A:H3'	1.99	0.44
1:5:1691:G:H5'	19:Q:15:ARG:HG3	2.00	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
1:5:153:G:H2'	1:5:154:G:H8	1.83	0.44
1:5:2848:G:O2'	1:5:3838:U:O4	2.30	0.44
1:5:4748:U:O4	1:5:4952:G:O6	2.35	0.44
1:5:659:G:H2'	1:5:660:A:H8	1.82	0.44
3:8:67:U:H2'	3:8:68:G:H8	1.82	0.44
51:K:5:U:H2'	51:K:6:G:C8	2.52	0.44
17:O:36:VAL:HG23	17:O:105:PHE:HB2	2.00	0.44
75:RR:48:HIS:HD2	75:RR:112:LYS:HG2	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
1:5:4760:G:H3'	17:O:12:ARG:HH22	1.81	0.44
1:5:951:G:H2'	1:5:952:G:H8	1.83	0.44
76:9:60:LEU:HD13	76:9:89:MET:HG3	1.99	0.44
5:B:331:VAL:HG21	5:B:347:LEU:HD21	1.99	0.44
11:H:167:VAL:HB	11:H:172:ILE:HG22	2.00	0.44
64:YY:31:ASN:HD21	64:YY:55:THR:HG22	1.83	0.44
51:K:1865:C:OP2	69:ZZ:5:ARG:NH2	2.49	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:5:4991:U:H2'	1:5:4992:G:C8	2.53	0.44
51:K:1623:A:H5''	77:II:133:GLY:HA3	2.00	0.44
51:K:305:U:H6	51:K:305:U:O5'	2.01	0.44
51:K:960:U:H5''	62:MM:149:ARG:HH21	1.83	0.44
17:O:44:SER:HB3	17:O:129:LEU:HD11	1.99	0.44
74:SS:93:THR:HG23	74:SS:94:LEU:HD12	1.99	0.44
12:I:27:PRO:HA	49:2:64:U:H4'	2.00	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
1:5:86:U:H2'	1:5:87:A:C8	2.53	0.43
59:XX:29:LEU:HD12	71:AA:115:PHE:HE2	1.83	0.43
8:E:153:HIS:HB3	8:E:156:LYS:HD2	1.99	0.43
60:EE:135:SER:O	60:EE:139:ARG:NH1	2.49	0.43
23:U:84:LYS:HG2	23:U:88:LYS:HE2	1.99	0.43
63:UU:41:MET:N	63:UU:41:MET:SD	2.91	0.43
1:5:53:C:O2'	1:5:2461:G:O2'	2.33	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
1:5:1593:A:H5''	1:5:2839:U:H5''	1.99	0.43
1:5:2903:G:H5'	1:5:3592:G:H1	1.84	0.43
84:6:258:ILE:HG13	84:6:267:VAL:HB	2.00	0.43
5:B:222:VAL:O	5:B:343:ARG:NH1	2.52	0.43
73:BB:50:PRO:HG2	73:BB:90:VAL:HG22	2.00	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
51:K:1691:U:H4'	69:ZZ:88:SER:HB3	1.99	0.43
23:U:65:ARG:HE	62:MM:50:LYS:HD3	146.05	0.43
24:V:18:LEU:HD13	24:V:54:ALA:HB3	2.00	0.43
1:5:4451:G:N9	48:1:256:TRP:HD1	2.06	0.43
1:5:2386:U:H2'	1:5:2387:G:H8	1.83	0.43
1:5:4274:A:H2'	1:5:4275:G:H8	1.83	0.43
8:E:161:LEU:HD21	8:E:253:ILE:HD11	2.00	0.43
51:K:1722:G:H2'	51:K:1723:G:C8	2.53	0.43
51:K:521:A:OP1	59:XX:45:ARG:NH1	2.49	0.43
51:K:90:G:OP1	51:K:445:A:N6	2.41	0.43
68:NN:78:SER:HB3	68:NN:81:TYR:HD2	1.83	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:5:3620:G:OP1	1:5:3622:C:N4	2.51	0.43
1:5:4748:U:H3	1:5:4952:G:H1	1.66	0.43
1:5:4737:G:H5''	1:5:5069:U:H2'	1.99	0.43
5:B:256:ALA:H	5:B:260:ALA:HB3	1.83	0.43
72:DD:93:THR:HG21	72:DD:198:ILE:HG13	1.99	0.43
51:K:104:A:H62	51:K:356:C:H5	1.65	0.43
51:K:603:C:N4	51:K:620:G:O6	2.52	0.43
28:Z:89:ILE:HG12	28:Z:91:LEU:HG	1.99	0.43
1:5:2520:C:H2'	1:5:2521:G:C8	2.52	0.43
1:5:695:G:OP1	8:E:219:ARG:NH2	2.52	0.43
2:7:63:C:H5'	2:7:64:G:H5''	2.01	0.43
73:BB:86:LYS:HA	73:BB:89:THR:HG22	2.01	0.43
13:J:56:THR:HG23	13:J:63:ARG:HA	2.01	0.43
51:K:919:A:O2'	51:K:1020:A:N1	2.41	0.43
62:MM:56:VAL:HG11	62:MM:80:ASP:HB3	2.01	0.43
16:N:181:HIS:O	16:N:195:ARG:NH2	2.44	0.43
68:NN:43:LYS:HA	68:NN:46:LYS:HG2	1.99	0.43
15:M:53:LYS:HE3	21:S:160:ARG:HG3	1.99	0.43
1:5:4421:C:H42	1:5:4475:G:H22	1.65	0.43
51:K:1401:A:H4'	79:GG:52:GLY:HA3	2.01	0.43
79:GG:48:LEU:HD11	79:GG:91:LEU:HD22	2.00	0.43
12:I:48:LEU:HD21	12:I:145:LYS:HG2	2.00	0.43
51:K:1417:C:N3	51:K:1423:C:N4	2.61	0.43
51:K:1674:G:OP1	73:BB:51:HIS:NE2	2.49	0.43
51:K:807:G:H2'	51:K:808:A:C8	2.53	0.43
15:M:38:VAL:HG21	15:M:50:MET:HB3	2.01	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
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
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
27:Y:27:ARG:HB2	27:Y:75:ARG:HH11	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:5:1240:G:OP2	1:5:1271:G:O2'	2.35	0.43
1:5:1417:C:OP2	4:A:119:LYS:NZ	118.24	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
4:A:117:GLU:O	4:A:162:ASN:ND2	2.52	0.43
60:EE:35:ARG:NE	60:EE:50:ALA:O	2.43	0.43
51:K:160:U:O2'	51:K:162:C:O5'	2.36	0.43
14:L:80:GLU:OE2	14:L:113:ASN:ND2	2.51	0.43
50:3:47:U:O2'	50:3:50:A:OP1	2.25	0.42
1:5:2338:C:OP1	20:R:19:LYS:NZ	92.62	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
1:5:724:C:OP2	6:C:350:ARG:NH2	2.49	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
1:5:2096:G:O6	9:F:48:ARG:NH1	2.52	0.42
19:Q:18:PRO:HG3	19:Q:29:VAL:HG21	2.00	0.42
1:5:1461:C:H2'	1:5:1462:A:C8	2.55	0.42
1:5:150:U:OP2	10:G:200:THR:OG1	2.37	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
51:K:490:C:O2'	51:K:574:A:N1	2.45	0.42
27:Y:72:GLN:HE22	27:Y:74:TYR:HB2	1.84	0.42
1:5:1348:U:OP2	19:Q:56:THR:OG1	2.34	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
1:5:363:A:N7	1:5:378:A:N6	2.67	0.42
1:5:1940:G:N2	1:5:4434:C:OP1	2.42	0.42
1:5:4520:G:N2	5:B:253:CYS:SG	2.92	0.42
1:5:4870:G:N2	1:5:4870:G:OP2	2.41	0.42
3:8:26:C:O2'	6:C:53:ALA:O	2.31	0.42
51:K:374:G:H4'	60:EE:84:ARG:HD2	2.01	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
51:K:1407:U:O2'	63:UU:11:GLN:NE2	2.52	0.42
14:L:64:VAL:HA	14:L:67:HIS:HB2	2.01	0.42
62:MM:150:ARG:H	62:MM:150:ARG:HD3	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:5:3619: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
51:K:1268:C:O2	76:9:97:TYR:OH	2.37	0.42
5:B:302:ASN:HB2	5:B:313:SER:HA	2.00	0.42
73:BB:73:THR:HG23	73:BB:89:THR:HG23	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
58:CC:190:LEU:HD12	58:CC:194:GLU:HB3	2.02	0.42
77:II:20:ILE:HD11	77:II:33:ILE:HD11	2.01	0.42
70:JJ:20:LYS:HE3	70:JJ:28:PRO:HA	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
23:U:44:GLN:HA	23:U:56:LEU:HD21	2.01	0.42
69:ZZ:28:ARG:NH1	69:ZZ:29:CYS:O	2.52	0.42
1:5:229:G:H5''	27:Y:11:ARG:HD2	2.01	0.42
1:5:4862:G:H2'	1:5:4863:G:H8	1.84	0.42
1:5:704:C:H2'	1:5:705:G:H8	1.84	0.42
4:A:33:ASP:H	4:A:36:GLU:HB2	1.84	0.42
73:BB:14:THR:OG1	73:BB:17:ILE:O	2.32	0.42
51:K:915:G:N2	51:K:915:G:OP2	2.40	0.42
16:N:68:ARG:NH1	16:N:124:ASP:O	2.46	0.42
78:PP:5:THR:HG23	78:PP:7:LYS:H	1.84	0.42
51:K:916:A:C5	61:QQ:73:ARG:HD3	2.55	0.42
24:V:87:SER:HB2	25:W:19:ARG:HH11	1.84	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
1:5:2890:C:H42	1:5:3611:A:H61	1.68	0.42
1:5:667:A:H4'	6:C:6:PRO:HB3	2.01	0.42
1:5:943:A:OP1	9:F:247:ARG:NH1	2.53	0.42
84:6:289:LEU:HD12	84:6:298:LEU:HD21	2.00	0.42
8:E:254:LEU:HA	8:E:257:ILE:HG12	2.01	0.42
51:K:1146:C:O2'	51:K:1150:A:N1	2.42	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
51:K:928:G:H2'	51:K:929:G:C8	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
68:NN:7:ILE:HG23	68:NN:25:ILE:HG23	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
1:5:4124:G:H5'	28:Z:135:ARG:HH21	1.84	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
77:II:6:PRO:HG2	77:II:58:GLU:HG2	2.01	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
1:5:2575:U:H3'	28:Z:48:ARG:HH22	1.85	0.42
1:5:2465:C:H1'	1:5:3672:G:H22	1.84	0.42
1:5:4336:A:H5''	1:5:4337:C:H5'	2.01	0.42
76:9:44:ARG:HG2	76:9:84:ILE:HD11	2.02	0.42
5:B:329:ASP:N	5:B:329:ASP:OD1	2.53	0.42
6:C:78:ARG:HB3	6:C:88:GLY:HA2	2.01	0.42
60:EE:57:ASP:HB3	60:EE:60:CYS:HB2	2.01	0.42
11:H:120:GLU:OE1	11:H:124:ARG:NH2	2.51	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
1:5:1364:U:H5''	14:L:36:ARG:HH22	1.85	0.42
78:PP:56:ARG:HH22	78:PP:99:VAL:HB	1.85	0.42
64:YY:57:LEU:HD23	64:YY:60:ARG:HD3	2.02	0.42
1:5:1245:C:H2'	1:5:1246:G:C8	2.54	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
1:5:1919:G:N2	21:S:163:HIS:O	2.41	0.42
1:5:1333:A:H2'	1:5:1334:A:H8	1.85	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
51:K:639:C:H5''	71:AA:114:ARG:HH21	1.85	0.42
73:BB:103:LEU:HD23	73:BB:178:ILE:HD13	2.02	0.42
73:BB:34:SER:HA	81:FF:55:VAL:HB	2.02	0.42
1:5:1907:A:H4'	9:F:225:LYS:HE3	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
51:K:1588:A:H2'	51:K:1589:A:H8	1.85	0.42
51:K:369:C:H41	51:K:1730:U:H5''	1.84	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
51:K:522:A:O3'	59:XX:131:ARG:NH2	2.53	0.42
50:3:41:U:H2'	50:3:42:G:H8	1.84	0.41
1:5:208:A:N3	1:5:232:G:O2'	2.47	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
84:6:238:ALA:H	84:6:251:ALA:HB3	1.85	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
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
78:PP:38:LYS:NZ	78:PP:40:ALA:O	2.40	0.41
24:V:16:ILE:HB	24:V:88:TYR:HB2	2.01	0.41
49:2:4:U:H3	49:2:69:G:H22	1.67	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
11:H:114:ILE:HB	11:H:124:ARG:HB2	2.00	0.41
75:RR:40:LYS:HE2	83:O:130:VAL:HG22	2.02	0.41
27:Y:80:ILE:HD11	27:Y:104:VAL:HG21	2.02	0.41
27:Y:52:ASP:OD2	27:Y:110:LYS:NZ	2.41	0.41
1:5:1064:G:H2'	1:5:1065:G:H8	1.85	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
76:9:98:ASN:HB3	76:9:122:THR:HA	2.02	0.41
5:B:302:ASN:HD22	5:B:330:PHE:HE1	1.68	0.41
1:5:2421:G:H1'	18:P:139:TYR:CE2	2.56	0.41
78:PP:6:VAL:O	78:PP:11:GLN:NE2	2.53	0.41
67:VV:93:PHE:O	67:VV:140:ARG:NH1	2.53	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
1:5:709:C:H2'	1:5:710:G:C8	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
77:II:36:VAL:HG23	77:II:40:TYR:HD2	1.84	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
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
59:XX:42:GLU:OE2	59:XX:109:ARG:NH1	2.53	0.41
28:Z:29:ILE:HD13	28:Z:40:HIS:CD2	2.56	0.41
1:5:4208:U:H2'	1:5:4209:G:H8	1.85	0.41
1:5:441:G:H2'	1:5:442:G:H8	1.85	0.41
77:II:124:ARG:HB2	77:II:131:VAL:HG23	2.03	0.41
77:II:61:GLU:HA	77:II:64:VAL:HG22	2.03	0.41
51:K:1711:U:H2'	51:K:1712:A:C8	2.56	0.41
51:K:902:G:H5''	51:K:902:G:C8	2.56	0.41
18:P:33:ALA:HA	18:P:36:ILE:HG22	2.03	0.41
51:K:1124:C:O2'	64:YY:126:MET:O	2.37	0.41
6:C:70:GLY:O	48:1:245:PHE:HE1	2.03	0.41
1:5:131:C:N4	1:5:138:G:O6	2.54	0.41
1:5:2411:C:O2'	1:5:2526:C:O2	2.31	0.41
1:5:2757:A:H2'	1:5:2758:G:C8	2.56	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
84:6:9:GLY:H	84:6:309:VAL:HG22	1.85	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
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
16:N:84:PRO:HA	16:N:87:HIS:ND1	2.36	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
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
70:JJ:67:THR:HG21	70:JJ:72:ARG:HG3	2.03	0.41
51:K:1345:G:OP1	51:K:1688:C:O2'	2.39	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
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
1:5:49:U:H2'	1:5:50:C:H6	1.85	0.41
1:5:659:G:H2'	1:5:660:A:C8	2.56	0.41
1:5:66:A:H61	1:5:282:C:HO2'	1.64	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:5:73:A:N7	14:L:103:ARG:NH1	2.69	0.41
3:8:142:U:OP1	16:N:38:ARG:NH2	2.45	0.41
1:5:5001:U:O2'	5:B:372:SER:OG	2.30	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
51:K:1711:U:H2'	51:K:1712:A:H8	1.85	0.41
51:K:649:U:H2'	51:K:650:A:H8	1.85	0.41
50:3:15:G:H21	50:3:21:A:H1'	1.86	0.41
1:5:1350:C:H2'	1:5:1351:G:H8	1.86	0.41
1:5:1942:A:H2'	1:5:1943:A:C8	2.56	0.41
1:5:2443:G:OP2	1:5:2516:G:N2	2.48	0.41
1:5:2909:C:H2'	1:5:2910:G:C8	2.56	0.41
1:5:456:C:H2'	1:5:457:G:H8	1.85	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
1:5:4579:U:H4'	5:B:117:ARG:HG3	2.02	0.41
73:BB:127:ARG:NE	73:BB:135:ARG:O	2.54	0.41
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
51:K:1103:C:N4	51:K:1104:G:O6	2.54	0.41
51:K:588:G:OP2	51:K:588:G:N2	2.50	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
1:5:1382:G:H2'	1:5:1383:G:H8	1.85	0.41
1:5:1265:G:O3'	1:5:2112:G:N2	2.54	0.41
1:5:2811:G:N1	1:5:2814:C:OP2	2.38	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
58:CC:67:TRP:NE1	58:CC:191:GLU:OE2	2.54	0.41
1:5:1461:C:H2'	1:5:1462:A:H8	1.86	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
84:6:40:ILE:HB	84:6:59:LEU:HB2	2.02	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
1:5:4250:G:O2'	13:J:129:ASP:OD1	2.37	0.41
51:K:1232:U:H2'	51:K:1233:G:H8	1.86	0.41
51:K:675:U:H2'	51:K:676:C:H6	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:Q:175:GLU:HB3	19:Q:176:ARG:H	1.71	0.41
66:TT:90:GLN:HB2	66:TT:94:LEU:HD12	2.02	0.41
59:XX:42:GLU:OE2	59:XX:45:ARG:NH2	2.54	0.41
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
1:5:175:C:H2'	1:5:176:G:H8	1.85	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
1:5:710:G:H21	8:E:132:HIS:HE1	1.68	0.40
3:8:141:C:H2'	3:8:142:U:C6	2.57	0.40
63:UU:50:LYS:HE2	73:BB:49:LEU:HB2	2.02	0.40
73:BB:59:LYS:HB3	73:BB:62:ARG:HB2	2.03	0.40
60:EE:104:LYS:O	67:VV:11:ARG:NH2	2.54	0.40
65:HH:20:SER:HB3	65:HH:59:ILE:HD11	2.03	0.40
51:K:1566:G:O3'	51:K:1567:G:N2	2.51	0.40
51:K:562:U:H2'	51:K:563:G:C8	2.56	0.40
75:RR:54:SER:OG	75:RR:55:ASN:N	2.54	0.40
51:K:616:A:OP1	67:VV:68:LYS:NZ	2.53	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
84:6:79:LEU:HA	84:6:88:ARG:O	2.21	0.40
76:9:79:HIS:HA	76:9:97:TYR:HB3	2.03	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
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
15:M:12:VAL:HB	15:M:60:PHE:HB2	2.02	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
23:U:35:ASP:N	23:U:35:ASP:OD1	2.53	0.40
59:XX:93:LYS:HB3	59:XX:96:TYR:HD2	1.87	0.40
49:2:74:C:O2	49:2:74:C:C2'	2.70	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
1:5:2029: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
3:8:30:U:H2'	3:8:31:G:C8	2.56	0.40
73:BB:39:ILE:HG23	73:BB:68:ILE:HD13	2.03	0.40
79:GG:61:LEU:HB2	79:GG:82:MET:HB3	2.03	0.40
13:J:87:LEU:HB3	13:J:92:TYR:HD1	1.86	0.40
51:K:386:C:H4'	58:CC:9:HIS:HE1	1.86	0.40
51:K:475:C:O2'	51:K:507:G:N3	2.40	0.40
51:K:663:C:OP2	67:VV:2:GLY:N	2.54	0.40
1:5:4769:G:OP1	17:O:176:ARG:NH1	2.54	0.40
74:SS:58:VAL:HG23	74:SS:71:LEU:HA	2.03	0.40
51:K:623:G:N7	67:VV:63:ASN:ND2	2.69	0.40
27:Y:55:VAL:HG13	27:Y:104:VAL:HG13	2.04	0.40
49:2:9:A:H62	49:2:23:C:H41	1.68	0.40
85:4:49:A:O5'	85:4:49:A:H8	2.04	0.40
1:5:1198:G:H2'	1:5:1199:G:C8	2.57	0.40
1:5:378:A:O2'	1:5:413:G:N2	2.47	0.40
1:5:64:A:H1'	1:5:76:A:H1'	2.03	0.40
1:5:676:C:H2'	1:5:677:G:H8	1.87	0.40
5:B:52:GLY:HA2	5:B:341:LYS:HE3	2.04	0.40
5:B:36:ASP:HA	5:B:37:PRO:HD3	2.30	0.40
1:5:452:A:H62	8:E:218:LEU:HD21	1.86	0.40
51:K:455:A:O2'	51:K:1735:A:N3	2.46	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
51:K:433:A:OP1	58:CC:25:ARG:NH1	2.55	0.40
61:QQ:136:PRO:HG2	61:QQ:139:TRP:HB2	2.03	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
64:YY:16:ILE:HG22	64:YY:24:LEU:HD11	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
5:B:189:THR:HG23	5:B:192:GLU:H	1.86	0.40
51:K:1332:A:O2'	72:DD:145:GLN:O	2.34	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
51:K:1053:C:H2'	51:K:1054:G:H8	1.86	0.40
51:K:474:G:N2	51:K:507:G:O2'	2.38	0.40
78:PP:104:LEU:HD22	78:PP:121:ARG:HG3	2.03	0.40
21:S:83:ARG:HE	22:T:156:TYR:HB2	1.87	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
67:VV:90:CYS:HA	67:VV:93:PHE:HD2	1.86	0.40
51:K:39:A:H5'	59:XX:7:TRP:HE1	1.87	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%)	43	77
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%)	31	68
15	M	136/138 (99%)	128 (94%)	8 (6%)	0	100	100
16	N	201/203 (99%)	190 (94%)	11 (6%)	0	100	100
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%)	27	64

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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%)	11	43
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%)	17	53
44	p	89/91 (98%)	84 (94%)	5 (6%)	0	100	100
45	r	123/125 (98%)	110 (89%)	11 (9%)	2 (2%)	11	41
46	s	196/198 (99%)	178 (91%)	18 (9%)	0	100	100
47	t	161/163 (99%)	124 (77%)	36 (22%)	1 (1%)	27	64
48	l	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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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%)	24	61
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
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%)	56	85

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%)	182 (97%)	5 (3%)	48	78
5	B	336/342 (98%)	334 (99%)	2 (1%)	87	94
6	C	302/302 (100%)	297 (98%)	5 (2%)	63	85
7	D	247/247 (100%)	247 (100%)	0	100	100
8	E	208/221 (94%)	206 (99%)	2 (1%)	78	91
9	F	194/195 (100%)	194 (100%)	0	100	100
10	G	206/206 (100%)	201 (98%)	5 (2%)	52	80
11	H	169/169 (100%)	167 (99%)	2 (1%)	74	89
12	I	174/180 (97%)	171 (98%)	3 (2%)	63	85
13	J	142/142 (100%)	140 (99%)	2 (1%)	69	88
14	L	176/176 (100%)	174 (99%)	2 (1%)	76	90
15	M	117/117 (100%)	117 (100%)	0	100	100
16	N	171/171 (100%)	170 (99%)	1 (1%)	87	94
17	O	171/171 (100%)	165 (96%)	6 (4%)	39	73
18	P	134/134 (100%)	133 (99%)	1 (1%)	85	94
19	Q	163/163 (100%)	163 (100%)	0	100	100
20	R	159/159 (100%)	157 (99%)	2 (1%)	71	88

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
21	S	156/156 (100%)	156 (100%)	0	100	100
22	T	139/139 (100%)	138 (99%)	1 (1%)	85	94
23	U	89/89 (100%)	89 (100%)	0	100	100
24	V	101/101 (100%)	100 (99%)	1 (1%)	78	91
25	W	55/55 (100%)	54 (98%)	1 (2%)	62	85
26	X	107/107 (100%)	106 (99%)	1 (1%)	81	92
27	Y	124/124 (100%)	123 (99%)	1 (1%)	83	93
28	Z	117/117 (100%)	116 (99%)	1 (1%)	81	92
29	a	119/119 (100%)	119 (100%)	0	100	100
30	b	62/62 (100%)	61 (98%)	1 (2%)	65	87
31	c	79/79 (100%)	78 (99%)	1 (1%)	71	88
32	d	98/98 (100%)	96 (98%)	2 (2%)	58	83
33	e	114/114 (100%)	113 (99%)	1 (1%)	81	92
34	f	88/88 (100%)	87 (99%)	1 (1%)	76	90
35	g	98/98 (100%)	96 (98%)	2 (2%)	58	83
36	h	109/109 (100%)	108 (99%)	1 (1%)	81	92
37	i	86/86 (100%)	85 (99%)	1 (1%)	74	89
38	j	73/73 (100%)	71 (97%)	2 (3%)	48	78
39	k	64/64 (100%)	64 (100%)	0	100	100
40	l	47/47 (100%)	44 (94%)	3 (6%)	19	52
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%)	89 (97%)	3 (3%)	41	74
44	p	74/74 (100%)	72 (97%)	2 (3%)	48	78
45	r	109/109 (100%)	105 (96%)	4 (4%)	37	71
46	s	166/166 (100%)	165 (99%)	1 (1%)	87	94
47	t	136/136 (100%)	133 (98%)	3 (2%)	55	81
48	l	22/22 (100%)	21 (96%)	1 (4%)	30	65
52	q	180/181 (99%)	179 (99%)	1 (1%)	87	94
53	u	194/194 (100%)	191 (98%)	3 (2%)	67	87
54	v	187/187 (100%)	185 (99%)	2 (1%)	76	90

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
55	x	224/224 (100%)	222 (99%)	2 (1%)	81	92
56	z	207/207 (100%)	205 (99%)	2 (1%)	78	91
57	y	165/169 (98%)	165 (100%)	0	100	100
58	CC	178/178 (100%)	175 (98%)	3 (2%)	63	85
59	XX	161/161 (100%)	158 (98%)	3 (2%)	60	84
60	EE	130/136 (96%)	127 (98%)	3 (2%)	53	80
61	QQ	130/130 (100%)	129 (99%)	1 (1%)	83	93
62	MM	106/106 (100%)	104 (98%)	2 (2%)	60	84
63	UU	117/117 (100%)	114 (97%)	3 (3%)	49	78
64	YY	119/119 (100%)	119 (100%)	0	100	100
65	HH	67/67 (100%)	66 (98%)	1 (2%)	67	87
66	TT	112/112 (100%)	112 (100%)	0	100	100
67	VV	113/113 (100%)	113 (100%)	0	100	100
68	NN	107/107 (100%)	106 (99%)	1 (1%)	81	92
69	ZZ	88/88 (100%)	88 (100%)	0	100	100
70	JJ	75/75 (100%)	74 (99%)	1 (1%)	71	88
71	AA	46/46 (100%)	44 (96%)	2 (4%)	32	66
72	DD	190/190 (100%)	185 (97%)	5 (3%)	49	78
73	BB	158/161 (98%)	158 (100%)	0	100	100
74	SS	87/87 (100%)	86 (99%)	1 (1%)	76	90
75	RR	99/99 (100%)	98 (99%)	1 (1%)	78	91
76	9	109/109 (100%)	108 (99%)	1 (1%)	81	92
77	II	125/125 (100%)	124 (99%)	1 (1%)	83	93
78	PP	111/111 (100%)	110 (99%)	1 (1%)	81	92
79	GG	92/92 (100%)	91 (99%)	1 (1%)	76	90
80	OO	66/66 (100%)	66 (100%)	0	100	100
81	FF	55/55 (100%)	54 (98%)	1 (2%)	62	85
82	w	48/48 (100%)	48 (100%)	0	100	100
83	0	61/61 (100%)	60 (98%)	1 (2%)	65	87
84	6	272/272 (100%)	270 (99%)	2 (1%)	85	94
All	All	10029/10069 (100%)	9911 (99%)	118 (1%)	75	89

All (118) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	A	64	ARG
4	A	128	ARG
4	A	163	ARG
4	A	193	ARG
4	A	242	ARG
5	B	24	ARG
5	B	62	ARG
6	C	38	ASN
6	C	100	ARG
6	C	114	ARG
6	C	188	ARG
6	C	321	ASN
8	E	52	ARG
8	E	178	ASN
10	G	38	ASN
10	G	81	ASN
10	G	189	ARG
10	G	196	ARG
10	G	240	ASN
11	H	1	MET
11	H	28	LYS
12	I	3	ARG
12	I	100	ASN
12	I	144	ASN
13	J	146	ARG
13	J	151	ILE
14	L	104	ASN
14	L	162	LYS
16	N	38	ARG
17	O	12	ARG
17	O	65	ASN
17	O	94	ARG
17	O	117	ARG
17	O	187	LYS
17	O	191	ARG
18	P	128	ARG
20	R	39	GLN
20	R	133	LYS
22	T	63	ARG
24	V	48	ARG
25	W	45	ASN
26	X	94	ASN

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Mol	Chain	Res	Type
27	Y	2	LYS
28	Z	97	ASN
30	b	60	ASN
31	c	90	ARG
32	d	18	ASN
32	d	23	ARG
33	e	43	ASN
34	f	16	ARG
35	g	21	ARG
35	g	29	ARG
36	h	96	ASN
37	i	29	ARG
38	j	20	ARG
38	j	45	ARG
40	l	21	ARG
40	l	33	ASN
40	l	36	ARG
43	o	9	ARG
43	o	69	ARG
43	o	82	MET
44	p	17	ARG
44	p	49	ARG
45	r	12	ASN
45	r	21	ASN
45	r	31	ASN
45	r	83	ASN
46	s	62	ARG
47	t	1	MET
47	t	40	LYS
47	t	123	ARG
48	l	260	MET
52	q	50	ASN
53	u	40	ASN
53	u	147	ASN
53	u	213	ARG
54	v	167	ARG
54	v	248	TYR
55	x	232	ASN
55	x	240	ARG
56	z	63	MET
56	z	191	ARG
58	CC	84	ASN

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Mol	Chain	Res	Type
58	CC	87	ASN
58	CC	99	ASN
59	XX	69	ARG
59	XX	70	ARG
59	XX	79	ARG
60	EE	20	LYS
60	EE	69	ARG
60	EE	97	ARG
61	QQ	27	LYS
62	MM	146	ARG
62	MM	150	ARG
63	UU	41	MET
63	UU	85	ARG
63	UU	146	ARG
65	HH	82	ASN
68	NN	101	LYS
70	JJ	81	ARG
71	AA	99	LYS
71	AA	104	ARG
72	DD	22	ASN
72	DD	76	ARG
72	DD	94	ARG
72	DD	106	ARG
72	DD	227	LYS
74	SS	96	ARG
75	RR	33	ARG
76	9	13	ARG
77	II	8	LYS
78	PP	62	ARG
79	GG	47	ASN
81	FF	40	ARG
83	0	138	ARG
84	6	159	ASN
84	6	178	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (110) such sidechains are listed below:

Mol	Chain	Res	Type
5	B	167	GLN
5	B	204	GLN
5	B	245	HIS
5	B	302	ASN

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Mol	Chain	Res	Type
5	B	354	GLN
6	C	38	ASN
6	C	50	GLN
7	D	225	GLN
8	E	178	ASN
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	112	GLN
10	G	240	ASN
11	H	8	GLN
11	H	39	ASN
12	I	95	HIS
12	I	144	ASN
14	L	19	GLN
16	N	181	HIS
16	N	201	HIS
17	O	50	ASN
17	O	65	ASN
17	O	199	HIS
18	P	75	GLN
18	P	80	GLN
20	R	58	HIS
20	R	130	ASN
21	S	50	GLN
21	S	163	HIS
22	T	3	ASN
22	T	95	HIS
22	T	127	GLN
24	V	77	HIS
25	W	17	HIS
25	W	45	ASN
26	X	93	ASN
26	X	94	ASN
26	X	111	GLN
28	Z	97	ASN
29	a	14	HIS

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Mol	Chain	Res	Type
31	c	15	ASN
31	c	51	ASN
32	d	18	ASN
32	d	30	HIS
33	e	43	ASN
33	e	52	GLN
34	f	80	ASN
34	f	99	HIS
35	g	100	GLN
35	g	112	GLN
36	h	63	GLN
36	h	96	ASN
40	l	33	ASN
44	p	92	GLN
45	r	12	ASN
45	r	21	ASN
45	r	31	ASN
45	r	83	ASN
46	s	191	GLN
48	l	253	GLN
52	q	50	ASN
52	q	111	GLN
52	q	141	ASN
53	u	101	HIS
53	u	124	HIS
53	u	147	ASN
53	u	157	GLN
54	v	113	GLN
54	v	272	HIS
55	x	36	HIS
55	x	67	GLN
55	x	232	ASN
56	z	81	HIS
56	z	202	ASN
57	y	186	ASN
58	CC	84	ASN
58	CC	87	ASN
58	CC	88	ASN
58	CC	99	ASN
58	CC	138	ASN
58	CC	165	GLN
60	EE	83	GLN

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Mol	Chain	Res	Type
62	MM	94	HIS
63	UU	11	GLN
63	UU	35	ASN
63	UU	80	GLN
63	UU	97	GLN
64	YY	62	GLN
65	HH	47	ASN
65	HH	82	ASN
66	TT	113	HIS
68	NN	15	ASN
68	NN	63	HIS
71	AA	117	ASN
72	DD	22	ASN
73	BB	114	ASN
74	SS	44	HIS
75	RR	48	HIS
75	RR	82	ASN
76	9	41	GLN
79	GG	47	ASN
81	FF	29	GLN
84	6	159	ASN
84	6	178	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	5	3649/3662 (99%)	841 (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%)	352 (20%)	22 (1%)
85	4	9/10 (90%)	4 (44%)	0
All	All	5764/5797 (99%)	1289 (22%)	97 (1%)

All (1289) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	5	2	G
1	5	8	U
1	5	11	G

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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	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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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	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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
51	K	1664	A

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates 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
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