wwPDB EM Map/Model Validation Report (i)

Apr 10, 2016 – 02:24 PM BST

PDB ID	:	4UY8
EMDB ID:	:	EMD-2773
Title	:	Molecular basis for the ribosome functioning as a L-tryptophan sensor - Cryo-EM structure of a TnaC stalled E.coli ribosome
Authors	:	Bischoff, L.; Berninghausen, O.; Beckmann, R.
Deposited on	:	2014-08-29
Resolution	:	3.80 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

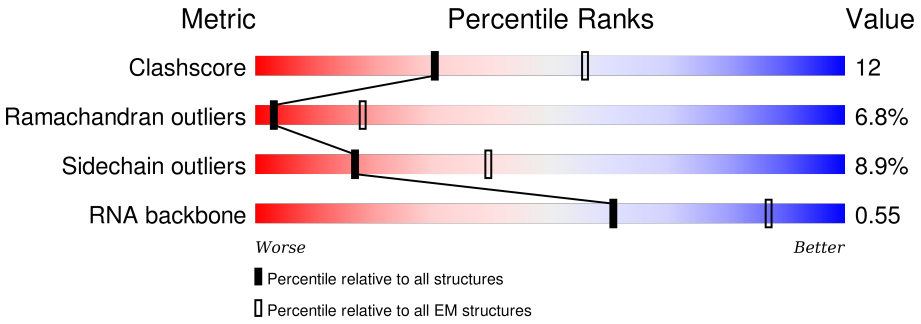
MolProbity	:	4.02b-467
Mogul	:	1.7.1 (RC1), CSD as537be (2016)
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk27241

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 3.80 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 <=5%

Mol	Chain	Length	Quality of chain
1	0	56	71% 25% • •
2	1	50	64% 28% 8%
3	2	46	76% 22% •
4	3	64	77% 19% 5%
5	4	38	55% 39% • •
6	5	148	29% 41% 20% 9%
7	6	30	60% 30% 10%
8	7	20	10% 25% 40% 25%

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Mol	Chain	Length	Quality of chain
9	8	94	77% 21%
10	A	2854	58% 32% 9%
11	B	118	66% 27% 7%
12	C	271	69% 27%
13	D	209	66% 28% 5%
14	E	201	69% 25% 5%
15	F	177	67% 29%
16	G	176	63% 29% 7%
17	H	50	58% 36% 6%
18	I	141	52% 42% 6%
19	J	142	61% 29% 9%
20	K	122	56% 34% 8%
21	L	143	70% 24%
22	M	136	63% 29% 7%
23	N	120	66% 31%
24	O	116	67% 30%
25	P	114	66% 25% 6%
26	Q	117	63% 31% 5%
27	R	103	63% 34%
28	S	110	61% 25% 11%
29	T	93	58% 35% 5%
30	U	102	63% 31% 5%
31	V	77	49% 36% 13%
32	W	79	37% 41% 20%
33	X	77	70% 23% 5%

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Mol	Chain	Length	Quality of chain
34	Y	63	60% 38%
35	Z	58	53% 36% 9%

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
36	TRP	7	1001	-	-	X	-
36	TRP	7	1002	-	-	X	-

2 Entry composition

There are 39 unique types of molecules in this entry. The entry contains 92995 atoms, of which 8 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 protein called 50S RIBOSOMAL PROTEIN L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	0	56	444	269	94	80	1	0	0

- Molecule 2 is a protein called 50S RIBOSOMAL PROTEIN L33.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
2	1	50	409	263	75	71	0	0

- Molecule 3 is a protein called 50S RIBOSOMAL PROTEIN L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	2	46	377	228	90	57	2	0	0

- Molecule 4 is a protein called 50S RIBOSOMAL PROTEIN L35.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	3	64	504	323	105	74	2	0	0

- Molecule 5 is a protein called 50S RIBOSOMAL PROTEIN L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	4	38	302	185	65	48	4	0	0

- Molecule 6 is a protein called 50S RIBOSOMAL PROTEIN L10.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	5	148	1117	705	196	209	7	0	0

- Molecule 7 is a protein called RIBOSOMAL L7 PROTEIN.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	6	30	Total	C	N	O	S	0	0
			227	144	33	47	3		

- Molecule 8 is a protein called TRYPTOPHANASE.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	7	20	Total	C	N	O	S	0	0
			170	109	32	28	1		

- Molecule 9 is a protein called 50S RIBOSOMAL PROTEIN L25.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	8	94	Total	C	N	O	S	0	0
			753	479	137	134	3		

- Molecule 10 is a RNA chain called RRNA-23S RIBOSOMAL RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	A	2854	Total	C	N	O	P	0	0
			61274	27334	11279	19807	2854		

- Molecule 11 is a RNA chain called RRNA-5S RIBOSOMAL RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	B	118	Total	C	N	O	P	0	0
			2529	1126	464	821	118		

- Molecule 12 is a protein called 50S RIBOSOMAL PROTEIN L2.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	C	271	Total	C	N	O	S	0	0
			2082	1288	423	364	7		

- Molecule 13 is a protein called 50S RIBOSOMAL PROTEIN L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	D	209	Total	C	N	O	S	0	0
			1565	979	288	294	4		

- Molecule 14 is a protein called 50S RIBOSOMAL PROTEIN L4.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	E	201	Total	C	N	O	S	0	0
			1552	974	283	290	5		

- Molecule 15 is a protein called 50S RIBOSOMAL PROTEIN L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	F	177	Total	C	N	O	S	0	0
			1410	899	249	256	6		

- Molecule 16 is a protein called 50S RIBOSOMAL PROTEIN L6.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	G	176	Total	C	N	O	S	0	0
			1323	832	243	246	2		

- Molecule 17 is a protein called RIBOSOMAL PROTEIN L9.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	H	50	Total	C	N	O	S	0	0
			384	247	68	68	1		

- Molecule 18 is a protein called 50S RIBOSOMAL PROTEIN L11.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	I	141	Total	C	N	O	S	0	0
			1032	651	179	196	6		

- Molecule 19 is a protein called 50S RIBOSOMAL PROTEIN L13.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	J	142	Total	C	N	O	S	0	0
			1129	714	212	199	4		

- Molecule 20 is a protein called 50S RIBOSOMAL PROTEIN L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	K	122	Total	C	N	O	S	0	0
			938	587	180	165	6		

- Molecule 21 is a protein called 50S RIBOSOMAL PROTEIN L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	L	143	Total	C	N	O	S	0	0
			1045	649	206	189	1		

- Molecule 22 is a protein called 50S RIBOSOMAL PROTEIN L16.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	M	136	Total	C	N	O	S	0	0
			1074	686	205	177	6		

- Molecule 23 is a protein called 50S RIBOSOMAL PROTEIN L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	N	120	Total	C	N	O	S	0	0
			960	593	196	166	5		

- Molecule 24 is a protein called 50S RIBOSOMAL PROTEIN L18.

Mol	Chain	Residues	Atoms				AltConf	Trace
24	O	116	Total	C	N	O	0	0
			892	552	178	162		

- Molecule 25 is a protein called 50S RIBOSOMAL PROTEIN L19.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	P	114	Total	C	N	O	S	0	0
			917	574	179	163	1		

- Molecule 26 is a protein called 50S RIBOSOMAL PROTEIN L20.

Mol	Chain	Residues	Atoms				AltConf	Trace
26	Q	117	Total	C	N	O	0	0
			947	604	192	151		

- Molecule 27 is a protein called 50S RIBOSOMAL PROTEIN L21.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	R	103	Total	C	N	O	S	0	0
			816	516	153	145	2		

- Molecule 28 is a protein called 50S RIBOSOMAL PROTEIN L22.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	S	110	Total	C	N	O	S	0	0
			857	532	166	156	3		

- Molecule 29 is a protein called 50S RIBOSOMAL PROTEIN L23.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	T	93	Total	C	N	O	S	0	0
			738	466	139	131	2		

- Molecule 30 is a protein called 50S RIBOSOMAL PROTEIN L24.

Mol	Chain	Residues	Atoms				AltConf	Trace
30	U	102	Total	C	N	O	0	0
			779	492	146	141		

- Molecule 31 is a RNA chain called RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	V	77	Total	C	N	O	P	0	0
			1649	733	297	542	77		

- Molecule 32 is a protein called 50S RIBOSOMAL PROTEIN L27.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	W	79	Total	C	N	O	S	0	0
			596	367	120	108	1		

- Molecule 33 is a protein called 50S RIBOSOMAL PROTEIN L28.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	X	77	Total	C	N	O	S	0	0
			625	388	129	106	2		

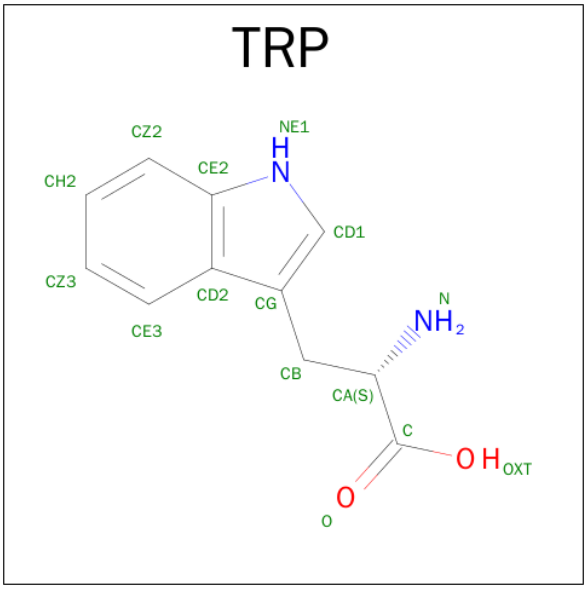
- Molecule 34 is a protein called 50S RIBOSOMAL PROTEIN L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	Y	63	Total	C	N	O	S	0	0
			509	313	99	95	2		

- Molecule 35 is a protein called 50S RIBOSOMAL PROTEIN L30.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	Z	58	Total	C	N	O	S	0	0
			449	281	87	79	2		

- Molecule 36 is TRYPTOPHAN (three-letter code: TRP) (formula: $C_{11}H_{12}N_2O_2$).



Mol	Chain	Residues	Atoms					AltConf
36	7	1	Total	C	H	N	O	0
			38	22	8	4	4	
36	7	1	Total	C	H	N	O	0
			38	22	8	4	4	

- Molecule 37 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
37	B	4	Total	Mg	0
			4	4	
37	A	135	Total	Mg	0
			135	135	
37	4	1	Total	Mg	0
			1	1	
37	C	2	Total	Mg	0
			2	2	
37	E	1	Total	Mg	0
			1	1	

- Molecule 38 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	AltConf
38	4	1	Total Zn 1 1	0

- Molecule 39 is water.

Mol	Chain	Residues	Atoms	AltConf
39	A	416	Total O 416 416	0
39	B	14	Total O 14 14	0
39	C	2	Total O 2 2	0
39	D	3	Total O 3 3	0
39	E	2	Total O 2 2	0
39	L	2	Total O 2 2	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: 50S RIBOSOMAL PROTEIN L32

Chain 0:

- Molecule 2: 50S RIBOSOMAL PROTEIN L33

Chain 1:

- Molecule 3: 50S RIBOSOMAL PROTEIN L34

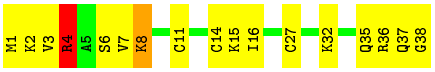
Chain 2:

- Molecule 4: 50S RIBOSOMAL PROTEIN L35

Chain 3:

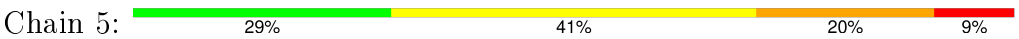
- Molecule 5: 50S RIBOSOMAL PROTEIN L36

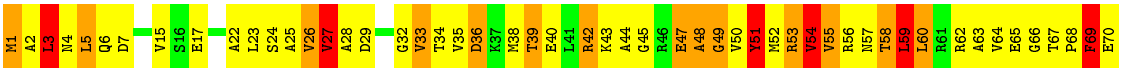
Chain 4:

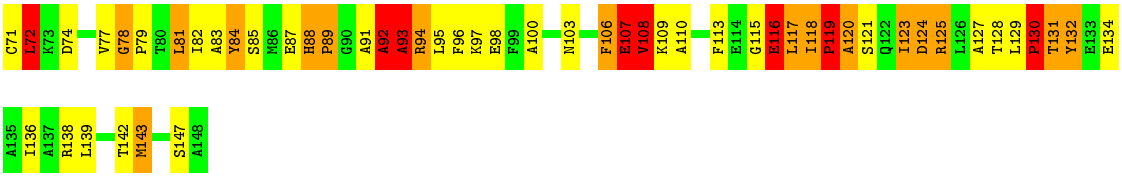


- Molecule 6: 50S RIBOSOMAL PROTEIN L10

Chain 5:







• Molecule 7: RIBOSOMAL L7 PROTEIN

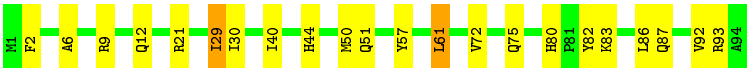
Chain 6:

• Molecule 8: TRYPTOPHANASE

Chain 7:

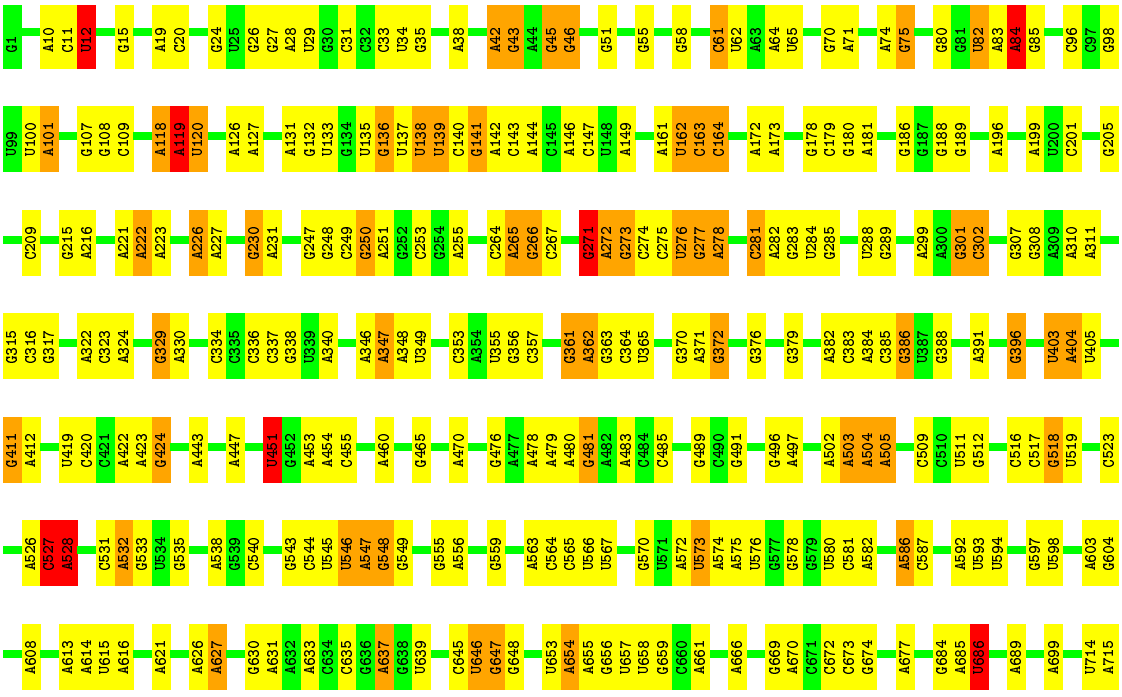
• Molecule 9: 50S RIBOSOMAL PROTEIN L25

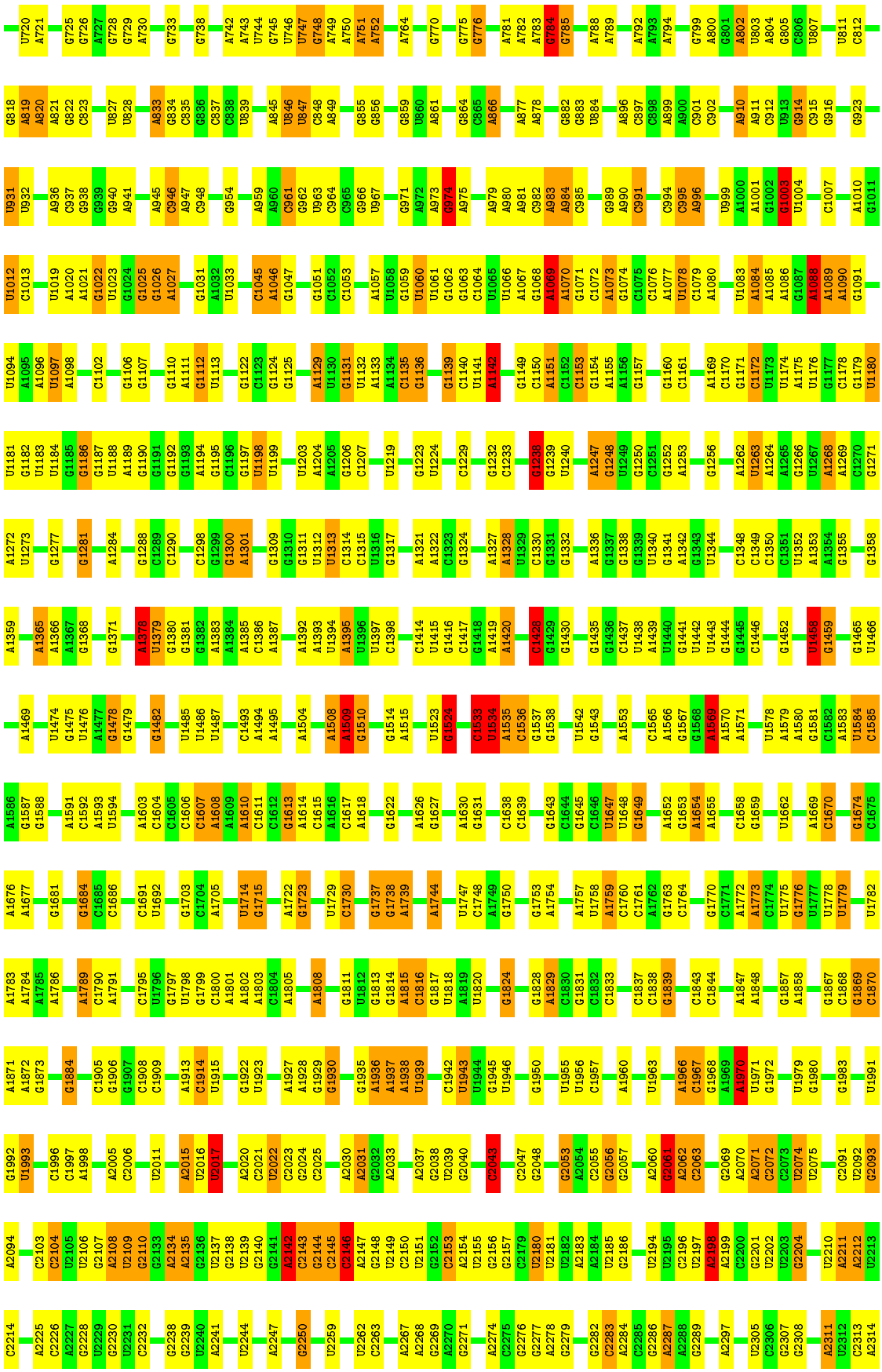
Chain 8:

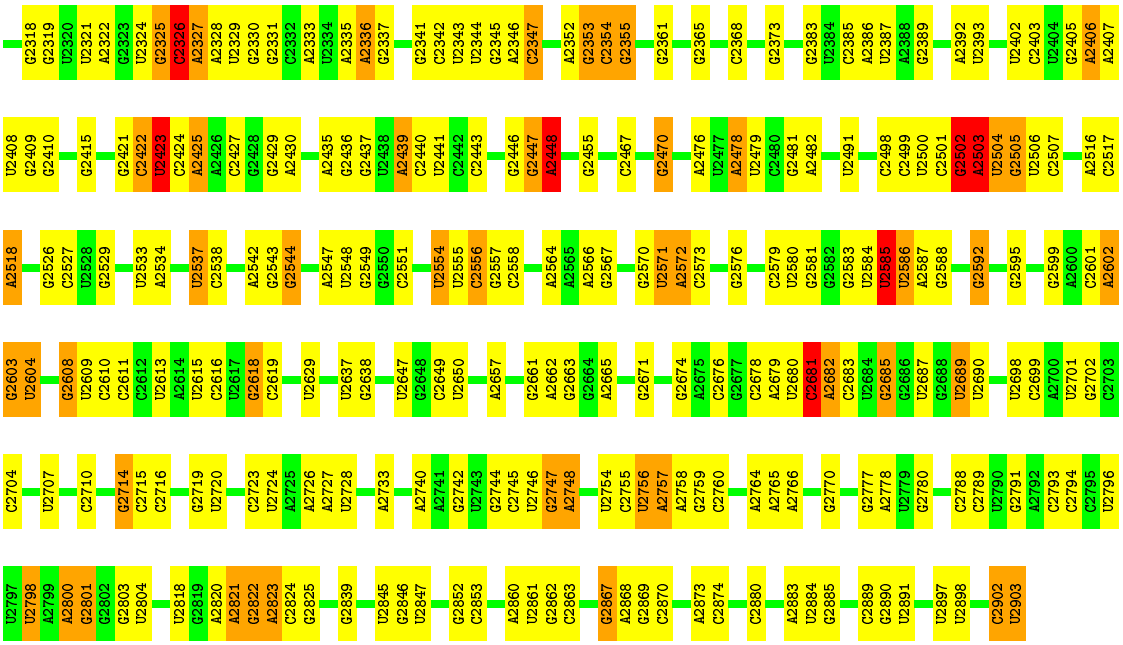


• Molecule 10: RRNA-23S RIBOSOMAL RNA

Chain A:

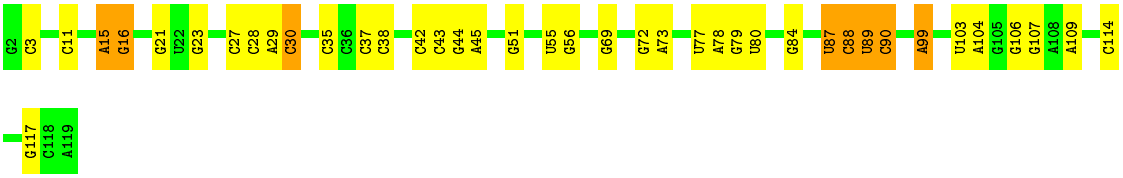






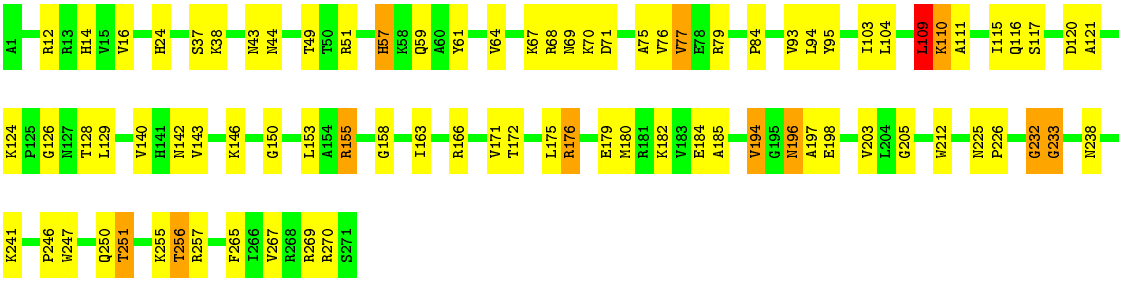
- Molecule 11: RRNA-5S RIBOSOMAL RNA

Chain B:



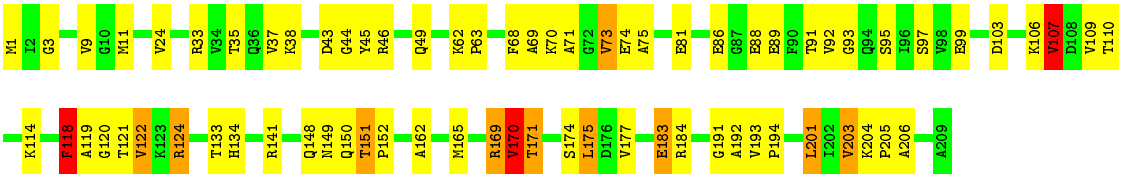
- Molecule 12: 50S RIBOSOMAL PROTEIN L2

Chain C:



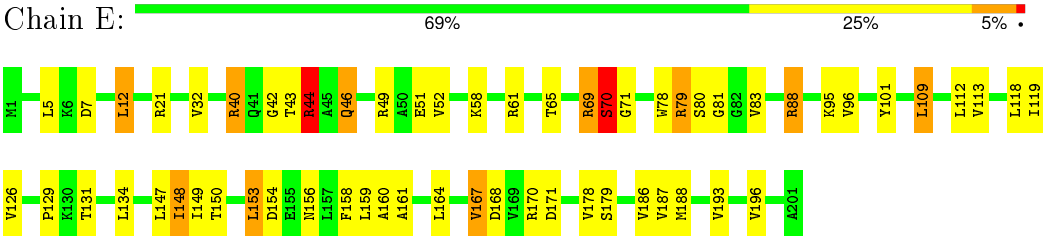
- Molecule 13: 50S RIBOSOMAL PROTEIN L3

Chain D:



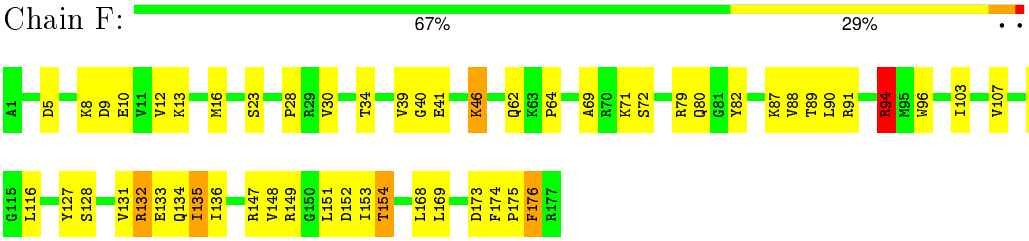
• Molecule 14: 50S RIBOSOMAL PROTEIN L4

Chain E:



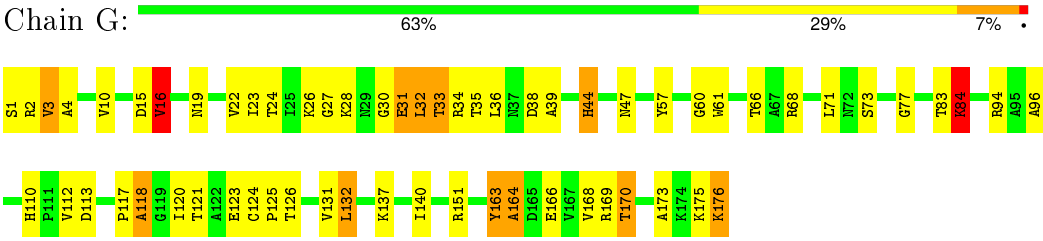
• Molecule 15: 50S RIBOSOMAL PROTEIN L5

Chain F:



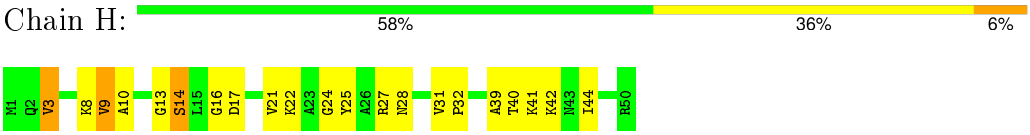
• Molecule 16: 50S RIBOSOMAL PROTEIN L6

Chain G:



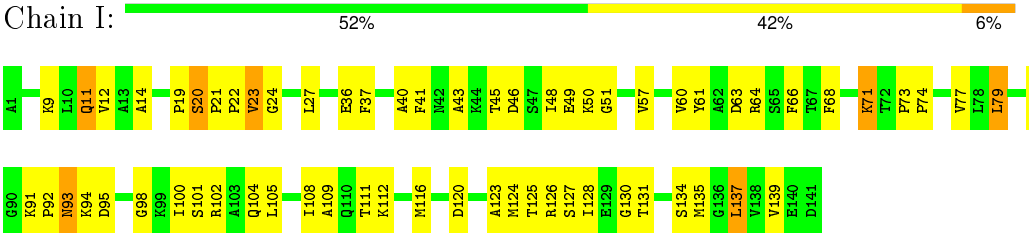
• Molecule 17: RIBOSOMAL PROTEIN L9

Chain H:



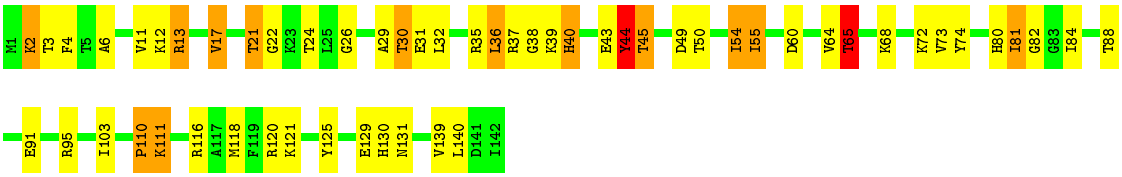
• Molecule 18: 50S RIBOSOMAL PROTEIN L11

Chain I:



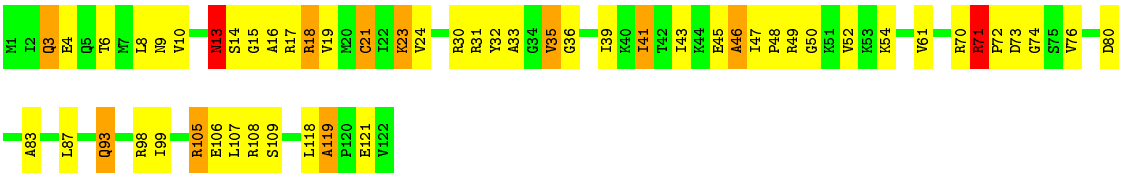
• Molecule 19: 50S RIBOSOMAL PROTEIN L13

Chain J:



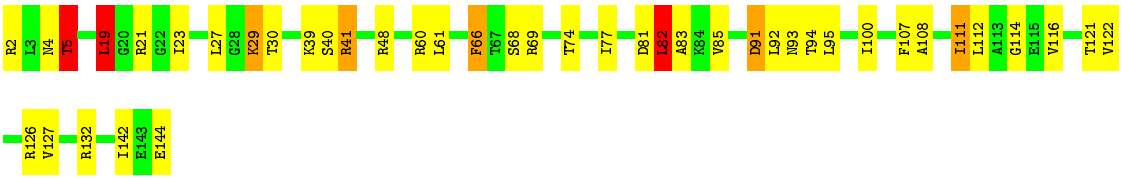
• Molecule 20: 50S RIBOSOMAL PROTEIN L14

Chain K:



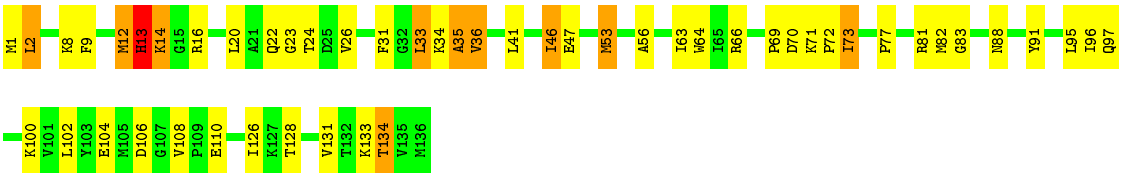
• Molecule 21: 50S RIBOSOMAL PROTEIN L15

Chain L:



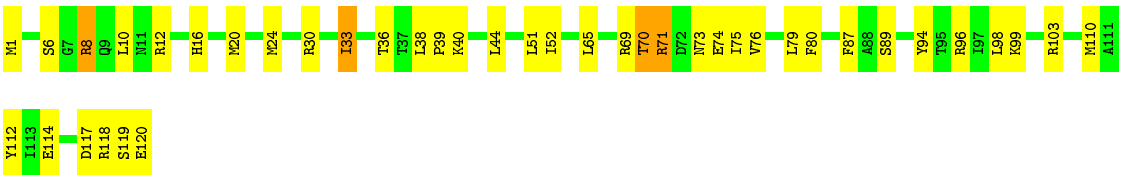
• Molecule 22: 50S RIBOSOMAL PROTEIN L16

Chain M:



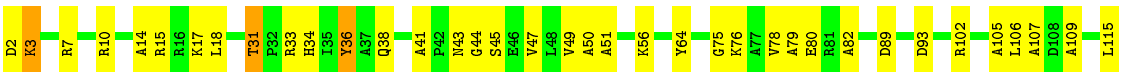
• Molecule 23: 50S RIBOSOMAL PROTEIN L17

Chain N:



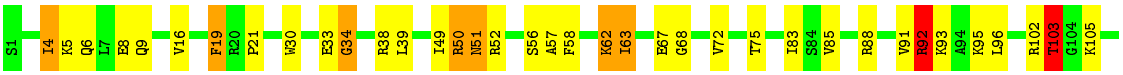
• Molecule 24: 50S RIBOSOMAL PROTEIN L18

Chain O:



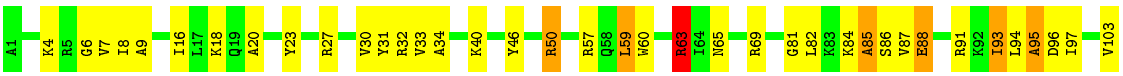
• Molecule 25: 50S RIBOSOMAL PROTEIN L19

Chain P:



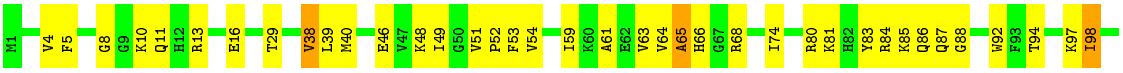
• Molecule 26: 50S RIBOSOMAL PROTEIN L20

Chain Q:



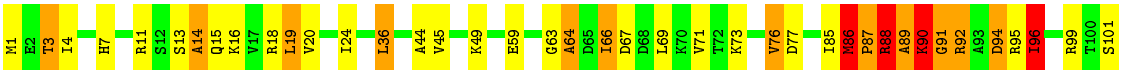
• Molecule 27: 50S RIBOSOMAL PROTEIN L21

Chain R:



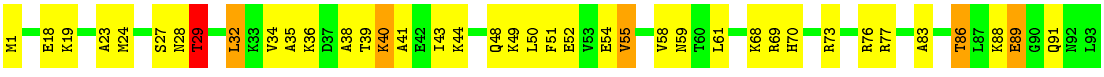
• Molecule 28: 50S RIBOSOMAL PROTEIN L22

Chain S:



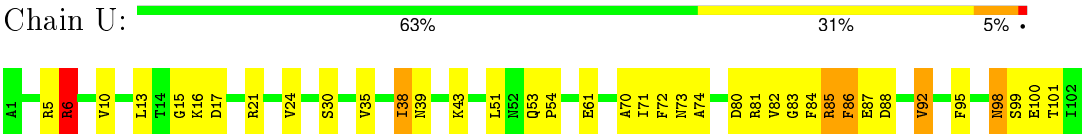
• Molecule 29: 50S RIBOSOMAL PROTEIN L23

Chain T:



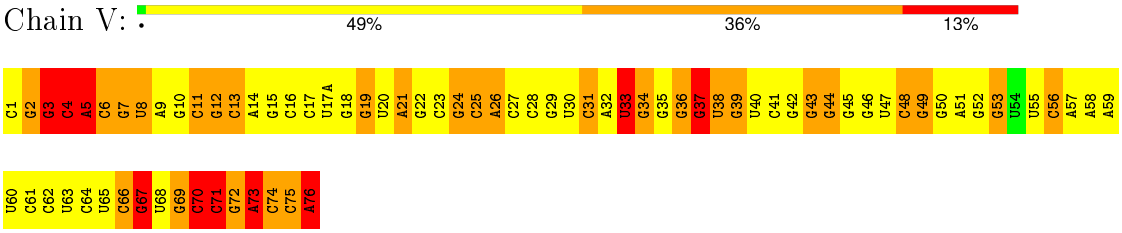
• Molecule 30: 50S RIBOSOMAL PROTEIN L24

Chain U:



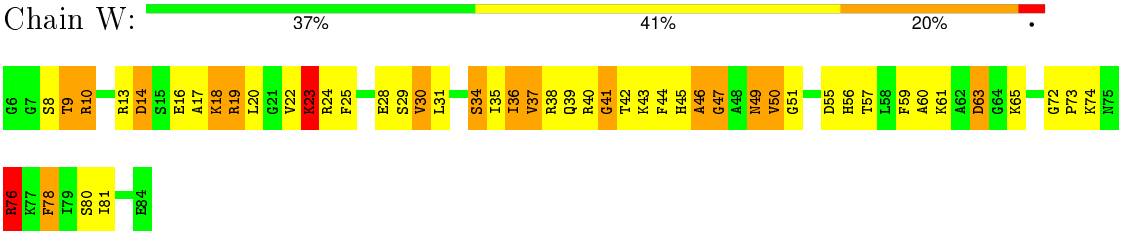
- Molecule 31: RNA

Chain V:



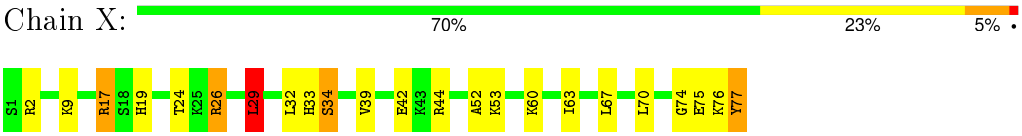
- Molecule 32: 50S RIBOSOMAL PROTEIN L27

Chain W:



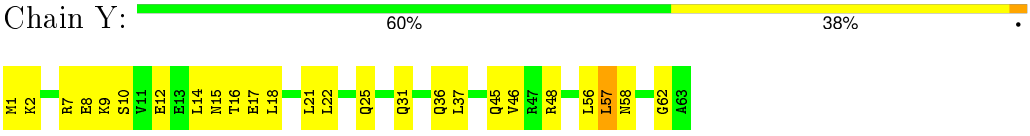
- Molecule 33: 50S RIBOSOMAL PROTEIN L28

Chain X:



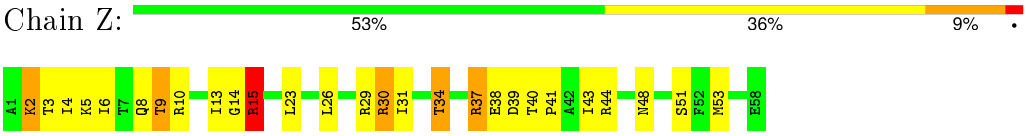
- Molecule 34: 50S RIBOSOMAL PROTEIN L29

Chain Y:



- Molecule 35: 50S RIBOSOMAL PROTEIN L30

Chain Z:



4 Experimental information (i)

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of images	Not provided	Depositor
Resolution determination method	Not provided	Depositor
CTF correction method	MICROGRAPH	Depositor
Microscope	OTHER	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	Not provided	Depositor
Minimum defocus (nm)	Not provided	Depositor
Maximum defocus (nm)	Not provided	Depositor
Magnification	Not provided	Depositor
Image detector	FEI FALCON II (4K X 4K)	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 5MU, 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	0	0.54	0/450	0.70	0/599
10	A	0.81	19/68626 (0.0%)	1.23	316/107056 (0.3%)
11	B	0.66	0/2828	1.10	2/4410 (0.0%)
12	C	0.54	0/2121	0.79	3/2852 (0.1%)
13	D	0.57	0/1586	0.77	1/2134 (0.0%)
14	E	0.53	0/1571	0.76	2/2113 (0.1%)
15	F	0.50	0/1434	0.71	1/1926 (0.1%)
16	G	0.55	0/1343	0.73	0/1816
17	H	0.53	0/389	0.73	0/523
18	I	0.62	0/1046	0.84	1/1410 (0.1%)
19	J	0.63	1/1152 (0.1%)	0.78	0/1551
2	1	0.53	0/416	0.74	0/554
20	K	0.65	1/947 (0.1%)	0.77	0/1268
21	L	0.56	0/1054	0.79	2/1403 (0.1%)
22	M	0.61	0/1093	0.77	0/1460
23	N	0.51	0/973	0.68	0/1301
24	O	0.46	0/902	0.70	0/1209
25	P	0.52	0/929	0.78	1/1242 (0.1%)
26	Q	0.62	0/960	0.71	1/1278 (0.1%)
27	R	0.61	1/829 (0.1%)	0.76	0/1107
28	S	0.88	3/864 (0.3%)	1.34	8/1156 (0.7%)
29	T	0.55	0/744	0.85	1/994 (0.1%)
3	2	0.53	0/380	0.70	0/498
30	U	0.56	0/787	0.78	0/1051
31	V	2.39	77/1820 (4.2%)	2.84	254/2836 (9.0%)
32	W	0.69	0/603	1.00	1/797 (0.1%)
33	X	0.50	0/635	0.79	1/848 (0.1%)
34	Y	0.46	0/510	0.75	0/677
35	Z	0.54	0/453	0.84	1/605 (0.2%)
4	3	0.53	0/513	0.75	0/676
5	4	0.59	0/303	0.84	0/397
6	5	0.74	0/1131	1.32	26/1524 (1.7%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >2	RMSZ	#|Z| >2
7	6	0.58	0/227	0.65	0/304
8	7	0.62	0/175	2.72	9/237 (3.8%)
9	8	0.48	0/766	0.67	1/1025 (0.1%)
All	All	0.81	102/100560 (0.1%)	1.20	632/150837 (0.4%)

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
12	C	0	1
13	D	0	1
19	J	0	1
20	K	0	1
28	S	0	3
31	V	0	13
6	5	0	1
8	7	0	4
All	All	0	25

All (102) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	V	39	G	N9-C4	15.38	1.50	1.38
31	V	69	G	C6-N1	13.21	1.48	1.39
31	V	5	A	C6-N1	12.91	1.44	1.35
31	V	39	G	C2-N3	12.19	1.42	1.32
31	V	39	G	N1-C2	11.42	1.46	1.37
31	V	5	A	C6-N6	10.61	1.42	1.33
31	V	67	G	N9-C4	10.41	1.46	1.38
31	V	67	G	N7-C5	10.08	1.45	1.39
10	A	2602	A	O3'-P	-10.05	1.49	1.61
31	V	37	G	C2-N3	9.96	1.40	1.32
31	V	5	A	N7-C5	-9.68	1.33	1.39
31	V	70	C	N1-C6	9.59	1.43	1.37
31	V	73	A	N7-C5	-9.48	1.33	1.39
31	V	1	C	C2-N3	9.36	1.43	1.35
31	V	69	G	N1-C2	8.94	1.45	1.37
31	V	7	G	C8-N7	-8.92	1.25	1.30
31	V	75	C	N1-C6	8.64	1.42	1.37
10	A	984	A	N9-C4	-8.39	1.32	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	V	38	U	C2'-C1'	-8.21	1.44	1.53
31	V	4	C	C2-N3	8.17	1.42	1.35
31	V	70	C	P-O5'	-8.07	1.51	1.59
31	V	32	A	N9-C8	8.06	1.44	1.37
31	V	2	G	C8-N7	-7.99	1.26	1.30
31	V	73	A	C5'-C4'	7.93	1.60	1.51
31	V	76	A	C5-C4	-7.86	1.33	1.38
31	V	72	G	C2'-C1'	-7.78	1.44	1.53
31	V	3	G	O3'-P	-7.70	1.51	1.61
31	V	6	C	C4-C5	-7.62	1.36	1.43
31	V	72	G	C2-N2	7.58	1.42	1.34
31	V	3	G	N9-C4	7.54	1.44	1.38
31	V	33	U	C4'-C3'	7.43	1.61	1.53
31	V	32	A	C4'-O4'	-7.18	1.36	1.45
31	V	13	C	C4'-O4'	7.09	1.54	1.45
31	V	75	C	N3-C4	7.06	1.38	1.33
31	V	6	C	C4-N4	6.79	1.40	1.33
31	V	76	A	C6-N6	6.76	1.39	1.33
31	V	37	G	C5-C4	-6.65	1.33	1.38
10	A	528	A	N9-C4	-6.64	1.33	1.37
31	V	71	C	C4'-O4'	6.63	1.54	1.45
31	V	7	G	N9-C8	6.57	1.42	1.37
31	V	3	G	C2'-C1'	-6.55	1.46	1.53
10	A	1142	A	N9-C4	-6.53	1.33	1.37
31	V	32	A	O3'-P	-6.47	1.53	1.61
31	V	38	U	C4'-C3'	-6.46	1.46	1.53
31	V	68	U	C4-O4	-6.42	1.18	1.23
31	V	76	A	C6-N1	6.33	1.40	1.35
31	V	34	G	C3'-C2'	-6.33	1.45	1.52
31	V	5	A	C2-N3	6.29	1.39	1.33
31	V	1	C	C2-O2	6.24	1.30	1.24
10	A	1569	A	N9-C4	-6.22	1.34	1.37
31	V	76	A	C8-N7	-6.21	1.27	1.31
31	V	32	A	N9-C4	6.18	1.41	1.37
31	V	2	G	N9-C4	6.15	1.42	1.38
10	A	2504	U	C4-O4	6.14	1.28	1.23
10	A	783	A	N3-C4	-6.07	1.31	1.34
10	A	783	A	N9-C4	-6.02	1.34	1.37
31	V	5	A	N1-C2	-5.91	1.29	1.34
31	V	5	A	C5-C6	5.85	1.46	1.41
10	A	1073	A	C5-C6	5.84	1.46	1.41
28	S	88	ARG	CA-C	-5.81	1.37	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	A	2504	U	N3-C4	5.79	1.43	1.38
31	V	69	G	C8-N7	-5.77	1.27	1.30
31	V	70	C	O3'-P	5.75	1.68	1.61
31	V	76	A	N1-C2	-5.74	1.29	1.34
31	V	2	G	C4'-C3'	-5.71	1.46	1.52
31	V	7	G	P-O5'	-5.71	1.54	1.59
31	V	6	C	C3'-C2'	5.67	1.59	1.52
19	J	44	TYR	CD2-CE2	-5.64	1.30	1.39
31	V	4	C	C4'-C3'	5.64	1.59	1.53
31	V	1	C	C3'-C2'	-5.62	1.46	1.52
31	V	32	A	C3'-C2'	5.58	1.59	1.52
31	V	76	A	N9-C4	5.56	1.41	1.37
31	V	69	G	C5-C6	-5.56	1.36	1.42
10	A	2504	U	C2-N3	5.55	1.41	1.37
10	A	783	A	N7-C5	-5.53	1.35	1.39
31	V	68	U	C2'-C1'	-5.50	1.47	1.53
31	V	38	U	N1-C6	5.50	1.42	1.38
10	A	528	A	N3-C4	-5.49	1.31	1.34
31	V	4	C	O4'-C1'	-5.46	1.34	1.41
10	A	1142	A	C5-C6	-5.44	1.36	1.41
31	V	67	G	P-O5'	-5.41	1.54	1.59
31	V	72	G	O3'-P	-5.39	1.54	1.61
31	V	36	G	C4'-C3'	-5.38	1.47	1.52
27	R	86	GLN	CB-CG	5.38	1.67	1.52
31	V	67	G	C5-C4	-5.34	1.34	1.38
31	V	73	A	N3-C4	-5.32	1.31	1.34
28	S	86	MET	CA-C	-5.25	1.39	1.52
31	V	37	G	C2'-C1'	-5.25	1.47	1.53
20	K	21	CYS	CB-SG	-5.24	1.73	1.81
10	A	2478	A	N9-C4	-5.20	1.34	1.37
31	V	70	C	O4'-C1'	5.20	1.48	1.41
10	A	2053	G	C6-O6	5.16	1.28	1.24
10	A	783	A	C5-C6	-5.14	1.36	1.41
28	S	91	GLY	C-O	-5.12	1.15	1.23
31	V	7	G	C2'-C1'	-5.11	1.47	1.53
10	A	1321	A	N9-C4	5.08	1.40	1.37
31	V	4	C	C2-O2	5.05	1.28	1.24
31	V	4	C	N1-C6	-5.05	1.34	1.37
10	A	2015	A	N3-C4	-5.04	1.31	1.34
31	V	5	A	C8-N7	5.03	1.35	1.31
31	V	7	G	N3-C4	5.03	1.39	1.35
31	V	73	A	C2-N3	5.00	1.38	1.33

All (632) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
28	S	86	MET	C-N-CD	-30.06	54.48	120.60
31	V	73	A	N1-C6-N6	22.84	132.30	118.60
10	A	1073	A	N1-C6-N6	-19.93	106.64	118.60
31	V	69	G	N1-C6-O6	19.71	131.73	119.90
31	V	69	G	C5-C6-O6	-19.59	116.85	128.60
8	7	14	ASN	N-CA-CB	15.73	138.91	110.60
31	V	73	A	C5-C6-N6	-15.38	111.40	123.70
8	7	5	HIS	CB-CA-C	14.92	140.24	110.40
10	A	2608	G	C4'-C3'-O3'	14.21	141.42	113.00
10	A	1073	A	C5-C6-N6	14.10	134.98	123.70
8	7	23	ARG	O-C-N	14.06	147.82	121.10
8	7	5	HIS	N-CA-C	-14.01	73.17	111.00
10	A	2053	G	N1-C6-O6	13.74	128.15	119.90
31	V	2	G	N1-C6-O6	13.60	128.06	119.90
31	V	3	G	C6-C5-N7	-13.52	122.29	130.40
31	V	4	C	N3-C4-N4	13.28	127.30	118.00
31	V	70	C	O4'-C1'-N1	13.17	118.74	108.20
31	V	67	G	N1-C6-O6	13.17	127.80	119.90
10	A	2504	U	N3-C4-O4	13.00	128.50	119.40
8	7	23	ARG	C-N-CD	12.74	155.15	128.40
31	V	4	C	C5-C4-N4	-12.69	111.32	120.20
31	V	39	G	C8-N9-C4	-12.66	101.34	106.40
31	V	6	C	C6-N1-C2	-12.57	115.27	120.30
31	V	26	A	N1-C6-N6	12.56	126.14	118.60
10	A	2585	U	C4'-C3'-O3'	-12.52	83.11	109.40
8	7	14	ASN	CB-CA-C	-12.40	85.61	110.40
31	V	21	A	N1-C6-N6	12.31	125.98	118.60
31	V	51	A	N1-C6-N6	12.31	125.98	118.60
31	V	5	A	O4'-C1'-N9	12.29	118.03	108.20
31	V	14	A	N1-C6-N6	12.27	125.96	118.60
31	V	9	A	N1-C6-N6	12.26	125.95	118.60
10	A	984	A	C2-N3-C4	-12.10	104.55	110.60
31	V	57	A	N1-C6-N6	12.04	125.82	118.60
31	V	7	G	N3-C2-N2	12.03	128.32	119.90
31	V	58	A	N1-C6-N6	11.84	125.70	118.60
10	A	961	C	O5'-P-OP2	-11.83	95.06	105.70
10	A	2053	G	C6-C5-N7	-11.60	123.44	130.40
31	V	72	G	P-O3'-C3'	11.52	133.53	119.70
31	V	32	A	P-O3'-C3'	11.47	133.47	119.70
31	V	59	A	N1-C6-N6	11.46	125.47	118.60
10	A	1073	A	C6-C5-N7	11.39	140.28	132.30
10	A	2053	G	C5-C6-N1	-11.34	105.83	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	A	1073	A	C4-C5-N7	-11.26	105.07	110.70
10	A	751	A	C4'-C3'-O3'	11.22	135.44	113.00
31	V	69	G	O4'-C1'-N9	11.19	117.15	108.20
31	V	67	G	C5-C6-O6	-11.00	122.00	128.60
31	V	6	C	C5-C6-N1	10.95	126.47	121.00
31	V	5	A	N1-C6-N6	10.94	125.17	118.60
8	7	16	ASP	N-CA-CB	-10.85	91.07	110.60
10	A	783	A	C5-N7-C8	-10.72	98.54	103.90
10	A	2504	U	C5-C6-N1	10.55	127.98	122.70
10	A	974	G	C6-C5-N7	-10.49	124.11	130.40
10	A	2586	U	C4'-C3'-O3'	-10.43	87.49	109.40
10	A	2053	G	C4-C5-C6	10.13	124.88	118.80
31	V	37	G	N3-C4-C5	-10.01	123.60	128.60
31	V	33	U	P-O3'-C3'	9.89	131.57	119.70
10	A	2504	U	C6-N1-C2	-9.85	115.09	121.00
31	V	53	G	N1-C6-O6	9.79	125.77	119.90
10	A	974	G	C4-C5-N7	9.78	114.71	110.80
31	V	34	G	P-O5'-C5'	9.76	136.52	120.90
31	V	4	C	O4'-C1'-N1	9.74	115.99	108.20
31	V	7	G	P-O3'-C3'	9.69	131.33	119.70
10	A	783	A	N7-C8-N9	9.65	118.62	113.80
6	5	92	ALA	C-N-CA	9.60	145.69	121.70
31	V	10	G	N1-C6-O6	9.56	125.64	119.90
31	V	32	A	N7-C8-N9	-9.55	109.03	113.80
31	V	65	U	P-O3'-C3'	9.41	130.99	119.70
31	V	22	G	N1-C6-O6	9.39	125.54	119.90
8	7	23	ARG	CA-C-N	-9.35	90.93	117.10
10	A	1534	U	C2-N1-C1'	9.33	128.90	117.70
31	V	37	G	C2-N3-C4	9.32	116.56	111.90
31	V	46	G	N1-C6-O6	9.32	125.49	119.90
10	A	528	A	C2-N3-C4	-9.32	105.94	110.60
28	S	88	ARG	N-CA-C	-9.28	85.94	111.00
10	A	1073	A	C5-N7-C8	9.28	108.54	103.90
31	V	72	G	O4'-C1'-N9	9.21	115.57	108.20
31	V	43	G	N1-C6-O6	9.18	125.41	119.90
31	V	39	G	N3-C4-C5	-9.16	124.02	128.60
31	V	31	C	O4'-C1'-N1	9.08	115.47	108.20
6	5	93	ALA	C-N-CA	9.07	144.38	121.70
31	V	50	G	N1-C6-O6	9.00	125.30	119.90
31	V	39	G	C6-C5-N7	-8.97	125.02	130.40
31	V	15	G	N1-C6-O6	8.96	125.28	119.90
31	V	24	G	N1-C6-O6	8.87	125.22	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	A	465	G	C8-N9-C4	-8.86	102.85	106.40
31	V	37	G	O4'-C1'-N9	8.86	115.28	108.20
31	V	42	G	N1-C6-O6	8.85	125.21	119.90
10	A	1950	G	N1-C6-O6	8.84	125.21	119.90
31	V	74	C	O4'-C1'-N1	8.83	115.26	108.20
10	A	783	A	C8-N9-C4	-8.82	102.27	105.80
31	V	29	G	N1-C6-O6	8.79	125.17	119.90
10	A	2061	G	C4'-C3'-O3'	-8.74	91.04	109.40
31	V	52	G	N1-C6-O6	8.72	125.13	119.90
31	V	12	G	N1-C6-O6	8.69	125.11	119.90
31	V	44	G	N1-C6-O6	8.66	125.10	119.90
10	A	1073	A	N9-C4-C5	8.65	109.26	105.80
10	A	2534	A	N1-C6-N6	8.64	123.78	118.60
31	V	39	G	O4'-C1'-N9	8.63	115.11	108.20
31	V	45	G	N1-C6-O6	8.61	125.07	119.90
31	V	73	A	C5'-C4'-C3'	8.59	129.74	116.00
10	A	2074	U	O5'-P-OP2	-8.53	98.02	105.70
31	V	18	G	N1-C6-O6	8.51	125.01	119.90
10	A	1533	C	N1-C2-O2	8.51	124.01	118.90
31	V	2	G	C5-C6-O6	-8.48	123.51	128.60
10	A	1936	A	C2-N3-C4	-8.47	106.36	110.60
10	A	1533	C	C2-N1-C1'	8.46	128.10	118.80
10	A	974	G	C4-N9-C1'	8.43	137.46	126.50
10	A	2572	A	N1-C6-N6	8.36	123.61	118.60
31	V	19	G	N1-C6-O6	8.35	124.91	119.90
31	V	34	G	OP1-P-OP2	-8.35	107.07	119.60
31	V	3	G	N1-C2-N3	-8.35	118.89	123.90
10	A	1142	A	C2-N3-C4	-8.29	106.46	110.60
31	V	56	C	O4'-C1'-N1	8.27	114.81	108.20
31	V	39	G	C6-N1-C2	-8.24	120.16	125.10
31	V	49	G	N1-C6-O6	8.22	124.83	119.90
6	5	27	VAL	CG1-CB-CG2	8.21	124.03	110.90
31	V	25	C	O4'-C1'-N1	8.12	114.69	108.20
10	A	586	A	O5'-P-OP1	-8.08	98.42	105.70
31	V	53	G	C5-C6-O6	-8.07	123.76	128.60
31	V	61	C	O4'-C1'-N1	8.06	114.65	108.20
10	A	1533	C	C6-N1-C2	-8.04	117.08	120.30
13	D	151	THR	C-N-CD	7.99	145.17	128.40
31	V	65	U	O4'-C1'-N1	7.98	114.58	108.20
31	V	39	G	C4-C5-C6	7.96	123.58	118.80
31	V	11	C	O4'-C1'-N1	7.96	114.57	108.20
10	A	1795	C	C6-N1-C2	-7.94	117.12	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	V	62	C	O4'-C1'-N1	7.93	114.54	108.20
10	A	783	A	C4-C5-N7	7.92	114.66	110.70
10	A	2609	U	C5'-C4'-O4'	7.92	118.61	109.10
10	A	2609	U	O4'-C1'-N1	7.91	114.53	108.20
28	S	86	MET	N-CA-C	-7.89	89.70	111.00
10	A	984	A	N3-C4-C5	7.85	132.29	126.80
31	V	71	C	O4'-C1'-N1	7.80	114.44	108.20
31	V	27	C	O4'-C1'-N1	7.78	114.43	108.20
31	V	64	C	O4'-C1'-N1	7.77	114.42	108.20
31	V	70	C	N1-C2-O2	7.76	123.55	118.90
31	V	10	G	C5-C6-O6	-7.72	123.97	128.60
31	V	23	C	O4'-C1'-N1	7.71	114.37	108.20
31	V	46	G	C5-C6-O6	-7.70	123.98	128.60
10	A	1478	G	N1-C6-O6	7.70	124.52	119.90
10	A	2504	U	N3-C4-C5	-7.69	109.99	114.60
10	A	465	G	N3-C4-C5	-7.68	124.76	128.60
6	5	51	TYR	C-N-CA	7.68	140.90	121.70
10	A	2609	U	P-O5'-C5'	7.68	133.19	120.90
10	A	2053	G	C4-N9-C1'	7.67	136.47	126.50
6	5	49	GLY	C-N-CA	7.66	140.86	121.70
31	V	20	U	O4'-C1'-N1	7.63	114.31	108.20
6	5	123	ILE	CG1-CB-CG2	7.62	128.17	111.40
31	V	28	C	O4'-C1'-N1	7.60	114.28	108.20
10	A	2146	C	N3-C4-C5	-7.60	118.86	121.90
10	A	974	G	C8-N9-C1'	-7.60	117.13	127.00
10	A	2053	G	C2-N3-C4	-7.57	108.11	111.90
31	V	30	U	O4'-C1'-N1	7.56	114.25	108.20
31	V	41	C	O4'-C1'-N1	7.56	114.25	108.20
10	A	783	A	N1-C6-N6	7.56	123.13	118.60
6	5	119	PRO	C-N-CA	7.54	140.56	121.70
14	E	44	ARG	NE-CZ-NH1	7.51	124.06	120.30
32	W	76	ARG	NE-CZ-NH1	7.48	124.04	120.30
10	A	1839	G	N1-C6-O6	7.48	124.39	119.90
10	A	783	A	C6-C5-N7	-7.48	127.07	132.30
10	A	776	G	C5-C6-O6	7.46	133.08	128.60
31	V	2	G	C6-N1-C2	7.45	129.57	125.10
31	V	17	C	O4'-C1'-N1	7.44	114.16	108.20
31	V	76	A	C8-N9-C4	-7.39	102.84	105.80
6	5	72	LEU	C-N-CA	7.36	140.09	121.70
31	V	22	G	C5-C6-O6	-7.36	124.19	128.60
31	V	43	G	C5-C6-O6	-7.35	124.19	128.60
10	A	1533	C	N3-C2-O2	-7.32	116.77	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	A	2504	U	C5-C4-O4	-7.32	121.51	125.90
6	5	81	LEU	CB-CG-CD2	7.29	123.39	111.00
31	V	3	G	N3-C2-N2	7.28	125.00	119.90
10	A	1073	A	O5'-P-OP2	7.28	119.43	110.70
10	A	974	G	C5-N7-C8	-7.27	100.67	104.30
31	V	3	G	C2-N3-C4	7.24	115.52	111.90
10	A	1534	U	C6-N1-C1'	-7.23	111.08	121.20
10	A	2447	G	O5'-P-OP1	-7.20	99.22	105.70
31	V	63	U	O4'-C1'-N1	7.19	113.95	108.20
10	A	2501	C	C2-N1-C1'	-7.19	110.89	118.80
10	A	2602	A	C4'-C3'-O3'	-7.19	94.31	109.40
10	A	2053	G	N1-C2-N3	7.17	128.20	123.90
10	A	1950	G	C6-C5-N7	-7.16	126.11	130.40
10	A	2053	G	C8-N9-C1'	-7.15	117.70	127.00
31	V	15	G	C5-C6-O6	-7.15	124.31	128.60
6	5	28	ALA	C-N-CA	7.14	139.55	121.70
31	V	37	G	C4-C5-C6	7.12	123.07	118.80
31	V	75	C	N3-C4-C5	-7.11	119.06	121.90
31	V	1	C	N3-C4-N4	7.09	122.96	118.00
28	S	94	ASP	N-CA-C	-7.09	91.87	111.00
10	A	2250	G	C6-C5-N7	-7.08	126.15	130.40
10	A	1142	A	N1-C6-N6	7.07	122.84	118.60
10	A	776	G	C5-C6-N1	-7.05	107.98	111.50
31	V	66	C	N3-C4-C5	-7.05	119.08	121.90
31	V	8	U	O4'-C1'-N1	7.04	113.84	108.20
6	5	47	GLU	C-N-CA	7.04	139.29	121.70
6	5	54	VAL	CG1-CB-CG2	7.00	122.10	110.90
31	V	37	G	N1-C2-N3	-7.00	119.70	123.90
31	V	67	G	C4-C5-C6	6.99	123.00	118.80
10	A	2423	U	P-O3'-C3'	6.99	128.09	119.70
31	V	7	G	OP1-P-O3'	6.97	120.54	105.20
31	V	7	G	N1-C2-N3	-6.97	119.72	123.90
10	A	2503	A	C5-C6-N6	-6.97	118.12	123.70
10	A	984	A	N3-C4-N9	-6.96	121.83	127.40
10	A	2448	A	N1-C6-N6	6.96	122.78	118.60
10	A	802	A	N1-C6-N6	-6.96	114.42	118.60
31	V	50	G	C5-C6-O6	-6.96	124.42	128.60
31	V	2	G	C6-C5-N7	-6.95	126.23	130.40
28	S	91	GLY	N-CA-C	-6.94	95.76	113.10
10	A	2602	A	P-O3'-C3'	6.93	128.02	119.70
10	A	1284	A	O5'-P-OP2	-6.92	99.47	105.70
31	V	37	G	C8-N9-C4	-6.90	103.64	106.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	V	3	G	O4'-C1'-N9	6.89	113.71	108.20
31	V	60	U	O4'-C1'-N1	6.89	113.71	108.20
10	A	1378	A	P-O3'-C3'	6.89	127.96	119.70
10	A	1935	G	O5'-P-OP2	-6.89	99.50	105.70
28	S	90	LYS	N-CA-C	-6.89	92.41	111.00
10	A	2250	G	N1-C6-O6	6.88	124.03	119.90
31	V	67	G	C6-C5-N7	-6.88	126.27	130.40
10	A	2504	U	C2-N1-C1'	6.88	125.95	117.70
10	A	1839	G	C6-C5-N7	-6.87	126.28	130.40
10	A	1654	A	O5'-P-OP1	-6.85	99.53	105.70
10	A	974	G	N1-C6-O6	6.83	124.00	119.90
10	A	2681	C	C6-N1-C2	6.83	123.03	120.30
31	V	42	G	C5-C6-O6	-6.82	124.51	128.60
31	V	76	A	N1-C6-N6	6.81	122.69	118.60
10	A	783	A	C2-N3-C4	-6.79	107.20	110.60
31	V	12	G	C5-C6-O6	-6.77	124.54	128.60
10	A	1192	G	C8-N9-C4	6.76	109.10	106.40
10	A	503	A	C8-N9-C4	-6.76	103.10	105.80
31	V	14	A	C4-C5-C6	6.76	120.38	117.00
8	7	23	ARG	C-N-CA	-6.74	93.68	122.00
10	A	974	G	N3-C4-N9	6.74	130.04	126.00
10	A	1815	A	N9-C4-C5	6.74	108.50	105.80
10	A	12	U	N3-C2-O2	-6.73	117.49	122.20
10	A	974	G	C5-C6-O6	-6.73	124.56	128.60
21	L	19	LEU	CA-CB-CG	6.72	130.75	115.30
31	V	47	U	O4'-C1'-N1	6.70	113.56	108.20
31	V	69	G	N3-C4-C5	6.70	131.95	128.60
31	V	6	C	C4'-C3'-C2'	-6.69	95.91	102.60
10	A	974	G	N7-C8-N9	6.69	116.44	113.10
10	A	1311	G	C8-N9-C4	-6.69	103.72	106.40
31	V	52	G	C5-C6-O6	-6.69	124.59	128.60
31	V	29	G	C5-C6-O6	-6.68	124.59	128.60
10	A	2823	A	C8-N9-C4	-6.66	103.14	105.80
31	V	1	C	O4'-C1'-N1	6.65	113.52	108.20
31	V	36	G	P-O5'-C5'	-6.65	110.26	120.90
15	F	94	ARG	NE-CZ-NH1	6.65	123.62	120.30
10	A	974	G	N9-C4-C5	-6.62	102.75	105.40
31	V	3	G	N9-C4-C5	-6.60	102.76	105.40
31	V	45	G	C5-C6-O6	-6.60	124.64	128.60
10	A	528	A	N1-C6-N6	6.59	122.56	118.60
31	V	39	G	N3-C4-N9	6.58	129.95	126.00
31	V	48	C	O4'-C1'-N1	6.58	113.46	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	C	233	GLY	N-CA-C	-6.58	96.66	113.10
31	V	44	G	C5-C6-O6	-6.57	124.66	128.60
10	A	2146	C	C2-N3-C4	6.55	123.18	119.90
10	A	670	A	O4'-C1'-N9	-6.54	102.97	108.20
31	V	24	G	C5-C6-O6	-6.53	124.68	128.60
31	V	69	G	N9-C4-C5	-6.51	102.80	105.40
31	V	40	U	O4'-C1'-N1	6.49	113.39	108.20
6	5	147	SER	C-N-CA	6.48	137.90	121.70
6	5	84	TYR	C-N-CA	6.46	137.85	121.70
10	A	820	A	O5'-P-OP1	-6.46	99.88	105.70
10	A	1263	U	N3-C4-C5	-6.46	110.73	114.60
31	V	55	U	O4'-C1'-N1	6.45	113.36	108.20
31	V	21	A	C4-C5-C6	6.45	120.23	117.00
31	V	3	G	P-O5'-C5'	-6.44	110.59	120.90
6	5	40	GLU	C-N-CA	6.43	137.77	121.70
31	V	72	G	N3-C2-N2	6.42	124.39	119.90
31	V	19	G	C5-C6-O6	-6.41	124.76	128.60
31	V	69	G	C5-N7-C8	6.40	107.50	104.30
31	V	6	C	C2-N3-C4	6.39	123.10	119.90
10	A	2689	U	C5-C4-O4	6.39	129.73	125.90
10	A	404	A	P-O3'-C3'	6.39	127.37	119.70
14	E	44	ARG	NE-CZ-NH2	-6.39	117.11	120.30
31	V	39	G	N7-C8-N9	6.39	116.29	113.10
10	A	2551	C	OP2-P-O3'	6.37	119.22	105.20
31	V	6	C	O4'-C1'-N1	6.37	113.30	108.20
6	5	50	VAL	C-N-CA	6.36	137.59	121.70
31	V	5	A	C5'-C4'-C3'	6.35	126.16	116.00
31	V	58	A	C4-C5-C6	6.35	120.18	117.00
28	S	85	ILE	O-C-N	-6.34	112.55	122.70
10	A	2770	G	N1-C6-O6	-6.34	116.09	119.90
31	V	2	G	N1-C2-N3	-6.34	120.10	123.90
31	V	9	A	C4-C5-C6	6.34	120.17	117.00
10	A	2754	U	N3-C4-O4	6.34	123.83	119.40
10	A	2142	A	OP2-P-O3'	6.33	119.13	105.20
28	S	94	ASP	CB-CG-OD2	6.32	123.98	118.30
31	V	18	G	C5-C6-O6	-6.32	124.81	128.60
31	V	37	G	N9-C4-C5	6.30	107.92	105.40
31	V	66	C	P-O3'-C3'	6.29	127.25	119.70
10	A	2267	A	C8-N9-C4	-6.28	103.29	105.80
10	A	1125	G	N1-C6-O6	6.27	123.66	119.90
31	V	70	C	P-O5'-C5'	6.26	130.92	120.90
10	A	1839	G	C5-C6-O6	-6.26	124.84	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	A	2447	G	N1-C6-O6	6.25	123.65	119.90
10	A	1142	A	N3-C4-C5	6.25	131.18	126.80
31	V	13	C	N3-C4-N4	6.25	122.37	118.00
31	V	49	G	C5-C6-O6	-6.25	124.85	128.60
31	V	39	G	C2'-C3'-O3'	6.24	123.68	113.70
6	5	108	VAL	CG1-CB-CG2	6.23	120.87	110.90
10	A	984	A	N1-C6-N6	6.23	122.34	118.60
6	5	39	THR	C-N-CA	6.22	137.24	121.70
6	5	60	LEU	CB-CG-CD1	6.20	121.55	111.00
10	A	748	G	O4'-C1'-N9	6.20	113.16	108.20
31	V	66	C	O4'-C1'-N1	6.20	113.16	108.20
31	V	26	A	C4-C5-C6	6.19	120.09	117.00
31	V	44	G	O4'-C1'-N9	6.19	113.15	108.20
31	V	2	G	C5-C6-N1	-6.18	108.41	111.50
31	V	57	A	C4-C5-C6	6.18	120.09	117.00
12	C	109	LEU	CA-CB-CG	6.17	129.49	115.30
31	V	52	G	O4'-C1'-N9	6.17	113.14	108.20
31	V	37	G	C5-N7-C8	6.15	107.37	104.30
31	V	26	A	C5-C6-N6	-6.14	118.78	123.70
31	V	1	C	C5-C4-N4	-6.14	115.90	120.20
10	A	1003	G	O5'-P-OP2	-6.14	100.18	105.70
10	A	567	U	N1-C2-O2	-6.13	118.51	122.80
10	A	1142	A	C5-N7-C8	-6.13	100.84	103.90
10	A	2592	G	O5'-P-OP2	-6.13	100.19	105.70
10	A	1950	G	C5-C6-O6	-6.12	124.92	128.60
31	V	38	U	C6-N1-C2	-6.10	117.34	121.00
10	A	1815	A	C8-N9-C4	-6.10	103.36	105.80
10	A	1142	A	C4-C5-N7	6.10	113.75	110.70
10	A	2241	A	C8-N9-C4	-6.09	103.37	105.80
31	V	21	A	C5-C6-N6	-6.08	118.84	123.70
10	A	784	G	P-O3'-C3'	6.07	126.99	119.70
6	5	59	LEU	C-N-CA	6.07	136.87	121.70
10	A	1328	A	O5'-P-OP2	-6.06	100.25	105.70
10	A	784	G	O4'-C1'-N9	-6.06	103.35	108.20
10	A	379	G	N1-C6-O6	6.06	123.53	119.90
21	L	82	LEU	CA-CB-CG	6.05	129.22	115.30
31	V	74	C	C3'-C2'-C1'	-6.05	96.66	101.50
10	A	2505	G	O5'-P-OP2	-6.04	100.26	105.70
10	A	1025	G	P-O3'-C3'	6.02	126.92	119.70
10	A	2250	G	C4-C5-N7	6.01	113.20	110.80
31	V	76	A	C1'-O4'-C4'	6.00	114.70	109.90
10	A	548	G	C8-N9-C4	-5.99	104.00	106.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	A	1069	A	OP2-P-O3'	5.99	118.38	105.20
31	V	59	A	O4'-C1'-N9	5.99	112.99	108.20
10	A	1358	G	C8-N9-C4	-5.98	104.01	106.40
10	A	2554	U	O5'-P-OP1	-5.98	100.32	105.70
10	A	119	A	O5'-P-OP2	-5.97	100.32	105.70
10	A	1073	A	N7-C8-N9	-5.96	110.82	113.80
10	A	1428	C	O5'-P-OP1	-5.96	100.34	105.70
10	A	2534	A	C4-C5-N7	5.96	113.68	110.70
31	V	49	G	O4'-C1'-N9	5.95	112.96	108.20
10	A	2250	G	C5-N7-C8	-5.95	101.33	104.30
31	V	70	C	C5-C4-N4	-5.94	116.04	120.20
31	V	51	A	C5-C6-N6	-5.94	118.94	123.70
10	A	1670	C	N1-C2-O2	-5.93	115.34	118.90
6	5	53	ARG	C-N-CA	5.92	136.50	121.70
10	A	1509	A	O4'-C1'-N9	5.92	112.93	108.20
31	V	75	C	C2-N3-C4	5.91	122.86	119.90
31	V	3	G	N3-C4-N9	5.90	129.54	126.00
10	A	1779	U	N3-C4-O4	-5.89	115.27	119.40
10	A	528	A	C5-C6-N1	-5.89	114.75	117.70
10	A	2715	C	C6-N1-C2	5.89	122.66	120.30
10	A	2747	G	OP2-P-O3'	5.89	118.16	105.20
10	A	2043	C	C6-N1-C2	-5.89	117.94	120.30
10	A	527	C	P-O3'-C3'	5.89	126.77	119.70
31	V	29	G	O4'-C1'-N9	5.87	112.89	108.20
31	V	36	G	O5'-C5'-C4'	5.86	122.84	111.70
10	A	964	C	O5'-P-OP2	-5.86	100.43	105.70
31	V	51	A	C4-C5-C6	5.85	119.93	117.00
31	V	68	U	C6-N1-C2	-5.85	117.49	121.00
10	A	1094	U	N3-C4-C5	-5.85	111.09	114.60
10	A	1837	C	O5'-P-OP1	-5.84	100.44	105.70
31	V	76	A	N7-C8-N9	5.84	116.72	113.80
31	V	32	A	C5-N7-C8	5.83	106.81	103.90
31	V	70	C	N3-C2-O2	-5.83	117.82	121.90
31	V	9	A	C5-C6-N6	-5.82	119.04	123.70
31	V	16	C	N3-C4-N4	5.82	122.07	118.00
10	A	2448	A	C6-C5-N7	-5.80	128.24	132.30
10	A	516	C	O5'-P-OP1	-5.80	100.48	105.70
31	V	59	A	C4-C5-C6	5.79	119.89	117.00
10	A	2241	A	N9-C4-C5	5.79	108.11	105.80
10	A	2447	G	C5-C6-O6	-5.79	125.13	128.60
31	V	16	C	O4'-C1'-N1	5.79	112.83	108.20
31	V	2	G	N7-C8-N9	5.78	115.99	113.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	V	14	A	C5-C6-N6	-5.77	119.08	123.70
31	V	42	G	O4'-C1'-N9	5.75	112.80	108.20
10	A	1088	A	O4'-C1'-N9	-5.74	103.61	108.20
31	V	48	C	N3-C4-N4	5.74	122.02	118.00
10	A	1645	G	N3-C4-C5	-5.72	125.74	128.60
31	V	7	G	N3-C4-C5	-5.72	125.74	128.60
10	A	1247	A	P-O3'-C3'	5.72	126.56	119.70
10	A	1606	C	C2-N3-C4	-5.72	117.04	119.90
10	A	2604	U	N3-C4-O4	-5.72	115.40	119.40
31	V	27	C	N3-C4-N4	5.72	122.00	118.00
6	5	117	LEU	C-N-CA	5.71	135.99	121.70
31	V	26	A	O4'-C1'-N9	5.71	112.77	108.20
10	A	2719	G	N1-C6-O6	5.70	123.32	119.90
31	V	16	C	N3-C4-C5	-5.69	119.62	121.90
10	A	1069	A	C8-N9-C4	-5.69	103.53	105.80
10	A	2501	C	N3-C4-C5	5.68	124.17	121.90
10	A	2719	G	C5-C6-N1	-5.68	108.66	111.50
10	A	866	A	N1-C6-N6	5.68	122.01	118.60
10	A	2271	G	C5-C6-O6	-5.68	125.19	128.60
31	V	45	G	O4'-C1'-N9	5.67	112.74	108.20
10	A	2534	A	C5-N7-C8	-5.67	101.06	103.90
10	A	1066	U	N3-C2-O2	-5.67	118.23	122.20
31	V	7	G	P-O5'-C5'	5.67	129.97	120.90
10	A	1263	U	C6-N1-C2	-5.66	117.61	121.00
10	A	1789	A	O5'-P-OP1	-5.65	100.61	105.70
31	V	61	C	N3-C4-N4	5.65	121.95	118.00
10	A	626	A	N1-C6-N6	5.65	121.99	118.60
10	A	1153	C	N1-C2-O2	-5.65	115.51	118.90
31	V	57	A	C5-C6-N6	-5.64	119.19	123.70
31	V	62	C	N3-C4-N4	5.62	121.93	118.00
10	A	271	G	OP1-P-O3'	5.61	117.55	105.20
31	V	31	C	N3-C4-N4	5.60	121.92	118.00
10	A	1207	C	C6-N1-C2	-5.60	118.06	120.30
31	V	76	A	OP1-P-OP2	-5.60	111.20	119.60
10	A	1979	U	C6-N1-C2	-5.59	117.64	121.00
10	A	1509	A	P-O3'-C3'	5.59	126.41	119.70
31	V	3	G	C4-C5-C6	5.59	122.16	118.80
10	A	1534	U	C5-C6-N1	5.58	125.49	122.70
31	V	12	G	O4'-C1'-N9	5.58	112.66	108.20
31	V	69	G	C6-N1-C2	-5.57	121.76	125.10
10	A	1611	C	N1-C2-O2	-5.57	115.56	118.90
31	V	48	C	N3-C4-C5	-5.56	119.67	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	A	1073	A	C4-N9-C1'	-5.56	116.30	126.30
10	A	1198	U	O5'-P-OP2	-5.56	100.70	105.70
31	V	22	G	O4'-C1'-N9	5.56	112.65	108.20
10	A	2586	U	O5'-C5'-C4'	5.55	122.25	111.70
10	A	2146	C	C6-N1-C2	-5.55	118.08	120.30
10	A	2053	G	N3-C2-N2	-5.54	116.02	119.90
31	V	58	A	C5-C6-N1	-5.54	114.93	117.70
10	A	989	G	O4'-C1'-N9	5.54	112.63	108.20
10	A	2544	G	C6-C5-N7	-5.54	127.08	130.40
31	V	43	G	O4'-C1'-N9	5.54	112.63	108.20
31	V	41	C	N3-C4-N4	5.54	121.88	118.00
10	A	2439	A	N1-C6-N6	5.53	121.92	118.60
10	A	1069	A	O4'-C1'-N9	5.53	112.62	108.20
31	V	57	A	O4'-C1'-N9	5.53	112.62	108.20
10	A	209	C	C6-N1-C2	5.52	122.51	120.30
31	V	25	C	N3-C4-C5	-5.52	119.69	121.90
31	V	28	C	N3-C4-N4	5.52	121.87	118.00
10	A	2326	C	C5-C4-N4	-5.52	116.33	120.20
10	A	1157	G	N1-C6-O6	5.52	123.21	119.90
10	A	2353	G	N1-C6-O6	-5.52	116.59	119.90
31	V	23	C	N3-C4-N4	5.51	121.86	118.00
31	V	62	C	N3-C4-C5	-5.50	119.70	121.90
10	A	2544	G	N1-C6-O6	5.50	123.20	119.90
31	V	33	U	O3'-P-O5'	5.50	114.44	104.00
31	V	28	C	N3-C4-C5	-5.49	119.70	121.90
31	V	23	C	N3-C4-C5	-5.49	119.70	121.90
31	V	14	A	C5-C6-N1	-5.49	114.96	117.70
10	A	2685	G	C5-C6-N1	-5.48	108.76	111.50
31	V	25	C	N3-C4-N4	5.48	121.84	118.00
10	A	84	A	N1-C6-N6	-5.47	115.32	118.60
31	V	17	C	N3-C4-N4	5.47	121.83	118.00
31	V	31	C	N3-C4-C5	-5.46	119.71	121.90
31	V	50	G	O4'-C1'-N9	5.46	112.57	108.20
10	A	2689	U	N3-C4-O4	-5.46	115.58	119.40
10	A	2355	G	C8-N9-C4	5.46	108.58	106.40
10	A	2604	U	C5-C4-O4	5.46	129.17	125.90
10	A	29	U	OP2-P-O3'	5.46	117.20	105.20
10	A	55	G	C5-C6-O6	-5.46	125.33	128.60
10	A	451	U	O4'-C1'-N1	5.45	112.56	108.20
10	A	1125	G	C6-C5-N7	-5.45	127.13	130.40
31	V	57	A	C5-C6-N1	-5.45	114.98	117.70
10	A	1129	A	O5'-P-OP1	-5.45	100.80	105.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	A	2446	G	OP2-P-O3'	5.45	117.18	105.20
11	B	80	U	N1-C2-N3	5.44	118.17	114.90
10	A	1355	G	C8-N9-C4	-5.44	104.22	106.40
10	A	1027	A	O4'-C1'-N9	-5.44	103.85	108.20
10	A	1824	G	N9-C4-C5	5.44	107.57	105.40
31	V	70	C	N3-C4-C5	5.43	124.07	121.90
10	A	1192	G	N9-C4-C5	-5.42	103.23	105.40
10	A	2271	G	N1-C6-O6	5.42	123.15	119.90
10	A	672	C	N1-C2-O2	5.42	122.15	118.90
31	V	58	A	C5-C6-N6	-5.42	119.36	123.70
10	A	2609	U	N1-C1'-C2'	5.42	121.04	114.00
31	V	7	G	C1'-O4'-C4'	5.42	114.23	109.90
31	V	11	C	N3-C4-C5	-5.41	119.73	121.90
10	A	598	U	OP2-P-O3'	5.41	117.10	105.20
10	A	1190	G	C5-N7-C8	-5.41	101.60	104.30
10	A	2244	U	C5-C4-O4	-5.41	122.66	125.90
10	A	532	A	C8-N9-C4	-5.40	103.64	105.80
10	A	1533	C	C5-C6-N1	5.39	123.70	121.00
10	A	2723	C	C6-N1-C2	-5.39	118.14	120.30
31	V	9	A	C5-C6-N1	-5.39	115.01	117.70
10	A	984	A	C5-C6-N1	-5.39	115.01	117.70
10	A	1073	A	C8-N9-C1'	5.38	137.38	127.70
10	A	1565	C	C6-N1-C2	-5.38	118.15	120.30
31	V	73	A	C2'-C3'-O3'	5.38	122.30	113.70
25	P	113	LEU	CA-CB-CG	5.37	127.66	115.30
10	A	250	G	O5'-P-OP2	-5.37	100.87	105.70
10	A	1229	C	C6-N1-C2	5.37	122.45	120.30
10	A	1950	G	C8-N9-C1'	-5.36	120.03	127.00
10	A	2153	C	O4'-C1'-N1	5.36	112.49	108.20
10	A	2037	A	N9-C4-C5	5.36	107.94	105.80
10	A	2263	C	N3-C4-C5	-5.36	119.76	121.90
10	A	2353	G	C2-N3-C4	5.35	114.58	111.90
10	A	991	C	C6-N1-C2	-5.35	118.16	120.30
10	A	837	C	N1-C2-O2	-5.35	115.69	118.90
10	A	2015	A	N1-C6-N6	-5.34	115.39	118.60
10	A	1420	A	O4'-C1'-N9	5.34	112.47	108.20
31	V	53	G	O4'-C1'-N9	5.33	112.47	108.20
31	V	61	C	N3-C4-C5	-5.33	119.77	121.90
10	A	1025	G	N3-C4-C5	-5.33	125.94	128.60
10	A	677	A	OP1-P-O3'	5.33	116.92	105.20
6	5	131	THR	N-CA-C	-5.33	96.62	111.00
10	A	2571	U	C2-N1-C1'	-5.33	111.31	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	A	1684	G	N3-C4-C5	-5.32	125.94	128.60
6	5	50	VAL	CG1-CB-CG2	5.32	119.41	110.90
31	V	59	A	C5-C6-N6	-5.32	119.45	123.70
31	V	68	U	C1'-O4'-C4'	5.31	114.15	109.90
31	V	56	C	N3-C4-C5	-5.31	119.78	121.90
31	V	64	C	N3-C4-N4	5.30	121.71	118.00
10	A	518	G	O5'-P-OP1	-5.29	100.94	105.70
31	V	15	G	O4'-C1'-N9	5.29	112.43	108.20
31	V	51	A	O4'-C1'-N9	5.29	112.43	108.20
10	A	1311	G	N7-C8-N9	5.29	115.75	113.10
31	V	2	G	N9-C4-C5	-5.29	103.28	105.40
10	A	2071	A	OP2-P-O3'	5.29	116.83	105.20
31	V	9	A	O4'-C1'-N9	5.29	112.43	108.20
10	A	1430	G	N1-C6-O6	5.28	123.07	119.90
10	A	2704	C	C6-N1-C2	5.28	122.41	120.30
10	A	2250	G	C2-N3-C4	-5.28	109.26	111.90
31	V	41	C	N3-C4-C5	-5.28	119.79	121.90
10	A	748	G	C4-C5-N7	-5.28	108.69	110.80
10	A	1458	U	P-O3'-C3'	5.28	126.03	119.70
10	A	1759	A	N1-C6-N6	5.27	121.77	118.60
26	Q	63	ARG	NE-CZ-NH2	-5.26	117.67	120.30
31	V	51	A	C5-C6-N1	-5.26	115.07	117.70
10	A	2470	G	OP2-P-O3'	5.26	116.77	105.20
6	5	50	VAL	CA-CB-CG1	5.26	118.79	110.90
10	A	776	G	C4-N9-C1'	5.26	133.34	126.50
10	A	1524	G	C8-N9-C4	-5.26	104.30	106.40
10	A	1970	A	C8-N9-C4	-5.26	103.70	105.80
10	A	2618	G	C5-C6-N1	-5.26	108.87	111.50
10	A	548	G	N3-C4-C5	-5.25	125.97	128.60
10	A	2368	C	C6-N1-C2	5.25	122.40	120.30
10	A	916	G	C6-C5-N7	-5.25	127.25	130.40
10	A	1131	G	OP1-P-O3'	5.25	116.76	105.20
10	A	1446	C	C6-N1-C2	-5.25	118.20	120.30
10	A	2501	C	C6-N1-C1'	5.25	127.10	120.80
35	Z	15	ARG	NE-CZ-NH1	5.25	122.93	120.30
10	A	404	A	C8-N9-C4	-5.25	103.70	105.80
31	V	59	A	C5-C6-N1	-5.25	115.08	117.70
31	V	26	A	C5-C6-N1	-5.25	115.08	117.70
10	A	1936	A	N3-C4-C5	5.24	130.47	126.80
31	V	10	G	O4'-C1'-N9	5.24	112.39	108.20
10	A	1206	G	N3-C4-C5	-5.24	125.98	128.60
10	A	1350	C	C6-N1-C2	5.24	122.40	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	V	6	C	N3-C4-C5	-5.24	119.80	121.90
31	V	13	C	C1'-O4'-C4'	-5.24	105.71	109.90
33	X	29	LEU	CA-CB-CG	5.24	127.35	115.30
10	A	1264	A	O5'-P-OP1	-5.24	100.99	105.70
10	A	733	G	C8-N9-C4	-5.23	104.31	106.40
10	A	2250	G	N7-C8-N9	5.22	115.71	113.10
10	A	1355	G	N3-C2-N2	-5.22	116.25	119.90
10	A	1943	U	C5-C4-O4	5.21	129.03	125.90
10	A	940	G	N1-C6-O6	5.20	123.02	119.90
10	A	2503	A	N1-C6-N6	5.20	121.72	118.60
10	A	1831	G	C8-N9-C4	-5.20	104.32	106.40
10	A	2537	U	C5-C4-O4	5.20	129.02	125.90
31	V	7	G	C2-N3-C4	5.19	114.50	111.90
10	A	833	A	C8-N9-C4	-5.18	103.73	105.80
31	V	7	G	N7-C8-N9	-5.18	110.51	113.10
10	A	2602	A	O4'-C1'-N9	5.17	112.33	108.20
10	A	119	A	P-O3'-C3'	5.17	125.90	119.70
10	A	1238	G	O5'-P-OP2	-5.17	101.05	105.70
11	B	114	C	C5-C4-N4	-5.17	116.58	120.20
10	A	2518	A	N1-C6-N6	5.16	121.70	118.60
10	A	807	U	N3-C4-O4	5.16	123.01	119.40
10	A	2534	A	C5-C6-N6	-5.16	119.57	123.70
6	5	130	PRO	CA-N-CD	-5.15	104.29	111.50
10	A	699	A	N1-C6-N6	5.14	121.69	118.60
10	A	2825	G	N3-C4-N9	5.14	129.09	126.00
10	A	2603	G	O4'-C4'-C3'	5.14	110.21	106.10
10	A	1639	C	C6-N1-C2	5.14	122.36	120.30
10	A	186	G	N3-C4-C5	5.13	131.16	128.60
31	V	56	C	N3-C4-N4	5.13	121.59	118.00
31	V	24	G	O4'-C1'-N9	5.12	112.30	108.20
10	A	1928	A	N1-C6-N6	5.12	121.67	118.60
31	V	17	C	N3-C4-C5	-5.12	119.85	121.90
10	A	2282	G	C8-N9-C4	-5.11	104.36	106.40
31	V	71	C	C2-N3-C4	5.11	122.46	119.90
9	8	61	LEU	CA-CB-CG	5.11	127.05	115.30
10	A	1395	A	O4'-C1'-N9	5.11	112.28	108.20
31	V	5	A	C5-C6-N6	-5.10	119.62	123.70
10	A	1534	U	N1-C2-O2	5.10	126.37	122.80
10	A	1025	G	C8-N9-C4	-5.09	104.36	106.40
10	A	1795	C	N3-C4-C5	-5.09	119.86	121.90
31	V	64	C	N3-C4-C5	-5.09	119.86	121.90
31	V	32	A	N1-C6-N6	5.09	121.66	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	A	465	G	C4-C5-C6	5.09	121.85	118.80
10	A	1659	G	N3-C4-C5	5.09	131.15	128.60
10	A	2198	A	O4'-C1'-N9	5.09	112.27	108.20
10	A	2422	C	N1-C2-O2	5.09	121.95	118.90
10	A	2443	C	N3-C4-N4	5.09	121.56	118.00
10	A	454	A	O5'-P-OP2	-5.08	101.12	105.70
10	A	403	U	P-O3'-C3'	5.08	125.80	119.70
10	A	2015	A	N9-C4-C5	5.08	107.83	105.80
10	A	1779	U	C5-C6-N1	-5.08	120.16	122.70
10	A	1122	G	N3-C4-N9	-5.07	122.96	126.00
10	A	2443	C	C6-N1-C2	-5.07	118.27	120.30
10	A	2537	U	N1-C2-N3	5.07	117.94	114.90
10	A	1533	C	C6-N1-C1'	-5.07	114.72	120.80
31	V	7	G	N1-C2-N2	-5.05	111.65	116.20
31	V	17(A)	U	O4'-C1'-N1	5.05	112.24	108.20
10	A	1606	C	P-O3'-C3'	5.05	125.76	119.70
18	I	79	LEU	CA-CB-CG	5.05	126.92	115.30
10	A	2448	A	C5-C6-N6	-5.05	119.66	123.70
10	A	984	A	N1-C2-N3	5.05	131.82	129.30
10	A	1538	G	N3-C4-C5	5.04	131.12	128.60
31	V	21	A	O4'-C1'-N9	5.04	112.24	108.20
31	V	21	A	C5-C6-N1	-5.04	115.18	117.70
10	A	776	G	C4-C5-C6	5.04	121.83	118.80
10	A	55	G	N1-C6-O6	5.04	122.92	119.90
31	V	5	A	C5-C6-N1	-5.04	115.18	117.70
10	A	376	G	C6-C5-N7	-5.04	127.38	130.40
10	A	686	U	C2-N1-C1'	-5.04	111.65	117.70
31	V	4	C	C4'-C3'-C2'	-5.03	97.57	102.60
29	T	29	THR	N-CA-C	5.03	124.58	111.00
10	A	2502	G	N3-C4-C5	-5.03	126.09	128.60
10	A	2551	C	O5'-P-OP1	-5.03	101.18	105.70
31	V	38	U	N3-C2-O2	5.03	125.72	122.20
10	A	2017	U	N3-C4-O4	5.02	122.92	119.40
10	A	2822	G	C6-C5-N7	-5.02	127.39	130.40
10	A	1358	G	N7-C8-N9	5.02	115.61	113.10
10	A	2455	G	O5'-P-OP2	-5.02	101.19	105.70
12	C	155	ARG	CG-CD-NE	5.02	122.33	111.80
10	A	752	A	C8-N9-C1'	5.01	136.73	127.70
10	A	1314	C	C2-N1-C1'	5.01	124.31	118.80
10	A	2439	A	C4-C5-N7	5.01	113.21	110.70
10	A	1659	G	C2-N3-C4	-5.01	109.39	111.90
10	A	2015	A	C5-C6-N6	5.01	127.71	123.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	V	3	G	C5-C6-N1	-5.01	109.00	111.50
10	A	1649	G	O5'-P-OP1	-5.01	101.19	105.70

There are no chirality outliers.

All (25) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
6	5	130	PRO	Peptide
8	7	15	ILE	Peptide
8	7	21	ASP	Peptide
8	7	23	ARG	Sidechain
8	7	6	ILE	Peptide
12	C	233	GLY	Peptide
13	D	9	VAL	Peptide
19	J	110	PRO	Peptide
20	K	71	ARG	Peptide
28	S	86	MET	Mainchain
28	S	88	ARG	Peptide
28	S	89	ALA	Peptide
31	V	13	C	Sidechain
31	V	3	G	Sidechain
31	V	33	U	Sidechain
31	V	37	G	Sidechain
31	V	39	G	Sidechain
31	V	4	C	Sidechain
31	V	5	A	Sidechain
31	V	66	C	Sidechain
31	V	67	G	Sidechain
31	V	69	G	Sidechain
31	V	70	C	Sidechain
31	V	71	C	Sidechain
31	V	75	C	Sidechain

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	0	444	0	461	19	0
2	1	409	0	440	15	0
3	2	377	0	418	9	0
4	3	504	0	574	10	0
5	4	302	0	340	16	0
6	5	1117	0	1155	121	0
7	6	227	0	237	7	0
8	7	170	0	166	94	0
9	8	753	0	780	14	0
10	A	61274	0	30816	829	0
11	B	2529	0	1281	21	0
12	C	2082	0	2157	54	0
13	D	1565	0	1616	47	0
14	E	1552	0	1619	41	0
15	F	1410	0	1445	45	0
16	G	1323	0	1374	38	0
17	H	384	0	405	13	0
18	I	1032	0	1088	51	0
19	J	1129	0	1162	53	0
20	K	938	0	1012	38	0
21	L	1045	0	1117	36	0
22	M	1074	0	1157	29	0
23	N	960	0	1000	30	0
24	O	892	0	923	20	0
25	P	917	0	965	40	0
26	Q	947	0	1022	51	0
27	R	816	0	839	35	0
28	S	857	0	922	53	0
29	T	738	0	807	35	0
30	U	779	0	834	26	0
31	V	1649	0	832	49	0
32	W	596	0	610	79	0
33	X	625	0	655	18	0
34	Y	509	0	543	13	0
35	Z	449	0	491	18	0
36	7	30	8	18	24	0
37	4	1	0	0	0	0
37	A	135	0	0	0	0
37	B	4	0	0	0	0
37	C	2	0	0	0	0
37	E	1	0	0	0	0
38	4	1	0	0	0	0
39	A	416	0	0	78	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
39	B	14	0	0	1	0
39	C	2	0	0	0	0
39	D	3	0	0	0	0
39	E	2	0	0	0	0
39	L	2	0	0	0	0
All	All	92987	8	61281	1783	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 12.

All (1783) 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)
8:7:11:LYS:CE	28:S:91:GLY:HA3	1.51	1.40
8:7:7:CYS:SG	28:S:95:ARG:NH2	2.05	1.29
15:F:79:ARG:NH2	31:V:56:C:O2	1.62	1.27
8:7:14:ASN:O	8:7:15:ILE:HD13	1.35	1.25
10:A:1923:U:H5"	31:V:24:G:O2'	1.04	1.19
10:A:912:C:OP1	22:M:8:LYS:NZ	1.79	1.13
8:7:6:ILE:HG13	8:7:7:CYS:N	1.57	1.10
8:7:11:LYS:HE3	28:S:91:GLY:HA3	1.13	1.10
10:A:1923:U:C5'	31:V:24:G:O2'	1.98	1.09
28:S:88:ARG:NH1	28:S:94:ASP:OD2	1.84	1.09
8:7:15:ILE:HD11	36:7:1002:TRP:HZ3	1.18	1.07
15:F:79:ARG:NH2	31:V:56:C:C2	2.25	1.05
6:5:71:CYS:HB3	6:5:117:LEU:HD12	1.33	1.04
8:7:21:ASP:HB2	36:7:1001:TRP:N	1.72	1.04
8:7:15:ILE:CD1	36:7:1002:TRP:CZ3	2.40	1.03
8:7:15:ILE:CD1	36:7:1002:TRP:HZ3	1.72	1.02
6:5:26:VAL:HG21	6:5:115:GLY:H	1.23	1.01
10:A:1782:U:C2'	10:A:2608:G:O2'	2.09	1.00
6:5:3:LEU:O	6:5:7:ASP:OD1	1.79	1.00
8:7:7:CYS:O	8:7:8:VAL:CG2	2.10	1.00
8:7:6:ILE:CG1	8:7:7:CYS:H	1.72	1.00
8:7:15:ILE:HD11	36:7:1002:TRP:CZ3	1.95	0.99
10:A:1782:U:H2'	10:A:2608:G:O2'	1.62	0.98
8:7:14:ASN:HB3	8:7:15:ILE:HD13	1.43	0.98
10:A:1923:U:H5"	31:V:24:G:C2'	1.92	0.97
8:7:16:ASP:O	8:7:17:ASN:HB2	1.65	0.96
8:7:11:LYS:HE2	28:S:91:GLY:HA3	1.46	0.95
8:7:6:ILE:HG13	8:7:7:CYS:H	0.81	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:A:1909:C:H4'	31:V:11:C:H4'	1.49	0.94
8:7:15:ILE:HG13	36:7:1002:TRP:CE3	2.03	0.94
10:A:576:U:OP1	39:A:3661:HOH:O	1.85	0.94
6:5:117:LEU:CD2	6:5:120:ALA:HA	1.97	0.93
3:2:3:ARG:NH2	10:A:752:A:P	2.42	0.93
8:7:11:LYS:CE	28:S:91:GLY:CA	2.45	0.92
10:A:1154:G:OP2	26:Q:57:ARG:NH1	2.03	0.92
8:7:19:ILE:O	8:7:20:VAL:HG23	1.69	0.92
10:A:1248:G:OP2	14:E:44:ARG:NH2	2.03	0.92
6:5:71:CYS:HB3	6:5:117:LEU:CD1	1.98	0.91
6:5:71:CYS:CB	6:5:117:LEU:HD12	2.00	0.91
10:A:1923:U:H5"	31:V:24:G:HO2'	1.32	0.91
8:7:22:HIS:C	8:7:23:ARG:HG3	1.91	0.90
10:A:2279:G:N7	32:W:10:ARG:NH2	2.20	0.90
8:7:7:CYS:O	8:7:8:VAL:HG22	1.70	0.90
10:A:2062:A:H2'	10:A:2063:C:C5	2.06	0.89
8:7:14:ASN:HB3	8:7:15:ILE:CD1	2.02	0.89
6:5:24:SER:HB2	6:5:116:GLU:HG2	1.54	0.89
11:B:43:C:O2	15:F:91:ARG:NH1	2.04	0.89
10:A:1922:G:O2'	31:V:25:C:H1'	1.73	0.89
8:7:14:ASN:O	8:7:15:ILE:CD1	2.20	0.89
8:7:14:ASN:OD1	14:E:61:ARG:CZ	2.19	0.89
30:U:98:ASN:O	30:U:100:GLU:N	2.06	0.88
6:5:71:CYS:CB	6:5:117:LEU:CD1	2.50	0.88
8:7:19:ILE:HD12	36:7:1001:TRP:CD1	2.08	0.88
10:A:996:A:OP2	26:Q:91:ARG:NH2	2.07	0.87
10:A:1336:A:OP2	29:T:68:LYS:NZ	2.06	0.87
10:A:2608:G:H5"	10:A:2608:G:H8	1.38	0.86
8:7:7:CYS:O	8:7:7:CYS:SG	2.34	0.86
29:T:39:THR:O	29:T:41:ALA:N	2.09	0.86
8:7:19:ILE:C	8:7:20:VAL:HG23	1.93	0.86
10:A:2611:C:OP2	39:A:3536:HOH:O	1.93	0.86
10:A:2053:G:N2	10:A:2616:C:N3	2.24	0.85
8:7:15:ILE:HG13	36:7:1002:TRP:CZ3	2.13	0.84
8:7:18:LYS:HE3	10:A:746:U:O2	1.78	0.84
8:7:19:ILE:HD12	36:7:1001:TRP:HD1	1.40	0.84
8:7:14:ASN:OD1	14:E:61:ARG:NH2	2.11	0.84
6:5:71:CYS:HA	6:5:117:LEU:HD13	1.60	0.84
10:A:1723:G:O6	10:A:1737:G:O2'	1.94	0.84
10:A:2608:G:H5"	10:A:2608:G:C8	2.12	0.83
10:A:1909:C:O4'	31:V:11:C:O2'	1.95	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:A:981:A:OP1	39:A:3588:HOH:O	1.95	0.83
10:A:1922:G:O3'	31:V:25:C:H4'	1.79	0.83
10:A:2585:U:O2'	10:A:2586:U:H5'	1.78	0.83
10:A:1069:A:N3	10:A:1073:A:N6	2.25	0.83
6:5:33:VAL:N	6:5:36:ASP:OD2	2.12	0.82
12:C:196:ASN:O	12:C:198:GLU:N	2.12	0.82
6:5:103:ASN:ND2	6:5:107:GLU:O	2.13	0.82
10:A:1923:U:OP1	31:V:25:C:H5'	1.79	0.82
6:5:71:CYS:HA	6:5:117:LEU:CD1	2.09	0.82
6:5:77:VAL:C	6:5:79:PRO:HD2	2.00	0.81
28:S:91:GLY:O	28:S:92:ARG:HG2	1.80	0.81
10:A:1783:A:OP1	39:A:3689:HOH:O	1.98	0.81
10:A:945:A:OP2	39:A:3342:HOH:O	1.98	0.81
10:A:1647:U:OP2	39:A:3416:HOH:O	1.98	0.81
10:A:526:A:OP1	39:A:3246:HOH:O	1.97	0.81
24:O:34:HIS:O	24:O:102:ARG:NH2	2.14	0.81
25:P:50:ARG:HB3	25:P:57:ALA:H	1.43	0.81
10:A:991:C:OP2	39:A:3593:HOH:O	1.97	0.81
10:A:2608:G:C5'	10:A:2608:G:H8	1.93	0.81
10:A:504:A:O2'	10:A:505:A:OP1	1.98	0.80
10:A:1371:G:N7	39:A:3398:HOH:O	2.13	0.80
8:7:21:ASP:CB	36:7:1001:TRP:N	2.44	0.80
10:A:1908:C:O2'	31:V:12:G:H5'	1.80	0.80
10:A:1268:A:OP1	39:A:3373:HOH:O	1.99	0.80
10:A:1012:U:OP2	26:Q:69:ARG:NH2	2.14	0.80
10:A:1614:A:C6	28:S:87:PRO:HB3	2.17	0.80
10:A:2448:A:OP2	39:A:3677:HOH:O	2.00	0.79
28:S:88:ARG:HD2	28:S:94:ASP:OD1	1.83	0.79
10:A:1799:G:OP2	12:C:269:ARG:NH2	2.16	0.79
6:5:33:VAL:HG12	6:5:34:THR:H	1.48	0.79
6:5:43:LYS:NZ	6:5:98:GLU:OE1	2.16	0.79
6:5:91:ALA:C	6:5:93:ALA:H	1.87	0.78
10:A:2720:U:OP1	25:P:52:ARG:NH2	2.15	0.78
10:A:1509:A:O2'	10:A:1510:G:OP2	2.01	0.78
10:A:975:A:OP2	39:A:3584:HOH:O	2.00	0.78
34:Y:18:LEU:O	34:Y:22:LEU:N	2.17	0.78
20:K:105:ARG:NH1	20:K:106:GLU:OE2	2.16	0.78
8:7:15:ILE:CG1	36:7:1002:TRP:CZ3	2.66	0.78
8:7:22:HIS:CD2	10:A:2503:A:H8	2.01	0.78
10:A:1782:U:O2	10:A:2608:G:O2'	2.02	0.77
6:5:117:LEU:HD23	6:5:120:ALA:HA	1.64	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:A:946:C:OP2	39:A:3342:HOH:O	2.02	0.77
10:A:2025:C:OP2	39:A:3471:HOH:O	2.03	0.77
10:A:2062:A:H2'	10:A:2063:C:C6	2.19	0.77
13:D:184:ARG:NH2	25:P:6:GLN:OE1	2.17	0.77
6:5:35:VAL:HA	6:5:38:MET:SD	2.24	0.77
6:5:71:CYS:CA	6:5:117:LEU:CD1	2.62	0.77
8:7:16:ASP:O	8:7:17:ASN:CB	2.34	0.76
3:2:3:ARG:NH2	10:A:752:A:OP2	2.18	0.76
8:7:19:ILE:HD13	10:A:2610:C:H5'	1.66	0.76
8:7:7:CYS:O	8:7:8:VAL:HG23	1.85	0.76
10:A:526:A:OP1	39:A:3248:HOH:O	2.03	0.76
12:C:68:ARG:NH2	12:C:126:GLY:O	2.18	0.76
12:C:69:ASN:O	12:C:71:ASP:N	2.18	0.76
8:7:14:ASN:O	8:7:15:ILE:HG23	1.86	0.75
10:A:2331:G:O2'	32:W:39:GLN:O	2.04	0.75
10:A:2588:G:OP2	39:A:3540:HOH:O	2.04	0.75
10:A:1380:G:OP2	39:A:3741:HOH:O	2.03	0.75
10:A:1187:G:OP1	27:R:85:LYS:NZ	2.20	0.75
8:7:18:LYS:O	8:7:19:ILE:HG22	1.87	0.75
10:A:2579:C:OP1	39:A:3537:HOH:O	2.05	0.75
10:A:1922:G:O2'	31:V:25:C:C1'	2.35	0.75
8:7:7:CYS:C	8:7:8:VAL:HG23	2.07	0.74
6:5:131:THR:O	6:5:134:GLU:N	2.20	0.74
5:4:11:CYS:SG	5:4:14:CYS:N	2.60	0.74
11:B:23:G:O6	39:B:1307:HOH:O	2.05	0.74
10:A:2006:C:OP1	39:A:3373:HOH:O	2.04	0.74
10:A:1186:G:OP2	39:A:3592:HOH:O	2.04	0.74
13:D:91:THR:O	13:D:93:GLY:N	2.21	0.74
6:5:1:MET:SD	6:5:2:ALA:N	2.58	0.74
10:A:2707:U:O2	23:N:71:ARG:NH2	2.20	0.74
10:A:1342:A:O2'	10:A:1344:U:OP2	2.04	0.74
10:A:2503:A:OP1	39:A:3661:HOH:O	2.04	0.74
10:A:990:A:OP2	39:A:3591:HOH:O	2.06	0.74
10:A:1153:C:OP2	39:A:3354:HOH:O	2.04	0.74
10:A:572:A:OP2	27:R:80:ARG:NH2	2.21	0.73
6:5:57:ASN:O	6:5:59:LEU:N	2.21	0.73
10:A:1782:U:C2	10:A:2586:U:O4	2.41	0.73
10:A:1782:U:N3	10:A:2586:U:N3	2.35	0.73
19:J:43:GLU:O	19:J:45:THR:N	2.22	0.73
10:A:2056:G:OP2	39:A:3482:HOH:O	2.06	0.73
8:7:11:LYS:HE3	28:S:91:GLY:CA	2.07	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:A:1970:A:OP2	39:A:3467:HOH:O	2.07	0.72
10:A:1998:A:OP2	13:D:141:ARG:NH2	2.21	0.72
10:A:2062:A:H2'	10:A:2063:C:H5	1.55	0.72
8:7:15:ILE:CG1	36:7:1002:TRP:HZ3	2.03	0.72
5:4:2:LYS:NZ	10:A:2478:A:OP2	2.23	0.72
16:G:22:VAL:HG12	16:G:36:LEU:CD1	2.19	0.72
6:5:106:PHE:O	6:5:108:VAL:N	2.22	0.71
10:A:1922:G:HO2'	31:V:25:C:C2'	2.00	0.71
10:A:1439:A:OP2	39:A:3624:HOH:O	2.07	0.71
8:7:22:HIS:CB	10:A:2062:A:H61	2.03	0.71
10:A:981:A:OP1	39:A:3586:HOH:O	2.08	0.71
10:A:621:A:OP2	39:A:3292:HOH:O	2.08	0.71
10:A:1993:U:H4'	13:D:133:THR:HG21	1.73	0.71
10:A:1776:G:OP2	39:A:3448:HOH:O	2.09	0.71
10:A:2353:G:H1'	32:W:30:VAL:HG12	1.72	0.71
25:P:5:LYS:NZ	25:P:9:GLN:OE1	2.23	0.70
10:A:2057:G:OP2	39:A:3482:HOH:O	2.08	0.70
10:A:1805:A:N3	12:C:49:THR:OG1	2.24	0.70
10:A:1010:A:OP2	39:A:3769:HOH:O	2.08	0.70
10:A:1938:A:OP2	39:A:3721:HOH:O	2.09	0.70
10:A:1604:C:OP1	39:A:3403:HOH:O	2.09	0.70
10:A:2324:U:H3'	10:A:2325:G:H5"	1.74	0.70
15:F:116:LEU:N	15:F:176:PHE:O	2.24	0.70
10:A:1799:G:O2'	12:C:179:GLU:OE2	2.07	0.70
10:A:1332:G:OP1	39:A:3752:HOH:O	2.09	0.70
10:A:1782:U:N3	10:A:2586:U:C4	2.59	0.70
10:A:587:C:OP2	21:L:21:ARG:NH2	2.25	0.70
10:A:161:A:H3'	10:A:162:U:H5"	1.72	0.69
10:A:971:G:OP2	10:A:974:G:N2	2.25	0.69
10:A:512:G:N7	39:A:3758:HOH:O	2.25	0.69
10:A:2247:A:OP1	39:A:3500:HOH:O	2.10	0.69
10:A:2091:C:O2	33:X:33:HIS:NE2	2.26	0.69
35:Z:8:GLN:O	35:Z:10:ARG:N	2.25	0.69
8:7:19:ILE:HG23	8:7:20:VAL:HG22	1.73	0.69
10:A:2269:G:OP1	39:A:3504:HOH:O	2.11	0.69
13:D:149:ASN:OD1	13:D:150:GLN:N	2.26	0.69
22:M:66:ARG:NH1	22:M:104:GLU:OE2	2.26	0.68
8:7:15:ILE:HG13	36:7:1002:TRP:HE3	1.59	0.68
6:5:25:ALA:O	6:5:26:VAL:HG13	1.94	0.68
6:5:117:LEU:HD22	6:5:120:ALA:HA	1.76	0.68
32:W:30:VAL:O	32:W:30:VAL:HG13	1.92	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:A:948:C:O2	10:A:984:A:O2'	2.12	0.68
10:A:42:A:C2'	10:A:43:G:H5'	2.24	0.68
10:A:1782:U:O2	10:A:2586:U:O4	2.11	0.67
10:A:301:G:OP2	30:U:81:ARG:NH2	2.26	0.67
10:A:2602:A:H4'	10:A:2603:G:H5'	1.74	0.67
21:L:93:ASN:O	21:L:95:LEU:N	2.27	0.67
10:A:1614:A:N6	28:S:87:PRO:HB3	2.10	0.67
8:7:22:HIS:CD2	10:A:2503:A:C8	2.82	0.67
20:K:76:VAL:HB	25:P:72:VAL:HG22	1.76	0.67
10:A:1936:A:N6	10:A:1963:U:O2	2.26	0.67
6:5:26:VAL:O	6:5:27:VAL:HB	1.93	0.67
8:7:19:ILE:HG23	8:7:20:VAL:CG2	2.25	0.67
10:A:324:A:N6	10:A:338:G:O2'	2.27	0.67
10:A:1820:U:OP1	12:C:176:ARG:NH1	2.27	0.67
11:B:73:A:C4	11:B:104:A:C2	2.82	0.67
18:I:100:ILE:HB	18:I:139:VAL:HA	1.76	0.67
10:A:2615:U:OP1	39:A:3738:HOH:O	2.12	0.67
20:K:18:ARG:HB2	20:K:45:GLU:HB2	1.77	0.66
19:J:4:PHE:N	19:J:44:TYR:OH	2.28	0.66
10:A:1658:C:OP1	39:A:3647:HOH:O	2.11	0.66
10:A:2602:A:O2'	31:V:74:C:OP1	2.12	0.66
10:A:120:U:OP1	39:A:3220:HOH:O	2.12	0.66
10:A:1417:C:HO2'	10:A:1587:G:HO2'	1.43	0.66
10:A:819:A:OP2	10:A:1187:G:N2	2.23	0.66
28:S:88:ARG:CZ	28:S:88:ARG:HB3	2.26	0.66
32:W:37:VAL:HG12	32:W:38:ARG:H	1.61	0.66
6:5:24:SER:CB	6:5:116:GLU:HG2	2.24	0.66
21:L:93:ASN:OD1	21:L:94:THR:N	2.28	0.66
6:5:39:THR:HA	6:5:42:ARG:HD2	1.78	0.66
8:7:21:ASP:O	8:7:23:ARG:N	2.29	0.65
10:A:2062:A:OP2	39:A:3490:HOH:O	2.14	0.65
10:A:363:G:H2'	10:A:364:C:C6	2.31	0.65
19:J:6:ALA:HB3	19:J:45:THR:HG21	1.78	0.65
8:7:11:LYS:HE2	28:S:91:GLY:CA	2.17	0.65
8:7:7:CYS:C	8:7:8:VAL:CG2	2.61	0.65
8:7:15:ILE:CG1	36:7:1002:TRP:CE3	2.78	0.65
20:K:71:ARG:HB3	20:K:72:PRO:HD3	1.78	0.65
10:A:1908:C:O2'	31:V:12:G:C5'	2.45	0.65
10:A:1482:G:H1'	10:A:1509:A:H61	1.62	0.65
10:A:1670:C:OP1	39:A:3432:HOH:O	2.14	0.65
10:A:1199:U:H5'	26:Q:4:LYS:HE3	1.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:A:999:U:OP2	39:A:3355:HOH:O	2.15	0.64
23:N:118:ARG:O	23:N:120:GLU:N	2.30	0.64
10:A:1669:A:OP2	39:A:3713:HOH:O	2.15	0.64
16:G:38:ASP:N	16:G:38:ASP:OD1	2.29	0.64
10:A:2602:A:H2'	31:V:74:C:H5"	1.80	0.64
16:G:1:SER:O	16:G:3:VAL:N	2.31	0.64
25:P:4:ILE:O	25:P:6:GLN:N	2.31	0.64
18:I:73:PRO:O	18:I:112:LYS:NZ	2.31	0.64
28:S:18:ARG:O	28:S:19:LEU:HB2	1.98	0.64
12:C:43:ASN:OD1	12:C:44:ASN:N	2.30	0.64
10:A:2608:G:C8	10:A:2608:G:C5'	2.76	0.64
10:A:1617:C:OP1	39:A:3417:HOH:O	2.15	0.64
10:A:2142:A:H4'	10:A:2143:C:OP2	1.96	0.64
25:P:50:ARG:HG3	25:P:57:ALA:O	1.97	0.64
32:W:35:ILE:O	32:W:37:VAL:N	2.31	0.63
19:J:44:TYR:HB2	26:Q:63:ARG:HB3	1.79	0.63
14:E:58:LYS:NZ	14:E:70:SER:O	2.31	0.63
30:U:73:ASN:ND2	30:U:80:ASP:OD2	2.31	0.63
11:B:87:U:H3'	11:B:88:C:H5'	1.80	0.63
10:A:1385:A:H1'	10:A:1386:C:C6	2.34	0.63
25:P:50:ARG:CB	25:P:57:ALA:H	2.11	0.63
10:A:42:A:H2'	10:A:43:G:H5'	1.80	0.63
29:T:32:LEU:H	29:T:83:ALA:HB3	1.63	0.63
10:A:1614:A:N1	28:S:87:PRO:HB3	2.13	0.63
10:A:2062:A:O2'	10:A:2063:C:H6	1.82	0.63
28:S:88:ARG:HH11	28:S:88:ARG:HG2	1.64	0.63
10:A:2588:G:OP2	39:A:3538:HOH:O	2.15	0.63
10:A:546:U:O2'	10:A:547:A:H4'	1.99	0.63
1:0:42:ILE:HD11	23:N:98:LEU:HB3	1.79	0.63
8:7:19:ILE:HG13	8:7:20:VAL:H	1.63	0.62
28:S:88:ARG:HG2	28:S:94:ASP:OD2	1.99	0.62
6:5:129:LEU:O	6:5:131:THR:N	2.26	0.62
10:A:1567:G:H5'	12:C:57:HIS:CD2	2.35	0.62
10:A:1813:G:H1'	12:C:49:THR:HG21	1.81	0.62
8:7:19:ILE:C	8:7:20:VAL:CG2	2.66	0.62
10:A:2061:G:OP2	39:A:3489:HOH:O	2.16	0.62
18:I:108:ILE:O	18:I:111:THR:OG1	2.17	0.62
30:U:15:GLY:O	30:U:17:ASP:N	2.32	0.62
10:A:1922:G:O2'	31:V:25:C:C2'	2.47	0.62
10:A:1938:A:OP2	39:A:3719:HOH:O	2.16	0.62
10:A:2346:A:H3'	10:A:2347:C:C5'	2.29	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:A:923:G:H1'	32:W:23:LYS:HD3	1.81	0.62
10:A:2011:U:OP2	28:S:16:LYS:NZ	2.31	0.62
8:7:21:ASP:OD2	36:7:1001:TRP:CZ3	2.53	0.62
10:A:861:A:N3	11:B:79:G:O2'	2.27	0.62
18:I:131:THR:O	18:I:134:SER:OG	2.16	0.62
10:A:163:C:O2'	10:A:164:C:O5'	2.17	0.61
10:A:1922:G:O3'	31:V:25:C:C4'	2.47	0.61
24:O:76:LYS:NZ	24:O:80:GLU:OE2	2.29	0.61
23:N:73:ASN:HA	23:N:76:VAL:HG12	1.81	0.61
10:A:2062:A:HO2'	10:A:2063:C:H6	1.49	0.61
6:5:27:VAL:HG13	6:5:83:ALA:HB3	1.83	0.61
6:5:29:ASP:HA	6:5:108:VAL:HG11	1.82	0.61
10:A:1248:G:N7	14:E:46:GLN:NE2	2.48	0.61
10:A:856:G:H21	32:W:19:ARG:NH2	1.97	0.61
19:J:6:ALA:CB	19:J:45:THR:HG21	2.31	0.61
5:4:36:ARG:HG2	5:4:37:GLN:H	1.66	0.61
10:A:963:U:OP2	39:A:3353:HOH:O	2.16	0.61
10:A:1803:A:O3'	12:C:256:THR:OG1	2.19	0.61
32:W:55:ASP:O	32:W:57:THR:N	2.34	0.60
7:6:18:ASP:N	7:6:18:ASP:OD1	2.32	0.60
18:I:100:ILE:HG22	18:I:101:SER:N	2.15	0.60
10:A:511:U:OP2	39:A:3759:HOH:O	2.15	0.60
10:A:1359:A:OP1	39:A:3608:HOH:O	2.16	0.60
23:N:98:LEU:O	23:N:112:TYR:N	2.34	0.60
10:A:2353:G:N3	32:W:30:VAL:CG1	2.65	0.60
13:D:118:PHE:HD1	13:D:119:ALA:H	1.49	0.60
32:W:63:ASP:N	32:W:63:ASP:OD1	2.35	0.60
10:A:983:A:C6	10:A:984:A:C2	2.90	0.60
24:O:89:ASP:HA	24:O:116:GLN:HB3	1.84	0.60
12:C:16:VAL:N	12:C:203:VAL:HG12	2.17	0.60
29:T:19:LYS:O	29:T:23:ALA:N	2.35	0.60
10:A:1828:G:OP2	39:A:3793:HOH:O	2.16	0.60
10:A:480:A:OP2	30:U:43:LYS:NZ	2.34	0.60
10:A:1262:A:OP2	28:S:99:ARG:NH2	2.35	0.59
10:A:616:A:H4'	14:E:101:TYR:CE2	2.36	0.59
30:U:38:ILE:CG2	30:U:39:ASN:N	2.64	0.59
10:A:1782:U:C4	10:A:2586:U:N3	2.70	0.59
8:7:22:HIS:HB2	10:A:2062:A:H61	1.67	0.59
10:A:1782:U:O2'	10:A:2608:G:O2'	2.21	0.59
10:A:1338:G:O2'	29:T:18:GLU:OE2	2.20	0.59
8:7:19:ILE:HA	36:7:1001:TRP:CD1	2.38	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:A:2062:A:C2'	10:A:2063:C:C6	2.85	0.59
6:5:26:VAL:HG21	6:5:115:GLY:N	2.06	0.59
10:A:800:A:OP1	39:A:3321:HOH:O	2.17	0.59
24:O:105:ALA:O	24:O:107:ALA:N	2.35	0.59
18:I:92:PRO:O	18:I:94:LYS:N	2.36	0.59
10:A:635:C:OP2	21:L:126:ARG:NH2	2.35	0.59
10:A:1922:G:O2'	31:V:25:C:O2'	1.73	0.59
6:5:15:VAL:HG22	6:5:66:GLY:HA3	1.84	0.59
18:I:93:ASN:ND2	18:I:135:MET:O	2.35	0.59
14:E:168:ASP:OD2	14:E:170:ARG:NH1	2.36	0.59
10:A:2800:A:H3'	10:A:2801:G:C5'	2.32	0.59
8:7:22:HIS:HB3	10:A:2062:A:H61	1.66	0.59
22:M:41:LEU:HD11	22:M:126:ILE:HD13	1.85	0.59
8:7:22:HIS:O	8:7:23:ARG:HG3	2.03	0.59
10:A:276:U:O2'	10:A:278:A:N7	2.34	0.59
10:A:673:C:OP1	14:E:49:ARG:NH1	2.36	0.59
10:A:1131:G:OP1	19:J:82:GLY:HA2	2.02	0.59
32:W:51:GLY:HA3	32:W:59:PHE:CZ	2.38	0.58
29:T:35:ALA:HB3	29:T:38:ALA:HB2	1.85	0.58
8:7:19:ILE:O	8:7:20:VAL:CG2	2.47	0.58
26:Q:84:LYS:O	26:Q:86:SER:N	2.36	0.58
10:A:370:G:OP2	39:A:3553:HOH:O	2.16	0.58
10:A:1654:A:O2'	13:D:118:PHE:CG	2.55	0.58
10:A:1386:C:H2'	10:A:1387:A:C8	2.39	0.58
10:A:1359:A:OP1	39:A:3611:HOH:O	2.17	0.58
12:C:77:VAL:HG23	12:C:111:ALA:HA	1.85	0.58
10:A:2780:G:OP2	19:J:120:ARG:NE	2.33	0.58
26:Q:63:ARG:NH1	26:Q:95:ALA:O	2.36	0.58
10:A:2499:C:O2	39:A:3524:HOH:O	2.13	0.58
10:A:1076:C:H2'	10:A:1077:A:O4'	2.04	0.58
10:A:370:G:O2'	10:A:424:G:OP1	2.15	0.58
18:I:37:PHE:O	18:I:41:PHE:HB3	2.04	0.58
25:P:63:ILE:HA	25:P:68:GLY:HA2	1.85	0.58
6:5:45:GLY:HA2	6:5:49:GLY:HA2	1.86	0.58
10:A:2579:C:OP1	39:A:3535:HOH:O	2.18	0.57
32:W:51:GLY:HA3	32:W:59:PHE:CE1	2.38	0.57
10:A:1930:G:O2'	10:A:1968:G:O6	2.17	0.57
26:Q:81:GLY:O	26:Q:85:ALA:N	2.37	0.57
32:W:39:GLN:HG2	32:W:41:GLY:H	1.69	0.57
10:A:2548:U:O2	20:K:23:LYS:NZ	2.37	0.57
25:P:50:ARG:HB3	25:P:57:ALA:N	2.17	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:A:1076:C:H1'	18:I:93:ASN:HB3	1.86	0.57
10:A:802:A:OP1	39:A:3327:HOH:O	2.17	0.57
10:A:2502:G:OP2	39:A:3488:HOH:O	2.18	0.57
32:W:9:THR:OG1	32:W:10:ARG:N	2.31	0.57
32:W:28:GLU:HB3	32:W:31:LEU:HD21	1.86	0.57
10:A:2517:C:C6	10:A:2542:A:N7	2.73	0.57
32:W:76:ARG:HH11	32:W:76:ARG:CG	2.17	0.57
6:5:3:LEU:CD1	6:5:5:LEU:HG	2.35	0.57
10:A:27:G:O2'	10:A:28:A:OP2	2.19	0.57
25:P:58:PHE:CD1	25:P:75:THR:HG22	2.40	0.57
10:A:1773:A:N7	10:A:1829:A:H1'	2.20	0.57
10:A:1019:U:H3	10:A:1142:A:H62	1.53	0.57
10:A:422:A:C2	10:A:423:A:C4	2.92	0.57
26:Q:105:PHE:O	26:Q:108:LEU:N	2.38	0.57
10:A:2331:G:O2'	10:A:2336:A:N1	2.38	0.57
6:5:62:ARG:NH2	10:A:1106:G:OP1	2.35	0.56
33:X:32:LEU:O	33:X:33:HIS:ND1	2.39	0.56
24:O:2:ASP:OD1	24:O:3:LYS:N	2.39	0.56
10:A:1923:U:H5'	31:V:25:C:O4'	2.04	0.56
6:5:132:TYR:CZ	7:6:23:ILE:HD11	2.40	0.56
29:T:54:GLU:HG3	29:T:88:LYS:HB2	1.86	0.56
10:A:2439:A:N6	31:V:76:A:OP1	2.39	0.56
14:E:150:THR:HG21	14:E:153:LEU:HA	1.87	0.56
28:S:88:ARG:HH11	28:S:88:ARG:CG	2.17	0.56
10:A:1936:A:H2	10:A:1943:U:C5	2.23	0.56
10:A:85:G:OP2	30:U:6:ARG:HG3	2.06	0.56
10:A:1676:A:OP2	39:A:3755:HOH:O	2.18	0.56
3:2:3:ARG:HH22	10:A:752:A:P	2.29	0.56
26:Q:63:ARG:HH22	26:Q:95:ALA:C	2.08	0.56
10:A:1315:C:OP2	39:A:3750:HOH:O	2.18	0.56
1:0:2:VAL:HG22	10:A:2015:A:C2	2.41	0.56
13:D:118:PHE:O	13:D:120:GLY:N	2.36	0.56
6:5:81:LEU:HA	10:A:1107:G:H4'	1.88	0.56
10:A:1353:A:C8	10:A:1378:A:N6	2.73	0.56
12:C:14:HIS:O	12:C:203:VAL:HG11	2.05	0.56
10:A:2681:C:OP2	13:D:114:LYS:NZ	2.33	0.56
10:A:910:A:N6	10:A:2277:G:O2'	2.36	0.56
20:K:121:GLU:OE2	25:P:62:LYS:NZ	2.36	0.56
8:7:14:ASN:C	8:7:15:ILE:CG1	2.74	0.56
8:7:19:ILE:HA	36:7:1001:TRP:NE1	2.20	0.56
6:5:56:ARG:O	6:5:57:ASN:ND2	2.39	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:J:81:ILE:HG13	19:J:82:GLY:N	2.21	0.56
10:A:1324:G:C4	10:A:1328:A:N6	2.74	0.56
5:4:36:ARG:NH1	10:A:2742:G:OP1	2.38	0.55
27:R:39:LEU:O	27:R:49:ILE:HG23	2.07	0.55
6:5:58:THR:CG2	10:A:1107:G:H5"	2.36	0.55
15:F:151:LEU:HD12	15:F:152:ASP:N	2.21	0.55
10:A:2757:A:N1	16:G:66:THR:HG21	2.21	0.55
10:A:2355:G:H4'	32:W:20:LEU:HD13	1.88	0.55
10:A:1482:G:C6	10:A:1508:A:C2	2.94	0.55
2:1:8:ILE:HD11	2:1:24:LYS:N	2.21	0.55
10:A:100:U:H4'	10:A:101:A:O5'	2.06	0.55
21:L:85:VAL:CG2	21:L:94:THR:HG22	2.36	0.55
28:S:89:ALA:HA	28:S:90:LYS:O	2.07	0.55
10:A:443:A:N7	14:E:40:ARG:HD3	2.21	0.55
25:P:33:GLU:HB2	25:P:38:ARG:HH21	1.71	0.55
6:5:129:LEU:C	6:5:131:THR:H	2.10	0.55
18:I:116:MET:SD	18:I:124:MET:HE2	2.46	0.55
6:5:64:VAL:O	6:5:68:PRO:HD2	2.07	0.55
32:W:18:LYS:HG3	32:W:19:ARG:N	2.21	0.55
10:A:283:G:C2	10:A:284:U:H1'	2.41	0.55
18:I:100:ILE:HD11	18:I:137:LEU:HG	1.88	0.55
10:A:163:C:O2'	10:A:164:C:P	2.65	0.55
10:A:1397:U:OP2	10:A:1398:C:N4	2.34	0.55
10:A:1909:C:H4'	31:V:11:C:C4'	2.30	0.55
10:A:2698:U:H2'	10:A:2699:C:H6	1.72	0.55
35:Z:5:LYS:H	35:Z:5:LYS:HD2	1.72	0.55
29:T:59:ASN:O	29:T:83:ALA:O	2.24	0.55
10:A:686:U:H2'	10:A:788:A:N1	2.21	0.55
19:J:17:VAL:HG23	19:J:139:VAL:HA	1.88	0.55
10:A:834:G:C6	10:A:835:C:C4	2.95	0.55
6:5:44:ALA:O	6:5:49:GLY:N	2.40	0.55
10:A:31:C:OP1	39:A:3696:HOH:O	2.18	0.55
10:A:1001:A:OP2	39:A:3726:HOH:O	2.18	0.55
12:C:68:ARG:CD	12:C:103:ILE:HD11	2.37	0.55
6:5:129:LEU:HB3	6:5:130:PRO:HD2	1.89	0.55
23:N:30:ARG:NH1	23:N:74:GLU:OE2	2.40	0.55
10:A:2335:A:C6	10:A:2337:G:H1'	2.42	0.55
10:A:1458:U:H4'	10:A:1459:G:O5'	2.07	0.55
10:A:811:U:C4	21:L:21:ARG:NH1	2.74	0.54
10:A:1936:A:N6	10:A:1963:U:H3	2.05	0.54
18:I:135:MET:HB3	18:I:137:LEU:HD22	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:A:1759:A:HO2'	10:A:2714:G:HO2'	1.49	0.54
20:K:43:ILE:CD1	20:K:52:VAL:HB	2.37	0.54
10:A:1824:G:N3	12:C:251:THR:HG21	2.21	0.54
8:7:15:ILE:CD1	36:7:1002:TRP:CE3	2.90	0.54
10:A:1909:C:C4'	31:V:11:C:O2'	2.55	0.54
1:0:2:VAL:HG11	10:A:2016:U:H1'	1.89	0.54
29:T:32:LEU:N	29:T:83:ALA:HB3	2.21	0.54
10:A:565:C:O3'	39:A:3329:HOH:O	2.18	0.54
26:Q:91:ARG:NH1	27:R:10:LYS:HB3	2.23	0.54
25:P:50:ARG:CG	25:P:57:ALA:O	2.55	0.54
10:A:784:G:O2'	10:A:785:G:OP2	2.15	0.54
13:D:107:VAL:CG2	13:D:203:VAL:HG23	2.37	0.54
10:A:2585:U:H2'	10:A:2585:U:O2	2.06	0.54
27:R:49:ILE:HB	27:R:51:VAL:O	2.08	0.54
6:5:60:LEU:O	6:5:64:VAL:HB	2.08	0.54
10:A:877:A:C2	10:A:899:A:C2	2.96	0.54
10:A:674:G:H1'	14:E:69:ARG:HE	1.72	0.54
28:S:73:LYS:HB3	28:S:106:VAL:HB	1.90	0.54
10:A:277:G:O2'	10:A:278:A:OP2	2.25	0.54
10:A:1786:A:H1'	10:A:1938:A:N6	2.22	0.54
10:A:855:G:H1'	32:W:23:LYS:HE3	1.89	0.54
30:U:38:ILE:HG22	30:U:39:ASN:H	1.73	0.54
6:5:43:LYS:HZ3	6:5:98:GLU:HB2	1.72	0.54
10:A:2680:U:H5'	13:D:194:PRO:HA	1.88	0.54
10:A:265:A:H4'	10:A:266:G:OP1	2.07	0.54
10:A:1772:A:N1	10:A:1980:G:C6	2.76	0.54
30:U:21:ARG:CZ	30:U:72:PHE:CE2	2.90	0.54
25:P:4:ILE:HG22	25:P:5:LYS:H	1.72	0.54
18:I:98:GLY:HA3	18:I:137:LEU:HB3	1.90	0.54
27:R:49:ILE:HG22	27:R:54:VAL:HG13	1.89	0.54
9:8:80:HIS:HD2	9:8:83:LYS:N	2.05	0.54
6:5:58:THR:HB	6:5:82:ILE:HB	1.89	0.54
1:0:12:ARG:NH1	10:A:1263:U:OP1	2.41	0.54
15:F:103:ILE:HG23	15:F:175:PRO:HD3	1.90	0.54
21:L:77:ILE:CD1	21:L:108:ALA:HB1	2.38	0.54
10:A:84:A:P	30:U:5:ARG:NH1	2.81	0.54
10:A:1754:A:H4'	25:P:102:ARG:NH2	2.22	0.54
8:7:12:TRP:O	8:7:13:PHE:O	2.26	0.54
10:A:1535:A:H4'	10:A:1536:C:OP2	2.08	0.54
10:A:1187:G:H5"	27:R:83:TYR:CE2	2.43	0.53
30:U:35:VAL:HB	30:U:38:ILE:HG21	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:A:1080:A:H1'	18:I:127:SER:HA	1.91	0.53
10:A:1750:G:O2'	10:A:2860:A:N1	2.37	0.53
6:5:4:ASN:O	6:5:6:GLN:N	2.41	0.53
6:5:23:LEU:HG	6:5:24:SER:N	2.22	0.53
13:D:106:LYS:HB3	13:D:206:ALA:HB3	1.89	0.53
6:5:54:VAL:HA	6:5:84:TYR:O	2.08	0.53
13:D:120:GLY:HA2	13:D:162:ALA:CB	2.38	0.53
10:A:1779:U:H5	10:A:1784:A:N7	2.06	0.53
20:K:80:ASP:HB2	25:P:67:GLU:HG3	1.90	0.53
10:A:1069:A:C4	10:A:1073:A:N7	2.77	0.53
10:A:954:G:OP2	22:M:16:ARG:NH2	2.42	0.53
5:4:1:MET:N	10:A:2526:G:N3	2.57	0.53
32:W:37:VAL:HG13	32:W:55:ASP:C	2.29	0.53
10:A:411:G:OP2	10:A:2406:A:O2'	2.25	0.53
29:T:50:LEU:H	29:T:50:LEU:HD12	1.74	0.53
29:T:50:LEU:C	29:T:52:GLU:H	2.11	0.53
10:A:2415:G:H4'	21:L:66:PHE:HB2	1.90	0.53
16:G:84:LYS:HB3	16:G:132:LEU:O	2.09	0.53
10:A:1614:A:N6	28:S:91:GLY:HA2	2.23	0.53
8:7:22:HIS:HD2	10:A:2503:A:H8	1.52	0.53
26:Q:93:ILE:O	26:Q:96:ASP:N	2.39	0.53
22:M:33:LEU:HD22	22:M:128:THR:HB	1.90	0.53
32:W:13:ARG:HG2	32:W:14:ASP:H	1.74	0.53
19:J:32:LEU:HD22	19:J:54:ILE:HD12	1.90	0.53
10:A:396:G:OP2	33:X:9:LYS:NZ	2.40	0.53
10:A:2425:A:H5"	10:A:2427:C:O4'	2.09	0.53
10:A:729:G:H2'	10:A:1775:U:H1'	1.91	0.53
10:A:2211:A:O2'	10:A:2212:A:OP1	2.25	0.53
19:J:39:LYS:HA	19:J:43:GLU:HB2	1.91	0.53
10:A:2602:A:H4'	10:A:2603:G:C5'	2.39	0.53
10:A:2547:A:H2'	10:A:2548:U:C6	2.43	0.53
10:A:2405:G:O2'	10:A:2406:A:OP1	2.26	0.53
16:G:84:LYS:HG3	16:G:132:LEU:H	1.73	0.53
20:K:107:LEU:O	20:K:109:SER:N	2.38	0.53
10:A:1378:A:O2'	10:A:1380:G:N7	2.27	0.53
32:W:46:ALA:HB3	32:W:80:SER:HB3	1.91	0.53
23:N:73:ASN:HA	23:N:76:VAL:CG1	2.39	0.53
26:Q:81:GLY:HA2	26:Q:116:LEU:CD1	2.38	0.53
26:Q:31:TYR:O	26:Q:34:ALA:N	2.42	0.53
10:A:2533:U:OP1	10:A:2665:A:O2'	2.20	0.53
24:O:31:THR:HG22	24:O:34:HIS:H	1.74	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:K:10:VAL:HG11	20:K:16:ALA:HB3	1.90	0.52
10:A:2232:C:P	33:X:26:ARG:HH22	2.33	0.52
6:5:25:ALA:HB3	6:5:85:SER:OG	2.09	0.52
10:A:1738:G:O2'	10:A:1739:A:O5'	2.25	0.52
10:A:947:A:HO2'	10:A:984:A:H2	1.58	0.52
10:A:1288:G:C4	10:A:1327:A:C2	2.98	0.52
10:A:2092:U:H4'	10:A:2093:G:O5'	2.09	0.52
10:A:2297:A:N1	10:A:2321:U:H5	2.07	0.52
10:A:384:A:H2'	10:A:385:C:H5'	1.90	0.52
10:A:299:A:OP2	39:A:3547:HOH:O	2.18	0.52
20:K:70:ARG:HD3	20:K:76:VAL:HG22	1.90	0.52
8:7:24:PRO:HG2	31:V:76:A:O3'	2.09	0.52
10:A:2134:A:HO2'	10:A:2135:A:H8	1.55	0.52
10:A:2502:G:H5'	10:A:2503:A:H5"	1.92	0.52
10:A:1509:A:HO2'	10:A:1510:G:P	2.29	0.52
10:A:1332:G:OP1	39:A:3750:HOH:O	2.18	0.52
10:A:1715:G:N2	10:A:1744:A:OP2	2.36	0.52
26:Q:63:ARG:HH12	26:Q:96:ASP:CA	2.22	0.52
1:0:2:VAL:CG1	10:A:2016:U:H1'	2.40	0.52
10:A:1417:C:O2'	10:A:1587:G:O2'	2.19	0.52
19:J:55:ILE:HD11	19:J:130:HIS:CG	2.45	0.52
10:A:38:A:O2'	14:E:43:THR:HA	2.09	0.52
34:Y:56:LEU:O	34:Y:58:ASN:N	2.39	0.52
6:5:118:ILE:HB	6:5:119:PRO:CD	2.39	0.52
30:U:82:VAL:HG12	30:U:83:GLY:N	2.25	0.52
10:A:2313:C:H5"	15:F:87:LYS:HD3	1.92	0.52
27:R:61:ALA:HB2	27:R:98:ILE:HA	1.92	0.52
29:T:69:ARG:CG	29:T:70:HIS:H	2.23	0.52
8:7:14:ASN:OD1	14:E:61:ARG:NH1	2.41	0.52
6:5:25:ALA:O	6:5:116:GLU:OE1	2.28	0.52
10:A:1776:G:OP2	39:A:3446:HOH:O	2.19	0.52
16:G:83:THR:HA	16:G:84:LYS:CE	2.39	0.52
35:Z:48:ASN:O	35:Z:51:SER:OG	2.27	0.52
8:7:15:ILE:HD12	36:7:1002:TRP:CZ3	2.41	0.52
10:A:2053:G:H1	10:A:2616:C:H42	1.57	0.52
10:A:1069:A:C5	10:A:1073:A:N7	2.77	0.52
6:5:43:LYS:NZ	6:5:98:GLU:HB2	2.24	0.52
10:A:273:G:N2	10:A:365:U:C2	2.77	0.52
6:5:81:LEU:HD23	6:5:82:ILE:N	2.24	0.52
5:4:3:VAL:HG23	5:4:4:ARG:H	1.74	0.52
29:T:44:LYS:HG3	29:T:55:VAL:HG11	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:W:8:SER:O	32:W:9:THR:HG22	2.10	0.51
32:W:37:VAL:HB	32:W:38:ARG:HH11	1.74	0.51
2:1:20:TYR:HH	10:A:2347:C:HO2'	1.56	0.51
10:A:1328:A:H2'	10:A:1330:C:C5	2.45	0.51
10:A:489:G:N7	28:S:49:LYS:NZ	2.58	0.51
19:J:39:LYS:HA	19:J:43:GLU:HG3	1.91	0.51
25:P:50:ARG:CD	25:P:51:ASN:N	2.72	0.51
25:P:33:GLU:CD	25:P:34:GLY:N	2.63	0.51
29:T:50:LEU:O	29:T:52:GLU:N	2.42	0.51
12:C:255:LYS:O	12:C:257:ARG:N	2.43	0.51
10:A:1277:G:C5'	23:N:20:MET:HE2	2.40	0.51
10:A:2039:U:H2'	10:A:2040:G:C8	2.45	0.51
26:Q:94:LEU:C	26:Q:96:ASP:H	2.14	0.51
6:5:36:ASP:O	6:5:39:THR:OG1	2.26	0.51
22:M:73:ILE:HG21	22:M:91:TYR:CZ	2.45	0.51
10:A:2803:G:H2'	10:A:2804:U:C6	2.45	0.51
10:A:460:A:C2	10:A:470:A:C4	2.99	0.51
17:H:41:LYS:HA	17:H:44:ILE:HG12	1.93	0.51
13:D:151:THR:HG22	13:D:152:PRO:HD3	1.92	0.51
22:M:8:LYS:HE3	22:M:9:PHE:CE2	2.45	0.51
10:A:2584:U:H6	10:A:2584:U:O5'	1.94	0.51
13:D:62:LYS:HB2	13:D:63:PRO:HD3	1.92	0.51
10:A:2387:U:O2'	32:W:38:ARG:NH2	2.43	0.51
6:5:94:ARG:O	6:5:97:LYS:N	2.43	0.51
10:A:1753:G:OP1	25:P:92:ARG:NE	2.38	0.51
15:F:132:ARG:O	15:F:133:GLU:HB3	2.10	0.51
10:A:2062:A:C2'	10:A:2063:C:H6	2.24	0.51
10:A:1647:U:OP2	39:A:3418:HOH:O	2.19	0.51
10:A:974:G:H8	10:A:990:A:H62	1.58	0.51
10:A:856:G:H21	32:W:19:ARG:HH22	1.58	0.51
10:A:1394:U:H4'	10:A:1603:A:H4'	1.92	0.51
31:V:33:U:C4	31:V:35:G:OP2	2.63	0.51
35:Z:6:ILE:O	35:Z:34:THR:HA	2.10	0.51
10:A:1783:A:N1	10:A:2587:A:H2'	2.25	0.51
19:J:44:TYR:O	19:J:45:THR:HB	2.11	0.51
10:A:26:G:C6	10:A:27:G:N1	2.79	0.51
10:A:1797:G:O2'	12:C:256:THR:CG2	2.59	0.51
32:W:76:ARG:HH11	32:W:76:ARG:HG2	1.76	0.51
23:N:20:MET:HE1	23:N:40:LYS:HE2	1.93	0.51
18:I:109:ALA:HB2	18:I:128:ILE:HG13	1.93	0.51
35:Z:41:PRO:HA	35:Z:44:ARG:HB3	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:8:9:ARG:NH2	9:8:12:GLN:HA	2.26	0.51
24:O:36:TYR:CD1	24:O:36:TYR:N	2.78	0.51
6:5:3:LEU:HD12	6:5:5:LEU:H	1.76	0.51
20:K:9:ASN:O	20:K:83:ALA:HA	2.11	0.51
22:M:20:LEU:HD22	22:M:20:LEU:N	2.26	0.51
10:A:2063:C:O2	10:A:2063:C:H2'	2.10	0.51
10:A:945:A:C5	10:A:2448:A:C2	2.98	0.51
32:W:16:GLU:O	32:W:17:ALA:HB3	2.10	0.51
19:J:81:ILE:CG1	19:J:82:GLY:N	2.74	0.51
10:A:954:G:O2'	10:A:2274:A:N1	2.41	0.51
10:A:1869:G:H3'	10:A:1870:C:H5"	1.94	0.51
16:G:16:VAL:HG21	16:G:44:HIS:CD2	2.46	0.51
10:A:2094:A:C2	10:A:2196:C:C2	2.99	0.51
10:A:1816:C:C5	12:C:61:TYR:CE2	2.98	0.51
21:L:81:ASP:O	21:L:83:ALA:N	2.41	0.51
21:L:91:ASP:OD1	21:L:92:LEU:N	2.43	0.51
35:Z:30:ARG:HH11	35:Z:30:ARG:HB3	1.76	0.51
8:7:19:ILE:HD13	10:A:2610:C:C5'	2.39	0.50
26:Q:94:LEU:C	26:Q:96:ASP:N	2.65	0.50
2:1:33:LEU:N	2:1:51:ALA:HB3	2.25	0.50
13:D:193:VAL:HG21	13:D:201:LEU:HD21	1.93	0.50
10:A:2314:A:OP1	15:F:87:LYS:NZ	2.44	0.50
28:S:86:MET:SD	28:S:96:ILE:HG21	2.51	0.50
9:8:51:GLN:OE1	9:8:57:TYR:OH	2.28	0.50
9:8:44:HIS:HE1	9:8:86:LEU:H	1.59	0.50
22:M:53:MET:HE3	22:M:63:ILE:HD13	1.93	0.50
15:F:71:LYS:HD3	15:F:72:SER:N	2.26	0.50
2:1:4:ILE:HG23	2:1:5:ARG:H	1.76	0.50
14:E:148:ILE:HA	14:E:187:VAL:HB	1.93	0.50
20:K:19:VAL:CG1	20:K:41:ILE:HG12	2.40	0.50
10:A:654:A:H3'	10:A:654:A:N3	2.26	0.50
26:Q:91:ARG:HE	26:Q:93:ILE:CG2	2.25	0.50
26:Q:65:ASN:OD1	26:Q:69:ARG:NH1	2.42	0.50
13:D:91:THR:O	13:D:91:THR:OG1	2.28	0.50
29:T:89:GLU:O	29:T:91:GLN:N	2.41	0.50
10:A:2329:U:H2'	10:A:2330:G:C8	2.47	0.50
23:N:52:ILE:HB	23:N:94:TYR:CD2	2.46	0.50
6:5:55:VAL:HG13	10:A:1084:A:H5'	1.93	0.50
10:A:223:A:C5	10:A:422:A:C8	3.00	0.50
10:A:1778:U:H2'	10:A:1784:A:N6	2.27	0.50
10:A:2571:U:O2'	13:D:151:THR:CG2	2.60	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:A:1300:G:H4'	10:A:1301:A:H5'	1.92	0.50
10:A:1203:U:O2'	21:L:4:ASN:OD1	2.28	0.50
16:G:96:ALA:HB3	16:G:103:ASN:HB2	1.93	0.50
3:2:34:ARG:NH1	3:2:41:ARG:O	2.45	0.50
10:A:1437:C:H2'	10:A:1438:U:C6	2.46	0.50
10:A:1533:C:H2'	10:A:1534:U:C6	2.46	0.50
10:A:1475:G:O2'	10:A:1514:G:O6	2.30	0.50
18:I:48:ILE:HG13	18:I:49:GLU:H	1.77	0.50
10:A:27:G:N2	10:A:512:G:H1'	2.26	0.50
10:A:565:C:H2'	10:A:566:U:O4'	2.11	0.50
10:A:322:A:H5'	10:A:340:A:H1'	1.94	0.50
22:M:35:ALA:O	22:M:36:VAL:HB	2.11	0.50
10:A:189:G:O6	10:A:205:G:O2'	2.19	0.50
10:A:750:A:OP1	10:A:1615:C:N4	2.40	0.50
10:A:139:U:O2'	29:T:1:MET:HA	2.12	0.50
10:A:141:G:N1	29:T:1:MET:O	2.44	0.50
10:A:2352:A:C6	32:W:30:VAL:HG11	2.47	0.50
21:L:19:LEU:HB2	21:L:27:LEU:HB3	1.94	0.50
28:S:13:SER:O	28:S:14:ALA:CB	2.60	0.50
5:4:7:VAL:O	5:4:35:GLN:NE2	2.42	0.50
11:B:55:U:O3'	15:F:23:SER:OG	2.21	0.50
10:A:2354:C:H4'	32:W:31:LEU:HD22	1.92	0.50
12:C:256:THR:O	12:C:256:THR:OG1	2.28	0.50
10:A:1533:C:C2	10:A:1534:U:C4	2.99	0.50
18:I:36:GLU:HB3	18:I:66:PHE:CE1	2.46	0.50
10:A:1022:G:C5	10:A:1140:C:C4	3.00	0.50
10:A:1808:A:O2'	33:X:2:ARG:NH2	2.45	0.50
20:K:13:ASN:O	20:K:15:GLY:N	2.43	0.50
3:2:27:GLY:O	3:2:30:VAL:HB	2.11	0.50
8:7:11:LYS:NZ	28:S:91:GLY:HA3	2.22	0.50
10:A:1923:U:C5'	31:V:24:G:C2'	2.76	0.50
27:R:39:LEU:HA	27:R:49:ILE:HG21	1.92	0.50
13:D:148:GLN:N	13:D:148:GLN:OE1	2.45	0.50
22:M:106:ASP:O	22:M:108:VAL:N	2.44	0.50
10:A:2074:U:H2'	10:A:2075:U:C6	2.46	0.50
14:E:112:LEU:HD13	14:E:186:VAL:HG11	1.94	0.50
10:A:118:A:N3	10:A:178:G:H1'	2.27	0.50
16:G:73:SER:O	16:G:77:GLY:N	2.45	0.50
10:A:1654:A:H2'	10:A:1655:A:H8	1.76	0.49
28:S:20:VAL:HG11	28:S:44:ALA:HA	1.93	0.49
16:G:30:GLY:O	16:G:32:LEU:N	2.38	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:A:391:A:C6	10:A:411:G:C2	3.00	0.49
10:A:1179:G:H2'	10:A:1180:U:O4'	2.12	0.49
10:A:2061:G:H21	10:A:2062:A:H2	1.59	0.49
10:A:1782:U:H2'	10:A:2608:G:HO2'	1.72	0.49
26:Q:63:ARG:NH1	26:Q:96:ASP:HA	2.28	0.49
6:5:138:ARG:NH2	7:6:26:MET:HA	2.28	0.49
10:A:1607:C:H4'	10:A:1608:A:O5'	2.13	0.49
34:Y:8:GLU:O	34:Y:12:GLU:HB2	2.12	0.49
10:A:2701:U:H3'	10:A:2702:G:C5'	2.42	0.49
10:A:2504:U:O5'	10:A:2504:U:H6	1.94	0.49
6:5:4:ASN:C	6:5:6:GLN:H	2.16	0.49
10:A:1474:U:H2'	10:A:1475:G:H5'	1.95	0.49
10:A:1730:C:OP1	10:A:1730:C:H4'	2.12	0.49
10:A:748:G:OP2	28:S:88:ARG:HB2	2.12	0.49
10:A:443:A:C5	14:E:40:ARG:HD3	2.47	0.49
10:A:2211:A:O2'	10:A:2212:A:P	2.70	0.49
13:D:151:THR:CG2	13:D:152:PRO:HD3	2.42	0.49
14:E:32:VAL:HG23	14:E:178:VAL:HG12	1.95	0.49
23:N:96:ARG:NH1	23:N:114:GLU:OE2	2.44	0.49
10:A:564:C:O2	10:A:578:G:N2	2.46	0.49
8:7:21:ASP:OD2	36:7:1001:TRP:CE3	2.66	0.49
10:A:308:G:O2'	10:A:329:G:N2	2.46	0.49
24:O:51:ALA:HB3	24:O:78:VAL:HG13	1.95	0.49
18:I:123:ALA:HA	18:I:126:ARG:CZ	2.43	0.49
4:3:4:LYS:NZ	10:A:253:C:OP2	2.38	0.49
33:X:70:LEU:O	33:X:75:GLU:N	2.45	0.49
6:5:95:LEU:H	6:5:95:LEU:HD22	1.77	0.49
10:A:1908:C:HO2'	31:V:12:G:H5'	1.74	0.49
10:A:923:G:H1'	32:W:23:LYS:CD	2.43	0.49
29:T:54:GLU:CG	29:T:88:LYS:HB2	2.42	0.49
10:A:995:C:O2	19:J:3:THR:HG23	2.13	0.49
28:S:24:ILE:HG22	28:S:71:VAL:HG11	1.95	0.49
10:A:2062:A:C2'	10:A:2062:A:N3	2.76	0.49
10:A:1567:G:H2'	12:C:84:PRO:HG3	1.95	0.49
18:I:60:VAL:HG22	18:I:66:PHE:HB3	1.95	0.49
19:J:21:THR:HG22	19:J:22:GLY:N	2.27	0.49
31:V:6:C:H2'	31:V:7:G:H8	1.78	0.49
4:3:30:HIS:HD2	10:A:2421:G:N7	2.10	0.49
10:A:2228:G:H22	33:X:33:HIS:HE2	1.61	0.49
18:I:135:MET:HB3	18:I:137:LEU:CD2	2.43	0.49
10:A:1417:C:N3	10:A:1581:G:N2	2.60	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:A:479:A:C2	10:A:480:A:C4	3.01	0.49
25:P:91:VAL:O	25:P:92:ARG:HG2	2.12	0.49
35:Z:26:LEU:O	35:Z:37:ARG:NH1	2.44	0.49
17:H:9:VAL:O	17:H:13:GLY:N	2.46	0.49
28:S:88:ARG:NH1	28:S:88:ARG:HB3	2.28	0.49
15:F:110:ILE:O	15:F:112:ASP:N	2.46	0.49
10:A:1022:G:C6	10:A:1140:C:C4	3.01	0.49
6:5:51:TYR:CD1	6:5:51:TYR:C	2.86	0.49
8:7:21:ASP:O	8:7:22:HIS:C	2.51	0.48
10:A:999:U:OP2	39:A:3356:HOH:O	2.19	0.48
10:A:2330:G:C2	10:A:2386:A:C2	3.01	0.48
30:U:85:ARG:HD3	30:U:86:PHE:N	2.28	0.48
3:2:10:LEU:HD23	10:A:770:G:H5"	1.95	0.48
10:A:2109:U:H2'	10:A:2110:G:H5'	1.93	0.48
1:0:24:VAL:O	1:0:25:THR:OG1	2.30	0.48
10:A:1922:G:H4'	31:V:25:C:O2'	2.13	0.48
10:A:2583:G:H3'	10:A:2584:U:C5	2.47	0.48
18:I:89:SER:OG	18:I:135:MET:SD	2.68	0.48
10:A:2016:U:H2'	10:A:2017:U:C6	2.48	0.48
10:A:1844:C:O3'	12:C:255:LYS:NZ	2.43	0.48
16:G:15:ASP:O	16:G:16:VAL:HG13	2.12	0.48
15:F:10:GLU:O	15:F:12:VAL:N	2.44	0.48
32:W:49:ASN:HA	32:W:61:LYS:HB2	1.94	0.48
13:D:68:PHE:C	13:D:73:VAL:HG12	2.33	0.48
10:A:2393:U:H5'	21:L:60:ARG:O	2.13	0.48
15:F:79:ARG:HB3	15:F:82:TYR:CZ	2.48	0.48
32:W:9:THR:HG23	32:W:10:ARG:HD3	1.95	0.48
10:A:301:G:H1'	10:A:302:C:C6	2.48	0.48
27:R:49:ILE:HD12	27:R:52:PRO:HA	1.95	0.48
10:A:1327:A:N6	10:A:1328:A:C2	2.81	0.48
6:5:4:ASN:C	6:5:6:GLN:N	2.66	0.48
10:A:107:G:H2'	10:A:108:G:H8	1.78	0.48
10:A:1485:U:H2'	10:A:1486:U:C6	2.49	0.48
29:T:34:VAL:O	29:T:34:VAL:CG2	2.61	0.48
1:0:2:VAL:CG2	10:A:2015:A:C2	2.96	0.48
32:W:49:ASN:C	32:W:49:ASN:ND2	2.66	0.48
10:A:1996:C:OP1	20:K:31:ARG:NE	2.46	0.48
25:P:105:LYS:HA	25:P:108:ARG:HD2	1.95	0.48
4:3:51:LYS:NZ	10:A:938:G:OP2	2.33	0.48
28:S:88:ARG:HG2	28:S:94:ASP:CG	2.34	0.48
10:A:1069:A:C1'	10:A:1073:A:H62	2.27	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:A:1268:A:OP1	39:A:3374:HOH:O	2.20	0.48
10:A:1778:U:H2'	10:A:1784:A:H62	1.78	0.48
10:A:250:G:C6	10:A:251:A:C6	3.01	0.48
10:A:2581:G:C2	10:A:2610:C:C6	3.02	0.48
10:A:747:U:O2'	28:S:88:ARG:NE	2.47	0.48
10:A:973:A:P	27:R:81:LYS:HZ3	2.36	0.48
10:A:856:G:O2'	32:W:22:VAL:HG23	2.14	0.48
6:5:58:THR:HG23	10:A:1107:G:H5"	1.94	0.48
18:I:40:ALA:O	18:I:43:ALA:HB3	2.14	0.48
10:A:528:A:C2	10:A:2043:C:H4'	2.49	0.48
5:4:6:SER:HB2	10:A:1031:G:H4'	1.95	0.48
22:M:1:MET:O	22:M:2:LEU:CB	2.62	0.48
10:A:846:U:HO2'	10:A:847:U:P	2.36	0.48
16:G:104:LEU:HB2	16:G:112:VAL:HG21	1.96	0.48
15:F:79:ARG:HB3	15:F:82:TYR:CE1	2.48	0.48
5:4:2:LYS:HZ1	10:A:2478:A:P	2.35	0.48
10:A:1199:U:H5'	26:Q:4:LYS:CE	2.42	0.48
16:G:84:LYS:HG3	16:G:132:LEU:N	2.28	0.48
19:J:32:LEU:CD2	19:J:54:ILE:HD12	2.44	0.48
12:C:225:ASN:HB3	12:C:226:PRO:HD2	1.96	0.48
6:5:39:THR:HA	6:5:42:ARG:CD	2.43	0.48
10:A:2800:A:H3'	10:A:2801:G:H5"	1.96	0.48
6:5:68:PRO:HA	6:5:72:LEU:HD11	1.94	0.48
10:A:2406:A:C2	21:L:69:ARG:NH2	2.82	0.48
34:Y:56:LEU:O	34:Y:57:LEU:HB3	2.14	0.48
18:I:14:ALA:HB3	18:I:51:GLY:H	1.79	0.48
27:R:68:ARG:HD3	27:R:92:TRP:CZ2	2.49	0.48
10:A:1135:C:N4	10:A:1139:G:C6	2.82	0.48
10:A:749:A:C6	10:A:1618:A:C2	3.01	0.48
10:A:1348:C:H2'	10:A:1349:C:H5'	1.96	0.48
4:3:63:TYR:HH	10:A:592:A:HO2'	1.61	0.48
14:E:164:LEU:HB3	14:E:167:VAL:CG1	2.44	0.48
10:A:1760:C:H2'	10:A:1761:C:O4'	2.14	0.48
25:P:19:PHE:CD1	25:P:19:PHE:N	2.82	0.48
8:7:14:ASN:O	8:7:15:ILE:CG1	2.61	0.48
19:J:44:TYR:CD1	26:Q:63:ARG:HG2	2.49	0.48
10:A:983:A:N6	10:A:984:A:C2	2.82	0.48
32:W:18:LYS:CG	32:W:19:ARG:N	2.77	0.48
6:5:51:TYR:HD1	6:5:52:MET:N	2.12	0.48
10:A:580:U:H2'	10:A:581:C:H6	1.79	0.48
10:A:11:C:C3'	10:A:12:U:H5'	2.44	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:A:2867:G:O2'	10:A:2868:A:OP2	2.28	0.48
16:G:23:ILE:HG21	16:G:71:LEU:HD11	1.95	0.48
8:7:11:LYS:NZ	10:A:1614:A:C5	2.81	0.48
8:7:14:ASN:C	8:7:15:ILE:HG12	2.34	0.48
10:A:1923:U:H5"	31:V:24:G:H2'	1.90	0.48
18:I:100:ILE:HD13	18:I:137:LEU:HD12	1.96	0.48
6:5:15:VAL:HG22	6:5:66:GLY:CA	2.44	0.48
10:A:2747:G:O2'	16:G:66:THR:HG22	2.14	0.48
10:A:2425:A:C5'	10:A:2427:C:O4'	2.62	0.48
15:F:79:ARG:CZ	31:V:56:C:C2	2.87	0.47
10:A:1799:G:C5	12:C:175:LEU:HD23	2.49	0.47
32:W:44:PHE:HD1	32:W:45:HIS:CE1	2.32	0.47
10:A:1814:G:C6	10:A:1815:A:N6	2.82	0.47
10:A:725:G:C6	10:A:726:G:N1	2.82	0.47
10:A:2678:C:H2'	10:A:2679:A:O4'	2.14	0.47
21:L:82:LEU:CD1	21:L:116:VAL:HG23	2.44	0.47
32:W:39:GLN:HG2	32:W:40:ARG:N	2.28	0.47
10:A:983:A:N6	10:A:984:A:N1	2.62	0.47
31:V:34:G:C2	31:V:35:G:C4	3.02	0.47
20:K:13:ASN:O	20:K:14:SER:OG	2.29	0.47
33:X:70:LEU:O	33:X:74:GLY:N	2.46	0.47
31:V:6:C:H2'	31:V:7:G:C8	2.49	0.47
12:C:232:GLY:H	12:C:241:LYS:HE3	1.79	0.47
22:M:34:LYS:HD2	22:M:131:VAL:HG11	1.95	0.47
15:F:64:PRO:HA	15:F:88:VAL:HG22	1.95	0.47
10:A:2862:G:C5	10:A:2863:C:C5	3.02	0.47
6:5:110:ALA:HB1	6:5:113:PHE:CZ	2.49	0.47
6:5:23:LEU:H	6:5:87:GLU:HB2	1.79	0.47
26:Q:63:ARG:HH22	26:Q:96:ASP:N	2.12	0.47
10:A:391:A:C5	10:A:411:G:C2	3.02	0.47
29:T:29:THR:OG1	29:T:86:THR:N	2.43	0.47
35:Z:38:GLU:O	35:Z:43:ILE:HG12	2.13	0.47
6:5:100:ALA:HB2	6:5:125:ARG:HE	1.79	0.47
10:A:2230:G:O3'	33:X:29:LEU:HD23	2.14	0.47
27:R:66:HIS:CG	27:R:94:THR:HG22	2.50	0.47
6:5:71:CYS:CA	6:5:117:LEU:HD13	2.31	0.47
6:5:54:VAL:HG22	6:5:83:ALA:HB1	1.97	0.47
6:5:60:LEU:HD23	6:5:78:GLY:HA3	1.96	0.47
17:H:8:LYS:O	17:H:9:VAL:HB	2.15	0.47
20:K:30:ARG:NH1	20:K:32:TYR:O	2.45	0.47
10:A:2902:C:C2'	10:A:2903:U:O5'	2.63	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:5:123:ILE:HG12	6:5:124:ASP:N	2.30	0.47
19:J:43:GLU:O	19:J:45:THR:HG22	2.13	0.47
26:Q:91:ARG:HH21	26:Q:93:ILE:HD13	1.80	0.47
10:A:2355:G:H4'	32:W:20:LEU:CD1	2.44	0.47
10:A:2335:A:C5	10:A:2337:G:C4	3.02	0.47
10:A:1088:A:HO2'	10:A:1089:A:P	2.37	0.47
18:I:19:PRO:CG	18:I:23:VAL:HG23	2.45	0.47
28:S:63:GLY:O	28:S:64:ALA:CB	2.62	0.47
32:W:9:THR:HG23	32:W:10:ARG:N	2.30	0.47
16:G:22:VAL:O	16:G:22:VAL:HG23	2.14	0.47
10:A:478:A:C6	10:A:480:A:C6	3.03	0.47
29:T:54:GLU:N	29:T:54:GLU:OE1	2.48	0.47
21:L:68:SER:O	21:L:69:ARG:HB3	2.15	0.47
13:D:174:SER:OG	13:D:175:LEU:N	2.46	0.47
13:D:38:LYS:NZ	13:D:81:GLU:OE2	2.26	0.47
10:A:451:U:C2	10:A:453:A:N7	2.83	0.47
8:7:19:ILE:HG13	8:7:20:VAL:N	2.30	0.47
28:S:88:ARG:NH1	28:S:88:ARG:CG	2.73	0.47
10:A:996:A:H4'	26:Q:91:ARG:NE	2.29	0.47
6:5:127:ALA:O	6:5:129:LEU:N	2.48	0.47
10:A:2346:A:H3'	10:A:2347:C:H5"	1.96	0.47
32:W:23:LYS:HE2	32:W:24:ARG:H	1.79	0.47
30:U:38:ILE:CG2	30:U:39:ASN:H	2.28	0.47
9:8:80:HIS:HD2	9:8:83:LYS:H	1.62	0.47
18:I:14:ALA:HB1	18:I:45:THR:HG23	1.97	0.47
10:A:2701:U:H3'	10:A:2702:G:H5"	1.96	0.47
33:X:67:LEU:HD23	33:X:70:LEU:HD12	1.96	0.47
16:G:112:VAL:HG23	16:G:113:ASP:N	2.28	0.47
6:5:110:ALA:HB1	6:5:113:PHE:CE1	2.49	0.47
9:8:2:PHE:HB3	9:8:50:MET:HE1	1.97	0.47
10:A:2889:C:N4	10:A:2890:G:C6	2.83	0.47
10:A:1817:G:H2'	10:A:1818:U:H5'	1.97	0.47
10:A:2839:G:N2	10:A:2880:C:C4	2.82	0.47
33:X:39:VAL:HG22	33:X:44:ARG:O	2.13	0.47
32:W:28:GLU:O	32:W:30:VAL:N	2.48	0.47
32:W:18:LYS:HA	32:W:36:ILE:HG13	1.95	0.47
10:A:1327:A:H2'	10:A:1328:A:O4'	2.14	0.47
10:A:1474:U:C2'	10:A:1475:G:H5'	2.44	0.47
20:K:24:VAL:HG13	20:K:33:ALA:HB2	1.95	0.47
10:A:1079:C:O2	18:I:130:GLY:HA3	2.15	0.47
32:W:72:GLY:N	32:W:73:PRO:CD	2.78	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:F:5:ASP:OD1	15:F:8:LYS:NZ	2.46	0.47
22:M:46:ILE:HD13	22:M:47:GLU:N	2.30	0.47
10:A:2601:C:H6	10:A:2601:C:O5'	1.97	0.47
15:F:69:ALA:N	15:F:82:TYR:O	2.47	0.47
32:W:9:THR:CG2	32:W:10:ARG:HD3	2.44	0.47
10:A:1392:A:N6	10:A:1393:A:N6	2.63	0.47
2:1:4:ILE:HD11	2:1:27:ARG:HB2	1.96	0.47
10:A:221:A:N1	10:A:265:A:O2'	2.45	0.47
10:A:2210:U:H4'	10:A:2211:A:H5'	1.97	0.47
32:W:47:GLY:H	32:W:80:SER:HB3	1.80	0.47
18:I:120:ASP:O	18:I:123:ALA:N	2.46	0.47
1:0:9:ARG:NH1	10:A:517:C:OP2	2.48	0.47
10:A:1939:U:O2	10:A:1967:C:H4'	2.15	0.47
21:L:23:ILE:HD12	27:R:84:ARG:CZ	2.45	0.47
12:C:265:PHE:N	12:C:265:PHE:CD1	2.82	0.47
10:A:2587:A:H8	10:A:2587:A:O5'	1.97	0.47
10:A:587:C:P	21:L:21:ARG:NH2	2.88	0.47
10:A:1198:U:O3'	26:Q:4:LYS:HE3	2.15	0.47
13:D:148:GLN:HB2	13:D:152:PRO:HG2	1.97	0.47
28:S:24:ILE:HD11	28:S:36:LEU:HD13	1.96	0.47
19:J:36:LEU:O	19:J:121:LYS:NZ	2.39	0.47
4:3:21:PHE:O	4:3:22:LYS:O	2.33	0.47
10:A:657:U:H2'	10:A:658:U:C6	2.50	0.47
13:D:169:ARG:O	13:D:170:VAL:HG13	2.15	0.47
15:F:134:GLN:O	15:F:136:ILE:N	2.47	0.47
19:J:84:ILE:O	19:J:84:ILE:HG23	2.15	0.47
3:2:3:ARG:NH2	10:A:752:A:OP1	2.48	0.46
10:A:1738:G:HO2'	10:A:1739:A:P	2.38	0.46
10:A:630:G:N2	10:A:633:A:OP2	2.37	0.46
21:L:19:LEU:HD23	21:L:19:LEU:C	2.35	0.46
10:A:995:C:N4	19:J:2:LYS:HB3	2.29	0.46
10:A:1219:U:OP2	26:Q:18:LYS:NZ	2.46	0.46
10:A:1161:C:H1'	27:R:8:GLY:O	2.15	0.46
12:C:246:PRO:HG2	12:C:247:TRP:CZ3	2.50	0.46
11:B:29:A:H2'	11:B:30:C:C6	2.50	0.46
6:5:77:VAL:O	6:5:79:PRO:HD2	2.13	0.46
25:P:72:VAL:HG23	25:P:72:VAL:O	2.15	0.46
30:U:73:ASN:HA	30:U:95:PHE:CE2	2.50	0.46
16:G:123:GLU:HG2	16:G:124:CYS:N	2.30	0.46
22:M:22:GLN:O	22:M:24:THR:N	2.48	0.46
29:T:61:LEU:C	29:T:61:LEU:HD12	2.35	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:A:923:G:N3	32:W:23:LYS:HD2	2.31	0.46
10:A:479:A:H4'	10:A:480:A:OP1	2.15	0.46
6:5:15:VAL:HG21	6:5:66:GLY:HA2	1.96	0.46
33:X:39:VAL:HG21	33:X:42:GLU:HB2	1.96	0.46
12:C:75:ALA:HB2	12:C:95:TYR:HA	1.97	0.46
10:A:2436:G:C2	10:A:2437:G:C8	3.04	0.46
10:A:504:A:HO2'	10:A:505:A:P	2.29	0.46
10:A:2478:A:H2'	10:A:2479:U:H5'	1.98	0.46
10:A:1567:G:C2'	12:C:84:PRO:HG3	2.46	0.46
32:W:17:ALA:O	32:W:18:LYS:CB	2.64	0.46
6:5:68:PRO:HA	6:5:72:LEU:CG	2.46	0.46
11:B:51:G:OP2	24:O:64:TYR:HD2	1.98	0.46
5:4:8:LYS:NZ	10:A:2467:C:OP1	2.48	0.46
10:A:2649:C:H2'	10:A:2650:U:C6	2.50	0.46
10:A:2897:U:H2'	10:A:2898:U:C6	2.51	0.46
15:F:39:VAL:HG13	15:F:40:GLY:N	2.31	0.46
10:A:523:C:H5"	10:A:540:C:O2'	2.15	0.46
27:R:64:VAL:HG21	27:R:97:LYS:HB2	1.97	0.46
19:J:12:LYS:O	19:J:13:ARG:CB	2.64	0.46
31:V:26:A:H61	31:V:44:G:H1	1.64	0.46
10:A:947:A:O2'	10:A:984:A:H2	1.98	0.46
27:R:49:ILE:HG22	27:R:53:PHE:C	2.36	0.46
20:K:24:VAL:CG1	20:K:30:ARG:HD3	2.45	0.46
18:I:24:GLY:O	18:I:27:LEU:HG	2.16	0.46
10:A:227:A:O2'	10:A:2407:A:O2'	2.19	0.46
10:A:419:U:H2'	10:A:420:C:C6	2.50	0.46
16:G:163:TYR:O	16:G:164:ALA:HB2	2.15	0.46
19:J:37:ARG:HA	19:J:118:MET:CE	2.45	0.46
12:C:93:VAL:HG12	12:C:94:LEU:N	2.31	0.46
12:C:67:LYS:HG2	12:C:150:GLY:HA2	1.97	0.46
25:P:50:ARG:HG2	25:P:57:ALA:N	2.30	0.46
10:A:2365:G:H4'	32:W:59:PHE:CZ	2.51	0.46
18:I:125:THR:O	18:I:128:ILE:N	2.48	0.46
16:G:23:ILE:H	16:G:23:ILE:HD12	1.81	0.46
10:A:1057:A:C6	10:A:1086:A:C2	3.04	0.46
10:A:959:A:H62	22:M:82:MET:CE	2.28	0.46
10:A:1090:A:C2	10:A:1102:C:H1'	2.50	0.46
10:A:1478:G:C2	10:A:1479:G:N7	2.83	0.46
10:A:2318:G:C6	10:A:2319:G:C6	3.03	0.46
10:A:1248:G:C5	14:E:46:GLN:NE2	2.84	0.46
10:A:1509:A:C4	10:A:1510:G:C8	3.04	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:W:60:ALA:HA	32:W:81:ILE:HD12	1.97	0.46
5:4:36:ARG:O	5:4:37:GLN:C	2.54	0.46
15:F:131:VAL:HG22	15:F:151:LEU:H	1.80	0.46
35:Z:39:ASP:OD2	35:Z:44:ARG:NH2	2.46	0.46
10:A:1313:U:H2'	10:A:1610:A:C2	2.51	0.46
10:A:2740:A:C6	10:A:2764:A:C8	3.04	0.46
6:5:88:HIS:CB	6:5:89:PRO:HD3	2.44	0.46
17:H:21:VAL:CG2	17:H:25:TYR:CD2	2.98	0.46
17:H:40:THR:C	17:H:42:LYS:H	2.19	0.46
10:A:2793:C:H2'	10:A:2794:C:C6	2.50	0.46
6:5:71:CYS:HA	6:5:117:LEU:HD11	1.96	0.46
6:5:33:VAL:HG12	6:5:34:THR:N	2.26	0.46
32:W:30:VAL:HG23	32:W:60:ALA:O	2.15	0.46
10:A:1936:A:C2	10:A:1943:U:C5	3.03	0.46
9:8:80:HIS:CD2	9:8:83:LYS:HB2	2.51	0.46
29:T:69:ARG:CD	29:T:70:HIS:H	2.28	0.46
6:5:48:ALA:HB3	6:5:51:TYR:HB3	1.98	0.46
2:1:16:THR:HG21	2:1:41:VAL:HG13	1.97	0.46
15:F:30:VAL:CG1	15:F:96:TRP:CH2	2.99	0.46
10:A:627:A:C6	10:A:637:A:C8	3.04	0.46
11:B:37:C:C5	11:B:38:C:C4	3.04	0.46
10:A:2326:C:H4'	10:A:2327:A:OP1	2.16	0.46
1:0:42:ILE:HD11	23:N:98:LEU:CB	2.46	0.46
10:A:2024:G:C4	10:A:2040:G:N2	2.84	0.46
10:A:11:C:H2'	10:A:12:U:H5'	1.98	0.46
10:A:1060:U:H3	10:A:1088:A:H2	1.64	0.46
20:K:98:ARG:HA	20:K:118:LEU:HD23	1.97	0.46
8:7:14:ASN:C	8:7:15:ILE:HD13	2.22	0.46
14:E:44:ARG:HH11	14:E:44:ARG:HG3	1.80	0.46
1:0:42:ILE:H	1:0:42:ILE:HD12	1.80	0.46
14:E:187:VAL:O	14:E:188:MET:HB3	2.16	0.46
29:T:29:THR:HB	29:T:86:THR:HG22	1.98	0.46
19:J:12:LYS:O	19:J:13:ARG:HB2	2.15	0.46
1:0:8:THR:HG21	10:A:2021:C:P	2.56	0.46
8:7:14:ASN:O	8:7:15:ILE:CG2	2.62	0.45
15:F:113:PHE:HE1	15:F:116:LEU:HD13	1.81	0.45
1:0:3:GLN:HA	10:A:2615:U:C2	2.51	0.45
35:Z:3:THR:HA	35:Z:37:ARG:O	2.16	0.45
27:R:68:ARG:HD3	27:R:92:TRP:CE2	2.50	0.45
15:F:147:ARG:HG3	15:F:148:VAL:N	2.30	0.45
20:K:99:ILE:HG21	20:K:119:ALA:HB2	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:A:751:A:C6	10:A:789:A:C5	3.04	0.45
23:N:103:ARG:CZ	23:N:110:MET:CE	2.95	0.45
17:H:31:VAL:HB	17:H:32:PRO:CD	2.46	0.45
18:I:61:TYR:N	18:I:61:TYR:CD1	2.82	0.45
18:I:137:LEU:HD23	18:I:137:LEU:H	1.81	0.45
13:D:193:VAL:HB	13:D:194:PRO:HD2	1.98	0.45
6:5:110:ALA:O	6:5:113:PHE:N	2.46	0.45
18:I:57:VAL:HG23	18:I:71:LYS:CE	2.46	0.45
10:A:1569:A:N6	10:A:1570:A:C6	2.84	0.45
17:H:14:SER:OG	17:H:17:ASP:CG	2.55	0.45
10:A:728:G:H4'	12:C:12:ARG:HD3	1.98	0.45
10:A:1662:U:O2	10:A:2687:U:H4'	2.17	0.45
6:5:71:CYS:CA	6:5:117:LEU:HD11	2.43	0.45
26:Q:91:ARG:HH21	26:Q:93:ILE:HG21	1.81	0.45
10:A:1936:A:N6	10:A:1963:U:C2	2.84	0.45
18:I:100:ILE:CG2	18:I:101:SER:N	2.79	0.45
26:Q:4:LYS:NZ	26:Q:7:VAL:CG1	2.79	0.45
32:W:19:ARG:CZ	32:W:22:VAL:HB	2.46	0.45
10:A:1141:U:H4'	10:A:1142:A:O4'	2.17	0.45
10:A:118:A:C8	10:A:119:A:C8	3.04	0.45
10:A:1171:G:C6	10:A:1172:C:C4	3.04	0.45
10:A:2108:A:C2'	10:A:2109:U:O5'	2.64	0.45
6:5:100:ALA:HB3	6:5:125:ARG:HD2	1.98	0.45
10:A:666:A:H4'	21:L:48:ARG:HD2	1.99	0.45
16:G:118:ALA:O	16:G:120:ILE:N	2.41	0.45
6:5:63:ALA:HB3	6:5:84:TYR:CE2	2.52	0.45
10:A:271:G:H4'	10:A:272:A:OP1	2.17	0.45
2:1:33:LEU:N	2:1:51:ALA:CB	2.80	0.45
10:A:2862:G:C6	10:A:2863:C:C4	3.04	0.45
25:P:21:PRO:HD3	25:P:49:ILE:HD12	1.98	0.45
31:V:70:C:H2'	31:V:71:C:H5'	1.98	0.45
10:A:1542:U:H2'	10:A:1543:G:O4'	2.16	0.45
11:B:11:C:O2'	11:B:15:A:N6	2.50	0.45
12:C:163:ILE:HG23	12:C:171:VAL:CG1	2.47	0.45
10:A:1593:A:H2'	10:A:1594:U:O4'	2.17	0.45
23:N:70:THR:HB	23:N:75:ILE:CD1	2.46	0.45
10:A:2144:G:N3	10:A:2144:G:H3'	2.30	0.45
14:E:154:ASP:OD1	14:E:154:ASP:N	2.50	0.45
26:Q:91:ARG:HH12	27:R:10:LYS:HB3	1.82	0.45
32:W:39:GLN:HG3	32:W:42:THR:H	1.81	0.45
35:Z:5:LYS:N	35:Z:5:LYS:HD2	2.32	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:Q:103:VAL:HG23	26:Q:104:ALA:N	2.32	0.45
10:A:281:C:H2'	10:A:282:A:C8	2.51	0.45
10:A:1482:G:H1'	10:A:1509:A:N6	2.30	0.45
10:A:2353:G:N3	32:W:30:VAL:HG12	2.32	0.45
10:A:855:G:H21	32:W:23:LYS:HG2	1.82	0.45
29:T:29:THR:CB	29:T:86:THR:H	2.29	0.45
20:K:98:ARG:HA	20:K:118:LEU:CD2	2.47	0.45
10:A:1686:C:C2	10:A:1703:G:C2	3.05	0.45
10:A:1992:G:OP1	39:A:3420:HOH:O	2.20	0.45
10:A:2852:G:C6	10:A:2853:C:N3	2.84	0.45
12:C:24:HIS:NE2	12:C:79:ARG:NH1	2.65	0.45
28:S:88:ARG:HD2	28:S:94:ASP:CG	2.35	0.45
19:J:44:TYR:HD1	26:Q:63:ARG:HG2	1.81	0.45
25:P:50:ARG:CB	25:P:57:ALA:N	2.78	0.45
23:N:33:ILE:CD1	23:N:118:ARG:NE	2.80	0.45
10:A:635:C:O2'	10:A:639:U:OP1	2.34	0.45
2:1:8:ILE:HG21	2:1:51:ALA:HA	1.98	0.45
19:J:49:ASP:OD1	19:J:121:LYS:NZ	2.32	0.45
10:A:2343:U:O2'	10:A:2373:G:O2'	2.28	0.45
10:A:2481:G:HO2'	10:A:2482:A:H8	1.64	0.45
10:A:1838:C:H4'	10:A:1839:G:C8	2.51	0.45
21:L:132:ARG:HG3	21:L:142:ILE:HD12	1.98	0.45
10:A:1186:G:P	39:A:3593:HOH:O	2.75	0.45
1:0:3:GLN:NE2	10:A:2016:U:O2	2.46	0.45
26:Q:4:LYS:NZ	26:Q:7:VAL:HG11	2.31	0.45
12:C:38:LYS:NZ	12:C:57:HIS:O	2.39	0.45
32:W:19:ARG:C	32:W:19:ARG:CD	2.85	0.45
2:1:4:ILE:HG23	2:1:5:ARG:N	2.32	0.45
31:V:2:G:C6	31:V:3:G:C5	3.05	0.45
4:3:12:ARG:HD3	21:L:61:LEU:O	2.16	0.45
6:5:136:ILE:HG13	6:5:139:LEU:HD12	1.98	0.45
10:A:2262:U:H4'	10:A:2328:A:C2	2.52	0.45
10:A:792:A:C6	10:A:2440:C:C6	3.05	0.45
10:A:1340:U:H4'	10:A:1341:G:OP2	2.17	0.45
13:D:121:THR:O	13:D:122:VAL:HB	2.17	0.45
10:A:593:U:H2'	10:A:594:U:C6	2.51	0.45
19:J:44:TYR:O	19:J:45:THR:CB	2.64	0.45
10:A:278:A:N1	10:A:362:A:C8	2.85	0.45
21:L:85:VAL:HG22	21:L:94:THR:HG22	1.97	0.45
16:G:83:THR:C	16:G:84:LYS:HD3	2.37	0.45
2:1:6:GLU:OE1	2:1:52:LYS:CE	2.64	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:A:979:A:H2'	10:A:982:C:H42	1.82	0.45
13:D:1:MET:HG2	13:D:205:PRO:HG3	1.98	0.45
10:A:33:C:O2	10:A:447:A:N6	2.50	0.45
34:Y:45:GLN:O	34:Y:46:VAL:HB	2.17	0.45
28:S:1:MET:O	28:S:108:SER:HB2	2.16	0.45
14:E:119:ILE:O	14:E:119:ILE:HG13	2.16	0.45
25:P:91:VAL:HG11	25:P:96:LEU:HD21	1.98	0.45
13:D:44:GLY:HA3	13:D:45:TYR:HD1	1.82	0.45
10:A:1150:C:H2'	10:A:1151:A:O5'	2.17	0.45
10:A:247:G:H4'	10:A:386:G:C5	2.51	0.45
10:A:2745:C:C4	10:A:2746:U:C4	3.05	0.45
10:A:2103:C:H2'	10:A:2104:C:C5'	2.47	0.45
10:A:820:A:H2'	10:A:821:A:O4'	2.16	0.45
10:A:288:U:H2'	10:A:289:G:C8	2.52	0.45
26:Q:7:VAL:HG13	26:Q:8:ILE:N	2.32	0.44
20:K:10:VAL:HG21	20:K:17:ARG:H	1.81	0.44
19:J:55:ILE:HD11	19:J:130:HIS:CD2	2.51	0.44
14:E:147:LEU:HB3	14:E:186:VAL:HG23	2.00	0.44
10:A:2407:A:C2	10:A:2408:U:C2	3.05	0.44
31:V:36:G:H2'	31:V:37:G:O4'	2.17	0.44
10:A:2564:A:C2	10:A:2647:U:H4'	2.53	0.44
13:D:70:LYS:O	13:D:71:ALA:HB3	2.16	0.44
10:A:2846:G:H2'	10:A:2847:U:O4'	2.17	0.44
10:A:2758:A:H2'	10:A:2759:G:H5'	1.99	0.44
10:A:597:G:C2	10:A:661:A:C2	3.04	0.44
10:A:980:A:C6	10:A:981:A:N1	2.86	0.44
10:A:973:A:O4'	10:A:1188:U:C6	2.70	0.44
10:A:85:G:OP1	30:U:6:ARG:N	2.49	0.44
29:T:48:GLN:O	29:T:52:GLU:HA	2.17	0.44
10:A:1428:C:C5	10:A:1569:A:H5"	2.52	0.44
10:A:2180:U:C2	10:A:2181:U:C5	3.06	0.44
24:O:79:ALA:O	24:O:82:ALA:N	2.49	0.44
13:D:3:GLY:HA3	13:D:204:LYS:HG2	1.99	0.44
4:3:3:ILE:HG21	4:3:62:PRO:HG3	1.98	0.44
14:E:160:ALA:O	14:E:161:ALA:HB3	2.18	0.44
10:A:748:G:OP2	28:S:88:ARG:CB	2.66	0.44
10:A:994:C:H1'	27:R:10:LYS:CE	2.47	0.44
10:A:996:A:H4'	26:Q:91:ARG:CD	2.47	0.44
10:A:2683:C:O2	20:K:70:ARG:NH2	2.38	0.44
6:5:125:ARG:CZ	6:5:125:ARG:HA	2.47	0.44
10:A:336:C:N3	10:A:337:C:C5	2.86	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:G:175:LYS:HA	16:G:176:LYS:HA	1.79	0.44
20:K:61:VAL:HG22	20:K:87:LEU:HD11	1.98	0.44
10:A:1181:U:H2'	10:A:1182:G:C8	2.52	0.44
15:F:128:SER:HA	15:F:154:THR:HA	1.99	0.44
4:3:31:ILE:HG13	4:3:31:ILE:O	2.17	0.44
10:A:2062:A:O2'	10:A:2063:C:O5'	2.31	0.44
10:A:819:A:C4	10:A:1189:A:C2	3.06	0.44
30:U:73:ASN:O	30:U:74:ALA:HB3	2.18	0.44
10:A:799:G:C6	10:A:800:A:C6	3.05	0.44
25:P:58:PHE:CE1	25:P:75:THR:HG22	2.51	0.44
9:8:80:HIS:CD2	9:8:82:TYR:H	2.35	0.44
31:V:34:G:H2'	31:V:35:G:C8	2.53	0.44
13:D:69:ALA:HA	13:D:73:VAL:CG1	2.47	0.44
12:C:265:PHE:N	12:C:265:PHE:HD1	2.15	0.44
15:F:127:TYR:O	15:F:128:SER:CB	2.65	0.44
10:A:2283:C:C2	10:A:2389:G:C2	3.06	0.44
12:C:76:VAL:HG22	12:C:76:VAL:O	2.17	0.44
13:D:86:GLU:N	13:D:86:GLU:CD	2.69	0.44
22:M:26:VAL:HB	22:M:133:LYS:HA	2.00	0.44
10:A:1387:A:H5'	10:A:1469:A:H1'	2.00	0.44
25:P:102:ARG:O	25:P:103:THR:HG22	2.17	0.44
31:V:34:G:C6	31:V:35:G:C6	3.05	0.44
18:I:45:THR:O	18:I:48:ILE:HG13	2.17	0.44
17:H:8:LYS:O	17:H:13:GLY:HA2	2.16	0.44
27:R:64:VAL:O	27:R:65:ALA:HB3	2.18	0.44
10:A:2326:C:C6	10:A:2326:C:H3'	2.52	0.44
20:K:118:LEU:O	20:K:119:ALA:HB3	2.17	0.44
21:L:122:VAL:CG1	21:L:142:ILE:HG12	2.47	0.44
10:A:1252:G:C2	26:Q:32:ARG:HG2	2.52	0.44
10:A:1523:U:O2'	10:A:1524:G:H5'	2.18	0.44
16:G:24:THR:HG23	16:G:34:ARG:HG2	1.99	0.44
30:U:53:GLN:N	30:U:54:PRO:CD	2.80	0.44
29:T:40:LYS:HG2	29:T:58:VAL:HG22	1.99	0.44
10:A:61:C:H2'	10:A:62:U:H5'	2.00	0.44
8:7:17:ASN:O	36:7:1002:TRP:CG	2.70	0.44
10:A:1737:G:H5"	10:A:1738:G:OP2	2.17	0.44
10:A:545:U:H2'	10:A:546:U:O3'	2.18	0.44
6:5:15:VAL:CG2	6:5:66:GLY:HA2	2.47	0.44
18:I:109:ALA:CB	18:I:128:ILE:HG13	2.48	0.44
5:4:6:SER:HB2	10:A:1031:G:C4'	2.47	0.44
10:A:2902:C:H2'	10:A:2903:U:O5'	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:F:134:GLN:OE1	15:F:149:ARG:HB3	2.18	0.44
10:A:315:G:H2'	10:A:316:C:C6	2.52	0.44
10:A:132:G:C2'	10:A:133:U:H5'	2.48	0.44
10:A:1045:C:C3'	10:A:1046:A:H5'	2.48	0.44
10:A:764:A:C6	10:A:781:A:C2	3.06	0.44
10:A:1443:U:H2'	10:A:1444:G:C8	2.53	0.44
10:A:1867:G:C5	10:A:1868:C:C5	3.05	0.44
24:O:43:ASN:O	24:O:45:SER:N	2.50	0.44
8:7:14:ASN:C	8:7:15:ILE:CD1	2.85	0.44
10:A:980:A:C4	10:A:1136:G:O4'	2.70	0.44
15:F:107:VAL:HG11	15:F:116:LEU:HD21	1.99	0.44
10:A:1197:G:H2'	10:A:1198:U:H6	1.83	0.44
32:W:19:ARG:NH2	32:W:22:VAL:HG21	2.33	0.44
10:A:800:A:OP1	39:A:3324:HOH:O	2.21	0.44
30:U:6:ARG:O	30:U:24:VAL:HB	2.17	0.44
10:A:2747:G:O6	10:A:2755:C:H5"	2.18	0.44
20:K:80:ASP:CB	25:P:67:GLU:HG3	2.47	0.44
16:G:104:LEU:HB2	16:G:112:VAL:CG2	2.47	0.44
10:A:222:A:N6	10:A:231:A:C2	2.86	0.44
11:B:90:C:H5"	11:B:90:C:H6	1.83	0.44
10:A:684:G:C2	10:A:794:A:C2	3.06	0.44
21:L:111:ILE:HD12	21:L:111:ILE:N	2.33	0.44
26:Q:91:ARG:HH11	27:R:11:GLN:H	1.64	0.44
6:5:129:LEU:CB	6:5:130:PRO:HD2	2.47	0.44
10:A:277:G:H2'	10:A:361:G:O6	2.17	0.44
28:S:18:ARG:HG3	28:S:76:VAL:HG13	1.98	0.44
10:A:855:G:H21	32:W:23:LYS:CG	2.31	0.44
29:T:69:ARG:HG3	29:T:70:HIS:H	1.83	0.44
31:V:37:G:C2	31:V:38:U:H1'	2.53	0.44
4:3:31:ILE:CG1	4:3:31:ILE:O	2.66	0.44
13:D:35:THR:N	13:D:49:GLN:O	2.41	0.44
12:C:109:LEU:HD23	12:C:110:LYS:H	1.83	0.44
13:D:110:THR:HG23	13:D:171:THR:HG22	2.00	0.44
21:L:2:ARG:HA	21:L:5:THR:CG2	2.48	0.44
11:B:27:C:C5	11:B:28:C:C5	3.06	0.44
10:A:476:G:H4'	10:A:502:A:N1	2.33	0.44
16:G:60:GLY:O	16:G:61:TRP:HB2	2.17	0.44
19:J:30:THR:HG22	19:J:31:GLU:N	2.31	0.44
32:W:19:ARG:HA	32:W:34:SER:HA	2.00	0.44
32:W:24:ARG:HD3	32:W:65:LYS:HG2	2.00	0.44
10:A:2276:G:P	22:M:83:GLY:O	2.76	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:F:72:SER:HB2	15:F:80:GLN:HB2	1.99	0.44
10:A:1171:G:N2	10:A:1179:G:C4	2.86	0.44
13:D:73:VAL:HG23	13:D:74:GLU:H	1.83	0.44
10:A:247:G:N7	10:A:249:C:C2	2.86	0.44
24:O:15:ARG:NE	24:O:93:ASP:OD2	2.44	0.44
10:A:818:G:H5'	10:A:839:U:OP1	2.18	0.44
10:A:2788:C:H2'	10:A:2789:C:C6	2.53	0.44
8:7:17:ASN:HA	36:7:1002:TRP:CE3	2.52	0.43
19:J:44:TYR:O	19:J:44:TYR:CD2	2.71	0.43
18:I:100:ILE:HD11	18:I:137:LEU:CG	2.48	0.43
11:B:78:A:H2'	11:B:79:G:O4'	2.18	0.43
19:J:80:HIS:O	19:J:82:GLY:N	2.50	0.43
14:E:42:GLY:O	14:E:43:THR:OG1	2.35	0.43
29:T:69:ARG:CG	29:T:70:HIS:N	2.81	0.43
10:A:581:C:H2'	10:A:582:A:C8	2.54	0.43
10:A:580:U:O3'	26:Q:30:VAL:HG13	2.18	0.43
10:A:1071:G:H1'	10:A:1089:A:C5	2.53	0.43
16:G:123:GLU:HG2	16:G:125:PRO:HD3	2.01	0.43
10:A:2283:C:H5"	10:A:2389:G:O2'	2.18	0.43
26:Q:27:ARG:HA	26:Q:33:VAL:HG12	1.99	0.43
22:M:13:HIS:O	22:M:14:LYS:CB	2.66	0.43
24:O:41:ALA:O	24:O:44:GLY:N	2.41	0.43
35:Z:15:ARG:HG2	35:Z:15:ARG:HH11	1.82	0.43
9:8:29:ILE:HD13	9:8:30:ILE:N	2.33	0.43
12:C:180:MET:O	12:C:267:VAL:N	2.43	0.43
22:M:102:LEU:HD12	22:M:102:LEU:N	2.32	0.43
8:7:13:PHE:CG	8:7:14:ASN:N	2.83	0.43
10:A:1923:U:C5'	31:V:24:G:H2'	2.48	0.43
17:H:8:LYS:O	17:H:9:VAL:CB	2.66	0.43
10:A:201:C:OP1	33:X:17:ARG:NH2	2.51	0.43
18:I:91:LYS:HB2	18:I:95:ASP:HB2	2.00	0.43
21:L:112:LEU:HD23	21:L:114:GLY:H	1.83	0.43
10:A:2307:G:N2	10:A:2311:A:C8	2.85	0.43
10:A:2682:A:C8	13:D:11:MET:HG3	2.53	0.43
28:S:66:ILE:HD13	28:S:67:ASP:N	2.32	0.43
15:F:94:ARG:CG	15:F:94:ARG:HH11	2.31	0.43
8:7:15:ILE:CG1	8:7:16:ASP:H	2.30	0.43
26:Q:91:ARG:HH11	27:R:11:GLN:N	2.16	0.43
10:A:948:C:H1'	10:A:984:A:O2'	2.17	0.43
10:A:2602:A:O2'	31:V:74:C:P	2.76	0.43
32:W:17:ALA:O	32:W:18:LYS:HB2	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:A:1779:U:C5	10:A:1784:A:N7	2.86	0.43
10:A:2134:A:O2'	10:A:2135:A:O4'	2.36	0.43
6:5:51:TYR:CE1	6:5:52:MET:HG2	2.53	0.43
18:I:40:ALA:O	18:I:68:PHE:CZ	2.71	0.43
10:A:1223:G:P	27:R:68:ARG:HH21	2.41	0.43
11:B:51:G:H5"	24:O:64:TYR:CD2	2.52	0.43
10:A:962:G:P	39:A:3352:HOH:O	2.77	0.43
10:A:720:U:H2'	10:A:721:A:C8	2.53	0.43
10:A:742:A:H2'	10:A:743:A:C8	2.53	0.43
6:5:87:GLU:OE2	6:5:95:LEU:HD23	2.18	0.43
10:A:2603:G:H2'	10:A:2604:U:O4'	2.18	0.43
10:A:1414:C:O2	10:A:1588:G:N2	2.44	0.43
32:W:37:VAL:HG11	32:W:55:ASP:HB2	1.99	0.43
10:A:2335:A:N6	10:A:2337:G:H1'	2.33	0.43
10:A:1171:G:H1	10:A:1178:C:H42	1.66	0.43
10:A:2043:C:OP1	10:A:2777:G:O2'	2.24	0.43
12:C:24:HIS:CE1	12:C:79:ARG:HH11	2.36	0.43
20:K:35:VAL:HG12	20:K:36:GLY:N	2.34	0.43
10:A:2197:U:O2	10:A:2198:A:O2'	2.21	0.43
10:A:1441:G:H2'	10:A:1442:U:C6	2.53	0.43
7:6:13:ALA:HB1	7:6:17:MET:CE	2.49	0.43
23:N:38:LEU:HB3	23:N:39:PRO:CD	2.48	0.43
10:A:1003:G:N2	10:A:1004:U:C2	2.86	0.43
10:A:1584:U:H2'	10:A:1585:C:H5'	1.99	0.43
20:K:72:PRO:O	20:K:74:GLY:N	2.43	0.43
1:0:42:ILE:HG22	1:0:43:THR:O	2.19	0.43
32:W:18:LYS:N	32:W:36:ILE:HG13	2.33	0.43
10:A:2517:C:C5	10:A:2542:A:C5	3.06	0.43
10:A:1536:C:H1'	10:A:1537:G:N2	2.34	0.43
10:A:2094:A:P	17:H:22:LYS:HD2	2.59	0.43
33:X:67:LEU:HD22	33:X:77:TYR:CE1	2.53	0.43
10:A:2108:A:H2'	10:A:2109:U:O5'	2.17	0.43
15:F:134:GLN:HG2	15:F:135:ILE:N	2.34	0.43
10:A:959:A:H62	22:M:82:MET:HE1	1.84	0.43
6:5:17:GLU:OE2	6:5:53:ARG:NH1	2.51	0.43
6:5:88:HIS:CB	6:5:89:PRO:CD	2.97	0.43
10:A:1638:C:H4'	10:A:2710:C:O2	2.19	0.43
18:I:87:SER:OG	18:I:88:GLY:N	2.43	0.43
10:A:172:A:H2'	10:A:173:A:C8	2.53	0.43
10:A:822:G:H2'	10:A:823:C:H6	1.83	0.43
10:A:2031:A:C6	10:A:2498:C:H1'	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:8:75:GLN:HB2	9:8:92:VAL:CG2	2.48	0.43
10:A:1494:A:C2	10:A:1495:A:C4	3.06	0.43
8:7:22:HIS:C	8:7:23:ARG:CG	2.75	0.43
14:E:44:ARG:HH11	14:E:44:ARG:CG	2.31	0.43
10:A:1439:A:C2	10:A:1553:A:C4	3.06	0.43
32:W:37:VAL:HB	32:W:38:ARG:NH1	2.34	0.43
32:W:24:ARG:HD3	32:W:65:LYS:CD	2.48	0.43
12:C:16:VAL:H	12:C:203:VAL:HG12	1.83	0.43
10:A:479:A:N3	10:A:481:G:H5"	2.34	0.43
32:W:49:ASN:ND2	32:W:50:VAL:N	2.67	0.43
23:N:70:THR:HB	23:N:75:ILE:HD11	2.00	0.43
10:A:1914:C:H2'	10:A:1915:U:O4'	2.18	0.43
10:A:936:A:H2'	10:A:937:C:C6	2.54	0.43
22:M:8:LYS:CE	22:M:9:PHE:CE2	3.02	0.43
6:5:54:VAL:O	6:5:55:VAL:C	2.57	0.43
10:A:1782:U:O2	10:A:2608:G:C2'	2.66	0.43
19:J:44:TYR:HA	26:Q:59:LEU:CD2	2.48	0.43
10:A:1942:C:OP2	10:A:1943:U:O2'	2.28	0.43
2:1:8:ILE:CD1	2:1:24:LYS:HG2	2.48	0.43
10:A:2698:U:H2'	10:A:2699:C:C6	2.51	0.43
10:A:1322:A:OP1	28:S:11:ARG:NE	2.38	0.43
10:A:348:A:C5	10:A:349:U:C5	3.07	0.43
23:N:8:ARG:HB3	23:N:10:LEU:CD2	2.48	0.43
10:A:2584:U:O2'	10:A:2585:U:C5	2.72	0.43
10:A:975:A:C5	10:A:990:A:N7	2.86	0.43
10:A:323:C:OP1	10:A:338:G:N2	2.51	0.43
26:Q:86:SER:O	27:R:51:VAL:HA	2.18	0.43
34:Y:56:LEU:H	34:Y:56:LEU:HD22	1.84	0.43
10:A:1485:U:H2'	10:A:1486:U:H6	1.83	0.43
10:A:226:A:C6	10:A:227:A:C6	3.07	0.43
10:A:1232:G:C5	10:A:1233:C:C5	3.06	0.43
10:A:1857:G:C2	10:A:1884:G:N3	2.86	0.43
10:A:1239:G:H2'	10:A:1240:U:O4'	2.19	0.43
16:G:39:ALA:HB2	16:G:57:TYR:CD2	2.54	0.43
9:8:72:VAL:HG12	9:8:93:ARG:HA	2.01	0.43
10:A:1281:G:C2	10:A:1290:C:C2	3.07	0.43
28:S:88:ARG:CZ	28:S:88:ARG:CB	2.92	0.43
32:W:39:GLN:HG2	32:W:41:GLY:N	2.34	0.43
26:Q:4:LYS:HZ3	26:Q:7:VAL:CG1	2.32	0.43
23:N:117:ASP:O	23:N:118:ARG:C	2.56	0.43
11:B:78:A:C2	11:B:99:A:C4	3.06	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:4:36:ARG:HG2	5:4:37:GLN:N	2.34	0.43
14:E:187:VAL:O	14:E:188:MET:CB	2.67	0.43
13:D:45:TYR:CD1	13:D:45:TYR:N	2.86	0.43
10:A:2344:U:H4'	10:A:2345:G:OP1	2.17	0.43
10:A:2070:A:H2'	10:A:2071:A:O4'	2.19	0.43
11:B:106:G:H2'	11:B:107:G:O4'	2.19	0.43
10:A:356:G:C6	10:A:357:C:C4	3.07	0.43
10:A:646:U:H3'	10:A:647:G:H5"	1.99	0.43
14:E:52:VAL:HG11	14:E:81:GLY:HA3	2.01	0.43
27:R:74:ILE:HB	27:R:87:GLN:O	2.18	0.43
10:A:744:U:H2'	10:A:745:G:O4'	2.19	0.43
10:A:1224:U:H4'	27:R:88:GLY:O	2.18	0.43
10:A:2423:U:H5'	10:A:2423:U:H6	1.83	0.43
10:A:945:A:C4	10:A:2448:A:C2	3.07	0.43
18:I:93:ASN:HB2	18:I:135:MET:SD	2.59	0.43
10:A:545:U:H6	10:A:545:U:O5'	2.02	0.43
32:W:36:ILE:O	32:W:36:ILE:HG22	2.18	0.43
10:A:2274:A:C5	10:A:2276:G:C8	3.07	0.43
10:A:2657:A:C2	10:A:2665:A:C4	3.06	0.43
29:T:70:HIS:HB3	29:T:73:ARG:O	2.19	0.43
10:A:1476:U:C5	10:A:1514:G:C2	3.07	0.43
32:W:44:PHE:O	32:W:78:PHE:HA	2.19	0.43
10:A:1204:A:C2	10:A:1240:U:N3	2.87	0.43
6:5:142:THR:OG1	6:5:143:MET:N	2.52	0.43
19:J:110:PRO:HB2	19:J:111:LYS:HG3	2.00	0.43
10:A:1096:A:H2'	10:A:1097:U:H5"	2.01	0.43
19:J:88:THR:HG22	19:J:91:GLU:CG	2.49	0.43
34:Y:1:MET:H3	34:Y:2:LYS:HD2	1.84	0.43
10:A:1747:U:H2'	10:A:1748:C:C6	2.54	0.43
10:A:2595:G:N1	10:A:2599:G:C6	2.87	0.43
13:D:124:ARG:HA	13:D:165:MET:SD	2.58	0.43
15:F:62:GLN:NE2	15:F:89:THR:O	2.46	0.43
6:5:71:CYS:SG	6:5:117:LEU:HD12	2.58	0.42
10:A:1188:U:H4'	27:R:81:LYS:O	2.19	0.42
16:G:36:LEU:HD22	16:G:36:LEU:N	2.33	0.42
18:I:82:ALA:HB1	18:I:108:ILE:HG21	2.00	0.42
12:C:16:VAL:N	12:C:203:VAL:CG1	2.82	0.42
10:A:2516:A:N6	10:A:2517:C:N4	2.67	0.42
6:5:67:THR:C	6:5:69:PHE:N	2.73	0.42
10:A:2661:G:C6	10:A:2662:A:C2	3.06	0.42
10:A:570:G:C4	10:A:2030:A:N7	2.87	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:I:46:ASP:HA	18:I:50:LYS:HD2	2.00	0.42
10:A:2062:A:N3	10:A:2063:C:C6	2.87	0.42
6:5:71:CYS:HB3	6:5:74:ASP:OD2	2.18	0.42
10:A:301:G:H2'	10:A:334:C:H2'	2.01	0.42
10:A:2602:A:H8	31:V:74:C:OP2	2.03	0.42
13:D:118:PHE:HZ	23:N:1:MET:HB2	1.85	0.42
30:U:38:ILE:HG23	30:U:39:ASN:N	2.33	0.42
25:P:58:PHE:HD1	25:P:75:THR:HG22	1.83	0.42
2:1:7:LYS:NZ	10:A:2421:G:P	2.92	0.42
10:A:528:A:P	19:J:116:ARG:HH21	2.42	0.42
23:N:103:ARG:HD3	23:N:110:MET:HE3	2.00	0.42
21:L:2:ARG:HA	21:L:5:THR:HG21	2.01	0.42
10:A:2661:G:H2'	10:A:2662:A:O4'	2.19	0.42
11:B:72:G:N2	11:B:103:U:C5	2.86	0.42
10:A:2287:A:C8	10:A:2289:G:C8	3.08	0.42
10:A:274:C:H2'	10:A:275:C:O4'	2.19	0.42
10:A:1465:G:H2'	10:A:1466:U:O4'	2.19	0.42
3:2:12:ARG:HH21	3:2:44:VAL:HG11	1.82	0.42
10:A:573:U:O2'	10:A:574:A:H3'	2.19	0.42
14:E:12:LEU:HD12	14:E:193:VAL:HG11	2.01	0.42
13:D:120:GLY:HA2	13:D:162:ALA:HA	2.00	0.42
30:U:35:VAL:O	30:U:38:ILE:HB	2.19	0.42
10:A:2755:C:O2'	10:A:2756:U:H2'	2.19	0.42
15:F:103:ILE:HG21	15:F:173:ASP:HB2	2.01	0.42
10:A:959:A:N6	22:M:82:MET:CE	2.82	0.42
6:5:17:GLU:HA	6:5:88:HIS:CE1	2.54	0.42
35:Z:15:ARG:HD3	35:Z:53:MET:SD	2.59	0.42
10:A:1966:A:N3	10:A:2592:G:O2'	2.47	0.42
14:E:158:PHE:HD2	14:E:159:LEU:HD12	1.83	0.42
34:Y:14:LEU:HA	34:Y:17:GLU:HB3	2.01	0.42
10:A:1782:U:N3	10:A:2587:A:C6	2.87	0.42
6:5:3:LEU:HD12	6:5:5:LEU:N	2.35	0.42
19:J:38:GLY:O	19:J:43:GLU:HB2	2.19	0.42
26:Q:60:TRP:CE2	26:Q:93:ILE:HB	2.54	0.42
26:Q:94:LEU:CD1	27:R:13:ARG:HB2	2.49	0.42
24:O:31:THR:HG22	24:O:34:HIS:N	2.33	0.42
32:W:42:THR:HG22	32:W:43:LYS:HZ2	1.83	0.42
10:A:1378:A:C4	10:A:1380:G:N7	2.87	0.42
13:D:149:ASN:CG	13:D:150:GLN:H	2.21	0.42
10:A:2748:A:H1'	16:G:66:THR:CG2	2.49	0.42
28:S:89:ALA:O	28:S:90:LYS:HG3	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:A:2803:G:H2'	10:A:2804:U:H6	1.84	0.42
10:A:2071:A:H2'	10:A:2072:C:C6	2.54	0.42
10:A:2557:G:H2'	10:A:2558:C:C6	2.54	0.42
10:A:1770:G:C6	10:A:1983:G:C6	3.07	0.42
10:A:2022:U:OP1	39:A:3657:HOH:O	2.20	0.42
10:A:1298:C:C2	10:A:1643:G:N2	2.88	0.42
23:N:24:MET:HE2	23:N:44:LEU:HD22	2.02	0.42
15:F:111:ARG:HA	15:F:111:ARG:NE	2.34	0.42
6:5:47:GLU:HG2	6:5:95:LEU:HD21	2.00	0.42
16:G:35:THR:HG22	16:G:36:LEU:N	2.33	0.42
10:A:2039:U:H2'	10:A:2040:G:H8	1.82	0.42
35:Z:39:ASP:CG	35:Z:44:ARG:HH21	2.23	0.42
10:A:1238:G:O2'	10:A:1239:G:H5'	2.19	0.42
10:A:146:A:H2'	10:A:147:C:C6	2.54	0.42
20:K:3:GLN:HG3	20:K:4:GLU:N	2.34	0.42
14:E:51:GLU:OE2	14:E:88:ARG:NH2	2.45	0.42
33:X:52:ALA:O	33:X:53:LYS:CB	2.67	0.42
10:A:2392:A:OP2	10:A:2422:C:N4	2.50	0.42
7:6:15:SER:OG	7:6:16:VAL:N	2.53	0.42
29:T:76:ARG:HG3	29:T:77:ARG:N	2.34	0.42
19:J:43:GLU:O	19:J:44:TYR:C	2.58	0.42
10:A:2845:U:H5"	25:P:51:ASN:O	2.20	0.42
10:A:2352:A:N1	32:W:30:VAL:HG21	2.35	0.42
16:G:1:SER:O	16:G:4:ALA:N	2.48	0.42
23:N:12:ARG:CZ	23:N:20:MET:HE1	2.50	0.42
14:E:188:MET:HE3	14:E:196:VAL:HG21	2.02	0.42
30:U:84:PHE:O	30:U:85:ARG:HB3	2.19	0.42
29:T:34:VAL:O	29:T:34:VAL:HG22	2.20	0.42
10:A:1937:A:N7	10:A:1939:U:H2'	2.35	0.42
10:A:1312:U:H4'	10:A:1313:U:O5'	2.20	0.42
10:A:2823:A:C5	10:A:2824:C:C5	3.07	0.42
10:A:1956:U:H2'	10:A:1957:C:H5'	2.01	0.42
34:Y:31:GLN:HG2	34:Y:36:GLN:HB2	2.01	0.42
24:O:14:ALA:O	24:O:17:LYS:N	2.52	0.42
2:1:18:HIS:CE1	2:1:40:PRO:HD3	2.54	0.42
10:A:2047:C:O2'	10:A:2048:G:H5'	2.19	0.42
6:5:22:ALA:N	6:5:87:GLU:O	2.53	0.42
6:5:131:THR:HA	6:5:134:GLU:CG	2.50	0.42
13:D:133:THR:HG23	13:D:134:HIS:N	2.34	0.42
10:A:272:A:HO2'	10:A:273:G:H8	1.65	0.42
10:A:84:A:N1	10:A:98:G:O2'	2.30	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:R:16:GLU:HA	27:R:98:ILE:HG22	2.01	0.42
6:5:51:TYR:CD1	6:5:52:MET:HG2	2.55	0.42
10:A:1814:G:C6	10:A:1815:A:C6	3.08	0.42
10:A:2674:G:H4'	20:K:30:ARG:HG3	2.02	0.42
4:3:22:LYS:HA	4:3:47:ALA:O	2.19	0.42
18:I:9:LYS:HB3	18:I:71:LYS:NZ	2.34	0.42
23:N:8:ARG:HB3	23:N:10:LEU:HD22	2.01	0.42
15:F:28:PRO:HB2	15:F:168:LEU:HD22	2.02	0.42
10:A:518:G:H2'	10:A:519:U:C6	2.55	0.42
20:K:47:ILE:HG13	20:K:48:PRO:HD2	2.00	0.42
10:A:1183:U:H2'	10:A:1184:U:C6	2.55	0.42
19:J:11:VAL:HG11	19:J:50:THR:HA	2.01	0.42
10:A:1112:G:C5	10:A:1113:U:C5	3.07	0.42
10:A:1084:A:C6	10:A:1085:A:C6	3.08	0.42
10:A:1909:C:C1'	31:V:11:C:O2'	2.68	0.42
27:R:80:ARG:O	27:R:81:LYS:HD3	2.20	0.42
10:A:1010:A:OP2	39:A:3767:HOH:O	2.20	0.42
15:F:107:VAL:HG13	15:F:110:ILE:HD12	2.02	0.42
11:B:16:G:C5	11:B:69:G:C2	3.07	0.42
20:K:39:ILE:HD12	20:K:41:ILE:HD11	2.02	0.42
10:A:1607:C:H42	10:A:1622:G:P	2.43	0.42
15:F:94:ARG:HH11	15:F:94:ARG:HB2	1.84	0.42
26:Q:6:GLY:HA2	26:Q:9:ALA:HB3	2.02	0.42
34:Y:21:LEU:HA	34:Y:25:GLN:HB3	2.01	0.42
26:Q:82:LEU:HD12	26:Q:112:ALA:HB2	2.02	0.42
8:7:17:ASN:O	36:7:1002:TRP:CD2	2.73	0.42
10:A:1782:U:C1'	10:A:2608:G:O2'	2.66	0.42
32:W:60:ALA:CB	32:W:81:ILE:CD1	2.98	0.42
10:A:479:A:C2	10:A:480:A:C5	3.08	0.42
27:R:38:VAL:O	27:R:53:PHE:HA	2.20	0.42
28:S:96:ILE:O	28:S:96:ILE:HG13	2.20	0.42
29:T:29:THR:HB	29:T:86:THR:HA	2.01	0.42
11:B:89:U:H3'	11:B:90:C:C5'	2.49	0.42
16:G:137:LYS:HA	16:G:140:ILE:HG22	2.02	0.42
26:Q:20:ALA:HA	26:Q:23:TYR:CE2	2.54	0.42
10:A:1691:C:C4	10:A:1692:U:C4	3.08	0.42
13:D:24:VAL:HA	13:D:191:GLY:H	1.85	0.42
10:A:2637:U:C2'	10:A:2638:G:H5'	2.50	0.42
10:A:2821:A:C2	10:A:2822:G:C4	3.08	0.42
10:A:126:A:C6	10:A:127:A:N1	2.88	0.42
27:R:5:PHE:HB3	27:R:59:ILE:HD12	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:A:833:A:OP1	21:L:39:LYS:HE3	2.19	0.42
10:A:685:A:C2	10:A:689:A:C6	3.08	0.42
8:7:17:ASN:ND2	8:7:17:ASN:C	2.73	0.42
8:7:22:HIS:O	8:7:23:ARG:O	2.37	0.42
10:A:996:A:C5	10:A:1160:G:C2	3.08	0.42
19:J:4:PHE:HB3	19:J:44:TYR:CE2	2.55	0.42
6:5:108:VAL:HG12	6:5:109:LYS:N	2.35	0.42
28:S:18:ARG:HG3	28:S:76:VAL:CG1	2.50	0.42
12:C:203:VAL:O	12:C:205:GLY:N	2.53	0.42
19:J:81:ILE:CG1	19:J:82:GLY:H	2.33	0.42
2:1:5:ARG:CZ	2:1:24:LYS:HA	2.49	0.42
6:5:67:THR:CG2	6:5:72:LEU:HA	2.49	0.42
10:A:1394:U:OP1	39:A:3405:HOH:O	2.22	0.42
28:S:59:GLU:HA	28:S:64:ALA:CB	2.50	0.42
27:R:74:ILE:HD12	27:R:74:ILE:N	2.34	0.42
10:A:1789:A:H2'	10:A:1790:C:O4'	2.20	0.42
24:O:75:GLY:HA3	24:O:109:ALA:HB3	2.00	0.42
10:A:179:C:C2	10:A:180:G:C8	3.08	0.42
10:A:75:G:H4'	34:Y:48:ARG:NH2	2.34	0.42
10:A:1194:A:C2'	10:A:1195:G:O5'	2.68	0.42
12:C:184:GLU:O	12:C:185:ALA:HB3	2.20	0.42
18:I:11:GLN:N	18:I:11:GLN:OE1	2.43	0.42
8:7:19:ILE:HA	8:7:19:ILE:HD12	1.89	0.41
19:J:4:PHE:O	19:J:44:TYR:OH	2.35	0.41
10:A:2526:G:C5	10:A:2527:C:C5	3.08	0.41
23:N:12:ARG:HB3	23:N:16:HIS:HB3	2.02	0.41
25:P:92:ARG:CG	25:P:92:ARG:O	2.68	0.41
10:A:864:G:OP2	22:M:22:GLN:NE2	2.52	0.41
31:V:3:G:C2	31:V:71:C:C2	3.08	0.41
10:A:109:C:H4'	10:A:348:A:H4'	2.02	0.41
24:O:49:VAL:HG12	24:O:50:ALA:N	2.35	0.41
19:J:64:VAL:HG13	19:J:65:THR:N	2.35	0.41
35:Z:13:ILE:HG22	35:Z:14:GLY:N	2.34	0.41
16:G:26:LYS:CG	16:G:27:GLY:N	2.83	0.41
6:5:27:VAL:O	6:5:83:ALA:N	2.52	0.41
10:A:1936:A:C2	10:A:1943:U:H5	2.38	0.41
17:H:39:ALA:HB1	17:H:44:ILE:HG22	2.01	0.41
25:P:92:ARG:HH11	25:P:92:ARG:HB2	1.85	0.41
10:A:653:U:H5	10:A:654:A:C2	2.38	0.41
10:A:201:C:O2'	10:A:251:A:N1	2.38	0.41
16:G:31:GLU:O	16:G:33:THR:N	2.52	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:A:555:G:O2'	10:A:556:A:OP2	2.31	0.41
10:A:1591:A:H2'	10:A:1592:C:C6	2.55	0.41
10:A:1945:G:C6	10:A:1946:U:C4	3.09	0.41
19:J:60:ASP:N	19:J:60:ASP:OD1	2.52	0.41
10:A:2576:G:H3'	10:A:2576:G:N3	2.35	0.41
6:5:108:VAL:CG1	6:5:109:LYS:N	2.82	0.41
10:A:1647:U:H3'	10:A:1647:U:P	2.60	0.41
10:A:1509:A:H1'	10:A:1510:G:O5'	2.20	0.41
10:A:1378:A:H4'	10:A:1379:U:OP1	2.20	0.41
10:A:1338:G:O2'	10:A:1393:A:N1	2.44	0.41
27:R:61:ALA:HB1	27:R:98:ILE:H	1.84	0.41
35:Z:4:ILE:HD13	35:Z:44:ARG:NH2	2.35	0.41
20:K:13:ASN:O	20:K:14:SER:CB	2.67	0.41
20:K:15:GLY:O	20:K:46:ALA:HA	2.20	0.41
10:A:1078:U:H5"	10:A:1079:C:OP1	2.20	0.41
19:J:35:ARG:HG2	19:J:40:HIS:HD2	1.84	0.41
14:E:79:ARG:HG2	14:E:80:SER:N	2.35	0.41
18:I:20:SER:HB3	18:I:21:PRO:HD3	2.01	0.41
10:A:2409:G:H2'	10:A:2410:G:O4'	2.20	0.41
10:A:1843:C:H5'	12:C:250:GLN:NE2	2.36	0.41
25:P:30:TRP:CE3	25:P:39:LEU:HD12	2.56	0.41
10:A:2580:U:C5	10:A:2581:G:C6	3.08	0.41
10:A:1923:U:H5'	31:V:25:C:C1'	2.50	0.41
10:A:1722:A:C2	10:A:1739:A:N3	2.89	0.41
18:I:100:ILE:CD1	18:I:137:LEU:HD12	2.50	0.41
1:0:42:ILE:HD12	23:N:99:LYS:O	2.20	0.41
32:W:24:ARG:HH11	32:W:65:LYS:HG2	1.85	0.41
28:S:89:ALA:O	28:S:90:LYS:CG	2.69	0.41
1:0:12:ARG:HD2	1:0:16:ARG:NH2	2.36	0.41
10:A:633:A:OP1	21:L:68:SER:OG	2.34	0.41
22:M:53:MET:CE	22:M:63:ILE:HG21	2.50	0.41
14:E:134:LEU:CD2	14:E:161:ALA:HB2	2.50	0.41
19:J:65:THR:HG22	19:J:68:LYS:NZ	2.36	0.41
11:B:117:G:OP1	24:O:56:LYS:NZ	2.49	0.41
10:A:966:G:C6	10:A:967:U:C4	3.07	0.41
10:A:2543:G:C6	10:A:2544:G:C6	3.08	0.41
10:A:803:U:C4	10:A:804:A:N7	2.88	0.41
10:A:19:A:H2'	10:A:20:C:O4'	2.20	0.41
12:C:172:THR:HG22	12:C:182:LYS:HG2	2.02	0.41
8:7:19:ILE:O	36:7:1002:TRP:HD1	2.03	0.41
8:7:19:ILE:CG1	8:7:20:VAL:H	2.32	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:A:2586:U:H2'	10:A:2587:A:C8	2.55	0.41
26:Q:63:ARG:HH12	26:Q:96:ASP:HA	1.86	0.41
6:5:33:VAL:HB	6:5:36:ASP:OD1	2.20	0.41
5:4:32:LYS:HD3	10:A:2478:A:H5'	2.02	0.41
10:A:2478:A:C2'	10:A:2479:U:H5'	2.51	0.41
10:A:1019:U:H3	10:A:1142:A:N6	2.17	0.41
15:F:151:LEU:CD1	15:F:153:ILE:HG23	2.51	0.41
20:K:13:ASN:OD1	20:K:13:ASN:N	2.48	0.41
10:A:2676:C:P	20:K:31:ARG:HH12	2.43	0.41
10:A:347:A:C2	10:A:348:A:C4	3.09	0.41
23:N:79:LEU:O	23:N:80:PHE:HB2	2.19	0.41
13:D:88:GLU:O	13:D:89:GLU:HG3	2.21	0.41
10:A:372:G:C4	33:X:60:LYS:HE2	2.54	0.41
10:A:2204:G:OP2	12:C:146:LYS:NZ	2.34	0.41
12:C:143:VAL:HB	12:C:153:LEU:HB2	2.02	0.41
9:8:21:ARG:NH1	11:B:77:U:OP1	2.54	0.41
10:A:1579:A:H2'	10:A:1580:A:C8	2.56	0.41
10:A:1681:G:N2	10:A:1763:G:OP2	2.45	0.41
10:A:669:G:C2'	10:A:669:G:N3	2.83	0.41
10:A:1301:A:H2'	10:A:1301:A:N3	2.35	0.41
10:A:138:U:H5'	10:A:139:U:C5'	2.51	0.41
10:A:1179:G:C6	10:A:1180:U:C4	3.08	0.41
10:A:749:A:C5	10:A:1618:A:C2	3.09	0.41
10:A:580:U:H2'	10:A:581:C:C6	2.54	0.41
10:A:1494:A:C6	10:A:1495:A:C5	3.08	0.41
15:F:111:ARG:HA	15:F:111:ARG:CZ	2.51	0.41
30:U:10:VAL:HG12	30:U:71:ILE:HA	2.01	0.41
9:8:6:ALA:HB1	9:8:40:ILE:CG2	2.50	0.41
10:A:2555:U:C5	10:A:2556:C:C2	3.09	0.41
14:E:129:PRO:HG3	14:E:156:ASN:OD1	2.21	0.41
10:A:2796:U:C4	10:A:2798:U:C5	3.08	0.41
15:F:46:LYS:H	15:F:46:LYS:HD3	1.86	0.41
30:U:98:ASN:ND2	30:U:100:GLU:OE1	2.53	0.41
10:A:1268:A:H2'	10:A:1269:A:O4'	2.20	0.41
15:F:112:ASP:OD1	15:F:112:ASP:N	2.54	0.41
32:W:19:ARG:NH1	32:W:22:VAL:CG2	2.83	0.41
10:A:635:C:P	21:L:126:ARG:HH21	2.44	0.41
10:A:1714:U:H5'	10:A:1715:G:H5'	2.02	0.41
35:Z:2:LYS:CB	35:Z:39:ASP:HB3	2.51	0.41
22:M:64:TRP:HZ3	22:M:106:ASP:HB2	1.86	0.41
22:M:63:ILE:HG22	22:M:64:TRP:N	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:E:187:VAL:HG12	14:E:188:MET:N	2.36	0.41
10:A:1365:A:N6	10:A:1366:A:C6	2.89	0.41
10:A:1365:A:OP1	33:X:2:ARG:NE	2.48	0.41
34:Y:12:GLU:O	34:Y:15:ASN:HB2	2.21	0.41
23:N:87:PHE:O	23:N:89:SER:N	2.54	0.41
21:L:40:SER:O	21:L:41:ARG:CB	2.67	0.41
10:A:58:G:N2	10:A:70:G:C4	2.89	0.41
8:7:19:ILE:HG23	8:7:20:VAL:HG23	2.01	0.41
10:A:2581:G:C4	10:A:2610:C:C5	3.09	0.41
19:J:4:PHE:CD2	19:J:44:TYR:CE2	3.08	0.41
10:A:1069:A:C2'	10:A:1070:A:OP2	2.68	0.41
10:A:1392:A:C6	10:A:1393:A:C6	3.09	0.41
12:C:77:VAL:O	12:C:77:VAL:HG23	2.20	0.41
10:A:2685:G:H1	10:A:2724:U:H3	1.68	0.41
10:A:84:A:P	30:U:5:ARG:HH12	2.42	0.41
29:T:69:ARG:HG3	29:T:70:HIS:N	2.36	0.41
19:J:88:THR:HG23	19:J:91:GLU:H	1.86	0.41
10:A:2727:A:C6	10:A:2728:U:O4	2.73	0.41
10:A:2201:G:C6	10:A:2202:U:C4	3.08	0.41
19:J:26:GLY:HA2	19:J:29:ALA:HB3	2.02	0.41
10:A:2145:C:N3	10:A:2146:C:N3	2.69	0.41
10:A:2581:G:C2	10:A:2610:C:C5	3.09	0.41
10:A:2583:G:N7	10:A:2584:U:C4	2.89	0.41
10:A:996:A:C6	10:A:1160:G:C2	3.08	0.41
25:P:50:ARG:CD	25:P:56:SER:HB3	2.51	0.41
10:A:1509:A:O2'	10:A:1510:G:P	2.76	0.41
10:A:1970:A:OP2	39:A:3464:HOH:O	2.21	0.41
10:A:1587:G:C4	10:A:1588:G:C8	3.09	0.41
10:A:1613:G:O6	10:A:1617:C:H2'	2.21	0.41
32:W:19:ARG:HG2	32:W:19:ARG:HH11	1.86	0.41
12:C:16:VAL:HB	12:C:203:VAL:HG12	2.02	0.41
10:A:2681:C:C2	10:A:2724:U:O4	2.74	0.41
10:A:2259:U:H1'	10:A:2427:C:C2	2.56	0.41
10:A:1486:U:H2'	10:A:1487:U:C6	2.55	0.41
10:A:528:A:H2	10:A:2043:C:H5'	1.85	0.41
10:A:527:C:H4'	10:A:528:A:O5'	2.21	0.41
28:S:63:GLY:O	28:S:64:ALA:HB3	2.21	0.41
10:A:1096:A:N6	10:A:1097:U:C4	2.89	0.41
23:N:24:MET:CE	23:N:36:THR:HG21	2.51	0.41
10:A:1063:G:H2'	10:A:1064:C:O4'	2.20	0.41
3:2:9:VAL:HG13	10:A:1309:G:OP1	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:A:1630:A:H2'	10:A:1631:G:H5'	2.03	0.41
10:A:2766:A:H2'	10:A:2766:A:N3	2.36	0.41
10:A:2618:G:C6	10:A:2619:C:C4	3.09	0.41
18:I:104:GLN:O	18:I:105:LEU:CB	2.69	0.41
15:F:169:LEU:O	15:F:174:PHE:HB2	2.21	0.41
10:A:307:G:N2	10:A:310:A:C8	2.89	0.41
10:A:866:A:N7	10:A:914:G:C6	2.88	0.41
10:A:659:G:H4'	14:E:95:LYS:HD3	2.02	0.41
28:S:69:LEU:HG	28:S:107:VAL:HG22	2.03	0.41
10:A:2341:G:H2'	10:A:2342:C:C6	2.56	0.41
10:A:996:A:C5	10:A:1160:G:N2	2.89	0.41
10:A:608:A:C8	10:A:621:A:N6	2.89	0.41
32:W:19:ARG:HG2	32:W:19:ARG:NH1	2.36	0.41
1:0:16:ARG:CZ	28:S:15:GLN:NE2	2.84	0.41
10:A:2038:G:H2'	10:A:2039:U:O4'	2.21	0.41
20:K:19:VAL:HG13	20:K:41:ILE:HG12	2.02	0.41
10:A:528:A:H2	10:A:2043:C:C5'	2.33	0.41
10:A:1381:G:H1'	10:A:1571:A:N1	2.35	0.41
23:N:51:LEU:HD21	23:N:70:THR:CG2	2.51	0.41
21:L:127:VAL:HG11	21:L:142:ILE:HG21	2.03	0.41
10:A:2103:C:H2'	10:A:2104:C:H5"	2.02	0.41
10:A:2180:U:N3	10:A:2181:U:C5	2.89	0.41
10:A:1638:C:H5"	10:A:2710:C:O2'	2.21	0.41
10:A:2537:U:C4	10:A:2538:C:N4	2.89	0.41
10:A:2447:G:C5	10:A:2500:U:C5	3.09	0.41
21:L:29:LYS:HG2	21:L:30:THR:N	2.36	0.41
26:Q:46:TYR:CZ	26:Q:50:ARG:NH2	2.89	0.41
5:4:38:GLY:OXT	10:A:1124:G:H1'	2.21	0.41
10:A:45:G:C5'	10:A:46:G:H5'	2.51	0.41
10:A:2869:G:C6	10:A:2870:C:C4	3.09	0.41
10:A:485:C:C2	10:A:496:G:N2	2.88	0.41
28:S:88:ARG:CD	28:S:94:ASP:OD2	2.70	0.40
6:5:47:GLU:CG	6:5:95:LEU:HD21	2.51	0.40
19:J:43:GLU:O	19:J:45:THR:CG2	2.70	0.40
10:A:1669:A:O2'	10:A:2549:G:OP1	2.36	0.40
32:W:22:VAL:O	32:W:23:LYS:HG3	2.22	0.40
10:A:2134:A:OP2	10:A:2134:A:C8	2.75	0.40
10:A:2570:G:H2'	10:A:2571:U:O4'	2.21	0.40
14:E:109:LEU:O	14:E:112:LEU:N	2.54	0.40
15:F:10:GLU:HG2	15:F:13:LYS:HD3	2.02	0.40
13:D:68:PHE:CE2	13:D:75:ALA:HB1	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:T:24:MET:HG3	29:T:29:THR:CG2	2.51	0.40
30:U:13:LEU:HD11	30:U:70:ALA:HB2	2.03	0.40
18:I:74:PRO:HG2	18:I:77:VAL:HB	2.02	0.40
10:A:901:C:C4	10:A:902:C:C4	3.09	0.40
17:H:24:GLY:O	17:H:28:ASN:HB2	2.21	0.40
16:G:10:VAL:HG22	16:G:47:ASN:C	2.41	0.40
22:M:12:MET:HE3	22:M:71:LYS:HG3	2.03	0.40
8:7:14:ASN:CG	14:E:61:ARG:NH2	2.74	0.40
6:5:23:LEU:HD22	6:5:92:ALA:O	2.21	0.40
10:A:2583:G:C5	10:A:2584:U:C4	3.09	0.40
6:5:106:PHE:CG	6:5:107:GLU:N	2.87	0.40
6:5:131:THR:HA	6:5:134:GLU:HG3	2.03	0.40
5:4:32:LYS:CD	10:A:2478:A:H5'	2.51	0.40
10:A:2780:G:P	19:J:120:ARG:HE	2.44	0.40
6:5:132:TYR:HE1	7:6:19:VAL:HG13	1.85	0.40
25:P:33:GLU:HB2	25:P:38:ARG:NH2	2.35	0.40
21:L:77:ILE:HD13	21:L:108:ALA:HB1	2.02	0.40
14:E:178:VAL:HG23	14:E:179:SER:N	2.36	0.40
1:0:47:TYR:CE1	1:0:52:LYS:HD3	2.57	0.40
7:6:7:ILE:HA	7:6:10:ALA:HB3	2.02	0.40
10:A:848:C:H2'	10:A:849:A:C8	2.56	0.40
32:W:39:GLN:OE1	32:W:43:LYS:HB2	2.21	0.40
10:A:1905:C:N4	10:A:1930:G:C2	2.89	0.40
8:7:24:PRO:HB2	31:V:76:A:O3'	2.21	0.40
9:8:44:HIS:CE1	9:8:86:LEU:H	2.39	0.40
10:A:580:U:O3'	26:Q:30:VAL:CG1	2.70	0.40
18:I:19:PRO:HG2	18:I:24:GLY:H	1.85	0.40
6:5:88:HIS:HB3	6:5:89:PRO:HD3	2.03	0.40
10:A:1570:A:C6	10:A:1571:A:C6	3.09	0.40
10:A:230:G:N2	10:A:231:A:C4	2.90	0.40
10:A:2447:G:C4	10:A:2500:U:C5	3.09	0.40
10:A:45:G:H5'	10:A:46:G:H5'	2.03	0.40
10:A:1684:G:C2	10:A:1705:A:C2	3.10	0.40
12:C:158:GLY:H	12:C:194:VAL:HG22	1.86	0.40
31:V:72:G:C3'	31:V:73:A:H5"	2.51	0.40
10:A:483:A:N7	10:A:497:A:H2	2.20	0.40
10:A:24:G:H1'	28:S:77:ASP:HB3	2.04	0.40
8:7:11:LYS:H	8:7:11:LYS:HG3	1.72	0.40
10:A:911:A:C5	22:M:9:PHE:CE2	3.10	0.40
25:P:4:ILE:HG22	25:P:8:GLU:HG3	2.04	0.40
12:C:68:ARG:NE	12:C:128:THR:OG1	2.55	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:A:1655:A:N6	10:A:2005:A:H1'	2.37	0.40
18:I:14:ALA:HB1	18:I:45:THR:CG2	2.52	0.40
15:F:148:VAL:HG23	15:F:149:ARG:N	2.36	0.40
10:A:1007:C:OP1	19:J:37:ARG:NH1	2.54	0.40
10:A:1149:G:H2'	10:A:1150:C:C6	2.57	0.40
10:A:1494:A:C6	10:A:1495:A:C6	3.08	0.40
10:A:2070:A:C2	10:A:2071:A:C4	3.09	0.40
10:A:136:G:H1	10:A:143:C:H42	1.69	0.40
25:P:88:ARG:HH22	25:P:113:LEU:HA	1.86	0.40
24:O:7:ARG:HA	24:O:10:ARG:NH1	2.36	0.40
1:0:33:SER:OG	1:0:35:GLU:HG3	2.21	0.40
10:A:64:A:C6	10:A:65:U:C4	3.10	0.40
2:1:35:LEU:HD22	2:1:35:LEU:N	2.37	0.40
10:A:82:U:H2'	10:A:83:A:C8	2.57	0.40
8:7:15:ILE:CG1	8:7:16:ASP:N	2.84	0.40
10:A:1068:G:H3'	10:A:1069:A:H5"	2.03	0.40
6:5:129:LEU:C	6:5:131:THR:N	2.73	0.40
6:5:59:LEU:HD23	6:5:62:ARG:HE	1.85	0.40
16:G:19:ASN:O	16:G:22:VAL:HG22	2.21	0.40
10:A:301:G:C6	10:A:317:G:C6	3.09	0.40
10:A:1798:U:OP1	12:C:255:LYS:O	2.40	0.40
10:A:1022:G:C5	10:A:1140:C:N4	2.89	0.40
10:A:2740:A:N6	10:A:2764:A:C8	2.90	0.40
10:A:2103:C:N4	10:A:2186:G:H1	2.19	0.40
34:Y:2:LYS:N	34:Y:2:LYS:HD2	2.36	0.40
12:C:115:ILE:HG22	12:C:116:GLN:N	2.36	0.40
10:A:535:G:C6	10:A:559:G:C6	3.09	0.40
10:A:931:U:OP1	35:Z:29:ARG:NH2	2.55	0.40
17:H:27:ARG:NH2	33:X:63:ILE:HG13	2.36	0.40
21:L:74:THR:HG22	21:L:107:PHE:HB2	2.03	0.40
10:A:1026:G:H2'	10:A:1027:A:C8	2.55	0.40
10:A:1674:G:N2	10:A:1677:A:N1	2.69	0.40
13:D:46:ARG:HB3	13:D:46:ARG:CZ	2.50	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	0	54/56 (96%)	43 (80%)	7 (13%)	4 (7%)	1 21
2	1	48/50 (96%)	42 (88%)	3 (6%)	3 (6%)	2 26
3	2	44/46 (96%)	41 (93%)	3 (7%)	0	100 100
4	3	62/64 (97%)	53 (86%)	7 (11%)	2 (3%)	5 44
5	4	36/38 (95%)	29 (81%)	4 (11%)	3 (8%)	1 18
6	5	146/148 (99%)	77 (53%)	41 (28%)	28 (19%)	0 3
7	6	28/30 (93%)	20 (71%)	7 (25%)	1 (4%)	4 41
8	7	18/20 (90%)	7 (39%)	1 (6%)	10 (56%)	0 0
9	8	92/94 (98%)	81 (88%)	11 (12%)	0	100 100
12	C	269/271 (99%)	211 (78%)	43 (16%)	15 (6%)	2 29
13	D	207/209 (99%)	163 (79%)	30 (14%)	14 (7%)	1 24
14	E	199/201 (99%)	162 (81%)	27 (14%)	10 (5%)	3 31
15	F	175/177 (99%)	141 (81%)	30 (17%)	4 (2%)	8 51
16	G	174/176 (99%)	127 (73%)	30 (17%)	17 (10%)	1 14
17	H	48/50 (96%)	29 (60%)	14 (29%)	5 (10%)	1 12
18	I	139/141 (99%)	97 (70%)	33 (24%)	9 (6%)	1 25
19	J	140/142 (99%)	113 (81%)	18 (13%)	9 (6%)	2 26
20	K	120/122 (98%)	95 (79%)	15 (12%)	10 (8%)	1 18
21	L	141/143 (99%)	104 (74%)	32 (23%)	5 (4%)	4 42
22	M	134/136 (98%)	107 (80%)	16 (12%)	11 (8%)	1 18
23	N	118/120 (98%)	101 (86%)	16 (14%)	1 (1%)	24 70
24	O	114/116 (98%)	95 (83%)	18 (16%)	1 (1%)	21 68
25	P	112/114 (98%)	86 (77%)	17 (15%)	9 (8%)	1 19
26	Q	115/117 (98%)	99 (86%)	12 (10%)	4 (4%)	4 42
27	R	101/103 (98%)	83 (82%)	15 (15%)	3 (3%)	5 46

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
28	S	108/110 (98%)	90 (83%)	10 (9%)	8 (7%)	1 21
29	T	91/93 (98%)	57 (63%)	24 (26%)	10 (11%)	0 10
30	U	100/102 (98%)	74 (74%)	16 (16%)	10 (10%)	1 13
32	W	77/79 (98%)	39 (51%)	21 (27%)	17 (22%)	0 1
33	X	75/77 (97%)	64 (85%)	8 (11%)	3 (4%)	4 38
34	Y	61/63 (97%)	39 (64%)	18 (30%)	4 (7%)	1 25
35	Z	56/58 (97%)	46 (82%)	8 (14%)	2 (4%)	4 41
All	All	3402/3466 (98%)	2615 (77%)	555 (16%)	232 (7%)	3 24

All (232) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	0	23	ALA
4	3	22	LYS
5	4	8	LYS
6	5	27	VAL
6	5	48	ALA
6	5	54	VAL
6	5	55	VAL
6	5	58	THR
6	5	69	PHE
6	5	93	ALA
6	5	107	GLU
6	5	108	VAL
6	5	120	ALA
6	5	124	ASP
6	5	130	PRO
8	7	8	VAL
8	7	13	PHE
8	7	15	ILE
8	7	17	ASN
8	7	19	ILE
12	C	70	LYS
12	C	104	LEU
12	C	121	ALA
12	C	140	VAL
13	D	43	ASP
13	D	73	VAL
13	D	170	VAL
14	E	79	ARG

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Mol	Chain	Res	Type
15	F	111	ARG
16	G	2	ARG
16	G	16	VAL
16	G	28	LYS
16	G	31	GLU
16	G	84	LYS
16	G	164	ALA
16	G	168	VAL
17	H	3	VAL
19	J	13	ARG
19	J	21	THR
19	J	44	TYR
19	J	45	THR
19	J	81	ILE
19	J	125	TYR
21	L	66	PHE
22	M	14	LYS
22	M	77	PRO
23	N	119	SER
25	P	50	ARG
25	P	51	ASN
25	P	93	LYS
28	S	3	THR
28	S	14	ALA
28	S	64	ALA
28	S	87	PRO
29	T	27	SER
29	T	29	THR
29	T	40	LYS
30	U	6	ARG
30	U	87	GLU
30	U	92	VAL
30	U	98	ASN
30	U	99	SER
32	W	9	THR
32	W	18	LYS
32	W	29	SER
32	W	36	ILE
32	W	56	HIS
35	Z	9	THR
1	0	35	GLU
2	1	4	ILE

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Mol	Chain	Res	Type
2	1	50	GLU
6	5	3	LEU
6	5	33	VAL
6	5	88	HIS
6	5	92	ALA
6	5	116	GLU
6	5	119	PRO
8	7	20	VAL
12	C	37	SER
12	C	77	VAL
12	C	238	ASN
12	C	256	THR
13	D	92	VAL
13	D	99	GLU
13	D	107	VAL
13	D	118	PHE
15	F	135	ILE
15	F	176	PHE
16	G	169	ARG
17	H	9	VAL
17	H	16	GLY
18	I	20	SER
18	I	79	LEU
19	J	111	LYS
20	K	35	VAL
20	K	71	ARG
21	L	111	ILE
22	M	2	LEU
22	M	36	VAL
22	M	56	ALA
27	R	65	ALA
28	S	19	LEU
28	S	96	ILE
29	T	36	LYS
29	T	49	LYS
30	U	51	LEU
32	W	14	ASP
32	W	47	GLY
32	W	50	VAL
32	W	74	LYS
34	Y	37	LEU
2	1	51	ALA

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Mol	Chain	Res	Type
5	4	4	ARG
6	5	5	LEU
6	5	78	GLY
6	5	118	ILE
7	6	14	MET
8	7	21	ASP
12	C	110	LYS
13	D	95	SER
13	D	109	VAL
13	D	192	ALA
14	E	7	ASP
14	E	70	SER
14	E	123	LYS
16	G	32	LEU
16	G	117	PRO
16	G	170	THR
17	H	10	ALA
18	I	11	GLN
20	K	13	ASN
20	K	46	ALA
20	K	93	GLN
22	M	69	PRO
24	O	3	LYS
25	P	113	LEU
27	R	98	ILE
28	S	92	ARG
29	T	28	ASN
30	U	85	ARG
30	U	101	THR
32	W	34	SER
33	X	17	ARG
33	X	34	SER
35	Z	34	THR
1	0	54	ILE
5	4	16	ILE
6	5	89	PRO
8	7	7	CYS
8	7	16	ASP
12	C	59	GLN
12	C	197	ALA
13	D	169	ARG
13	D	175	LEU

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Mol	Chain	Res	Type
15	F	132	ARG
16	G	33	THR
16	G	173	ALA
18	I	64	ARG
19	J	74	TYR
20	K	119	ALA
21	L	29	LYS
22	M	23	GLY
22	M	134	THR
25	P	4	ILE
25	P	103	THR
26	Q	87	VAL
26	Q	88	GLU
26	Q	95	ALA
28	S	90	LYS
29	T	51	PHE
29	T	55	VAL
32	W	37	VAL
33	X	76	LYS
34	Y	7	ARG
6	5	36	ASP
6	5	72	LEU
6	5	128	THR
8	7	23	ARG
12	C	64	VAL
12	C	120	ASP
12	C	196	ASN
13	D	183	GLU
14	E	46	GLN
14	E	96	VAL
16	G	97	VAL
16	G	163	TYR
16	G	166	GLU
18	I	12	VAL
18	I	71	LYS
19	J	65	THR
20	K	49	ARG
20	K	108	ARG
21	L	5	THR
21	L	41	ARG
22	M	35	ALA
22	M	73	ILE

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Mol	Chain	Res	Type
25	P	34	GLY
25	P	92	ARG
26	Q	85	ALA
29	T	86	THR
29	T	89	GLU
30	U	88	ASP
32	W	10	ARG
32	W	46	ALA
34	Y	9	LYS
6	5	59	LEU
6	5	94	ARG
14	E	83	VAL
14	E	153	LEU
16	G	118	ALA
17	H	14	SER
18	I	93	ASN
20	K	6	THR
20	K	50	GLY
22	M	13	HIS
27	R	40	MET
30	U	16	LYS
32	W	23	LYS
32	W	76	ARG
32	W	78	PHE
25	P	63	ILE
32	W	41	GLY
6	5	32	GLY
14	E	148	ILE
34	Y	62	GLY
4	3	6	VAL
12	C	232	GLY
13	D	122	VAL
18	I	22	PRO
18	I	88	GLY
1	0	24	VAL
14	E	71	GLY

5.3.2 Protein sidechains (i)

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
1	0	47/47 (100%)	46 (98%)	1 (2%)	61 86
2	1	45/45 (100%)	42 (93%)	3 (7%)	20 62
3	2	38/38 (100%)	35 (92%)	3 (8%)	15 55
4	3	51/51 (100%)	46 (90%)	5 (10%)	10 44
5	4	34/34 (100%)	31 (91%)	3 (9%)	12 50
6	5	112/112 (100%)	93 (83%)	19 (17%)	2 19
7	6	26/26 (100%)	22 (85%)	4 (15%)	3 24
8	7	20/20 (100%)	15 (75%)	5 (25%)	1 6
9	8	78/78 (100%)	75 (96%)	3 (4%)	40 76
12	C	216/216 (100%)	202 (94%)	14 (6%)	21 62
13	D	164/164 (100%)	151 (92%)	13 (8%)	15 55
14	E	165/165 (100%)	146 (88%)	19 (12%)	7 37
15	F	148/148 (100%)	138 (93%)	10 (7%)	20 61
16	G	137/137 (100%)	122 (89%)	15 (11%)	8 40
17	H	40/40 (100%)	39 (98%)	1 (2%)	55 83
18	I	109/109 (100%)	105 (96%)	4 (4%)	41 76
19	J	116/116 (100%)	100 (86%)	16 (14%)	4 30
20	K	103/103 (100%)	92 (89%)	11 (11%)	8 41
21	L	102/102 (100%)	95 (93%)	7 (7%)	19 60
22	M	109/109 (100%)	93 (85%)	16 (15%)	4 27
23	N	100/100 (100%)	93 (93%)	7 (7%)	19 60
24	O	86/86 (100%)	78 (91%)	8 (9%)	11 47
25	P	99/99 (100%)	91 (92%)	8 (8%)	15 54
26	Q	89/89 (100%)	81 (91%)	8 (9%)	12 49
27	R	84/84 (100%)	78 (93%)	6 (7%)	18 59
28	S	93/93 (100%)	83 (89%)	10 (11%)	8 41
29	T	80/80 (100%)	78 (98%)	2 (2%)	55 83
30	U	83/83 (100%)	77 (93%)	6 (7%)	18 58
32	W	59/59 (100%)	53 (90%)	6 (10%)	9 43
33	X	67/67 (100%)	61 (91%)	6 (9%)	12 49

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
34	Y	55/55 (100%)	52 (94%)	3 (6%)	27 68
35	Z	48/48 (100%)	40 (83%)	8 (17%)	3 20
All	All	2803/2803 (100%)	2553 (91%)	250 (9%)	17 50

All (250) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	0	24	VAL
2	1	8	ILE
2	1	35	LEU
2	1	47	ILE
3	2	8	SER
3	2	9	VAL
3	2	24	THR
4	3	7	ARG
4	3	30	HIS
4	3	31	ILE
4	3	49	VAL
4	3	56	LEU
5	4	4	ARG
5	4	15	LYS
5	4	27	CYS
6	5	1	MET
6	5	3	LEU
6	5	26	VAL
6	5	42	ARG
6	5	51	TYR
6	5	54	VAL
6	5	59	LEU
6	5	65	GLU
6	5	69	PHE
6	5	70	GLU
6	5	96	PHE
6	5	106	PHE
6	5	107	GLU
6	5	116	GLU
6	5	121	SER
6	5	125	ARG
6	5	130	PRO
6	5	132	TYR
6	5	143	MET

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Mol	Chain	Res	Type
7	6	17	MET
7	6	18	ASP
7	6	24	SER
7	6	26	MET
8	7	11	LYS
8	7	13	PHE
8	7	15	ILE
8	7	21	ASP
8	7	23	ARG
9	8	29	ILE
9	8	61	LEU
9	8	87	GLN
12	C	51	ARG
12	C	57	HIS
12	C	109	LEU
12	C	117	SER
12	C	124	LYS
12	C	129	LEU
12	C	142	ASN
12	C	155	ARG
12	C	166	ARG
12	C	176	ARG
12	C	194	VAL
12	C	212	TRP
12	C	251	THR
12	C	270	ARG
13	D	33	ARG
13	D	37	VAL
13	D	97	SER
13	D	103	ASP
13	D	107	VAL
13	D	118	PHE
13	D	124	ARG
13	D	170	VAL
13	D	171	THR
13	D	177	VAL
13	D	183	GLU
13	D	201	LEU
13	D	203	VAL
14	E	5	LEU
14	E	12	LEU
14	E	21	ARG

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Mol	Chain	Res	Type
14	E	40	ARG
14	E	44	ARG
14	E	65	THR
14	E	69	ARG
14	E	70	SER
14	E	78	TRP
14	E	88	ARG
14	E	109	LEU
14	E	113	VAL
14	E	118	LEU
14	E	120	VAL
14	E	126	VAL
14	E	131	THR
14	E	149	ILE
14	E	167	VAL
14	E	171	ASP
15	F	9	ASP
15	F	16	MET
15	F	34	THR
15	F	41	GLU
15	F	46	LYS
15	F	90	LEU
15	F	94	ARG
15	F	111	ARG
15	F	114	ARG
15	F	154	THR
16	G	3	VAL
16	G	16	VAL
16	G	44	HIS
16	G	68	ARG
16	G	84	LYS
16	G	94	ARG
16	G	103	ASN
16	G	110	HIS
16	G	121	THR
16	G	126	THR
16	G	131	VAL
16	G	132	LEU
16	G	151	ARG
16	G	170	THR
16	G	176	LYS
17	H	3	VAL

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Mol	Chain	Res	Type
18	I	23	VAL
18	I	63	ASP
18	I	102	ARG
18	I	137	LEU
19	J	2	LYS
19	J	17	VAL
19	J	24	THR
19	J	30	THR
19	J	36	LEU
19	J	40	HIS
19	J	54	ILE
19	J	55	ILE
19	J	65	THR
19	J	72	LYS
19	J	73	VAL
19	J	95	ARG
19	J	103	ILE
19	J	129	GLU
19	J	131	ASN
19	J	140	LEU
20	K	3	GLN
20	K	8	LEU
20	K	13	ASN
20	K	18	ARG
20	K	21	CYS
20	K	23	LYS
20	K	41	ILE
20	K	54	LYS
20	K	73	ASP
20	K	93	GLN
20	K	105	ARG
21	L	5	THR
21	L	19	LEU
21	L	82	LEU
21	L	91	ASP
21	L	100	ILE
21	L	121	THR
21	L	144	GLU
22	M	12	MET
22	M	13	HIS
22	M	31	PHE
22	M	33	LEU

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Mol	Chain	Res	Type
22	M	46	ILE
22	M	53	MET
22	M	70	ASP
22	M	72	PRO
22	M	81	ARG
22	M	88	ASN
22	M	95	LEU
22	M	96	ILE
22	M	97	GLN
22	M	100	LYS
22	M	110	GLU
22	M	134	THR
23	N	6	SER
23	N	8	ARG
23	N	33	ILE
23	N	65	LEU
23	N	69	ARG
23	N	70	THR
23	N	71	ARG
24	O	18	LEU
24	O	31	THR
24	O	33	ARG
24	O	36	TYR
24	O	38	GLN
24	O	47	VAL
24	O	106	LEU
24	O	115	LEU
25	P	16	VAL
25	P	19	PHE
25	P	62	LYS
25	P	83	ILE
25	P	85	VAL
25	P	92	ARG
25	P	95	LYS
25	P	103	THR
26	Q	16	ILE
26	Q	40	LYS
26	Q	50	ARG
26	Q	59	LEU
26	Q	63	ARG
26	Q	88	GLU
26	Q	93	ILE

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Mol	Chain	Res	Type
26	Q	97	ILE
27	R	4	VAL
27	R	29	THR
27	R	38	VAL
27	R	46	GLU
27	R	48	LYS
27	R	63	VAL
28	S	3	THR
28	S	4	ILE
28	S	7	HIS
28	S	36	LEU
28	S	45	VAL
28	S	66	ILE
28	S	76	VAL
28	S	88	ARG
28	S	96	ILE
28	S	101	SER
29	T	32	LEU
29	T	43	ILE
30	U	6	ARG
30	U	30	SER
30	U	38	ILE
30	U	61	GLU
30	U	86	PHE
30	U	92	VAL
32	W	19	ARG
32	W	23	LYS
32	W	25	PHE
32	W	30	VAL
32	W	49	ASN
32	W	63	ASP
33	X	19	HIS
33	X	24	THR
33	X	26	ARG
33	X	29	LEU
33	X	34	SER
33	X	77	TYR
34	Y	10	SER
34	Y	16	THR
34	Y	57	LEU
35	Z	2	LYS
35	Z	9	THR

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Mol	Chain	Res	Type
35	Z	15	ARG
35	Z	23	LEU
35	Z	30	ARG
35	Z	31	ILE
35	Z	37	ARG
35	Z	40	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
4	3	30	HIS
8	7	17	ASN
8	7	22	HIS
9	8	44	HIS
9	8	80	HIS
15	F	4	HIS
15	F	26	GLN
24	O	34	HIS
34	Y	41	HIS

5.3.3 RNA

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
10	A	2850/2854 (99%)	453 (15%)	40 (1%)
11	B	117/118 (99%)	17 (14%)	0
31	V	76/77 (98%)	15 (19%)	0
All	All	3043/3049 (99%)	485 (15%)	40 (1%)

All (485) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
10	A	10	A
10	A	12	U
10	A	15	G
10	A	34	U
10	A	35	G
10	A	42	A
10	A	43	G
10	A	45	G
10	A	46	G

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Mol	Chain	Res	Type
10	A	51	G
10	A	61	C
10	A	71	A
10	A	74	A
10	A	75	G
10	A	80	G
10	A	82	U
10	A	84	A
10	A	96	C
10	A	101	A
10	A	118	A
10	A	119	A
10	A	120	U
10	A	131	A
10	A	135	U
10	A	136	G
10	A	137	U
10	A	138	U
10	A	139	U
10	A	140	C
10	A	141	G
10	A	142	A
10	A	144	A
10	A	149	A
10	A	162	U
10	A	163	C
10	A	164	C
10	A	181	A
10	A	188	G
10	A	196	A
10	A	199	A
10	A	215	G
10	A	216	A
10	A	222	A
10	A	226	A
10	A	230	G
10	A	248	G
10	A	255	A
10	A	264	C
10	A	265	A
10	A	266	G
10	A	267	C

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Mol	Chain	Res	Type
10	A	272	A
10	A	273	G
10	A	276	U
10	A	277	G
10	A	278	A
10	A	281	C
10	A	285	G
10	A	302	C
10	A	311	A
10	A	329	G
10	A	330	A
10	A	346	A
10	A	347	A
10	A	353	C
10	A	355	U
10	A	361	G
10	A	362	A
10	A	371	A
10	A	372	G
10	A	382	A
10	A	383	C
10	A	386	G
10	A	388	G
10	A	396	G
10	A	404	A
10	A	405	U
10	A	411	G
10	A	412	A
10	A	424	G
10	A	451	U
10	A	455	C
10	A	481	G
10	A	491	G
10	A	503	A
10	A	504	A
10	A	505	A
10	A	509	C
10	A	528	A
10	A	531	C
10	A	532	A
10	A	533	G
10	A	538	A

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Mol	Chain	Res	Type
10	A	543	G
10	A	544	C
10	A	546	U
10	A	547	A
10	A	548	G
10	A	549	G
10	A	563	A
10	A	573	U
10	A	575	A
10	A	586	A
10	A	603	A
10	A	604	G
10	A	613	A
10	A	614	A
10	A	615	U
10	A	627	A
10	A	631	A
10	A	637	A
10	A	645	C
10	A	646	U
10	A	647	G
10	A	648	G
10	A	654	A
10	A	655	A
10	A	656	G
10	A	686	U
10	A	714	U
10	A	715	A
10	A	730	A
10	A	738	G
10	A	747	U
10	A	775	G
10	A	776	G
10	A	782	A
10	A	784	G
10	A	785	G
10	A	805	G
10	A	812	C
10	A	819	A
10	A	827	U
10	A	828	U
10	A	845	A

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Mol	Chain	Res	Type
10	A	846	U
10	A	847	U
10	A	859	G
10	A	878	A
10	A	883	G
10	A	884	U
10	A	896	A
10	A	897	C
10	A	910	A
10	A	914	G
10	A	915	C
10	A	932	U
10	A	941	A
10	A	946	C
10	A	961	C
10	A	974	G
10	A	983	A
10	A	985	C
10	A	995	C
10	A	996	A
10	A	1003	G
10	A	1012	U
10	A	1013	C
10	A	1021	A
10	A	1022	G
10	A	1023	U
10	A	1025	G
10	A	1026	G
10	A	1033	U
10	A	1045	C
10	A	1046	A
10	A	1047	G
10	A	1051	G
10	A	1053	C
10	A	1059	G
10	A	1060	U
10	A	1061	U
10	A	1062	G
10	A	1067	A
10	A	1069	A
10	A	1070	A
10	A	1072	C

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Mol	Chain	Res	Type
10	A	1074	G
10	A	1078	U
10	A	1083	U
10	A	1084	A
10	A	1088	A
10	A	1089	A
10	A	1090	A
10	A	1091	G
10	A	1097	U
10	A	1098	A
10	A	1110	G
10	A	1111	A
10	A	1112	G
10	A	1129	A
10	A	1132	U
10	A	1133	A
10	A	1135	C
10	A	1136	G
10	A	1139	G
10	A	1142	A
10	A	1151	A
10	A	1155	A
10	A	1169	A
10	A	1170	C
10	A	1172	C
10	A	1174	U
10	A	1175	A
10	A	1176	U
10	A	1180	U
10	A	1186	G
10	A	1238	G
10	A	1248	G
10	A	1250	G
10	A	1253	A
10	A	1256	G
10	A	1266	G
10	A	1268	A
10	A	1271	G
10	A	1272	A
10	A	1273	U
10	A	1281	G
10	A	1300	G

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Mol	Chain	Res	Type
10	A	1301	A
10	A	1313	U
10	A	1317	G
10	A	1352	U
10	A	1365	A
10	A	1368	G
10	A	1378	A
10	A	1379	U
10	A	1383	A
10	A	1395	A
10	A	1415	U
10	A	1416	G
10	A	1419	A
10	A	1420	A
10	A	1428	C
10	A	1435	G
10	A	1452	G
10	A	1459	G
10	A	1482	G
10	A	1493	C
10	A	1504	A
10	A	1508	A
10	A	1510	G
10	A	1515	A
10	A	1524	G
10	A	1533	C
10	A	1534	U
10	A	1535	A
10	A	1536	C
10	A	1566	A
10	A	1569	A
10	A	1578	U
10	A	1583	A
10	A	1584	U
10	A	1585	C
10	A	1607	C
10	A	1608	A
10	A	1610	A
10	A	1613	G
10	A	1627	G
10	A	1647	U
10	A	1648	U

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Mol	Chain	Res	Type
10	A	1649	G
10	A	1652	A
10	A	1653	G
10	A	1674	G
10	A	1714	U
10	A	1715	G
10	A	1723	G
10	A	1729	U
10	A	1730	C
10	A	1737	G
10	A	1738	G
10	A	1739	A
10	A	1744	A
10	A	1758	U
10	A	1764	C
10	A	1773	A
10	A	1776	G
10	A	1791	A
10	A	1800	C
10	A	1801	A
10	A	1802	A
10	A	1808	A
10	A	1811	G
10	A	1816	C
10	A	1829	A
10	A	1833	C
10	A	1847	A
10	A	1848	A
10	A	1858	A
10	A	1869	G
10	A	1870	C
10	A	1871	A
10	A	1872	A
10	A	1873	G
10	A	1884	G
10	A	1906	G
10	A	1913	A
10	A	1914	C
10	A	1927	A
10	A	1929	G
10	A	1930	G
10	A	1937	A

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Mol	Chain	Res	Type
10	A	1938	A
10	A	1955	U
10	A	1960	A
10	A	1966	A
10	A	1967	C
10	A	1970	A
10	A	1971	U
10	A	1972	G
10	A	1991	U
10	A	1993	U
10	A	1997	C
10	A	2017	U
10	A	2020	A
10	A	2022	U
10	A	2023	C
10	A	2031	A
10	A	2033	A
10	A	2043	C
10	A	2055	C
10	A	2056	G
10	A	2060	A
10	A	2061	G
10	A	2062	A
10	A	2063	C
10	A	2069	G
10	A	2072	C
10	A	2093	G
10	A	2104	C
10	A	2106	U
10	A	2107	G
10	A	2108	A
10	A	2109	U
10	A	2110	G
10	A	2134	A
10	A	2135	A
10	A	2137	U
10	A	2138	G
10	A	2139	U
10	A	2140	G
10	A	2142	A
10	A	2143	C
10	A	2144	G

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Mol	Chain	Res	Type
10	A	2145	C
10	A	2146	C
10	A	2147	A
10	A	2148	G
10	A	2149	U
10	A	2150	C
10	A	2151	U
10	A	2153	C
10	A	2154	A
10	A	2155	U
10	A	2156	G
10	A	2157	G
10	A	2180	U
10	A	2183	A
10	A	2185	U
10	A	2194	U
10	A	2198	A
10	A	2199	A
10	A	2204	G
10	A	2211	A
10	A	2212	A
10	A	2214	C
10	A	2225	A
10	A	2226	C
10	A	2238	G
10	A	2239	G
10	A	2250	G
10	A	2268	A
10	A	2278	A
10	A	2283	C
10	A	2284	A
10	A	2286	G
10	A	2287	A
10	A	2305	U
10	A	2308	G
10	A	2311	A
10	A	2322	A
10	A	2325	G
10	A	2327	A
10	A	2333	A
10	A	2336	A
10	A	2347	C

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Mol	Chain	Res	Type
10	A	2354	C
10	A	2361	G
10	A	2383	G
10	A	2385	C
10	A	2402	U
10	A	2403	C
10	A	2406	A
10	A	2423	U
10	A	2424	C
10	A	2425	A
10	A	2429	G
10	A	2430	A
10	A	2435	A
10	A	2441	U
10	A	2448	A
10	A	2470	G
10	A	2476	A
10	A	2491	U
10	A	2502	G
10	A	2503	A
10	A	2505	G
10	A	2506	U
10	A	2507	C
10	A	2518	A
10	A	2529	G
10	A	2554	U
10	A	2556	C
10	A	2566	A
10	A	2567	G
10	A	2572	A
10	A	2573	C
10	A	2585	U
10	A	2613	U
10	A	2629	U
10	A	2663	G
10	A	2671	G
10	A	2681	C
10	A	2682	A
10	A	2689	U
10	A	2690	U
10	A	2714	G
10	A	2716	C

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Mol	Chain	Res	Type
10	A	2726	A
10	A	2733	A
10	A	2744	G
10	A	2748	A
10	A	2757	A
10	A	2760	C
10	A	2765	A
10	A	2778	A
10	A	2791	G
10	A	2798	U
10	A	2800	A
10	A	2801	G
10	A	2818	U
10	A	2820	A
10	A	2821	A
10	A	2861	U
10	A	2867	G
10	A	2873	A
10	A	2874	C
10	A	2883	A
10	A	2884	U
10	A	2885	G
10	A	2891	U
10	A	2903	U
11	B	3	C
11	B	15	A
11	B	16	G
11	B	21	G
11	B	30	C
11	B	35	C
11	B	42	C
11	B	44	G
11	B	45	A
11	B	56	G
11	B	84	G
11	B	87	U
11	B	88	C
11	B	89	U
11	B	90	C
11	B	99	A
11	B	109	A
31	V	4	C

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Mol	Chain	Res	Type
31	V	5	A
31	V	8	U
31	V	19	G
31	V	21	A
31	V	31	C
31	V	33	U
31	V	43	G
31	V	48	C
31	V	49	G
31	V	53	G
31	V	67	G
31	V	71	C
31	V	73	A
31	V	76	A

All (40) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
10	A	119	A
10	A	271	G
10	A	277	G
10	A	301	G
10	A	403	U
10	A	404	A
10	A	503	A
10	A	527	C
10	A	613	A
10	A	655	A
10	A	784	G
10	A	827	U
10	A	846	U
10	A	882	G
10	A	931	U
10	A	1020	A
10	A	1025	G
10	A	1069	A
10	A	1088	A
10	A	1110	G
10	A	1247	A
10	A	1378	A
10	A	1458	U
10	A	1509	A

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Mol	Chain	Res	Type
10	A	1535	A
10	A	1626	A
10	A	1738	G
10	A	1757	A
10	A	1847	A
10	A	1870	C
10	A	1939	U
10	A	2108	A
10	A	2142	A
10	A	2211	A
10	A	2286	G
10	A	2326	C
10	A	2423	U
10	A	2756	U
10	A	2873	A
10	A	2902	C

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

1 non-standard protein/DNA/RNA residue is modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
31	5MU	V	54	31	13,21,23	1.53	2 (15%)	17,30,35	3.31	3 (17%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
31	5MU	V	54	31	-	0/3/25/26	0/2/2/2

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	V	54	5MU	C6-N1	2.26	1.38	1.35
31	V	54	5MU	C4-N3	4.32	1.40	1.33

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	V	54	5MU	C5-C4-N3	-3.97	113.54	123.28
31	V	54	5MU	O4'-C1'-N1	3.06	113.91	108.10
31	V	54	5MU	C4-N3-C2	12.44	127.32	114.21

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

Of 146 ligands modelled in this entry, 144 are monoatomic - leaving 2 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
36	TRP	7	1001	-	11,16,16	0.55	0	9,22,22	0.81	0
36	TRP	7	1002	-	11,16,16	0.54	0	9,22,22	0.86	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
36	TRP	7	1001	-	-	0/3/8/8	0/2/2/2
36	TRP	7	1002	-	-	0/3/8/8	0/2/2/2

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.

2 monomers are involved in 24 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
36	7	1001	TRP	8	0
36	7	1002	TRP	16	0

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.