



wwPDB EM Map/Model Validation Report ⓘ

Apr 10, 2016 – 02:17 PM BST

PDB ID : 3J6B
EMDB ID: : EMD-2566
Title : Structure of the yeast mitochondrial large ribosomal subunit
Authors : Amunts, A.; Brown, A.; Bai, X.C.; Llacer, J.L.; Hussain, T.; Emsley, P.; Long, F.; Murshudov, G.; Scheres, S.H.W.; Ramakrishnan, V.
Deposited on : 2014-01-22
Resolution : 3.20 Å(reported)

This is a wwPDB EM Map/Model Validation Report for a publicly released PDB/EMDB entry.
For rigid body fitted models, validation errors reported here could stem from errors in the original structure(s) used in the fitting.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/EMValidationReportHelp>

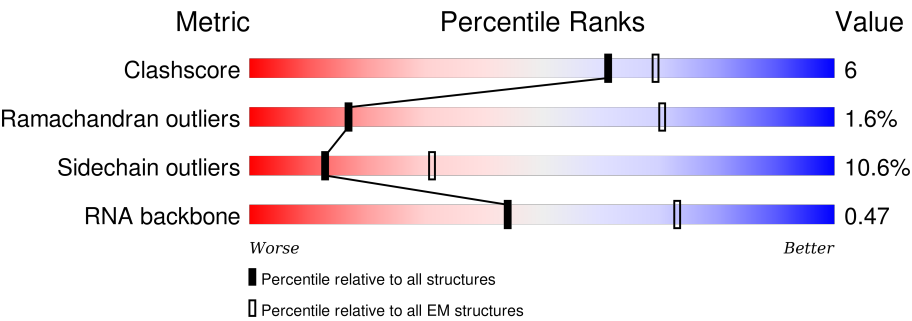
MolProbity : 4.02b-467
Mogul : unknown
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : trunk27241

1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 3.20 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.













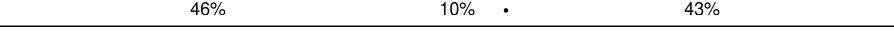
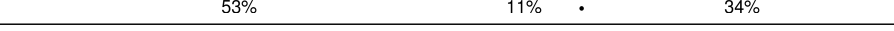





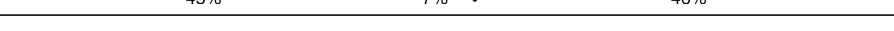

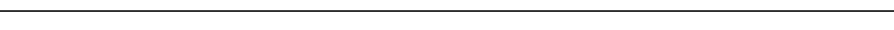

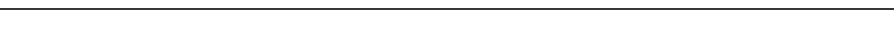
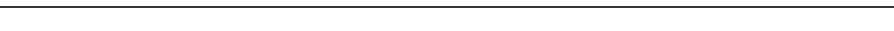


Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	114402	924
Ramachandran outliers	111179	726
Sidechain outliers	111093	686
RNA backbone	3027	244

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	A	3296	<div><div>48%</div><div>26%</div><div>8%</div><div>18%</div></div>
2	B	393	<div><div>55%</div><div>18%</div><div>•</div><div>25%</div></div>
3	C	269	<div><div>74%</div><div>16%</div><div>•</div><div>7%</div></div>
4	D	286	<div><div>62%</div><div>18%</div><div>•</div><div>16%</div></div>
5	E	292	<div><div>78%</div><div>15%</div><div>•</div><div>6%</div></div>
6	F	214	<div><div>66%</div><div>17%</div><div>•</div><div>14%</div></div>
7	G	139	<div><div>35%</div><div>5%</div><div>60%</div></div>
8	H	163	<div><div>74%</div><div>14%</div><div>• •</div><div>9%</div></div>

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Mol	Chain	Length	Quality of chain
9	I	138	
10	J	322	
11	K	232	
12	L	238	
13	M	169	
14	N	161	
15	O	309	
16	P	263	
17	Q	297	
18	R	371	
19	S	258	
20	T	319	
21	U	86	
22	V	177	
23	W	183	
24	X	70	
25	Y	105	
26	Z	115	
27	0	93	
28	1	367	
29	2	147	
30	3	146	
31	4	140	
32	5	390	
33	6	281	

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Mol	Chain	Length	Quality of chain
34	7	146	
35	8	264	
36	9	253	
37	a	195	
38	b	157	
39	c	131	
40	d	226	
41	e	20	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
44	ZN	0	100	-	-	X	-

2 Entry composition

There are 44 unique types of molecules in this entry. The entry contains 195137 atoms, of which 83818 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 21S ribosomal RNA.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	A	2713	Total	C	H	N	O	P	0	0
			86569	25948	28898	10265	18752	2706		

- Molecule 2 is a protein called 54S ribosomal protein RML2, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
2	B	295	Total	C	H	N	O	S	0	0
			4603	1405	2343	459	387	9		

- Molecule 3 is a protein called 54S ribosomal protein L9, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
3	C	249	Total	C	H	N	O	S	0	0
			3906	1217	1976	360	343	10		

- Molecule 4 is a protein called 54S ribosomal protein YmL6, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
4	D	239	Total	C	H	N	O	S	0	0
			3780	1187	1914	337	339	3		

- Molecule 5 is a protein called 54S ribosomal protein L7, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
5	E	274	Total	C	H	N	O	S	0	0
			4294	1363	2169	387	369	6		

- Molecule 6 is a protein called 54S ribosomal protein L6, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
6	F	185	Total	C	H	N	O	S	0	0
			2747	870	1392	236	246	3		

- Molecule 7 is a protein called 54S ribosomal protein L50, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
7	G	55	Total	C	H	N	O	S	0	0
			929	293	471	86	78	1		

- Molecule 8 is a protein called 54S ribosomal protein L23, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
8	H	148	Total	C	H	N	O	S	0	0
			2394	742	1218	225	205	4		

- Molecule 9 is a protein called 54S ribosomal protein L38, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
9	I	125	Total	C	H	N	O	S	0	0
			1952	583	1015	175	168	11		

- Molecule 10 is a protein called 54S ribosomal protein L10, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
10	J	220	Total	C	H	N	O	S	0	0
			3555	1109	1828	325	290	3		

- Molecule 11 is a protein called 54S ribosomal protein L16, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
11	K	195	Total	C	H	N	O	S	0	0
			3208	1001	1635	297	270	5		

- Molecule 12 is a protein called 54S ribosomal protein L8, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
12	L	229	Total	C	H	N	O	S	0	0
			3698	1139	1883	333	335	8		

- Molecule 13 is a protein called 54S ribosomal protein IMG1, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
13	M	151	Total	C	H	N	O	S	0	0
			2492	766	1286	220	217	3		

- Molecule 14 is a protein called 54S ribosomal protein L49, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
14	N	118	Total	C	H	N	O	S	0	0
			1958	598	1010	177	171	2		

- Molecule 15 is a protein called 54S ribosomal protein L22, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
15	O	223	Total	C	H	N	O	S	0	0
			3684	1147	1895	328	309	5		

- Molecule 16 is a protein called 54S ribosomal protein L41, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
16	P	207	Total	C	H	N	O	S	0	0
			3450	1101	1728	310	305	6		

- Molecule 17 is a protein called 54S ribosomal protein L40, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
17	Q	279	Total	C	H	N	O	S	0	0
			4287	1368	2161	375	375	8		

- Molecule 18 is a protein called 54S ribosomal protein L2, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
18	R	318	Total	C	H	N	O	S	0	0
			4981	1571	2500	452	454	4		

- Molecule 19 is a protein called 54S ribosomal protein L24, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
19	S	146	Total	C	H	N	O	S	0	0
			2440	763	1249	220	207	1		

- Molecule 20 is a protein called 54S ribosomal protein L4, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
20	T	209	Total	C	H	N	O	S	0	0
			3264	1044	1618	307	292	3		

- Molecule 21 is a protein called 54S ribosomal protein L33, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	U	82	Total	C	H	N	O	0	0
			1341	410	702	116	113		

- Molecule 22 is a protein called 54S ribosomal protein L36, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
22	V	64	Total	C	H	N	O	S	0	0
			1083	332	555	105	90	1		

- Molecule 23 is a protein called 54S ribosomal protein L32, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
23	W	112	Total	C	H	N	O	S	0	0
			1922	587	985	181	163	6		

- Molecule 24 is a protein called 54S ribosomal protein L39, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	X	64	Total	C	H	N	O	0	0
			1077	330	565	96	86		

- Molecule 25 is a protein called 54S ribosomal protein L34, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	Y	45	Total	C	H	N	O	0	0
			788	239	412	80	57		

- Molecule 26 is a protein called mitochondrial ribosomal protein YNL122C.

Mol	Chain	Residues	Atoms						AltConf	Trace
26	Z	62	Total	C	H	N	O	S	0	0
			1054	322	546	111	74	1		

- Molecule 27 is a protein called 54S ribosomal protein RTC6, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace	
27	0	38	Total	C	H	N	O	S	0	0
			673	205	349	66	50	3		

- Molecule 28 is a protein called 54S ribosomal protein L35, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
28	1	332	Total	C	H	N	O	S	0	0
			5397	1744	2690	467	490	6		

- Molecule 29 is a protein called 54S ribosomal protein L28, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
29	2	113	Total	C	H	N	O	S	0	0
			1858	583	939	169	162	5		

- Molecule 30 is a protein called 54S ribosomal protein L27, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
30	3	126	Total	C	H	N	O	S	0	0
			2025	643	1030	181	168	3		

- Molecule 31 is a protein called 54S ribosomal protein L51, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
31	4	138	Total	C	H	N	O	S	0	0
			2263	700	1146	219	193	5		

- Molecule 32 is a protein called 54S ribosomal protein L3, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
32	5	326	Total	C	H	N	O	S	0	0
			5026	1596	2541	425	453	11		

- Molecule 33 is a protein called 54S ribosomal protein L17, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
33	6	209	Total	C	H	N	O	S	0	0
			3187	1046	1595	273	271	2		

- Molecule 34 is a protein called 54S ribosomal protein IMG2, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
34	7	106	Total	C	H	N	O	S	0	0
			1755	550	901	150	152	2		

- Molecule 35 is a protein called 54S ribosomal protein L13, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
35	8	182	Total	C	H	N	O	S	0	0
			2829	898	1416	241	271	3		

- Molecule 36 is a protein called 54S ribosomal protein L15, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
36	9	195	Total	C	H	N	O	S	0	0
			2865	919	1437	250	254	5		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
9	169	GLY	ASP	CONFLICT	UNP P36523

- Molecule 37 is a protein called 54S ribosomal protein L20, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
37	a	176	Total	C	H	N	O	S	0	0
			2882	898	1455	264	259	6		

- Molecule 38 is a protein called 54S ribosomal protein L25, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
38	b	155	Total	C	H	N	O	S	0	0
			2671	850	1372	225	221	3		

- Molecule 39 is a protein called 54S ribosomal protein L31, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
39	c	118	Total	C	H	N	O	S	0	0
			2066	643	1066	190	163	4		

- Molecule 40 is a protein called Mitochondrial homologous recombination protein 1.

Mol	Chain	Residues	Atoms						AltConf	Trace
40	d	204	Total	C	H	N	O	S	0	0
			3423	1099	1706	313	299	6		

- Molecule 41 is a RNA chain called E-site tRNA.

Mol	Chain	Residues	Atoms						AltConf	Trace
41	e	20	Total	C	H	N	O	P	0	0
			648	191	221	81	136	19		

- Molecule 42 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
42	A	109	Total	Mg	0
			109	109	
42	N	1	Total	Mg	0
			1	1	

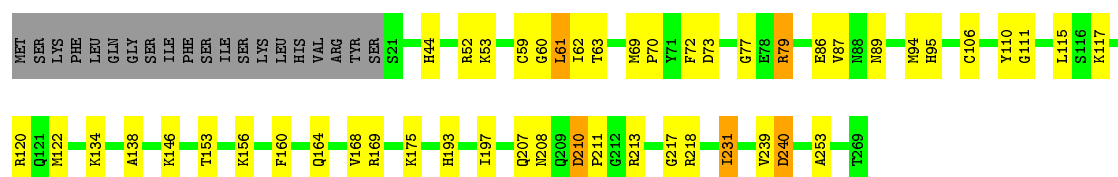
- Molecule 43 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		AltConf
43	B	1	Total	Na	0
			1	1	

- Molecule 44 is ZINC ION (three-letter code: ZN) (formula: Zn).

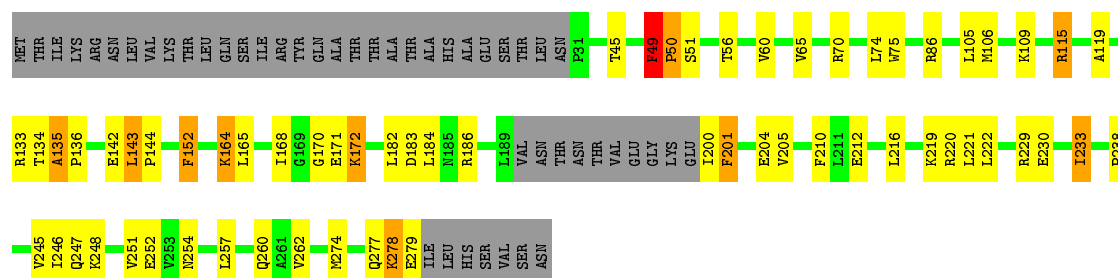
Mol	Chain	Residues	Atoms		AltConf
44	0	1	Total	Zn	0
			1	1	
44	W	1	Total	Zn	0
			1	1	



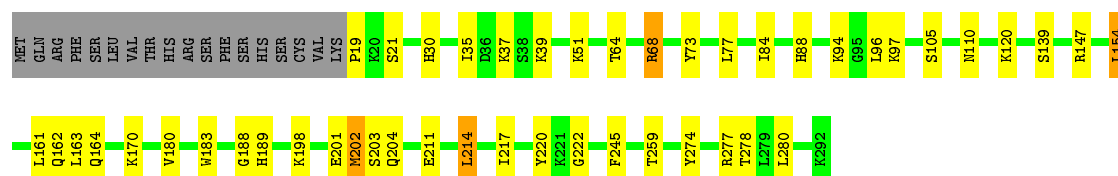
- Molecule 4: 54S ribosomal protein YmL6, mitochondrial

Chain D: 62% 18% 16%



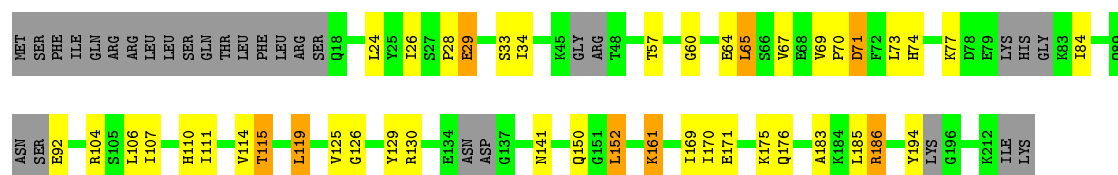
- Molecule 5: 54S ribosomal protein L7, mitochondrial

Chain E: 78% 15% 6%



- Molecule 6: 54S ribosomal protein L6, mitochondrial

Chain F: 66% 17% 14%



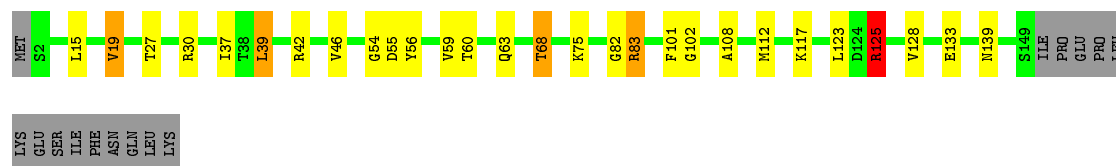
- Molecule 7: 54S ribosomal protein L50, mitochondrial

Chain G: 35% 5% 60%




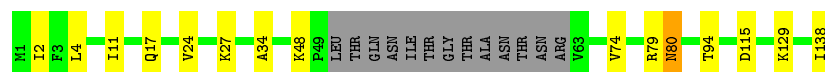
- Molecule 8: 54S ribosomal protein L23, mitochondrial

Chain H: 



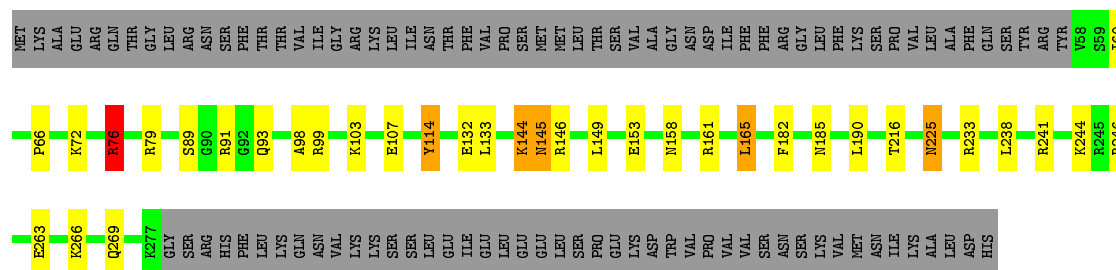
- Molecule 9: 54S ribosomal protein L38, mitochondrial

Chain I: 



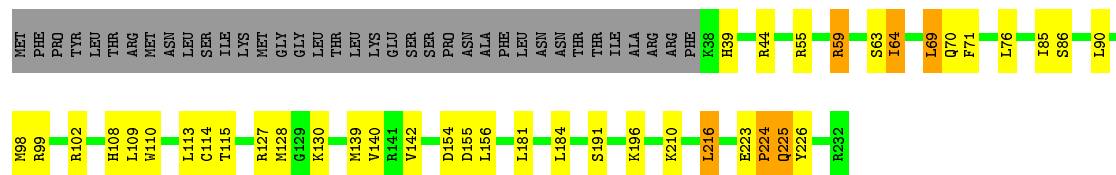
- Molecule 10: 54S ribosomal protein L10, mitochondrial

Chain J: 




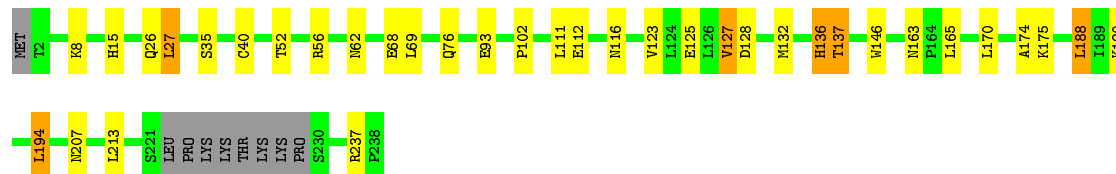
- Molecule 11: 54S ribosomal protein L16, mitochondrial

Chain K: 



- Molecule 12: 54S ribosomal protein L8, mitochondrial

Chain L: 

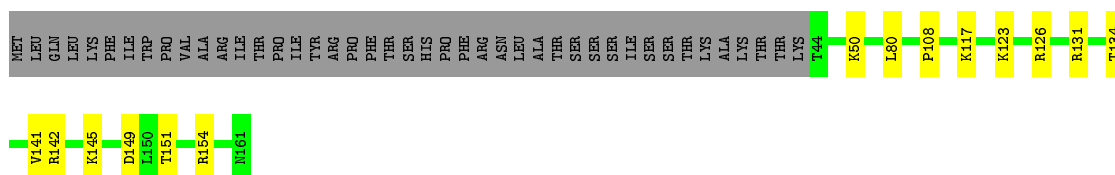


- Molecule 13: 54S ribosomal protein IMG1, mitochondrial

Chain M: 

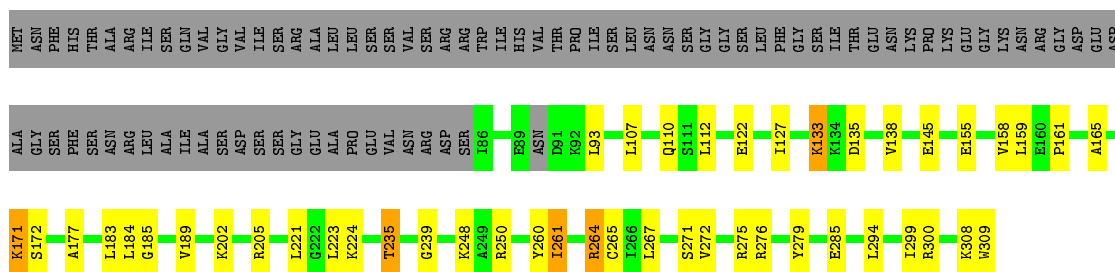
- Molecule 14: 54S ribosomal protein L49, mitochondrial

Chain N: 65% 9% 27%



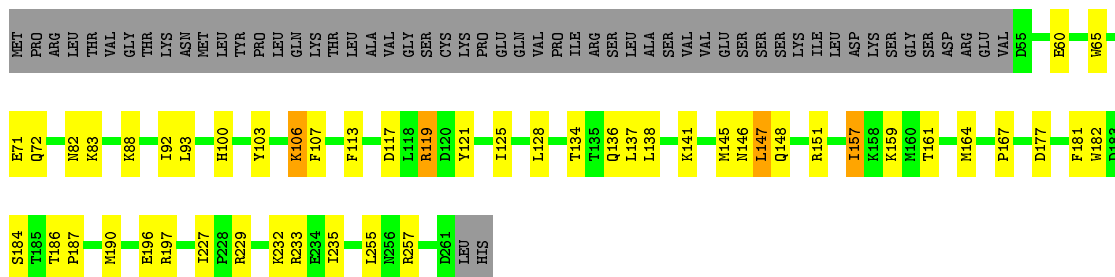
- Molecule 15: 54S ribosomal protein L22, mitochondrial

Chain 0:  57% 14% • 28%




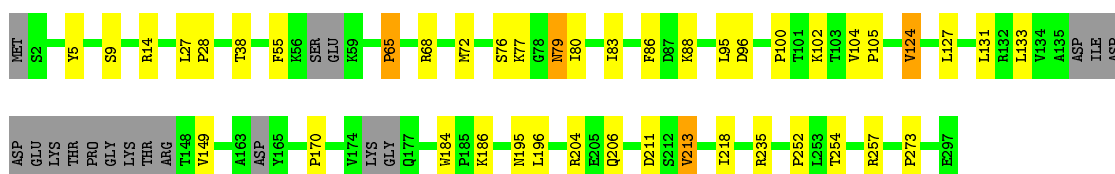
- Molecule 16: 54S ribosomal protein L41, mitochondrial

Chain P:  60% 17% • 21%

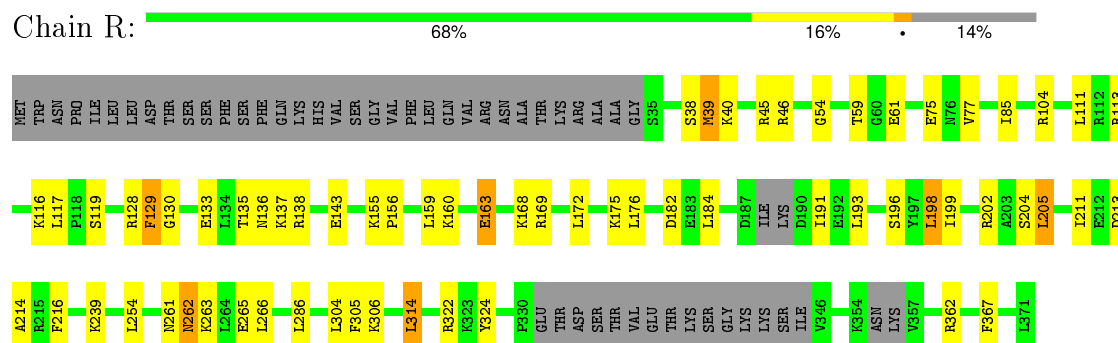


- Molecule 17: 54S ribosomal protein L40, mitochondrial

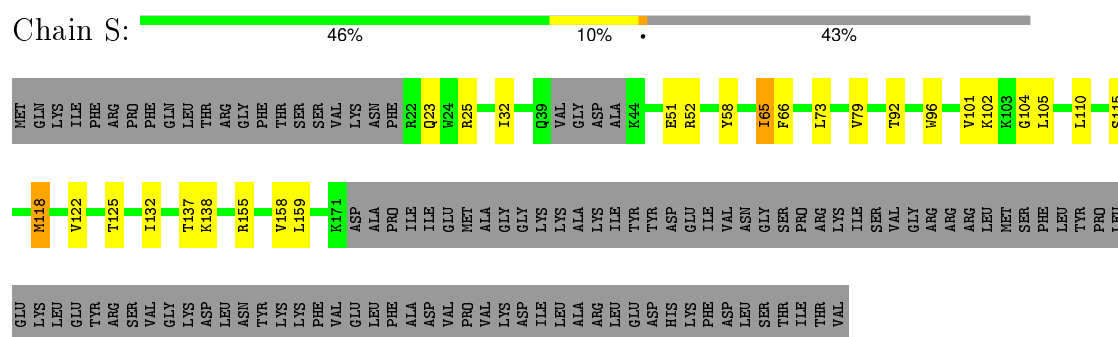
Chain Q:  79% 13% • 6%



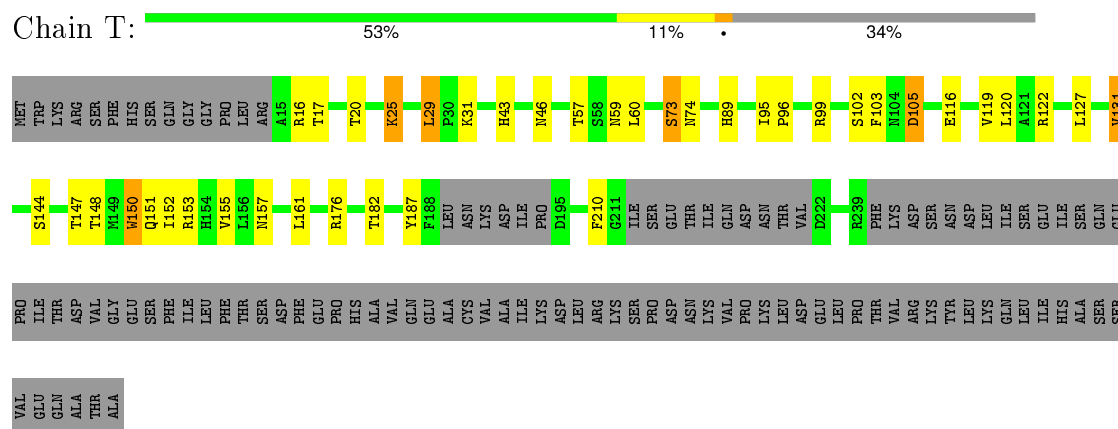
- Molecule 18: 54S ribosomal protein L2, mitochondrial



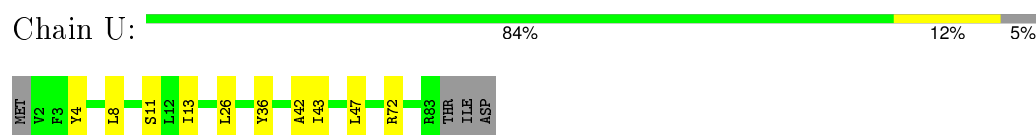
- Molecule 19: 54S ribosomal protein L24, mitochondrial



- Molecule 20: 54S ribosomal protein L4, mitochondrial



- Molecule 21: 54S ribosomal protein L33, mitochondrial

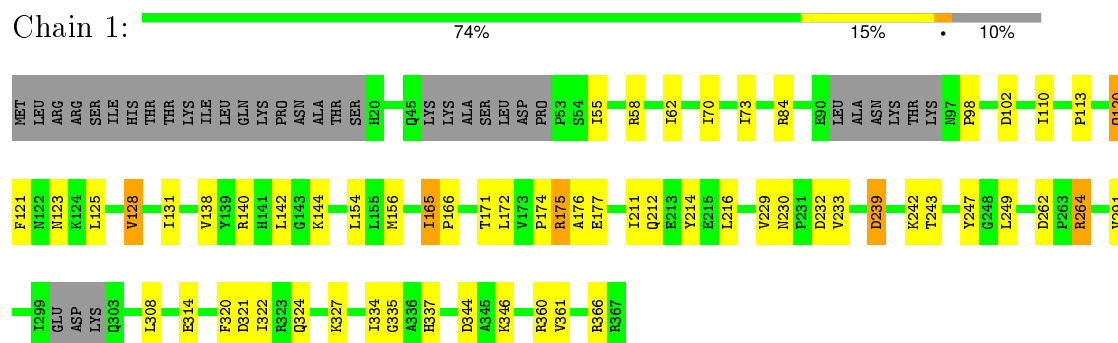


- Molecule 22: 54S ribosomal protein L36, mitochondrial

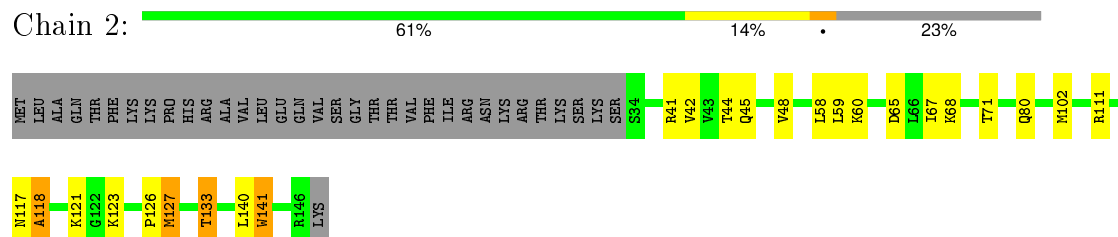


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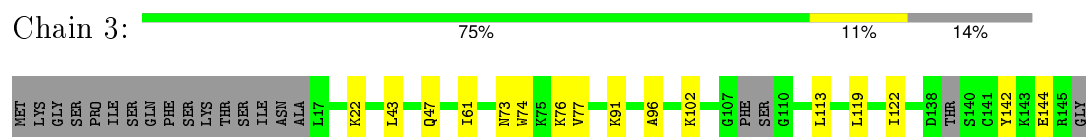
- Molecule 28: 54S ribosomal protein L35, mitochondrial



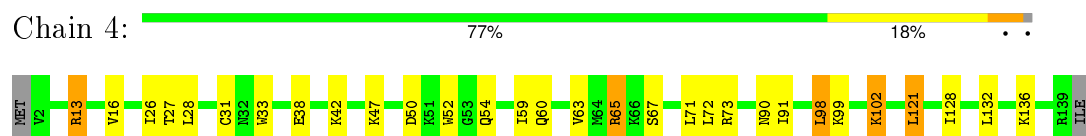
- Molecule 29: 54S ribosomal protein L28, mitochondrial



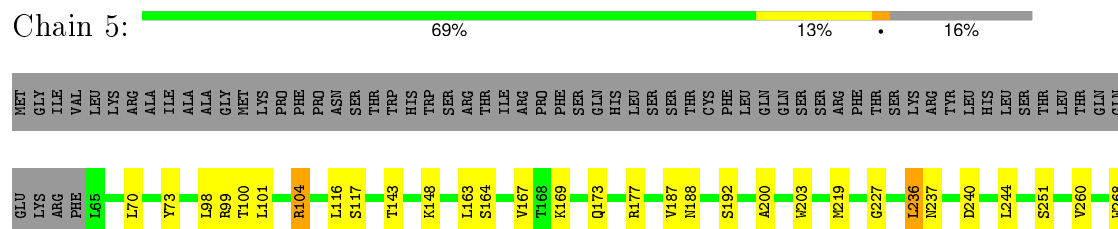
- Molecule 30: 54S ribosomal protein L27, mitochondrial



- Molecule 31: 54S ribosomal protein L51, mitochondrial



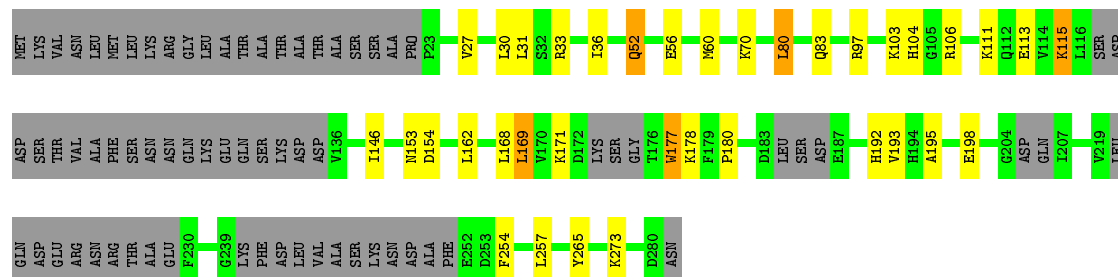
- Molecule 32: 54S ribosomal protein L3, mitochondrial





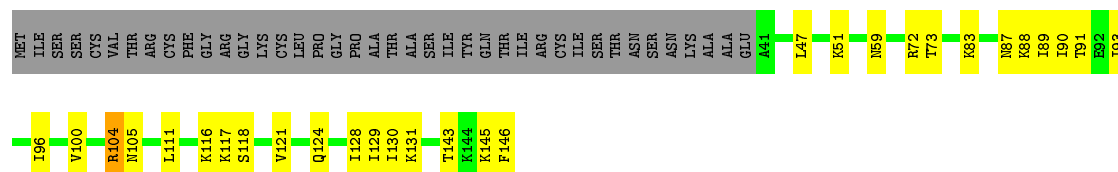
- Molecule 33: 54S ribosomal protein L17, mitochondrial

Chain 6: 62% 11% 26%



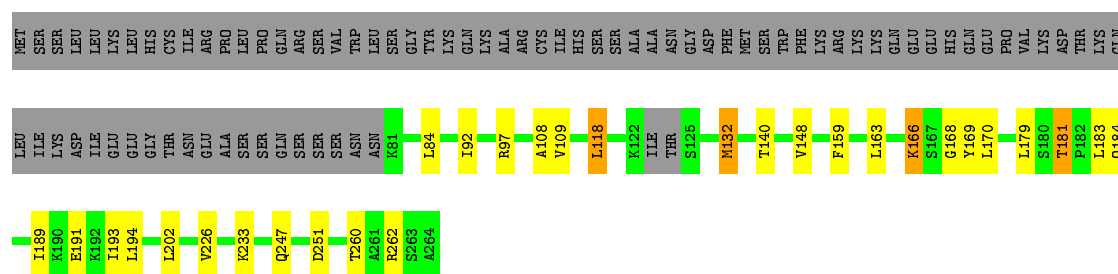
- Molecule 34: 54S ribosomal protein IMG2, mitochondrial

Chain 7: 53% 19% 27%



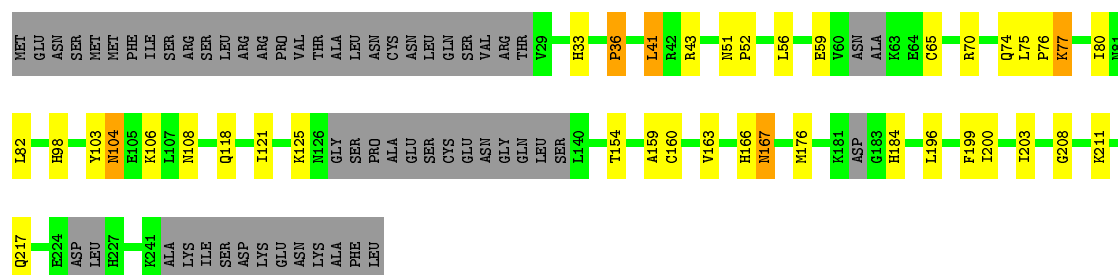
- Molecule 35: 54S ribosomal protein L13, mitochondrial

Chain 8: 58% 10% 31%

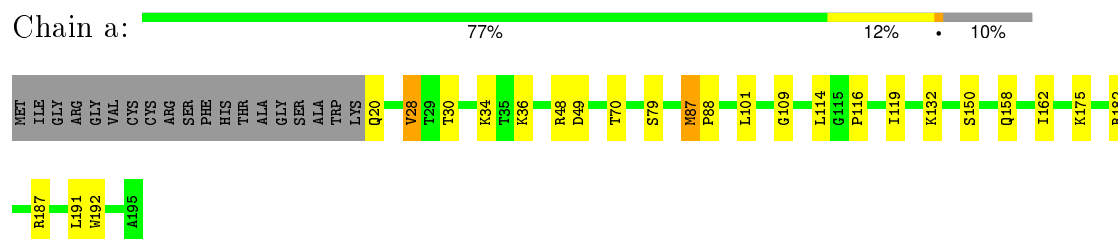


- Molecule 36: 54S ribosomal protein L15, mitochondrial

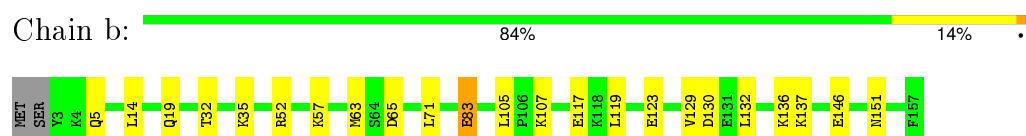
Chain 9: 62% 13% 23%



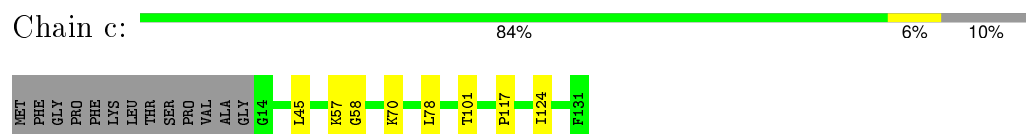
- Molecule 37: 54S ribosomal protein L20, mitochondrial



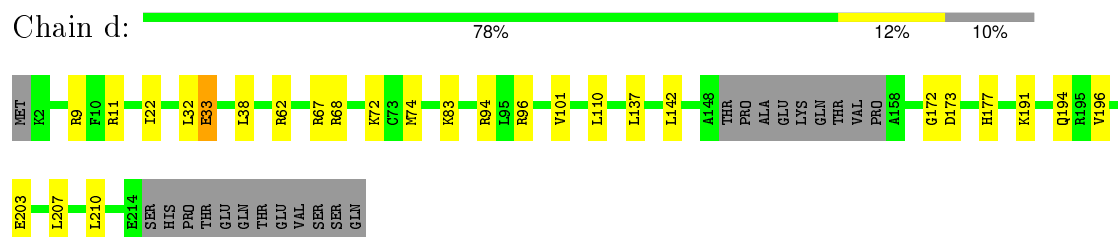
- Molecule 38: 54S ribosomal protein L25, mitochondrial



- Molecule 39: 54S ribosomal protein L31, mitochondrial



- Molecule 40: Mitochondrial homologous recombination protein 1



- Molecule 41: E-site tRNA



4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of images	47124	Depositor
Resolution determination method	FSC 0.143 gold-standard	Depositor
CTF correction method	Each particle	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	25	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	4700	Depositor
Magnification	59000	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: NA, ZN, MG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 2$	RMSZ	# $ Z > 2$
1	A	0.24	0/64599	0.70	13/100487 (0.0%)
10	J	0.33	0/1764	0.66	2/2360 (0.1%)
11	K	0.33	0/1606	0.65	0/2148
12	L	0.35	0/1843	0.64	0/2486
13	M	0.30	0/1224	0.64	0/1651
14	N	0.30	0/961	0.61	0/1295
15	O	0.35	0/1821	0.68	0/2444
16	P	0.34	0/1766	0.63	0/2381
17	Q	0.31	0/2174	0.57	0/2946
18	R	0.36	0/2522	0.68	0/3392
19	S	0.34	0/1216	0.58	0/1626
2	B	0.32	0/2305	0.66	0/3102
20	T	0.36	0/1689	0.69	0/2297
21	U	0.38	0/648	0.67	0/870
22	V	0.28	0/539	0.54	0/726
23	W	0.33	0/955	0.65	0/1273
24	X	0.33	0/520	0.62	0/696
25	Y	0.44	0/383	0.69	0/504
26	Z	0.38	0/522	0.71	0/695
27	0	0.32	0/329	0.56	0/432
28	1	0.32	0/2777	0.61	0/3772
29	2	0.37	0/938	0.70	0/1264
3	C	0.32	0/1973	0.59	0/2654
30	3	0.31	0/1018	0.57	0/1368
31	4	0.33	0/1138	0.65	0/1526
32	5	0.34	0/2538	0.66	1/3451 (0.0%)
33	6	0.30	0/1631	0.54	0/2214
34	7	0.31	0/869	0.57	0/1166
35	8	0.35	0/1438	0.61	0/1945
36	9	0.34	0/1453	0.61	0/1969
37	a	0.33	0/1458	0.63	0/1961
38	b	0.34	0/1333	0.63	0/1783

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >2	RMSZ	# Z >2
39	c	0.35	0/1024	0.63	0/1367
4	D	0.33	0/1904	0.65	0/2579
40	d	0.34	0/1762	0.65	0/2381
41	e	0.21	0/476	0.73	2/739 (0.3%)
5	E	0.31	0/2181	0.54	0/2955
6	F	0.31	0/1376	0.58	0/1869
7	G	0.32	0/468	0.57	0/628
8	H	0.36	0/1200	0.63	1/1610 (0.1%)
9	I	0.30	0/943	0.58	0/1260
All	All	0.29	0/119284	0.67	19/174272 (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
1	A	1	0
10	J	0	1
20	T	0	1
3	C	0	1
37	a	0	1
4	D	0	1
All	All	1	5

There are no bond length outliers.

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	2897	A	C2'-C3'-O3'	7.88	126.83	109.50
1	A	1892	G	C2'-C3'-O3'	7.84	126.75	109.50
1	A	733	A	C2'-C3'-O3'	7.69	126.42	109.50
10	J	76	ARG	NE-CZ-NH1	7.44	124.02	120.30
8	H	125	ARG	NE-CZ-NH1	7.28	123.94	120.30
1	A	2906	U	C2'-C3'-O3'	6.62	124.30	113.70
1	A	1312	G	C2'-C3'-O3'	6.52	124.13	113.70
1	A	3268	A	C2'-C3'-O3'	6.46	124.03	113.70
41	e	1	G	C5'-C4'-O4'	6.41	116.79	109.10
1	A	840	C	C2'-C3'-O3'	6.08	123.43	113.70
1	A	3020	U	C2'-C3'-O3'	6.04	123.37	113.70
1	A	1409	C	C2'-C3'-O3'	5.97	123.26	113.70
1	A	44	U	C2'-C3'-O3'	5.96	123.24	113.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	326	A	C2'-C3'-O3'	5.85	123.05	113.70
41	e	1	G	C5'-C4'-C3'	5.78	125.25	116.00
32	5	236	LEU	CA-CB-CG	5.51	127.98	115.30
1	A	2359	U	C2'-C3'-O3'	5.06	121.79	113.70
10	J	76	ARG	NE-CZ-NH2	-5.06	117.77	120.30
1	A	2586	U	C2'-C3'-O3'	5.04	121.77	113.70

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	1665	G	C1'

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	C	210	ASP	Peptide
4	D	49	PHE	Peptide
10	J	93	GLN	Peptide
20	T	43	HIS	Peptide
37	a	87	MET	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	57671	28898	28934	625	0
2	B	2260	2343	2303	47	0
3	C	1930	1976	1964	21	0
4	D	1866	1914	1898	30	0
5	E	2125	2169	2125	23	0
6	F	1355	1392	1338	22	0
7	G	458	471	467	2	0
8	H	1176	1218	1210	19	0
9	I	937	1015	1013	10	0
10	J	1727	1828	1812	12	0
11	K	1573	1635	1629	9	0
12	L	1815	1883	1873	21	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
13	M	1206	1286	1283	13	0
14	N	948	1010	1006	2	0
15	O	1789	1895	1877	21	0
16	P	1722	1728	1718	22	0
17	Q	2126	2161	2092	19	0
18	R	2481	2500	2413	25	0
19	S	1191	1249	1234	16	0
20	T	1646	1618	1557	22	0
21	U	639	702	699	11	0
22	V	528	555	553	3	0
23	W	937	985	974	9	0
24	X	512	565	563	3	0
25	Y	376	412	410	4	0
26	Z	508	546	539	6	0
27	0	324	349	345	4	0
28	1	2707	2690	2661	24	0
29	2	919	939	923	14	0
30	3	995	1030	1012	10	0
31	4	1117	1146	1142	18	0
32	5	2485	2541	2488	26	0
33	6	1592	1595	1511	13	0
34	7	854	901	897	10	0
35	8	1413	1416	1381	14	0
36	9	1428	1437	1368	19	0
37	a	1427	1455	1449	0	0
38	b	1299	1372	1367	0	0
39	c	1000	1066	1062	0	0
40	d	1717	1706	1691	0	0
41	e	427	221	222	0	0
42	A	109	0	0	0	0
42	N	1	0	0	0	0
43	B	1	0	0	0	0
44	0	1	0	0	2	0
44	W	1	0	0	0	0
All	All	111319	83818	83003	1022	0

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

All (1022) 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:A:45:U:O4	1:A:2895:A:N1	1.58	1.36
1:A:114:U:O4	1:A:118:A:N1	1.68	1.25
1:A:1913:A:N1	1:A:2880:U:O4	1.73	1.21
1:A:122:A:N6	1:A:139:U:N3	1.91	1.19
1:A:274:U:O4	1:A:367:A:N1	1.78	1.15
1:A:1344:U:O4	1:A:1555:A:N1	1.85	1.09
1:A:1344:U:C4	1:A:1555:A:N1	2.23	1.06
1:A:45:U:H3	1:A:2895:A:H61	1.04	1.00
1:A:123:A:C2	1:A:139:U:O2	2.20	0.94
1:A:1689:U:H3	1:A:2853:A:H61	1.15	0.94
1:A:230:A:H8	1:A:588:C:HO2'	1.08	0.93
27:0:66:CYS:SG	44:0:100:ZN:ZN	1.57	0.92
1:A:1913:A:N6	1:A:2880:U:H3	1.68	0.91
1:A:1361:C:O2'	1:A:1362:C:H6	1.53	0.91
1:A:2941:A:H2'	1:A:2942:A:C8	2.06	0.91
1:A:45:U:H3	1:A:2895:A:N6	1.67	0.90
1:A:944:U:HO2'	1:A:946:A:H2	1.20	0.89
1:A:274:U:H3	1:A:367:A:N6	1.70	0.88
1:A:315:A:H4'	1:A:315:A:OP1	1.72	0.88
1:A:1360:G:C6	1:A:1361:C:N3	2.43	0.87
1:A:1689:U:H3	1:A:2853:A:N6	1.73	0.86
1:A:2949:C:O2	3:C:79:ARG:NH2	2.08	0.86
26:Z:60:GLY:O	26:Z:64:ARG:HD2	1.75	0.86
1:A:152:G:O2'	1:A:153:G:O5'	1.94	0.85
1:A:1583:G:C2'	1:A:1585:G:H22	1.89	0.85
1:A:1361:C:O2'	1:A:1362:C:O5'	1.95	0.85
1:A:3160:U:H5''	12:L:52:THR:HG21	1.58	0.84
6:F:24:LEU:HD13	6:F:107:ILE:HD11	1.57	0.84
1:A:3242:A:H2'	1:A:3243:A:C8	2.14	0.82
1:A:1360:G:C5	1:A:1361:C:N3	2.48	0.82
32:5:104:ARG:NH1	32:5:203:TRP:O	2.13	0.82
1:A:274:U:H3	1:A:367:A:H61	1.24	0.81
1:A:2359:U:O3'	18:R:169:ARG:NH2	2.13	0.81
1:A:268:C:N4	1:A:2674:U:O2	2.13	0.81
1:A:122:A:N6	1:A:139:U:C2	2.48	0.81
1:A:3156:U:H2'	1:A:3157:A:C8	2.17	0.80
1:A:3162:U:H2'	1:A:3163:U:C6	2.15	0.80
1:A:2792:G:HO2'	27:0:56:PHE:N	1.79	0.80
1:A:114:U:C4	1:A:118:A:N1	2.50	0.80
1:A:45:U:O4	1:A:2895:A:C2	2.34	0.80
1:A:164:U:O2	16:P:82:ASN:HA	1.81	0.80
1:A:1913:A:N6	1:A:2880:U:N3	2.26	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2612:A:C8	1:A:2648:A:H2'	2.18	0.78
1:A:164:U:O2'	1:A:165:A:OP1	2.00	0.78
13:M:144:GLN:O	13:M:145:ARG:HB2	1.83	0.78
27:0:66:CYS:HG	44:0:100:ZN:ZN	0.95	0.78
1:A:238:C:H5	1:A:288:G:H1	1.32	0.78
1:A:1681:C:O2	1:A:1681:C:O5'	2.02	0.77
1:A:307:G:O2'	1:A:308:U:O5'	2.03	0.76
1:A:122:A:N6	1:A:139:U:H3	1.80	0.76
1:A:45:U:C4	1:A:2895:A:N1	2.53	0.76
1:A:1360:G:C2	1:A:1361:C:O2	2.39	0.76
33:6:36:ILE:HD11	33:6:162:LEU:HD22	1.68	0.75
1:A:849:U:H2'	1:A:850:A:C8	2.21	0.75
1:A:1583:G:H2'	1:A:1585:G:H22	1.54	0.73
1:A:3271:A:HO2'	13:M:16:TYR:N	1.86	0.73
1:A:307:G:HO2'	1:A:308:U:P	2.12	0.73
1:A:1913:A:N1	1:A:2880:U:C4	2.57	0.72
1:A:1313:G:H5'	1:A:1314:U:H2'	1.70	0.71
1:A:727:G:C6	1:A:728:C:N3	2.58	0.71
1:A:3159:G:N2	1:A:3248:C:C2	2.58	0.71
2:B:155:ILE:HD11	2:B:157:PHE:CZ	2.26	0.71
1:A:1344:U:C4	1:A:1555:A:C2	2.78	0.71
15:O:294:LEU:HD21	32:5:335:VAL:HG12	1.73	0.70
1:A:2373:U:O2'	1:A:2374:A:OP2	2.09	0.70
1:A:3159:G:N2	12:L:102:PRO:O	2.24	0.70
1:A:2597:G:N2	1:A:2652:C:C2	2.59	0.70
1:A:2957:A:H1'	1:A:2958:U:H5''	1.74	0.70
1:A:3025:U:H2'	1:A:3026:A:C8	2.26	0.70
1:A:1583:G:H2'	1:A:1585:G:N2	2.06	0.70
1:A:563:U:O2'	1:A:564:A:OP1	2.08	0.70
1:A:1075:A:C6	1:A:1076:U:H1'	2.27	0.69
1:A:2913:U:O4	1:A:2941:A:N1	2.26	0.69
6:F:119:LEU:HD11	6:F:169:ILE:HD11	1.73	0.69
1:A:114:U:N3	1:A:118:A:N6	2.39	0.69
31:4:60:GLN:HB3	32:5:100:THR:HG21	1.74	0.68
1:A:1312:G:H2'	1:A:1313:G:H5''	1.74	0.68
1:A:2913:U:H3	1:A:2941:A:H2	1.42	0.68
1:A:616:A:O2'	1:A:617:A:OP1	2.09	0.68
1:A:841:G:OP1	5:E:110:ASN:HB2	1.94	0.68
1:A:2670:C:N3	1:A:2682:G:C2	2.62	0.67
13:M:61:LEU:O	13:M:62:ILE:HB	1.95	0.67
1:A:2613:A:O2'	1:A:2614:U:OP1	2.12	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1361:C:O2'	1:A:1362:C:C5'	2.42	0.67
9:I:2:ILE:HD11	9:I:94:THR:HG21	1.76	0.67
1:A:268:C:O2'	1:A:269:A:OP2	2.12	0.67
1:A:1361:C:O2'	1:A:1362:C:C6	2.33	0.67
1:A:2814:U:H5'	1:A:2833:A:C2	2.30	0.66
16:P:181:PHE:HB3	20:T:127:LEU:HD11	1.78	0.66
1:A:1180:C:OP1	21:U:72:ARG:NH1	2.29	0.66
1:A:115:A:OP2	17:Q:9:SER:OG	2.14	0.66
1:A:3247:A:C2	1:A:3250:A:N6	2.63	0.66
3:C:59:CYS:SG	3:C:60:GLY:N	2.68	0.66
1:A:1892:G:O2'	1:A:1893:U:OP2	2.10	0.66
1:A:2913:U:C5	1:A:3068:U:H2'	2.30	0.66
1:A:486:G:H22	10:J:91:ARG:NE	1.94	0.66
17:Q:27:LEU:N	17:Q:28:PRO:HD2	2.10	0.66
1:A:1913:A:C2	1:A:2880:U:O4	2.49	0.66
1:A:3160:U:C5'	12:L:52:THR:HG21	2.26	0.66
1:A:743:A:O2'	21:U:42:ALA:O	2.15	0.65
1:A:1424:U:H2'	1:A:1425:U:O4'	1.96	0.65
1:A:1312:G:O2'	1:A:1313:G:OP1	2.13	0.65
1:A:1343:U:H1'	1:A:1344:U:C5	2.32	0.65
4:D:133:ARG:O	4:D:134:THR:HG22	1.97	0.65
9:I:79:ARG:O	9:I:80:ASN:CB	2.45	0.65
20:T:151:GLN:O	20:T:155:VAL:HG13	1.97	0.65
1:A:1392:A:O2'	1:A:1393:U:O5'	2.13	0.64
1:A:275:A:C2	1:A:367:A:C2	2.86	0.64
1:A:2094:A:N6	1:A:2250:G:O2'	2.30	0.64
1:A:1064:A:O2'	1:A:1065:A:OP2	2.12	0.64
30:3:61:ILE:HG23	30:3:77:VAL:HG22	1.78	0.64
17:Q:83:ILE:HG22	17:Q:95:LEU:HD22	1.79	0.64
1:A:1696:A:OP2	2:B:334:ARG:NH1	2.31	0.64
33:6:171:LYS:HA	33:6:177:TRP:HB2	1.79	0.64
1:A:114:U:O4	1:A:118:A:C2	2.50	0.64
1:A:2612:A:H5''	1:A:2612:A:N3	2.13	0.64
1:A:3247:A:H2	1:A:3250:A:H61	1.46	0.64
12:L:190:LYS:O	12:L:194:LEU:HD22	1.98	0.64
1:A:608:A:C2	1:A:1585:G:H8	2.15	0.63
1:A:608:A:C2	1:A:1585:G:C8	2.87	0.63
1:A:3159:G:C2	1:A:3248:C:N3	2.66	0.63
18:R:198:LEU:HD21	18:R:254:LEU:HD22	1.79	0.63
1:A:1344:U:O4	1:A:1555:A:C6	2.52	0.63
5:E:84:ILE:HD11	29:2:123:LYS:CB	2.29	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:39:LEU:O	8:H:54:GLY:HA3	1.98	0.63
16:P:255:LEU:HD21	32:5:73:TYR:CE2	2.33	0.62
1:A:3242:A:H2'	1:A:3243:A:H8	1.60	0.62
14:N:80:LEU:HD12	14:N:151:THR:HG21	1.79	0.62
1:A:1761:A:H2'	1:A:1762:A:C8	2.35	0.62
34:7:96:ILE:HG21	34:7:100:VAL:HG12	1.82	0.62
1:A:2331:U:O2	1:A:2367:A:H1'	1.99	0.62
11:K:63:SER:O	11:K:64:ILE:HG22	1.98	0.62
1:A:1343:U:C1'	1:A:1344:U:C5	2.83	0.62
36:9:76:PRO:O	36:9:77:LYS:CB	2.48	0.61
31:4:13:ARG:NH1	32:5:289:SER:O	2.33	0.61
1:A:2913:U:H5	1:A:3068:U:H2'	1.64	0.61
3:C:213:ARG:NH2	8:H:82:GLY:O	2.33	0.61
10:J:76:ARG:HG3	10:J:76:ARG:HH11	1.64	0.61
1:A:2446:U:O2'	1:A:2447:A:O5'	2.17	0.61
1:A:238:C:O2	1:A:238:C:O5'	2.18	0.61
16:P:227:ILE:HD13	16:P:232:LYS:HD3	1.82	0.61
1:A:314:A:N6	1:A:361:G:C8	2.69	0.61
28:1:243:THR:OG1	28:1:320:PHE:O	2.18	0.61
1:A:2958:U:H3'	1:A:2958:U:O2	2.00	0.61
1:A:2670:C:C2	1:A:2682:G:N2	2.68	0.61
1:A:271:A:H2'	1:A:272:G:O4'	2.01	0.61
6:F:69:VAL:HG11	6:F:73:LEU:HD23	1.83	0.61
15:O:177:ALA:HB3	15:O:235:THR:HG21	1.83	0.60
5:E:217:ILE:HG23	5:E:220:TYR:HB2	1.81	0.60
12:L:111:LEU:HD21	12:L:123:VAL:HG23	1.83	0.60
12:L:111:LEU:HD22	23:W:118:MET:HE1	1.81	0.60
18:R:176:LEU:HD13	18:R:198:LEU:HB3	1.82	0.60
1:A:2913:U:N3	1:A:2941:A:C2	2.66	0.60
1:A:1696:A:H2'	1:A:1697:C:O4'	2.01	0.60
1:A:1361:C:O2	1:A:1361:C:O4'	2.19	0.60
18:R:77:VAL:HG13	18:R:85:ILE:HG23	1.84	0.60
1:A:486:G:H22	10:J:91:ARG:HE	1.48	0.60
1:A:274:U:C4	1:A:367:A:N1	2.66	0.60
31:4:99:LYS:O	31:4:102:LYS:HG3	2.02	0.59
1:A:1107:U:H2'	8:H:68:THR:HG21	1.84	0.59
2:B:254:ASN:O	2:B:303:ALA:HA	2.02	0.59
1:A:34:U:O2'	1:A:35:U:P	2.60	0.59
1:A:34:U:HO2'	1:A:35:U:P	2.25	0.59
1:A:671:G:H2'	1:A:673:A:N7	2.18	0.59
2:B:241:LEU:HD11	2:B:305:ILE:HD11	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2670:C:C2	1:A:2682:G:C2	2.91	0.59
24:X:35:THR:HB	24:X:48:LEU:HD11	1.85	0.59
1:A:346:G:C2	1:A:357:C:O2	2.55	0.59
1:A:1944:C:C2	1:A:2892:G:N2	2.71	0.59
18:R:54:GLY:O	18:R:113:ARG:NH2	2.35	0.59
1:A:461:U:H5'	1:A:461:U:H6	1.68	0.59
1:A:1358:C:H2'	1:A:1358:C:O2	2.03	0.59
1:A:2585:A:H4'	1:A:2586:U:OP1	2.03	0.59
1:A:1361:C:HO2'	1:A:1362:C:H6	0.72	0.58
1:A:1583:G:N3	1:A:1585:G:N2	2.51	0.58
16:P:227:ILE:HD12	16:P:227:ILE:O	2.03	0.58
2:B:278:LYS:HG2	2:B:299:LEU:HD11	1.85	0.58
1:A:1313:G:N2	1:A:1321:C:C2	2.71	0.58
1:A:122:A:N6	1:A:140:U:C4	2.72	0.58
1:A:543:A:N1	1:A:550:A:N1	2.51	0.58
1:A:850:A:H2'	1:A:851:A:C8	2.39	0.58
1:A:1564:C:C2	1:A:1572:G:C2	2.92	0.58
1:A:615:U:C2'	1:A:616:A:OP1	2.51	0.58
1:A:2597:G:C2	1:A:2652:C:C2	2.92	0.58
1:A:331:A:O2'	1:A:332:A:P	2.62	0.58
36:9:51:ASN:HB2	36:9:52:PRO:HD2	1.86	0.58
1:A:1549:U:OP1	16:P:119:ARG:NH2	2.36	0.58
36:9:103:TYR:O	36:9:104:ASN:CB	2.51	0.58
1:A:1173:U:H2'	1:A:1174:G:O4'	2.04	0.57
1:A:2835:U:H2'	1:A:2836:G:O4'	2.05	0.57
1:A:966:A:C2	1:A:1059:A:C2	2.92	0.57
1:A:2593:A:H2'	1:A:2594:A:C8	2.39	0.57
7:G:21:VAL:HG12	7:G:57:TYR:HA	1.86	0.57
9:I:24:VAL:HG22	9:I:34:ALA:HB2	1.85	0.57
6:F:28:PRO:O	6:F:29:GLU:CB	2.51	0.57
1:A:122:A:C6	1:A:139:U:N3	2.62	0.57
20:T:95:ILE:N	20:T:96:PRO:CD	2.68	0.57
1:A:1944:C:C2	1:A:2892:G:C2	2.92	0.57
11:K:85:ILE:HD12	11:K:142:VAL:HG21	1.87	0.57
1:A:23:U:H2'	1:A:24:G:C8	2.40	0.57
12:L:170:LEU:HD13	12:L:213:LEU:HD11	1.85	0.57
1:A:3107:U:OP1	3:C:52:ARG:NH1	2.37	0.57
1:A:2590:U:H3'	1:A:2591:A:H5'	1.86	0.57
4:D:135:ALA:CB	4:D:136:PRO:CD	2.83	0.56
1:A:1755:A:H2'	1:A:1756:U:C6	2.40	0.56
1:A:1360:G:N2	1:A:1552:C:C2	2.73	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1344:U:H2'	1:A:1562:A:C2	2.40	0.56
1:A:2612:A:H2	1:A:2638:G:H1	1.52	0.56
1:A:1074:U:O4	1:A:1075:A:N6	2.38	0.56
1:A:3031:U:C4	1:A:3032:U:C4	2.92	0.56
23:W:123:GLN:O	23:W:127:ILE:HG23	2.05	0.56
1:A:3035:U:O2	1:A:3035:U:O4'	2.23	0.56
8:H:102:GLY:HA2	8:H:128:VAL:HG11	1.87	0.56
21:U:26:LEU:HD21	21:U:47:LEU:HD23	1.87	0.56
16:P:184:SER:HA	20:T:131:VAL:HG23	1.86	0.56
1:A:2733:A:N6	1:A:2734:A:C6	2.73	0.56
31:4:27:THR:HB	31:4:73:ARG:HG3	1.87	0.56
1:A:847:U:O4'	1:A:847:U:O2	2.23	0.56
15:O:133:LYS:HE3	15:O:279:TYR:CZ	2.40	0.56
1:A:1343:U:C2	1:A:1344:U:O4	2.59	0.56
1:A:1725:G:OP1	2:B:176:ARG:NH2	2.39	0.56
1:A:34:U:O2'	1:A:35:U:O5'	2.23	0.56
6:F:152:LEU:HD21	6:F:185:LEU:HD23	1.88	0.56
1:A:2335:U:O2	1:A:2335:U:O4'	2.23	0.56
1:A:1362:C:H2'	1:A:1363:C:H6	1.70	0.56
1:A:2958:U:O2'	1:A:2959:C:O4'	2.20	0.56
1:A:1952:A:H4'	3:C:207:GLN:O	2.06	0.56
1:A:1261:U:H5'	31:4:71:LEU:HD21	1.87	0.56
1:A:1344:U:C5	1:A:1555:A:C2	2.93	0.56
32:5:283:ILE:O	32:5:287:ILE:N	2.38	0.56
1:A:878:G:H22	1:A:891:A:H2	1.53	0.55
1:A:1360:G:C2	1:A:1552:C:C2	2.94	0.55
1:A:2711:G:OP1	4:D:115:ARG:NH2	2.38	0.55
31:4:16:VAL:HG23	32:5:289:SER:HB2	1.88	0.55
8:H:108:ALA:O	8:H:112:MET:HG2	2.06	0.55
1:A:23:U:HO2'	36:9:98:HIS:HD1	1.40	0.55
4:D:233:ILE:HG22	4:D:245:VAL:HG11	1.89	0.55
35:8:132:MET:SD	35:8:166:LYS:HB3	2.47	0.55
1:A:2597:G:C2	1:A:2652:C:N3	2.75	0.55
4:D:70:ARG:NH1	34:7:124:GLN:O	2.40	0.55
1:A:2360:U:P	18:R:169:ARG:HH22	2.30	0.55
1:A:238:C:O2	1:A:238:C:O4'	2.24	0.55
1:A:2958:U:H2'	1:A:2959:C:C6	2.42	0.55
4:D:205:VAL:HG11	35:8:108:ALA:HB1	1.87	0.55
1:A:1833:G:C6	1:A:1834:C:C4	2.94	0.55
1:A:386:U:O2	1:A:386:U:O4'	2.25	0.55
19:S:132:ILE:N	19:S:132:ILE:HD12	2.22	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:T:144:SER:O	20:T:147:THR:OG1	2.22	0.54
1:A:595:U:O4	25:Y:73:ARG:HB2	2.05	0.54
1:A:1698:C:O3'	2:B:318:LEU:O	2.26	0.54
1:A:1743:G:N2	1:A:1744:C:C2	2.75	0.54
1:A:2426:A:O2'	1:A:2427:U:O5'	2.20	0.54
1:A:3279:U:H2'	1:A:3280:C:C6	2.43	0.54
1:A:602:A:O2'	1:A:1366:A:N3	2.37	0.54
17:Q:218:ILE:HG22	20:T:103:PHE:CD1	2.43	0.54
1:A:509:A:H2'	1:A:510:A:O4'	2.07	0.54
31:4:28:LEU:HD13	31:4:72:LEU:CD2	2.38	0.54
12:L:146:TRP:CZ3	23:W:127:ILE:HD11	2.43	0.54
1:A:2707:G:N1	1:A:2708:C:C4	2.76	0.54
3:C:62:ILE:HD11	3:C:138:ALA:HB3	1.90	0.54
1:A:1358:C:H5	1:A:1553:G:H1	1.56	0.54
8:H:37:ILE:HG23	8:H:42:ARG:HB2	1.90	0.54
18:R:204:SER:CB	18:R:214:ALA:HB1	2.38	0.54
1:A:857:U:O4'	1:A:857:U:O2	2.22	0.54
5:E:214:LEU:O	5:E:217:ILE:HG22	2.08	0.54
1:A:1313:G:C2	1:A:1321:C:C2	2.95	0.53
1:A:1561:G:H3'	1:A:1561:G:N3	2.22	0.53
6:F:125:VAL:O	6:F:125:VAL:HG12	2.09	0.53
1:A:3160:U:H5''	12:L:52:THR:CG2	2.33	0.53
1:A:2720:G:C6	1:A:2765:C:N3	2.77	0.53
1:A:1405:U:O4'	1:A:1405:U:O2	2.26	0.53
1:A:2707:G:N2	1:A:2708:C:C2	2.77	0.53
1:A:176:U:H2'	1:A:177:A:C8	2.44	0.53
6:F:65:LEU:N	6:F:65:LEU:HD22	2.24	0.53
1:A:3156:U:H2'	1:A:3157:A:H8	1.70	0.53
32:5:163:LEU:HD12	32:5:283:ILE:HD11	1.90	0.53
8:H:27:THR:HG22	8:H:30:ARG:HD2	1.90	0.53
1:A:536:A:H4'	1:A:537:U:OP1	2.07	0.53
20:T:102:SER:N	20:T:105:ASP:OD2	2.42	0.53
1:A:2952:G:H1'	1:A:3062:A:C2	2.44	0.53
1:A:331:A:O2'	1:A:332:A:OP2	2.25	0.53
3:C:61:LEU:HD21	3:C:160:PHE:CE2	2.44	0.53
1:A:554:U:H2'	1:A:556:A:C8	2.44	0.53
1:A:870:C:O4'	1:A:870:C:O2	2.22	0.53
5:E:161:LEU:HD22	29:2:45:GLN:HB3	1.91	0.53
1:A:1750:G:C6	1:A:1751:C:C4	2.97	0.53
16:P:92:ILE:HG23	20:T:122:ARG:HA	1.91	0.53
1:A:595:U:O2	1:A:595:U:H2'	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:S:138:LYS:O	19:S:155:ARG:NH2	2.42	0.53
1:A:2382:A:H4'	33:6:80:LEU:HD11	1.91	0.53
34:7:83:LYS:HB2	34:7:88:LYS:HG2	1.91	0.53
1:A:2287:A:OP1	18:R:45:ARG:NH2	2.41	0.53
1:A:2913:U:OP2	1:A:3069:A:OP1	2.27	0.52
32:5:324:VAL:HG21	32:5:339:HIS:ND1	2.24	0.52
1:A:28:U:O2'	1:A:29:A:OP1	2.26	0.52
1:A:1720:U:HO2'	2:B:135:ASN:H	1.57	0.52
28:1:233:VAL:HG22	28:1:242:LYS:O	2.09	0.52
15:O:172:SER:O	15:O:261:ILE:HG23	2.08	0.52
29:2:140:LEU:O	29:2:141:TRP:CB	2.56	0.52
1:A:1373:U:O4'	1:A:1373:U:O2	2.25	0.52
16:P:186:THR:HG22	16:P:187:PRO:HD3	1.91	0.52
1:A:3247:A:H2	1:A:3250:A:N6	2.06	0.52
1:A:33:A:N6	1:A:34:U:C4	2.77	0.52
1:A:915:G:C5	21:U:13:ILE:HD12	2.44	0.52
1:A:1493:U:H2'	1:A:1494:A:C8	2.45	0.52
18:R:204:SER:HB3	18:R:214:ALA:HB1	1.91	0.52
1:A:3264:C:O2'	32:5:332:LYS:O	2.26	0.52
5:E:202:MET:HG3	5:E:203:SER:N	2.24	0.52
3:C:240:ASP:OD1	3:C:240:ASP:N	2.43	0.52
20:T:96:PRO:O	20:T:99:ARG:HB2	2.09	0.52
17:Q:213:VAL:HG22	30:3:122:ILE:HD13	1.91	0.52
1:A:1486:U:H2'	1:A:1487:A:C8	2.45	0.52
20:T:57:THR:HG21	23:W:148:LEU:HD12	1.92	0.52
1:A:2913:U:N3	1:A:2941:A:H2	2.06	0.52
1:A:247:A:H2'	1:A:248:A:O4'	2.09	0.52
25:Y:71:LEU:HD11	25:Y:75:ARG:NH2	2.24	0.52
1:A:1392:A:HO2'	1:A:1393:U:C5'	2.22	0.52
32:5:188:ASN:O	32:5:192:SER:N	2.43	0.52
1:A:581:C:C2	1:A:700:G:C2	2.97	0.52
1:A:3162:U:N3	1:A:3163:U:C4	2.78	0.52
10:J:76:ARG:CG	10:J:76:ARG:HH11	2.23	0.52
1:A:27:A:HO2'	1:A:28:U:P	2.32	0.52
1:A:1681:C:O2	1:A:1681:C:O4'	2.26	0.51
20:T:144:SER:O	20:T:148:THR:HG23	2.10	0.51
1:A:2720:G:C2	1:A:2765:C:O2	2.63	0.51
1:A:511:G:H2'	1:A:512:U:C6	2.46	0.51
6:F:126:GLY:HA3	6:F:129:TYR:CD2	2.45	0.51
1:A:2741:G:N2	1:A:2796:G:H1	2.06	0.51
1:A:2601:A:O2'	1:A:2602:A:C8	2.63	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:261:A:C4	1:A:307:G:N7	2.79	0.51
1:A:2427:U:H3'	1:A:2427:U:O2	2.10	0.51
14:N:134:THR:HB	14:N:141:VAL:HG22	1.92	0.51
6:F:183:ALA:O	6:F:186:ARG:HG3	2.10	0.51
16:P:92:ILE:O	16:P:107:PHE:HA	2.11	0.51
1:A:2364:U:H2'	1:A:2365:A:H8	1.75	0.51
1:A:527:A:H62	1:A:539:U:H5'	1.74	0.51
29:2:117:ASN:O	29:2:118:ALA:C	2.48	0.51
1:A:2258:C:OP1	19:S:96:TRP:CZ3	2.64	0.51
20:T:89:HIS:O	30:3:96:ALA:HB2	2.11	0.51
1:A:441:A:N1	1:A:448:U:H5	2.09	0.51
15:O:155:GLU:O	15:O:158:VAL:HG12	2.10	0.51
1:A:3068:U:H4'	1:A:3069:A:OP2	2.10	0.51
1:A:23:U:O2'	36:9:98:HIS:ND1	2.33	0.51
1:A:904:G:C2	1:A:912:C:C2	2.98	0.51
1:A:2435:A:H3'	1:A:2436:A:H5''	1.91	0.51
1:A:1355:G:O2'	1:A:1356:U:P	2.69	0.51
1:A:2594:A:H2'	1:A:2595:U:C6	2.46	0.51
32:5:169:LYS:O	32:5:173:GLN:HG2	2.11	0.51
36:9:82:LEU:HD11	36:9:203:ILE:HG22	1.92	0.51
13:M:108:LEU:HG	13:M:125:LEU:HD23	1.93	0.51
1:A:1960:A:C2	1:A:1961:G:C8	2.99	0.51
17:Q:83:ILE:HG22	17:Q:95:LEU:CD2	2.41	0.51
23:W:124:ILE:O	23:W:127:ILE:HG12	2.10	0.51
1:A:834:A:HO2'	1:A:835:A:H8	1.58	0.51
1:A:122:A:N6	1:A:139:U:C4	2.56	0.51
1:A:1582:A:H2'	1:A:1583:G:O4'	2.11	0.51
4:D:70:ARG:HH11	4:D:70:ARG:HG2	1.76	0.51
19:S:105:LEU:HB3	19:S:132:ILE:HD11	1.93	0.51
11:K:69:LEU:HD23	11:K:69:LEU:H	1.76	0.51
1:A:3233:A:O5'	1:A:3233:A:H8	1.94	0.51
1:A:164:U:HO2'	1:A:165:A:P	2.30	0.51
1:A:1830:G:O2'	1:A:1868:G:N1	2.44	0.51
9:I:79:ARG:O	9:I:80:ASN:HB3	2.10	0.50
28:1:120:GLN:HB3	28:1:121:PHE:CD1	2.47	0.50
1:A:117:U:O4'	1:A:117:U:O2	2.30	0.50
1:A:1392:A:O2'	1:A:1393:U:P	2.69	0.50
15:O:127:ILE:HD12	15:O:138:VAL:HG23	1.93	0.50
16:P:138:LEU:HD11	16:P:159:LYS:HD2	1.92	0.50
11:K:223:GLU:HG2	11:K:224:PRO:HD2	1.93	0.50
1:A:2612:A:OP1	24:X:46:HIS:NE2	2.42	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:143:LEU:HD23	4:D:144:PRO:HD2	1.93	0.50
1:A:1386:A:O2'	19:S:65:ILE:O	2.15	0.50
4:D:246:ILE:HG21	4:D:251:VAL:HA	1.93	0.50
23:W:118:MET:HE2	23:W:118:MET:HA	1.94	0.50
2:B:209:PHE:HB2	2:B:241:LEU:HB3	1.94	0.50
1:A:1806:C:H2'	1:A:1830:G:C8	2.46	0.50
1:A:1535:A:H2'	1:A:1536:A:C8	2.47	0.50
1:A:419:U:H2'	1:A:420:U:O4'	2.12	0.50
1:A:2898:U:H2'	1:A:2899:U:C6	2.45	0.50
1:A:2317:A:O2'	1:A:2318:U:P	2.69	0.50
1:A:2258:C:OP1	19:S:96:TRP:HZ3	1.95	0.50
18:R:286:LEU:HD12	18:R:324:TYR:CG	2.46	0.50
1:A:1993:U:H1'	19:S:101:VAL:HG11	1.93	0.50
1:A:488:A:H2'	1:A:489:A:C8	2.47	0.50
1:A:3069:A:O2'	1:A:3070:A:OP2	2.21	0.50
33:6:171:LYS:HA	33:6:177:TRP:CB	2.41	0.50
2:B:286:ILE:HD11	2:B:296:TYR:CE1	2.46	0.50
1:A:3192:A:H2'	1:A:3193:A:O4'	2.11	0.50
1:A:502:A:C8	1:A:563:U:C5	3.00	0.50
1:A:1972:G:C6	1:A:1973:C:C4	3.00	0.50
1:A:275:A:N6	1:A:276:U:O4	2.45	0.49
1:A:3069:A:C8	1:A:3108:U:H1'	2.46	0.49
1:A:2958:U:O2	1:A:2958:U:C3'	2.60	0.49
1:A:346:G:C6	1:A:357:C:N3	2.80	0.49
8:H:139:ASN:HB3	32:5:329:ARG:O	2.12	0.49
1:A:645:U:H2'	1:A:646:C:C6	2.47	0.49
1:A:3159:G:C2	1:A:3248:C:C2	3.00	0.49
4:D:200:ILE:O	4:D:201:PHE:CB	2.59	0.49
1:A:238:C:O2	1:A:238:C:C5'	2.60	0.49
1:A:365:A:N3	1:A:365:A:H2'	2.28	0.49
33:6:27:VAL:HG11	33:6:195:ALA:HB2	1.94	0.49
1:A:1318:A:N7	12:L:116:ASN:ND2	2.59	0.49
36:9:118:GLN:O	36:9:121:ILE:HG22	2.13	0.49
1:A:2648:A:O3'	5:E:19:PRO:N	2.45	0.49
15:O:271:SER:O	15:O:275:ARG:HD3	2.13	0.49
1:A:2706:C:OP2	2:B:349:ARG:NH2	2.42	0.49
1:A:3164:A:N1	1:A:3233:A:C2	2.81	0.49
29:2:41:ARG:O	29:2:44:THR:OG1	2.27	0.49
32:5:167:VAL:HG13	32:5:288:MET:HE1	1.94	0.49
1:A:366:A:C6	1:A:367:A:N6	2.81	0.49
1:A:789:A:N7	1:A:840:C:C4	2.80	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:61:LEU:O	13:M:62:ILE:CB	2.60	0.49
1:A:2814:U:C2	1:A:2815:U:C5	3.01	0.49
20:T:147:THR:HA	20:T:150:TRP:CD1	2.48	0.49
20:T:116:GLU:O	20:T:119:VAL:HG22	2.13	0.49
1:A:2607:G:C6	1:A:2608:C:C4	3.00	0.49
1:A:538:A:N1	1:A:556:A:C2	2.81	0.49
1:A:207:U:C2	1:A:208:A:C8	3.01	0.49
35:8:189:ILE:HG22	35:8:194:LEU:HD23	1.95	0.49
15:O:294:LEU:HD21	32:5:335:VAL:CG1	2.42	0.49
1:A:543:A:C2	1:A:550:A:N1	2.81	0.49
1:A:304:A:H1'	1:A:365:A:H2	1.78	0.49
26:Z:65:TRP:CZ3	26:Z:100:ALA:HB2	2.48	0.49
1:A:133:A:C6	1:A:134:U:C2	3.00	0.49
15:O:112:LEU:HD21	16:P:227:ILE:HG21	1.95	0.49
34:7:104:ARG:HG3	34:7:105:ASN:N	2.26	0.49
11:K:225:GLN:HG2	11:K:226:TYR:N	2.28	0.49
15:O:171:LYS:HD2	15:O:260:TYR:CZ	2.48	0.49
1:A:1846:G:C6	1:A:1847:C:C4	3.00	0.49
1:A:1743:G:N1	1:A:1744:C:C4	2.81	0.48
16:P:186:THR:N	16:P:187:PRO:CD	2.76	0.48
33:6:192:HIS:CE1	33:6:193:VAL:HG23	2.48	0.48
1:A:735:A:H4'	1:A:736:A:OP1	2.11	0.48
6:F:77:LYS:HA	6:F:84:ILE:HG22	1.95	0.48
36:9:200:ILE:O	36:9:203:ILE:HG12	2.13	0.48
1:A:2468:A:OP1	5:E:97:LYS:NZ	2.46	0.48
1:A:119:A:H2'	1:A:119:A:N3	2.28	0.48
34:7:93:ILE:HD12	34:7:128:ILE:HD11	1.95	0.48
18:R:155:LYS:N	18:R:156:PRO:CD	2.76	0.48
1:A:3158:G:H2'	1:A:3159:G:O4'	2.13	0.48
1:A:2590:U:H3'	1:A:2591:A:C5'	2.43	0.48
1:A:708:U:O2'	1:A:730:U:H5''	2.14	0.48
35:8:118:LEU:HB3	35:8:168:GLY:HA2	1.95	0.48
23:W:137:ILE:HG23	23:W:137:ILE:O	2.13	0.48
1:A:1360:G:H2'	1:A:1361:C:H5'	1.95	0.48
10:J:114:TYR:O	26:Z:64:ARG:HD3	2.13	0.48
1:A:3163:U:C2	1:A:3164:A:C8	3.02	0.48
1:A:1382:A:C6	1:A:1392:A:N6	2.81	0.48
29:2:44:THR:O	29:2:48:VAL:HG23	2.13	0.48
1:A:1901:U:OP1	12:L:8:LYS:NZ	2.46	0.48
30:3:74:TRP:C	30:3:76:LYS:H	2.16	0.48
31:4:121:LEU:N	31:4:121:LEU:HD23	2.28	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:364:U:O2'	1:A:365:A:C8	2.66	0.48
8:H:19:VAL:HG13	8:H:59:VAL:HG22	1.94	0.48
1:A:409:A:H2'	1:A:409:A:N3	2.29	0.48
1:A:2802:G:C6	1:A:2803:C:C4	3.02	0.48
1:A:448:U:O2	1:A:448:U:O4'	2.28	0.48
5:E:274:TYR:HA	5:E:277:ARG:HG2	1.95	0.48
5:E:154:LEU:HG	29:2:42:VAL:HG11	1.95	0.48
4:D:50:PRO:CD	4:D:183:ASP:HB2	2.43	0.48
1:A:3122:U:O2'	1:A:3123:A:OP2	2.29	0.48
18:R:205:LEU:HD21	18:R:211:ILE:HG22	1.95	0.48
28:1:174:PRO:O	28:1:334:ILE:O	2.31	0.48
1:A:945:A:N1	1:A:1107:U:O2'	2.32	0.48
1:A:27:A:O2'	1:A:28:U:P	2.72	0.48
1:A:364:U:O2'	1:A:365:A:H8	1.97	0.48
1:A:25:A:O2'	1:A:26:A:P	2.71	0.48
2:B:180:ILE:HD12	2:B:193:TYR:CD1	2.49	0.48
6:F:24:LEU:CD1	6:F:107:ILE:HD11	2.37	0.48
1:A:615:U:O2'	1:A:616:A:OP1	2.29	0.48
36:9:103:TYR:O	36:9:104:ASN:HB2	2.13	0.48
1:A:1969:G:C6	1:A:1970:C:C4	3.02	0.48
1:A:2601:A:HO2'	1:A:2602:A:H8	1.60	0.48
1:A:119:A:C2'	1:A:119:A:N3	2.76	0.48
1:A:1981:U:O4	1:A:2263:U:C4	2.67	0.48
1:A:1555:A:H2'	1:A:1556:A:O4'	2.13	0.47
18:R:77:VAL:CG1	18:R:85:ILE:HG23	2.44	0.47
1:A:2707:G:C2	1:A:2708:C:C6	3.02	0.47
1:A:880:G:OP2	11:K:55:ARG:NH1	2.44	0.47
32:5:98:LEU:HG	32:5:227:GLY:HA2	1.96	0.47
1:A:2452:U:H2'	1:A:2453:G:O4'	2.14	0.47
32:5:340:VAL:HG23	32:5:362:ALA:HB1	1.95	0.47
1:A:651:G:H2'	1:A:652:A:O4'	2.14	0.47
16:P:103:TYR:CE1	16:P:167:PRO:HB3	2.49	0.47
8:H:56:TYR:CD2	8:H:125:ARG:HG3	2.49	0.47
1:A:275:A:C6	1:A:276:U:O4	2.67	0.47
4:D:135:ALA:HB1	4:D:136:PRO:HD3	1.95	0.47
21:U:11:SER:OG	21:U:13:ILE:HG22	2.14	0.47
3:C:63:THR:HG22	3:C:87:VAL:HG22	1.96	0.47
1:A:169:A:H2'	1:A:170:U:O4'	2.14	0.47
1:A:1541:U:H2'	1:A:1542:U:C6	2.49	0.47
1:A:2947:C:H5'	3:C:253:ALA:HA	1.96	0.47
5:E:245:PHE:CD1	5:E:245:PHE:N	2.82	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:9:166:HIS:O	36:9:167:ASN:CB	2.62	0.47
1:A:274:U:O4	1:A:367:A:C2	2.62	0.47
1:A:1756:U:C2	1:A:1757:A:C8	3.02	0.47
2:B:173:ASP:OD2	2:B:176:ARG:NH1	2.44	0.47
36:9:199:PHE:O	36:9:203:ILE:HG23	2.13	0.47
36:9:118:GLN:HA	36:9:121:ILE:HG22	1.95	0.47
1:A:880:G:C6	1:A:881:C:C4	3.02	0.47
1:A:1142:U:H2'	1:A:1143:A:O4'	2.15	0.47
15:O:299:ILE:HD11	31:4:128:ILE:HG23	1.97	0.47
1:A:275:A:N1	1:A:367:A:C2	2.81	0.47
1:A:3261:U:O4'	1:A:3261:U:O2	2.31	0.47
28:1:176:ALA:HB3	28:1:334:ILE:HD12	1.95	0.47
1:A:954:A:O2'	1:A:955:A:OP2	2.27	0.47
1:A:3137:A:H1'	1:A:3143:A:C2	2.50	0.47
17:Q:195:ASN:O	30:3:91:LYS:HG2	2.14	0.47
1:A:231:A:H2'	1:A:232:C:C6	2.50	0.47
1:A:718:G:H2'	1:A:1968:U:C2	2.48	0.47
2:B:268:SER:O	2:B:271:THR:HG22	2.13	0.47
1:A:2885:G:C6	1:A:2886:C:C4	3.02	0.47
1:A:1630:A:O2'	1:A:1891:U:H4'	2.14	0.47
1:A:832:U:H4'	11:K:70:GLN:HG3	1.97	0.47
6:F:60:GLY:HA3	6:F:114:VAL:HB	1.97	0.47
15:O:183:LEU:HD11	23:W:97:MET:HG3	1.97	0.47
19:S:66:PHE:CE1	19:S:79:VAL:HG23	2.50	0.47
6:F:24:LEU:HB2	6:F:84:ILE:HG13	1.95	0.47
1:A:2951:U:O2'	9:I:80:ASN:HA	2.15	0.47
8:H:125:ARG:CG	8:H:125:ARG:HH11	2.28	0.47
8:H:46:VAL:HG13	15:O:299:ILE:HG23	1.96	0.47
1:A:643:U:H4'	1:A:644:A:O5'	2.13	0.47
1:A:2785:U:C5	1:A:2808:A:C6	3.02	0.47
2:B:385:ARG:HG3	2:B:386:PRO:HD2	1.96	0.47
1:A:1258:A:H2'	1:A:1259:A:O4'	2.15	0.47
1:A:2741:G:N2	1:A:2796:G:N1	2.62	0.47
1:A:1535:A:OP1	2:B:151:ARG:NH2	2.47	0.47
18:R:117:LEU:O	18:R:119:SER:N	2.47	0.47
1:A:1116:A:N6	1:A:1117:G:C6	2.82	0.47
1:A:3122:U:O2'	1:A:3123:A:P	2.73	0.47
1:A:328:A:H2'	1:A:329:A:H5'	1.96	0.47
1:A:716:A:H2'	1:A:717:U:O4'	2.14	0.47
1:A:2954:U:H2'	1:A:2955:G:O4'	2.15	0.47
1:A:3109:U:OP1	3:C:169:ARG:NH2	2.47	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1938:A:H2'	1:A:1939:U:O4'	2.15	0.47
1:A:789:A:H2'	1:A:790:A:C8	2.50	0.47
18:R:196:SER:HA	18:R:199:ILE:HG12	1.96	0.47
1:A:221:A:H2'	1:A:222:A:C8	2.50	0.47
5:E:161:LEU:HD22	29:2:45:GLN:CB	2.45	0.46
1:A:1805:G:C6	1:A:1806:C:C4	3.03	0.46
1:A:1995:G:H2'	1:A:1996:A:O4'	2.14	0.46
1:A:3254:U:OP1	23:W:102:ASN:HB2	2.15	0.46
1:A:2446:U:H4'	1:A:2447:A:OP1	2.15	0.46
19:S:132:ILE:N	19:S:132:ILE:CD1	2.78	0.46
1:A:2207:A:C5	1:A:2208:A:N7	2.83	0.46
2:B:183:LEU:HG	2:B:194:ILE:HG12	1.97	0.46
1:A:2597:G:N1	1:A:2652:C:C4	2.84	0.46
1:A:1392:A:HO2'	1:A:1393:U:P	2.39	0.46
1:A:1833:G:C5	1:A:1834:C:C5	3.04	0.46
1:A:1493:U:O2'	1:A:1494:A:OP1	2.32	0.46
1:A:3029:U:C4	1:A:3030:U:C4	3.03	0.46
1:A:2732:G:OP1	27:0:59:ARG:HB2	2.16	0.46
18:R:216:PHE:CZ	28:1:264:ARG:HD2	2.51	0.46
28:1:171:THR:HG22	28:1:172:LEU:N	2.30	0.46
33:6:30:LEU:O	33:6:30:LEU:HD12	2.14	0.46
1:A:308:U:C2'	1:A:309:C:O5'	2.63	0.46
1:A:28:U:O2'	1:A:29:A:P	2.73	0.46
1:A:2317:A:C2	1:A:2318:U:C2	3.04	0.46
35:8:169:TYR:CD2	35:8:193:ILE:HG21	2.50	0.46
1:A:1245:U:O4	1:A:1267:A:N1	2.49	0.46
1:A:1808:G:C6	1:A:1809:C:C4	3.04	0.46
1:A:1706:G:O2'	2:B:295:ARG:NH1	2.48	0.46
1:A:914:A:C5	21:U:13:ILE:HD13	2.50	0.46
1:A:3120:A:N1	1:A:3261:U:C4	2.84	0.46
16:P:146:ASN:O	16:P:147:LEU:CB	2.63	0.46
1:A:836:A:N3	1:A:2290:A:O2'	2.40	0.46
1:A:1765:A:C6	1:A:1786:A:C2	3.03	0.46
1:A:840:C:O2	1:A:840:C:H3'	2.16	0.46
4:D:230:GLU:O	4:D:233:ILE:HG13	2.15	0.46
3:C:69:MET:HB2	3:C:70:PRO:CD	2.45	0.46
3:C:115:LEU:HD11	13:M:28:VAL:HG21	1.97	0.46
1:A:1362:C:H2'	1:A:1363:C:C6	2.51	0.46
1:A:1312:G:C2'	1:A:1313:G:H5''	2.45	0.46
1:A:1261:U:C5'	31:4:71:LEU:HD21	2.46	0.46
1:A:1364:C:C2	1:A:1402:G:C2	3.03	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3268:A:H2'	1:A:3269:U:H6	1.81	0.46
1:A:123:A:C2	1:A:139:U:C2	3.02	0.46
20:T:147:THR:O	20:T:151:GLN:HG2	2.16	0.46
18:R:128:ARG:O	28:1:239:ASP:O	2.33	0.46
12:L:127:VAL:HG12	12:L:128:ASP:N	2.31	0.46
1:A:2874:G:H2'	1:A:2875:G:O4'	2.16	0.46
6:F:161:LYS:HG2	6:F:169:ILE:CG2	2.46	0.46
1:A:673:A:C2	2:B:338:MET:HG2	2.51	0.46
1:A:328:A:C2'	1:A:329:A:H5'	2.45	0.46
1:A:1759:A:H2'	1:A:1760:U:O4'	2.16	0.46
2:B:294:HIS:O	2:B:382:VAL:HG23	2.16	0.46
1:A:581:C:C2	1:A:700:G:N2	2.83	0.46
1:A:2730:G:C6	1:A:2731:C:C4	3.03	0.46
22:V:57:VAL:HB	29:2:133:THR:HG22	1.98	0.46
1:A:1274:A:C8	31:4:33:TRP:CH2	3.04	0.46
34:7:118:SER:HB2	34:7:131:LYS:HB2	1.97	0.46
32:5:200:ALA:HB2	32:5:260:VAL:HG23	1.97	0.46
1:A:549:U:O2	1:A:2635:C:O2'	2.16	0.46
1:A:2796:G:H2'	1:A:2797:U:OP1	2.15	0.45
1:A:2898:U:H2'	1:A:2899:U:H6	1.79	0.45
1:A:3143:A:H2'	1:A:3144:A:O4'	2.16	0.45
18:R:129:PHE:HB3	28:1:239:ASP:O	2.16	0.45
5:E:73:TYR:HA	5:E:77:LEU:HB2	1.97	0.45
1:A:1220:G:H2'	1:A:1221:G:O4'	2.16	0.45
13:M:95:LEU:HD12	13:M:109:LEU:HD13	1.97	0.45
1:A:1360:G:N3	1:A:1361:C:O2	2.48	0.45
1:A:1392:A:H2'	1:A:1392:A:N3	2.31	0.45
1:A:346:G:N1	1:A:357:C:C2	2.85	0.45
1:A:1356:U:OP2	1:A:1358:C:O2	2.33	0.45
15:O:155:GLU:HG2	16:P:235:ILE:HD11	1.98	0.45
1:A:2607:G:C2	1:A:2608:C:C2	3.04	0.45
1:A:416:U:H2'	1:A:417:U:C6	2.52	0.45
1:A:1702:C:H2'	1:A:1703:U:O4'	2.15	0.45
16:P:121:TYR:O	16:P:125:ILE:HG12	2.16	0.45
1:A:1925:U:H2'	1:A:1926:A:C8	2.51	0.45
13:M:76:VAL:HG21	13:M:94:ILE:HD11	1.97	0.45
1:A:910:G:H2'	1:A:910:G:N3	2.32	0.45
1:A:114:U:H3	1:A:118:A:N6	2.13	0.45
1:A:275:A:C2	1:A:367:A:N3	2.84	0.45
1:A:3160:U:OP1	12:L:52:THR:HG21	2.15	0.45
6:F:26:ILE:HD11	6:F:84:ILE:HG12	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2373:U:O2'	1:A:2374:A:P	2.73	0.45
1:A:1116:A:H2'	1:A:1117:G:H5'	1.98	0.45
1:A:1245:U:H2'	1:A:1246:A:C8	2.52	0.45
1:A:2631:G:H2'	1:A:2632:A:O4'	2.16	0.45
36:9:159:ALA:HB1	36:9:196:LEU:HD23	1.97	0.45
19:S:137:THR:OG1	19:S:159:LEU:HD11	2.16	0.45
1:A:291:A:P	26:Z:58:HIS:HE2	2.39	0.45
36:9:36:PRO:O	36:9:43:ARG:NH2	2.49	0.45
2:B:240:CYS:CB	2:B:304:THR:HG22	2.46	0.45
1:A:2777:U:H2'	1:A:2778:C:O4'	2.16	0.45
1:A:1111:U:H3'	1:A:1112:A:H5''	1.98	0.45
1:A:3281:U:C2	1:A:3282:A:C8	3.04	0.45
1:A:2324:U:H4'	1:A:2325:A:OP1	2.17	0.45
1:A:2913:U:C4	1:A:2941:A:N1	2.85	0.45
1:A:1391:U:H2'	1:A:1392:A:H5'	1.98	0.45
1:A:1825:A:H3'	1:A:1826:U:H5''	1.99	0.45
1:A:2586:U:H1'	1:A:2587:U:C6	2.52	0.45
1:A:779:A:N1	1:A:847:U:H5	2.13	0.45
1:A:2730:G:C2	1:A:2731:C:C2	3.05	0.45
2:B:270:GLY:HA2	2:B:311:ILE:HG22	1.98	0.45
1:A:1678:C:O2'	1:A:1693:A:H1'	2.16	0.45
1:A:261:A:C8	1:A:307:G:O6	2.70	0.45
1:A:536:A:C2	1:A:557:A:C2	3.05	0.45
1:A:1364:C:O2'	1:A:1536:A:N3	2.42	0.45
1:A:3138:U:H2'	1:A:3139:A:H5''	1.98	0.45
34:7:91:THR:OG1	34:7:130:ILE:HB	2.17	0.45
1:A:1371:A:H3'	1:A:1372:A:C5'	2.47	0.45
19:S:32:ILE:HD12	19:S:32:ILE:N	2.32	0.45
35:8:181:THR:HG23	35:8:184:GLN:HB2	1.99	0.45
20:T:152:ILE:O	20:T:155:VAL:HG22	2.17	0.45
16:P:186:THR:CG2	16:P:187:PRO:HD3	2.47	0.45
1:A:603:U:OP2	2:B:149:ARG:NH1	2.50	0.45
1:A:685:G:H2'	1:A:686:U:O4'	2.17	0.45
19:S:104:GLY:HA2	19:S:115:SER:HA	1.99	0.45
1:A:58:A:OP1	15:O:264:ARG:NH2	2.49	0.45
1:A:482:G:C6	1:A:483:C:C4	3.05	0.45
12:L:132:MET:HB3	12:L:188:LEU:HD13	1.99	0.45
26:Z:92:LYS:HA	26:Z:92:LYS:HE2	1.99	0.45
1:A:3279:U:H2'	1:A:3280:C:H6	1.81	0.45
1:A:355:U:H2'	1:A:356:U:O4'	2.17	0.45
1:A:2811:G:H2'	1:A:2812:G:O4'	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1750:G:C2	1:A:1751:C:C2	3.05	0.44
2:B:194:ILE:HG22	2:B:195:ILE:N	2.32	0.44
1:A:2872:A:C6	1:A:2873:U:O4	2.70	0.44
1:A:2915:A:H2'	1:A:2916:U:C6	2.52	0.44
18:R:38:SER:O	18:R:39:MET:CB	2.65	0.44
1:A:840:C:H2'	1:A:841:G:H5''	1.99	0.44
5:E:68:ARG:NH2	22:V:57:VAL:HG21	2.32	0.44
2:B:240:CYS:HA	2:B:304:THR:HA	1.99	0.44
28:1:229:VAL:HG21	28:1:322:ILE:HD12	2.00	0.44
1:A:551:U:H2'	1:A:552:A:H8	1.81	0.44
1:A:2860:A:C6	1:A:2861:U:C4	3.05	0.44
1:A:307:G:O2'	1:A:308:U:C5'	2.65	0.44
1:A:2951:U:O2	9:I:80:ASN:OD1	2.36	0.44
4:D:60:VAL:HG21	4:D:65:VAL:HG21	1.99	0.44
34:7:90:ILE:HD13	34:7:129:ILE:HG23	1.99	0.44
32:5:268:TRP:HA	32:5:279:VAL:CG2	2.47	0.44
1:A:2584:A:C2	1:A:2585:A:H1'	2.52	0.44
1:A:1743:G:C6	1:A:1744:C:C4	3.05	0.44
1:A:918:U:H2'	1:A:919:A:O4'	2.18	0.44
22:V:43:HIS:HA	33:6:60:MET:SD	2.58	0.44
2:B:125:VAL:HG23	2:B:154:LEU:HD11	1.99	0.44
21:U:13:ILE:HG23	21:U:13:ILE:O	2.17	0.44
8:H:125:ARG:HG2	8:H:125:ARG:HH11	1.82	0.44
2:B:158:ASN:O	2:B:210:ARG:NH1	2.50	0.44
1:A:1430:U:H2'	1:A:1431:U:O4'	2.18	0.44
31:4:63:VAL:HB	35:8:226:VAL:HG22	1.99	0.44
5:E:30:HIS:HB2	28:1:165:ILE:HD12	2.00	0.44
19:S:110:LEU:HD23	19:S:158:VAL:HG22	1.99	0.44
1:A:276:U:H1'	1:A:277:U:OP1	2.17	0.44
1:A:727:G:C5	1:A:728:C:C4	3.06	0.44
1:A:461:U:C6	1:A:461:U:C5'	3.01	0.44
1:A:3268:A:H2'	1:A:3269:U:C6	2.53	0.44
20:T:73:SER:OG	20:T:74:ASN:N	2.50	0.44
1:A:2601:A:O2'	1:A:2602:A:H8	1.99	0.44
28:1:121:PHE:CE1	29:2:67:ILE:HD11	2.53	0.44
1:A:640:C:O2	1:A:1570:A:H2'	2.17	0.44
6:F:67:VAL:HG22	6:F:110:HIS:CE1	2.52	0.44
1:A:2696:A:H2'	1:A:2696:A:N3	2.33	0.44
17:Q:27:LEU:N	17:Q:28:PRO:CD	2.77	0.44
1:A:583:G:O2'	4:D:115:ARG:HD2	2.18	0.44
8:H:139:ASN:CB	32:5:329:ARG:O	2.66	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:6:168:LEU:HD23	33:6:169:LEU:N	2.33	0.44
1:A:1848:C:C2	1:A:1859:G:C2	3.06	0.44
1:A:315:A:O2'	1:A:317:U:C1'	2.65	0.44
1:A:2373:U:HO2'	1:A:2374:A:P	2.37	0.44
1:A:1833:G:C2	1:A:1834:C:C2	3.06	0.44
1:A:208:A:H2'	1:A:209:U:C6	2.53	0.44
1:A:2787:C:C2	1:A:2812:G:N2	2.86	0.44
1:A:2905:A:O2'	3:C:44:HIS:O	2.35	0.44
2:B:253:HIS:O	2:B:255:VAL:HG23	2.18	0.44
1:A:74:A:O2'	4:D:238:PRO:O	2.36	0.44
1:A:2814:U:C5'	1:A:2833:A:C2	3.00	0.43
1:A:673:A:N3	2:B:338:MET:HG2	2.33	0.43
1:A:1366:A:O4'	1:A:1534:G:N2	2.51	0.43
32:5:324:VAL:HG21	32:5:339:HIS:CG	2.53	0.43
16:P:157:ILE:HD12	17:Q:5:TYR:HB3	1.99	0.43
1:A:136:A:H2'	1:A:137:A:C8	2.53	0.43
10:J:91:ARG:HD3	10:J:98:ALA:HA	1.99	0.43
1:A:2584:A:H3'	1:A:2585:A:H5''	1.99	0.43
1:A:1754:A:N1	1:A:1755:A:C6	2.86	0.43
1:A:2364:U:H2'	1:A:2365:A:C8	2.52	0.43
1:A:3193:A:H2'	1:A:3194:U:H4'	2.00	0.43
4:D:164:LYS:HG2	4:D:260:GLN:O	2.18	0.43
1:A:2336:G:C4	28:1:62:ILE:HD13	2.53	0.43
1:A:466:U:H2'	1:A:467:U:O4'	2.18	0.43
1:A:1210:A:O2'	31:4:90:ASN:ND2	2.51	0.43
6:F:26:ILE:HD11	6:F:84:ILE:HG23	1.99	0.43
1:A:1846:G:C2	1:A:1847:C:C2	3.07	0.43
28:1:113:PRO:HG3	29:2:71:THR:HG21	1.99	0.43
1:A:443:U:H4'	1:A:445:U:OP1	2.19	0.43
1:A:1631:G:N2	1:A:1671:A:O2'	2.51	0.43
1:A:1279:A:H2'	1:A:1280:A:O4'	2.18	0.43
1:A:915:G:OP2	21:U:11:SER:OG	2.31	0.43
34:7:89:ILE:O	34:7:131:LYS:O	2.36	0.43
1:A:1693:A:N6	1:A:2873:U:O4'	2.50	0.43
1:A:2722:G:C2	1:A:2762:C:C2	3.05	0.43
1:A:1763:A:H2'	1:A:1990:A:H1'	2.00	0.43
1:A:1717:A:H2'	1:A:1718:A:C8	2.52	0.43
1:A:827:U:C2	1:A:828:A:C8	3.06	0.43
7:G:44:LEU:CD2	7:G:49:LEU:HD13	2.48	0.43
1:A:1698:C:H5	1:A:1736:G:H21	1.65	0.43
1:A:95:A:H2'	1:A:96:C:C6	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:146:ARG:CZ	34:7:73:THR:HG23	2.48	0.43
1:A:1769:U:C2'	1:A:1770:U:OP1	2.66	0.43
2:B:344:PRO:HB3	2:B:356:LYS:HD3	2.01	0.43
1:A:866:G:H5'	1:A:867:A:OP2	2.18	0.43
4:D:165:LEU:HD12	4:D:262:VAL:HG23	2.00	0.43
1:A:1113:A:N3	1:A:1113:A:O5'	2.52	0.43
35:8:247:GLN:O	35:8:251:ASP:HB2	2.18	0.43
35:8:166:LYS:N	35:8:166:LYS:HD2	2.33	0.43
36:9:80:ILE:HG22	36:9:82:LEU:CD1	2.49	0.43
4:D:152:PHE:HZ	4:D:251:VAL:HG13	1.84	0.43
1:A:1786:A:H2'	1:A:1787:A:C8	2.53	0.43
1:A:3231:A:OP1	12:L:56:ARG:NH2	2.52	0.43
25:Y:95:ARG:CZ	25:Y:100:ARG:HD3	2.48	0.43
1:A:1949:G:C6	1:A:1950:C:C4	3.07	0.43
1:A:2607:G:H2'	1:A:2608:C:O4'	2.19	0.43
12:L:237:ARG:NH1	13:M:30:PRO:O	2.52	0.43
5:E:64:THR:HA	33:6:52:GLN:HB3	2.00	0.43
6:F:111:ILE:O	6:F:115:THR:HG22	2.19	0.43
1:A:3159:G:N1	1:A:3248:C:C4	2.87	0.43
4:D:229:ARG:O	4:D:233:ILE:HG23	2.18	0.43
1:A:1750:G:H2'	1:A:1751:C:O4'	2.19	0.43
1:A:3118:U:C4	1:A:3119:A:N7	2.87	0.43
1:A:3058:G:C6	1:A:3059:C:C4	3.06	0.43
28:1:247:TYR:CZ	28:1:249:LEU:HD21	2.53	0.43
1:A:577:U:C4	1:A:579:A:C8	3.06	0.43
1:A:676:A:H4'	1:A:1686:U:H4'	2.00	0.43
1:A:1104:A:O2'	8:H:108:ALA:O	2.37	0.43
32:5:268:TRP:HA	32:5:279:VAL:HG21	2.01	0.43
1:A:1113:A:O2'	1:A:1114:U:OP1	2.29	0.43
1:A:3058:G:H2'	1:A:3059:C:O4'	2.18	0.43
1:A:2440:G:H2'	1:A:2441:U:O4'	2.19	0.43
3:C:73:ASP:O	3:C:77:GLY:N	2.52	0.43
1:A:2292:C:H1'	1:A:2298:U:O4	2.19	0.43
28:1:128:VAL:HG23	28:1:131:ILE:HB	2.00	0.43
17:Q:80:ILE:HD11	35:8:84:LEU:CD1	2.49	0.43
2:B:94:LYS:HB2	2:B:110:ILE:HD11	2.00	0.43
1:A:486:G:H4'	1:A:487:U:O5'	2.18	0.43
1:A:1848:C:C2	1:A:1859:G:N2	2.87	0.43
2:B:246:ILE:HG22	2:B:250:THR:HG21	2.01	0.43
1:A:1374:U:C6	1:A:1374:U:OP1	2.72	0.43
1:A:2651:G:H5'	5:E:19:PRO:CG	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2586:U:H4'	1:A:2587:U:OP1	2.19	0.42
1:A:536:A:C2	1:A:557:A:H2	2.37	0.42
5:E:245:PHE:HD1	5:E:245:PHE:N	2.15	0.42
1:A:657:U:H2'	1:A:658:U:O4'	2.19	0.42
1:A:1743:G:C2	1:A:1744:C:C2	3.08	0.42
1:A:294:G:H4'	1:A:328:A:C5	2.54	0.42
1:A:142:A:H2'	1:A:143:A:O4'	2.18	0.42
1:A:1490:A:C2	1:A:1523:A:H2	2.37	0.42
12:L:35:SER:HG	12:L:40:CYS:HG	1.64	0.42
18:R:143:GLU:HB3	28:1:361:VAL:HG11	2.01	0.42
1:A:121:A:H3'	1:A:122:A:H5''	2.02	0.42
1:A:2674:U:H2'	1:A:2675:U:C6	2.53	0.42
1:A:1314:U:O2	1:A:1316:U:H2'	2.18	0.42
1:A:1516:U:C2	1:A:3022:G:N2	2.87	0.42
21:U:11:SER:CB	21:U:13:ILE:HG22	2.49	0.42
2:B:257:ILE:CD1	2:B:265:PHE:CE2	3.03	0.42
15:O:165:ALA:HB3	15:O:265:CYS:SG	2.60	0.42
28:1:211:ILE:N	28:1:211:ILE:HD12	2.34	0.42
15:O:107:LEU:HD21	15:O:161:PRO:HB3	2.01	0.42
1:A:1680:A:H2'	1:A:1681:C:O4'	2.19	0.42
17:Q:65:PRO:HA	17:Q:83:ILE:HG13	2.00	0.42
4:D:50:PRO:HG2	4:D:183:ASP:CB	2.50	0.42
1:A:3147:U:OP2	3:C:117:LYS:HE3	2.18	0.42
9:I:11:ILE:HD11	9:I:74:VAL:HG21	2.01	0.42
1:A:951:A:O2'	1:A:952:A:O5'	2.32	0.42
1:A:2858:C:OP1	2:B:351:LYS:HD3	2.19	0.42
2:B:197:CYS:SG	2:B:198:ASP:N	2.92	0.42
1:A:720:A:N3	1:A:720:A:H2'	2.34	0.42
1:A:268:C:OP1	10:J:216:THR:HG21	2.19	0.42
1:A:1605:U:O4	12:L:8:LYS:HB3	2.19	0.42
2:B:294:HIS:HB2	2:B:383:LYS:HB2	2.02	0.42
21:U:4:TYR:O	21:U:36:TYR:HA	2.19	0.42
1:A:1946:U:H2'	1:A:1947:C:C6	2.54	0.42
1:A:1589:A:C5	1:A:1590:U:C5	3.07	0.42
1:A:1869:A:O2'	1:A:1872:G:N3	2.45	0.42
1:A:230:A:N3	1:A:230:A:O4'	2.51	0.42
6:F:161:LYS:HG2	6:F:169:ILE:HG23	2.01	0.42
19:S:105:LEU:HD12	19:S:118:MET:CE	2.50	0.42
1:A:904:G:N2	1:A:912:C:C2	2.88	0.42
1:A:231:A:H2'	1:A:232:C:H6	1.83	0.42
1:A:1706:G:O2'	1:A:1707:C:OP2	2.29	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1826:U:H4'	1:A:1826:U:OP1	2.20	0.42
2:B:145:GLY:HA3	2:B:330:ARG:HG3	2.02	0.42
3:C:168:VAL:HB	3:C:231:ILE:HG23	2.01	0.42
1:A:2751:G:C6	1:A:2752:C:C4	3.08	0.42
13:M:46:LEU:O	13:M:49:ILE:HG13	2.19	0.42
1:A:2418:U:H2'	1:A:2419:U:O4'	2.19	0.42
1:A:587:G:C6	1:A:588:C:C4	3.07	0.42
1:A:1581:U:H2'	1:A:1582:A:H5'	2.01	0.42
1:A:2669:A:H4'	1:A:2670:C:H5''	2.01	0.42
1:A:720:A:C2'	1:A:720:A:N3	2.82	0.42
1:A:274:U:N3	1:A:367:A:N6	2.43	0.42
6:F:26:ILE:HD11	6:F:84:ILE:CG2	2.50	0.42
1:A:261:A:H4'	1:A:262:A:O5'	2.19	0.42
2:B:125:VAL:CG2	2:B:154:LEU:HD11	2.50	0.42
9:I:24:VAL:HG11	9:I:27:LYS:HD2	2.01	0.42
1:A:2707:G:C6	1:A:2708:C:C4	3.07	0.42
4:D:74:LEU:HG	4:D:257:LEU:HD11	2.00	0.42
1:A:3019:U:O4	1:A:3033:A:C2	2.72	0.42
1:A:3127:U:OP1	3:C:120:ARG:HB2	2.20	0.42
1:A:1181:U:C4	1:A:1182:A:N7	2.88	0.42
17:Q:149:VAL:HG13	35:8:92:ILE:HD12	2.01	0.42
1:A:204:A:C2	1:A:205:A:C8	3.08	0.42
1:A:315:A:H2'	1:A:317:U:C6	2.55	0.42
1:A:3163:U:C4	1:A:3164:A:N7	2.87	0.42
1:A:1391:U:C2'	1:A:1392:A:H5'	2.50	0.42
5:E:220:TYR:CZ	5:E:222:GLY:HA2	2.54	0.42
1:A:536:A:H2	1:A:557:A:C2	2.37	0.42
1:A:551:U:H2'	1:A:552:A:C8	2.55	0.42
1:A:3015:U:C4	1:A:3016:A:N6	2.88	0.42
1:A:1127:A:OP2	1:A:1169:A:O3'	2.37	0.42
4:D:75:TRP:CZ3	10:J:66:PRO:HB3	2.55	0.42
29:2:126:PRO:O	29:2:127:MET:CB	2.67	0.42
1:A:2434:A:N3	5:E:188:GLY:HA2	2.35	0.42
1:A:1360:G:H2'	1:A:1361:C:C5'	2.49	0.42
1:A:3162:U:C2	1:A:3243:A:N1	2.88	0.42
1:A:2359:U:C2'	1:A:2360:U:O5'	2.68	0.42
31:4:52:TRP:HH2	31:4:99:LYS:HA	1.85	0.42
29:2:140:LEU:O	29:2:141:TRP:HB2	2.19	0.42
1:A:2802:G:C2	1:A:2803:C:C2	3.08	0.42
18:R:128:ARG:O	18:R:130:GLY:N	2.52	0.42
33:6:83:GLN:OE1	33:6:115:LYS:N	2.48	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:217:GLY:HA3	8:H:83:ARG:NH1	2.35	0.42
11:K:115:THR:HA	11:K:140:VAL:HB	2.01	0.42
28:1:321:ASP:HB2	28:1:324:GLN:HB3	2.01	0.42
12:L:27:LEU:HD21	12:L:125:GLU:HA	2.01	0.42
6:F:119:LEU:HA	6:F:170:ILE:O	2.20	0.41
20:T:95:ILE:HB	20:T:96:PRO:HD3	2.02	0.41
1:A:1697:C:H2'	1:A:1698:C:C6	2.55	0.41
4:D:49:PHE:HB2	4:D:168:ILE:HG12	2.01	0.41
28:1:334:ILE:HG13	28:1:335:GLY:N	2.35	0.41
1:A:1769:U:H3'	1:A:1770:U:H5''	2.01	0.41
1:A:578:G:N2	1:A:579:A:C2	2.88	0.41
10:J:144:LYS:O	10:J:145:ASN:HB2	2.19	0.41
31:4:31:CYS:SG	31:4:67:SER:HA	2.60	0.41
15:O:189:VAL:HG11	15:O:267:LEU:HD13	2.01	0.41
11:K:216:LEU:HD22	11:K:216:LEU:HA	1.93	0.41
1:A:308:U:H2'	1:A:309:C:O5'	2.20	0.41
1:A:22:U:C4	1:A:23:U:C5	3.08	0.41
1:A:162:U:C2	30:3:76:LYS:HE2	2.56	0.41
2:B:198:ASP:HA	2:B:309:SER:HA	2.01	0.41
1:A:1663:A:H3'	13:M:150:TYR:CD1	2.55	0.41
1:A:1530:U:H3	1:A:1533:G:H1	1.68	0.41
1:A:1594:G:H2'	1:A:1595:G:O4'	2.20	0.41
1:A:84:A:H2'	1:A:85:A:C8	2.55	0.41
30:3:119:LEU:HA	30:3:122:ILE:HD12	2.02	0.41
36:9:118:GLN:O	36:9:121:ILE:CG2	2.69	0.41
1:A:2787:C:C2	1:A:2812:G:C2	3.07	0.41
1:A:434:U:O3'	15:O:300:ARG:HB2	2.20	0.41
1:A:620:G:C5	2:B:320:LYS:HB2	2.56	0.41
1:A:1521:U:H2'	1:A:1522:A:C8	2.56	0.41
1:A:350:A:H2'	1:A:351:C:C6	2.55	0.41
1:A:1344:U:C5	1:A:1555:A:H2	2.36	0.41
1:A:1735:U:OP2	2:B:334:ARG:NE	2.51	0.41
1:A:1564:C:C2	1:A:1572:G:N2	2.88	0.41
21:U:26:LEU:HD21	21:U:47:LEU:CD2	2.51	0.41
1:A:119:A:N6	20:T:153:ARG:HH11	2.19	0.41
2:B:257:ILE:HD11	2:B:265:PHE:CZ	2.54	0.41
10:J:225:ASN:O	10:J:225:ASN:CG	2.58	0.41
1:A:1846:G:C6	1:A:1847:C:N3	2.88	0.41
1:A:1112:A:OP1	1:A:1112:A:O4'	2.38	0.41
18:R:261:ASN:HD21	18:R:265:GLU:HB2	1.85	0.41
16:P:100:HIS:CE1	16:P:106:LYS:HD2	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2828:A:H2'	1:A:2829:U:O4'	2.20	0.41
17:Q:76:SER:O	17:Q:79:ASN:HB2	2.20	0.41
19:S:122:VAL:O	19:S:125:THR:OG1	2.28	0.41
16:P:148:GLN:OE1	16:P:148:GLN:N	2.54	0.41
17:Q:131:LEU:O	17:Q:131:LEU:HD12	2.20	0.41
20:T:127:LEU:O	20:T:131:VAL:HG13	2.19	0.41
1:A:1493:U:O2'	1:A:1494:A:P	2.78	0.41
17:Q:213:VAL:CG2	30:3:122:ILE:HD13	2.51	0.41
1:A:955:A:H2'	1:A:956:A:C8	2.55	0.41
1:A:1808:G:C2	1:A:1809:C:C2	3.09	0.41
17:Q:252:PRO:HG2	19:S:159:LEU:HB3	2.03	0.41
1:A:1768:A:H2'	1:A:1769:U:C6	2.55	0.41
12:L:174:ALA:O	12:L:175:LYS:C	2.59	0.41
1:A:1249:U:H2'	1:A:1250:U:C6	2.56	0.41
1:A:3152:A:OP1	1:A:3152:A:H4'	2.20	0.41
1:A:874:U:H2'	1:A:875:U:C6	2.55	0.41
5:E:217:ILE:HG23	5:E:220:TYR:CB	2.46	0.41
2:B:278:LYS:C	2:B:279:LEU:HD12	2.40	0.41
1:A:425:A:H5''	8:H:117:LYS:HG3	2.02	0.41
8:H:63:GLN:HA	8:H:101:PHE:CD1	2.55	0.41
1:A:1265:A:H2'	1:A:1266:U:C6	2.56	0.41
4:D:212:GLU:OE1	35:8:109:VAL:HG13	2.21	0.41
25:Y:103:LEU:O	25:Y:104:SER:CB	2.68	0.41
35:8:140:THR:HG21	35:8:159:PHE:HA	2.02	0.41
12:L:136:HIS:O	12:L:137:THR:CB	2.69	0.41
6:F:24:LEU:HD11	6:F:104:ARG:HG2	2.02	0.41
1:A:2358:A:C6	1:A:2359:U:C4	3.09	0.41
4:D:171:GLU:O	4:D:172:LYS:CB	2.69	0.41
30:3:74:TRP:C	30:3:76:LYS:N	2.74	0.41
1:A:2001:U:H2'	1:A:2002:U:O4'	2.21	0.41
1:A:228:U:H2'	1:A:229:G:O4'	2.21	0.41
2:B:155:ILE:HD11	2:B:157:PHE:CE1	2.55	0.41
1:A:564:A:O2'	1:A:565:A:C8	2.69	0.41
1:A:1959:A:N6	1:A:1960:A:C2	2.89	0.41
1:A:26:A:C6	36:9:41:LEU:HD12	2.55	0.41
2:B:378:ASN:O	2:B:381:LYS:HB2	2.21	0.41
29:2:68:LYS:O	29:2:71:THR:OG1	2.29	0.41
1:A:2441:U:H2'	1:A:2442:A:C8	2.55	0.41
15:O:107:LEU:HD13	15:O:221:LEU:HD13	2.03	0.41
18:R:160:LYS:O	18:R:163:GLU:HG3	2.21	0.41
1:A:449:A:H2'	1:A:450:U:C6	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:X:66:LEU:O	24:X:67:ARG:C	2.58	0.41
1:A:2772:U:O2'	1:A:2773:C:OP2	2.29	0.41
4:D:45:THR:HG23	4:D:45:THR:O	2.21	0.41
1:A:1609:U:H2'	1:A:1610:A:C8	2.56	0.41
1:A:1433:A:H2'	1:A:1434:A:C8	2.56	0.41
4:D:105:LEU:HD11	4:D:119:ALA:HB2	2.02	0.41
3:C:110:TYR:CD1	3:C:110:TYR:C	2.94	0.41
1:A:402:A:H2'	1:A:403:A:O4'	2.20	0.41
1:A:1963:C:H2'	1:A:1964:C:O4'	2.20	0.41
1:A:602:A:H1'	1:A:1367:A:H1'	2.03	0.41
31:4:28:LEU:HD13	31:4:72:LEU:HD21	2.02	0.41
1:A:3090:U:H2'	1:A:3092:U:OP1	2.21	0.41
1:A:214:A:H2'	1:A:215:A:C4'	2.51	0.41
17:Q:104:VAL:HG13	17:Q:105:PRO:HD2	2.02	0.41
1:A:2628:A:OP1	26:Z:74:ARG:NH1	2.54	0.41
32:5:70:LEU:O	32:5:70:LEU:HD23	2.21	0.41
17:Q:170:PRO:O	17:Q:184:TRP:NE1	2.52	0.41
1:A:274:U:C2'	1:A:274:U:O2	2.68	0.40
1:A:2796:G:O2'	1:A:2797:U:P	2.80	0.40
36:9:80:ILE:HG22	36:9:82:LEU:HD12	2.02	0.40
1:A:1808:G:N2	1:A:1809:C:C2	2.89	0.40
5:E:180:VAL:O	5:E:183:TRP:O	2.39	0.40
13:M:151:ILE:O	13:M:154:THR:HG22	2.20	0.40
1:A:337:A:N6	1:A:338:G:C2	2.89	0.40
1:A:3020:U:C2'	1:A:3021:A:O5'	2.69	0.40
28:1:140:ARG:HG3	28:1:214:TYR:HD1	1.86	0.40
17:Q:100:PRO:HB2	17:Q:124:VAL:HG23	2.01	0.40
8:H:15:LEU:O	8:H:55:ASP:HB3	2.22	0.40
1:A:2779:A:H2'	1:A:2780:A:C8	2.56	0.40
1:A:1849:U:H2'	1:A:1850:A:O4'	2.20	0.40
1:A:1361:C:H2'	1:A:1362:C:C5	2.56	0.40
1:A:2941:A:H2'	1:A:2942:A:H8	1.75	0.40
1:A:164:U:H3	16:P:82:ASN:C	2.25	0.40
32:5:163:LEU:CD1	32:5:283:ILE:HD11	2.51	0.40
1:A:1833:G:C4	1:A:1834:C:C6	3.09	0.40
1:A:1404:A:C2'	1:A:1405:U:OP1	2.69	0.40
1:A:248:A:H2'	1:A:249:C:C6	2.56	0.40
4:D:152:PHE:CZ	4:D:251:VAL:HG13	2.56	0.40
1:A:1972:G:C2	1:A:1973:C:C2	3.09	0.40
28:1:174:PRO:O	28:1:176:ALA:N	2.54	0.40
1:A:1707:C:H4'	1:A:1708:A:H3'	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:257:LEU:HD22	10:J:60:ILE:CG2	2.51	0.40
1:A:1609:U:H2'	1:A:1610:A:H8	1.86	0.40
1:A:638:U:O2'	15:O:248:LYS:HE3	2.21	0.40
30:3:102:LYS:O	30:3:142:TYR:HB2	2.21	0.40
3:C:72:PHE:CE1	3:C:79:ARG:HG3	2.56	0.40
1:A:3233:A:C8	1:A:3233:A:O5'	2.73	0.40
1:A:2379:U:O2'	1:A:2380:U:O5'	2.33	0.40
32:5:338:VAL:HG21	32:5:359:LYS:HA	2.03	0.40
1:A:1747:C:C4	1:A:1748:A:N7	2.90	0.40
1:A:3252:U:O2'	1:A:3253:U:OP2	2.24	0.40
18:R:135:THR:O	18:R:136:ASN:C	2.58	0.40
1:A:326:A:N3	1:A:326:A:H3'	2.37	0.40
1:A:1829:U:O4'	1:A:1829:U:O2	2.36	0.40
1:A:859:U:O2	1:A:859:U:O4'	2.37	0.40
1:A:1361:C:C2'	1:A:1362:C:C6	3.04	0.40
20:T:95:ILE:HG23	20:T:155:VAL:HG12	2.03	0.40
33:6:27:VAL:CG1	33:6:195:ALA:HB2	2.51	0.40
5:E:30:HIS:CD2	28:1:166:PRO:HB3	2.56	0.40
1:A:3058:G:C2	1:A:3059:C:C2	3.09	0.40
1:A:142:A:O3'	20:T:157:ASN:ND2	2.54	0.40
9:I:138:ILE:HG22	13:M:121:ILE:HD11	2.02	0.40
1:A:1388:A:N6	1:A:1715:A:C2	2.89	0.40
31:4:26:ILE:HD13	31:4:98:LEU:CD2	2.51	0.40
1:A:3069:A:H4'	1:A:3070:A:O5'	2.22	0.40
1:A:2952:G:H4'	9:I:79:ARG:HG3	2.04	0.40
35:8:189:ILE:HG22	35:8:194:LEU:CD2	2.50	0.40
2:B:159:ARG:NE	2:B:194:ILE:HD12	2.37	0.40
2:B:381:LYS:O	2:B:382:VAL:C	2.60	0.40
1:A:1308:A:OP2	1:A:1597:G:O2'	2.34	0.40
33:6:257:LEU:HD21	33:6:265:TYR:CD2	2.57	0.40
36:9:70:ARG:HG2	36:9:75:LEU:HD12	2.03	0.40
28:1:291:VAL:CG1	28:1:337:HIS:HB3	2.52	0.40
1:A:599:A:H2'	1:A:600:C:O4'	2.21	0.40
1:A:2961:A:H2'	1:A:2962:U:O4'	2.21	0.40
18:R:262:ASN:ND2	18:R:314:LEU:HA	2.37	0.40
31:4:65:ARG:HD2	31:4:65:ARG:C	2.42	0.40
32:5:310:LEU:HD11	32:5:370:TRP:CG	2.56	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	
2	B	291/393 (74%)	272 (94%)	16 (6%)	3 (1%)	19	65
3	C	247/269 (92%)	226 (92%)	15 (6%)	6 (2%)	7	43
4	D	235/286 (82%)	211 (90%)	15 (6%)	9 (4%)	4	28
5	E	272/292 (93%)	246 (90%)	22 (8%)	4 (2%)	13	55
6	F	173/214 (81%)	163 (94%)	7 (4%)	3 (2%)	11	52
7	G	53/139 (38%)	50 (94%)	3 (6%)	0	100	100
8	H	146/163 (90%)	138 (94%)	8 (6%)	0	100	100
9	I	121/138 (88%)	110 (91%)	10 (8%)	1 (1%)	24	69
10	J	218/322 (68%)	202 (93%)	14 (6%)	2 (1%)	21	67
11	K	193/232 (83%)	182 (94%)	7 (4%)	4 (2%)	9	46
12	L	225/238 (94%)	208 (92%)	14 (6%)	3 (1%)	15	59
13	M	149/169 (88%)	138 (93%)	9 (6%)	2 (1%)	15	59
14	N	116/161 (72%)	109 (94%)	6 (5%)	1 (1%)	21	67
15	O	219/309 (71%)	199 (91%)	18 (8%)	2 (1%)	21	67
16	P	205/263 (78%)	189 (92%)	14 (7%)	2 (1%)	19	65
17	Q	269/297 (91%)	243 (90%)	22 (8%)	4 (2%)	13	55
18	R	310/371 (84%)	288 (93%)	17 (6%)	5 (2%)	12	54
19	S	142/258 (55%)	136 (96%)	6 (4%)	0	100	100
20	T	203/319 (64%)	184 (91%)	13 (6%)	6 (3%)	5	35
21	U	80/86 (93%)	77 (96%)	3 (4%)	0	100	100
22	V	62/177 (35%)	57 (92%)	5 (8%)	0	100	100
23	W	110/183 (60%)	100 (91%)	6 (6%)	4 (4%)	4	30
24	X	62/70 (89%)	55 (89%)	6 (10%)	1 (2%)	12	54
25	Y	43/105 (41%)	41 (95%)	1 (2%)	1 (2%)	8	44
26	Z	60/115 (52%)	57 (95%)	3 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
27	0	36/93 (39%)	34 (94%)	2 (6%)	0	100	100
28	1	324/367 (88%)	293 (90%)	26 (8%)	5 (2%)	13	55
29	2	111/147 (76%)	103 (93%)	5 (4%)	3 (3%)	6	39
30	3	120/146 (82%)	103 (86%)	16 (13%)	1 (1%)	24	69
31	4	136/140 (97%)	128 (94%)	8 (6%)	0	100	100
32	5	324/390 (83%)	299 (92%)	23 (7%)	2 (1%)	30	75
33	6	195/281 (69%)	179 (92%)	12 (6%)	4 (2%)	9	46
34	7	104/146 (71%)	99 (95%)	5 (5%)	0	100	100
35	8	178/264 (67%)	168 (94%)	10 (6%)	0	100	100
36	9	185/253 (73%)	163 (88%)	14 (8%)	8 (4%)	3	25
37	a	174/195 (89%)	161 (92%)	7 (4%)	6 (3%)	5	31
38	b	153/157 (98%)	139 (91%)	12 (8%)	2 (1%)	15	59
39	c	116/131 (88%)	108 (93%)	5 (4%)	3 (3%)	7	40
40	d	200/226 (88%)	179 (90%)	16 (8%)	5 (2%)	7	41
All	All	6560/8505 (77%)	6037 (92%)	421 (6%)	102 (2%)	17	54

All (102) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	382	VAL
3	C	211	PRO
4	D	49	PHE
4	D	50	PRO
4	D	135	ALA
4	D	248	LYS
6	F	70	PRO
6	F	71	ASP
10	J	165	LEU
11	K	154	ASP
13	M	62	ILE
13	M	145	ARG
14	N	108	PRO
20	T	31	LYS
23	W	100	HIS
28	1	55	ILE
29	2	141	TRP
36	9	77	LYS

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Mol	Chain	Res	Type
38	b	83	GLU
38	b	151	ASN
3	C	193	HIS
3	C	208	ASN
4	D	172	LYS
4	D	278	LYS
6	F	29	GLU
10	J	145	ASN
11	K	59	ARG
12	L	127	VAL
12	L	137	THR
15	O	185	GLY
15	O	239	GLY
16	P	177	ASP
17	Q	96	ASP
18	R	129	PHE
18	R	262	ASN
20	T	20	THR
20	T	29	LEU
20	T	46	ASN
24	X	67	ARG
28	1	110	ILE
28	1	125	LEU
28	1	175	ARG
29	2	127	MET
36	9	33	HIS
36	9	104	ASN
36	9	167	ASN
37	a	79	SER
40	d	67	ARG
40	d	172	GLY
40	d	196	VAL
4	D	201	PHE
5	E	37	LYS
9	I	80	ASN
12	L	136	HIS
16	P	147	LEU
18	R	184	LEU
18	R	306	LYS
20	T	73	SER
25	Y	104	SER
29	2	118	ALA

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Mol	Chain	Res	Type
32	5	219	MET
33	6	153	ASN
33	6	180	PRO
36	9	59	GLU
37	a	88	PRO
37	a	109	GLY
2	B	355	ASN
4	D	51	SER
5	E	21	SER
5	E	88	HIS
11	K	64	ILE
17	Q	211	ASP
17	Q	235	ARG
23	W	136	GLU
39	c	124	ILE
40	d	33	GLU
40	d	68	ARG
4	D	170	GLY
17	Q	273	PRO
18	R	39	MET
20	T	25	LYS
23	W	107	CYS
23	W	137	ILE
30	3	144	GLU
36	9	36	PRO
36	9	74	GLN
39	c	117	PRO
2	B	386	PRO
3	C	197	ILE
3	C	210	ASP
5	E	35	ILE
32	5	381	PRO
33	6	154	ASP
37	a	116	PRO
28	1	98	PRO
3	C	111	GLY
11	K	224	PRO
33	6	146	ILE
37	a	28	VAL
37	a	87	MET
36	9	208	GLY
39	c	58	GLY

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	B	233/337 (69%)	210 (90%)	23 (10%)	10	38
3	C	209/229 (91%)	190 (91%)	19 (9%)	12	42
4	D	200/248 (81%)	173 (86%)	27 (14%)	5	22
5	E	225/260 (86%)	201 (89%)	24 (11%)	8	34
6	F	141/190 (74%)	120 (85%)	21 (15%)	4	17
7	G	50/129 (39%)	47 (94%)	3 (6%)	24	65
8	H	126/141 (89%)	117 (93%)	9 (7%)	18	57
9	I	106/117 (91%)	101 (95%)	5 (5%)	32	73
10	J	175/274 (64%)	147 (84%)	28 (16%)	3	14
11	K	167/200 (84%)	138 (83%)	29 (17%)	2	12
12	L	202/212 (95%)	188 (93%)	14 (7%)	19	59
13	M	136/153 (89%)	124 (91%)	12 (9%)	12	45
14	N	107/147 (73%)	98 (92%)	9 (8%)	14	48
15	O	191/270 (71%)	169 (88%)	22 (12%)	7	30
16	P	183/236 (78%)	155 (85%)	28 (15%)	3	17
17	Q	219/268 (82%)	198 (90%)	21 (10%)	10	39
18	R	250/337 (74%)	218 (87%)	32 (13%)	5	25
19	S	126/231 (54%)	116 (92%)	10 (8%)	15	53
20	T	171/298 (57%)	156 (91%)	15 (9%)	12	45
21	U	73/77 (95%)	71 (97%)	2 (3%)	52	85
22	V	59/161 (37%)	58 (98%)	1 (2%)	68	90
23	W	104/167 (62%)	90 (86%)	14 (14%)	5	22
24	X	56/62 (90%)	52 (93%)	4 (7%)	18	57
25	Y	39/93 (42%)	37 (95%)	2 (5%)	29	70
26	Z	50/100 (50%)	45 (90%)	5 (10%)	9	37
27	0	36/84 (43%)	36 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
28	1	299/341 (88%)	269 (90%)	30 (10%)	9	37
29	2	99/137 (72%)	90 (91%)	9 (9%)	12	42
30	3	102/126 (81%)	97 (95%)	5 (5%)	31	72
31	4	121/123 (98%)	107 (88%)	14 (12%)	7	30
32	5	263/345 (76%)	234 (89%)	29 (11%)	8	33
33	6	153/252 (61%)	134 (88%)	19 (12%)	6	27
34	7	94/128 (73%)	81 (86%)	13 (14%)	4	21
35	8	149/240 (62%)	134 (90%)	15 (10%)	9	36
36	9	140/221 (63%)	127 (91%)	13 (9%)	11	41
37	a	156/171 (91%)	136 (87%)	20 (13%)	5	25
38	b	144/146 (99%)	122 (85%)	22 (15%)	3	17
39	c	110/120 (92%)	105 (96%)	5 (4%)	34	74
40	d	185/210 (88%)	162 (88%)	23 (12%)	6	27
All	All	5649/7581 (74%)	5053 (89%)	596 (11%)	13	34

All (596) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	94	LYS
2	B	95	ARG
2	B	107	ARG
2	B	127	ARG
2	B	128	LYS
2	B	140	THR
2	B	153	ARG
2	B	159	ARG
2	B	169	ARG
2	B	195	ILE
2	B	204	ASP
2	B	205	VAL
2	B	210	ARG
2	B	237	ARG
2	B	241	LEU
2	B	246	ILE
2	B	316	ARG
2	B	339	ASN
2	B	351	LYS

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Mol	Chain	Res	Type
2	B	364	GLN
2	B	375	LYS
2	B	376	ASN
2	B	382	VAL
3	C	53	LYS
3	C	61	LEU
3	C	79	ARG
3	C	86	GLU
3	C	89	ASN
3	C	94	MET
3	C	95	HIS
3	C	106	CYS
3	C	122	MET
3	C	134	LYS
3	C	146	LYS
3	C	153	THR
3	C	156	LYS
3	C	164	GLN
3	C	175	LYS
3	C	218	ARG
3	C	231	ILE
3	C	239	VAL
3	C	240	ASP
4	D	56	THR
4	D	86	ARG
4	D	106	MET
4	D	109	LYS
4	D	115	ARG
4	D	142	GLU
4	D	143	LEU
4	D	152	PHE
4	D	164	LYS
4	D	182	LEU
4	D	184	LEU
4	D	186	ARG
4	D	204	GLU
4	D	210	PHE
4	D	216	LEU
4	D	219	LYS
4	D	220	ARG
4	D	221	LEU
4	D	222	LEU

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Mol	Chain	Res	Type
4	D	233	ILE
4	D	247	GLN
4	D	252	GLU
4	D	254	ASN
4	D	274	MET
4	D	277	GLN
4	D	278	LYS
4	D	279	GLU
5	E	39	LYS
5	E	51	LYS
5	E	68	ARG
5	E	94	LYS
5	E	96	LEU
5	E	105	SER
5	E	120	LYS
5	E	139	SER
5	E	147	ARG
5	E	154	LEU
5	E	162	GLN
5	E	163	LEU
5	E	164	GLN
5	E	170	LYS
5	E	189	HIS
5	E	198	LYS
5	E	201	GLU
5	E	202	MET
5	E	204	GLN
5	E	211	GLU
5	E	214	LEU
5	E	259	THR
5	E	278	THR
5	E	280	LEU
6	F	33	SER
6	F	34	ILE
6	F	57	THR
6	F	64	GLU
6	F	65	LEU
6	F	71	ASP
6	F	74	HIS
6	F	92	GLU
6	F	106	LEU
6	F	115	THR

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Mol	Chain	Res	Type
6	F	119	LEU
6	F	130	ARG
6	F	141	ASN
6	F	150	GLN
6	F	152	LEU
6	F	161	LYS
6	F	171	GLU
6	F	175	LYS
6	F	176	GLN
6	F	186	ARG
6	F	194	TYR
7	G	22	GLN
7	G	34	LYS
7	G	45	MET
8	H	19	VAL
8	H	39	LEU
8	H	60	THR
8	H	68	THR
8	H	75	LYS
8	H	83	ARG
8	H	123	LEU
8	H	125	ARG
8	H	133	GLU
9	I	4	LEU
9	I	17	GLN
9	I	48	LYS
9	I	115	ASP
9	I	129	LYS
10	J	72	LYS
10	J	76	ARG
10	J	79	ARG
10	J	89	SER
10	J	99	ARG
10	J	103	LYS
10	J	107	GLU
10	J	114	TYR
10	J	132	GLU
10	J	133	LEU
10	J	144	LYS
10	J	149	LEU
10	J	153	GLU
10	J	158	ASN

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Mol	Chain	Res	Type
10	J	161	ARG
10	J	165	LEU
10	J	182	PHE
10	J	185	ASN
10	J	190	LEU
10	J	225	ASN
10	J	233	ARG
10	J	238	LEU
10	J	241	ARG
10	J	244	LYS
10	J	246	ARG
10	J	263	GLU
10	J	266	LYS
10	J	269	GLN
11	K	39	HIS
11	K	44	ARG
11	K	59	ARG
11	K	69	LEU
11	K	71	PHE
11	K	76	LEU
11	K	86	SER
11	K	90	LEU
11	K	98	MET
11	K	99	ARG
11	K	102	ARG
11	K	108	HIS
11	K	109	LEU
11	K	110	TRP
11	K	113	LEU
11	K	114	CYS
11	K	127	ARG
11	K	128	MET
11	K	130	LYS
11	K	139	MET
11	K	155	ASP
11	K	156	LEU
11	K	181	LEU
11	K	184	LEU
11	K	191	SER
11	K	196	LYS
11	K	210	LYS
11	K	216	LEU

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Mol	Chain	Res	Type
11	K	225	GLN
12	L	15	HIS
12	L	26	GLN
12	L	27	LEU
12	L	62	ASN
12	L	68	GLU
12	L	69	LEU
12	L	76	GLN
12	L	93	GLU
12	L	112	GLU
12	L	163	ASN
12	L	165	LEU
12	L	188	LEU
12	L	194	LEU
12	L	207	ASN
13	M	24	LYS
13	M	34	ARG
13	M	39	GLN
13	M	49	ILE
13	M	50	GLU
13	M	65	LYS
13	M	108	LEU
13	M	110	LEU
13	M	125	LEU
13	M	145	ARG
13	M	155	ARG
13	M	166	ARG
14	N	50	LYS
14	N	117	LYS
14	N	123	LYS
14	N	126	ARG
14	N	131	ARG
14	N	142	ARG
14	N	145	LYS
14	N	149	ASP
14	N	154	ARG
15	O	93	LEU
15	O	110	GLN
15	O	122	GLU
15	O	133	LYS
15	O	135	ASP
15	O	145	GLU

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Mol	Chain	Res	Type
15	O	159	LEU
15	O	171	LYS
15	O	184	LEU
15	O	202	LYS
15	O	205	ARG
15	O	223	LEU
15	O	224	LYS
15	O	235	THR
15	O	250	ARG
15	O	261	ILE
15	O	264	ARG
15	O	272	VAL
15	O	276	ARG
15	O	285	GLU
15	O	308	LYS
15	O	309	TRP
16	P	60	GLU
16	P	65	TRP
16	P	71	GLU
16	P	72	GLN
16	P	83	LYS
16	P	88	LYS
16	P	93	LEU
16	P	106	LYS
16	P	113	PHE
16	P	117	ASP
16	P	119	ARG
16	P	128	LEU
16	P	134	THR
16	P	136	GLN
16	P	137	LEU
16	P	141	LYS
16	P	145	MET
16	P	151	ARG
16	P	157	ILE
16	P	161	THR
16	P	164	MET
16	P	182	TRP
16	P	190	MET
16	P	196	GLU
16	P	197	ARG
16	P	229	ARG

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Mol	Chain	Res	Type
16	P	233	ARG
16	P	257	ARG
17	Q	14	ARG
17	Q	38	THR
17	Q	55	PHE
17	Q	65	PRO
17	Q	68	ARG
17	Q	72	MET
17	Q	77	LYS
17	Q	79	ASN
17	Q	86	PHE
17	Q	88	LYS
17	Q	102	LYS
17	Q	124	VAL
17	Q	127	LEU
17	Q	133	LEU
17	Q	186	LYS
17	Q	196	LEU
17	Q	204	ARG
17	Q	206	GLN
17	Q	213	VAL
17	Q	254	THR
17	Q	257	ARG
18	R	40	LYS
18	R	46	ARG
18	R	59	THR
18	R	61	GLU
18	R	75	GLU
18	R	104	ARG
18	R	111	LEU
18	R	116	LYS
18	R	133	GLU
18	R	137	LYS
18	R	138	ARG
18	R	159	LEU
18	R	163	GLU
18	R	168	LYS
18	R	172	LEU
18	R	175	LYS
18	R	182	ASP
18	R	191	ILE
18	R	193	LEU

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Mol	Chain	Res	Type
18	R	198	LEU
18	R	202	ARG
18	R	205	LEU
18	R	213	ASP
18	R	239	LYS
18	R	263	LYS
18	R	266	LEU
18	R	304	LEU
18	R	305	PHE
18	R	314	LEU
18	R	322	ARG
18	R	362	ARG
18	R	367	PHE
19	S	23	GLN
19	S	25	ARG
19	S	51	GLU
19	S	52	ARG
19	S	58	TYR
19	S	65	ILE
19	S	73	LEU
19	S	92	THR
19	S	102	LYS
19	S	118	MET
20	T	16	ARG
20	T	17	THR
20	T	25	LYS
20	T	29	LEU
20	T	59	ASN
20	T	60	LEU
20	T	105	ASP
20	T	120	LEU
20	T	131	VAL
20	T	150	TRP
20	T	161	LEU
20	T	176	ARG
20	T	182	THR
20	T	187	TYR
20	T	210	PHE
21	U	8	LEU
21	U	43	ILE
22	V	27	ARG
23	W	82	LYS

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Mol	Chain	Res	Type
23	W	84	ARG
23	W	86	LYS
23	W	101	LEU
23	W	103	LYS
23	W	107	CYS
23	W	111	LYS
23	W	134	LYS
23	W	140	ARG
23	W	141	GLN
23	W	157	ARG
23	W	163	THR
23	W	169	LYS
23	W	178	ARG
24	X	29	LYS
24	X	33	LEU
24	X	37	VAL
24	X	45	ARG
25	Y	73	ARG
25	Y	80	LEU
26	Z	64	ARG
26	Z	74	ARG
26	Z	95	THR
26	Z	111	LEU
26	Z	112	LEU
28	1	58	ARG
28	1	70	ILE
28	1	73	ILE
28	1	84	ARG
28	1	102	ASP
28	1	120	GLN
28	1	123	ASN
28	1	128	VAL
28	1	138	VAL
28	1	142	LEU
28	1	144	LYS
28	1	154	LEU
28	1	156	MET
28	1	165	ILE
28	1	175	ARG
28	1	177	GLU
28	1	212	GLN
28	1	216	LEU

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Mol	Chain	Res	Type
28	1	230	ASN
28	1	232	ASP
28	1	239	ASP
28	1	262	ASP
28	1	264	ARG
28	1	308	LEU
28	1	314	GLU
28	1	327	LYS
28	1	344	ASP
28	1	346	LYS
28	1	360	ARG
28	1	366	ARG
29	2	58	LEU
29	2	59	LEU
29	2	60	LYS
29	2	65	ASP
29	2	80	GLN
29	2	102	MET
29	2	111	ARG
29	2	121	LYS
29	2	133	THR
30	3	22	LYS
30	3	43	LEU
30	3	47	GLN
30	3	73	ASN
30	3	113	LEU
31	4	13	ARG
31	4	38	GLU
31	4	42	LYS
31	4	47	LYS
31	4	50	ASP
31	4	54	GLN
31	4	59	ILE
31	4	65	ARG
31	4	91	ILE
31	4	98	LEU
31	4	102	LYS
31	4	121	LEU
31	4	132	LEU
31	4	136	LYS
32	5	99	ARG
32	5	101	LEU

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Mol	Chain	Res	Type
32	5	104	ARG
32	5	116	LEU
32	5	117	SER
32	5	143	THR
32	5	148	LYS
32	5	164	SER
32	5	177	ARG
32	5	187	VAL
32	5	236	LEU
32	5	237	ASN
32	5	240	ASP
32	5	244	LEU
32	5	251	SER
32	5	271	THR
32	5	281	ARG
32	5	283	ILE
32	5	296	LYS
32	5	297	MET
32	5	310	LEU
32	5	312	ARG
32	5	314	GLU
32	5	320	VAL
32	5	335	VAL
32	5	339	HIS
32	5	368	MET
32	5	369	LYS
32	5	390	VAL
33	6	31	LEU
33	6	33	ARG
33	6	52	GLN
33	6	56	GLU
33	6	70	LYS
33	6	80	LEU
33	6	97	ARG
33	6	103	LYS
33	6	104	HIS
33	6	106	ARG
33	6	111	LYS
33	6	113	GLU
33	6	115	LYS
33	6	169	LEU
33	6	177	TRP

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Mol	Chain	Res	Type
33	6	178	LYS
33	6	198	GLU
33	6	254	PHE
33	6	273	LYS
34	7	47	LEU
34	7	51	LYS
34	7	59	ASN
34	7	72	ARG
34	7	87	ASN
34	7	104	ARG
34	7	111	LEU
34	7	116	LYS
34	7	117	LYS
34	7	121	VAL
34	7	143	THR
34	7	145	LYS
34	7	146	PHE
35	8	97	ARG
35	8	118	LEU
35	8	132	MET
35	8	148	VAL
35	8	163	LEU
35	8	166	LYS
35	8	170	LEU
35	8	179	LEU
35	8	181	THR
35	8	183	LEU
35	8	191	GLU
35	8	202	LEU
35	8	233	LYS
35	8	260	THR
35	8	262	ARG
36	9	41	LEU
36	9	56	LEU
36	9	65	CYS
36	9	106	LYS
36	9	108	ASN
36	9	125	LYS
36	9	154	THR
36	9	160	CYS
36	9	163	VAL
36	9	176	MET

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Mol	Chain	Res	Type
36	9	184	HIS
36	9	211	LYS
36	9	217	GLN
37	a	20	GLN
37	a	28	VAL
37	a	30	THR
37	a	34	LYS
37	a	36	LYS
37	a	48	ARG
37	a	49	ASP
37	a	70	THR
37	a	101	LEU
37	a	114	LEU
37	a	119	ILE
37	a	132	LYS
37	a	150	SER
37	a	158	GLN
37	a	162	ILE
37	a	175	LYS
37	a	182	ARG
37	a	187	ARG
37	a	191	LEU
37	a	192	TRP
38	b	5	GLN
38	b	14	LEU
38	b	19	GLN
38	b	32	THR
38	b	35	LYS
38	b	52	ARG
38	b	57	LYS
38	b	63	MET
38	b	65	ASP
38	b	71	LEU
38	b	83	GLU
38	b	105	LEU
38	b	107	LYS
38	b	117	GLU
38	b	119	LEU
38	b	123	GLU
38	b	129	VAL
38	b	130	ASP
38	b	132	LEU

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Mol	Chain	Res	Type
38	b	136	LYS
38	b	137	LYS
38	b	146	GLU
39	c	45	LEU
39	c	57	LYS
39	c	70	LYS
39	c	78	LEU
39	c	101	THR
40	d	9	ARG
40	d	11	ARG
40	d	22	ILE
40	d	32	LEU
40	d	33	GLU
40	d	38	LEU
40	d	62	ARG
40	d	72	LYS
40	d	74	MET
40	d	83	LYS
40	d	94	ARG
40	d	96	ARG
40	d	101	VAL
40	d	110	LEU
40	d	137	LEU
40	d	142	LEU
40	d	173	ASP
40	d	177	HIS
40	d	191	LYS
40	d	194	GLN
40	d	203	GLU
40	d	207	LEU
40	d	210	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	378	ASN
3	C	207	GLN
16	P	256	ASN
19	S	84	ASN
22	V	81	ASN
35	8	235	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	2682/3296 (81%)	692 (25%)	132 (4%)
41	e	18/20 (90%)	6 (33%)	0
All	All	2700/3316 (81%)	698 (25%)	132 (4%)

All (698) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	22	U
1	A	26	A
1	A	27	A
1	A	28	U
1	A	29	A
1	A	30	U
1	A	31	U
1	A	32	U
1	A	35	U
1	A	38	A
1	A	41	G
1	A	43	U
1	A	45	U
1	A	48	A
1	A	49	G
1	A	68	A
1	A	69	U
1	A	70	A
1	A	85	A
1	A	93	U
1	A	94	A
1	A	106	A
1	A	112	G
1	A	115	A
1	A	116	C
1	A	117	U
1	A	118	A
1	A	119	A
1	A	120	U
1	A	122	A
1	A	134	U
1	A	135	U
1	A	139	U
1	A	149	A

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Mol	Chain	Res	Type
1	A	150	A
1	A	151	A
1	A	152	G
1	A	153	G
1	A	155	A
1	A	161	U
1	A	162	U
1	A	163	A
1	A	164	U
1	A	165	A
1	A	204	A
1	A	209	U
1	A	215	A
1	A	216	U
1	A	217	A
1	A	218	A
1	A	219	U
1	A	222	A
1	A	236	A
1	A	239	A
1	A	244	A
1	A	245	G
1	A	246	U
1	A	253	A
1	A	255	G
1	A	256	A
1	A	261	A
1	A	262	A
1	A	264	U
1	A	266	A
1	A	269	A
1	A	270	G
1	A	276	U
1	A	277	U
1	A	281	A
1	A	288	G
1	A	290	G
1	A	292	G
1	A	301	A
1	A	307	G
1	A	308	U
1	A	309	C

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Mol	Chain	Res	Type
1	A	311	A
1	A	312	A
1	A	313	U
1	A	314	A
1	A	315	A
1	A	316	G
1	A	327	A
1	A	328	A
1	A	329	A
1	A	330	A
1	A	331	A
1	A	332	A
1	A	336	A
1	A	337	A
1	A	342	A
1	A	343	U
1	A	344	A
1	A	348	U
1	A	349	A
1	A	355	U
1	A	359	A
1	A	365	A
1	A	366	A
1	A	380	G
1	A	382	A
1	A	384	A
1	A	386	U
1	A	387	A
1	A	401	A
1	A	425	A
1	A	427	G
1	A	428	C
1	A	429	A
1	A	430	A
1	A	433	A
1	A	435	G
1	A	442	U
1	A	445	U
1	A	448	U
1	A	450	U
1	A	455	A
1	A	461	U

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Mol	Chain	Res	Type
1	A	462	A
1	A	472	U
1	A	474	A
1	A	486	G
1	A	487	U
1	A	494	U
1	A	498	A
1	A	502	A
1	A	503	A
1	A	507	A
1	A	508	U
1	A	510	A
1	A	516	A
1	A	526	A
1	A	527	A
1	A	536	A
1	A	537	U
1	A	546	A
1	A	548	A
1	A	551	U
1	A	554	U
1	A	561	U
1	A	562	U
1	A	563	U
1	A	564	A
1	A	565	A
1	A	578	G
1	A	595	U
1	A	604	G
1	A	614	A
1	A	615	U
1	A	616	A
1	A	617	A
1	A	618	A
1	A	619	C
1	A	620	G
1	A	621	A
1	A	637	U
1	A	638	U
1	A	644	A
1	A	655	A
1	A	656	A

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Mol	Chain	Res	Type
1	A	661	G
1	A	666	G
1	A	667	U
1	A	673	A
1	A	674	A
1	A	675	G
1	A	676	A
1	A	681	U
1	A	682	C
1	A	683	U
1	A	684	G
1	A	696	G
1	A	703	U
1	A	706	U
1	A	707	A
1	A	710	A
1	A	718	G
1	A	719	U
1	A	720	A
1	A	733	A
1	A	734	U
1	A	736	A
1	A	737	A
1	A	747	U
1	A	755	U
1	A	767	A
1	A	776	A
1	A	777	G
1	A	778	A
1	A	782	G
1	A	783	U
1	A	789	A
1	A	790	A
1	A	797	U
1	A	798	A
1	A	803	A
1	A	833	U
1	A	835	A
1	A	840	C
1	A	841	G
1	A	843	A
1	A	845	U

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Mol	Chain	Res	Type
1	A	854	A
1	A	855	U
1	A	856	A
1	A	857	U
1	A	858	A
1	A	866	G
1	A	867	A
1	A	871	A
1	A	872	G
1	A	884	U
1	A	887	G
1	A	891	A
1	A	900	A
1	A	901	A
1	A	909	A
1	A	910	G
1	A	912	C
1	A	916	A
1	A	919	A
1	A	925	U
1	A	928	A
1	A	929	G
1	A	938	A
1	A	939	A
1	A	942	A
1	A	947	G
1	A	948	U
1	A	951	A
1	A	952	A
1	A	953	U
1	A	961	A
1	A	966	A
1	A	967	U
1	A	1058	U
1	A	1063	A
1	A	1065	A
1	A	1075	A
1	A	1077	A
1	A	1078	U
1	A	1086	U
1	A	1087	U
1	A	1094	U

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Mol	Chain	Res	Type
1	A	1095	A
1	A	1096	A
1	A	1097	U
1	A	1099	U
1	A	1101	C
1	A	1102	G
1	A	1105	U
1	A	1110	A
1	A	1111	U
1	A	1112	A
1	A	1113	A
1	A	1114	U
1	A	1115	A
1	A	1117	G
1	A	1118	A
1	A	1119	A
1	A	1126	A
1	A	1127	A
1	A	1130	C
1	A	1161	A
1	A	1169	A
1	A	1170	U
1	A	1171	A
1	A	1182	A
1	A	1191	U
1	A	1206	A
1	A	1213	A
1	A	1242	A
1	A	1243	U
1	A	1244	A
1	A	1255	A
1	A	1256	U
1	A	1257	U
1	A	1258	A
1	A	1260	U
1	A	1267	A
1	A	1269	G
1	A	1271	A
1	A	1272	U
1	A	1273	U
1	A	1279	A
1	A	1280	A

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Mol	Chain	Res	Type
1	A	1281	U
1	A	1283	G
1	A	1286	A
1	A	1287	A
1	A	1289	G
1	A	1298	A
1	A	1304	G
1	A	1305	A
1	A	1306	A
1	A	1307	A
1	A	1308	A
1	A	1313	G
1	A	1314	U
1	A	1315	A
1	A	1316	U
1	A	1317	A
1	A	1331	A
1	A	1332	A
1	A	1333	A
1	A	1337	U
1	A	1342	U
1	A	1344	U
1	A	1346	A
1	A	1349	A
1	A	1350	U
1	A	1352	A
1	A	1356	U
1	A	1357	A
1	A	1358	C
1	A	1359	G
1	A	1360	G
1	A	1361	C
1	A	1362	C
1	A	1365	U
1	A	1368	U
1	A	1371	A
1	A	1372	A
1	A	1374	U
1	A	1386	A
1	A	1387	A
1	A	1389	U
1	A	1392	A

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Mol	Chain	Res	Type
1	A	1393	U
1	A	1396	A
1	A	1399	A
1	A	1400	U
1	A	1404	A
1	A	1405	U
1	A	1406	A
1	A	1409	C
1	A	1410	U
1	A	1411	A
1	A	1412	U
1	A	1418	U
1	A	1423	A
1	A	1424	U
1	A	1477	A
1	A	1490	A
1	A	1493	U
1	A	1494	A
1	A	1500	U
1	A	1501	A
1	A	1507	U
1	A	1516	U
1	A	1523	A
1	A	1528	G
1	A	1531	C
1	A	1534	G
1	A	1537	A
1	A	1546	G
1	A	1548	A
1	A	1549	U
1	A	1560	A
1	A	1562	A
1	A	1563	C
1	A	1568	U
1	A	1569	C
1	A	1578	A
1	A	1579	A
1	A	1583	G
1	A	1598	A
1	A	1599	A
1	A	1600	U
1	A	1603	G

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Mol	Chain	Res	Type
1	A	1604	A
1	A	1605	U
1	A	1606	A
1	A	1612	A
1	A	1616	A
1	A	1618	G
1	A	1626	G
1	A	1632	A
1	A	1633	U
1	A	1634	A
1	A	1635	G
1	A	1648	U
1	A	1649	C
1	A	1653	A
1	A	1655	A
1	A	1661	A
1	A	1662	U
1	A	1663	A
1	A	1664	A
1	A	1665	G
1	A	1666	A
1	A	1671	A
1	A	1672	G
1	A	1680	A
1	A	1687	A
1	A	1689	U
1	A	1693	A
1	A	1694	A
1	A	1706	G
1	A	1707	C
1	A	1708	A
1	A	1709	G
1	A	1715	A
1	A	1716	U
1	A	1717	A
1	A	1720	U
1	A	1724	A
1	A	1727	A
1	A	1728	U
1	A	1737	A
1	A	1740	U
1	A	1743	G

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Mol	Chain	Res	Type
1	A	1746	C
1	A	1755	A
1	A	1764	U
1	A	1767	A
1	A	1768	A
1	A	1769	U
1	A	1770	U
1	A	1777	C
1	A	1778	G
1	A	1782	A
1	A	1786	A
1	A	1789	U
1	A	1790	A
1	A	1797	G
1	A	1807	A
1	A	1813	A
1	A	1814	U
1	A	1815	U
1	A	1818	G
1	A	1820	G
1	A	1824	U
1	A	1825	A
1	A	1826	U
1	A	1829	U
1	A	1830	G
1	A	1831	U
1	A	1836	A
1	A	1837	A
1	A	1838	A
1	A	1851	U
1	A	1855	U
1	A	1863	C
1	A	1867	U
1	A	1869	A
1	A	1870	A
1	A	1871	U
1	A	1872	G
1	A	1875	G
1	A	1882	U
1	A	1891	U
1	A	1892	G
1	A	1893	U

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Mol	Chain	Res	Type
1	A	1897	C
1	A	1920	A
1	A	1923	C
1	A	1930	A
1	A	1931	A
1	A	1933	A
1	A	1936	C
1	A	1943	C
1	A	1949	G
1	A	1951	A
1	A	1952	A
1	A	1955	C
1	A	1956	G
1	A	1959	A
1	A	1961	G
1	A	1963	C
1	A	1964	C
1	A	1969	G
1	A	1980	G
1	A	1989	U
1	A	1990	A
1	A	1991	G
1	A	1995	G
1	A	2005	U
1	A	2009	U
1	A	2084	G
1	A	2093	A
1	A	2094	A
1	A	2095	U
1	A	2251	A
1	A	2253	A
1	A	2263	U
1	A	2264	G
1	A	2276	G
1	A	2293	A
1	A	2301	C
1	A	2305	A
1	A	2306	U
1	A	2309	G
1	A	2310	U
1	A	2313	A
1	A	2315	A

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Mol	Chain	Res	Type
1	A	2316	A
1	A	2317	A
1	A	2318	U
1	A	2323	A
1	A	2324	U
1	A	2325	A
1	A	2330	A
1	A	2332	U
1	A	2349	A
1	A	2356	A
1	A	2358	A
1	A	2360	U
1	A	2361	A
1	A	2362	U
1	A	2363	A
1	A	2369	U
1	A	2372	U
1	A	2373	U
1	A	2374	A
1	A	2379	U
1	A	2380	U
1	A	2419	U
1	A	2423	G
1	A	2424	U
1	A	2425	A
1	A	2427	U
1	A	2428	A
1	A	2430	A
1	A	2431	U
1	A	2435	A
1	A	2436	A
1	A	2438	A
1	A	2439	U
1	A	2444	A
1	A	2447	A
1	A	2453	G
1	A	2455	A
1	A	2458	G
1	A	2461	A
1	A	2462	A
1	A	2467	A
1	A	2468	A

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Mol	Chain	Res	Type
1	A	2469	U
1	A	2470	A
1	A	2575	A
1	A	2580	A
1	A	2585	A
1	A	2586	U
1	A	2587	U
1	A	2588	A
1	A	2591	A
1	A	2597	G
1	A	2599	A
1	A	2601	A
1	A	2603	C
1	A	2610	A
1	A	2612	A
1	A	2613	A
1	A	2614	U
1	A	2616	G
1	A	2618	A
1	A	2638	G
1	A	2650	G
1	A	2652	C
1	A	2656	A
1	A	2659	A
1	A	2660	A
1	A	2666	A
1	A	2670	C
1	A	2671	U
1	A	2672	G
1	A	2673	A
1	A	2674	U
1	A	2691	A
1	A	2695	A
1	A	2696	A
1	A	2700	A
1	A	2701	A
1	A	2705	A
1	A	2707	G
1	A	2711	G
1	A	2713	G
1	A	2714	A
1	A	2720	G

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Mol	Chain	Res	Type
1	A	2725	A
1	A	2737	A
1	A	2740	A
1	A	2741	G
1	A	2742	A
1	A	2744	A
1	A	2750	A
1	A	2753	U
1	A	2760	G
1	A	2766	U
1	A	2773	C
1	A	2774	G
1	A	2779	A
1	A	2784	U
1	A	2791	U
1	A	2795	U
1	A	2796	G
1	A	2797	U
1	A	2802	G
1	A	2813	U
1	A	2814	U
1	A	2815	U
1	A	2821	U
1	A	2823	C
1	A	2826	C
1	A	2829	U
1	A	2833	A
1	A	2834	A
1	A	2836	G
1	A	2840	C
1	A	2852	U
1	A	2853	A
1	A	2869	A
1	A	2870	G
1	A	2876	U
1	A	2877	U
1	A	2880	U
1	A	2881	A
1	A	2894	A
1	A	2896	U
1	A	2897	A
1	A	2898	U

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Mol	Chain	Res	Type
1	A	2907	U
1	A	2909	A
1	A	2913	U
1	A	2928	A
1	A	2930	G
1	A	2940	G
1	A	2950	A
1	A	2956	U
1	A	2957	A
1	A	2958	U
1	A	2959	C
1	A	2980	A
1	A	3016	A
1	A	3017	U
1	A	3021	A
1	A	3023	U
1	A	3024	U
1	A	3037	A
1	A	3038	U
1	A	3039	A
1	A	3043	U
1	A	3050	G
1	A	3060	U
1	A	3062	A
1	A	3069	A
1	A	3070	A
1	A	3080	A
1	A	3092	U
1	A	3093	U
1	A	3094	A
1	A	3098	A
1	A	3102	A
1	A	3103	G
1	A	3106	G
1	A	3122	U
1	A	3123	A
1	A	3124	A
1	A	3125	U
1	A	3126	C
1	A	3127	U
1	A	3134	U
1	A	3135	U

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Mol	Chain	Res	Type
1	A	3136	U
1	A	3141	U
1	A	3148	A
1	A	3150	U
1	A	3151	A
1	A	3152	A
1	A	3153	U
1	A	3155	A
1	A	3159	G
1	A	3168	A
1	A	3169	U
1	A	3171	A
1	A	3172	U
1	A	3173	U
1	A	3193	A
1	A	3194	U
1	A	3248	C
1	A	3251	A
1	A	3252	U
1	A	3253	U
1	A	3255	A
1	A	3256	U
1	A	3257	C
1	A	3264	C
1	A	3265	U
1	A	3268	A
1	A	3269	U
1	A	3274	U
41	e	2	C
41	e	6	G
41	e	68	C
41	e	71	G
41	e	74	C
41	e	76	A

All (132) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	25	A
1	A	27	A
1	A	34	U
1	A	44	U

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Mol	Chain	Res	Type
1	A	93	U
1	A	134	U
1	A	162	U
1	A	164	U
1	A	216	U
1	A	217	A
1	A	236	A
1	A	239	A
1	A	261	A
1	A	268	C
1	A	276	U
1	A	306	G
1	A	313	U
1	A	326	A
1	A	329	A
1	A	365	A
1	A	409	A
1	A	426	A
1	A	429	A
1	A	454	A
1	A	461	U
1	A	486	G
1	A	507	A
1	A	526	A
1	A	536	A
1	A	561	U
1	A	563	U
1	A	564	A
1	A	578	G
1	A	614	A
1	A	615	U
1	A	616	A
1	A	617	A
1	A	637	U
1	A	643	U
1	A	655	A
1	A	666	G
1	A	675	G
1	A	682	C
1	A	696	G
1	A	733	A
1	A	735	A

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Mol	Chain	Res	Type
1	A	746	A
1	A	781	G
1	A	840	C
1	A	856	A
1	A	909	A
1	A	951	A
1	A	1062	U
1	A	1064	A
1	A	1093	A
1	A	1113	A
1	A	1126	A
1	A	1272	U
1	A	1306	A
1	A	1312	G
1	A	1313	G
1	A	1316	U
1	A	1331	A
1	A	1349	A
1	A	1409	C
1	A	1410	U
1	A	1422	A
1	A	1489	U
1	A	1493	U
1	A	1522	A
1	A	1547	U
1	A	1560	A
1	A	1591	G
1	A	1662	U
1	A	1663	A
1	A	1664	A
1	A	1665	G
1	A	1693	A
1	A	1706	G
1	A	1707	C
1	A	1708	A
1	A	1727	A
1	A	1818	G
1	A	1829	U
1	A	1830	G
1	A	1854	U
1	A	1892	G
1	A	1990	A

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Mol	Chain	Res	Type
1	A	2301	C
1	A	2304	A
1	A	2309	G
1	A	2314	U
1	A	2316	A
1	A	2324	U
1	A	2329	A
1	A	2357	U
1	A	2359	U
1	A	2372	U
1	A	2373	U
1	A	2378	A
1	A	2426	A
1	A	2427	U
1	A	2437	U
1	A	2446	U
1	A	2467	A
1	A	2585	A
1	A	2587	U
1	A	2591	A
1	A	2612	A
1	A	2613	A
1	A	2713	G
1	A	2783	U
1	A	2796	G
1	A	2880	U
1	A	2897	A
1	A	2906	U
1	A	2956	U
1	A	3020	U
1	A	3023	U
1	A	3036	U
1	A	3068	U
1	A	3069	A
1	A	3122	U
1	A	3124	A
1	A	3125	U
1	A	3126	C
1	A	3135	U
1	A	3150	U
1	A	3171	A
1	A	3193	A

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Mol	Chain	Res	Type
1	A	3252	U
1	A	3268	A

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 113 ligands modelled in this entry, 113 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.