



Full wwPDB/EMDatabank EM Map/Model Validation Report ⓘ

Jan 30, 2018 – 11:36 AM EST

PDB ID : 6ELZ
EMDB ID: : EMD-3891
Title : State E (TAP-Flag-Ytm1 E80A) - Visualizing the assembly pathway of nucleolar pre-60S ribosomes
Authors : Kater, L.; Cheng, J.; Barrio-Garcia, C.; Hurt, E.; Beckmann, R.
Deposited on : 2017-09-30
Resolution : 3.30 Å(reported)

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
<http://wwpdb.org/validation/2016/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

MolProbity : 4.02b-467
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20030736

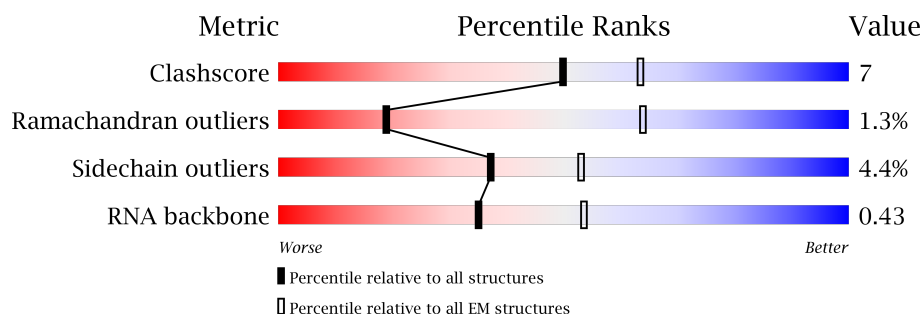
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.30 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.









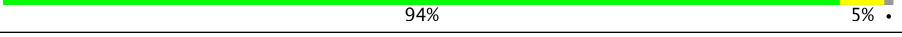

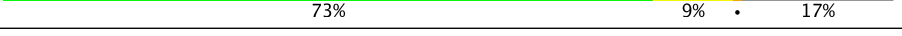

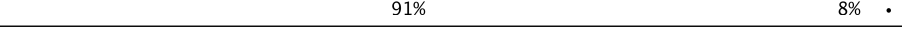
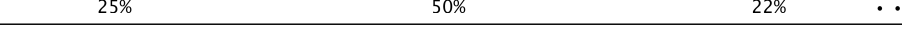

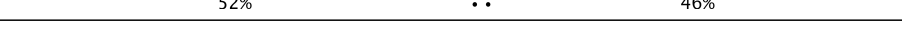


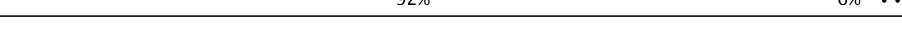
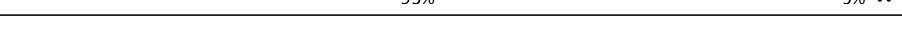
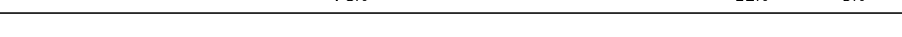






Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	125131	1336
Ramachandran outliers	121729	1120
Sidechain outliers	121581	1026
RNA backbone	3398	335

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	1	3396	35% 29% 8% 28%
2	2	158	58% 38% .
3	6	232	12% 10% 6% 72%
4	L	199	50% 10% . 39%
5	N	204	71% 18% . 9%
6	Q	186	61% 10% . 28%
7	R	189	52% 11% . 37%
8	S	172	81% 15% ...








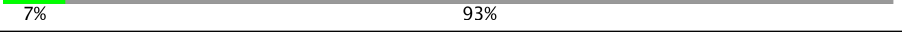
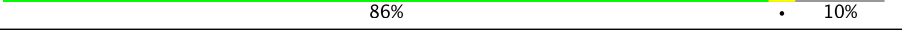
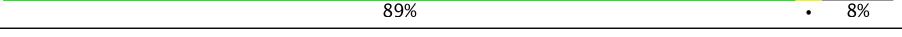
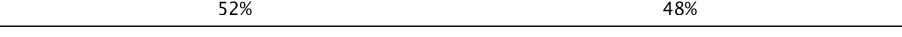

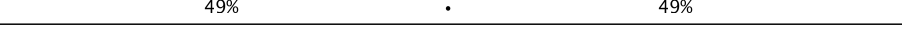
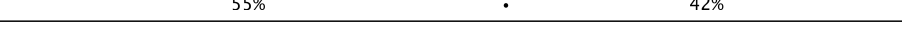
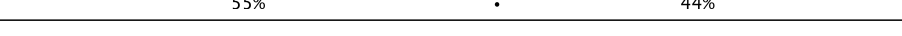
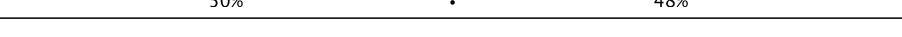

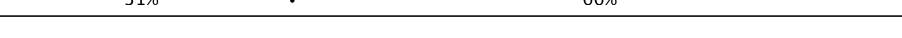
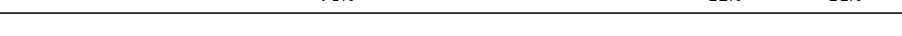


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Mol	Chain	Length	Quality of chain
9	T	160	
10	U	121	
11	Z	136	
12	c	105	
13	d	113	
14	e	130	
15	f	107	
16	g	121	
17	i	100	
18	j	88	
19	k	78	
20	O	199	
21	V	137	
22	a	149	
23	P	184	
24	X	142	
25	Y	127	
26	h	120	
27	F	244	
28	B	387	
29	C	362	
30	H	191	
31	A	291	
32	K	376	
33	m	807	

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Mol	Chain	Length	Quality of chain
34	D	505	
35	W	236	
36	l	181	
37	b	647	
38	o	220	
39	n	605	
40	r	261	
41	s	520	
42	t	322	
43	y	245	
44	z	106	
45	p	460	
46	q	618	
47	u	199	
48	v	231	
49	w	841	
50	I	663	
51	J	427	
52	E	176	
53	G	256	
54	M	138	

2 Entry composition

There are 55 unique types of molecules in this entry. The entry contains 134887 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 25S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	1	2457	Total	C	N	O	P	0	0
			52595	23485	9508	17146	2456		

- Molecule 2 is a RNA chain called 5.8S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	2	158	Total	C	N	O	P	0	0
			3353	1500	586	1109	158		

- Molecule 3 is a RNA chain called Internal transcribed spacer 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	6	65	Total	C	N	O	P	0	0
			1370	614	228	463	65		

- Molecule 4 is a protein called 60S ribosomal protein L13-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
4	L	122	Total	C	N	O	0	0
			998	628	209	161		

- Molecule 5 is a protein called 60S ribosomal protein L15-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	N	186	Total	C	N	O	S	0	0
			1587	994	333	259	1		

- Molecule 6 is a protein called 60S ribosomal protein L18-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	Q	134	Total	C	N	O	S	0	0
			1035	659	196	179	1		

- Molecule 7 is a protein called 60S ribosomal protein L19-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
7	R	120	Total	C	N	O	0	0
			964	610	194	160		

- Molecule 8 is a protein called 60S ribosomal protein L20-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	S	170	Total	C	N	O	S	0	0
			1432	922	265	242	3		

- Molecule 9 is a protein called 60S ribosomal protein L21-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	T	55	Total	C	N	O	S	0	0
			422	259	85	77	1		

- Molecule 10 is a protein called 60S ribosomal protein L22-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
10	U	98	Total	C	N	O	0	0
			778	505	127	146		

- Molecule 11 is a protein called 60S ribosomal protein L27-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
11	Z	135	Total	C	N	O	0	0
			1092	710	202	180		

- Molecule 12 is a protein called 60S ribosomal protein L30.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	c	97	Total	C	N	O	S	0	0
			743	479	124	139	1		

- Molecule 13 is a protein called 60S ribosomal protein L31-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	d	107	Total	C	N	O	S	0	0
			873	553	165	154	1		

- Molecule 14 is a protein called 60S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	e	125	Total	C	N	O	S	0	0
			1009	641	203	164	1		

- Molecule 15 is a protein called 60S ribosomal protein L33-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	f	106	Total	C	N	O	S	0	0
			850	540	165	144	1		

- Molecule 16 is a protein called 60S ribosomal protein L34-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	g	112	Total	C	N	O	S	0	0
			881	546	179	152	4		

- Molecule 17 is a protein called 60S ribosomal protein L36-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	i	83	Total	C	N	O	S	0	0
			658	408	135	113	2		

- Molecule 18 is a protein called 60S ribosomal protein L37-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	j	73	Total	C	N	O	S	0	0
			580	353	126	96	5		

- Molecule 19 is a protein called 60S ribosomal protein L38.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	k	77	Total	C	N	O	S	0	0
			612	391	115	106			

- Molecule 20 is a protein called 60S ribosomal protein L16-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	O	197	Total	C	N	O	S	0	0
			1555	1003	289	262	1		

- Molecule 21 is a protein called 60S ribosomal protein L23-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	V	134	Total	C	N	O	S	0	0
			993	623	187	176	7		

- Molecule 22 is a protein called 60S ribosomal protein L28.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	a	81	Total	C	N	O		0	0
			626	408	108	110			

- Molecule 23 is a protein called 60S ribosomal protein L17-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	P	183	Total	C	N	O		0	0
			1442	896	287	259			

- Molecule 24 is a protein called 60S ribosomal protein L25.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	X	141	Total	C	N	O	S	0	0
			1100	705	196	197	2		

- Molecule 25 is a protein called 60S ribosomal protein L26-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	Y	126	Total	C	N	O		0	0
			993	625	192	176			

- Molecule 26 is a protein called 60S ribosomal protein L35-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	h	119	Total	C	N	O	S	0	0
			969	615	186	167	1		

- Molecule 27 is a protein called 60S ribosomal protein L7-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	F	222	Total	C	N	O	S	0	0
			1784	1151	324	308	1		

- Molecule 28 is a protein called 60S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	B	341	Total	C	N	O	S	0	0
			2702	1715	501	480	6		

- Molecule 29 is a protein called 60S ribosomal protein L4-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	C	359	Total	C	N	O	S	0	0
			2731	1720	518	490	3		

- Molecule 30 is a protein called 60S ribosomal protein L9-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	H	190	Total	C	N	O	S	0	0
			1510	957	273	276	4		

- Molecule 31 is a protein called Ribosome biogenesis protein BRX1.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	A	198	Total	C	N	O	S	0	0
			1623	1043	284	290	6		

- Molecule 32 is a protein called Proteasome-interacting protein CIC1.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	K	257	Total	C	N	O	S	0	0
			2073	1337	341	392	3		

- Molecule 33 is a protein called Ribosome biogenesis protein ERB1.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	m	645	Total	C	N	O	S	0	0
			5223	3322	907	979	15		

- Molecule 34 is a protein called ATP-dependent RNA helicase HAS1.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	D	194	Total	C	N	O	S	0	0
			1590	1030	268	287	5		

- Molecule 35 is a protein called Ribosome assembly factor MRT4.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	W	232	Total	C	N	O	S	0	0
			1870	1184	321	360	5		

- Molecule 36 is a protein called 60S ribosome subunit biogenesis protein NIP7.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	l	174	Total	C	N	O	S	0	0
			1377	887	242	241	7		

- Molecule 37 is a protein called Nucleolar GTP-binding protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	b	421	Total	C	N	O	S	0	0
			3410	2180	585	627	18		

- Molecule 38 is a protein called Ribosome biogenesis protein 15.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	o	133	Total	C	N	O	S	0	0
			1107	716	198	189	4		

- Molecule 39 is a protein called Pescadillo homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	n	411	Total	C	N	O	S	0	0
			3369	2179	585	592	13		

- Molecule 40 is a protein called Ribosome biogenesis protein NSA2.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	r	176	Total	C	N	O	S	0	0
			1438	906	279	248	5		

- Molecule 41 is a protein called Nuclear GTP-binding protein NUG1.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	s	36	Total	C	N	O	S	0	0
			301	184	69	46	2		

- Molecule 42 is a protein called Ribosome biogenesis protein RLP7.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	t	290	Total	C	N	O	S	0	0
			2328	1472	431	422	3		

- Molecule 43 is a protein called Eukaryotic translation initiation factor 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	y	225	Total	C	N	O	S	0	0
			1701	1056	295	343	7		

- Molecule 44 is a protein called UPF0642 protein YBL028C.

Mol	Chain	Residues	Atoms				AltConf	Trace
44	z	55	Total	C	N	O	0	0
			444	273	88	83		

- Molecule 45 is a protein called Ribosome biogenesis protein YTM1.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	p	298	Total	C	N	O	S	0	0
			2321	1448	410	457	6		

- Molecule 46 is a protein called 25S rRNA (cytosine(2870)-C(5))-methyltransferase.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	q	317	Total	C	N	O	S	0	0
			2485	1591	429	455	10		

- Molecule 47 is a protein called Ribosome biogenesis protein RLP24.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	u	116	Total	C	N	O	S	0	0
			976	612	200	155	9		

- Molecule 48 is a protein called Nucleolar protein 16.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	v	130	Total	C	N	O	S	0	0
			1087	678	211	195	3		

- Molecule 49 is a protein called 27S pre-rRNA (guanosine(2922)-2'-O)-methyltransferase.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	w	436	Total	C	N	O	S	0	0
			3511	2235	628	630	18		

- Molecule 50 is a protein called Nucleolar complex-associated protein 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	I	433	Total	C	N	O	S	0	1
			3470	2217	591	645	17		

- Molecule 51 is a protein called rRNA-processing protein EBP2.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	J	145	Total	C	N	O	S	0	0
			1215	759	225	228	3		

- Molecule 52 is a protein called 60S ribosomal protein L6-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	E	156	Total	C	N	O	S	0	0
			1239	800	222	216	1		

- Molecule 53 is a protein called 60S ribosomal protein L8-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	G	184	Total	C	N	O	S	0	0
			1438	930	249	257	2		

- Molecule 54 is a protein called 60S ribosomal protein L14-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	M	136	Total	C	N	O	S	0	0
			1053	675	199	177	2		

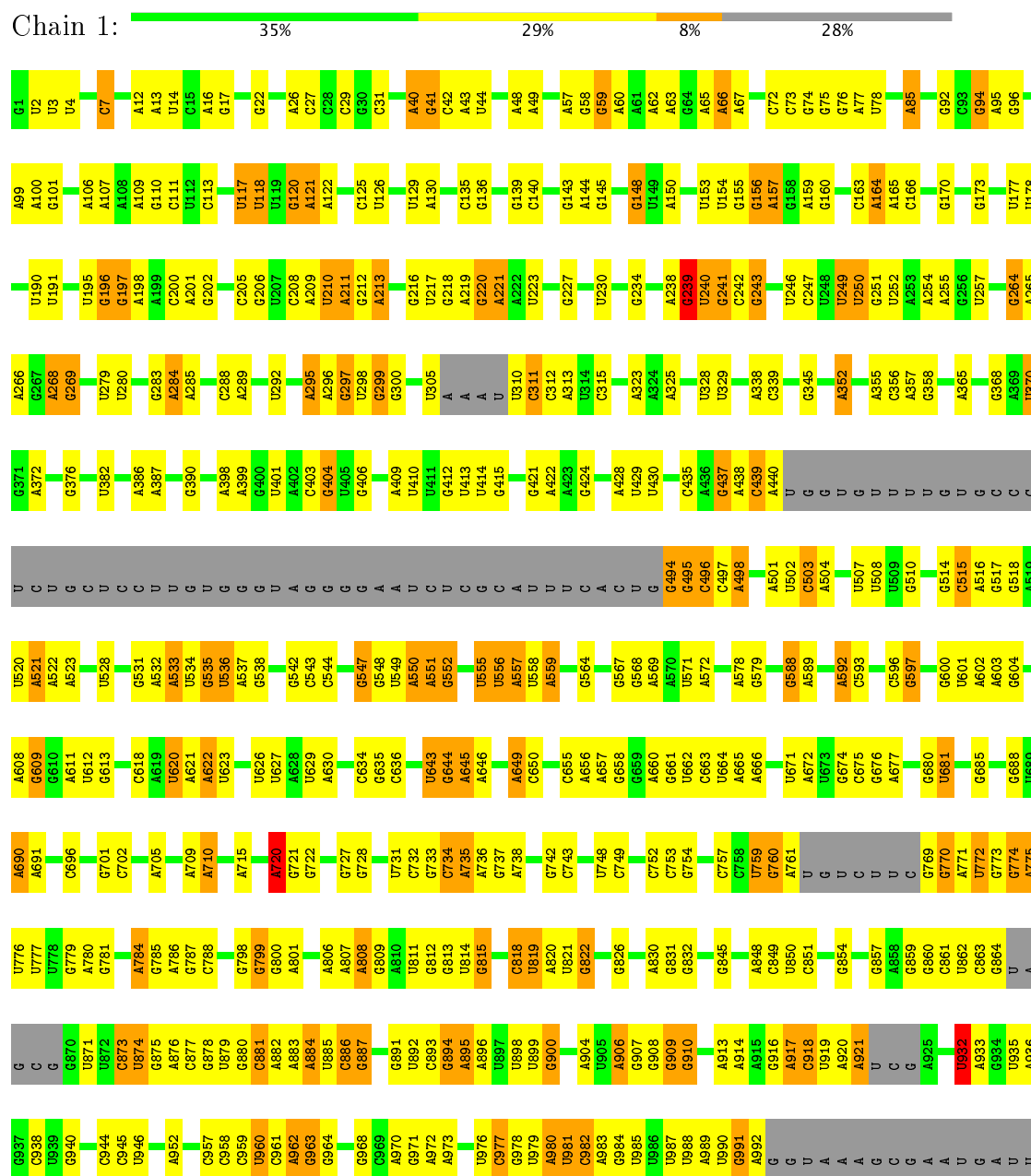
- Molecule 55 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
55	j	1	Total	Zn	0
			1	1	

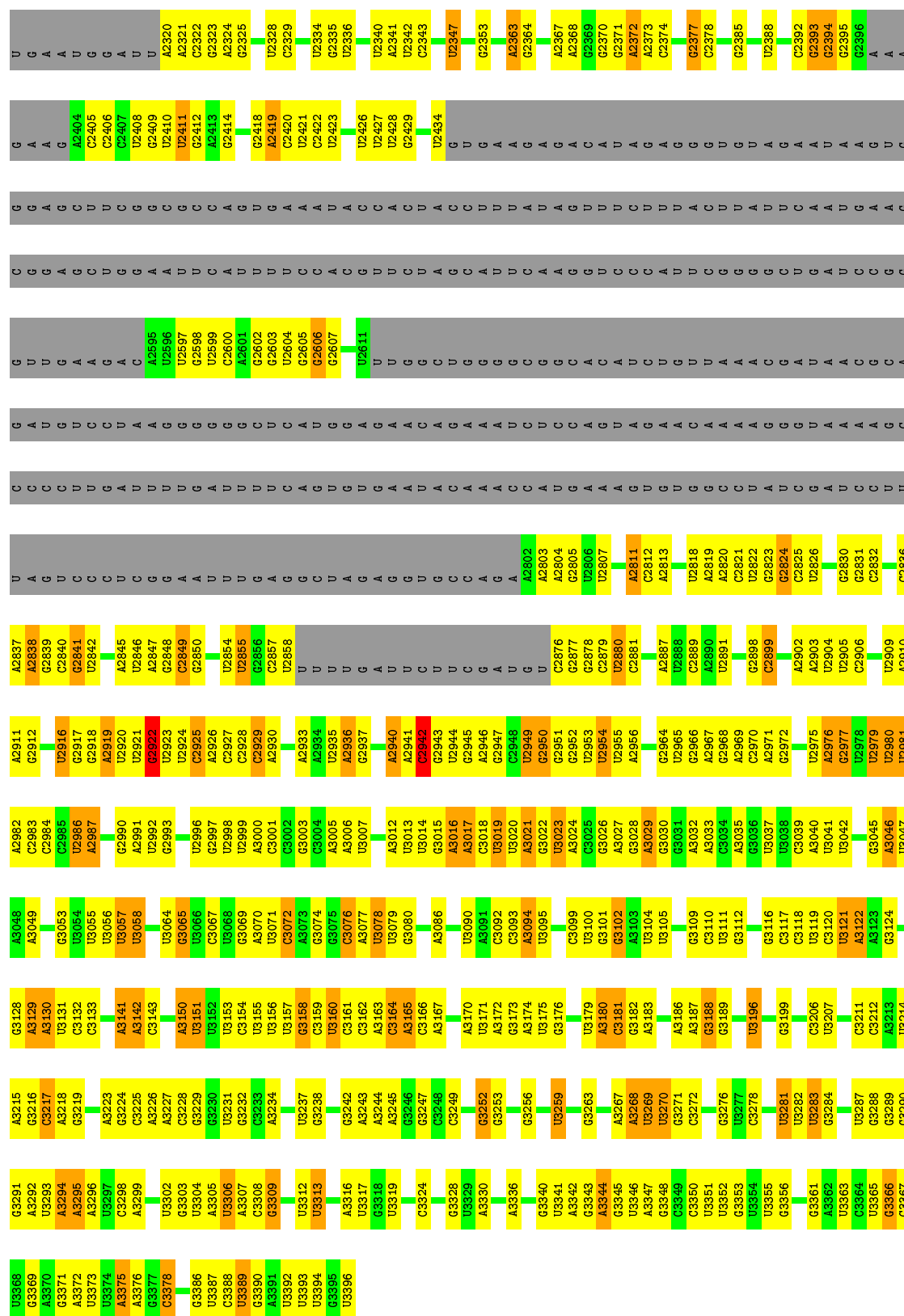
3 Residue-property plots

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: 25S ribosomal RNA

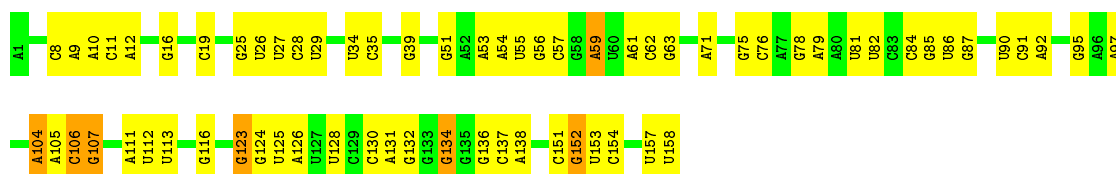




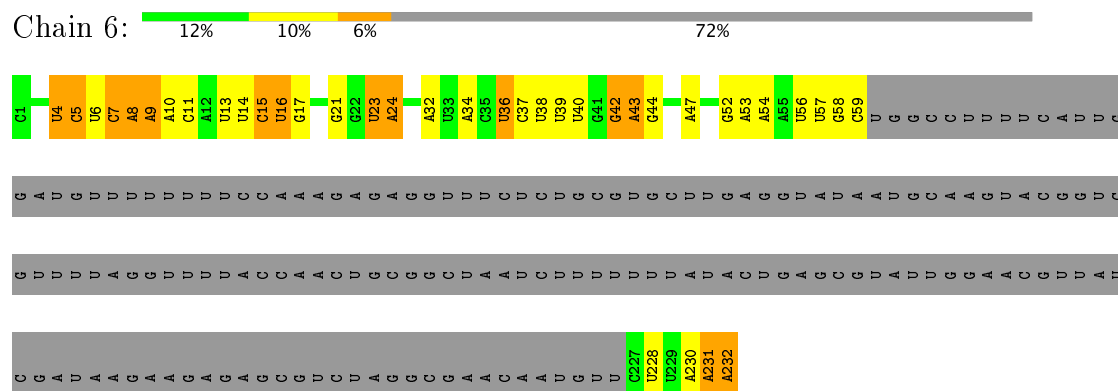



- Molecule 2: 5.8S ribosomal RNA

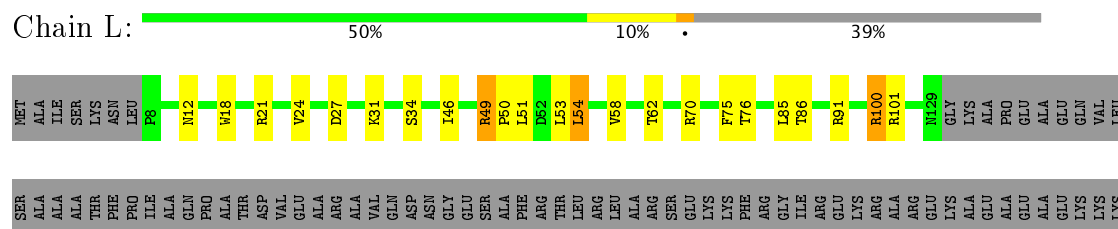




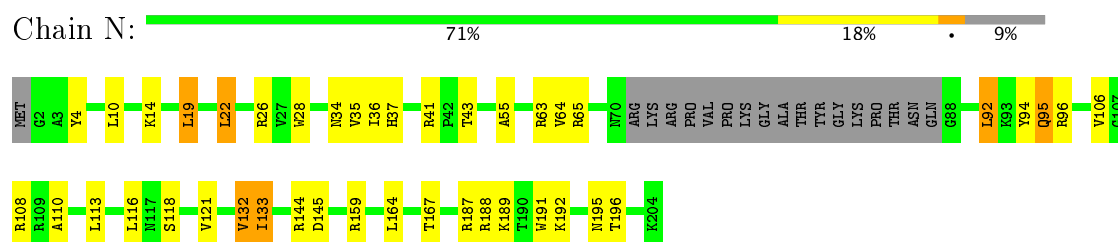
- Molecule 3: Internal transcribed spacer 2



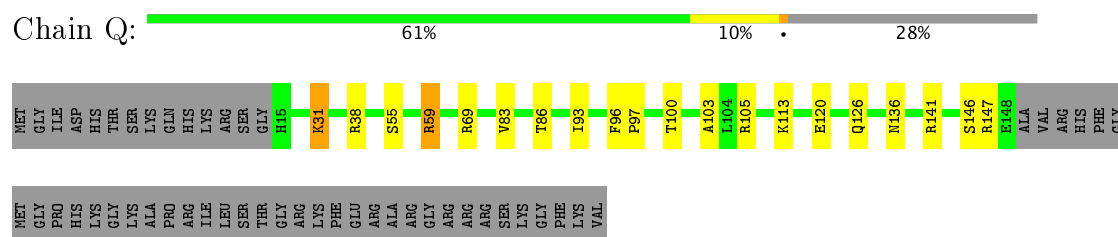
- Molecule 4: 60S ribosomal protein L13-A



- Molecule 5: 60S ribosomal protein L15-A




- Molecule 6: 60S ribosomal protein L18-A



- Molecule 7: 60S ribosomal protein L19-A



Chain d:  89% . . 5%



- Molecule 14: 60S ribosomal protein L32

Chain e:  92% 5% .




- Molecule 15: 60S ribosomal protein L33-A

Chain f:  94% 5% .



- Molecule 16: 60S ribosomal protein L34-A

Chain g:  84% 8% 7%



- Molecule 17: 60S ribosomal protein L36-A

Chain i:  73% 9% 17%



- Molecule 18: 60S ribosomal protein L37-A

Chain j:  73% 10% 17%



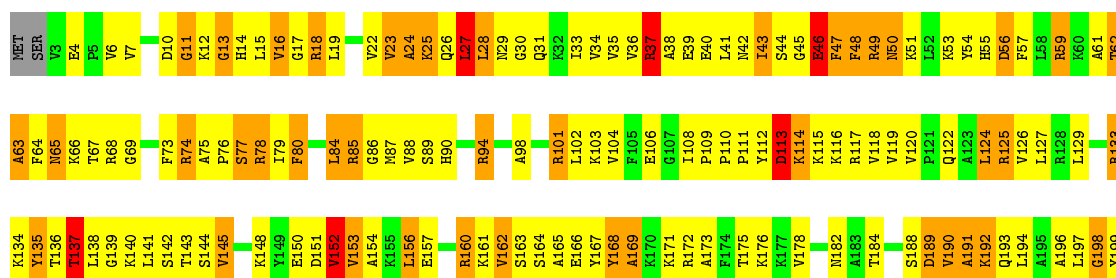
- Molecule 19: 60S ribosomal protein L38

Chain k:  91% 8% .



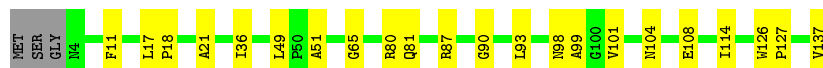
- Molecule 20: 60S ribosomal protein L16-A

Chain O:  25% 50% 22% . .



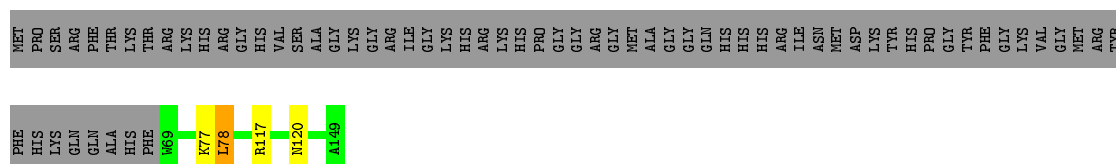
- Molecule 21: 60S ribosomal protein L23-A

Chain V: 82% 16%



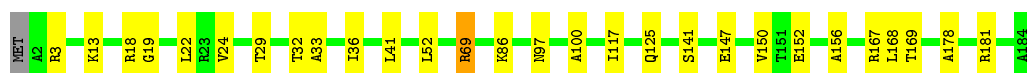
- Molecule 22: 60S ribosomal protein L28

Chain a: 52% 46%



- Molecule 23: 60S ribosomal protein L17-A

Chain P: 84% 15%



- Molecule 24: 60S ribosomal protein L25

Chain X: 90% 9%



- Molecule 25: 60S ribosomal protein L26-A

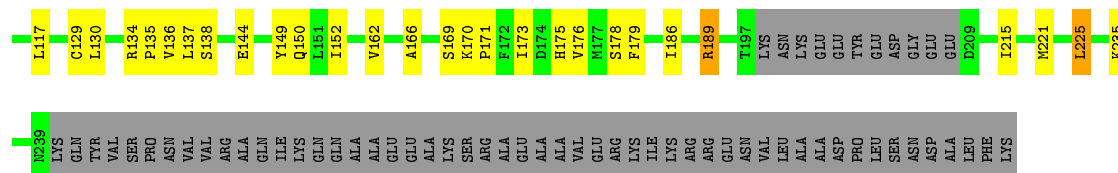
Chain Y: 92% 6%



- Molecule 26: 60S ribosomal protein L35-A

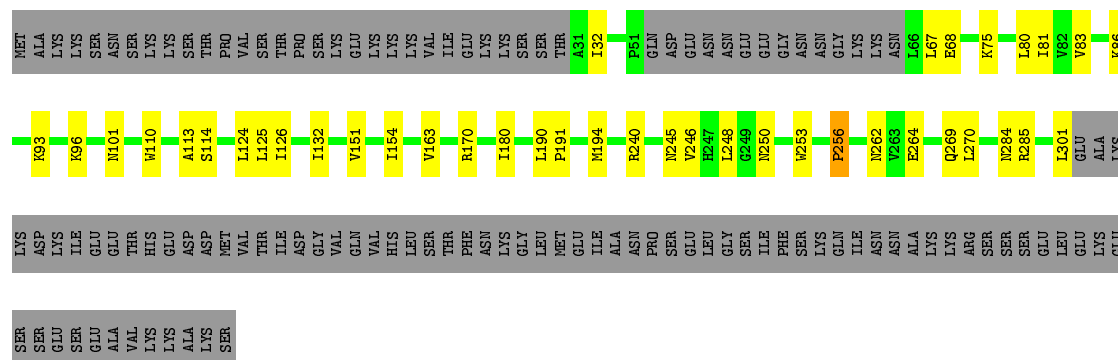
Chain h: 93% 5%





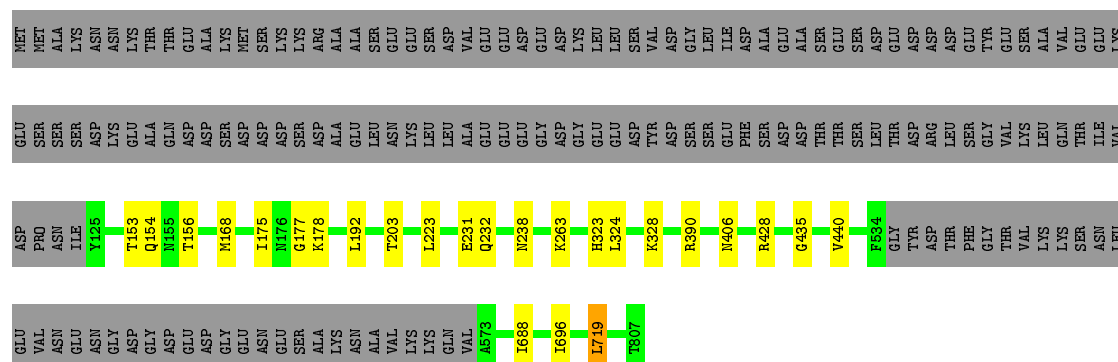
- Molecule 32: Proteasome-interacting protein CIC1

Chain K: 



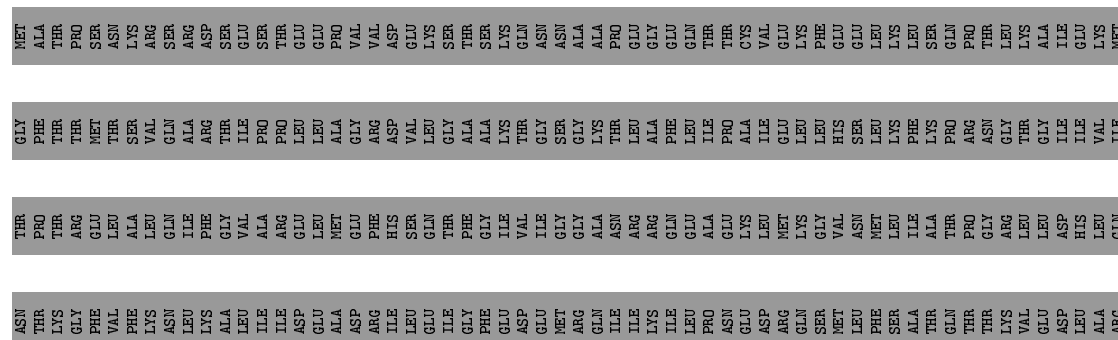
- Molecule 33: Ribosome biogenesis protein ERB1

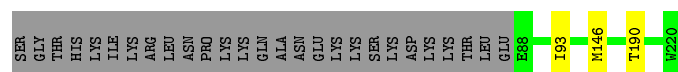
Chain m: 77% . 20%



- Molecule 34: ATP-dependent RNA helicase HAS1

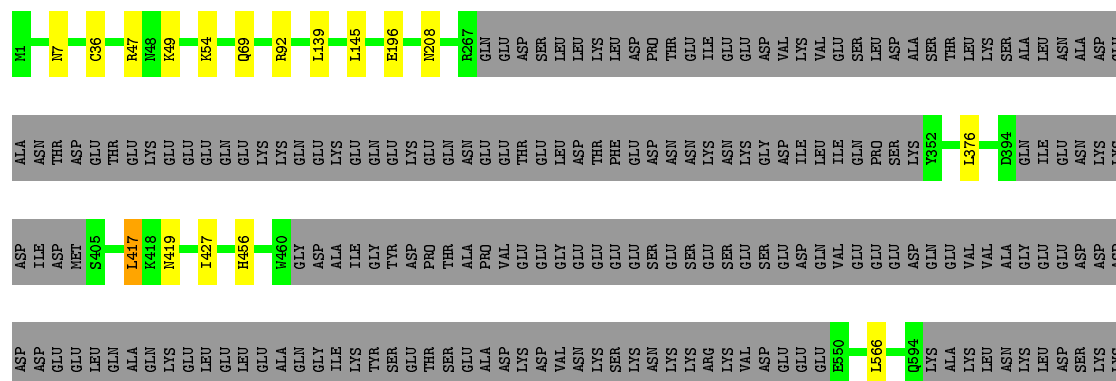
Chain D:  34% 5% 62%





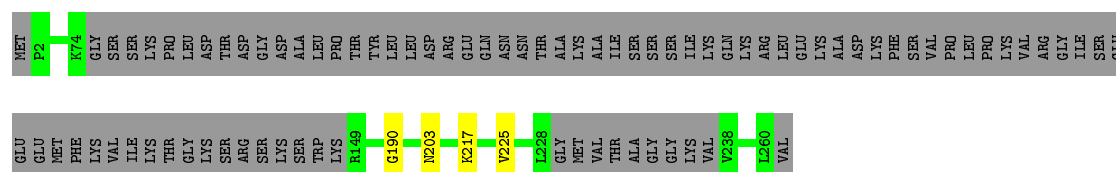
- Molecule 39: Pescadillo homolog

Chain n: 65% 32%



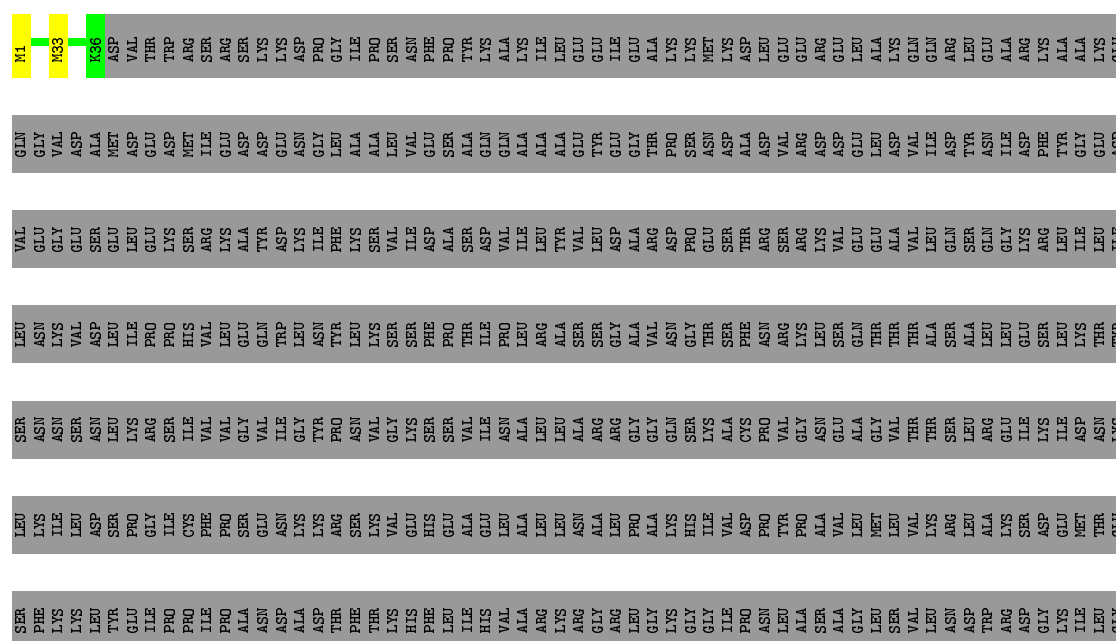
- Molecule 40: Ribosome biogenesis protein NSA2

Chain r: 66% 33%



- Molecule 41: Nuclear GTP-binding protein NUG1

Chain s: 7% 93%



- Molecule 42: Ribosome biogenesis protein RLP7

Chain t: 86% 10%

ME1	SER	SER	THR	GLN	ASP	SER	LYS	ALA	GLN	THR	L142	M15	L166	E105	LYS	ALA	ASN	GLY	ALA	GLU	GLI	ASN	ASP	VAL	LEU	GLI	GLU	THR	GLU	GLU	GLU	GLI	ASP	ASP	G127	L151	M157	L187	I227	G240	Q269	P270	R275	E276	V277	Q291
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- Molecule 43: Eukaryotic translation initiation factor 6

Chain y: 89% • 8%

W1	I58	R100	L101	V114	N145	I146	L154	L173	Q225	ASP	ALA	GLN	PRO	GLU	SER	SER	SER	GLY	ASN	LEU	ARG	ASP	ASP	THR	THR	LEU	ILE	GLU	THR	TYR	SER
----	-----	------	------	------	------	------	------	------	------	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

- Molecule 44: UPF0642 protein YBL028C

Chain z:  52% 48%

MET	A2	G56	ILE	ASP	ASP	MET	ASP	VAL	ASP	GLU	LYS	LYS	SER	ASN	GLU	GLU	ALA	PRO	ARG	ARG	LYS	LYS	ILE	SER	THR	SER	SER	GLY	TRP	ARG	ASP	GLY	ARG	HIS	HIS	THR	TYP	LYS	LYS	ALA	LYS	LEU	MET	MET	LYS	GLN	SER	SER	LYS	LYS	LYS	THR	LYS	THR	PHE	SER	SER	THR	THR	ARG	DHF
-----	----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

- Molecule 45: Ribosome biogenesis protein YTM1

Chain p:  63% . 35%

[illegible][illegible]

ASP	GLU	VAL	ASP	ILE	GLU	D197	V244	PRO	LEU	GLU	ASP	ASN	ASN	PRO	ASN	ASN	LYS	ILE	SER	THR	ALA	ALA	ARG	ARG	LYS	LEU	THR	ILE	R276	R276	R351	R359	VAL	GLY	ALA	SER	SER	LYS	VAL	T667	D418	K419	S420	VAL	ILE
-----	-----	-----	-----	-----	-----	------	------	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	------	------	------	------	-----	-----	-----	-----	-----	-----	-----	------	------	------	------	-----	-----

LYS	G424	K453	GLY	ASP	ASN	ILE	PHE	LYS	ASN
-----	------	------	-----	-----	-----	-----	-----	-----	-----

- Molecule 46: 25S rRNA (cytosine(2870)-C(5))-methyltransferase

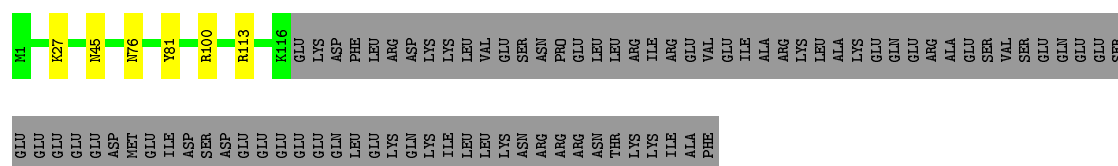
Chain q:

[illegible]



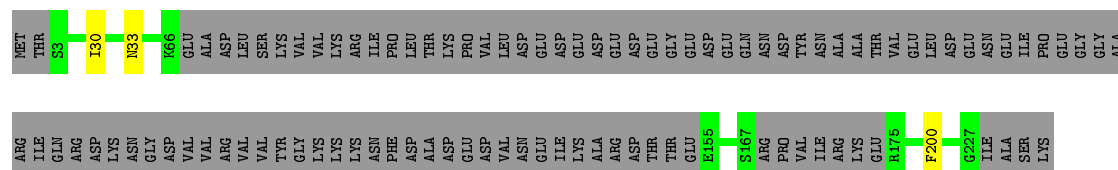
• Molecule 47: Ribosome biogenesis protein RLP24

Chain u: 55% 42%



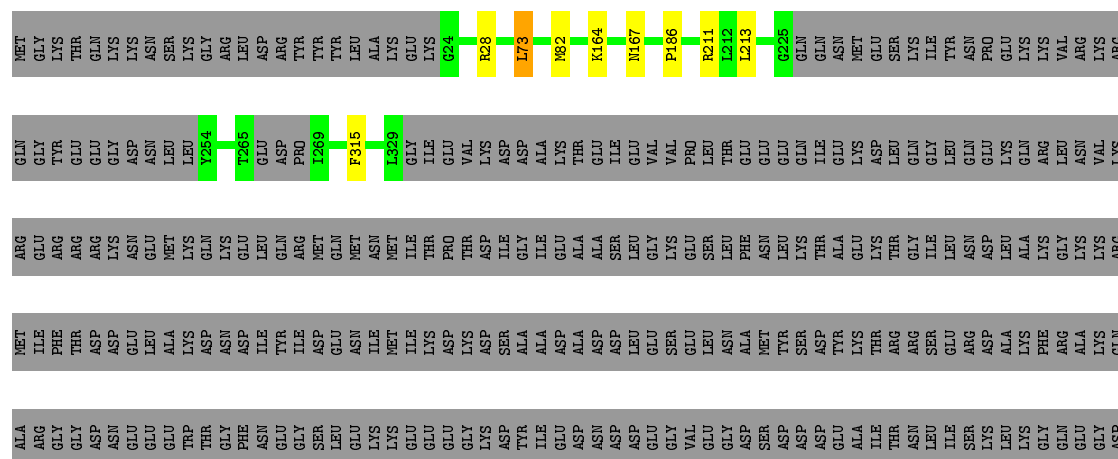
• Molecule 48: Nucleolar protein 16

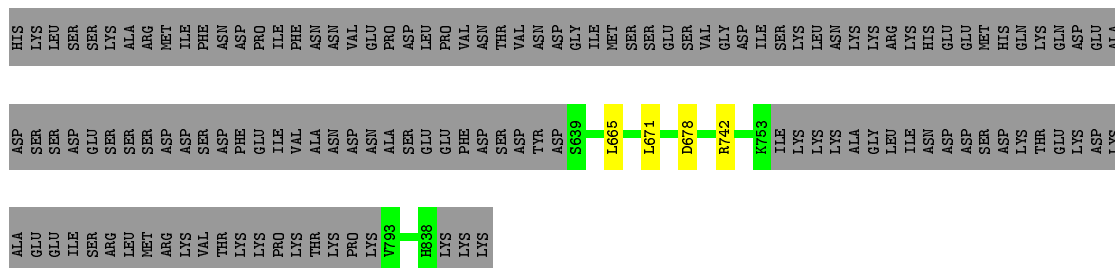
Chain v: 55% 44%



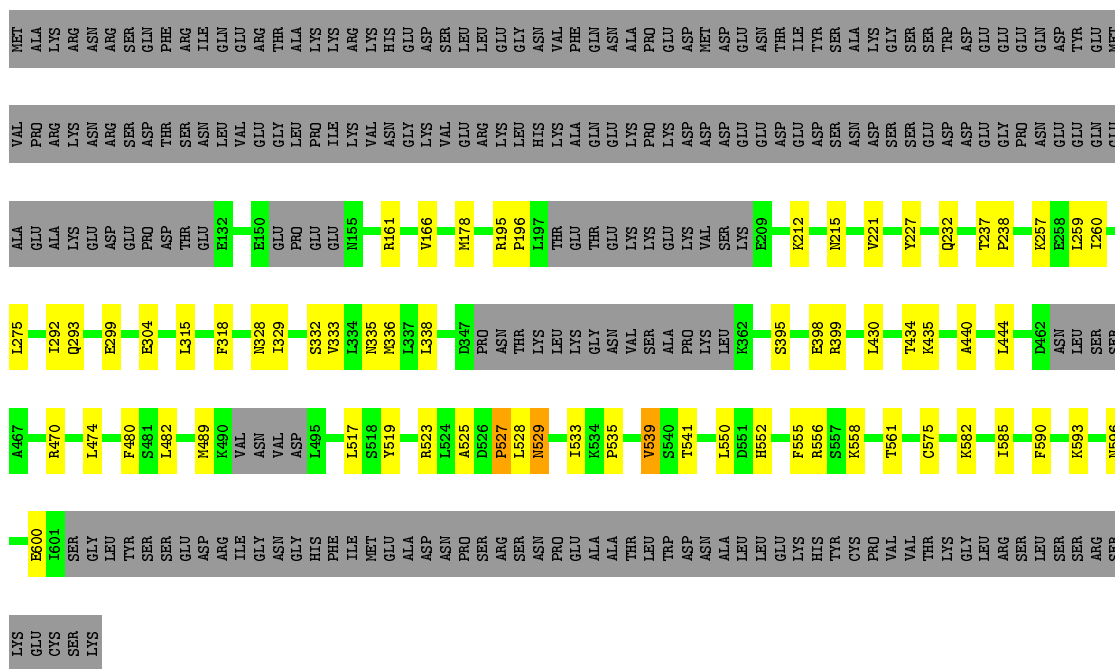
• Molecule 49: 27S pre-rRNA (guanosine(2922)-2'-O)-methyltransferase

Chain w: 50% 48%

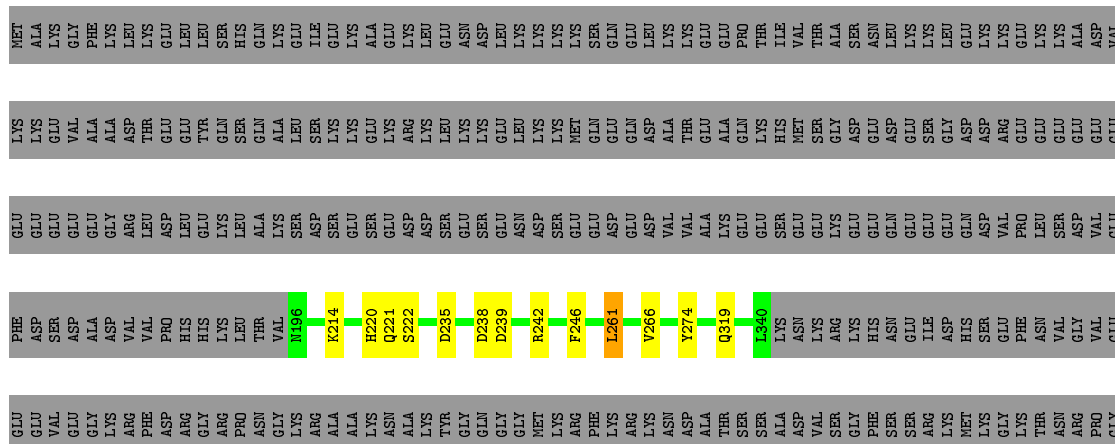




- Molecule 50: Nucleolar complex-associated protein 3



- Molecule 51: rRNA-processing protein EBP2



MET	SR	T3	V7	K8	V15	E16	V17	K25	A29	I38	V44	L45	I46	R55	Q66	N69	G61	Q62	V63	L72	P73	R74	R77	V81	M85	R124	R128	V131	L135	L138
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4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	112099	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 ($e^-/\text{\AA}^2$)	27	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

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	1	0.26	2/58862 (0.0%)	0.70	18/91746 (0.0%)
10	U	0.45	0/794	0.59	0/1076
11	Z	0.41	0/1118	0.65	0/1497
12	c	0.42	0/751	0.63	0/1008
13	d	0.38	0/887	0.64	1/1191 (0.1%)
14	e	0.38	0/1030	0.65	1/1379 (0.1%)
15	f	0.37	0/868	0.63	0/1168
16	g	0.37	0/891	0.65	0/1191
17	i	0.40	0/665	0.76	1/884 (0.1%)
18	j	0.39	0/592	0.68	0/785
19	k	0.39	0/618	0.66	0/826
2	2	0.25	0/3746	0.67	1/5832 (0.0%)
20	O	0.28	0/1585	0.44	0/2128
21	V	0.39	0/1008	0.63	0/1356
22	a	0.41	0/637	0.63	0/862
23	P	0.38	0/1464	0.62	0/1965
24	X	0.39	0/1116	0.64	1/1503 (0.1%)
25	Y	0.37	0/1004	0.66	0/1341
26	h	0.37	0/978	0.63	1/1301 (0.1%)
27	F	0.40	0/1821	0.63	0/2451
28	B	0.41	0/2756	0.66	0/3702
29	C	0.38	0/2782	0.64	1/3766 (0.0%)
3	6	0.27	0/1527	0.75	0/2371
30	H	0.38	0/1531	0.60	0/2062
31	A	0.40	0/1663	0.67	0/2248
32	K	0.42	0/2107	0.65	0/2845
33	m	0.40	0/5356	0.65	1/7264 (0.0%)
34	D	0.44	0/1626	0.65	0/2193
35	W	0.42	0/1902	0.64	0/2564
36	l	0.42	0/1407	0.66	1/1896 (0.1%)
37	b	0.42	0/3474	0.63	1/4683 (0.0%)
38	o	0.42	0/1129	0.65	0/1502

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >2	RMSZ	# Z >2
39	n	0.40	0/3441	0.61	1/4625 (0.0%)
4	L	0.39	0/1016	0.70	0/1363
40	r	0.37	0/1462	0.60	0/1952
41	s	0.32	0/301	0.60	0/386
42	t	0.39	0/2355	0.65	0/3158
43	y	0.40	0/1722	0.62	0/2343
44	z	0.36	0/445	0.62	0/585
45	p	0.42	0/2362	0.67	1/3200 (0.0%)
46	q	0.44	0/2536	0.64	0/3433
47	u	0.41	0/996	0.61	0/1324
48	v	0.38	0/1100	0.59	0/1456
49	w	0.40	0/3571	0.63	2/4789 (0.0%)
5	N	0.38	0/1619	0.69	0/2166
50	I	0.41	0/3515	0.63	0/4725
51	J	0.39	0/1232	0.62	0/1642
52	E	0.39	0/1260	0.66	0/1694
53	G	0.41	0/1463	0.70	0/1978
54	M	0.38	0/1068	0.63	0/1438
6	Q	0.40	0/1050	0.68	0/1419
7	R	0.38	0/977	0.66	0/1310
8	S	0.41	0/1468	0.64	0/1973
9	T	0.41	0/427	0.70	0/576
All	All	0.34	2/143081 (0.0%)	0.67	32/206121 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
5	N	0	1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1	2981	U	C1'-N1	5.54	1.57	1.48
1	1	2942	C	C1'-N1	5.06	1.56	1.48

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	649	A	C2'-C3'-O3'	8.32	127.80	109.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	932	U	N1-C1'-C2'	7.62	123.90	114.00
33	m	719	LEU	CA-CB-CG	7.58	132.74	115.30
17	i	57	LEU	CA-CB-CG	7.46	132.46	115.30
37	b	277	LEU	CA-CB-CG	6.73	130.77	115.30
45	p	109	LEU	CA-CB-CG	6.72	130.75	115.30
1	1	1227	C	C2'-C3'-O3'	6.68	124.39	113.70
1	1	644	G	C2'-C3'-O3'	6.41	123.95	113.70
36	l	54	LEU	CA-CB-CG	6.25	129.67	115.30
1	1	2922	G	C2'-C3'-O3'	6.25	123.69	113.70
39	n	417	LEU	CA-CB-CG	6.10	129.32	115.30
14	e	82	LEU	CA-CB-CG	6.03	129.18	115.30
2	2	123	G	C2'-C3'-O3'	5.95	123.21	113.70
29	C	313	LEU	CA-CB-CG	5.85	128.75	115.30
1	1	1307	G	C2'-C3'-O3'	5.81	123.00	113.70
1	1	239	G	C2'-C3'-O3'	5.79	122.97	113.70
1	1	292	U	O4'-C1'-N1	5.59	112.67	108.20
49	w	213	LEU	CA-CB-CG	5.59	128.15	115.30
1	1	2954	U	C2'-C3'-O3'	5.54	122.57	113.70
26	h	28	LEU	CA-CB-CG	5.46	127.86	115.30
1	1	221	A	O4'-C1'-N9	5.35	112.48	108.20
49	w	73	LEU	CA-CB-CG	5.26	127.41	115.30
1	1	1203	A	N9-C1'-C2'	5.22	120.78	114.00
1	1	1299	U	N1-C1'-C2'	-5.19	106.29	112.00
1	1	720	A	C2'-C3'-O3'	5.14	121.93	113.70
1	1	2940	A	C4'-C3'-O3'	5.12	123.24	113.00
1	1	1861	G	C2'-C3'-O3'	5.12	121.89	113.70
1	1	1299	U	C5'-C4'-O4'	5.10	115.22	109.10
13	d	87	ASN	C-N-CD	-5.10	109.38	120.60
24	X	40	LEU	CA-CB-CG	5.06	126.93	115.30
1	1	1820	U	C2'-C3'-O3'	5.02	121.72	113.70
1	1	1108	U	O4'-C1'-N1	5.00	112.20	108.20

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
5	N	92	LEU	Peptide

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	1	52595	0	26437	649	0
2	2	3353	0	1695	34	0
3	6	1370	0	692	17	0
4	L	998	0	1051	14	0
5	N	1587	0	1635	21	0
6	Q	1035	0	1115	9	0
7	R	964	0	1039	10	0
8	S	1432	0	1470	15	0
9	T	422	0	441	7	0
10	U	778	0	791	7	0
11	Z	1092	0	1155	10	0
12	c	743	0	797	0	0
13	d	873	0	914	0	0
14	e	1009	0	1080	0	0
15	f	850	0	880	0	0
16	g	881	0	945	0	0
17	i	658	0	712	0	0
18	j	580	0	584	0	0
19	k	612	0	682	0	0
20	O	1555	0	1659	318	0
21	V	993	0	1040	11	0
22	a	626	0	676	0	0
23	P	1442	0	1484	16	0
24	X	1100	0	1187	5	0
25	Y	993	0	1081	5	0
26	h	969	0	1078	0	0
27	F	1784	0	1862	15	0
28	B	2702	0	2779	35	0
29	C	2731	0	2852	38	0
30	H	1510	0	1576	12	0
31	A	1623	0	1624	27	0
32	K	2073	0	2155	24	0
33	m	5223	0	5201	0	0
34	D	1590	0	1598	10	0
35	W	1870	0	1902	12	0
36	l	1377	0	1415	0	0
37	b	3410	0	3463	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
38	o	1107	0	1159	0	0
39	n	3369	0	3496	0	0
40	r	1438	0	1515	0	0
41	s	301	0	359	0	0
42	t	2328	0	2476	0	0
43	y	1701	0	1697	0	0
44	z	444	0	478	0	0
45	p	2321	0	2294	0	0
46	q	2485	0	2516	0	0
47	u	976	0	1011	0	0
48	v	1087	0	1133	0	0
49	w	3511	0	3639	0	0
50	I	3470	0	3611	27	0
51	J	1215	0	1245	7	0
52	E	1239	0	1326	15	0
53	G	1438	0	1520	34	0
54	M	1053	0	1148	14	0
55	j	1	0	0	0	0
All	All	134887	0	109370	1313	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 7.

All (1313) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:1190:A:N6	1:1:1315:U:H3	1.16	1.41
1:1:78:U:H3	1:1:325:A:N6	1.18	1.40
1:1:808:A:N1	1:1:932:U:O4	1.57	1.37
20:O:65:ASN:ND2	20:O:67:THR:HG22	1.36	1.35
1:1:1188:U:H3	1:1:1317:A:N6	1.26	1.34
20:O:10:ASP:OD1	20:O:37:ARG:HD3	1.21	1.28
1:1:1554:U:H3	1:1:1559:A:N6	1.28	1.27
20:O:198:GLY:O	20:O:199:TYR:CD2	1.89	1.26
20:O:160:ARG:HD2	20:O:160:ARG:O	1.28	1.25
20:O:65:ASN:HD21	20:O:67:THR:CG2	1.47	1.25
20:O:76:PRO:O	20:O:79:ILE:HG22	1.38	1.23
20:O:143:THR:OG1	20:O:150:GLU:OE1	1.60	1.20
20:O:125:ARG:NE	20:O:135:TYR:CE2	2.06	1.20
20:O:14:HIS:O	20:O:15:LEU:HD12	1.40	1.18
1:1:533:A:N6	1:1:556:U:H5	1.42	1.17

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:O:125:ARG:HH11	20:O:125:ARG:HG2	1.04	1.14
20:O:43:ILE:HG22	20:O:44:SER:H	1.02	1.14
1:1:1205:A:C2	1:1:1299:U:C5	2.33	1.13
20:O:84:LEU:O	20:O:84:LEU:HD23	1.50	1.12
20:O:76:PRO:C	20:O:79:ILE:HG22	1.70	1.12
1:1:78:U:O4	1:1:325:A:N1	1.84	1.11
20:O:23:VAL:HG11	20:O:84:LEU:HD12	1.33	1.10
20:O:160:ARG:HD2	20:O:160:ARG:C	1.68	1.09
1:1:808:A:N6	1:1:932:U:H3	1.51	1.08
1:1:1205:A:H2	1:1:1299:U:C5	1.58	1.08
20:O:64:PHE:HZ	20:O:68:ARG:NH2	1.49	1.08
20:O:27:LEU:O	20:O:30:GLY:N	1.87	1.08
20:O:49:ARG:HH11	20:O:49:ARG:CG	1.66	1.08
20:O:102:LEU:HD12	20:O:103:LYS:H	1.16	1.07
20:O:37:ARG:HG2	20:O:37:ARG:HH11	0.90	1.06
20:O:84:LEU:C	20:O:84:LEU:HD23	1.74	1.06
20:O:56:ASP:O	20:O:59:ARG:HG2	1.51	1.06
20:O:49:ARG:HG3	20:O:49:ARG:NH1	1.57	1.05
20:O:76:PRO:O	20:O:79:ILE:CG2	2.05	1.04
20:O:152:VAL:HG12	20:O:153:VAL:H	1.22	1.03
1:1:1188:U:O4	1:1:1317:A:N1	1.91	1.02
20:O:12:LYS:HE3	20:O:40:GLU:OE2	1.57	1.02
20:O:168:TYR:O	20:O:171:LYS:N	1.93	1.00
1:1:1554:U:N3	1:1:1559:A:N6	1.93	1.00
1:1:976:U:C5	1:1:1105:A:C2	2.46	1.00
20:O:76:PRO:HA	20:O:79:ILE:CG2	1.91	1.00
20:O:125:ARG:CG	20:O:125:ARG:HH11	1.73	1.00
53:G:146:LYS:HE3	53:G:173:MET:O	1.63	0.99
20:O:39:GLU:HG2	20:O:40:GLU:N	1.74	0.98
1:1:536:U:H2'	1:1:537:A:H8	1.27	0.98
20:O:10:ASP:OD1	20:O:37:ARG:CD	2.12	0.98
20:O:16:VAL:HG22	20:O:41:LEU:CD2	1.94	0.98
20:O:190:VAL:HG13	20:O:191:ALA:H	1.27	0.97
20:O:23:VAL:O	20:O:27:LEU:HD23	1.64	0.97
20:O:161:LYS:O	20:O:164:SER:OG	1.82	0.97
1:1:973:A:H2	1:1:1108:U:C5	1.78	0.96
20:O:37:ARG:CG	20:O:37:ARG:HH11	1.79	0.96
20:O:43:ILE:HG22	20:O:44:SER:N	1.81	0.96
20:O:125:ARG:NE	20:O:135:TYR:HE2	1.60	0.95
20:O:152:VAL:CG1	20:O:153:VAL:N	2.27	0.95
1:1:249:U:H3'	1:1:250:U:H5''	1.48	0.95

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:O:27:LEU:O	20:O:29:ASN:N	2.00	0.95
20:O:37:ARG:HG2	20:O:37:ARG:NH1	1.72	0.94
20:O:102:LEU:HD12	20:O:103:LYS:N	1.81	0.94
1:1:976:U:C5	1:1:1105:A:H2	1.67	0.94
20:O:198:GLY:O	20:O:199:TYR:HD2	1.48	0.94
20:O:14:HIS:C	20:O:15:LEU:HD12	1.87	0.93
20:O:76:PRO:HA	20:O:79:ILE:HG21	1.48	0.93
20:O:49:ARG:HH11	20:O:49:ARG:HG3	0.77	0.93
1:1:536:U:H2'	1:1:537:A:C8	2.04	0.93
20:O:77:SER:N	20:O:106:GLU:OE2	2.01	0.93
20:O:114:LYS:O	20:O:115:LYS:HG2	1.68	0.93
1:1:1200:A:H2	1:1:2824:G:H1	1.15	0.93
1:1:1205:A:H2	1:1:1299:U:H5	1.15	0.92
1:1:808:A:H61	1:1:932:U:H3	0.98	0.91
20:O:45:GLY:O	20:O:136:THR:OG1	1.89	0.90
1:1:1554:U:O4	1:1:1559:A:N1	2.05	0.89
20:O:108:ILE:HB	20:O:160:ARG:HH12	1.37	0.89
20:O:111:PRO:O	20:O:115:LYS:HG3	1.72	0.89
20:O:64:PHE:CZ	20:O:68:ARG:NH2	2.28	0.89
1:1:533:A:N6	1:1:556:U:C5	2.25	0.88
20:O:56:ASP:C	20:O:56:ASP:OD2	2.09	0.88
20:O:142:SER:O	20:O:145:VAL:HG12	1.73	0.88
1:1:1190:A:N1	1:1:1315:U:O4	2.05	0.88
1:1:819:U:H3	1:1:906:A:H61	1.14	0.88
20:O:12:LYS:HG3	20:O:40:GLU:HG2	1.56	0.88
1:1:799:G:HO2'	4:L:18:TRP:HE1	1.21	0.88
20:O:125:ARG:NE	20:O:135:TYR:CD2	2.41	0.88
20:O:11:GLY:O	20:O:41:LEU:HD12	1.74	0.87
20:O:47:PHE:O	20:O:49:ARG:N	2.08	0.87
20:O:22:VAL:CG1	20:O:122:GLN:HE21	1.89	0.86
20:O:85:ARG:O	20:O:87:MET:N	2.07	0.86
20:O:152:VAL:HG12	20:O:153:VAL:N	1.88	0.86
20:O:76:PRO:CA	20:O:79:ILE:HG22	2.05	0.86
30:H:21:LYS:HG3	54:M:8:LYS:HG3	1.57	0.85
20:O:108:ILE:HB	20:O:160:ARG:NH1	1.90	0.85
53:G:91:PHE:HE2	53:G:185:ARG:HG2	1.41	0.84
20:O:84:LEU:HD13	20:O:102:LEU:HD21	1.59	0.84
20:O:56:ASP:O	20:O:59:ARG:CG	2.26	0.84
20:O:28:LEU:HD21	20:O:88:VAL:HG13	1.60	0.83
20:O:23:VAL:HG11	20:O:84:LEU:CD1	2.08	0.83
20:O:135:TYR:H	20:O:135:TYR:HD1	1.26	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:807:A:N6	1:1:935:U:H3	1.77	0.82
20:O:84:LEU:C	20:O:84:LEU:CD2	2.47	0.82
20:O:15:LEU:HD11	20:O:125:ARG:CB	2.10	0.81
20:O:39:GLU:HG2	20:O:40:GLU:H	1.39	0.81
20:O:125:ARG:CD	20:O:135:TYR:CD2	2.64	0.81
1:1:807:A:N6	1:1:935:U:N3	2.28	0.81
1:1:1187:C:H5	1:1:1319:G:H1	1.28	0.81
1:1:1385:C:O2'	52:E:2:SER:HB2	1.81	0.81
1:1:533:A:N6	1:1:555:U:O2	2.14	0.80
1:1:808:A:N1	1:1:932:U:C4	2.50	0.80
20:O:16:VAL:HG22	20:O:41:LEU:HD23	1.62	0.80
20:O:85:ARG:C	20:O:87:MET:H	1.84	0.80
1:1:894:G:H5''	1:1:895:A:H8	1.46	0.80
20:O:56:ASP:OD2	20:O:57:PHE:N	2.15	0.79
20:O:125:ARG:HG2	20:O:125:ARG:NH1	1.86	0.79
1:1:973:A:C2	1:1:1108:U:C5	2.59	0.79
20:O:108:ILE:HG21	20:O:117:ARG:HH21	1.47	0.79
5:N:110:ALA:HB1	5:N:113:LEU:HD23	1.63	0.79
20:O:37:ARG:HD2	20:O:108:ILE:HD11	1.65	0.79
20:O:188:SER:O	20:O:190:VAL:HG12	1.83	0.79
1:1:2928:C:H2'	1:1:2928:C:O2	1.80	0.78
20:O:36:VAL:HG23	20:O:37:ARG:HG3	1.64	0.78
20:O:88:VAL:O	20:O:90:HIS:N	2.15	0.78
53:G:141:ALA:O	53:G:145:ASN:OD1	2.01	0.78
5:N:106:VAL:HG21	5:N:132:VAL:HG11	1.64	0.78
20:O:12:LYS:HG3	20:O:40:GLU:CG	2.14	0.78
20:O:190:VAL:HG13	20:O:191:ALA:N	1.98	0.78
1:1:1419:A:H5''	29:C:193:LYS:NZ	1.99	0.77
20:O:23:VAL:CG1	20:O:84:LEU:HD12	2.12	0.77
20:O:16:VAL:HG22	20:O:41:LEU:HD21	1.66	0.77
3:6:38:U:O2	3:6:42:G:N1	2.17	0.77
1:1:909:G:H1	1:1:918:C:H42	1.33	0.76
1:1:807:A:N1	1:1:935:U:O4	2.19	0.76
20:O:14:HIS:C	20:O:15:LEU:CD1	2.54	0.76
20:O:160:ARG:CD	20:O:160:ARG:C	2.50	0.76
20:O:18:ARG:O	20:O:22:VAL:HG13	1.86	0.76
1:1:424:G:O6	1:1:635:G:N2	2.18	0.75
1:1:536:U:O2	1:1:557:A:N7	2.19	0.75
1:1:916:G:H2'	1:1:917:A:C8	2.20	0.75
1:1:818:C:H5	1:1:907:G:H22	1.34	0.75
20:O:125:ARG:HD3	20:O:135:TYR:HD2	1.50	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:3049:A:H5'	28:B:53:MET:HB3	1.68	0.75
20:O:74:ARG:HD3	20:O:74:ARG:N	2.02	0.75
1:1:3016:A:HO2'	1:1:3017:A:H8	1.35	0.74
20:O:50:ASN:N	20:O:50:ASN:HD22	1.84	0.74
20:O:125:ARG:CD	20:O:135:TYR:HD2	2.00	0.74
1:1:1190:A:N6	1:1:1315:U:N3	1.94	0.74
1:1:909:G:H1	1:1:918:C:N4	1.86	0.74
20:O:84:LEU:HD13	20:O:102:LEU:CD2	2.17	0.74
1:1:1786:G:H2'	1:1:1787:A:C8	2.23	0.74
1:1:2831:G:H2'	1:1:2832:C:C6	2.22	0.73
20:O:125:ARG:CZ	20:O:135:TYR:HE2	2.01	0.73
1:1:1387:G:HO2'	52:E:2:SER:N	1.87	0.73
20:O:16:VAL:CG2	20:O:41:LEU:HD23	2.17	0.73
20:O:152:VAL:CG1	20:O:153:VAL:H	1.91	0.73
20:O:47:PHE:O	20:O:48:PHE:C	2.24	0.72
20:O:161:LYS:C	20:O:164:SER:HG	1.90	0.72
1:1:662:U:H2'	1:1:663:C:C6	2.24	0.72
20:O:19:LEU:O	20:O:22:VAL:HG22	1.90	0.72
1:1:531:G:H2'	1:1:532:A:C8	2.25	0.72
20:O:27:LEU:CD2	20:O:33:ILE:HD12	2.20	0.71
20:O:188:SER:O	20:O:190:VAL:N	2.23	0.71
20:O:36:VAL:HG23	20:O:37:ARG:N	2.04	0.71
20:O:23:VAL:CG1	20:O:84:LEU:CD1	2.68	0.71
1:1:808:A:C2	1:1:932:U:O4	2.41	0.71
20:O:84:LEU:HD11	20:O:102:LEU:HD22	1.73	0.70
1:1:1546:A:H1'	5:N:96:ARG:HH12	1.56	0.70
1:1:63:A:H2	1:1:78:U:O2	1.75	0.70
1:1:1188:U:C4	1:1:1317:A:N1	2.59	0.70
20:O:152:VAL:HG13	20:O:153:VAL:N	2.06	0.70
1:1:528:U:H3	1:1:564:G:H1	1.40	0.70
20:O:110:PRO:CA	20:O:113:ASP:OD2	2.40	0.70
20:O:16:VAL:CG2	20:O:41:LEU:CD2	2.69	0.70
1:1:876:A:H2	1:1:881:C:H41	1.38	0.70
20:O:65:ASN:C	20:O:65:ASN:HD22	1.94	0.70
20:O:113:ASP:O	20:O:115:LYS:N	2.24	0.69
1:1:808:A:H2'	1:1:809:G:C8	2.28	0.69
20:O:76:PRO:CA	20:O:79:ILE:CG2	2.63	0.69
1:1:249:U:H3'	1:1:250:U:C5'	2.21	0.69
1:1:818:C:H41	1:1:907:G:H1	1.41	0.69
20:O:137:THR:CG2	20:O:138:LEU:N	2.56	0.69
1:1:873:C:H3'	1:1:874:U:H4'	1.74	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:2602:G:C6	1:1:2603:G:N7	2.61	0.69
1:1:533:A:H2	1:1:559:A:N6	1.90	0.69
1:1:3105:U:C5	1:1:3128:G:N2	2.61	0.68
20:O:38:ALA:O	20:O:41:LEU:HB2	1.94	0.68
20:O:198:GLY:O	20:O:199:TYR:CG	2.45	0.68
1:1:1419:A:H5''	29:C:193:LYS:HZ2	1.57	0.68
20:O:15:LEU:HD11	20:O:125:ARG:HB2	1.76	0.68
24:X:103:TYR:HB3	24:X:135:ILE:HD11	1.75	0.68
20:O:172:ARG:O	20:O:175:THR:OG1	2.12	0.68
20:O:74:ARG:CD	20:O:74:ARG:N	2.57	0.68
1:1:3021:A:H2	1:1:3033:A:H62	1.40	0.68
1:1:3371:G:H2'	1:1:3372:A:H8	1.58	0.68
20:O:43:ILE:CG2	20:O:44:SER:H	1.87	0.68
1:1:2406:C:H1'	51:J:319:GLN:HG2	1.76	0.68
20:O:161:LYS:O	20:O:164:SER:N	2.27	0.67
1:1:1105:A:H2'	1:1:1106:G:C8	2.29	0.67
1:1:1661:G:H2'	1:1:1662:G:C8	2.30	0.67
52:E:54:TYR:HA	52:E:65:ILE:HG22	1.77	0.67
1:1:1200:A:H2	1:1:2824:G:N1	1.90	0.67
31:A:103:LYS:HB2	31:A:107:GLY:HA3	1.76	0.67
20:O:94:ARG:O	20:O:94:ARG:HD3	1.94	0.67
20:O:23:VAL:HG12	20:O:24:ALA:N	2.09	0.67
1:1:78:U:C4	1:1:325:A:N1	2.63	0.66
20:O:84:LEU:CD1	20:O:102:LEU:CD2	2.72	0.66
20:O:125:ARG:CG	20:O:125:ARG:NH1	2.43	0.66
1:1:720:A:H2'	6:Q:69:ARG:HH22	1.59	0.66
1:1:1201:C:H2'	1:1:1202:A:N3	2.11	0.66
1:1:2838:A:N6	1:1:2850:G:O2'	2.28	0.66
20:O:76:PRO:HA	20:O:79:ILE:HG22	1.66	0.66
1:1:121:A:N1	53:G:129:PRO:HG2	2.09	0.66
20:O:26:GLN:HB3	20:O:33:ILE:HD11	1.77	0.66
3:6:7:C:H5	3:6:21:G:H1	1.43	0.66
1:1:1609:C:H2'	1:1:1610:G:C8	2.31	0.66
20:O:14:HIS:O	20:O:15:LEU:CD1	2.33	0.66
1:1:1949:G:H5''	7:R:101:VAL:HG11	1.77	0.66
20:O:22:VAL:HG21	20:O:120:VAL:HG11	1.76	0.66
1:1:1233:G:H1	1:1:1255:C:H5	1.41	0.65
1:1:1105:A:H2'	1:1:1106:G:H8	1.61	0.65
20:O:168:TYR:O	20:O:169:ALA:C	2.35	0.65
1:1:1385:C:O2'	52:E:2:SER:CB	2.44	0.65
1:1:2830:G:H2'	1:1:2831:G:C8	2.31	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:C:84:ARG:HH11	29:C:87:GLN:HE21	1.43	0.65
20:O:22:VAL:HG12	20:O:122:GLN:NE2	2.11	0.65
1:1:3234:A:H2	1:1:3253:G:H1	1.41	0.65
1:1:3366:G:H2'	1:1:3367:C:C6	2.32	0.65
1:1:799:G:O2'	4:L:18:TRP:NE1	2.20	0.65
1:1:1724:U:H1'	1:1:1725:C:C6	2.31	0.65
1:1:144:A:H2'	1:1:145:G:O4'	1.96	0.64
20:O:22:VAL:HG12	20:O:122:GLN:HE21	1.63	0.64
1:1:107:A:H1'	1:1:325:A:N3	2.12	0.64
1:1:643:U:HO2'	1:1:645:A:H2	1.46	0.64
1:1:495:G:N2	1:1:620:U:O4	2.30	0.64
1:1:910:G:O6	1:1:917:A:N1	2.31	0.64
1:1:1253:U:H5''	1:1:1254:C:H5'	1.80	0.64
20:O:27:LEU:C	20:O:29:ASN:N	2.51	0.64
53:G:90:THR:HA	53:G:214:LEU:HD21	1.80	0.64
28:B:41:VAL:HA	28:B:185:GLY:HA3	1.80	0.63
28:B:219:ALA:HB2	28:B:336:VAL:HG12	1.80	0.63
23:P:18:ARG:HG3	23:P:147:GLU:HB3	1.79	0.63
1:1:240:U:H4'	1:1:241:G:H5'	1.80	0.63
1:1:567:G:H2'	1:1:568:G:C8	2.34	0.63
1:1:1609:C:H2'	1:1:1610:G:H8	1.63	0.63
20:O:7:VAL:HG23	20:O:31:GLN:HE21	1.62	0.63
20:O:6:VAL:HG12	20:O:7:VAL:N	2.13	0.63
1:1:352:A:H61	1:1:365:A:H5''	1.64	0.63
1:1:501:A:H2'	1:1:502:U:C6	2.34	0.63
20:O:135:TYR:CD1	20:O:135:TYR:N	2.63	0.63
1:1:2891:U:HO2'	11:Z:2:ALA:N	152.01	0.63
1:1:532:A:HO2'	1:1:533:A:H8	1.46	0.63
20:O:80:PHE:O	20:O:80:PHE:CG	2.52	0.63
20:O:54:TYR:CE2	20:O:145:VAL:HG21	2.34	0.63
20:O:114:LYS:C	20:O:115:LYS:HG2	2.19	0.62
1:1:536:U:O2	1:1:557:A:C5	2.52	0.62
20:O:62:THR:OG1	20:O:69:GLY:CA	2.47	0.62
20:O:98:ALA:HA	20:O:101:ARG:NH1	2.15	0.62
25:Y:55:GLU:HB2	25:Y:108:LYS:HB3	1.81	0.62
20:O:12:LYS:HG3	20:O:40:GLU:CD	2.19	0.62
20:O:46:GLU:O	20:O:49:ARG:HB2	2.00	0.62
5:N:116:LEU:HD23	5:N:133:ILE:HD11	1.81	0.62
20:O:12:LYS:HG2	20:O:13:GLY:N	2.14	0.62
53:G:158:ASP:HB3	53:G:159:PRO:HD3	1.82	0.62
20:O:12:LYS:CE	20:O:40:GLU:OE2	2.42	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:O:190:VAL:CG1	20:O:191:ALA:H	2.06	0.62
1:1:197:G:H2'	1:1:198:A:C8	2.35	0.62
20:O:27:LEU:N	20:O:27:LEU:CD2	2.62	0.62
20:O:36:VAL:O	20:O:37:ARG:C	2.39	0.62
31:A:186:ILE:HG23	31:A:221:MET:HB2	1.81	0.62
31:A:189:ARG:HH12	51:J:246:PHE:HB3	1.64	0.62
1:1:1060:U:H2'	1:1:1061:A:C8	2.35	0.61
1:1:894:G:H5''	1:1:895:A:C8	2.32	0.61
11:Z:17:ARG:HG3	11:Z:17:ARG:HH11	1.64	0.61
1:1:1949:G:N2	1:1:2097:U:O2	2.33	0.61
1:1:2340:U:H2'	1:1:2341:A:H8	1.64	0.61
1:1:774:G:C6	1:1:775:A:N6	2.68	0.61
20:O:23:VAL:CG1	20:O:24:ALA:N	2.63	0.61
20:O:14:HIS:O	20:O:42:ASN:HB2	1.99	0.61
1:1:1495:U:H3'	1:1:1495:U:H6	1.65	0.61
20:O:137:THR:HG23	20:O:138:LEU:N	2.15	0.61
20:O:46:GLU:O	20:O:47:PHE:O	2.18	0.61
29:C:138:ARG:HE	29:C:240:PRO:HD2	1.66	0.61
20:O:22:VAL:CG1	20:O:122:GLN:NE2	2.62	0.61
1:1:1510:G:H2'	1:1:1512:U:C5	2.35	0.61
1:1:2979:U:H5'	1:1:2980:U:H5'	1.82	0.61
3:6:43:A:H2'	3:6:44:G:C8	2.36	0.61
20:O:171:LYS:O	20:O:175:THR:HG23	1.99	0.61
1:1:3344:A:N6	1:1:3361:G:O2'	2.33	0.61
1:1:894:G:H8	1:1:895:A:H5'	1.65	0.61
1:1:40:A:H4'	1:1:41:G:OP1	2.00	0.61
1:1:1786:G:H2'	1:1:1787:A:H8	1.65	0.60
20:O:84:LEU:CD1	20:O:102:LEU:HD22	2.29	0.60
1:1:909:G:H2'	1:1:910:G:C8	2.36	0.60
1:1:94:G:H2'	1:1:95:A:C8	2.36	0.60
53:G:81:THR:HG21	53:G:181:LYS:HE3	1.83	0.60
20:O:108:ILE:HG21	20:O:117:ARG:NH2	2.17	0.60
20:O:54:TYR:CD2	20:O:145:VAL:HG21	2.36	0.60
1:1:808:A:N6	1:1:932:U:N3	2.20	0.60
20:O:191:ALA:O	20:O:192:LYS:C	2.40	0.60
20:O:35:VAL:HG12	20:O:104:VAL:HA	1.84	0.60
1:1:1889:G:H2'	1:1:1890:U:C6	2.37	0.60
20:O:41:LEU:HD23	20:O:138:LEU:HD22	1.84	0.60
1:1:973:A:H2	1:1:1108:U:H5	1.43	0.60
27:F:98:LYS:HB3	27:F:99:PRO:HD3	1.83	0.60
35:W:99:VAL:HG12	35:W:100:THR:H	1.66	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:6:23:U:H3	32:K:96:LYS:HE2	1.67	0.59
20:O:15:LEU:O	20:O:16:VAL:C	2.40	0.59
1:1:1608:C:C2	1:1:1609:C:C5	2.90	0.59
1:1:1764:U:H4'	1:1:1765:U:H5''	1.84	0.59
31:A:41:VAL:HG13	31:A:45:HIS:HB2	1.82	0.59
20:O:136:THR:O	20:O:137:THR:O	2.20	0.59
1:1:1250:G:H2'	1:1:1251:A:C8	2.37	0.59
35:W:46:ASP:HA	35:W:99:VAL:HG21	1.85	0.59
1:1:2917:G:H1	1:1:2929:C:H5	1.50	0.59
20:O:160:ARG:HG3	20:O:160:ARG:HH11	1.68	0.59
20:O:27:LEU:HD23	20:O:27:LEU:H	1.68	0.59
1:1:3371:G:H2'	1:1:3372:A:C8	2.38	0.59
20:O:126:VAL:HG13	20:O:127:LEU:HD23	1.84	0.59
1:1:117:U:O4	53:G:147:LYS:HD2	2.03	0.59
2:2:10:A:H2'	2:2:11:C:C6	2.38	0.59
31:A:136:VAL:HB	31:A:176:VAL:HG12	1.84	0.59
53:G:146:LYS:CE	53:G:173:MET:O	2.46	0.59
4:L:100:ARG:HD3	4:L:100:ARG:H	1.67	0.59
1:1:503:C:N3	1:1:504:A:N7	2.50	0.58
1:1:503:C:N4	1:1:504:A:H62	2.01	0.58
52:E:4:GLN:HG3	52:E:4:GLN:O	2.02	0.58
20:O:73:PHE:HB3	20:O:78:ARG:HB2	1.85	0.58
29:C:35:VAL:HG21	29:C:244:LEU:HD21	1.85	0.58
1:1:1696:A:H2'	1:1:1697:A:C8	2.38	0.58
1:1:3217:C:C2'	1:1:3217:C:O2	2.52	0.58
1:1:735:A:H2'	1:1:736:A:C8	2.39	0.58
1:1:3117:C:H2'	1:1:3118:C:O4'	2.02	0.58
50:I:232:GLN:HA	50:I:275:LEU:HD21	1.84	0.58
20:O:25:LYS:HA	20:O:28:LEU:HD12	1.86	0.58
1:1:2604:U:H2'	1:1:2605:G:O4'	2.04	0.58
20:O:49:ARG:CG	20:O:49:ARG:NH1	2.38	0.58
6:Q:55:SER:O	6:Q:59:ARG:HG3	2.04	0.58
1:1:406:G:H1'	2:2:16:G:N2	2.18	0.57
20:O:160:ARG:HG3	20:O:160:ARG:NH1	2.19	0.57
20:O:109:PRO:O	20:O:112:TYR:HB2	2.05	0.57
20:O:7:VAL:HG23	20:O:31:GLN:NE2	2.19	0.57
3:6:15:C:H4'	3:6:16:U:OP2	2.04	0.57
32:K:81:ILE:HG23	32:K:246:VAL:HB	1.86	0.57
20:O:6:VAL:CG1	20:O:7:VAL:N	2.68	0.57
1:1:1277:C:HO2'	1:1:1278:A:H8	1.51	0.57
1:1:1597:C:H5'	1:1:1696:A:H1'	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:A:134:ARG:HB2	31:A:173:ILE:HG22	1.85	0.57
52:E:92:SER:HB3	52:E:148:GLU:HG2	1.86	0.57
20:O:78:ARG:HE	20:O:78:ARG:HA	1.70	0.57
1:1:1744:G:H2'	1:1:1745:C:C6	2.40	0.57
1:1:1619:A:H61	1:1:1825:G:H1	1.53	0.57
1:1:533:A:C6	1:1:556:U:C5	2.72	0.57
32:K:113:ALA:HB3	32:K:253:TRP:CH2	2.40	0.57
20:O:22:VAL:HG11	20:O:122:GLN:HE21	1.65	0.57
1:1:3064:U:H2'	1:1:3065:G:O4'	2.05	0.57
20:O:125:ARG:HG3	20:O:126:VAL:N	2.20	0.57
20:O:135:TYR:HD1	20:O:135:TYR:N	1.98	0.57
1:1:414:U:N3	1:1:415:G:N7	2.53	0.57
1:1:620:U:H4'	23:P:167:ARG:HH12	1.70	0.57
1:1:1597:C:H2'	1:1:1598:G:C8	2.40	0.56
20:O:65:ASN:ND2	20:O:65:ASN:C	2.58	0.56
1:1:1777:U:H2'	1:1:1778:G:C8	2.41	0.56
1:1:2426:U:H3	1:1:2603:G:H1	1.53	0.56
1:1:709:A:H2'	1:1:710:A:C8	2.40	0.56
29:C:206:LEU:HD11	29:C:237:GLN:HB3	1.87	0.56
20:O:65:ASN:ND2	20:O:67:THR:H	2.03	0.56
1:1:12:A:H2'	1:1:13:A:C8	2.41	0.56
53:G:147:LYS:O	53:G:201:THR:HG23	2.05	0.56
32:K:124:LEU:HD21	32:K:126:ILE:HG13	1.87	0.56
1:1:156:G:H22	4:L:91:ARG:HH12	1.53	0.56
20:O:61:ALA:O	20:O:63:ALA:N	2.38	0.56
1:1:1498:A:H2'	1:1:1499:C:C6	2.40	0.56
1:1:1766:G:H2'	1:1:1767:C:C6	2.41	0.56
1:1:502:U:H4'	52:E:26:ARG:HB3	1.85	0.56
20:O:188:SER:O	20:O:190:VAL:CG1	2.54	0.56
28:B:82:PRO:HB2	28:B:165:GLN:HB2	1.88	0.56
20:O:12:LYS:HE3	20:O:40:GLU:CD	2.25	0.56
1:1:1798:A:H2'	1:1:1799:A:C8	2.40	0.56
1:1:197:G:N2	1:1:372:A:C8	2.74	0.56
1:1:760:G:N1	1:1:770:G:N3	2.53	0.56
11:Z:95:VAL:HG21	11:Z:113:VAL:HG11	1.88	0.56
2:2:26:U:H2'	2:2:27:U:C6	2.41	0.56
1:1:933:A:N6	29:C:98:ARG:HD2	2.20	0.56
54:M:81:VAL:O	54:M:85:TRP:HB2	2.06	0.56
20:O:46:GLU:OE1	20:O:47:PHE:N	2.39	0.56
1:1:3165:A:H2'	1:1:3166:C:C6	2.41	0.55
1:1:2839:G:H2'	1:1:2840:C:C6	2.41	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
50:I:430:LEU:HD12	50:I:474:LEU:HB3	1.87	0.55
20:O:10:ASP:O	20:O:12:LYS:N	2.39	0.55
20:O:74:ARG:O	20:O:75:ALA:C	2.44	0.55
1:1:1290:A:H2'	1:1:1291:A:C8	2.41	0.55
1:1:1188:U:N3	1:1:1317:A:N6	2.11	0.55
1:1:662:U:H2'	1:1:663:C:H6	1.71	0.55
2:2:9:A:H2'	2:2:10:A:C8	2.42	0.55
28:B:222:LYS:HD3	28:B:331:ASN:HB3	1.88	0.55
1:1:3078:U:OP1	1:1:3080:G:H5'	2.07	0.55
20:O:98:ALA:O	20:O:101:ARG:HG3	2.06	0.55
1:1:1643:A:H2'	1:1:1644:C:C2	2.41	0.55
1:1:1722:U:H5''	7:R:99:LEU:HD22	1.88	0.55
1:1:1124:U:H2'	1:1:1125:U:C6	2.42	0.55
1:1:209:A:H4'	1:1:211:A:N7	2.21	0.55
1:1:1136:A:H2'	1:1:1137:C:C6	2.41	0.55
1:1:3217:C:H2'	1:1:3217:C:O2	2.06	0.55
1:1:952:A:H4'	1:1:968:G:H21	1.72	0.55
8:S:167:ARG:HE	20:O:119:VAL:HG11	1.72	0.55
20:O:161:LYS:O	20:O:164:SER:CB	2.54	0.55
21:V:81:GLN:O	21:V:98:ASN:ND2	2.40	0.55
1:1:2411:U:H3	1:1:2811:A:H61	1.54	0.55
1:1:148:G:O6	53:G:135:GLY:HA3	2.07	0.55
20:O:12:LYS:O	20:O:14:HIS:N	2.39	0.55
20:O:156:LEU:HB2	53:G:217:THR:HG21	192.22	0.55
8:S:8:GLN:HB2	8:S:64:ILE:HD11	1.89	0.55
1:1:345:G:O2'	2:2:25:G:N3	2.39	0.55
31:A:129:CYS:SG	31:A:215:ILE:HD11	2.47	0.55
20:O:137:THR:HG23	20:O:138:LEU:H	1.72	0.55
20:O:78:ARG:CA	20:O:78:ARG:HE	2.19	0.54
1:1:818:C:O2'	1:1:819:U:O4'	2.26	0.54
1:1:1611:G:H2'	1:1:1612:A:O4'	2.07	0.54
1:1:1724:U:H1'	1:1:1725:C:C5	2.43	0.54
1:1:643:U:O2'	1:1:645:A:H2	1.91	0.54
28:B:305:ILE:HG22	28:B:359:ILE:HG21	1.90	0.54
29:C:47:ARG:HD3	29:C:109:TRP:HE3	1.71	0.54
3:6:24:A:H1'	32:K:93:LYS:HE2	1.88	0.54
20:O:151:ASP:O	20:O:154:ALA:HB3	2.07	0.54
20:O:76:PRO:O	20:O:79:ILE:HG23	2.03	0.54
1:1:3223:A:H2'	1:1:3224:G:O4'	2.07	0.54
1:1:976:U:H5	1:1:1105:A:H2	1.45	0.54
1:1:2831:G:H2'	1:1:2832:C:H6	1.72	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:2922:G:H2'	1:1:2922:G:N3	2.22	0.54
1:1:3252:G:H2'	1:1:3253:G:H8	1.71	0.54
27:F:162:PRO:HB3	29:C:314:LYS:HD2	1.90	0.54
20:O:126:VAL:HG13	20:O:127:LEU:N	2.22	0.54
1:1:620:U:H5'	23:P:167:ARG:HH22	1.72	0.54
1:1:571:U:H2'	1:1:572:A:H8	1.73	0.54
3:6:10:A:H2'	3:6:11:C:O4'	2.07	0.54
1:1:118:U:O2	1:1:121:A:H5''	2.07	0.53
1:1:2909:U:H2'	1:1:2910:A:O4'	2.08	0.53
1:1:601:U:H2'	1:1:602:A:C8	2.43	0.53
1:1:66:A:H61	1:1:76:G:H1'	1.72	0.53
31:A:48:LEU:HD11	31:A:117:LEU:HD22	1.90	0.53
2:2:152:G:H5''	53:G:63:LYS:HD2	1.89	0.53
1:1:727:G:N7	1:1:728:G:C8	2.76	0.53
1:1:3330:A:H4'	28:B:366:GLY:HA3	1.90	0.53
32:K:250:ASN:HB3	32:K:253:TRP:CD1	2.43	0.53
20:O:27:LEU:C	20:O:29:ASN:H	2.11	0.53
1:1:1766:G:H2'	1:1:1767:C:H6	1.73	0.53
1:1:257:U:H5''	4:L:86:THR:HG21	1.89	0.53
29:C:3:ARG:HB3	29:C:22:LEU:HB2	1.90	0.53
20:O:85:ARG:C	20:O:87:MET:N	2.51	0.53
23:P:41:LEU:HD23	23:P:150:VAL:HG11	1.90	0.53
1:1:2936:A:H2'	1:1:2937:G:C8	2.44	0.53
1:1:2993:G:H2'	1:1:3142:A:N6	2.24	0.53
1:1:655:C:H2'	1:1:656:A:H8	1.72	0.53
31:A:166:ALA:HB3	31:A:169:SER:HB2	1.91	0.53
50:I:338:LEU:HD22	50:I:435:LYS:HD2	1.91	0.53
1:1:3166:C:H2'	1:1:3167:A:C8	2.44	0.53
1:1:3182:G:H2'	1:1:3183:A:C8	2.44	0.53
1:1:618:C:H5'	23:P:169:THR:HG22	1.91	0.53
29:C:283:THR:HG22	29:C:285:ASP:H	1.74	0.53
20:O:27:LEU:O	20:O:28:LEU:C	2.46	0.53
1:1:1205:A:C2	1:1:1299:U:H5	1.99	0.53
1:1:2830:G:H2'	1:1:2831:G:H8	1.71	0.53
1:1:310:U:H2'	1:1:311:C:O4'	2.08	0.53
2:2:9:A:H2'	2:2:10:A:H8	1.74	0.53
1:1:3129:A:H2'	1:1:3130:A:H5''	1.91	0.53
1:1:850:U:H2'	1:1:851:C:C6	2.44	0.53
28:B:216:ASP:HB3	28:B:278:ILE:HA	1.91	0.53
20:O:37:ARG:CG	20:O:37:ARG:NH1	2.48	0.53
29:C:338:LYS:O	29:C:340:GLY:N	2.41	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
54:M:59:ASN:HB2	54:M:62:GLN:HG3	1.91	0.52
1:1:1240:A:N6	1:1:1241:U:O4	2.42	0.52
1:1:3252:G:H2'	1:1:3253:G:C8	2.44	0.52
8:S:70:THR:HG22	54:M:55:ARG:HG2	1.90	0.52
20:O:76:PRO:N	20:O:106:GLU:OE2	2.42	0.52
20:O:110:PRO:N	20:O:113:ASP:OD2	2.42	0.52
8:S:26:ARG:HH22	8:S:28:ARG:HH21	1.57	0.52
1:1:533:A:HO2'	1:1:535:G:H8	1.54	0.52
32:K:113:ALA:HB3	32:K:253:TRP:HH2	1.74	0.52
20:O:46:GLU:O	20:O:49:ARG:CB	2.57	0.52
1:1:3045:G:H2'	1:1:3046:A:O4'	2.10	0.52
28:B:57:VAL:HG23	28:B:357:LYS:HB3	1.91	0.52
27:F:45:LEU:HD12	29:C:329:PRO:HB2	1.91	0.52
53:G:152:LEU:HD22	53:G:180:VAL:HB	1.92	0.52
23:P:178:ALA:HA	23:P:181:ARG:HE	1.75	0.52
1:1:962:A:H3'	1:1:963:G:H8	1.74	0.52
28:B:90:VAL:HG13	28:B:104:THR:HG22	1.91	0.52
28:B:34:LYS:O	28:B:35:ASP:HB2	2.08	0.52
27:F:123:THR:HA	27:F:126:LEU:HD12	1.91	0.52
35:W:188:VAL:HG11	35:W:202:ILE:HG21	1.91	0.52
1:1:1485:G:H5''	1:1:1875:G:H1'	1.91	0.52
32:K:68:GLU:HA	34:D:286:ARG:HH12	1.73	0.52
20:O:47:PHE:CD2	20:O:48:PHE:N	2.77	0.52
1:1:2353:G:H5''	23:P:86:LYS:HB2	1.91	0.52
1:1:29:C:H4'	1:1:62:A:H4'	1.91	0.52
1:1:980:A:H1'	1:1:981:U:H5	1.73	0.52
20:O:27:LEU:HD21	20:O:33:ILE:HD12	1.92	0.52
1:1:2428:U:H2'	1:1:2429:G:C8	2.45	0.52
52:E:2:SER:O	52:E:2:SER:OG	2.22	0.52
20:O:51:LYS:HE3	20:O:144:SER:O	2.08	0.52
1:1:1250:G:H2'	1:1:1251:A:H8	1.74	0.52
1:1:1799:A:H2'	1:1:1800:A:H8	1.75	0.52
1:1:2942:C:O2	1:1:2942:C:H2'	2.10	0.52
1:1:2986:U:H2'	1:1:2987:A:H8	1.74	0.52
1:1:3027:A:H2'	1:1:3028:G:O4'	2.09	0.52
1:1:3162:C:N4	1:1:3163:A:H62	2.08	0.52
31:A:88:PHE:HB3	31:A:100:TRP:HB2	1.91	0.52
32:K:132:ILE:HG12	32:K:154:ILE:HD12	1.91	0.52
20:O:27:LEU:HD22	20:O:33:ILE:HD12	1.90	0.52
1:1:1348:U:H5	6:Q:31:LYS:HE2	1.72	0.52
1:1:3283:U:H2'	1:1:3284:G:C8	2.45	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:629:U:H2'	1:1:630:A:H8	1.74	0.52
25:Y:112:ASP:H	25:Y:115:ARG:HB3	1.73	0.52
1:1:1495:U:H3'	1:1:1495:U:C6	2.45	0.51
1:1:1569:U:H6	1:1:1571:A:H62	1.57	0.51
1:1:26:A:N3	1:1:328:U:O2'	2.42	0.51
20:O:153:VAL:O	20:O:154:ALA:C	2.48	0.51
1:1:2428:U:H2'	1:1:2429:G:H8	1.74	0.51
1:1:3040:A:H5'	21:V:11:PHE:HA	1.92	0.51
50:I:257:LYS:HE3	50:I:293:GLN:HB3	1.92	0.51
20:O:77:SER:OG	20:O:106:GLU:OE2	2.26	0.51
1:1:3166:C:H2'	1:1:3167:A:H8	1.73	0.51
7:R:102:LEU:HD22	7:R:138:LEU:HD13	1.92	0.51
7:R:17:VAL:HG21	7:R:52:LYS:HE2	1.91	0.51
10:U:22:PRO:HB2	10:U:28:PHE:HB3	1.93	0.51
1:1:1437:C:O2	1:1:1437:C:H2'	2.09	0.51
1:1:1549:U:H2'	1:1:1550:C:C6	2.45	0.51
1:1:3294:A:H2'	1:1:3295:A:O4'	2.11	0.51
28:B:48:GLY:HA3	28:B:81:THR:HG22	1.93	0.51
20:O:125:ARG:CZ	20:O:135:TYR:CE2	2.80	0.51
1:1:989:A:O2'	9:T:104:GLU:HB3	2.10	0.51
1:1:1168:U:O2	1:1:1169:A:C8	2.64	0.51
1:1:1290:A:H2'	1:1:1291:A:H8	1.76	0.51
1:1:2408:U:H2'	1:1:2409:G:C8	2.46	0.51
1:1:2427:U:H4'	4:L:54:LEU:HA	123.95	0.51
1:1:2841:G:N2	1:1:2847:A:H8	2.08	0.51
1:1:886:C:H2'	1:1:887:G:C8	2.45	0.51
1:1:629:U:H2'	1:1:630:A:C8	2.46	0.51
1:1:3047:U:H5'	28:B:329:PRO:HA	1.92	0.51
32:K:86:LYS:HE3	32:K:301:LEU:HB2	1.93	0.51
1:1:1190:A:N1	1:1:1315:U:C4	2.78	0.51
1:1:1255:C:O2	1:1:1255:C:O4'	2.29	0.51
1:1:3181:C:H2'	1:1:3182:G:C8	2.46	0.51
1:1:596:C:H2'	1:1:597:G:O4'	2.11	0.51
20:O:49:ARG:HD2	20:O:49:ARG:C	2.31	0.51
7:R:92:GLN:O	7:R:96:ILE:HG13	2.11	0.51
32:K:124:LEU:HD22	32:K:180:ILE:HG23	1.93	0.50
32:K:101:ASN:HB2	32:K:269:GLN:HE22	1.75	0.50
20:O:125:ARG:HD3	20:O:135:TYR:CD2	2.34	0.50
20:O:178:VAL:O	20:O:182:ASN:ND2	2.44	0.50
20:O:34:VAL:HG22	20:O:103:LYS:HB2	1.91	0.50
1:1:1324:U:H2'	1:1:1325:U:O4'	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:O:54:TYR:O	20:O:57:PHE:HB3	2.11	0.50
20:O:27:LEU:CD2	20:O:27:LEU:H	2.23	0.50
28:B:376:LYS:O	28:B:380:MET:HB2	2.11	0.50
20:O:15:LEU:N	20:O:15:LEU:CD1	2.74	0.50
1:1:3375:A:O2'	1:1:3378:C:OP2	2.26	0.50
2:2:132:G:H5''	24:X:94:GLN:HE21	1.77	0.50
50:I:333:VAL:HA	50:I:336:MET:HG2	1.93	0.50
30:H:47:LYS:HB2	54:M:7:VAL:HB	1.92	0.50
2:2:8:C:N4	2:2:9:A:H62	2.10	0.50
50:I:434:THR:HG22	50:I:482:LEU:HG	1.93	0.50
20:O:110:PRO:HA	20:O:113:ASP:OD2	2.11	0.50
11:Z:23:VAL:HG12	11:Z:45:GLY:HA3	1.94	0.50
1:1:129:U:H2'	1:1:130:A:C8	2.47	0.50
1:1:1596:C:H2'	1:1:1597:C:C6	2.47	0.50
1:1:1742:U:C2	1:1:1743:G:C8	3.00	0.50
28:B:286:GLY:HA3	28:B:321:PHE:CE1	2.46	0.50
20:O:140:LYS:O	20:O:141:LEU:C	2.50	0.50
8:S:13:ARG:HA	8:S:56:GLY:HA2	1.93	0.50
1:1:1717:U:H2'	1:1:1718:G:H8	1.77	0.50
1:1:238:A:H2'	1:1:239:G:O4'	2.12	0.50
1:1:664:U:H2'	1:1:665:A:C8	2.47	0.50
1:1:759:U:H3'	1:1:760:G:H5''	1.94	0.50
32:K:110:TRP:O	32:K:114:SER:HB2	2.12	0.50
20:O:26:GLN:HB3	20:O:33:ILE:CD1	2.41	0.50
20:O:50:ASN:HD22	20:O:50:ASN:H	1.57	0.50
24:X:132:ALA:HA	24:X:135:ILE:HG22	1.93	0.50
1:1:1278:A:HO2'	1:1:1279:C:H6	1.55	0.49
1:1:3016:A:O2'	1:1:3017:A:H8	1.94	0.49
34:D:362:ILE:HG22	34:D:391:LEU:HG	1.93	0.49
23:P:13:LYS:HB3	23:P:152:GLU:HB2	1.94	0.49
10:U:77:LYS:HG2	10:U:81:LYS:HE2	1.94	0.49
1:1:1680:G:H1	1:1:1688:U:H3	1.59	0.49
1:1:2949:U:H2'	1:1:2950:G:C8	2.47	0.49
1:1:3057:U:C6	1:1:3376:A:N6	2.80	0.49
1:1:3188:G:C2	1:1:3189:G:C8	3.00	0.49
1:1:908:G:N2	1:1:921:A:N1	2.60	0.49
28:B:57:VAL:HG22	28:B:358:TRP:HB3	1.93	0.49
1:1:680:G:H5''	29:C:114:ASN:HD22	1.77	0.49
1:1:976:U:H5	1:1:1105:A:C2	2.22	0.49
1:1:125:C:H2'	1:1:126:U:C6	2.48	0.49
1:1:1554:U:C2	1:1:1559:A:N6	2.73	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:3162:C:H42	1:1:3163:A:N6	2.10	0.49
1:1:3268:A:H1'	52:E:75:PRO:HG3	1.94	0.49
27:F:176:TYR:CZ	27:F:197:GLN:HG2	2.47	0.49
20:O:133:ARG:HH11	20:O:133:ARG:CG	2.25	0.49
20:O:15:LEU:HD11	20:O:125:ARG:HB3	1.92	0.49
1:1:1676:A:C6	1:1:1677:G:N7	2.81	0.49
1:1:3165:A:H2'	1:1:3166:C:H6	1.76	0.49
2:2:10:A:H2'	2:2:11:C:H6	1.78	0.49
20:O:46:GLU:O	20:O:47:PHE:C	2.51	0.49
1:1:1696:A:H2'	1:1:1697:A:H8	1.77	0.49
1:1:1948:G:H2'	1:1:1949:G:C8	2.48	0.49
1:1:2367:A:H2'	1:1:2368:A:C8	2.47	0.49
1:1:2904:U:H2'	1:1:2905:U:H6	1.76	0.49
1:1:3295:A:H2'	1:1:3296:A:C8	2.48	0.49
1:1:382:U:H4'	23:P:100:ALA:HB1	1.94	0.49
1:1:3312:U:H4'	28:B:25:ILE:HD13	1.95	0.49
1:1:1278:A:O2'	1:1:1279:C:C6	2.66	0.49
1:1:1495:U:C3'	1:1:1495:U:C6	2.96	0.49
1:1:1744:G:H2'	1:1:1745:C:H6	1.77	0.49
1:1:1810:A:H2'	1:1:1811:G:C8	2.47	0.49
2:2:106:C:H4'	2:2:107:G:H5''	1.92	0.49
1:1:1278:A:O2'	1:1:1279:C:H6	1.96	0.49
1:1:1466:G:N2	1:1:1510:G:H5''	2.28	0.49
1:1:3019:U:H5	1:1:3035:A:H61	1.56	0.49
1:1:831:G:H2'	1:1:832:G:H8	1.78	0.49
20:O:112:TYR:O	20:O:113:ASP:C	2.51	0.49
20:O:152:VAL:O	20:O:153:VAL:C	2.51	0.49
20:O:36:VAL:HG23	20:O:37:ARG:CG	2.38	0.49
1:1:201:A:H2'	1:1:202:G:H8	1.78	0.49
1:1:664:U:H2'	1:1:665:A:H8	1.78	0.49
1:1:884:A:H4'	1:1:885:U:H5'	1.95	0.49
20:O:56:ASP:C	20:O:59:ARG:HG2	2.27	0.49
25:Y:119:ILE:HG22	25:Y:124:GLY:HA3	1.95	0.49
1:1:1949:G:N1	1:1:2097:U:N3	2.60	0.49
1:1:2905:U:H2'	1:1:2906:C:H6	1.77	0.49
1:1:3076:C:H2'	1:1:3077:A:C8	2.48	0.49
20:O:111:PRO:O	20:O:115:LYS:CG	2.53	0.49
20:O:161:LYS:O	20:O:162:VAL:C	2.51	0.49
20:O:51:LYS:HA	20:O:141:LEU:HD11	1.95	0.49
23:P:29:THR:HA	23:P:32:THR:HG22	1.95	0.49
1:1:1245:A:C8	1:1:1272:C:H4'	2.48	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:250:U:O2	1:1:250:U:O4'	2.29	0.49
1:1:3019:U:O2	1:1:3019:U:O4'	2.31	0.49
1:1:3132:C:H2'	1:1:3133:C:C6	2.48	0.49
1:1:3159:C:H2'	1:1:3160:U:C6	2.48	0.49
1:1:66:A:N6	1:1:76:G:H1'	2.28	0.49
1:1:3118:C:H2'	1:1:3119:U:O4'	2.13	0.48
1:1:78:U:N3	1:1:325:A:N6	2.04	0.48
3:6:38:U:O2	3:6:42:G:C2	2.65	0.48
1:1:284:A:H5''	31:A:42:ASN:HA	1.95	0.48
50:I:550:LEU:HB3	50:I:590:PHE:CZ	2.48	0.48
32:K:163:VAL:HG23	53:G:205:ALA:HB3	1.94	0.48
9:T:148:PRO:HG2	29:C:358:THR:HG21	1.95	0.48
1:1:1278:A:H5''	35:W:11:THR:HG21	1.95	0.48
11:Z:17:ARG:NH1	11:Z:17:ARG:HG3	2.28	0.48
1:1:1229:G:H2'	1:1:1230:G:H8	1.78	0.48
53:G:95:ASN:HD22	53:G:98:ARG:HE	1.60	0.48
20:O:50:ASN:O	20:O:53:LYS:N	2.46	0.48
1:1:1234:G:H3'	1:1:1235:U:H6	1.78	0.48
1:1:201:A:H2'	1:1:202:G:C8	2.48	0.48
29:C:237:GLN:O	29:C:246:ARG:HD3	2.13	0.48
1:1:1554:U:C4	1:1:1559:A:N1	2.80	0.48
1:1:1659:U:H2'	1:1:1660:C:H6	1.77	0.48
1:1:2904:U:C2	1:1:2905:U:C5	3.01	0.48
1:1:787:G:H2'	1:1:788:C:C6	2.47	0.48
28:B:332:ARG:HD3	28:B:332:ARG:H	1.79	0.48
29:C:145:ILE:HD11	29:C:148:ILE:HD11	1.94	0.48
20:O:35:VAL:CG1	20:O:104:VAL:HG22	2.43	0.48
20:O:39:GLU:CG	20:O:40:GLU:N	2.61	0.48
1:1:1659:U:H2'	1:1:1660:C:C6	2.48	0.48
1:1:268:A:H61	1:1:295:A:H3'	1.79	0.48
1:1:29:C:OP1	5:N:189:LYS:HB2	2.13	0.48
1:1:7:C:H2'	1:1:7:C:O2	2.14	0.48
1:1:655:C:H2'	1:1:656:A:C8	2.47	0.48
1:1:771:A:N3	1:1:771:A:H2'	2.29	0.48
1:1:2841:G:H21	1:1:2847:A:H8	1.61	0.48
1:1:296:A:H3'	1:1:297:G:H21	1.79	0.48
1:1:987:U:H2'	1:1:988:U:C6	2.49	0.48
1:1:990:U:H3'	1:1:991:G:H5''	1.95	0.48
34:D:369:ASP:HB3	34:D:372:ASP:HB2	1.96	0.48
5:N:159:ARG:HB3	5:N:164:LEU:HB2	1.96	0.48
20:O:42:ASN:ND2	20:O:137:THR:HA	2.27	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:P:125:GLN:HB2	23:P:141:SER:HB2	1.94	0.48
1:1:3392:U:H2'	1:1:3393:U:C6	2.48	0.48
1:1:592:A:H2'	1:1:592:A:N3	2.28	0.48
3:6:230:A:H4'	3:6:231:A:C2	2.49	0.48
32:K:80:LEU:HD22	32:K:245:ASN:HD22	1.79	0.48
54:M:60:LEU:HA	54:M:63:VAL:HG12	1.96	0.48
20:O:110:PRO:HB3	20:O:113:ASP:OD2	2.13	0.48
20:O:23:VAL:CG2	20:O:33:ILE:HG21	2.44	0.48
20:O:77:SER:H	20:O:106:GLU:CD	2.08	0.48
1:1:2347:U:O2	1:1:2347:U:H2'	2.13	0.48
1:1:514:G:H2'	1:1:515:C:O4'	2.14	0.48
4:L:27:ASP:O	4:L:31:LYS:HB2	2.13	0.48
20:O:12:LYS:HD2	20:O:40:GLU:OE1	2.14	0.48
20:O:4:GLU:HB2	20:O:6:VAL:O	2.13	0.48
1:1:1187:C:O2	1:1:1187:C:O4'	2.29	0.48
1:1:1595:U:C2	1:1:1596:C:C5	3.02	0.48
1:1:1806:A:H2'	1:1:1807:G:O4'	2.14	0.48
1:1:3231:U:H2'	1:1:3232:G:H8	1.79	0.48
28:B:51:ALA:HB2	28:B:333:LYS:H	1.78	0.48
1:1:3005:A:H5'	28:B:98:GLY:HA3	1.95	0.48
20:O:62:THR:O	20:O:63:ALA:C	2.52	0.48
20:O:110:PRO:CB	20:O:113:ASP:OD2	2.62	0.47
20:O:188:SER:O	20:O:189:ASP:C	2.51	0.47
20:O:90:HIS:CD2	20:O:90:HIS:O	2.67	0.47
23:P:33:ALA:HB1	23:P:117:ILE:HG12	1.95	0.47
1:1:1596:C:H2'	1:1:1597:C:H6	1.78	0.47
28:B:348:ARG:HH21	28:B:351:LEU:HG	1.79	0.47
29:C:150:LEU:HD21	29:C:172:VAL:HG11	1.96	0.47
34:D:299:CYS:HB2	34:D:320:HIS:HB2	1.95	0.47
20:O:160:ARG:CD	20:O:160:ARG:O	2.25	0.47
20:O:46:GLU:HB2	20:O:134:LYS:HD3	1.95	0.47
20:O:47:PHE:HA	20:O:136:THR:HG23	1.96	0.47
8:S:167:ARG:HH12	20:O:12:LYS:HD3	1.79	0.47
1:1:100:A:H3'	1:1:101:G:H21	1.80	0.47
1:1:1229:G:H2'	1:1:1230:G:C8	2.49	0.47
1:1:1449:A:H2'	1:1:1450:G:O4'	2.14	0.47
1:1:1799:A:H2'	1:1:1800:A:C8	2.49	0.47
1:1:3159:C:H2'	1:1:3160:U:H6	1.79	0.47
1:1:3298:C:C4	1:1:3299:A:N7	2.83	0.47
1:1:3308:C:H2'	1:1:3309:G:O4'	2.15	0.47
3:6:43:A:H2'	3:6:44:G:H8	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:K:190:LEU:N	32:K:191:PRO:HD2	2.29	0.47
20:O:116:LYS:HD2	20:O:117:ARG:H	1.79	0.47
20:O:153:VAL:O	20:O:157:GLU:N	2.48	0.47
1:1:1124:U:H2'	1:1:1125:U:H6	1.79	0.47
50:I:292:ILE:HG23	50:I:525:ALA:HB2	1.96	0.47
1:1:1169:A:H2'	1:1:1170:A:C8	2.50	0.47
1:1:1620:U:H2'	1:1:1621:A:H8	1.79	0.47
1:1:727:G:C8	1:1:728:G:C8	3.02	0.47
50:I:440:ALA:HB1	50:I:444:LEU:HD12	1.97	0.47
20:O:126:VAL:CG1	20:O:127:LEU:N	2.77	0.47
20:O:172:ARG:HG3	20:O:173:ALA:N	2.30	0.47
20:O:19:LEU:HD23	20:O:41:LEU:HD11	1.97	0.47
21:V:104:ASN:HD21	21:V:108:GLU:HB2	1.78	0.47
1:1:1688:U:C2	1:1:1689:U:C5	3.03	0.47
1:1:1742:U:N3	1:1:1743:G:C8	2.82	0.47
1:1:507:U:H2'	1:1:508:U:C6	2.49	0.47
1:1:548:G:H2'	1:1:549:U:O4'	2.14	0.47
1:1:962:A:H3'	1:1:963:G:C8	2.50	0.47
20:O:74:ARG:HD3	20:O:74:ARG:H	1.75	0.47
8:S:14:LEU:HA	8:S:15:PRO:HD3	1.81	0.47
8:S:52:LYS:HE3	8:S:54:ALA:HB3	1.97	0.47
21:V:87:ARG:HH22	21:V:137:VAL:HG13	1.80	0.47
1:1:1458:U:H2'	1:1:1459:C:C6	2.49	0.47
1:1:299:G:H3'	1:1:300:G:H8	1.80	0.47
2:2:27:U:H2'	2:2:28:C:H6	1.79	0.47
1:1:297:G:H1'	1:1:299:G:H1'	1.96	0.47
1:1:550:A:N6	1:1:551:A:H62	2.13	0.47
1:1:845:G:N2	1:1:848:A:OP2	2.48	0.47
1:1:1362:G:O2'	27:F:159:GLN:HA	2.15	0.47
7:R:43:LYS:HA	7:R:46:LYS:HE3	1.97	0.47
1:1:551:A:O2'	1:1:552:G:O5'	2.31	0.47
1:1:63:A:C2	1:1:78:U:O2	2.61	0.47
29:C:126:ILE:HD11	29:C:233:LEU:HD13	1.97	0.47
1:1:516:A:H4'	27:F:60:ARG:HH22	1.79	0.47
50:I:582:LYS:HA	50:I:585:ILE:HD12	1.96	0.47
54:M:7:VAL:O	54:M:7:VAL:HG12	2.14	0.47
20:O:136:THR:O	20:O:137:THR:C	2.54	0.47
1:1:1883:A:H2'	1:1:1884:A:O4'	2.15	0.46
1:1:2408:U:H2'	1:1:2409:G:H8	1.79	0.46
1:1:3013:U:H2'	1:1:3014:U:C6	2.51	0.46
35:W:60:TRP:CD1	35:W:63:SER:HB2	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:1134:G:H2'	1:1:1135:A:H8	1.80	0.46
1:1:157:A:H62	1:1:264:G:H21	1.63	0.46
1:1:355:A:H2'	1:1:356:C:O4'	2.16	0.46
1:1:952:A:H4'	1:1:968:G:N2	2.30	0.46
31:A:134:ARG:HE	31:A:162:VAL:HG13	1.79	0.46
34:D:348:VAL:HG12	34:D:351:ARG:HH22	1.79	0.46
52:E:31:ARG:HD3	52:E:31:ARG:H	1.80	0.46
50:I:212:LYS:HD2	50:I:215:ASN:HB2	1.96	0.46
32:K:170:ARG:HD2	32:K:194:MET:HA	1.98	0.46
3:6:32:A:C5	32:K:285:ARG:NH2	2.83	0.46
11:Z:87:LEU:HD11	11:Z:121:ARG:HD3	1.97	0.46
1:1:1590:G:O2'	1:1:1797:A:N6	2.48	0.46
1:1:1836:C:H2'	1:1:1837:U:C6	2.50	0.46
1:1:1857:C:N4	1:1:1858:A:C6	2.84	0.46
1:1:2127:U:H2'	1:1:2128:C:C6	2.50	0.46
31:A:134:ARG:HE	31:A:162:VAL:CG1	2.29	0.46
29:C:22:LEU:HA	29:C:23:PRO:HD3	1.81	0.46
1:1:1439:U:OP1	29:C:87:GLN:HB2	2.15	0.46
32:K:67:LEU:HD13	34:D:283:PHE:HZ	1.79	0.46
1:1:666:A:H1'	4:L:12:ASN:HD21	1.80	0.46
8:S:25:PHE:HB3	9:T:151:LEU:HD22	1.97	0.46
1:1:1226:G:H1	1:1:1283:C:H42	1.63	0.46
1:1:1581:C:H4'	1:1:1582:C:OP1	2.15	0.46
1:1:2933:A:OP1	1:1:3015:G:H4'	2.16	0.46
29:C:23:PRO:HG2	29:C:258:LEU:HD23	1.98	0.46
20:O:35:VAL:HG12	20:O:104:VAL:HG22	1.98	0.46
21:V:18:PRO:HA	21:V:51:ALA:HA	1.96	0.46
1:1:1178:G:N3	1:1:1328:C:O2'	2.47	0.46
1:1:2095:G:H2'	1:1:2096:A:C8	2.51	0.46
1:1:661:G:H4'	1:1:662:U:H6	1.80	0.46
31:A:225:LEU:HD21	31:A:235:LYS:HD3	1.96	0.46
28:B:26:ARG:HD3	28:B:177:HIS:HB3	1.96	0.46
53:G:217:THR:O	53:G:221:ASN:HB2	2.16	0.46
5:N:35:VAL:HG13	5:N:65:ARG:HB3	1.97	0.46
20:O:12:LYS:CD	20:O:40:GLU:CD	2.84	0.46
20:O:19:LEU:CD2	20:O:41:LEU:HD11	2.46	0.46
23:P:19:GLY:HA3	23:P:22:LEU:HD11	1.98	0.46
1:1:2377:G:H5'	1:1:2378:C:H5	1.80	0.46
1:1:3306:U:O4'	1:1:3306:U:O2	2.31	0.46
31:A:41:VAL:HG12	31:A:46:ARG:HG3	1.97	0.46
54:M:17:VAL:HG21	54:M:74:ARG:HG3	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:O:120:VAL:O	20:O:120:VAL:HG12	2.15	0.46
1:1:1697:A:H2'	1:1:1698:C:O4'	2.15	0.46
1:1:1949:G:N1	1:1:2097:U:C2	2.84	0.46
1:1:208:C:H2'	1:1:209:A:O4'	2.16	0.46
2:2:91:C:H2'	2:2:92:A:H8	1.80	0.46
30:H:137:SER:HB3	30:H:143:GLU:HB3	1.97	0.46
50:I:195:ARG:HB2	50:I:221:VAL:HG21	1.98	0.46
20:O:35:VAL:CG1	20:O:104:VAL:HG13	2.45	0.46
1:1:1116:G:N7	1:1:1117:G:C8	2.84	0.46
1:1:1497:C:H2'	1:1:1498:A:H8	1.80	0.46
1:1:1348:U:O2	1:1:1349:G:N2	2.49	0.46
1:1:1717:U:H2'	1:1:1718:G:C8	2.51	0.46
1:1:3017:A:H2'	1:1:3018:C:C6	2.50	0.46
1:1:771:A:C2	1:1:772:U:C4	3.04	0.46
29:C:217:LYS:HA	29:C:220:ARG:HG2	1.96	0.46
29:C:205:PRO:HB3	29:C:247:PHE:CD2	2.51	0.46
9:T:133:ALA:HB3	27:F:121:LYS:HB2	1.96	0.46
4:L:24:VAL:HG21	29:C:106:TRP:HB3	1.97	0.46
5:N:22:LEU:O	5:N:26:ARG:HG3	2.16	0.46
20:O:189:ASP:O	20:O:190:VAL:C	2.55	0.46
20:O:43:ILE:CG2	20:O:44:SER:N	2.55	0.46
1:1:1176:C:H2'	1:1:1177:G:N2	2.31	0.46
1:1:220:G:O2'	1:1:221:A:H5'	2.15	0.46
1:1:2328:U:H2'	1:1:2329:C:H6	1.81	0.46
1:1:2422:C:H2'	1:1:2423:U:O4'	2.16	0.46
29:C:169:LEU:HD22	29:C:249:ILE:HD13	1.97	0.46
52:E:42:LEU:HD22	52:E:79:VAL:HG21	1.99	0.46
20:O:42:ASN:HD22	20:O:137:THR:HA	1.81	0.46
1:1:1190:A:N6	1:1:1315:U:C2	2.77	0.45
1:1:1289:G:H2'	1:1:1290:A:C8	2.51	0.45
2:2:91:C:H2'	2:2:92:A:C8	2.51	0.45
52:E:68:PRO:HG3	52:E:145:LEU:HD23	1.98	0.45
1:1:2942:C:C2'	1:1:2942:C:O2	2.64	0.45
31:A:173:ILE:HG21	51:J:221:GLN:HE22	1.80	0.45
32:K:32:ILE:HD11	32:K:264:GLU:HA	1.99	0.45
20:O:184:THR:HG22	20:O:184:THR:O	2.16	0.45
1:1:1622:U:C2	1:1:1623:G:C8	3.05	0.45
1:1:2341:A:H2'	1:1:2342:U:C6	2.52	0.45
1:1:242:C:HO2'	1:1:243:G:H8	1.62	0.45
1:1:2998:U:H2'	1:1:2999:U:O4'	2.16	0.45
2:2:107:G:H4'	2:2:138:A:H5'	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:B:71:GLU:HG2	28:B:357:LYS:HE3	1.98	0.45
1:1:1574:C:C2	1:1:1575:A:N7	2.84	0.45
1:1:2928:C:O2	1:1:2928:C:C2'	2.52	0.45
1:1:3101:G:H2'	1:1:3102:G:C8	2.51	0.45
1:1:3110:C:H2'	1:1:3111:U:C6	2.51	0.45
1:1:3196:U:O2	1:1:3196:U:O4'	2.35	0.45
28:B:84:VAL:HG13	28:B:162:VAL:HB	1.99	0.45
30:H:67:ALA:O	30:H:70:THR:HG22	2.16	0.45
20:O:137:THR:HG23	20:O:139:GLY:H	1.81	0.45
7:R:8:LYS:HD3	7:R:24:LEU:HD13	1.99	0.45
7:R:10:LEU:HB3	7:R:41:ILE:HG13	1.97	0.45
1:1:159:A:H2'	1:1:160:G:H8	1.82	0.45
1:1:3295:A:H2'	1:1:3296:A:H8	1.81	0.45
1:1:3365:U:H2'	1:1:3366:G:H8	1.82	0.45
53:G:133:LYS:HG2	53:G:138:HIS:NE2	2.31	0.45
1:1:1060:U:H2'	1:1:1061:A:H8	1.81	0.45
1:1:1597:C:H2'	1:1:1598:G:H8	1.81	0.45
1:1:3039:C:C2	1:1:3040:A:C8	3.04	0.45
1:1:3180:A:C6	20:O:114:LYS:HG3	2.51	0.45
20:O:38:ALA:O	20:O:41:LEU:CB	2.63	0.45
6:Q:83:VAL:O	6:Q:103:ALA:HA	2.16	0.45
1:1:1619:A:H5'	1:1:1620:U:OP2	2.17	0.45
1:1:3006:A:H2'	1:1:3007:U:O4'	2.16	0.45
1:1:3278:C:O2	1:1:3278:C:H2'	2.17	0.45
1:1:977:C:O2	1:1:977:C:O4'	2.35	0.45
31:A:86:VAL:HG13	31:A:102:SER:HB3	1.99	0.45
27:F:165:ASP:HB3	27:F:168:ILE:HD12	1.99	0.45
20:O:37:ARG:CD	20:O:108:ILE:HD11	2.41	0.45
20:O:162:VAL:O	20:O:163:SER:C	2.55	0.45
1:1:1439:U:H2'	1:1:1440:G:O4'	2.17	0.45
1:1:1549:U:H2'	1:1:1550:C:H6	1.81	0.45
1:1:658:G:N2	29:C:93:MET:HB2	2.32	0.45
1:1:1339:C:H2'	1:1:1340:G:O4'	2.17	0.45
1:1:2599:U:H2'	1:1:2600:C:C6	2.52	0.45
1:1:370:U:H4'	1:1:404:G:H5'	1.98	0.45
20:O:137:THR:CG2	20:O:139:GLY:H	2.29	0.45
20:O:48:PHE:O	20:O:49:ARG:C	2.56	0.45
1:1:1525:G:H2'	1:1:1525:G:N3	2.32	0.45
1:1:900:G:H1'	1:1:1589:A:N6	2.32	0.45
1:1:2342:U:H2'	1:1:2343:C:H6	1.81	0.45
1:1:3305:A:H2'	1:1:3306:U:O4'	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:612:U:H2'	1:1:613:G:H8	1.82	0.45
1:1:674:G:H2'	1:1:675:C:O4'	2.17	0.45
29:C:138:ARG:HH21	29:C:240:PRO:HG2	1.82	0.45
20:O:156:LEU:HD12	53:G:89:GLU:HG3	193.67	0.45
20:O:47:PHE:HA	20:O:136:THR:CG2	2.46	0.45
6:Q:100:THR:HG23	6:Q:120:GLU:HB3	1.99	0.45
1:1:1236:G:N2	1:1:1244:A:OP1	2.49	0.44
1:1:3211:C:H2'	1:1:3212:C:C6	2.52	0.44
1:1:656:A:H2'	1:1:657:A:C8	2.53	0.44
21:V:17:LEU:HD21	21:V:98:ASN:HB3	1.99	0.44
1:1:148:G:H5''	5:N:55:ALA:HB3	1.98	0.44
1:1:1551:C:H2'	1:1:1552:G:O4'	2.18	0.44
1:1:3028:G:H2'	1:1:3029:A:C8	2.53	0.44
1:1:2909:U:O2'	1:1:3105:U:O2	2.24	0.44
1:1:881:C:H42	1:1:886:C:H1'	1.83	0.44
30:H:16:VAL:HG12	30:H:29:GLY:HA3	1.99	0.44
20:O:12:LYS:CG	20:O:13:GLY:N	2.80	0.44
20:O:166:GLU:O	20:O:167:TYR:C	2.55	0.44
25:Y:51:ARG:HG2	25:Y:115:ARG:HH22	1.83	0.44
1:1:16:A:H2'	1:1:17:G:O4'	2.17	0.44
1:1:3017:A:H2'	1:1:3018:C:H6	1.82	0.44
1:1:3343:G:C2	1:1:3361:G:C2	3.05	0.44
1:1:496:C:H2'	1:1:497:C:O4'	2.17	0.44
29:C:122:THR:HG22	29:C:235:LEU:HB2	1.99	0.44
27:F:88:ARG:HA	27:F:134:VAL:HG12	1.99	0.44
20:O:30:GLY:HA2	20:O:101:ARG:CZ	2.48	0.44
20:O:27:LEU:HD11	20:O:102:LEU:HB2	1.99	0.44
20:O:112:TYR:O	20:O:113:ASP:O	2.36	0.44
35:W:22:ASN:HD21	35:W:25:ARG:HH21	1.64	0.44
1:1:1594:A:H1'	1:1:1615:C:H1'	1.99	0.44
1:1:210:U:C2	1:1:230:U:H4'	2.52	0.44
1:1:3041:U:H2'	1:1:3042:U:H6	1.81	0.44
1:1:3162:C:N4	1:1:3163:A:N6	2.64	0.44
1:1:3346:U:H2'	1:1:3347:A:C8	2.52	0.44
1:1:556:U:O2	1:1:559:A:N7	2.50	0.44
1:1:814:U:H2'	1:1:815:G:O4'	2.17	0.44
1:1:3:U:H2'	1:1:4:U:C6	2.52	0.44
28:B:159:ARG:HA	28:B:182:GLN:HA	1.99	0.44
28:B:28:ARG:HH22	28:B:30:LYS:HE2	1.82	0.44
20:O:46:GLU:HB2	20:O:134:LYS:CD	2.47	0.44
1:1:1145:G:O6	1:1:1158:A:H2	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:1289:G:H2'	1:1:1290:A:H8	1.83	0.44
1:1:3105:U:C5	1:1:3128:G:C2	3.06	0.44
1:1:409:A:H1'	1:1:655:C:H1'	1.98	0.44
2:2:130:C:H2'	2:2:131:A:O4'	2.18	0.44
50:I:166:VAL:HG21	50:I:178:MET:HG2	1.99	0.44
50:I:332:SER:HA	50:I:335:ASN:HD22	1.81	0.44
32:K:83:VAL:HG21	32:K:270:LEU:HD13	1.99	0.44
20:O:114:LYS:C	20:O:115:LYS:CG	2.85	0.44
20:O:27:LEU:N	20:O:27:LEU:HD22	2.30	0.44
1:1:1200:A:C2	1:1:2824:G:N1	2.63	0.44
1:1:279:U:H2'	1:1:280:U:H6	1.82	0.44
1:1:2991:A:H2	23:P:69:ARG:HH22	1.66	0.44
1:1:3346:U:H2'	1:1:3347:A:H8	1.83	0.44
34:D:433:ILE:HG23	34:D:434:LYS:HG3	1.99	0.44
50:I:335:ASN:HB3	50:I:527:PRO:HB3	2.00	0.44
20:O:194:LEU:O	20:O:197:LEU:N	2.42	0.44
20:O:45:GLY:O	20:O:46:GLU:C	2.55	0.44
1:1:2916:U:H2'	1:1:2917:G:C8	2.52	0.44
29:C:84:ARG:O	29:C:87:GLN:HG2	2.18	0.44
20:O:65:ASN:HD22	20:O:67:THR:H	1.65	0.44
1:1:2127:U:H2'	1:1:2128:C:H6	1.83	0.44
1:1:3072:C:H5'	1:1:3336:A:H5''	1.99	0.44
1:1:3150:A:H5''	1:1:3151:U:OP2	2.17	0.44
2:2:26:U:H2'	2:2:27:U:H6	1.81	0.44
20:O:59:ARG:HB2	20:O:59:ARG:HE	1.68	0.44
1:1:1471:U:H2'	1:1:1472:U:C6	2.53	0.43
1:1:1498:A:H2'	1:1:1499:C:H6	1.81	0.43
1:1:497:C:H2'	1:1:498:A:O4'	2.18	0.43
1:1:990:U:HO2'	9:T:101:CYS:N	2.16	0.43
31:A:179:PHE:HB3	31:A:186:ILE:HD11	2.00	0.43
30:H:21:LYS:CG	54:M:8:LYS:HG3	2.40	0.43
8:S:14:LEU:H	8:S:56:GLY:HA2	1.82	0.43
1:1:246:U:H2'	1:1:247:C:C6	2.53	0.43
1:1:3057:U:H3'	1:1:3058:U:H4'	1.99	0.43
1:1:3347:A:H2'	1:1:3348:G:O4'	2.18	0.43
31:A:135:PRO:HB3	31:A:175:HIS:CE1	2.53	0.43
20:O:172:ARG:CG	20:O:173:ALA:N	2.81	0.43
1:1:1263:A:N3	1:1:1263:A:H2'	2.32	0.43
1:1:1435:A:C8	1:1:1437:C:C6	3.06	0.43
1:1:1488:G:C2	1:1:1489:A:C8	3.06	0.43
1:1:148:G:OP2	5:N:4:TYR:OH	2.32	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:A:112:PHE:CD1	31:A:221:MET:HB3	2.53	0.43
34:D:268:TYR:HA	34:D:392:MET:H	1.83	0.43
50:I:593:LYS:HA	50:I:596:ASN:HD22	1.83	0.43
7:R:92:GLN:HE21	7:R:96:ILE:HD11	1.83	0.43
9:T:154:VAL:N	9:T:155:PRO:HA	2.33	0.43
1:1:139:G:H2'	1:1:140:C:C6	2.53	0.43
1:1:3214:U:O4'	1:1:3214:U:O2	2.35	0.43
1:1:620:U:H4'	23:P:167:ARG:NH1	2.32	0.43
1:1:960:U:H5''	1:1:963:G:O6	2.19	0.43
50:I:517:LEU:HD13	50:I:519:TYR:H	1.82	0.43
4:L:58:VAL:HG12	4:L:70:ARG:HG3	2.00	0.43
20:O:10:ASP:C	20:O:12:LYS:H	2.20	0.43
20:O:165:ALA:O	20:O:168:TYR:HB3	2.17	0.43
20:O:191:ALA:O	20:O:193:GLN:N	2.52	0.43
20:O:12:LYS:CG	20:O:40:GLU:CD	2.86	0.43
1:1:2839:G:H2'	1:1:2840:C:H6	1.82	0.43
1:1:3121:U:H1'	1:1:3122:A:H5''	2.00	0.43
3:6:4:U:H3'	3:6:5:C:H5'	1.99	0.43
30:H:87:LYS:HD3	30:H:89:LYS:HE3	2.01	0.43
51:J:220:HIS:CE1	51:J:222:SER:HB3	2.53	0.43
5:N:28:TRP:HH2	53:G:61:GLN:HB3	1.83	0.43
20:O:102:LEU:CD1	20:O:103:LYS:N	2.67	0.43
20:O:108:ILE:HD13	20:O:117:ARG:HE	1.83	0.43
20:O:34:VAL:O	20:O:34:VAL:HG12	2.19	0.43
1:1:221:A:O2'	1:1:223:U:OP2	2.37	0.43
1:1:2411:U:H3	1:1:2811:A:N6	2.16	0.43
1:1:2803:A:H2'	1:1:2804:A:H8	1.83	0.43
1:1:2803:A:H2'	1:1:2804:A:C8	2.53	0.43
1:1:2976:A:HO2'	1:1:2977:G:H8	1.64	0.43
1:1:504:A:N6	1:1:588:G:O6	2.52	0.43
1:1:600:G:N2	1:1:602:A:H3'	2.34	0.43
1:1:800:G:H22	29:C:101:ALA:HA	1.83	0.43
1:1:818:C:H2'	1:1:818:C:O2	2.17	0.43
2:2:104:A:C8	2:2:105:A:C8	3.06	0.43
2:2:27:U:H4'	29:C:51:ALA:HB3	2.01	0.43
54:M:38:ILE:HG13	54:M:38:ILE:H	1.65	0.43
5:N:118:SER:HB3	5:N:132:VAL:HG23	1.99	0.43
1:1:1141:C:H2'	1:1:1142:G:O4'	2.18	0.43
1:1:1569:U:O2	1:1:1569:U:H2'	2.18	0.43
1:1:1895:A:O2'	1:1:3053:G:H4'	2.18	0.43
1:1:2599:U:H2'	1:1:2600:C:H6	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:406:G:H1'	2:2:16:G:H22	1.83	0.43
2:2:27:U:H2'	2:2:28:C:C6	2.53	0.43
53:G:112:GLU:O	53:G:116:VAL:HB	2.19	0.43
1:1:120:G:C5	53:G:128:LYS:HB3	2.54	0.43
20:O:151:ASP:O	20:O:152:VAL:C	2.57	0.43
20:O:76:PRO:HB2	20:O:106:GLU:HG2	2.01	0.43
21:V:80:ARG:HB2	21:V:99:ALA:HB3	2.01	0.43
1:1:1468:A:N1	1:1:1880:U:O2'	2.42	0.43
1:1:288:C:H2'	1:1:289:A:H8	1.83	0.43
1:1:3211:C:H2'	1:1:3212:C:H6	1.84	0.43
1:1:894:G:C8	1:1:895:A:H5'	2.49	0.43
53:G:144:GLU:HA	53:G:173:MET:CE	2.48	0.43
20:O:98:ALA:HA	20:O:101:ARG:HH11	1.84	0.43
35:W:130:LYS:HD2	35:W:192:GLY:HA2	2.00	0.43
1:1:2320:A:H2'	1:1:2321:A:C8	2.54	0.43
1:1:3041:U:H2'	1:1:3042:U:C6	2.53	0.43
1:1:3163:A:C6	1:1:3164:C:N4	2.86	0.43
1:1:3388:C:H5''	1:1:3389:U:H5'	2.01	0.43
1:1:507:U:H2'	1:1:508:U:H6	1.84	0.43
1:1:753:C:N4	1:1:754:G:O6	2.51	0.43
28:B:46:PHE:HE2	28:B:81:THR:HB	1.83	0.43
29:C:193:LYS:HE3	29:C:193:LYS:HB2	1.82	0.43
1:1:1458:U:H2'	1:1:1459:C:H6	1.83	0.43
1:1:1794:G:O2'	1:1:1796:G:N2	2.52	0.43
1:1:976:U:O2	1:1:976:U:O4'	2.37	0.43
31:A:112:PHE:HZ	31:A:152:ILE:HD11	1.83	0.43
34:D:472:LYS:HB2	34:D:477:TYR:HB2	2.00	0.43
53:G:175:VAL:HA	53:G:176:PRO:HD3	1.90	0.43
54:M:46:ILE:HD11	54:M:56:GLN:HE21	1.84	0.43
1:1:279:U:H2'	1:1:280:U:C6	2.54	0.42
1:1:2367:A:H2'	1:1:2368:A:H8	1.84	0.42
1:1:2993:G:H2'	1:1:3142:A:H61	1.84	0.42
1:1:3237:U:H2'	1:1:3238:G:O4'	2.19	0.42
1:1:3393:U:H2'	1:1:3394:U:C6	2.54	0.42
1:1:549:U:H3'	1:1:550:A:H8	1.84	0.42
1:1:671:U:C2	1:1:672:A:C8	3.08	0.42
30:H:86:TYR:CE2	30:H:151:VAL:HG22	2.53	0.42
51:J:239:ASP:HA	51:J:242:ARG:HB3	2.00	0.42
6:Q:93:ILE:HD11	6:Q:113:LYS:HD3	2.01	0.42
8:S:38:LYS:HG2	8:S:58:ILE:HG13	2.01	0.42
35:W:55:GLU:HA	35:W:58:THR:HG22	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:1117:G:H2'	1:1:1118:C:C6	2.54	0.42
1:1:1886:A:H2'	1:1:1887:A:C8	2.54	0.42
2:2:75:G:H2'	2:2:76:C:C6	2.54	0.42
52:E:42:LEU:HD11	52:E:52:VAL:HG21	2.01	0.42
1:1:3272:C:H5''	52:E:77:ARG:HH21	1.84	0.42
5:N:95:GLN:HB2	5:N:95:GLN:HE21	1.58	0.42
20:O:34:VAL:HG22	20:O:103:LYS:CB	2.49	0.42
20:O:77:SER:O	20:O:80:PHE:N	2.34	0.42
21:V:21:ALA:HB3	21:V:36:ILE:HD12	2.00	0.42
1:1:195:U:H2'	1:1:196:G:O4'	2.18	0.42
1:1:2419:A:H5''	1:1:2606:G:H22	1.84	0.42
1:1:2904:U:H2'	1:1:2905:U:C6	2.53	0.42
1:1:2905:U:H2'	1:1:2906:C:C6	2.54	0.42
1:1:3023:U:H2'	1:1:3024:A:H8	1.84	0.42
1:1:3158:G:H2'	1:1:3158:G:N3	2.34	0.42
1:1:3291:G:H2'	1:1:3292:A:C8	2.55	0.42
1:1:772:U:H2'	1:1:773:G:O4'	2.20	0.42
53:G:139:VAL:O	53:G:143:ILE:HG13	2.19	0.42
50:I:315:LEU:HA	50:I:318:PHE:HB3	2.01	0.42
6:Q:96:PHE:HA	6:Q:97:PRO:HD3	1.94	0.42
1:1:1214:U:H2'	1:1:1215:U:C6	2.54	0.42
1:1:1622:U:H2'	1:1:1623:G:H8	1.85	0.42
1:1:2912:G:C6	1:1:3130:A:N7	2.88	0.42
1:1:357:A:H2'	1:1:358:G:O4'	2.19	0.42
1:1:556:U:O4'	1:1:557:A:C5	2.72	0.42
3:6:23:U:H1'	32:K:191:PRO:HG3	2.00	0.42
28:B:56:ILE:HG21	28:B:356:LEU:HD22	2.01	0.42
50:I:395:SER:HA	50:I:398:GLU:HB2	2.02	0.42
4:L:46:ILE:HG22	4:L:49:ARG:HB2	2.00	0.42
1:1:269:G:H5''	5:N:14:LYS:HZ3	1.85	0.42
20:O:136:THR:C	20:O:137:THR:O	2.57	0.42
20:O:178:VAL:HG12	20:O:182:ASN:ND2	2.34	0.42
1:1:2854:U:H2'	1:1:2855:U:C6	2.54	0.42
1:1:2918:G:H2'	1:1:2919:A:C8	2.55	0.42
50:I:299:GLU:HB3	50:I:528:LEU:HD11	2.00	0.42
20:O:108:ILE:HD13	20:O:117:ARG:NE	2.35	0.42
1:1:1060:U:H1'	9:T:101:CYS:HB2	2.01	0.42
1:1:1162:U:C4	1:1:1163:A:N7	2.88	0.42
1:1:1231:A:H5''	1:1:1232:C:H5'	2.02	0.42
1:1:1797:A:H2'	1:1:1798:A:C8	2.55	0.42
1:1:429:U:H2'	1:1:430:U:H6	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:533:A:H61	1:1:556:U:H5	0.63	0.42
3:6:7:C:O2'	3:6:8:A:O5'	2.36	0.42
53:G:75:ILE:HG22	53:G:76:ALA:H	1.85	0.42
54:M:38:ILE:HG22	54:M:44:VAL:HG12	2.02	0.42
1:1:2880:U:H2'	1:1:2881:C:H6	1.85	0.42
1:1:3141:A:H3'	1:1:3142:A:H4'	2.00	0.42
1:1:3:U:O2'	3:6:232:A:H8	2.01	0.42
1:1:428:A:H2'	1:1:429:U:C6	2.55	0.42
1:1:544:C:N4	1:1:547:G:O6	2.53	0.42
1:1:737:G:H2'	1:1:738:A:H8	1.85	0.42
1:1:808:A:H2'	1:1:809:G:H8	1.78	0.42
31:A:138:SER:HB2	31:A:178:SER:HA	2.01	0.42
52:E:23:LYS:HD3	52:E:23:LYS:HA	1.94	0.42
53:G:136:LEU:HD11	53:G:163:VAL:HG22	2.02	0.42
20:O:124:LEU:HA	20:O:124:LEU:HD13	1.74	0.42
20:O:61:ALA:HB3	20:O:66:LYS:HD3	2.01	0.42
1:1:2341:A:H2'	1:1:2342:U:H6	1.84	0.42
1:1:2876:C:H4'	1:1:2925:C:H5	1.85	0.42
1:1:685:G:H21	21:V:65:GLY:H	146.09	0.42
1:1:784:A:H8	6:Q:69:ARG:HE	1.66	0.42
2:2:154:C:H5'	53:G:181:LYS:HD3	2.01	0.42
50:I:227:TYR:HE2	50:I:259:LEU:HD11	1.85	0.42
50:I:552:HIS:CE1	50:I:556:ARG:HD2	2.55	0.42
1:1:216:G:H2'	1:1:217:U:O4'	2.19	0.42
1:1:2420:C:H2'	1:1:2421:U:C6	2.55	0.42
1:1:2848:G:H2'	1:1:2849:C:C6	2.55	0.42
1:1:3117:C:N4	35:W:6:ARG:HD2	2.35	0.42
1:1:501:A:H2'	1:1:502:U:H6	1.84	0.42
1:1:503:C:C2	1:1:504:A:C8	3.07	0.42
1:1:748:U:H2'	1:1:749:C:C6	2.54	0.42
53:G:75:ILE:C	53:G:77:GLN:H	2.23	0.42
32:K:86:LYS:HD2	32:K:301:LEU:HD13	2.02	0.42
5:N:192:LYS:O	5:N:196:THR:OG1	2.38	0.42
5:N:191:TRP:O	5:N:195:ASN:HB2	2.19	0.42
20:O:85:ARG:HH21	20:O:90:HIS:CE1	2.36	0.42
35:W:175:ILE:HG22	35:W:180:ILE:HA	2.02	0.42
25:Y:37:LYS:H	25:Y:37:LYS:HD2	1.85	0.42
11:Z:103:GLN:HG3	11:Z:103:GLN:O	2.20	0.42
1:1:1238:C:H2'	1:1:1239:C:C6	2.55	0.41
1:1:2340:U:H2'	1:1:2341:A:C8	2.51	0.41
1:1:2420:C:H2'	1:1:2421:U:H6	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:2598:G:H2'	1:1:2599:U:C6	2.55	0.41
1:1:3112:G:O6	1:1:3120:C:H5''	2.20	0.41
1:1:715:A:H4'	1:1:752:C:O2'	2.19	0.41
1:1:811:U:H2'	1:1:812:G:O4'	2.20	0.41
1:1:850:U:H2'	1:1:851:C:H6	1.83	0.41
53:G:141:ALA:O	53:G:145:ASN:CG	2.57	0.41
50:I:555:PHE:HZ	50:I:593:LYS:HB3	1.85	0.41
20:O:47:PHE:C	20:O:49:ARG:N	2.73	0.41
21:V:101:VAL:HG11	21:V:114:ILE:HG12	2.02	0.41
24:X:105:VAL:HG21	24:X:135:ILE:HD12	2.02	0.41
1:1:1734:G:H2'	1:1:1735:G:O4'	2.19	0.41
1:1:646:A:H1'	1:1:2372:A:C2	2.56	0.41
2:2:59:A:H5''	2:2:61:A:C8	2.55	0.41
28:B:215:ILE:HD13	28:B:338:LEU:HD23	2.02	0.41
29:C:23:PRO:HB2	29:C:25:VAL:HG23	2.01	0.41
50:I:529:ASN:H	50:I:533:ILE:HD12	1.84	0.41
5:N:36:ILE:HG12	5:N:64:VAL:HG23	2.01	0.41
20:O:78:ARG:HG2	20:O:78:ARG:H	1.57	0.41
8:S:8:GLN:HG3	8:S:26:ARG:HE	1.85	0.41
1:1:1316:C:H5''	1:1:1317:A:C2	2.55	0.41
1:1:1341:U:H2'	1:1:1342:C:H6	1.86	0.41
1:1:1362:G:H2'	1:1:1363:A:C8	2.55	0.41
1:1:1561:G:HO2'	1:1:1562:C:P	2.44	0.41
1:1:3000:A:H2'	1:1:3001:C:C6	2.56	0.41
1:1:312:C:H2'	1:1:313:A:H8	1.85	0.41
1:1:439:C:H5'	1:1:494:G:N2	2.36	0.41
1:1:688:G:H2'	1:1:690:A:C8	2.54	0.41
1:1:881:C:H42	1:1:886:C:C1'	2.33	0.41
1:1:940:G:O2'	1:1:1435:A:H4'	2.20	0.41
3:6:8:A:H2'	3:6:9:A:C8	2.56	0.41
4:L:46:ILE:O	4:L:46:ILE:HG22	2.20	0.41
20:O:175:THR:HG1	20:O:176:LYS:H	1.66	0.41
10:U:89:LEU:HB3	10:U:93:ILE:HD12	2.02	0.41
2:2:134:G:OP1	24:X:56:ARG:HD3	2.20	0.41
1:1:1124:U:O4'	1:1:1124:U:O2	2.38	0.41
1:1:1242:G:H2'	1:1:1243:G:C8	2.56	0.41
1:1:1231:A:H4'	1:1:1261:G:C8	2.54	0.41
1:1:3281:U:H2'	1:1:3282:U:C6	2.55	0.41
1:1:701:G:H2'	1:1:702:C:C6	2.55	0.41
27:F:178:ILE:HG23	27:F:183:ASP:HB2	2.02	0.41
5:N:22:LEU:HD11	53:G:160:ILE:HB	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
50:I:237:THR:HA	50:I:238:PRO:HD3	1.94	0.41
50:I:535:PRO:HG2	50:I:539:VAL:HA	2.03	0.41
20:O:36:VAL:CG2	20:O:108:ILE:HG12	2.50	0.41
20:O:50:ASN:N	20:O:50:ASN:ND2	2.55	0.41
10:U:41:ILE:HB	10:U:50:LEU:HD11	2.02	0.41
35:W:157:MET:HB2	35:W:180:ILE:HD13	2.03	0.41
1:1:1061:A:H2'	1:1:1062:A:C8	2.55	0.41
1:1:1222:G:H21	1:1:1286:A:H2	1.68	0.41
1:1:177:U:C4	1:1:178:U:C5	3.08	0.41
1:1:1836:C:H2'	1:1:1837:U:H6	1.84	0.41
1:1:2363:A:H2'	1:1:2364:G:O4'	2.20	0.41
1:1:3015:G:OP2	11:Z:2:ALA:N	150.60	0.41
1:1:3150:A:H4'	28:B:128:LYS:O	2.20	0.41
2:2:153:U:H2'	2:2:154:C:O4'	2.21	0.41
31:A:189:ARG:CZ	31:A:189:ARG:HB2	2.51	0.41
29:C:295:ILE:O	29:C:299:ILE:HG12	2.21	0.41
27:F:85:PHE:HB2	27:F:139:PRO:HG3	2.03	0.41
20:O:168:TYR:O	20:O:171:LYS:CA	2.66	0.41
1:1:2899:C:O2	1:1:2899:C:O4'	2.39	0.41
1:1:3094:A:H2'	1:1:3095:U:C6	2.56	0.41
1:1:386:A:C5	1:1:387:A:H1'	2.55	0.41
1:1:412:G:H2'	1:1:413:U:C6	2.56	0.41
1:1:503:C:H42	1:1:504:A:H62	1.65	0.41
53:G:205:ALA:HA	53:G:208:GLU:HB2	2.03	0.41
30:H:36:LYS:HZ3	30:H:74:LEU:HD22	1.86	0.41
1:1:1452:A:H1'	1:1:1453:A:H4'	2.02	0.41
1:1:2393:G:H1'	1:1:2394:G:N7	2.36	0.41
1:1:557:A:H8	1:1:557:A:H2'	1.72	0.41
1:1:58:G:H2'	1:1:59:G:C8	2.55	0.41
1:1:862:U:H2'	1:1:863:C:C6	2.56	0.41
1:1:971:G:C6	1:1:972:A:C5	3.09	0.41
2:2:55:U:C2	2:2:56:G:C8	3.09	0.41
3:6:36:U:H2'	3:6:37:C:C6	2.56	0.41
28:B:216:ASP:HB3	28:B:278:ILE:HG22	2.02	0.41
29:C:151:VAL:HG22	29:C:250:TRP:HB2	2.03	0.41
20:O:161:LYS:O	20:O:164:SER:CA	2.68	0.41
1:1:1293:U:C2	1:1:1294:A:C8	3.09	0.41
1:1:1758:G:H5'	10:U:104:ARG:NH2	2.36	0.41
1:1:2328:U:H2'	1:1:2329:C:C6	2.55	0.41
1:1:2340:U:C2	1:1:2341:A:C8	3.09	0.41
1:1:769:G:H5''	1:1:770:G:C5	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:881:C:N4	1:1:885:U:O2	2.54	0.41
2:2:107:G:C8	2:2:137:C:N4	2.88	0.41
2:2:91:C:C2	2:2:92:A:C8	3.08	0.41
31:A:137:LEU:HD12	31:A:179:PHE:HE2	1.86	0.41
50:I:480:PHE:HB3	50:I:552:HIS:HB3	2.02	0.41
20:O:193:GLN:O	20:O:196:ALA:N	2.54	0.41
2:2:12:A:H5''	23:P:3:ARG:HG3	2.03	0.41
1:1:1497:C:H2'	1:1:1498:A:C8	2.54	0.41
1:1:163:C:N4	1:1:164:A:H62	2.19	0.41
1:1:645:A:H8	1:1:2372:A:C2	2.39	0.41
1:1:2902:A:H2'	1:1:2903:A:O4'	2.21	0.41
1:1:532:A:O2'	1:1:533:A:H8	2.02	0.41
1:1:85:A:N1	1:1:99:A:H5''	2.36	0.41
53:G:144:GLU:HA	53:G:173:MET:HG3	2.01	0.41
51:J:235:ASP:HB3	51:J:238:ASP:HB2	2.02	0.41
20:O:51:LYS:HA	20:O:141:LEU:CD1	2.51	0.41
20:O:51:LYS:NZ	20:O:144:SER:HB2	2.35	0.41
20:O:80:PHE:O	20:O:80:PHE:CD2	2.74	0.41
1:1:1699:A:N6	1:1:1700:G:O6	2.54	0.41
1:1:1837:U:H2'	1:1:1838:G:O4'	2.21	0.41
1:1:1870:C:O2'	1:1:3067:C:H5'	2.20	0.41
1:1:246:U:H2'	1:1:247:C:H6	1.86	0.41
1:1:521:A:H2'	1:1:522:A:O4'	2.21	0.41
1:1:608:A:H5'	29:C:322:GLN:HB3	2.02	0.41
1:1:731:U:H2'	1:1:732:C:C6	2.56	0.41
2:2:53:A:C2	2:2:54:A:H1'	2.56	0.41
28:B:116:ARG:NH1	28:B:174:LYS:HB3	2.36	0.41
28:B:56:ILE:HD12	28:B:359:ILE:HG12	2.03	0.41
27:F:159:GLN:O	27:F:160:ARG:C	2.59	0.41
32:K:125:LEU:HD13	32:K:151:VAL:HG13	2.02	0.41
20:O:118:VAL:HG23	20:O:119:VAL:N	2.36	0.41
7:R:99:LEU:HD21	7:R:103:ARG:CZ	2.51	0.41
1:1:1295:G:H1'	8:S:113:ARG:O	2.20	0.41
1:1:437:G:H1	1:1:622:A:H61	1.68	0.41
1:1:900:G:H1'	1:1:1589:A:H62	1.85	0.41
31:A:130:LEU:HD12	31:A:170:LYS:HD3	2.03	0.41
27:F:214:TRP:CE2	27:F:219:LYS:HE2	2.56	0.41
20:O:16:VAL:CG2	20:O:41:LEU:HD21	2.40	0.41
1:1:3077:A:H2'	1:1:3080:G:O4'	2.21	0.40
1:1:735:A:H2'	1:1:736:A:H8	1.85	0.40
1:1:798:G:H2'	1:1:799:G:O4'	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:807:A:H3'	1:1:807:A:N3	2.36	0.40
34:D:300:ASN:HA	34:D:303:LYS:HE3	2.03	0.40
30:H:10:ILE:HB	30:H:53:ILE:HB	2.02	0.40
5:N:14:LYS:HA	5:N:19:LEU:HD22	2.02	0.40
20:O:39:GLU:O	20:O:138:LEU:HB3	2.21	0.40
20:O:188:SER:H	20:O:191:ALA:HB3	1.86	0.40
6:Q:86:THR:HG22	6:Q:105:ARG:HB2	2.02	0.40
1:1:1167:U:H2'	1:1:1168:U:O4'	2.21	0.40
1:1:2421:U:H2'	1:1:2422:C:C6	2.56	0.40
1:1:3014:U:H2'	1:1:3015:G:H8	1.86	0.40
1:1:3269:U:H4'	1:1:3270:U:O5'	2.22	0.40
1:1:536:U:O2	1:1:557:A:C6	2.55	0.40
1:1:67:A:O2'	1:1:315:C:O2	2.39	0.40
1:1:681:U:O2'	1:1:696:C:N4	2.54	0.40
1:1:734:C:O3'	1:1:735:A:H8	2.04	0.40
1:1:821:U:H2'	1:1:822:G:O4'	2.21	0.40
1:1:913:A:H2'	1:1:914:A:C8	2.56	0.40
53:G:91:PHE:CE2	53:G:185:ARG:HG2	2.34	0.40
30:H:45:PHE:CD1	30:H:55:VAL:HG12	2.56	0.40
54:M:124:ARG:O	54:M:128:ARG:HB2	2.22	0.40
1:1:31:C:H4'	5:N:96:ARG:HD3	2.03	0.40
20:O:36:VAL:CG2	20:O:37:ARG:HG3	2.44	0.40
10:U:50:LEU:HD22	10:U:54:VAL:HG22	2.03	0.40
10:U:33:TYR:HE1	10:U:80:THR:HG22	1.84	0.40
1:1:1394:A:N3	2:2:19:C:O2'	2.51	0.40
1:1:1713:G:H22	1:1:1730:G:H1'	1.87	0.40
1:1:213:A:N6	1:1:227:G:H2'	2.36	0.40
1:1:26:A:H2'	1:1:27:C:C6	2.57	0.40
1:1:288:C:H2'	1:1:289:A:C8	2.56	0.40
1:1:3215:A:HO2'	1:1:3259:U:H3	1.68	0.40
1:1:3225:C:C2	1:1:3226:A:C8	3.10	0.40
1:1:609:G:N7	29:C:308:LYS:HE2	2.36	0.40
1:1:945:C:H2'	1:1:946:U:H6	1.85	0.40
1:1:982:C:H2'	1:1:983:A:C8	2.56	0.40
28:B:37:ARG:HA	28:B:186:GLY:HA3	2.03	0.40
51:J:261:LEU:HG	51:J:266:VAL:HG13	2.04	0.40
2:2:29:U:H5''	4:L:27:ASP:HB3	2.03	0.40
11:Z:51:LEU:HB3	11:Z:65:ARG:HD2	2.02	0.40
1:1:106:A:H2'	1:1:107:A:O4'	2.21	0.40
1:1:1134:G:H2'	1:1:1135:A:C8	2.56	0.40
1:1:254:A:H2'	1:1:255:A:O4'	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:2598:G:H2'	1:1:2599:U:H6	1.86	0.40
1:1:2936:A:H2'	1:1:2937:G:H8	1.83	0.40
1:1:3302:U:H1'	1:1:3313:U:O2	2.21	0.40
1:1:3372:A:H2'	1:1:3373:U:C6	2.56	0.40
1:1:409:A:H3'	1:1:410:U:H6	1.86	0.40
1:1:537:A:C2	1:1:538:G:H1'	2.56	0.40
1:1:661:G:H4'	1:1:662:U:C6	2.54	0.40
1:1:680:G:H2'	1:1:681:U:H5'	2.03	0.40
2:2:56:G:H2'	2:2:57:C:O4'	2.21	0.40
31:A:144:GLU:HG2	31:A:150:GLN:HE22	1.86	0.40
28:B:89:VAL:HG21	28:B:195:ALA:HB2	2.03	0.40
1:1:1334:U:H5''	27:F:206:LYS:HB3	2.03	0.40
20:O:110:PRO:HA	20:O:112:TYR:N	2.35	0.40
20:O:87:MET:C	20:O:88:VAL:HG23	2.41	0.40
21:V:126:TRP:HA	21:V:127:PRO:HD3	1.95	0.40
35:W:45:LEU:HB3	35:W:215:VAL:HG23	2.03	0.40
11:Z:61:LYS:O	11:Z:65:ARG:HG2	2.22	0.40
1:1:109:A:H5''	4:L:53:LEU:HD11	2.03	0.40
1:1:435:C:O2'	1:1:1401:A:H5'	2.21	0.40
1:1:571:U:H2'	1:1:572:A:C8	2.56	0.40
1:1:626:U:H2'	1:1:627:U:O4'	2.21	0.40
31:A:149:TYR:HA	31:A:152:ILE:HG22	2.02	0.40
30:H:90:MET:HB2	30:H:144:ILE:HG23	2.03	0.40
8:S:148:LEU:HD23	54:M:38:ILE:HD13	2.04	0.40
5:N:37:HIS:HE1	5:N:63:ARG:HH11	1.68	0.40
20:O:148:LYS:HB3	20:O:148:LYS:HE2	1.81	0.40
8:S:94:ILE:HD11	8:S:106:LEU:HD12	2.02	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	L	119/199 (60%)	107 (90%)	8 (7%)	4 (3%)	4	27
5	N	182/204 (89%)	166 (91%)	13 (7%)	3 (2%)	11	43
6	Q	132/186 (71%)	123 (93%)	9 (7%)	0	100	100
7	R	116/189 (61%)	109 (94%)	6 (5%)	1 (1%)	20	55
8	S	168/172 (98%)	151 (90%)	13 (8%)	4 (2%)	7	35
9	T	53/160 (33%)	46 (87%)	6 (11%)	1 (2%)	9	41
10	U	96/121 (79%)	90 (94%)	6 (6%)	0	100	100
11	Z	133/136 (98%)	117 (88%)	13 (10%)	3 (2%)	7	36
12	c	95/105 (90%)	92 (97%)	3 (3%)	0	100	100
13	d	105/113 (93%)	96 (91%)	7 (7%)	2 (2%)	9	41
14	e	123/130 (95%)	120 (98%)	3 (2%)	0	100	100
15	f	104/107 (97%)	100 (96%)	4 (4%)	0	100	100
16	g	110/121 (91%)	106 (96%)	4 (4%)	0	100	100
17	i	81/100 (81%)	68 (84%)	12 (15%)	1 (1%)	15	50
18	j	71/88 (81%)	67 (94%)	3 (4%)	1 (1%)	13	46
19	k	75/78 (96%)	69 (92%)	5 (7%)	1 (1%)	14	48
20	O	195/199 (98%)	125 (64%)	38 (20%)	32 (16%)	0	1
21	V	132/137 (96%)	123 (93%)	8 (6%)	1 (1%)	22	57
22	a	79/149 (53%)	72 (91%)	5 (6%)	2 (2%)	6	34
23	P	179/184 (97%)	164 (92%)	14 (8%)	1 (1%)	28	63
24	X	139/142 (98%)	122 (88%)	15 (11%)	2 (1%)	13	46
25	Y	124/127 (98%)	115 (93%)	9 (7%)	0	100	100
26	h	117/120 (98%)	108 (92%)	6 (5%)	3 (3%)	6	33
27	F	220/244 (90%)	204 (93%)	11 (5%)	5 (2%)	7	36
28	B	337/387 (87%)	293 (87%)	38 (11%)	6 (2%)	10	42
29	C	357/362 (99%)	317 (89%)	33 (9%)	7 (2%)	9	39
30	H	188/191 (98%)	173 (92%)	14 (7%)	1 (0%)	32	66
31	A	192/291 (66%)	174 (91%)	16 (8%)	2 (1%)	18	53
32	K	253/376 (67%)	231 (91%)	20 (8%)	2 (1%)	22	57
33	m	641/807 (79%)	576 (90%)	58 (9%)	7 (1%)	17	52
34	D	188/505 (37%)	167 (89%)	21 (11%)	0	100	100
35	W	230/236 (98%)	214 (93%)	14 (6%)	2 (1%)	20	55

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
36	l	170/181 (94%)	156 (92%)	14 (8%)	0	100	100
37	b	413/647 (64%)	387 (94%)	24 (6%)	2 (0%)	32	66
38	o	131/220 (60%)	121 (92%)	9 (7%)	1 (1%)	22	57
39	n	403/605 (67%)	372 (92%)	29 (7%)	2 (0%)	32	66
40	r	170/261 (65%)	149 (88%)	20 (12%)	1 (1%)	28	63
41	s	34/520 (6%)	33 (97%)	1 (3%)	0	100	100
42	t	286/322 (89%)	260 (91%)	20 (7%)	6 (2%)	8	38
43	y	223/245 (91%)	211 (95%)	11 (5%)	1 (0%)	38	71
44	z	53/106 (50%)	53 (100%)	0	0	100	100
45	p	288/460 (63%)	262 (91%)	24 (8%)	2 (1%)	25	60
46	q	313/618 (51%)	270 (86%)	36 (12%)	7 (2%)	8	37
47	u	114/199 (57%)	107 (94%)	6 (5%)	1 (1%)	20	55
48	v	124/231 (54%)	118 (95%)	6 (5%)	0	100	100
49	w	426/841 (51%)	389 (91%)	37 (9%)	0	100	100
50	I	421/663 (64%)	380 (90%)	35 (8%)	6 (1%)	13	46
51	J	143/427 (34%)	135 (94%)	8 (6%)	0	100	100
52	E	152/176 (86%)	132 (87%)	20 (13%)	0	100	100
53	G	180/256 (70%)	166 (92%)	12 (7%)	2 (1%)	17	52
54	M	134/138 (97%)	124 (92%)	9 (7%)	1 (1%)	25	60
All	All	9512/13782 (69%)	8630 (91%)	756 (8%)	126 (1%)	19	48

All (126) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	L	51	LEU
5	N	145	ASP
8	S	13	ARG
11	Z	103	GLN
19	k	33	LYS
20	O	28	LEU
20	O	47	PHE
20	O	48	PHE
20	O	62	THR
20	O	63	ALA
20	O	86	GLY

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Mol	Chain	Res	Type
20	O	89	SER
20	O	113	ASP
20	O	114	LYS
20	O	137	THR
20	O	145	VAL
20	O	162	VAL
20	O	189	ASP
21	V	90	GLY
26	h	91	ALA
27	F	160	ARG
28	B	34	LYS
28	B	222	LYS
29	C	4	PRO
29	C	140	HIS
29	C	339	LEU
33	m	231	GLU
38	o	190	THR
42	t	227	ILE
42	t	269	GLN
50	I	558	LYS
4	L	50	PRO
5	N	144	ARG
11	Z	125	GLY
13	d	87	ASN
17	i	30	LYS
20	O	13	GLY
20	O	16	VAL
20	O	17	GLY
20	O	27	LEU
20	O	77	SER
20	O	190	VAL
20	O	191	ALA
20	O	198	GLY
27	F	191	VAL
28	B	35	ASP
28	B	138	ALA
29	C	269	SER
30	H	22	SER
33	m	177	GLY
33	m	232	GLN
33	m	328	LYS
42	t	277	VAL

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Mol	Chain	Res	Type
46	q	300	GLY
46	q	427	THR
46	q	429	VAL
54	M	29	ALA
4	L	62	THR
4	L	75	PHE
7	R	53	LYS
20	O	11	GLY
20	O	168	TYR
20	O	169	ALA
20	O	192	LYS
22	a	77	LYS
24	X	4	SER
26	h	119	LYS
27	F	157	ASN
27	F	158	LYS
27	F	164	SER
28	B	187	SER
31	A	171	PRO
33	m	406	ASN
37	b	198	ALA
47	u	81	TYR
50	I	541	THR
53	G	232	HIS
5	N	94	TYR
8	S	24	LEU
9	T	127	GLN
18	j	85	LYS
20	O	24	ALA
20	O	37	ARG
20	O	85	ARG
20	O	152	VAL
22	a	78	LEU
23	P	156	ALA
24	X	5	ALA
26	h	84	LYS
28	B	155	ALA
29	C	268	ALA
31	A	63	PRO
32	K	284	ASN
33	m	154	GLN
33	m	435	GLY

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Mol	Chain	Res	Type
42	t	240	GLY
42	t	270	PRO
46	q	317	GLY
50	I	600	GLU
8	S	14	LEU
13	d	88	PRO
29	C	311	HIS
32	K	256	PRO
37	b	432	MET
39	n	196	GLU
39	n	456	HIS
42	t	151	LEU
45	p	351	ARG
45	p	418	ASP
50	I	527	PRO
50	I	561	THR
53	G	79	GLN
20	O	46	GLU
46	q	268	ALA
20	O	43	ILE
35	W	146	GLY
46	q	269	ARG
11	Z	16	GLY
29	C	146	PRO
35	W	101	GLY
50	I	196	PRO
8	S	167	ARG
40	r	190	GLY
43	y	58	ILE
46	q	423	PRO
20	O	153	VAL

5.3.2 Protein sidechains ⓘ

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

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

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	L	101/159 (64%)	93 (92%)	8 (8%)	14	45
5	N	161/176 (92%)	146 (91%)	15 (9%)	10	36
6	Q	110/151 (73%)	102 (93%)	8 (7%)	16	49
7	R	101/154 (66%)	95 (94%)	6 (6%)	23	58
8	S	155/156 (99%)	143 (92%)	12 (8%)	15	47
9	T	44/137 (32%)	41 (93%)	3 (7%)	18	53
10	U	85/107 (79%)	84 (99%)	1 (1%)	75	87
11	Z	115/116 (99%)	112 (97%)	3 (3%)	51	77
12	c	81/88 (92%)	76 (94%)	5 (6%)	21	56
13	d	94/97 (97%)	90 (96%)	4 (4%)	33	68
14	e	108/111 (97%)	103 (95%)	5 (5%)	31	67
15	f	90/91 (99%)	85 (94%)	5 (6%)	25	60
16	g	95/103 (92%)	85 (90%)	10 (10%)	8	31
17	i	69/82 (84%)	60 (87%)	9 (13%)	5	22
18	j	60/71 (84%)	52 (87%)	8 (13%)	4	21
19	k	68/69 (99%)	63 (93%)	5 (7%)	16	48
20	O	160/162 (99%)	132 (82%)	28 (18%)	2	10
21	V	103/105 (98%)	101 (98%)	2 (2%)	62	81
22	a	66/119 (56%)	63 (96%)	3 (4%)	32	67
23	P	145/146 (99%)	139 (96%)	6 (4%)	35	69
24	X	117/118 (99%)	113 (97%)	4 (3%)	42	73
25	Y	109/110 (99%)	106 (97%)	3 (3%)	49	76
26	h	104/105 (99%)	100 (96%)	4 (4%)	38	70
27	F	186/205 (91%)	181 (97%)	5 (3%)	50	77
28	B	284/323 (88%)	266 (94%)	18 (6%)	21	56
29	C	286/289 (99%)	280 (98%)	6 (2%)	59	81
30	H	170/171 (99%)	162 (95%)	8 (5%)	30	66
31	A	185/263 (70%)	181 (98%)	4 (2%)	57	80
32	K	238/346 (69%)	233 (98%)	5 (2%)	59	81
33	m	582/723 (80%)	564 (97%)	18 (3%)	45	75

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
34	D	175/440 (40%)	170 (97%)	5 (3%)	48	75
35	W	209/213 (98%)	200 (96%)	9 (4%)	33	68
36	l	149/156 (96%)	143 (96%)	6 (4%)	36	70
37	b	377/573 (66%)	360 (96%)	17 (4%)	32	67
38	o	118/199 (59%)	116 (98%)	2 (2%)	66	83
39	n	371/548 (68%)	356 (96%)	15 (4%)	36	70
40	r	156/229 (68%)	153 (98%)	3 (2%)	62	81
41	s	32/445 (7%)	30 (94%)	2 (6%)	21	56
42	t	259/287 (90%)	252 (97%)	7 (3%)	50	77
43	y	193/211 (92%)	186 (96%)	7 (4%)	40	72
44	z	48/95 (50%)	48 (100%)	0	100	100
45	p	265/413 (64%)	260 (98%)	5 (2%)	62	81
46	q	268/535 (50%)	262 (98%)	6 (2%)	57	80
47	u	101/180 (56%)	96 (95%)	5 (5%)	28	64
48	v	116/205 (57%)	113 (97%)	3 (3%)	51	77
49	w	383/745 (51%)	371 (97%)	12 (3%)	45	75
50	I	393/602 (65%)	381 (97%)	12 (3%)	45	75
51	J	133/383 (35%)	130 (98%)	3 (2%)	56	79
52	E	134/153 (88%)	123 (92%)	11 (8%)	13	44
53	G	150/208 (72%)	136 (91%)	14 (9%)	10	36
54	M	107/109 (98%)	99 (92%)	8 (8%)	16	48
All	All	8409/11982 (70%)	8036 (96%)	373 (4%)	37	67

All (373) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	L	21	ARG
4	L	34	SER
4	L	49	ARG
4	L	54	LEU
4	L	76	THR
4	L	85	LEU
4	L	100	ARG
4	L	101	ARG
5	N	10	LEU

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Mol	Chain	Res	Type
5	N	19	LEU
5	N	22	LEU
5	N	34	ASN
5	N	41	ARG
5	N	43	THR
5	N	92	LEU
5	N	95	GLN
5	N	108	ARG
5	N	121	VAL
5	N	132	VAL
5	N	133	ILE
5	N	167	THR
5	N	187	ARG
5	N	188	ARG
6	Q	31	LYS
6	Q	38	ARG
6	Q	59	ARG
6	Q	126	GLN
6	Q	136	ASN
6	Q	141	ARG
6	Q	146	SER
6	Q	147	ARG
7	R	10	LEU
7	R	19	LYS
7	R	30	SER
7	R	98	ARG
7	R	106	LEU
7	R	140	GLU
8	S	12	ARG
8	S	13	ARG
8	S	24	LEU
8	S	48	LEU
8	S	71	LYS
8	S	80	ARG
8	S	97	VAL
8	S	100	VAL
8	S	120	SER
8	S	125	LYS
8	S	147	ASP
8	S	155	ARG
9	T	106	LEU
9	T	139	ARG

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Mol	Chain	Res	Type
9	T	151	LEU
10	U	18	ASP
11	Z	17	ARG
11	Z	51	LEU
11	Z	105	SER
12	c	10	ILE
12	c	18	ILE
12	c	50	VAL
12	c	84	LEU
12	c	104	LEU
13	d	13	THR
13	d	61	LYS
13	d	106	THR
13	d	109	VAL
14	e	27	ARG
14	e	33	ARG
14	e	61	LYS
14	e	75	LEU
14	e	85	LEU
15	f	49	ILE
15	f	59	VAL
15	f	60	ARG
15	f	81	VAL
15	f	107	ILE
16	g	10	ARG
16	g	16	ARG
16	g	29	ILE
16	g	44	CYS
16	g	49	SER
16	g	51	LEU
16	g	55	SER
16	g	59	PRO
16	g	83	ASN
16	g	108	GLN
17	i	20	MET
17	i	36	ARG
17	i	47	ILE
17	i	56	ARG
17	i	57	LEU
17	i	60	LEU
17	i	76	ARG
17	i	77	LEU

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Mol	Chain	Res	Type
17	i	79	SER
18	j	24	ARG
18	j	26	SER
18	j	30	GLN
18	j	52	LYS
18	j	58	THR
18	j	67	LEU
18	j	79	GLN
18	j	82	SER
19	k	6	THR
19	k	12	LEU
19	k	22	THR
19	k	46	ARG
19	k	65	LEU
20	O	18	ARG
20	O	23	VAL
20	O	25	LYS
20	O	27	LEU
20	O	37	ARG
20	O	46	GLU
20	O	49	ARG
20	O	50	ASN
20	O	55	HIS
20	O	56	ASP
20	O	59	ARG
20	O	65	ASN
20	O	74	ARG
20	O	78	ARG
20	O	80	PHE
20	O	84	LEU
20	O	94	ARG
20	O	101	ARG
20	O	113	ASP
20	O	124	LEU
20	O	125	ARG
20	O	129	LEU
20	O	133	ARG
20	O	135	TYR
20	O	137	THR
20	O	152	VAL
20	O	156	LEU
20	O	160	ARG

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Mol	Chain	Res	Type
21	V	49	LEU
21	V	93	LEU
22	a	78	LEU
22	a	117	ARG
22	a	120	ASN
23	P	24	VAL
23	P	36	ILE
23	P	52	LEU
23	P	69	ARG
23	P	97	ASN
23	P	168	LEU
24	X	12	LYS
24	X	16	LYS
24	X	38	LEU
24	X	63	ILE
25	Y	37	LYS
25	Y	51	ARG
25	Y	74	TYR
26	h	28	LEU
26	h	49	LYS
26	h	62	GLN
26	h	93	THR
27	F	88	ARG
27	F	89	ILE
27	F	93	ASN
27	F	124	LEU
27	F	244	ASN
28	B	28	ARG
28	B	50	LYS
28	B	55	THR
28	B	70	ARG
28	B	85	VAL
28	B	89	VAL
28	B	100	ARG
28	B	114	VAL
28	B	148	LEU
28	B	152	LYS
28	B	164	THR
28	B	168	LYS
28	B	178	LEU
28	B	216	ASP
28	B	325	LYS

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Mol	Chain	Res	Type
28	B	332	ARG
28	B	380	MET
28	B	385	LYS
29	C	52	VAL
29	C	154	THR
29	C	179	LEU
29	C	194	TYR
29	C	206	LEU
29	C	259	ASP
30	H	26	LYS
30	H	41	ILE
30	H	63	LYS
30	H	118	LEU
30	H	138	THR
30	H	151	VAL
30	H	157	ASN
30	H	161	LEU
31	A	84	ASN
31	A	106	ASN
31	A	189	ARG
31	A	225	LEU
32	K	75	LYS
32	K	240	ARG
32	K	248	LEU
32	K	256	PRO
32	K	262	ASN
33	m	153	THR
33	m	156	THR
33	m	168	MET
33	m	175	ILE
33	m	178	LYS
33	m	192	LEU
33	m	203	THR
33	m	223	LEU
33	m	238	ASN
33	m	263	LYS
33	m	323	HIS
33	m	324	LEU
33	m	390	ARG
33	m	428	ARG
33	m	440	VAL
33	m	688	ILE

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Mol	Chain	Res	Type
33	m	696	ILE
33	m	719	LEU
34	D	294	VAL
34	D	394	LEU
34	D	429	LEU
34	D	448	ARG
34	D	451	LEU
35	W	15	THR
35	W	22	ASN
35	W	48	VAL
35	W	49	ARG
35	W	57	ARG
35	W	113	LYS
35	W	128	ASN
35	W	174	LYS
35	W	232	ASN
36	l	22	ARG
36	l	47	VAL
36	l	51	VAL
36	l	54	LEU
36	l	63	LEU
36	l	70	LEU
37	b	3	LEU
37	b	15	ASN
37	b	31	THR
37	b	39	ILE
37	b	48	ARG
37	b	70	ASN
37	b	175	TYR
37	b	177	ASN
37	b	180	LYS
37	b	221	THR
37	b	277	LEU
37	b	281	LYS
37	b	384	ASN
37	b	415	ASN
37	b	440	ASN
37	b	445	LEU
37	b	456	LEU
38	o	93	ILE
38	o	146	MET
39	n	7	ASN

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Mol	Chain	Res	Type
39	n	36	CYS
39	n	47	ARG
39	n	49	LYS
39	n	54	LYS
39	n	69	GLN
39	n	92	ARG
39	n	139	LEU
39	n	145	LEU
39	n	208	ASN
39	n	376	LEU
39	n	417	LEU
39	n	419	ASN
39	n	427	ILE
39	n	566	LEU
40	r	203	ASN
40	r	217	LYS
40	r	225	VAL
41	s	1	MET
41	s	33	MET
42	t	15	ASN
42	t	66	LEU
42	t	151	LEU
42	t	157	ASN
42	t	187	LEU
42	t	275	ARG
42	t	291	GLN
43	y	100	ARG
43	y	101	LEU
43	y	114	VAL
43	y	145	ASN
43	y	146	ILE
43	y	154	LEU
43	y	173	LEU
45	p	109	LEU
45	p	111	VAL
45	p	165	ARG
45	p	167	LEU
45	p	326	ARG
46	q	273	ILE
46	q	274	ARG
46	q	280	THR
46	q	282	ARG

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Mol	Chain	Res	Type
46	q	299	ILE
46	q	534	HIS
47	u	27	LYS
47	u	45	ASN
47	u	76	ASN
47	u	100	ARG
47	u	113	ARG
48	v	30	ILE
48	v	33	ASN
48	v	200	PHE
49	w	28	ARG
49	w	73	LEU
49	w	82	MET
49	w	164	LYS
49	w	167	ASN
49	w	186	PRO
49	w	211	ARG
49	w	315	PHE
49	w	665	LEU
49	w	671	LEU
49	w	678	ASP
49	w	742	ARG
50	I	161	ARG
50	I	260	ILE
50	I	304	GLU
50	I	328	ASN
50	I	329	ILE
50	I	399	ARG
50	I	470	ARG
50	I	489	MET
50	I	523	ARG
50	I	529	ASN
50	I	539	VAL
50	I	575	CYS
51	J	214	LYS
51	J	261	LEU
51	J	274	TYR
52	E	4	GLN
52	E	19	LYS
52	E	26	ARG
52	E	30	LEU
52	E	31	ARG

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Mol	Chain	Res	Type
52	E	78	ARG
52	E	84	VAL
52	E	140	VAL
52	E	154	LEU
52	E	155	LEU
52	E	167	ASN
53	G	65	LEU
53	G	77	GLN
53	G	84	ARG
53	G	136	LEU
53	G	150	LEU
53	G	166	LEU
53	G	169	LEU
53	G	190	VAL
53	G	197	VAL
53	G	200	LEU
53	G	204	ARG
53	G	213	LYS
53	G	214	LEU
53	G	229	VAL
54	M	15	VAL
54	M	25	LYS
54	M	38	ILE
54	M	63	VAL
54	M	72	LEU
54	M	77	ARG
54	M	131	VAL
54	M	135	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (94) such sidechains are listed below:

Mol	Chain	Res	Type
4	L	12	ASN
4	L	37	ASN
4	L	120	GLN
5	N	34	ASN
5	N	37	HIS
5	N	95	GLN
6	Q	58	ASN
6	Q	73	GLN
6	Q	136	ASN
7	R	92	GLN

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Mol	Chain	Res	Type
8	S	89	ASN
11	Z	57	HIS
15	f	42	GLN
19	k	40	GLN
20	O	26	GLN
20	O	31	GLN
20	O	42	ASN
20	O	50	ASN
20	O	65	ASN
20	O	72	HIS
20	O	122	GLN
21	V	98	ASN
22	a	120	ASN
23	P	34	GLN
23	P	37	ASN
23	P	96	GLN
24	X	111	ASN
26	h	59	ASN
27	F	209	ASN
28	B	182	GLN
28	B	184	ASN
28	B	279	ASN
28	B	345	ASN
29	C	48	GLN
29	C	87	GLN
29	C	114	ASN
29	C	291	ASN
30	H	58	HIS
31	A	73	GLN
31	A	75	ASN
31	A	150	GLN
31	A	175	HIS
32	K	42	ASN
32	K	262	ASN
33	m	232	GLN
33	m	238	ASN
33	m	629	HIS
33	m	748	HIS
34	D	310	ASN
35	W	128	ASN
35	W	205	GLN
35	W	232	ASN

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Mol	Chain	Res	Type
36	l	50	HIS
36	l	82	HIS
36	l	112	HIS
37	b	70	ASN
37	b	78	HIS
37	b	217	GLN
37	b	415	ASN
38	o	113	GLN
39	n	73	HIS
39	n	164	ASN
39	n	419	ASN
39	n	437	ASN
40	r	4	ASN
42	t	51	ASN
42	t	238	GLN
43	y	9	ASN
43	y	11	ASN
45	p	139	GLN
45	p	337	GLN
45	p	452	ASN
46	q	447	GLN
47	u	45	ASN
47	u	76	ASN
48	v	33	ASN
48	v	39	ASN
49	w	118	HIS
49	w	130	GLN
49	w	137	GLN
49	w	167	ASN
49	w	276	ASN
49	w	694	ASN
50	I	155	ASN
50	I	335	ASN
50	I	344	HIS
50	I	596	ASN
51	J	215	HIS
51	J	220	HIS
51	J	221	GLN
52	E	4	GLN
53	G	95	ASN
53	G	137	ASN
54	M	56	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	1	2439/3396 (71%)	742 (30%)	70 (2%)
2	2	157/158 (99%)	35 (22%)	3 (1%)
3	6	63/232 (27%)	30 (47%)	2 (3%)
All	All	2659/3786 (70%)	807 (30%)	75 (2%)

All (807) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	1	2	U
1	1	7	C
1	1	14	U
1	1	22	G
1	1	40	A
1	1	41	G
1	1	42	C
1	1	43	A
1	1	44	U
1	1	48	A
1	1	49	A
1	1	57	A
1	1	59	G
1	1	60	A
1	1	65	A
1	1	66	A
1	1	72	C
1	1	73	C
1	1	74	G
1	1	75	G
1	1	77	A
1	1	85	A
1	1	92	G
1	1	94	G
1	1	96	G
1	1	110	G
1	1	111	C
1	1	113	C
1	1	117	U
1	1	118	U
1	1	120	G
1	1	121	A
1	1	122	A

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Mol	Chain	Res	Type
1	1	135	C
1	1	136	G
1	1	143	G
1	1	148	G
1	1	150	A
1	1	154	U
1	1	155	G
1	1	156	G
1	1	157	A
1	1	164	A
1	1	165	A
1	1	166	C
1	1	170	G
1	1	173	G
1	1	190	U
1	1	191	U
1	1	196	G
1	1	197	G
1	1	200	C
1	1	205	C
1	1	206	G
1	1	210	U
1	1	211	A
1	1	212	G
1	1	213	A
1	1	218	G
1	1	219	A
1	1	220	G
1	1	234	G
1	1	240	U
1	1	241	G
1	1	243	G
1	1	249	U
1	1	250	U
1	1	251	G
1	1	252	U
1	1	264	G
1	1	265	A
1	1	266	A
1	1	268	A
1	1	269	G
1	1	283	G

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Mol	Chain	Res	Type
1	1	284	A
1	1	285	A
1	1	295	A
1	1	298	U
1	1	299	G
1	1	305	U
1	1	311	C
1	1	323	A
1	1	329	U
1	1	338	A
1	1	339	C
1	1	352	A
1	1	368	G
1	1	370	U
1	1	376	G
1	1	390	G
1	1	398	A
1	1	399	A
1	1	401	U
1	1	403	C
1	1	404	G
1	1	421	G
1	1	422	A
1	1	437	G
1	1	438	A
1	1	439	C
1	1	440	A
1	1	495	G
1	1	496	C
1	1	498	A
1	1	503	C
1	1	510	G
1	1	515	C
1	1	517	G
1	1	518	G
1	1	520	U
1	1	521	A
1	1	523	A
1	1	533	A
1	1	534	U
1	1	535	G
1	1	536	U

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Mol	Chain	Res	Type
1	1	542	G
1	1	543	C
1	1	547	G
1	1	550	A
1	1	551	A
1	1	552	G
1	1	555	U
1	1	556	U
1	1	557	A
1	1	558	U
1	1	559	A
1	1	569	A
1	1	578	A
1	1	579	G
1	1	589	A
1	1	592	A
1	1	593	C
1	1	597	G
1	1	603	A
1	1	604	G
1	1	609	G
1	1	611	A
1	1	620	U
1	1	621	A
1	1	622	A
1	1	623	U
1	1	634	C
1	1	636	C
1	1	643	U
1	1	644	G
1	1	645	A
1	1	649	A
1	1	650	C
1	1	660	A
1	1	676	G
1	1	677	A
1	1	681	U
1	1	690	A
1	1	691	A
1	1	705	A
1	1	710	A
1	1	720	A

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Mol	Chain	Res	Type
1	1	721	G
1	1	722	G
1	1	733	G
1	1	734	C
1	1	735	A
1	1	742	G
1	1	743	C
1	1	757	C
1	1	759	U
1	1	760	G
1	1	761	A
1	1	770	G
1	1	772	U
1	1	774	G
1	1	775	A
1	1	776	U
1	1	777	U
1	1	779	G
1	1	780	A
1	1	781	G
1	1	784	A
1	1	785	G
1	1	786	A
1	1	799	G
1	1	801	A
1	1	806	A
1	1	808	A
1	1	813	G
1	1	815	G
1	1	818	C
1	1	819	U
1	1	820	A
1	1	822	G
1	1	826	G
1	1	830	A
1	1	849	C
1	1	854	G
1	1	857	G
1	1	859	G
1	1	860	G
1	1	861	C
1	1	864	G

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Mol	Chain	Res	Type
1	1	871	U
1	1	874	U
1	1	875	G
1	1	877	C
1	1	878	G
1	1	879	U
1	1	880	G
1	1	881	C
1	1	882	A
1	1	883	A
1	1	884	A
1	1	886	C
1	1	887	G
1	1	891	G
1	1	892	U
1	1	893	C
1	1	894	G
1	1	895	A
1	1	896	A
1	1	898	U
1	1	899	U
1	1	900	G
1	1	904	A
1	1	906	A
1	1	909	G
1	1	910	G
1	1	918	C
1	1	919	U
1	1	920	A
1	1	921	A
1	1	932	U
1	1	936	A
1	1	938	C
1	1	944	C
1	1	957	C
1	1	958	C
1	1	959	C
1	1	960	U
1	1	961	C
1	1	962	A
1	1	963	G
1	1	964	G

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Mol	Chain	Res	Type
1	1	970	A
1	1	977	C
1	1	978	G
1	1	979	U
1	1	980	A
1	1	981	U
1	1	982	C
1	1	984	G
1	1	985	U
1	1	991	G
1	1	992	A
1	1	1059	G
1	1	1060	U
1	1	1098	A
1	1	1103	A
1	1	1104	G
1	1	1105	A
1	1	1108	U
1	1	1111	U
1	1	1112	A
1	1	1116	G
1	1	1117	G
1	1	1126	G
1	1	1127	G
1	1	1129	A
1	1	1132	C
1	1	1135	A
1	1	1136	A
1	1	1139	G
1	1	1142	G
1	1	1144	U
1	1	1151	U
1	1	1153	A
1	1	1155	C
1	1	1159	A
1	1	1160	C
1	1	1174	G
1	1	1177	G
1	1	1180	A
1	1	1181	U
1	1	1186	G
1	1	1192	C

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Mol	Chain	Res	Type
1	1	1193	A
1	1	1196	C
1	1	1197	A
1	1	1198	C
1	1	1199	C
1	1	1200	A
1	1	1201	C
1	1	1204	A
1	1	1213	G
1	1	1217	A
1	1	1218	U
1	1	1221	A
1	1	1222	G
1	1	1227	C
1	1	1228	C
1	1	1233	G
1	1	1235	U
1	1	1237	G
1	1	1241	U
1	1	1242	G
1	1	1244	A
1	1	1245	A
1	1	1250	G
1	1	1251	A
1	1	1252	A
1	1	1253	U
1	1	1258	U
1	1	1259	A
1	1	1262	G
1	1	1263	A
1	1	1264	G
1	1	1266	G
1	1	1272	C
1	1	1273	A
1	1	1277	C
1	1	1278	A
1	1	1279	C
1	1	1283	C
1	1	1284	C
1	1	1286	A
1	1	1287	A
1	1	1299	U

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Mol	Chain	Res	Type
1	1	1300	G
1	1	1302	A
1	1	1303	A
1	1	1304	A
1	1	1305	U
1	1	1307	G
1	1	1308	A
1	1	1309	U
1	1	1325	U
1	1	1330	A
1	1	1331	U
1	1	1332	A
1	1	1348	U
1	1	1349	G
1	1	1350	A
1	1	1351	U
1	1	1352	A
1	1	1353	U
1	1	1354	G
1	1	1355	A
1	1	1356	U
1	1	1357	G
1	1	1364	C
1	1	1367	G
1	1	1380	G
1	1	1386	A
1	1	1391	C
1	1	1397	C
1	1	1399	A
1	1	1400	G
1	1	1419	A
1	1	1421	G
1	1	1429	G
1	1	1434	G
1	1	1437	C
1	1	1443	G
1	1	1446	A
1	1	1450	G
1	1	1452	A
1	1	1453	A
1	1	1454	A
1	1	1455	U

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Mol	Chain	Res	Type
1	1	1477	A
1	1	1481	A
1	1	1483	G
1	1	1484	U
1	1	1485	G
1	1	1487	G
1	1	1495	U
1	1	1503	A
1	1	1508	C
1	1	1512	U
1	1	1533	U
1	1	1536	G
1	1	1539	A
1	1	1544	G
1	1	1546	A
1	1	1547	G
1	1	1555	U
1	1	1556	C
1	1	1557	A
1	1	1560	G
1	1	1561	G
1	1	1562	C
1	1	1566	A
1	1	1567	U
1	1	1568	U
1	1	1569	U
1	1	1571	A
1	1	1573	G
1	1	1574	C
1	1	1575	A
1	1	1580	A
1	1	1581	C
1	1	1582	C
1	1	1587	A
1	1	1589	A
1	1	1590	G
1	1	1593	A
1	1	1596	C
1	1	1605	A
1	1	1608	C
1	1	1613	A
1	1	1619	A

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Mol	Chain	Res	Type
1	1	1620	U
1	1	1627	U
1	1	1628	C
1	1	1630	U
1	1	1639	C
1	1	1641	U
1	1	1642	A
1	1	1643	A
1	1	1647	A
1	1	1656	A
1	1	1657	C
1	1	1658	G
1	1	1683	A
1	1	1685	C
1	1	1687	U
1	1	1688	U
1	1	1713	G
1	1	1715	A
1	1	1716	U
1	1	1717	U
1	1	1724	U
1	1	1725	C
1	1	1730	G
1	1	1736	G
1	1	1741	A
1	1	1742	U
1	1	1743	G
1	1	1749	A
1	1	1750	A
1	1	1751	G
1	1	1756	C
1	1	1764	U
1	1	1765	U
1	1	1766	G
1	1	1768	U
1	1	1770	G
1	1	1775	G
1	1	1780	G
1	1	1792	C
1	1	1794	G
1	1	1795	U
1	1	1796	G

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Mol	Chain	Res	Type
1	1	1797	A
1	1	1808	G
1	1	1813	A
1	1	1814	A
1	1	1815	U
1	1	1816	A
1	1	1817	G
1	1	1820	U
1	1	1821	U
1	1	1852	G
1	1	1853	U
1	1	1862	U
1	1	1865	A
1	1	1866	C
1	1	1867	A
1	1	1868	G
1	1	1869	C
1	1	1871	U
1	1	1878	G
1	1	1879	A
1	1	1880	U
1	1	1881	A
1	1	1884	A
1	1	1886	A
1	1	1900	A
1	1	1906	G
1	1	1947	G
1	1	1948	G
1	1	1951	C
1	1	1952	G
1	1	1953	G
1	1	2095	G
1	1	2098	C
1	1	2100	A
1	1	2101	C
1	1	2123	G
1	1	2130	G
1	1	2322	C
1	1	2323	G
1	1	2324	A
1	1	2325	G
1	1	2334	U

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Mol	Chain	Res	Type
1	1	2335	G
1	1	2336	U
1	1	2347	U
1	1	2363	A
1	1	2370	G
1	1	2371	G
1	1	2372	A
1	1	2373	A
1	1	2374	C
1	1	2377	G
1	1	2385	G
1	1	2388	U
1	1	2392	C
1	1	2393	G
1	1	2394	G
1	1	2395	G
1	1	2405	C
1	1	2410	U
1	1	2411	U
1	1	2412	G
1	1	2414	G
1	1	2418	G
1	1	2419	A
1	1	2434	U
1	1	2597	U
1	1	2606	G
1	1	2607	G
1	1	2805	G
1	1	2807	U
1	1	2811	A
1	1	2812	C
1	1	2813	A
1	1	2818	U
1	1	2819	A
1	1	2820	A
1	1	2821	C
1	1	2822	U
1	1	2823	G
1	1	2824	G
1	1	2825	C
1	1	2826	U
1	1	2836	C

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Mol	Chain	Res	Type
1	1	2837	A
1	1	2838	A
1	1	2841	G
1	1	2842	U
1	1	2845	A
1	1	2846	U
1	1	2849	C
1	1	2855	U
1	1	2857	C
1	1	2858	U
1	1	2877	G
1	1	2878	G
1	1	2879	C
1	1	2880	U
1	1	2887	A
1	1	2889	C
1	1	2898	G
1	1	2899	C
1	1	2911	A
1	1	2916	U
1	1	2919	A
1	1	2920	U
1	1	2921	U
1	1	2922	G
1	1	2923	U
1	1	2924	U
1	1	2925	C
1	1	2926	A
1	1	2927	C
1	1	2929	C
1	1	2930	A
1	1	2935	U
1	1	2936	A
1	1	2941	A
1	1	2942	C
1	1	2943	G
1	1	2944	U
1	1	2945	G
1	1	2946	A
1	1	2947	G
1	1	2949	U
1	1	2950	G

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Mol	Chain	Res	Type
1	1	2951	G
1	1	2952	G
1	1	2953	U
1	1	2954	U
1	1	2955	U
1	1	2956	A
1	1	2964	G
1	1	2965	U
1	1	2966	G
1	1	2967	A
1	1	2968	G
1	1	2969	A
1	1	2970	C
1	1	2971	A
1	1	2972	G
1	1	2975	U
1	1	2976	A
1	1	2977	G
1	1	2979	U
1	1	2980	U
1	1	2981	U
1	1	2982	A
1	1	2983	C
1	1	2984	C
1	1	2987	A
1	1	2990	G
1	1	2992	U
1	1	2996	U
1	1	2997	G
1	1	3003	G
1	1	3012	A
1	1	3017	A
1	1	3019	U
1	1	3020	U
1	1	3021	A
1	1	3022	G
1	1	3023	U
1	1	3026	G
1	1	3029	A
1	1	3030	G
1	1	3032	A
1	1	3037	U

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Mol	Chain	Res	Type
1	1	3046	A
1	1	3056	U
1	1	3057	U
1	1	3058	U
1	1	3065	G
1	1	3069	G
1	1	3070	A
1	1	3071	U
1	1	3072	C
1	1	3074	G
1	1	3076	C
1	1	3078	U
1	1	3079	U
1	1	3086	A
1	1	3090	U
1	1	3092	C
1	1	3093	C
1	1	3094	A
1	1	3099	C
1	1	3100	U
1	1	3102	G
1	1	3104	U
1	1	3109	G
1	1	3116	G
1	1	3122	A
1	1	3124	G
1	1	3129	A
1	1	3130	A
1	1	3131	U
1	1	3141	A
1	1	3142	A
1	1	3143	C
1	1	3150	A
1	1	3151	U
1	1	3153	U
1	1	3154	C
1	1	3155	U
1	1	3156	U
1	1	3157	U
1	1	3158	G
1	1	3160	U
1	1	3161	C

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Mol	Chain	Res	Type
1	1	3164	C
1	1	3165	A
1	1	3170	A
1	1	3172	A
1	1	3173	G
1	1	3174	A
1	1	3175	U
1	1	3176	G
1	1	3179	U
1	1	3180	A
1	1	3181	C
1	1	3186	A
1	1	3187	A
1	1	3188	G
1	1	3196	U
1	1	3199	G
1	1	3206	C
1	1	3207	U
1	1	3216	G
1	1	3217	C
1	1	3218	A
1	1	3219	G
1	1	3227	A
1	1	3228	C
1	1	3229	G
1	1	3242	G
1	1	3243	A
1	1	3244	A
1	1	3245	A
1	1	3247	G
1	1	3249	C
1	1	3252	G
1	1	3256	G
1	1	3259	U
1	1	3263	G
1	1	3268	A
1	1	3269	U
1	1	3270	U
1	1	3271	G
1	1	3276	G
1	1	3281	U
1	1	3283	U

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Mol	Chain	Res	Type
1	1	3287	U
1	1	3288	G
1	1	3289	G
1	1	3290	G
1	1	3293	U
1	1	3294	A
1	1	3295	A
1	1	3303	G
1	1	3304	U
1	1	3306	U
1	1	3307	A
1	1	3309	G
1	1	3313	U
1	1	3316	A
1	1	3317	U
1	1	3319	U
1	1	3324	C
1	1	3328	G
1	1	3341	U
1	1	3342	A
1	1	3344	A
1	1	3345	G
1	1	3350	C
1	1	3351	U
1	1	3352	U
1	1	3353	G
1	1	3355	U
1	1	3356	G
1	1	3363	U
1	1	3366	G
1	1	3369	G
1	1	3375	A
1	1	3378	C
1	1	3386	G
1	1	3387	U
1	1	3390	G
1	1	3396	U
2	2	34	U
2	2	35	C
2	2	39	G
2	2	51	G
2	2	59	A

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Mol	Chain	Res	Type
2	2	62	C
2	2	63	G
2	2	71	A
2	2	78	G
2	2	79	A
2	2	81	U
2	2	82	U
2	2	84	C
2	2	85	G
2	2	86	U
2	2	87	G
2	2	90	U
2	2	95	G
2	2	97	A
2	2	104	A
2	2	106	C
2	2	107	G
2	2	111	A
2	2	113	U
2	2	116	G
2	2	124	G
2	2	125	U
2	2	126	A
2	2	128	U
2	2	134	G
2	2	136	G
2	2	151	C
2	2	152	G
2	2	157	U
2	2	158	U
3	6	4	U
3	6	5	C
3	6	6	U
3	6	7	C
3	6	8	A
3	6	9	A
3	6	13	U
3	6	14	U
3	6	15	C
3	6	16	U
3	6	17	G
3	6	23	U

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Mol	Chain	Res	Type
3	6	24	A
3	6	34	A
3	6	36	U
3	6	39	U
3	6	40	U
3	6	42	G
3	6	43	A
3	6	47	A
3	6	52	G
3	6	53	A
3	6	54	A
3	6	56	U
3	6	57	U
3	6	58	G
3	6	59	C
3	6	228	U
3	6	231	A
3	6	232	A

All (75) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	1	40	A
1	1	153	U
1	1	154	U
1	1	165	A
1	1	239	G
1	1	297	G
1	1	376	G
1	1	494	G
1	1	518	G
1	1	533	A
1	1	556	U
1	1	557	A
1	1	588	G
1	1	644	G
1	1	649	A
1	1	720	A
1	1	734	C
1	1	818	C
1	1	873	C
1	1	878	G

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Mol	Chain	Res	Type
1	1	899	U
1	1	917	A
1	1	978	G
1	1	1102	A
1	1	1103	A
1	1	1104	G
1	1	1128	U
1	1	1159	A
1	1	1227	C
1	1	1241	U
1	1	1299	U
1	1	1302	A
1	1	1307	G
1	1	1329	U
1	1	1331	U
1	1	1355	A
1	1	1428	A
1	1	1451	C
1	1	1481	A
1	1	1502	C
1	1	1574	C
1	1	1581	C
1	1	1641	U
1	1	1716	U
1	1	1813	A
1	1	1820	U
1	1	1861	G
1	1	1947	G
1	1	2323	G
1	1	2837	A
1	1	2857	C
1	1	2878	G
1	1	2922	G
1	1	2940	A
1	1	2946	A
1	1	2954	U
1	1	2986	U
1	1	3016	A
1	1	3055	U
1	1	3093	C
1	1	3116	G
1	1	3121	U

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Mol	Chain	Res	Type
1	1	3171	U
1	1	3218	A
1	1	3228	C
1	1	3267	A
1	1	3269	U
1	1	3340	G
1	1	3350	C
1	1	3389	U
2	2	85	G
2	2	112	U
2	2	123	G
3	6	16	U
3	6	56	U

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 1 ligands modelled in this entry, 1 is 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 ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	1	2
23	P	1
4	L	1
36	1	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	1	135:ALA	C	136:MET	N	6.21
1	1	1792:C	O3'	1793:C	P	5.60
1	L	8:PRO	C	9:ILE	N	4.88
1	1	966:U	O3'	967:A	P	4.55
1	P	131:ARG	C	132:ALA	N	3.63