



Full wwPDB/EMDataBank EM Map/Model Validation Report ⓘ

Jul 24, 2017 – 07:19 AM EDT

PDB ID : 5LMQ
EMDB ID: : EMD-4076
Title : Structure of bacterial 30S-IF1-IF3-mRNA-tRNA translation pre-initiation complex, open form (state-2A)
Authors : Hussain, T.; Llacer, J.L.; Wimberly, B.T.; Ramakrishnan, V.
Deposited on : unknown
Resolution : 4.20 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

MolProbity : 4.02b-467
Mogul : 1.7.2 (RC1), CSD as538be (2017)
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20029824

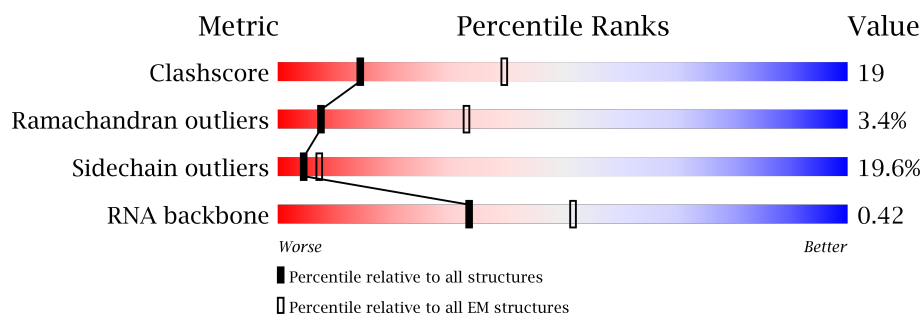
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.20 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.




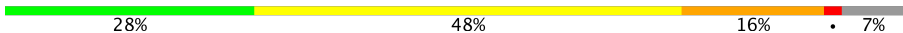



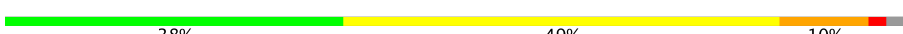











Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	125131	1336
Ramachandran outliers	121729	1120
Sidechain outliers	121581	1026
RNA backbone	3398	335

The table below summarises the geometric issues observed across the polymeric chains. The red, orange, yellow and green segments on the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	A	1522	26% 57% 16% ..
2	B	256	45% 38% 7% • 9%
3	C	239	50% 33% • 14%
4	D	209	53% 39% 8%
5	E	162	52% 33% 7% 7%
6	F	101	58% 37% • •
7	G	156	65% 33% • •
8	H	138	65% 28% 7%

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Mol	Chain	Length	Quality of chain
9	I	128	
10	J	105	
11	K	129	
12	L	132	
13	M	126	
14	N	61	
15	O	89	
16	P	88	
17	Q	105	
18	R	88	
19	S	93	
20	T	106	
21	V	27	
22	W	72	
23	X	171	
24	Y	42	
25	Z	77	

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
27	ZN	D	300	-	-	X	-

2 Entry composition

There are 27 unique types of molecules in this entry. The entry contains 55841 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a RNA chain called 16S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1514	Total	C	N	O	P	0	0
			32522	14481	6019	10512	1510		

- Molecule 2 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	234	Total	C	N	O	S	0	0
			1900	1213	341	341	5		

- Molecule 3 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	206	Total	C	N	O	S	0	0
			1612	1016	314	281	1		

- Molecule 4 is a protein called 30S ribosomal protein S4.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	208	Total	C	N	O	S	0	0
			1703	1066	339	291	7		

- Molecule 5 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	150	Total	C	N	O	S	0	0
			1146	724	217	201	4		

- Molecule 6 is a protein called 30S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	101	Total	C	N	O	S	0	0
			843	531	155	154	3		

- Molecule 7 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	155	Total	C	N	O	S	0	0
			1257	781	252	218	6		

- Molecule 8 is a protein called 30S ribosomal protein S8.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	138	Total	C	N	O	S	0	0
			1116	705	215	193	3		

- Molecule 9 is a protein called 30S ribosomal protein S9.

Mol	Chain	Residues	Atoms				AltConf	Trace
9	I	127	Total	C	N	O	0	0
			1010	639	197	174		

- Molecule 10 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	98	Total	C	N	O	S	0	0
			792	498	156	137	1		

- Molecule 11 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	K	122	Total	C	N	O	S	0	0
			906	563	172	168	3		

- Molecule 12 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	L	124	Total	C	N	O	S	0	0
			970	611	195	163	1		

- Molecule 13 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	M	125	Total	C	N	O	S	0	0
			997	617	207	171	2		

- Molecule 14 is a protein called 30S ribosomal protein S14 type Z.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	N	60	Total	C	N	O	S	0	0
			492	312	104	72	4		

- Molecule 15 is a protein called 30S ribosomal protein S15.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	O	88	Total	C	N	O	S	0	0
			734	459	147	126	2		

- Molecule 16 is a protein called 30S ribosomal protein S16.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	P	83	Total	C	N	O	S	0	0
			700	443	139	117	1		

- Molecule 17 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	Q	99	Total	C	N	O	S	0	0
			823	528	151	142	2		

- Molecule 18 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms				AltConf	Trace
18	R	73	Total	C	N	O	0	0
			598	381	118	99		

- Molecule 19 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	S	82	Total	C	N	O	S	0	0
			655	419	120	114	2		

- Molecule 20 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	T	99	Total	C	N	O	S	0	0
			763	470	162	129	2		

- Molecule 21 is a protein called 30S ribosomal protein Thx.

Mol	Chain	Residues	Atoms				AltConf	Trace
21	V	24	Total	C	N	O	0	0
			208	128	50	30		

- Molecule 22 is a protein called Translation initiation factor IF-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	W	71	Total	C	N	O	S	0	0
			570	362	103	103	2		

- Molecule 23 is a protein called Translation initiation factor IF-3.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	X	168	Total	C	N	O	S	0	0
			1356	853	249	245	9		

- Molecule 24 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	Y	21	Total	C	N	O	P	0	0
			459	205	91	142	21		

- Molecule 25 is a RNA chain called tRNA.

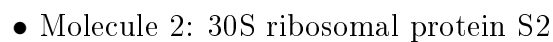
Mol	Chain	Residues	Atoms						AltConf	Trace
25	Z	77	Total	C	N	O	P	S	0	0
			1643	735	297	534	76	1		

- Molecule 26 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
26	W	1	Total	Mg	0
			1	1	
26	A	63	Total	Mg	0
			63	63	

- Molecule 27 is ZINC ION (three-letter code: ZN) (formula: Zn).

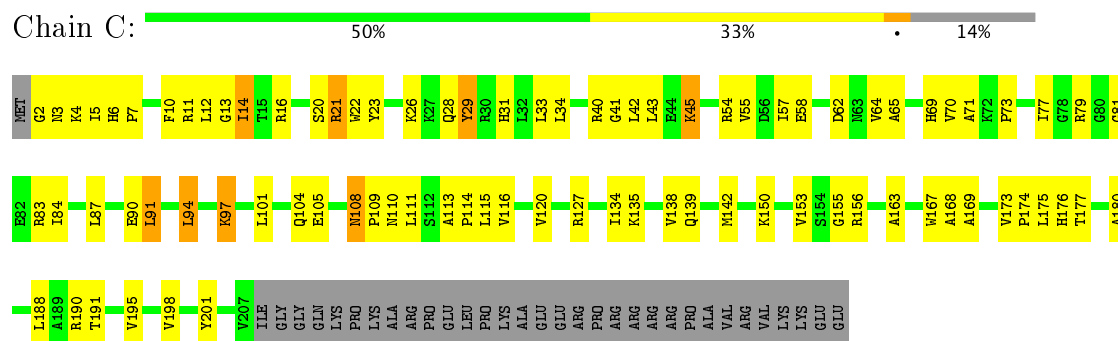
Mol	Chain	Residues	Atoms		AltConf
27	D	1	Total	Zn	0
			1	1	
27	N	1	Total	Zn	0
			1	1	



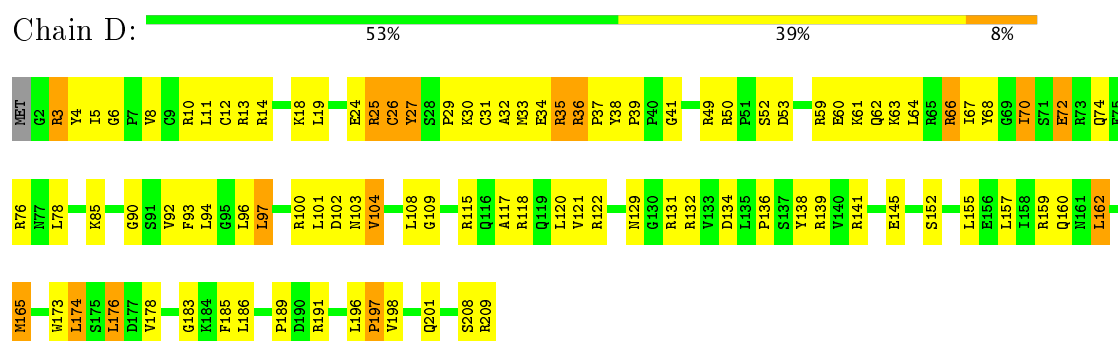
Frequency	Percentage
Daily	45%
Often	38%
Sometimes	7%
Never	9%



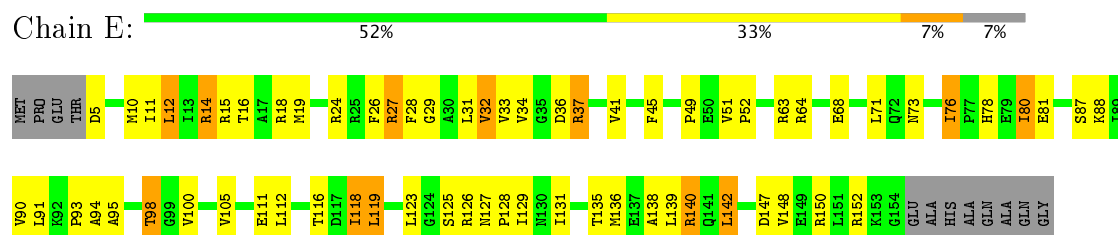
- Molecule 3: 30S ribosomal protein S3



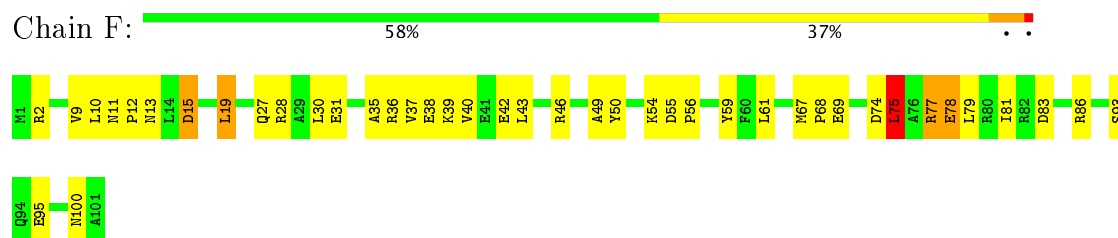
- Molecule 4: 30S ribosomal protein S4



- Molecule 5: 30S ribosomal protein S5

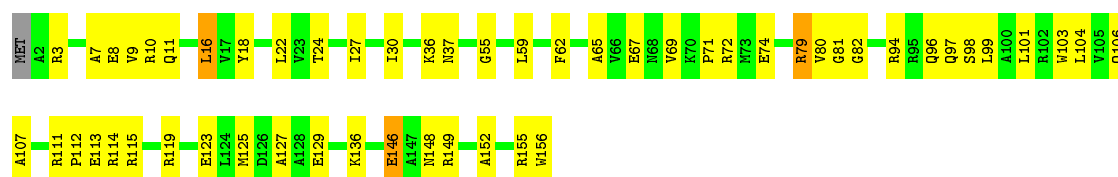


- Molecule 6: 30S ribosomal protein S6



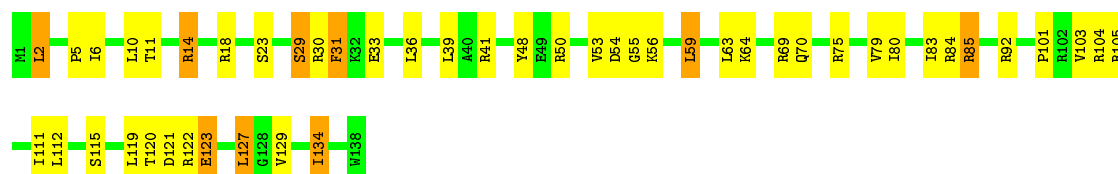
- Molecule 7: 30S ribosomal protein S7





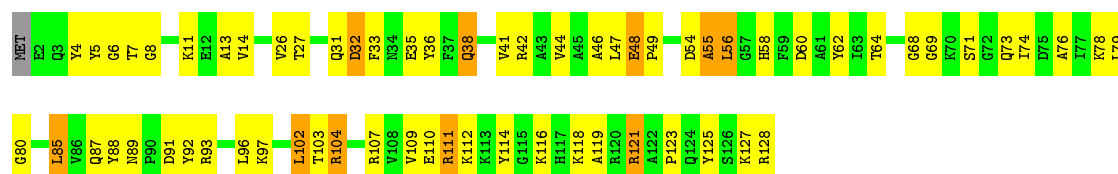
• Molecule 8: 30S ribosomal protein S8

Chain H: 65% 28% 7%



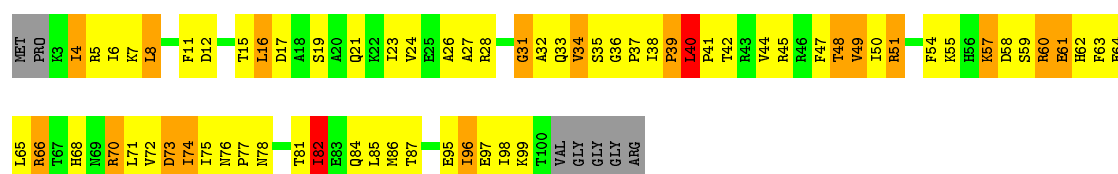
• Molecule 9: 30S ribosomal protein S9

Chain I: 48% 43% 8%



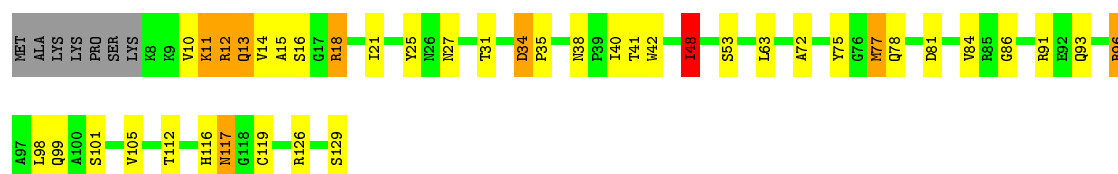
• Molecule 10: 30S ribosomal protein S10

Chain J: 28% 48% 16% 7%



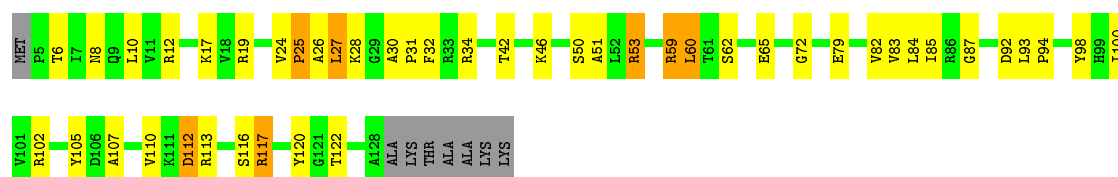
• Molecule 11: 30S ribosomal protein S11

Chain K: 63% 25% 6% 5%



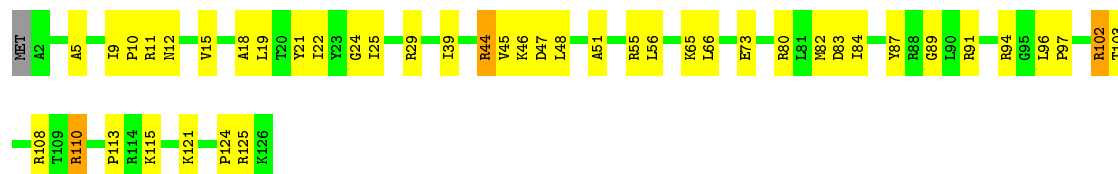
• Molecule 12: 30S ribosomal protein S12

Chain L: 59% 30% 5% 6%



- Molecule 13: 30S ribosomal protein S13

Chain M: 64% 33% ..



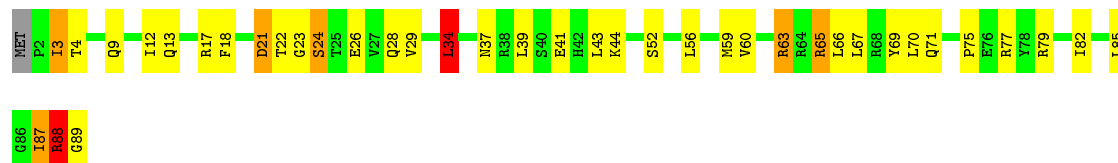
- Molecule 14: 30S ribosomal protein S14 type Z

Chain N: 38% 49% 10% ..



- Molecule 15: 30S ribosomal protein S15

Chain O: 55% 35% 7% ..



- Molecule 16: 30S ribosomal protein S16

Chain P: 57% 34% 6% ..



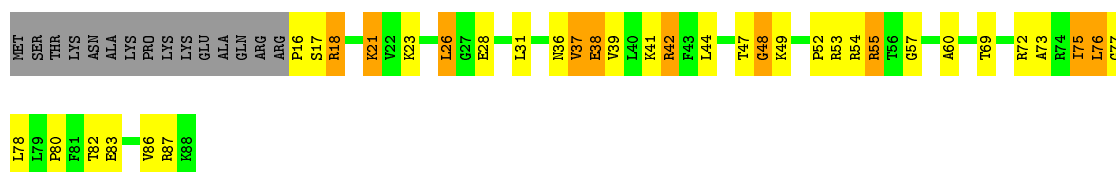
- Molecule 17: 30S ribosomal protein S17

Chain Q: 69% 20% 6% 6%



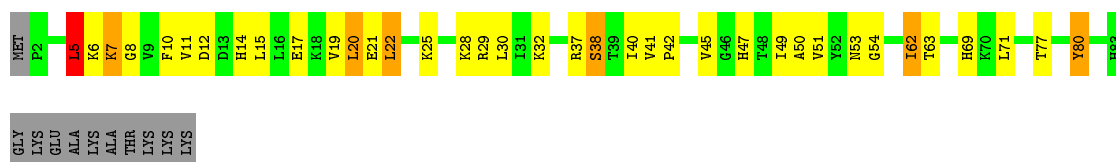
- Molecule 18: 30S ribosomal protein S18

Chain R: 42% 30% 11% 17%



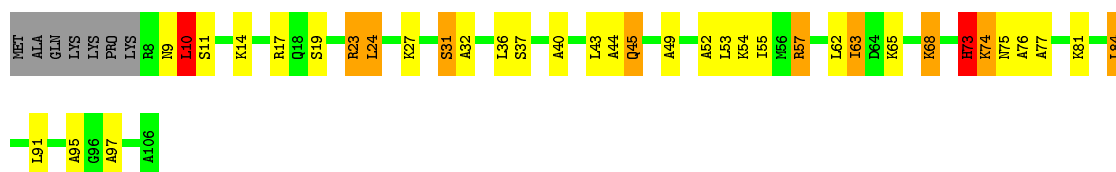
- Molecule 19: 30S ribosomal protein S19

Chain S: 



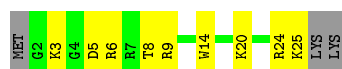
- Molecule 20: 30S ribosomal protein S20

Chain T: 



- Molecule 21: 30S ribosomal protein Thx

Chain V: 



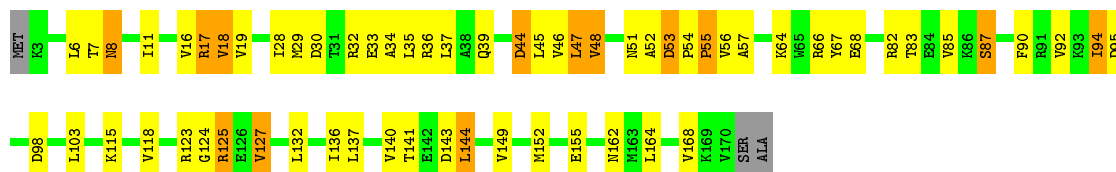
- Molecule 22: Translation initiation factor IF-1

Chain W: 



- Molecule 23: Translation initiation factor IF-3

Chain X: 



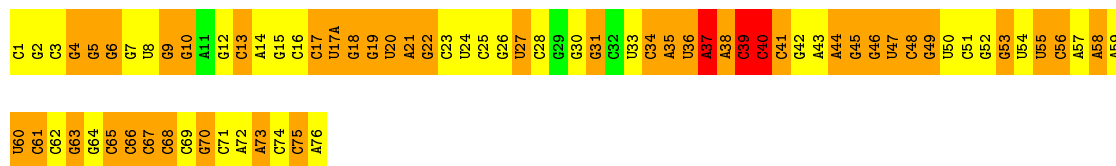
- Molecule 24: mRNA

Chain Y: 14% 21% 14% 50%



- Molecule 25: tRNA

Chain Z:  40% 52%



4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of particles used	31888	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI POLARA 300	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	30	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	3500	Depositor
Magnification	104478	Depositor
Image detector	OTHER	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, OMC, ZN, G7M, MG, 4SU, PSU

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >2	RMSZ	# Z >2
1	A	0.37	2/36394 (0.0%)	0.74	24/56779 (0.0%)
10	J	0.51	0/805	0.76	0/1082
11	K	0.49	0/921	0.82	0/1241
12	L	0.44	0/986	0.77	0/1320
13	M	0.53	0/1008	0.82	1/1347 (0.1%)
14	N	0.44	0/501	0.80	1/664 (0.2%)
15	O	0.52	1/745 (0.1%)	0.89	1/992 (0.1%)
16	P	0.44	0/716	0.74	0/963
17	Q	0.43	0/836	0.79	0/1117
18	R	0.51	0/604	0.86	1/801 (0.1%)
19	S	0.55	0/670	0.82	1/903 (0.1%)
2	B	0.57	0/1935	0.86	1/2609 (0.0%)
20	T	0.50	0/765	0.96	1/1007 (0.1%)
21	V	0.47	0/212	0.77	0/277
22	W	0.51	0/580	0.99	4/782 (0.5%)
23	X	0.56	0/1375	0.86	1/1844 (0.1%)
24	Y	0.56	0/516	0.83	0/804
25	Z	0.55	0/1718	0.90	3/2678 (0.1%)
3	C	0.48	0/1636	0.85	2/2205 (0.1%)
4	D	0.46	0/1733	0.85	0/2318
5	E	0.47	0/1162	0.82	0/1564
6	F	0.47	0/856	0.88	1/1154 (0.1%)
7	G	0.46	0/1276	0.79	0/1709
8	H	0.43	0/1136	0.82	0/1527
9	I	0.49	0/1029	0.79	1/1379 (0.1%)
All	All	0.43	3/60115 (0.0%)	0.78	43/89066 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
12	L	0	1
2	B	0	2
23	X	0	2
8	H	0	1
All	All	0	6

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	999	C	O3'-P	-6.98	1.52	1.61
1	A	1001	A	O3'-P	-6.75	1.53	1.61
15	O	24	SER	CB-OG	5.23	1.49	1.42

All (43) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	W	23	ARG	N-CA-C	-10.10	83.74	111.00
22	W	23	ARG	CB-CA-C	-8.69	93.02	110.40
6	F	75	LEU	CA-CB-CG	8.65	135.20	115.30
1	A	1001	A	O4'-C4'-C3'	-8.10	95.90	104.00
1	A	575	G	C2'-C3'-O3'	7.99	127.07	109.50
22	W	34	ALA	N-CA-CB	-7.90	99.04	110.10
25	Z	37	A	C2'-C3'-O3'	7.40	125.78	109.50
1	A	1001	A	C2'-C3'-O3'	7.33	125.63	109.50
1	A	1534	A	C2'-C3'-O3'	7.32	125.61	109.50
20	T	10	LEU	CA-CB-CG	7.29	132.08	115.30
1	A	1301	U	C2'-C3'-O3'	7.28	125.52	109.50
14	N	44	LEU	CA-CB-CG	7.10	131.63	115.30
1	A	1212	U	C2'-C3'-O3'	6.91	124.75	113.70
3	C	34	LEU	CA-CB-CG	6.90	131.17	115.30
1	A	266	G	C2'-C3'-O3'	6.88	124.70	113.70
1	A	1498	U	C2'-C3'-O3'	6.86	124.67	113.70
3	C	91	LEU	CA-CB-CG	6.63	130.55	115.30
1	A	197	A	C2'-C3'-O3'	6.58	124.23	113.70
1	A	1000	U	C2'-C3'-O3'	6.58	124.22	113.70
1	A	328	C	C2'-C3'-O3'	6.24	123.68	113.70
22	W	24	VAL	N-CA-CB	-6.20	97.85	111.50
1	A	1145	C	C2'-C3'-O3'	6.05	123.38	113.70
15	O	34	LEU	CA-CB-CG	6.05	129.21	115.30
23	X	103	LEU	CA-CB-CG	6.04	129.19	115.30
25	Z	39	C	C4'-C3'-O3'	5.96	124.92	113.00
1	A	748	C	C2'-C3'-O3'	5.95	123.22	113.70
2	B	51	LEU	CA-CB-CG	5.79	128.62	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1190	G	C2'-C3'-O3'	5.71	122.83	113.70
1	A	1067	A	C2'-C3'-O3'	5.69	122.81	113.70
25	Z	40	C	C2'-C3'-O3'	5.67	122.76	113.70
1	A	960	U	C2'-C3'-O3'	5.66	122.76	113.70
19	S	20	LEU	CA-CB-CG	5.60	128.19	115.30
18	R	26	LEU	CA-CB-CG	5.47	127.88	115.30
1	A	428	G	C2'-C3'-O3'	5.37	122.29	113.70
1	A	1065	U	C2'-C3'-O3'	5.32	122.21	113.70
9	I	85	LEU	CA-CB-CG	5.27	127.43	115.30
13	M	56	LEU	CA-CB-CG	5.27	127.42	115.30
1	A	965	A	C2'-C3'-O3'	5.17	121.97	113.70
1	A	792	A	C2'-C3'-O3'	5.16	121.95	113.70
1	A	181	G	C2'-C3'-O3'	5.12	121.90	113.70
1	A	51	A	C4'-C3'-O3'	5.11	123.22	113.00
1	A	372	C	C2'-C3'-O3'	5.10	121.86	113.70
1	A	60	A	C2'-C3'-O3'	5.08	121.82	113.70

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	11	LEU	Peptide
2	B	130	ARG	Peptide
8	H	2	LEU	Peptide
12	L	112	ASP	Peptide
23	X	53	ASP	Peptide
23	X	55	PRO	Peptide

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	32522	0	16435	1114	0
2	B	1900	0	1951	55	0
3	C	1612	0	1677	81	0
4	D	1703	0	1765	77	0
5	E	1146	0	1207	74	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	F	843	0	857	18	0
7	G	1257	0	1296	25	0
8	H	1116	0	1177	17	0
9	I	1010	0	1037	47	0
10	J	792	0	835	83	0
11	K	906	0	928	21	0
12	L	970	0	1057	23	0
13	M	997	0	1072	27	0
14	N	492	0	530	47	0
15	O	734	0	771	20	0
16	P	700	0	720	18	0
17	Q	823	0	891	20	0
18	R	598	0	670	25	0
19	S	655	0	672	17	0
20	T	763	0	861	20	0
21	V	208	0	221	6	0
22	W	570	0	599	24	0
23	X	1356	0	1401	33	0
24	Y	459	0	228	15	0
25	Z	1643	0	844	128	0
26	A	63	0	0	0	0
26	W	1	0	0	0	0
27	D	1	0	0	4	0
27	N	1	0	0	0	0
All	All	55841	0	39702	1833	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 19.

All (1833) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1080:A:H4'	5:E:16:THR:CG2	1.32	1.59
1:A:1080:A:C5'	5:E:16:THR:HG21	1.42	1.46
1:A:247:G:OP2	17:Q:100:LYS:CG	1.64	1.44
1:A:1080:A:C4'	5:E:16:THR:CG2	2.00	1.40
10:J:61:GLU:CD	14:N:58:LYS:HD3	1.39	1.39
10:J:38:ILE:CG2	10:J:71:LEU:O	1.81	1.29
10:J:61:GLU:OE2	14:N:58:LYS:HD3	1.25	1.28
10:J:36:GLY:O	10:J:72:VAL:HG22	1.10	1.28
1:A:413:G:O6	4:D:35:ARG:NH1	1.67	1.28

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:827:U:H3	1:A:872:A:N6	1.33	1.26
1:A:1080:A:C5'	5:E:16:THR:CG2	2.12	1.23
22:W:23:ARG:NH2	22:W:33:LEU:HD11	1.54	1.22
5:E:15:ARG:HG3	5:E:28:PHE:CE1	1.77	1.20
1:A:1113:C:H4'	3:C:14:ILE:CD1	1.70	1.20
10:J:38:ILE:HG23	10:J:71:LEU:O	1.32	1.18
5:E:15:ARG:CG	5:E:28:PHE:HE1	1.57	1.17
1:A:961:U:O4	1:A:974:A:N1	1.77	1.16
3:C:29:TYR:OH	14:N:54:PRO:HD2	1.44	1.16
1:A:92:C:H2'	1:A:93:G:C8	1.78	1.16
1:A:827:U:N3	1:A:872:A:N6	1.90	1.15
1:A:1080:A:H5''	5:E:16:THR:CG2	1.74	1.15
3:C:29:TYR:OH	14:N:54:PRO:CG	1.96	1.14
3:C:62:ASP:C	3:C:97:LYS:HD3	1.67	1.13
10:J:37:PRO:HA	10:J:72:VAL:CG2	1.78	1.13
1:A:1125:U:C5	10:J:73:ASP:OD2	2.02	1.13
10:J:37:PRO:HA	10:J:72:VAL:HG23	1.30	1.13
3:C:29:TYR:OH	14:N:54:PRO:CD	1.95	1.13
1:A:1081:G:OP2	5:E:27:ARG:NE	1.81	1.12
1:A:1080:A:H4'	5:E:16:THR:HG22	1.27	1.12
3:C:29:TYR:OH	14:N:54:PRO:HG2	1.45	1.11
3:C:64:VAL:HG23	3:C:97:LYS:CD	1.80	1.11
1:A:1113:C:H4'	3:C:14:ILE:HD13	1.30	1.11
3:C:62:ASP:O	3:C:97:LYS:HD3	1.48	1.11
1:A:413:G:C6	4:D:35:ARG:NH1	2.15	1.11
22:W:23:ARG:HH21	22:W:33:LEU:CD1	1.64	1.10
4:D:29:PRO:O	4:D:35:ARG:HD3	1.51	1.10
3:C:64:VAL:CG2	3:C:97:LYS:CE	2.31	1.09
1:A:1080:A:H4'	5:E:16:THR:HG23	1.12	1.08
3:C:64:VAL:HG21	3:C:97:LYS:HE2	1.31	1.07
1:A:247:G:OP2	17:Q:100:LYS:HG3	1.33	1.07
3:C:64:VAL:HG23	3:C:97:LYS:HD2	1.30	1.07
3:C:64:VAL:CG2	3:C:97:LYS:HE2	1.86	1.06
25:Z:5:G:H1	25:Z:68:C:N4	1.52	1.05
3:C:29:TYR:HE1	3:C:33:LEU:HD12	1.19	1.05
1:A:1081:G:OP1	5:E:27:ARG:HD2	1.55	1.05
1:A:247:G:OP2	17:Q:100:LYS:HG2	1.47	1.05
10:J:61:GLU:OE1	14:N:58:LYS:HD3	1.54	1.04
10:J:36:GLY:O	10:J:72:VAL:CG2	2.06	1.04
3:C:29:TYR:CE1	3:C:33:LEU:HD12	1.92	1.03
10:J:61:GLU:CD	14:N:58:LYS:CD	2.26	1.02

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:61:GLU:OE2	14:N:58:LYS:CD	2.09	1.01
4:D:201:GLN:NE2	5:E:116:THR:OG1	1.93	1.00
1:A:664:G:H22	1:A:741:G:H1	1.04	1.00
1:A:827:U:O4	1:A:872:A:N1	1.95	1.00
22:W:23:ARG:NH2	22:W:33:LEU:CD1	2.23	0.99
5:E:15:ARG:HG3	5:E:28:PHE:HE1	1.11	0.99
23:X:52:ALA:HB2	25:Z:19:G:N2	1.77	0.99
25:Z:44:A:O2'	25:Z:45:G:H5'	1.62	0.98
1:A:92:C:H2'	1:A:93:G:H8	1.16	0.98
1:A:80:G:H3'	1:A:81:U:H5''	1.45	0.98
4:D:29:PRO:O	4:D:35:ARG:CD	2.12	0.98
1:A:864:A:H2'	1:A:865:A:C8	1.98	0.97
1:A:1081:G:P	5:E:27:ARG:CD	2.52	0.97
25:Z:72:A:H3'	25:Z:73:A:H5''	1.41	0.97
10:J:61:GLU:OE1	14:N:58:LYS:CD	2.13	0.96
1:A:413:G:C5	4:D:35:ARG:NH1	2.33	0.96
10:J:38:ILE:HG22	10:J:71:LEU:O	1.64	0.95
4:D:31:CYS:SG	27:D:300:ZN:ZN	1.56	0.94
1:A:413:G:N7	4:D:35:ARG:NH1	2.17	0.93
25:Z:7:G:H2'	25:Z:49:G:H5'	1.50	0.93
1:A:1081:G:OP2	5:E:27:ARG:CD	2.15	0.93
1:A:1219:U:H2'	1:A:1220:G:C8	2.04	0.93
1:A:1458:G:OP1	20:T:32:ALA:HA	1.67	0.93
1:A:1219:U:H2'	1:A:1220:G:H8	1.33	0.93
1:A:1125:U:H5'	1:A:1126:U:H5	1.34	0.92
2:B:186:ALA:HB2	2:B:197:VAL:HG11	1.52	0.92
5:E:15:ARG:CG	5:E:28:PHE:CE1	2.44	0.92
1:A:1080:A:C4'	5:E:16:THR:HG21	1.86	0.91
1:A:736:C:H2'	1:A:737:A:C8	2.06	0.91
25:Z:5:G:N2	25:Z:68:C:N3	2.20	0.90
3:C:64:VAL:HG23	3:C:97:LYS:CE	2.00	0.90
1:A:1113:C:C4'	3:C:14:ILE:CD1	2.48	0.90
4:D:26:CYS:SG	27:D:300:ZN:ZN	1.60	0.89
1:A:1001:A:H2'	1:A:1001(A):G:C8	2.06	0.89
3:C:62:ASP:O	3:C:97:LYS:CD	2.20	0.89
4:D:35:ARG:NH2	4:D:35:ARG:HB3	1.88	0.89
9:I:125:TYR:CE1	9:I:128:ARG:HB3	2.07	0.89
23:X:52:ALA:HB2	25:Z:19:G:H22	1.33	0.88
1:A:1348:U:H2'	1:A:1349:A:H8	1.37	0.88
1:A:1080:A:C4'	5:E:16:THR:HG23	1.88	0.87
25:Z:4:G:H1	25:Z:69:C:H42	1.23	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1386:G:H2'	1:A:1387:G:H8	1.40	0.86
5:E:15:ARG:HG2	5:E:15:ARG:HH21	1.38	0.86
5:E:15:ARG:NH2	5:E:26:PHE:CG	2.42	0.86
25:Z:9:G:O2'	25:Z:45:G:H1'	1.75	0.86
1:A:18:C:H2'	1:A:19:C:O4'	1.74	0.86
1:A:1403:C:O2	1:A:1499:A:N6	2.08	0.85
1:A:729:A:H2'	1:A:730:G:H8	1.41	0.85
1:A:1079:G:H2'	1:A:1080:A:C8	2.12	0.85
4:D:36:ARG:HD2	4:D:38:TYR:CZ	2.11	0.85
5:E:15:ARG:HA	5:E:28:PHE:CD1	2.12	0.84
10:J:24:VAL:HG13	10:J:28:ARG:HE	1.42	0.84
24:Y:34:A:H2'	24:Y:35:A:C8	2.12	0.84
1:A:1280:A:H3'	1:A:1281:U:H5''	1.58	0.84
1:A:920:U:H2'	1:A:921:U:C6	2.12	0.84
1:A:312:C:H2'	1:A:313:A:C8	2.13	0.84
5:E:27:ARG:CB	5:E:27:ARG:HH11	1.89	0.84
1:A:1488:G:H2'	1:A:1489:G:H8	1.43	0.83
10:J:36:GLY:C	10:J:72:VAL:HG22	1.97	0.83
9:I:5:TYR:CE2	9:I:7:THR:OG1	2.31	0.83
1:A:1125:U:H5	10:J:73:ASP:OD2	1.59	0.83
3:C:29:TYR:CE1	3:C:33:LEU:CD1	2.61	0.83
5:E:15:ARG:HA	5:E:28:PHE:CE1	2.14	0.83
1:A:1081:G:OP1	5:E:27:ARG:CD	2.27	0.82
4:D:18:LYS:NZ	4:D:34:GLU:HG3	1.94	0.82
1:A:1081:G:P	5:E:27:ARG:HD3	2.19	0.81
24:Y:33:A:O2'	24:Y:34:A:C8	2.34	0.81
9:I:97:LYS:HG3	9:I:102:LEU:HD13	1.62	0.81
1:A:1113:C:O2'	3:C:14:ILE:HD11	1.81	0.80
1:A:662:G:H2'	1:A:663:A:C8	2.17	0.80
25:Z:37:A:H3'	25:Z:38:A:H8	1.46	0.80
1:A:917:G:H2'	1:A:918:A:C8	2.16	0.80
3:C:29:TYR:HH	14:N:54:PRO:HG2	1.46	0.80
1:A:1123:A:H4'	10:J:36:GLY:HA3	1.64	0.80
1:A:1080:A:H5''	5:E:16:THR:HG21	0.81	0.79
25:Z:40:C:H2'	25:Z:41:C:H6	1.45	0.79
1:A:76:C:C2'	1:A:77:G:H5'	2.12	0.79
1:A:312:C:H2'	1:A:313:A:H8	1.46	0.79
22:W:23:ARG:HH21	22:W:33:LEU:HD13	1.45	0.79
25:Z:10:G:O6	25:Z:45:G:N2	2.14	0.79
1:A:1071:C:H2'	1:A:1072:G:H8	1.46	0.79
1:A:501:C:H2'	1:A:502:G:C8	2.18	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:Y:33:A:O2'	24:Y:34:A:H8	1.66	0.79
25:Z:21:A:N6	25:Z:46:G7M:H2'	1.98	0.78
1:A:1256:A:N6	1:A:1278:U:O2	2.15	0.78
1:A:1127:G:H21	1:A:1147:C:N4	1.81	0.78
1:A:439:A:P	1:A:493:G:H1	2.06	0.78
4:D:36:ARG:HD2	4:D:38:TYR:OH	1.82	0.78
25:Z:68:C:H2'	25:Z:69:C:C6	2.18	0.78
18:R:47:THR:HA	18:R:83:GLU:HB2	1.65	0.78
1:A:1542:U:H4'	18:R:18:ARG:H	1.46	0.78
1:A:1080:A:O3'	5:E:16:THR:HG22	1.83	0.78
10:J:60:ARG:HH11	10:J:60:ARG:HG3	1.49	0.78
1:A:714:G:H2'	1:A:715:A:C8	2.20	0.77
3:C:62:ASP:CA	3:C:97:LYS:HD3	2.13	0.77
25:Z:21:A:H61	25:Z:46:G7M:H2'	1.49	0.77
25:Z:49:G:N2	25:Z:66:C:C2	2.52	0.77
4:D:35:ARG:HH21	4:D:35:ARG:HB3	1.49	0.77
1:A:748:C:H1'	1:A:749:C:H5	1.50	0.76
5:E:15:ARG:HH22	5:E:26:PHE:CB	1.99	0.76
10:J:6:ILE:HA	10:J:97:GLU:O	1.84	0.76
1:A:1113:C:H4'	3:C:14:ILE:HD12	1.65	0.76
2:B:186:ALA:CB	2:B:197:VAL:HG11	2.15	0.76
1:A:1342:C:H2'	1:A:1343:G:H8	1.49	0.76
10:J:5:ARG:HA	10:J:73:ASP:OD1	1.85	0.76
1:A:1102:A:H2'	1:A:1103:C:C6	2.20	0.76
1:A:736:C:H2'	1:A:737:A:H8	1.49	0.76
1:A:90:U:H2'	1:A:91:C:C6	2.20	0.76
3:C:23:TYR:HA	10:J:11:PHE:CE2	2.21	0.76
10:J:60:ARG:NH1	10:J:60:ARG:HG3	2.01	0.76
1:A:247:G:OP2	17:Q:100:LYS:CD	2.34	0.76
3:C:29:TYR:CZ	14:N:54:PRO:HG2	2.20	0.75
1:A:80:G:H3'	1:A:81:U:C5'	2.17	0.75
4:D:68:TYR:HB2	4:D:70:ILE:HD11	1.67	0.75
1:A:918:A:H2'	1:A:919:A:C8	2.22	0.75
3:C:64:VAL:CG2	3:C:97:LYS:HD2	2.14	0.74
4:D:36:ARG:CD	4:D:38:TYR:CZ	2.69	0.74
12:L:117:ARG:HB2	12:L:122:THR:HB	1.68	0.74
9:I:26:VAL:HB	9:I:33:PHE:HB2	1.69	0.74
22:W:33:LEU:O	22:W:64:ARG:HA	1.88	0.74
11:K:18:ARG:HG3	11:K:81:ASP:HB2	1.68	0.74
3:C:64:VAL:CG2	3:C:97:LYS:CD	2.61	0.74
10:J:33:GLN:HB3	10:J:75:ILE:HD12	1.68	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1172:C:H2'	1:A:1173:G:H8	1.52	0.74
6:F:49:ALA:HB1	18:R:80:PRO:HA	1.68	0.74
1:A:1342:C:H2'	1:A:1343:G:C8	2.22	0.74
10:J:39:PRO:O	10:J:40:LEU:HB2	1.88	0.73
6:F:100:ASN:HA	18:R:23:LYS:HE2	1.69	0.73
10:J:37:PRO:CA	10:J:72:VAL:CG2	2.63	0.73
23:X:19:VAL:HG21	25:Z:56:C:N4	2.03	0.73
25:Z:6:G:N2	25:Z:68:C:C2	2.56	0.73
1:A:78:G:H2'	1:A:79:G:O4'	1.88	0.73
1:A:880:C:H2'	1:A:881:G:H8	1.52	0.73
9:I:55:ALA:HB1	9:I:58:HIS:HB3	1.71	0.73
20:T:14:LYS:HA	20:T:17:ARG:HD2	1.71	0.73
1:A:1007:C:H42	1:A:1022:G:H1	1.36	0.73
1:A:24:U:H2'	1:A:25:C:C6	2.24	0.73
4:D:29:PRO:O	4:D:35:ARG:CG	2.35	0.73
1:A:664:G:N2	1:A:741:G:H1	1.85	0.73
1:A:973:G:H3'	1:A:974:A:H5''	1.70	0.73
2:B:20:GLU:HB3	2:B:23:ARG:HD2	1.70	0.73
1:A:524:G:C6	1:A:525:C:N4	2.56	0.73
25:Z:49:G:C2	25:Z:66:C:N3	2.57	0.73
25:Z:12:G:H1	25:Z:23:C:H42	1.36	0.72
1:A:814:A:H2'	1:A:816:A:H5''	1.70	0.72
1:A:946:A:H2'	1:A:947:G:C8	2.23	0.72
18:R:37:VAL:HG22	18:R:78:LEU:HD13	1.71	0.72
5:E:27:ARG:HH11	5:E:27:ARG:HB2	1.52	0.72
23:X:64:LYS:O	23:X:68:GLU:HG2	1.89	0.72
9:I:8:GLY:HA2	9:I:79:LEU:HD12	1.72	0.72
1:A:1287:A:H2'	1:A:1288:A:C8	2.25	0.72
1:A:1384:C:H2'	1:A:1385:G:C8	2.24	0.72
1:A:76:C:H2'	1:A:77:G:H5'	1.71	0.72
1:A:1105:A:H2'	1:A:1106:G:H8	1.53	0.72
11:K:15:ALA:HA	11:K:77:MET:HA	1.69	0.71
1:A:1427:U:H2'	1:A:1428:A:C8	2.25	0.71
1:A:961:U:C4	1:A:974:A:N1	2.58	0.71
1:A:1081:G:OP2	5:E:27:ARG:HD3	1.88	0.71
1:A:1226:C:H2'	13:M:103:THR:HB	1.72	0.71
3:C:29:TYR:HE1	3:C:33:LEU:CD1	2.00	0.71
25:Z:39:C:H2'	25:Z:40:C:C6	2.26	0.71
1:A:745:C:H2'	1:A:746:A:C8	2.25	0.71
25:Z:48:C:H5''	25:Z:50:U:OP1	1.91	0.71
2:B:84:GLU:HB3	2:B:219:VAL:HG21	1.73	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1099:G:C6	1:A:1100:C:N3	2.59	0.70
1:A:868:C:H2'	1:A:869:G:O4'	1.91	0.70
3:C:77:ILE:HA	3:C:84:ILE:HB	1.72	0.70
4:D:18:LYS:HZ2	4:D:34:GLU:HG3	1.56	0.70
1:A:1014:A:H5''	19:S:14:HIS:HB3	1.72	0.70
1:A:1530:G:H2'	1:A:1531:A:C8	2.27	0.70
1:A:1518:A:H2'	1:A:1519:A:C8	2.26	0.70
10:J:27:ALA:HB2	10:J:85:LEU:HD21	1.74	0.70
1:A:1128:C:H1'	1:A:1146:A:H61	1.57	0.70
3:C:77:ILE:HG22	3:C:81:GLY:HA2	1.74	0.70
11:K:126:ARG:HH12	11:K:129:SER:HA	1.56	0.70
1:A:1071:C:H2'	1:A:1072:G:C8	2.27	0.69
1:A:501:C:H2'	1:A:502:G:H8	1.55	0.69
3:C:73:PRO:O	3:C:77:ILE:HG12	1.92	0.69
25:Z:69:C:H2'	25:Z:70:G:O4'	1.91	0.69
1:A:1022:G:H2'	1:A:1023:G:H8	1.56	0.69
1:A:1513:A:H2'	1:A:1514:C:C6	2.27	0.69
1:A:79:G:H2'	1:A:80:G:H8	1.56	0.69
1:A:834:C:H5''	18:R:60:ALA:CB	2.23	0.69
4:D:36:ARG:CD	4:D:38:TYR:OH	2.39	0.69
5:E:15:ARG:HG3	5:E:28:PHE:CZ	2.28	0.69
1:A:975:A:H4'	1:A:976:G:H5'	1.73	0.69
16:P:59:TRP:O	16:P:62:VAL:HG22	1.92	0.69
1:A:524:G:C2	1:A:525:C:N3	2.61	0.69
1:A:1076:C:H2'	1:A:1077:G:C8	2.28	0.69
1:A:1488:G:H2'	1:A:1489:G:C8	2.26	0.69
1:A:1125:U:H5'	1:A:1126:U:C5	2.25	0.69
1:A:1151:A:O2'	1:A:1152:A:H8	1.76	0.69
1:A:1348:U:H2'	1:A:1349:A:C8	2.25	0.68
1:A:56:U:H2'	1:A:57:G:C8	2.28	0.68
1:A:13:U:H3	1:A:915:A:N6	1.90	0.68
4:D:31:CYS:HG	27:D:300:ZN:ZN	0.40	0.68
1:A:1218:C:H2'	1:A:1219:U:C6	2.27	0.68
1:A:34:C:H2'	1:A:35:G:C8	2.27	0.68
1:A:579:G:H2'	1:A:580:U:C6	2.29	0.68
1:A:778:G:HO2'	11:K:119:CYS:HG	1.32	0.68
1:A:877:C:H2'	1:A:878:G:H8	1.59	0.68
1:A:1060:C:C5	3:C:2:GLY:HA2	2.29	0.68
1:A:67:C:H2'	1:A:68:G:C8	2.29	0.68
25:Z:72:A:H3'	25:Z:73:A:C5'	2.19	0.68
1:A:729:A:H2'	1:A:730:G:C8	2.29	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1080:A:C5'	5:E:16:THR:HG23	2.13	0.68
1:A:1080:A:C4'	5:E:16:THR:HG22	1.98	0.68
3:C:116:VAL:O	3:C:120:VAL:HG23	1.94	0.68
4:D:96:LEU:HG	4:D:139:ARG:HE	1.59	0.68
1:A:987:G:H1	1:A:1218:C:H42	1.41	0.67
5:E:100:VAL:HG13	5:E:118:ILE:HD11	1.75	0.67
1:A:269:C:H2'	1:A:270:A:C8	2.28	0.67
1:A:313:A:H2'	1:A:314:C:C6	2.29	0.67
1:A:1386:G:H2'	1:A:1387:G:C8	2.28	0.67
5:E:15:ARG:NH2	5:E:26:PHE:CD1	2.62	0.67
3:C:23:TYR:HA	10:J:11:PHE:HE2	1.58	0.67
1:A:34:C:H2'	1:A:35:G:H8	1.58	0.67
1:A:576:G:H3'	1:A:577:G:H5''	1.76	0.67
25:Z:66:C:H2'	25:Z:67:C:O4'	1.93	0.67
1:A:45:U:H2'	1:A:46:G:C8	2.30	0.67
10:J:51:ARG:HD3	10:J:59:SER:HB3	1.76	0.67
1:A:1113:C:C4'	3:C:14:ILE:HD12	2.24	0.67
1:A:1405:G:H2'	1:A:1406:U:C6	2.30	0.67
10:J:62:HIS:HB2	14:N:59:ALA:HB3	1.76	0.67
1:A:1523:G:H2'	1:A:1524:C:C6	2.30	0.67
1:A:1223:C:H5''	1:A:1224:G:H5''	1.76	0.66
1:A:1384:C:H2'	1:A:1385:G:H8	1.60	0.66
10:J:5:ARG:CA	10:J:73:ASP:OD1	2.42	0.66
1:A:1445:C:C2	1:A:1458:G:C2	2.84	0.66
1:A:1353:G:N2	1:A:1354:C:C2	2.64	0.66
1:A:1318:A:H1'	19:S:37:ARG:HH11	1.61	0.66
25:Z:40:C:H2'	25:Z:41:C:C6	2.29	0.66
1:A:750:G:N3	15:O:23:GLY:HA3	2.11	0.66
25:Z:5:G:H1	25:Z:68:C:H42	0.74	0.66
15:O:26:GLU:O	15:O:29:VAL:HG12	1.95	0.66
16:P:58:TYR:O	16:P:62:VAL:HG13	1.96	0.66
1:A:1404:C:H2'	1:A:1405:G:C8	2.31	0.66
2:B:219:VAL:HA	2:B:222:ILE:HD12	1.76	0.66
15:O:12:ILE:HG21	15:O:22:THR:HG22	1.78	0.66
1:A:398:C:H2'	1:A:399:G:H8	1.59	0.66
7:G:65:ALA:HB1	7:G:127:ALA:HB3	1.78	0.66
1:A:1405:G:H2'	1:A:1406:U:H6	1.60	0.66
1:A:725:G:N2	1:A:726:C:C2	2.64	0.66
1:A:92:C:C2'	1:A:93:G:H8	2.02	0.66
1:A:381:C:H2'	1:A:382:A:O4'	1.95	0.65
1:A:457:C:H2'	1:A:458:C:C6	2.31	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:Z:38:A:H3'	25:Z:39:C:H6	1.61	0.65
25:Z:8:4SU:H6	25:Z:8:4SU:O5'	1.95	0.65
1:A:774:G:N2	1:A:806:C:C2	2.64	0.65
1:A:243:A:H4'	1:A:244:U:O5'	1.95	0.65
1:A:1281:U:H4'	1:A:1282:C:OP2	1.96	0.65
2:B:21:ARG:HA	2:B:39:ILE:HA	1.78	0.65
8:H:64:LYS:HB3	8:H:79:VAL:HG11	1.77	0.65
1:A:975:A:H4'	1:A:976:G:C5'	2.26	0.65
19:S:47:HIS:O	19:S:62:ILE:HG22	1.97	0.65
25:Z:71:C:H2'	25:Z:72:A:O4'	1.96	0.65
1:A:880:C:H2'	1:A:881:G:C8	2.31	0.65
1:A:910:C:H4'	1:A:1413:A:H4'	1.78	0.65
1:A:1084:G:H5''	1:A:1085:U:H2'	1.77	0.65
1:A:1172:C:H2'	1:A:1173:G:C8	2.31	0.65
25:Z:4:G:H1	25:Z:69:C:N4	1.93	0.65
4:D:11:LEU:HD13	4:D:66:ARG:HG3	1.78	0.65
5:E:15:ARG:NH2	5:E:15:ARG:HG2	2.11	0.65
1:A:289:G:N2	1:A:290:C:C2	2.65	0.65
5:E:140:ARG:HB2	5:E:140:ARG:HH11	1.62	0.65
24:Y:23:C:H2'	24:Y:24:A:O4'	1.97	0.65
1:A:1048:G:N2	1:A:1210:C:C2	2.66	0.64
25:Z:49:G:C2	25:Z:66:C:C2	2.86	0.64
1:A:16:A:H2	1:A:1080:A:N3	1.95	0.64
1:A:1475:G:H2'	1:A:1476:G:H8	1.61	0.64
10:J:5:ARG:HG2	10:J:71:LEU:HD21	1.79	0.64
11:K:99:GLN:HA	11:K:105:VAL:HG21	1.79	0.64
18:R:38:GLU:CD	18:R:38:GLU:H	1.99	0.64
1:A:132:C:C2	1:A:231:G:N2	2.65	0.64
25:Z:10:G:H1	25:Z:25:C:H42	1.45	0.64
1:A:992:U:H1'	1:A:993:G:C2	2.33	0.64
1:A:662:G:H2'	1:A:663:A:H8	1.58	0.64
1:A:737:A:H2'	1:A:738:C:C6	2.33	0.64
1:A:839:U:O2	1:A:839:U:H2'	1.97	0.64
1:A:123:C:H2'	1:A:124:G:H8	1.63	0.64
2:B:72:GLY:HA3	2:B:81:VAL:HG21	1.80	0.64
10:J:82:ILE:HG22	10:J:86:MET:HB2	1.78	0.64
1:A:45:U:H2'	1:A:46:G:H8	1.63	0.64
1:A:254:G:H1	1:A:272:C:H42	1.46	0.63
1:A:999:C:O2	1:A:1043:C:O2	2.15	0.63
10:J:34:VAL:HG22	10:J:74:ILE:HG23	1.80	0.63
1:A:354:G:N2	1:A:355:C:C2	2.67	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1507:A:H2'	1:A:1508:G:C8	2.32	0.63
1:A:1523:G:H2'	1:A:1524:C:H6	1.63	0.63
2:B:223:ILE:HG21	2:B:230:VAL:HB	1.79	0.63
4:D:18:LYS:HZ3	4:D:34:GLU:HG3	1.64	0.63
8:H:111:ILE:HG22	8:H:134:ILE:HD12	1.80	0.63
9:I:46:ALA:HB2	9:I:74:ILE:HG23	1.80	0.63
1:A:748:C:H1'	1:A:749:C:C5	2.33	0.63
17:Q:11:VAL:HG12	17:Q:85:VAL:HG22	1.80	0.63
25:Z:38:A:H3'	25:Z:39:C:C6	2.33	0.63
1:A:1354:C:H2'	1:A:1355:G:H8	1.63	0.63
25:Z:56:C:H2'	25:Z:57:A:C8	2.33	0.63
1:A:1496:C:H2'	1:A:1497:G:O4'	1.98	0.62
1:A:695:A:H2'	1:A:696:A:C8	2.34	0.62
1:A:1166:G:N2	1:A:1170:A:OP2	2.31	0.62
10:J:6:ILE:CD1	10:J:23:ILE:HG21	2.29	0.62
1:A:1125:U:C4	10:J:73:ASP:OD2	2.53	0.62
1:A:24:U:H2'	1:A:25:C:H6	1.63	0.62
5:E:15:ARG:HG2	5:E:28:PHE:HE1	1.57	0.62
6:F:12:PRO:HA	6:F:59:TYR:HB2	1.82	0.62
9:I:5:TYR:HE2	9:I:7:THR:OG1	1.82	0.62
25:Z:67:C:C2	25:Z:68:C:C5	2.87	0.62
1:A:253:U:H2'	1:A:254:G:H8	1.63	0.62
1:A:890:G:O2'	1:A:906:G:O6	2.16	0.62
12:L:25:PRO:C	12:L:27:LEU:H	2.00	0.62
1:A:1076:C:H2'	1:A:1077:G:H8	1.65	0.62
1:A:779:C:H2'	1:A:780:A:O4'	1.99	0.62
1:A:1118:C:P	9:I:104:ARG:HE	2.22	0.62
1:A:1278:U:H5''	1:A:1279:A:O4'	2.00	0.62
1:A:1493:A:H4'	1:A:1494:G:OP1	1.99	0.62
1:A:258:G:N2	1:A:269:C:C2	2.68	0.62
25:Z:37:A:H3'	25:Z:38:A:C8	2.32	0.62
25:Z:52:G:HO2'	25:Z:53:G:H8	1.47	0.62
22:W:17:LEU:HB3	22:W:18:PRO:HD2	1.81	0.62
1:A:1255:G:H2'	1:A:1279:A:H62	1.65	0.62
1:A:911:U:H2'	1:A:912:C:C6	2.35	0.62
5:E:51:VAL:HB	5:E:52:PRO:HD3	1.81	0.62
19:S:11:VAL:HA	19:S:38:SER:HB2	1.82	0.62
1:A:1367:C:H5'	10:J:60:ARG:NH1	2.14	0.62
6:F:75:LEU:O	6:F:79:LEU:HG	2.00	0.62
9:I:112:LYS:HA	9:I:119:ALA:HB2	1.80	0.62
1:A:32:A:H2'	1:A:33:A:C8	2.35	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:840:C:H4'	1:A:841:U:O5'	2.00	0.61
1:A:917:G:H2'	1:A:918:A:H8	1.62	0.61
1:A:961:U:H2'	1:A:962:C:C6	2.35	0.61
3:C:29:TYR:HD1	3:C:29:TYR:O	1.82	0.61
23:X:34:ALA:HA	23:X:37:LEU:HD12	1.81	0.61
1:A:1062:U:H2'	1:A:1063:C:C6	2.35	0.61
1:A:457:C:H2'	1:A:458:C:H6	1.66	0.61
1:A:652:U:O4	1:A:752:G:O2'	2.15	0.61
1:A:132:C:N3	1:A:231:G:C2	2.69	0.61
1:A:992:U:H2'	1:A:992:U:O2	2.00	0.61
1:A:827:U:C2	1:A:872:A:N6	2.65	0.61
10:J:50:ILE:HG13	10:J:60:ARG:HD3	1.82	0.61
11:K:96:ARG:HH11	11:K:96:ARG:HG2	1.65	0.61
21:V:24:ARG:O	21:V:25:LYS:HB2	1.99	0.61
1:A:1264:C:H2'	1:A:1265:G:H8	1.64	0.61
10:J:21:GLN:HA	10:J:24:VAL:HB	1.83	0.61
25:Z:56:C:H2'	25:Z:57:A:H8	1.64	0.61
1:A:718:G:H21	18:R:49:LYS:HE3	1.65	0.61
1:A:1105:A:H2'	1:A:1106:G:C8	2.33	0.61
5:E:27:ARG:HH11	5:E:27:ARG:CG	2.14	0.61
8:H:119:LEU:HD13	8:H:123:GLU:HB3	1.81	0.61
1:A:69:G:H1	1:A:100:C:H42	1.49	0.61
1:A:1189:C:H5'	14:N:58:LYS:HZ1	1.65	0.61
23:X:11:ILE:HG12	23:X:47:LEU:HB2	1.82	0.61
1:A:755:G:N2	1:A:756:C:C2	2.69	0.60
1:A:1539:C:H42	24:Y:26:G:H1	1.50	0.60
25:Z:44:A:C2'	25:Z:45:G:H5'	2.31	0.60
1:A:1255:G:H2'	1:A:1279:A:N6	2.17	0.60
1:A:1356:G:H2'	1:A:1357:A:C8	2.36	0.60
1:A:1514:C:H2'	1:A:1515:C:C6	2.36	0.60
1:A:170:U:H2'	1:A:171:A:H8	1.66	0.60
1:A:17:U:O2	1:A:1079:G:N2	2.35	0.60
1:A:513:C:H2'	1:A:514:C:C6	2.37	0.60
7:G:65:ALA:O	7:G:69:VAL:HG23	2.00	0.60
1:A:56:U:H2'	1:A:57:G:H8	1.67	0.60
4:D:102:ASP:HB3	4:D:136:PRO:HB3	1.84	0.60
12:L:32:PHE:HB3	12:L:84:LEU:HD11	1.84	0.60
24:Y:21:G:H2'	24:Y:22:G:C8	2.37	0.60
1:A:413:G:O6	4:D:35:ARG:CZ	2.48	0.60
25:Z:9:G:N3	25:Z:45:G:H2'	2.16	0.60
1:A:1025:U:H2'	1:A:1026:G:C8	2.35	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:64:VAL:CG2	3:C:97:LYS:HE3	2.29	0.60
1:A:537:G:H5''	12:L:113:ARG:HH12	1.66	0.60
22:W:23:ARG:HH22	22:W:33:LEU:HD11	1.62	0.60
23:X:7:THR:HG22	23:X:46:VAL:HG22	1.84	0.60
1:A:129(A):G:H4'	1:A:130:A:O5'	2.02	0.60
1:A:17:U:H2'	1:A:18:C:C6	2.37	0.60
1:A:902:G:H2'	1:A:903:G:H8	1.66	0.60
3:C:150:LYS:HB3	3:C:201:TYR:HB2	1.84	0.60
22:W:32:ILE:HB	22:W:63:THR:O	2.02	0.60
25:Z:21:A:H61	25:Z:46:G7M:C2'	2.15	0.60
25:Z:58:A:O3'	25:Z:60:U:H5	1.84	0.60
1:A:1283:G:N2	1:A:1284:C:C2	2.70	0.59
1:A:1458:G:OP1	20:T:32:ALA:CA	2.49	0.59
1:A:613:C:H2'	1:A:614:A:H8	1.66	0.59
10:J:50:ILE:HG13	10:J:60:ARG:CD	2.32	0.59
25:Z:62:C:H2'	25:Z:63:G:O4'	2.02	0.59
1:A:439:A:C4	1:A:496:A:C2	2.90	0.59
12:L:72:GLY:HA3	12:L:102:ARG:HH11	1.67	0.59
18:R:48:GLY:HA3	18:R:82:THR:HA	1.84	0.59
1:A:229:U:H2'	1:A:230:G:C8	2.37	0.59
2:B:19:HIS:CD2	2:B:20:GLU:HG2	2.37	0.59
4:D:25:ARG:C	4:D:27:TYR:H	2.03	0.59
25:Z:35:A:H2'	25:Z:36:U:C6	2.37	0.59
1:A:1070:U:H2'	1:A:1071:C:C6	2.37	0.59
1:A:643:C:H4'	8:H:31:PHE:CE2	2.37	0.59
1:A:948:C:H2'	1:A:949:A:H8	1.67	0.59
4:D:36:ARG:HD2	4:D:38:TYR:CE1	2.38	0.59
15:O:82:ILE:HA	15:O:87:ILE:HD12	1.83	0.59
14:N:41:ARG:HG3	14:N:42:ILE:N	2.18	0.59
1:A:1192:C:H2'	1:A:1193:G:O4'	2.03	0.59
1:A:266:G:O2'	17:Q:67:LYS:HD2	2.03	0.59
1:A:313:A:H2'	1:A:314:C:H6	1.64	0.59
1:A:546:G:OP2	4:D:72:GLU:HB3	2.03	0.59
1:A:975:A:N7	10:J:60:ARG:NH2	2.51	0.59
25:Z:20:U:H5'	25:Z:21:A:OP2	2.03	0.59
1:A:588:G:N2	1:A:589:C:C2	2.71	0.59
1:A:926:G:H3'	1:A:1505:G:H21	1.68	0.59
3:C:156:ARG:H	3:C:163:ALA:HA	1.68	0.59
1:A:636:U:H2'	1:A:637:G:C8	2.38	0.58
10:J:50:ILE:HD12	10:J:50:ILE:H	1.68	0.58
25:Z:50:U:O2	25:Z:64:G:O6	2.20	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:542:G:H5'	4:D:41:GLY:HA3	1.85	0.58
8:H:33:GLU:HA	8:H:36:LEU:HD12	1.85	0.58
12:L:24:VAL:HG12	12:L:26:ALA:H	1.67	0.58
1:A:222:U:H2'	1:A:223:U:C6	2.38	0.58
12:L:83:VAL:HG23	12:L:107:ALA:HB2	1.85	0.58
1:A:671:G:C2	1:A:736:C:N3	2.71	0.58
1:A:69:G:H1	1:A:100:C:N4	2.01	0.58
1:A:1411:C:H2'	1:A:1412:C:O4'	2.03	0.58
1:A:500:G:C6	1:A:501:C:N4	2.71	0.58
1:A:757:U:H2'	1:A:758:G:O4'	2.02	0.58
1:A:926:G:H2'	1:A:1505:G:N3	2.18	0.58
7:G:125:MET:O	7:G:129:GLU:HG2	2.03	0.58
11:K:11:LYS:O	11:K:13:GLN:N	2.34	0.58
25:Z:18:G:N2	25:Z:57:A:H2'	2.19	0.58
1:A:1225:A:N3	1:A:1225:A:H2'	2.18	0.58
1:A:1287:A:H2'	1:A:1288:A:H8	1.67	0.58
1:A:520:A:H62	1:A:529:G:H21	1.52	0.58
10:J:60:ARG:HH11	10:J:60:ARG:CG	2.14	0.58
1:A:110:C:H2'	1:A:111:G:O4'	2.03	0.58
1:A:1418:A:N6	1:A:1482:G:O2'	2.37	0.58
1:A:521:G:N2	1:A:522:C:C2	2.71	0.58
1:A:617:G:N1	1:A:618:C:C4	2.72	0.58
2:B:105:PHE:HA	2:B:108:ILE:HG22	1.85	0.58
2:B:222:ILE:O	2:B:226:ARG:HG3	2.03	0.58
4:D:129:ASN:HD21	4:D:145:GLU:H	1.50	0.58
24:Y:21:G:H2'	24:Y:22:G:H8	1.69	0.58
1:A:1225:A:OP1	13:M:102:ARG:HA	2.03	0.58
1:A:1127:G:H21	1:A:1147:C:H41	1.49	0.57
1:A:1427:U:H2'	1:A:1428:A:H8	1.69	0.57
1:A:335:C:H2'	1:A:336:C:C6	2.39	0.57
1:A:441:A:H8	1:A:441:A:H5''	1.69	0.57
1:A:522:C:H41	12:L:53:ARG:NH2	2.01	0.57
1:A:734:G:H21	18:R:75:ILE:HD11	1.69	0.57
1:A:1141:C:H2'	1:A:1142:G:H8	1.68	0.57
1:A:114:U:H2'	1:A:115:G:C8	2.39	0.57
1:A:1221:G:H2'	1:A:1222:G:H8	1.68	0.57
1:A:1443:G:N2	1:A:1444:C:C2	2.72	0.57
1:A:1443:G:C6	1:A:1444:C:N4	2.72	0.57
1:A:575:G:H4'	1:A:576:G:H5'	1.85	0.57
9:I:114:TYR:CE2	10:J:58:ASP:O	2.57	0.57
1:A:61:G:H2'	1:A:62:U:O4'	2.03	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:794:A:H2'	1:A:795:C:C6	2.39	0.57
4:D:101:LEU:HB2	4:D:138:TYR:HB3	1.85	0.57
5:E:15:ARG:HA	5:E:28:PHE:HD1	1.65	0.57
14:N:24:CYS:HB3	14:N:29:ARG:H	1.68	0.57
1:A:1530:G:H2'	1:A:1531:A:H8	1.66	0.57
1:A:262:A:H5''	20:T:76:ALA:HB2	1.86	0.57
3:C:40:ARG:HG2	3:C:55:VAL:HG11	1.86	0.57
9:I:114:TYR:CD2	10:J:58:ASP:O	2.58	0.57
1:A:1069:C:H42	1:A:1106:G:H1	1.51	0.57
1:A:1258:G:C6	1:A:1259:C:N4	2.72	0.57
1:A:142:G:H2'	1:A:143:A:C8	2.39	0.57
1:A:67:C:H2'	1:A:68:G:H8	1.69	0.57
3:C:134:ILE:O	3:C:138:VAL:HG23	2.05	0.57
1:A:1495:U:H1'	23:X:95:ASP:HB2	1.87	0.57
1:A:1075:C:H5'	1:A:1101:A:N6	2.20	0.57
1:A:874:G:N2	1:A:875:C:C2	2.73	0.57
1:A:684:A:H4'	11:K:12:ARG:CZ	2.34	0.57
25:Z:65:C:C2	25:Z:66:C:C5	2.93	0.57
1:A:1005:A:O4'	1:A:1036:G:N2	2.38	0.57
1:A:1438:G:N2	1:A:1439:C:C2	2.73	0.57
1:A:434:U:H2'	1:A:435:C:C6	2.39	0.57
20:T:37:SER:HB3	20:T:84:LEU:HD21	1.86	0.57
1:A:1391:U:H2'	1:A:1392:G:C8	2.40	0.57
1:A:70:G:C2	1:A:100:C:O2	2.58	0.57
25:Z:9:G:H2'	25:Z:10:G:N7	2.20	0.57
1:A:1509:C:H2'	1:A:1510:U:O4'	2.04	0.57
1:A:256:U:H2'	1:A:257:G:C8	2.40	0.57
13:M:121:LYS:HG2	13:M:125:ARG:HG2	1.87	0.57
18:R:48:GLY:H	18:R:83:GLU:H	1.51	0.57
20:T:54:LYS:HA	20:T:57:ARG:HD3	1.87	0.57
1:A:1001:A:H2'	1:A:1001(A):G:H8	1.67	0.56
1:A:10:A:H2'	1:A:11:G:C8	2.40	0.56
1:A:598:U:H2'	1:A:599:C:C6	2.39	0.56
3:C:57:ILE:HA	3:C:65:ALA:O	2.05	0.56
4:D:26:CYS:HG	27:D:300:ZN:ZN	1.17	0.56
13:M:97:PRO:HA	13:M:110:ARG:HH11	1.70	0.56
1:A:1296:C:H5''	13:M:44:ARG:HH22	1.70	0.56
10:J:61:GLU:OE2	14:N:58:LYS:CG	2.53	0.56
1:A:674:G:H2'	1:A:675:A:H8	1.70	0.56
1:A:84:U:H2'	1:A:88:A:O4'	2.04	0.56
23:X:140:VAL:O	23:X:144:LEU:HG	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:X:16:VAL:HG23	23:X:18:VAL:HG23	1.87	0.56
1:A:1314:C:H2'	1:A:1315:U:C6	2.40	0.56
1:A:509:A:H4'	1:A:510:A:OP1	2.05	0.56
1:A:769:G:N2	1:A:770:C:C2	2.73	0.56
23:X:90:PHE:HD2	23:X:94:ILE:HD13	1.70	0.56
3:C:41:GLY:O	3:C:45:LYS:HG2	2.05	0.56
3:C:62:ASP:HA	3:C:97:LYS:HD3	1.87	0.56
1:A:1371:G:OP1	9:I:11:LYS:O	2.24	0.56
1:A:122:G:C6	1:A:123:C:C4	2.94	0.56
1:A:663:A:H2'	1:A:664:G:O4'	2.05	0.56
1:A:1068:G:N2	1:A:1069:C:C2	2.74	0.56
1:A:1354:C:H2'	1:A:1355:G:C8	2.41	0.56
7:G:115:ARG:O	7:G:119:ARG:HG3	2.06	0.56
10:J:47:PHE:HB2	10:J:63:PHE:HB2	1.87	0.56
1:A:247:G:N2	1:A:248:C:C2	2.74	0.56
5:E:14:ARG:HG2	5:E:29:GLY:HA3	1.86	0.56
12:L:110:VAL:HG23	12:L:120:TYR:HB3	1.88	0.56
12:L:60:LEU:HD11	12:L:85:ILE:CD1	2.35	0.56
25:Z:74:C:H2'	25:Z:75:C:H5'	1.86	0.56
1:A:1409:C:H2'	1:A:1410:G:C8	2.41	0.56
1:A:352:C:H4'	1:A:354:G:OP1	2.05	0.56
1:A:827:U:C4	1:A:872:A:N1	2.73	0.56
4:D:64:LEU:HA	4:D:67:ILE:HD12	1.86	0.56
1:A:447:G:H3'	1:A:485:G:H22	1.70	0.56
1:A:725:G:N1	1:A:726:C:C4	2.74	0.56
4:D:67:ILE:HD13	4:D:196:LEU:HD22	1.87	0.56
1:A:1080:A:C3'	5:E:16:THR:HG22	2.35	0.56
14:N:37:PHE:HB3	14:N:39:LEU:HD12	1.86	0.56
1:A:397:A:N3	1:A:397:A:H3'	2.20	0.56
1:A:695:A:H2'	1:A:696:A:H8	1.71	0.56
1:A:701:C:H4'	1:A:702:A:O5'	2.05	0.56
1:A:935:A:H2'	1:A:936:C:C6	2.41	0.56
1:A:1180:A:H5'	9:I:103:THR:HG23	1.88	0.56
13:M:19:LEU:HA	13:M:22:ILE:HD12	1.86	0.56
22:W:32:ILE:HD13	22:W:32:ILE:H	1.70	0.56
1:A:1016:A:H2'	1:A:1017:G:O4'	2.05	0.55
1:A:1125:U:C5'	1:A:1126:U:H5	2.13	0.55
1:A:448:A:OP2	1:A:485:G:N2	2.39	0.55
1:A:1366:C:H2'	1:A:1367:C:C6	2.41	0.55
1:A:264:U:H2'	1:A:265:G:O4'	2.07	0.55
1:A:299:G:H2'	1:A:300:A:C8	2.41	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:560:U:O2'	1:A:561:U:OP2	2.16	0.55
23:X:149:VAL:HG13	23:X:168:VAL:HG22	1.88	0.55
25:Z:48:C:C5'	25:Z:50:U:OP1	2.54	0.55
1:A:235:C:H2'	1:A:236:G:H8	1.71	0.55
1:A:337:C:H2'	1:A:338:A:H8	1.71	0.55
1:A:370:C:C2	1:A:392:G:N2	2.75	0.55
25:Z:64:G:H2'	25:Z:65:C:O4'	2.07	0.55
1:A:414:A:H2'	1:A:415:A:O4'	2.07	0.55
1:A:877:C:H2'	1:A:878:G:C8	2.41	0.55
1:A:1409:C:H2'	1:A:1410:G:H8	1.71	0.55
1:A:60:A:H4'	1:A:61:G:O5'	2.07	0.55
6:F:27:GLN:HA	6:F:30:LEU:HD12	1.88	0.55
1:A:1323:G:H2'	1:A:1324:A:C8	2.42	0.55
1:A:1339:A:H2'	1:A:1340:A:O4'	2.07	0.55
1:A:590:C:N3	1:A:650:G:C2	2.74	0.55
15:O:18:PHE:O	15:O:21:ASP:HB3	2.06	0.55
17:Q:88:TYR:O	17:Q:92:ARG:HG2	2.06	0.55
1:A:519:C:OP1	22:W:66:ARG:HD3	2.07	0.55
1:A:1022:G:H2'	1:A:1023:G:C8	2.39	0.55
1:A:1485:U:H2'	1:A:1486:G:H8	1.71	0.55
1:A:216:G:C6	1:A:217:C:N4	2.74	0.55
1:A:671:G:N2	1:A:736:C:C2	2.75	0.55
1:A:743:U:H2'	1:A:744:C:C6	2.42	0.55
3:C:43:LEU:HD12	3:C:55:VAL:HG13	1.89	0.55
13:M:10:PRO:HG2	13:M:18:ALA:HB1	1.89	0.55
1:A:16:A:C2	1:A:1080:A:N3	2.74	0.55
1:A:1241:G:N2	1:A:1242:C:C2	2.75	0.55
1:A:613:C:H2'	1:A:614:A:C8	2.41	0.55
1:A:987:G:H1	1:A:1218:C:N4	2.05	0.55
20:T:40:ALA:HB2	20:T:55:ILE:HG22	1.87	0.55
1:A:1221:G:H2'	1:A:1222:G:C8	2.41	0.55
1:A:182:U:OP2	1:A:183:G:C8	2.60	0.55
1:A:333:G:N2	1:A:334:C:C2	2.74	0.55
1:A:571:U:H3'	1:A:572:A:H5''	1.88	0.55
5:E:139:LEU:HA	5:E:142:LEU:HD12	1.87	0.55
10:J:81:THR:HG22	10:J:85:LEU:HD12	1.89	0.55
25:Z:69:C:H2'	25:Z:70:G:C1'	2.36	0.55
1:A:325:A:H2'	1:A:326:G:C8	2.42	0.55
1:A:761:G:C2	1:A:762:C:C2	2.95	0.55
9:I:125:TYR:HE1	9:I:128:ARG:HB3	1.69	0.55
9:I:48:GLU:N	9:I:49:PRO:HD2	2.21	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:S:6:LYS:HG3	19:S:8:GLY:H	1.71	0.55
1:A:1353:G:N1	1:A:1354:C:C4	2.74	0.54
2:B:61:LEU:HD13	2:B:66:GLY:HA3	1.88	0.54
7:G:65:ALA:HB1	7:G:127:ALA:CB	2.37	0.54
9:I:4:TYR:CE2	9:I:88:TYR:HD1	2.24	0.54
10:J:16:LEU:HD13	10:J:68:HIS:HB2	1.88	0.54
25:Z:6:G:H2'	25:Z:7:G:C8	2.42	0.54
1:A:753:A:H5''	15:O:69:TYR:HE1	1.71	0.54
22:W:16:ALA:HA	22:W:22:PHE:HD1	1.71	0.54
25:Z:30:G:C2	25:Z:41:C:C2	2.95	0.54
23:X:56:VAL:HG21	25:Z:56:C:C2	2.42	0.54
1:A:1521:G:H2'	1:A:1522:U:C6	2.43	0.54
1:A:181:G:H4'	1:A:182:U:H5'	1.88	0.54
1:A:824:C:H2'	1:A:825:G:H8	1.72	0.54
1:A:838:G:C2	1:A:849:C:C2	2.95	0.54
18:R:42:ARG:HH11	18:R:42:ARG:HB3	1.70	0.54
6:F:35:ALA:HA	6:F:67:MET:HB3	1.89	0.54
20:T:65:LYS:O	20:T:68:LYS:HB3	2.06	0.54
1:A:1074:G:O2'	1:A:1101:A:N1	2.37	0.54
1:A:1262:C:H42	1:A:1273:G:H1	1.55	0.54
1:A:1542:U:H4'	18:R:18:ARG:N	2.21	0.54
1:A:170:U:H2'	1:A:171:A:C8	2.42	0.54
1:A:961:U:H3	1:A:974:A:H61	1.56	0.54
4:D:33:MET:HA	4:D:36:ARG:O	2.08	0.54
9:I:6:GLY:HA3	9:I:80:GLY:O	2.07	0.54
23:X:52:ALA:CB	25:Z:19:G:H22	2.13	0.54
25:Z:27:U:H2'	25:Z:28:C:C6	2.43	0.54
1:A:1234:C:H2'	1:A:1235:U:C6	2.42	0.54
8:H:6:ILE:O	8:H:10:LEU:HG	2.07	0.54
24:Y:35:A:O3'	24:Y:36:A:H8	1.89	0.54
1:A:373:A:H2'	1:A:374:A:H8	1.73	0.54
2:B:215:LEU:O	2:B:219:VAL:HG23	2.07	0.54
25:Z:6:G:C2	25:Z:68:C:C2	2.96	0.54
1:A:914:A:H2'	1:A:915:A:H8	1.72	0.54
10:J:5:ARG:CG	10:J:71:LEU:HD21	2.38	0.54
11:K:11:LYS:O	11:K:75:TYR:CD2	2.61	0.54
1:A:1431:C:C2	1:A:1470:G:N2	2.76	0.54
1:A:559:A:O2'	1:A:560:U:OP2	2.24	0.54
1:A:575:G:H4'	1:A:576:G:C5'	2.38	0.54
5:E:27:ARG:O	5:E:27:ARG:HG2	2.05	0.54
7:G:24:THR:HA	7:G:27:ILE:HD12	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1534:A:H2'	1:A:1535:C:C6	2.43	0.53
1:A:189(D):C:H3'	1:A:189(E):U:C6	2.43	0.53
1:A:437:U:H3'	1:A:438:G:H8	1.71	0.53
1:A:864:A:C2	1:A:865:A:C2	2.96	0.53
1:A:391:G:H2'	1:A:392:G:O4'	2.08	0.53
1:A:922:G:H3'	1:A:923:A:H8	1.72	0.53
3:C:174:PRO:HB2	3:C:177:THR:HG22	1.90	0.53
1:A:1342:C:H5''	9:I:125:TYR:CZ	2.43	0.53
1:A:947:G:H2'	1:A:948:C:O4'	2.08	0.53
1:A:752:G:H4'	15:O:69:TYR:OH	2.07	0.53
1:A:1537:U:N3	24:Y:28:A:N6	2.57	0.53
1:A:450:G:H5''	1:A:451:A:H3'	1.90	0.53
1:A:621:A:H2'	1:A:622:A:O4'	2.09	0.53
25:Z:47:U:H6	25:Z:47:U:O5'	1.91	0.53
1:A:122:G:C2	1:A:123:C:C2	2.96	0.53
1:A:289:G:N1	1:A:290:C:C4	2.76	0.53
16:P:42:ARG:HB3	16:P:44:THR:HG23	1.89	0.53
1:A:100:C:H2'	1:A:101:A:C8	2.43	0.53
1:A:1361:G:C6	1:A:1362:C:N3	2.76	0.53
1:A:19:C:O2	1:A:917:G:C2	2.62	0.53
1:A:553:A:H2'	1:A:554:C:C6	2.43	0.53
10:J:31:GLY:HA3	10:J:78:ASN:HD22	1.71	0.53
1:A:1347:G:N2	1:A:1373:G:H2'	2.23	0.53
1:A:137:C:C2	1:A:227:G:C2	2.96	0.53
1:A:253:U:H2'	1:A:254:G:C8	2.42	0.53
1:A:615:C:H2'	1:A:616:G:H8	1.73	0.53
1:A:522:C:H41	12:L:53:ARG:HH21	1.54	0.53
14:N:3:ARG:H	14:N:6:LEU:HD12	1.74	0.53
1:A:1541:U:H3	24:Y:24:A:H61	1.57	0.53
1:A:1264:C:H2'	1:A:1265:G:C8	2.44	0.53
1:A:1464:G:C2	1:A:1465:C:N3	2.77	0.53
10:J:6:ILE:HD11	10:J:23:ILE:HG21	1.90	0.53
1:A:1248:A:H2'	1:A:1249:C:C6	2.44	0.53
1:A:1456:G:N2	1:A:1457:G:C8	2.76	0.53
1:A:767:A:H2'	1:A:768:A:O4'	2.09	0.53
1:A:777:A:H2'	1:A:778:G:C8	2.44	0.53
2:B:69:LEU:HD13	2:B:155:LEU:HD11	1.90	0.53
1:A:774:G:C2	1:A:806:C:N3	2.77	0.53
1:A:976:G:H4'	1:A:977:A:OP1	2.08	0.53
1:A:112:G:OP2	16:P:27:LYS:HE3	2.09	0.53
1:A:1106:G:C6	1:A:1107:C:N4	2.78	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1327:C:H5''	21:V:20:LYS:HB2	1.91	0.52
1:A:279:A:H5''	1:A:280:C:H3'	1.91	0.52
1:A:333:G:C6	1:A:334:C:N4	2.78	0.52
1:A:456:C:C2	1:A:476:G:N2	2.77	0.52
1:A:66:G:N2	1:A:67:C:C2	2.77	0.52
12:L:60:LEU:HD11	12:L:85:ILE:HD11	1.90	0.52
17:Q:92:ARG:O	17:Q:95:TYR:HB2	2.09	0.52
1:A:1101:A:H5'	2:B:172:ILE:HG21	1.92	0.52
1:A:1137:C:H4'	1:A:1138:G:C2	2.44	0.52
22:W:37:SER:HB3	22:W:40:MET:HG3	1.90	0.52
23:X:137:LEU:O	23:X:141:THR:HG23	2.08	0.52
25:Z:58:A:C2	25:Z:60:U:H2'	2.44	0.52
1:A:1404:C:H2'	1:A:1405:G:H8	1.75	0.52
1:A:1475:G:H2'	1:A:1476:G:C8	2.43	0.52
1:A:159:G:N2	1:A:163:C:C2	2.77	0.52
1:A:20:U:H2'	1:A:21:G:O4'	2.09	0.52
1:A:577:G:N2	1:A:578:C:C2	2.77	0.52
1:A:636:U:H5'	17:Q:2:PRO:HG3	1.90	0.52
1:A:124:G:H2'	1:A:125:U:O4'	2.09	0.52
1:A:1437:C:H2'	1:A:1438:G:H8	1.74	0.52
1:A:628:G:H2'	1:A:629:G:C8	2.45	0.52
2:B:201:ILE:HG21	2:B:214:ILE:HG21	1.91	0.52
25:Z:12:G:H1	25:Z:23:C:N4	2.06	0.52
1:A:1382:C:H2'	1:A:1383:C:C6	2.44	0.52
1:A:216:G:C2	1:A:217:C:N3	2.77	0.52
1:A:236:G:C2	1:A:237:C:C2	2.98	0.52
1:A:403:C:H2'	1:A:404:U:H6	1.75	0.52
1:A:97:G:H2'	1:A:98:G:C8	2.44	0.52
2:B:91:PRO:HB3	2:B:154:LEU:HB2	1.92	0.52
24:Y:30:G:H2'	24:Y:31:U:H5''	1.91	0.52
1:A:1000:U:H6	1:A:1000:U:H3'	1.75	0.52
1:A:1464:G:C6	1:A:1465:C:N4	2.77	0.52
1:A:1048:G:C2	1:A:1210:C:C2	2.98	0.52
1:A:1258:G:C2	1:A:1259:C:N3	2.78	0.52
1:A:217:C:H2'	1:A:218:C:C6	2.45	0.52
1:A:21:G:H2'	1:A:22:G:C8	2.45	0.52
1:A:571:U:C3'	1:A:572:A:H5''	2.40	0.52
1:A:722:A:H2'	1:A:724:G:C8	2.45	0.52
4:D:63:LYS:HD3	4:D:197:PRO:HB2	1.91	0.52
5:E:88:LYS:HB3	5:E:123:LEU:HB2	1.92	0.52
10:J:50:ILE:HA	10:J:59:SER:O	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:O:67:LEU:HD11	15:O:87:ILE:HG21	1.92	0.52
25:Z:30:G:N2	25:Z:41:C:C2	2.77	0.52
1:A:823:G:H2'	1:A:824:C:C6	2.45	0.52
2:B:71:VAL:HB	2:B:164:VAL:HA	1.92	0.52
10:J:61:GLU:OE1	14:N:58:LYS:HD2	2.04	0.52
15:O:75:PRO:O	15:O:79:ARG:HG3	2.10	0.52
1:A:1500:A:H5''	1:A:1508:G:H5''	1.92	0.52
1:A:233:C:H2'	1:A:234:C:C6	2.45	0.52
1:A:601:C:H42	1:A:637:G:H1	1.57	0.52
1:A:590:C:C2	1:A:650:G:C2	2.97	0.52
4:D:209:ARG:HG2	4:D:209:ARG:HH11	1.74	0.52
25:Z:67:C:H2'	25:Z:68:C:C6	2.45	0.52
1:A:1082:G:H2'	1:A:1083:U:O4'	2.10	0.52
1:A:321:A:H2'	1:A:322:C:C6	2.45	0.52
1:A:504:C:C2	1:A:542:G:C2	2.98	0.52
1:A:657:G:H4'	15:O:28:GLN:HG3	1.91	0.52
1:A:70:G:C6	1:A:100:C:N3	2.78	0.52
1:A:761:G:C6	1:A:762:C:C4	2.98	0.52
1:A:1000:U:C6	1:A:1000:U:H3'	2.44	0.51
1:A:189(K):U:H2'	1:A:189(L):G:C8	2.45	0.51
1:A:939:G:C6	1:A:940:C:N4	2.78	0.51
4:D:196:LEU:HB3	4:D:198:VAL:HG12	1.91	0.51
5:E:80:ILE:HD12	5:E:91:LEU:HB2	1.90	0.51
1:A:674:G:H5'	6:F:50:TYR:CE2	2.45	0.51
1:A:309:G:H2'	1:A:310:G:H8	1.75	0.51
1:A:599:C:O2'	8:H:129:VAL:HG23	2.09	0.51
1:A:1190:G:H5'	3:C:176:HIS:CE1	2.45	0.51
4:D:60:GLU:HG3	4:D:198:VAL:HG23	1.91	0.51
1:A:1103:C:H2'	1:A:1104:G:O4'	2.10	0.51
1:A:22:G:C6	1:A:23:C:C4	2.98	0.51
1:A:257:G:H1	1:A:269:C:H42	1.58	0.51
1:A:339:C:H2'	1:A:340:U:C6	2.45	0.51
1:A:441:A:C8	1:A:441:A:H5''	2.45	0.51
1:A:617:G:N2	1:A:618:C:C2	2.78	0.51
9:I:89:ASN:HB3	9:I:92:TYR:CD2	2.45	0.51
1:A:1106:G:H2'	1:A:1107:C:C6	2.46	0.51
1:A:1466:C:H2'	1:A:1467:G:O4'	2.11	0.51
1:A:598:U:H2'	1:A:599:C:H6	1.74	0.51
4:D:64:LEU:HD12	4:D:198:VAL:HG21	1.93	0.51
7:G:97:GLN:O	7:G:101:LEU:HG	2.10	0.51
25:Z:2:G:C2	25:Z:3:C:C2	2.98	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1125:U:O4	10:J:5:ARG:HB2	2.11	0.51
1:A:337:C:H2'	1:A:338:A:C8	2.46	0.51
1:A:568:G:C6	1:A:569:C:N4	2.78	0.51
3:C:29:TYR:C	3:C:29:TYR:HD1	2.14	0.51
25:Z:49:G:C2	25:Z:50:U:H1'	2.45	0.51
1:A:1050:G:C6	1:A:1051:C:N4	2.79	0.51
1:A:1164:G:N2	1:A:1165:C:C2	2.79	0.51
1:A:250:A:H4'	1:A:251:G:O5'	2.10	0.51
1:A:785:G:H1	1:A:797:C:H42	1.59	0.51
3:C:42:LEU:HD11	3:C:94:LEU:HG	1.93	0.51
9:I:8:GLY:HA3	9:I:76:ALA:O	2.10	0.51
1:A:520:A:N1	1:A:536:C:H1'	2.26	0.51
1:A:823:G:N2	1:A:824:C:C2	2.79	0.51
5:E:127:ASN:O	5:E:131:ILE:HG12	2.10	0.51
7:G:71:PRO:HD2	7:G:96:GLN:HG3	1.93	0.51
9:I:41:VAL:O	9:I:44:VAL:HG22	2.10	0.51
10:J:7:LYS:HB3	10:J:97:GLU:HB2	1.92	0.51
20:T:63:ILE:HG23	20:T:77:ALA:HB1	1.93	0.51
1:A:794:A:H2'	1:A:795:C:H6	1.75	0.51
1:A:834:C:C2	1:A:853:G:C2	2.99	0.51
2:B:158:LEU:HD21	2:B:180:LEU:HD22	1.93	0.51
3:C:21:ARG:HG2	3:C:58:GLU:HG2	1.93	0.51
1:A:1424:C:H42	1:A:1476:G:H1	1.59	0.51
6:F:2:ARG:HG3	6:F:69:GLU:HG3	1.92	0.51
14:N:41:ARG:HG3	14:N:42:ILE:H	1.76	0.51
25:Z:18:G:C2	25:Z:58:A:C5	2.99	0.51
25:Z:6:G:H2'	25:Z:7:G:H8	1.74	0.51
1:A:1235:U:H2'	1:A:1236:A:O4'	2.11	0.51
1:A:255:G:H2'	1:A:256:U:C6	2.46	0.51
1:A:320:C:H2'	1:A:321:A:C8	2.46	0.51
1:A:444:C:H42	1:A:490:G:H1	1.57	0.51
1:A:540:G:H2'	1:A:541:G:C8	2.46	0.51
1:A:756:C:H2'	1:A:757:U:O4'	2.11	0.51
2:B:97:TRP:HZ2	2:B:102:LEU:HD13	1.76	0.51
10:J:28:ARG:HH22	10:J:36:GLY:HA2	1.74	0.51
23:X:90:PHE:CD2	23:X:94:ILE:HD13	2.46	0.51
25:Z:12:G:N1	25:Z:13:C:C2	2.79	0.51
1:A:1077:G:N1	1:A:1081:G:C6	2.78	0.50
1:A:1416:G:H2'	1:A:1417:G:O4'	2.12	0.50
1:A:1512:U:H2'	1:A:1513:A:H8	1.76	0.50
1:A:521:G:N1	1:A:522:C:C4	2.80	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:29:PRO:O	4:D:35:ARG:HG2	2.11	0.50
1:A:1151:A:O2'	1:A:1152:A:C8	2.61	0.50
1:A:1312:G:C2	1:A:1326:C:C2	2.99	0.50
1:A:217:C:H2'	1:A:218:C:H6	1.75	0.50
1:A:289:G:C2	1:A:290:C:C4	2.99	0.50
1:A:385:C:N4	1:A:386:C:N4	2.59	0.50
1:A:444:C:C2	1:A:491:G:N2	2.80	0.50
1:A:784:C:C2	1:A:799:G:N2	2.79	0.50
1:A:908:A:H2'	1:A:909:A:C8	2.46	0.50
3:C:26:LYS:HD3	14:N:36:PHE:CE1	2.47	0.50
18:R:26:LEU:HD21	18:R:39:VAL:HG22	1.94	0.50
25:Z:51:C:N3	25:Z:63:G:O6	2.44	0.50
1:A:1148:U:H5'	9:I:7:THR:HG21	1.94	0.50
1:A:946:A:H2'	1:A:947:G:H8	1.73	0.50
7:G:71:PRO:HG3	7:G:103:TRP:HH2	1.74	0.50
11:K:16:SER:O	11:K:35:PRO:HD3	2.11	0.50
15:O:63:ARG:HA	15:O:66:LEU:HD12	1.93	0.50
1:A:1132:C:H2'	1:A:1133:G:C8	2.47	0.50
1:A:270:A:H2'	1:A:271:C:C6	2.46	0.50
1:A:410:G:H21	1:A:432:A:H62	1.58	0.50
1:A:500:G:C2	1:A:501:C:N3	2.79	0.50
1:A:579:G:H5'	1:A:728:A:H1'	1.92	0.50
1:A:971:G:C8	1:A:1365:G:H4'	2.47	0.50
2:B:68:ILE:HG12	2:B:161:ALA:HB3	1.92	0.50
2:B:96:ARG:HB3	2:B:148:TYR:CE2	2.46	0.50
3:C:108:ASN:HD21	3:C:110:ASN:HB2	1.76	0.50
3:C:28:GLN:HA	3:C:31:HIS:CD2	2.46	0.50
25:Z:52:G:O2'	25:Z:53:G:H8	1.94	0.50
1:A:1050:G:N2	1:A:1051:C:C2	2.79	0.50
1:A:369:C:H2'	1:A:370:C:C6	2.47	0.50
1:A:392:G:H2'	1:A:393:A:C8	2.46	0.50
1:A:576:G:H3'	1:A:577:G:C5'	2.41	0.50
1:A:64:G:H4'	1:A:65:U:H5''	1.94	0.50
1:A:670:G:H1	1:A:736:C:H42	1.59	0.50
1:A:908:A:H2'	1:A:909:A:H8	1.77	0.50
3:C:150:LYS:HD2	3:C:173:VAL:HG11	1.94	0.50
3:C:5:ILE:HD13	3:C:10:PHE:HB2	1.94	0.50
13:M:18:ALA:HA	13:M:21:TYR:HD2	1.77	0.50
1:A:1280:A:C3'	1:A:1281:U:H5''	2.37	0.50
1:A:629:G:H2'	1:A:630:G:O4'	2.11	0.50
1:A:902:G:H2'	1:A:903:G:C8	2.45	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:129:ASN:HD21	4:D:145:GLU:N	2.09	0.50
10:J:32:ALA:CB	10:J:74:ILE:HG22	2.41	0.50
19:S:22:LEU:HD22	19:S:28:LYS:HB2	1.93	0.50
1:A:665:A:N3	1:A:732:C:H2'	2.27	0.50
4:D:108:LEU:HG	4:D:174:LEU:HD22	1.94	0.50
1:A:544:G:OP1	4:D:62:GLN:HG3	2.11	0.50
1:A:192:U:H2'	1:A:193:C:C6	2.47	0.50
1:A:542:G:N2	1:A:543:C:C2	2.80	0.50
4:D:121:VAL:O	4:D:134:ASP:HA	2.12	0.50
6:F:30:LEU:HD13	6:F:37:VAL:HG21	1.94	0.50
10:J:44:VAL:HG22	10:J:66:ARG:HB3	1.93	0.50
14:N:24:CYS:HB3	14:N:28:GLY:H	1.77	0.50
1:A:1537:U:C4	24:Y:28:A:N6	2.80	0.50
25:Z:2:G:H3'	25:Z:3:C:H6	1.75	0.50
1:A:584:G:H2'	1:A:585:G:H8	1.76	0.50
1:A:745:C:H2'	1:A:746:A:H8	1.73	0.50
1:A:945:G:H2'	1:A:945:G:N3	2.27	0.50
2:B:75:LYS:HA	2:B:78:GLN:HB2	1.94	0.50
1:A:1216:G:N2	1:A:1217:C:C2	2.80	0.49
1:A:602:A:H2'	1:A:603:U:O4'	2.12	0.49
10:J:5:ARG:O	10:J:98:ILE:HA	2.11	0.49
3:C:29:TYR:HH	14:N:54:PRO:CG	2.13	0.49
25:Z:36:U:H2'	25:Z:37:A:O4'	2.12	0.49
1:A:573:A:H2'	1:A:574:A:O4'	2.12	0.49
16:P:57:ARG:NE	16:P:79:VAL:O	2.45	0.49
25:Z:6:G:C2	25:Z:68:C:N3	2.79	0.49
3:C:71:ALA:HB2	3:C:115:LEU:HD13	1.94	0.49
5:E:27:ARG:CG	5:E:27:ARG:NH1	2.73	0.49
17:Q:60:ILE:HG22	17:Q:72:ARG:HB2	1.94	0.49
25:Z:2:G:N2	25:Z:3:C:C2	2.81	0.49
1:A:1129:C:H1'	1:A:1132:C:H5	1.77	0.49
1:A:1127:G:N2	1:A:1147:C:N4	2.57	0.49
1:A:1220:G:H2'	1:A:1221:G:O4'	2.12	0.49
1:A:1353:G:C2	1:A:1354:C:C4	3.00	0.49
1:A:559:A:H4'	1:A:560:U:H5''	1.93	0.49
1:A:731:G:N2	1:A:732:C:C2	2.80	0.49
1:A:988:G:N1	1:A:989:C:C2	2.80	0.49
3:C:135:LYS:O	3:C:139:GLN:HG2	2.11	0.49
11:K:86:GLY:HA2	11:K:112:THR:HG23	1.94	0.49
25:Z:35:A:H4'	25:Z:36:U:OP1	2.12	0.49
1:A:123:C:H2'	1:A:124:G:C8	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1338:G:H2'	1:A:1339:A:C8	2.47	0.49
1:A:192:U:H2'	1:A:193:C:H6	1.77	0.49
1:A:861:G:N2	1:A:862:C:C2	2.81	0.49
3:C:29:TYR:C	3:C:29:TYR:CD1	2.86	0.49
1:A:1435:G:H2'	1:A:1436:U:C6	2.47	0.49
1:A:28:G:H2'	1:A:29:G:O4'	2.13	0.49
1:A:623:C:H2'	1:A:624:C:O4'	2.12	0.49
3:C:70:VAL:O	3:C:105:GLU:HA	2.12	0.49
9:I:32:ASP:HB3	9:I:35:GLU:HB2	1.95	0.49
1:A:1525:G:H2'	1:A:1526:G:H8	1.77	0.49
1:A:524:G:C2	1:A:525:C:C4	3.01	0.49
1:A:967:C:H2'	1:A:968:A:C8	2.48	0.49
2:B:115:LEU:HD21	2:B:153:ARG:HE	1.78	0.49
18:R:17:SER:HB3	18:R:55:ARG:HD3	1.94	0.49
22:W:12:VAL:HG22	22:W:52:ARG:HD3	1.94	0.49
1:A:1392:G:H21	1:A:1502:A:H8	1.61	0.49
1:A:137:C:C2	1:A:227:G:N2	2.80	0.49
1:A:233:C:H2'	1:A:234:C:H6	1.78	0.49
1:A:601:C:H2'	1:A:602:A:H8	1.77	0.49
1:A:914:A:C4	1:A:915:A:N7	2.81	0.49
1:A:945:G:C2	1:A:946:A:C8	3.01	0.49
1:A:1015:A:H2'	1:A:1016:A:C8	2.47	0.49
1:A:1027:C:H2'	1:A:1028:C:H5'	1.94	0.49
1:A:1347:G:O2'	1:A:1348:U:OP2	2.22	0.49
1:A:258:G:C2	1:A:269:C:N3	2.81	0.49
1:A:109:A:C6	1:A:326:G:C6	3.00	0.49
1:A:354:G:N1	1:A:355:C:C4	2.80	0.49
1:A:382:A:H2'	1:A:383:A:C8	2.48	0.49
1:A:753:A:H5''	15:O:69:TYR:CE1	2.46	0.49
3:C:177:THR:HG23	3:C:180:ALA:HB2	1.95	0.49
7:G:16:LEU:HD12	9:I:41:VAL:HG12	1.95	0.49
9:I:93:ARG:HH21	9:I:97:LYS:HE3	1.77	0.49
9:I:96:LEU:HB3	9:I:102:LEU:HD12	1.95	0.49
11:K:34:ASP:OD1	11:K:38:ASN:N	2.42	0.49
25:Z:10:G:H1	25:Z:25:C:N4	2.11	0.49
1:A:19:C:N3	1:A:917:G:C6	2.81	0.49
1:A:22:G:C2	1:A:23:C:C2	3.01	0.49
1:A:971:G:OP1	1:A:971:G:H3'	2.13	0.49
1:A:1349:A:H5''	9:I:121:ARG:HB2	1.95	0.49
10:J:5:ARG:N	10:J:73:ASP:OD1	2.45	0.49
16:P:2:VAL:HG13	16:P:64:ALA:HA	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1049:U:H4'	1:A:1050:G:OP2	2.13	0.48
1:A:677:U:H2'	1:A:678:U:O4'	2.12	0.48
3:C:150:LYS:HG3	3:C:169:ALA:HB2	1.95	0.48
25:Z:52:G:C4	25:Z:53:G:C8	3.00	0.48
1:A:1283:G:N1	1:A:1284:C:C4	2.81	0.48
1:A:1347:G:HO2'	1:A:1348:U:P	2.36	0.48
1:A:1468:A:H2'	1:A:1469:G:O4'	2.12	0.48
1:A:17:U:H2'	1:A:18:C:C5	2.47	0.48
2:B:19:HIS:CG	2:B:20:GLU:HG2	2.47	0.48
9:I:31:GLN:HB3	9:I:35:GLU:HB3	1.95	0.48
1:A:1347:G:O2'	1:A:1373:G:N1	2.43	0.48
1:A:1443:G:C2	1:A:1444:C:C4	3.01	0.48
1:A:42:G:C2	1:A:43:C:C2	3.01	0.48
1:A:838:G:N2	1:A:849:C:C2	2.81	0.48
1:A:898:G:C2	1:A:902:G:C6	3.01	0.48
1:A:961:U:O4	1:A:974:A:C2	2.59	0.48
5:E:76:ILE:HG22	5:E:93:PRO:HB3	1.93	0.48
19:S:40:ILE:HD12	19:S:69:HIS:HB2	1.94	0.48
25:Z:34:C:H2'	25:Z:35:A:C8	2.48	0.48
1:A:504:C:C2	1:A:542:G:N2	2.82	0.48
1:A:540:G:H2'	1:A:541:G:H8	1.78	0.48
1:A:579:G:H2'	1:A:580:U:H6	1.74	0.48
1:A:947:G:C2	1:A:948:C:C2	3.02	0.48
1:A:1134:G:N2	1:A:1141:C:C2	2.81	0.48
1:A:1281:U:H3'	1:A:1282:C:C6	2.48	0.48
1:A:1438:G:N1	1:A:1439:C:C4	2.80	0.48
1:A:148:G:H2'	1:A:149:A:C8	2.48	0.48
1:A:518:C:O2'	1:A:519:C:OP2	2.28	0.48
1:A:872:A:C8	1:A:874:G:C8	3.01	0.48
1:A:992:U:H4'	1:A:993:G:O5'	2.13	0.48
7:G:107:ALA:HB3	7:G:123:GLU:HG2	1.95	0.48
8:H:10:LEU:HD22	8:H:83:ILE:HD11	1.94	0.48
22:W:33:LEU:O	22:W:65:GLY:N	2.44	0.48
1:A:1163:C:C2	1:A:1174:G:N2	2.82	0.48
1:A:1233:G:C6	1:A:1234:C:N4	2.82	0.48
1:A:344:A:H4'	1:A:345:C:OP2	2.13	0.48
1:A:939:G:H2'	1:A:940:C:C6	2.48	0.48
2:B:15:VAL:HG11	2:B:209:ARG:HB3	1.95	0.48
3:C:26:LYS:HA	14:N:36:PHE:HE1	1.78	0.48
10:J:24:VAL:HG13	10:J:28:ARG:NE	2.21	0.48
11:K:11:LYS:O	11:K:75:TYR:HD2	1.97	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:Z:1:C:H2'	25:Z:2:G:C8	2.49	0.48
1:A:1106:G:N2	1:A:1107:C:C2	2.82	0.48
1:A:189(A):C:H2'	1:A:189(B):C:C6	2.49	0.48
1:A:189(K):U:H2'	1:A:189(L):G:H8	1.79	0.48
1:A:504:C:N3	1:A:542:G:C2	2.81	0.48
1:A:928:G:H1	1:A:1389:C:H42	1.60	0.48
1:A:977:A:H2'	1:A:978:A:H5''	1.94	0.48
13:M:10:PRO:HB3	13:M:21:TYR:CD2	2.48	0.48
1:A:1074:G:C6	1:A:1075:C:C4	3.01	0.48
1:A:505:G:H5'	1:A:534:U:H2'	1.95	0.48
1:A:734:G:C2	1:A:735:C:C2	3.01	0.48
1:A:1080:A:C3'	5:E:16:THR:CG2	2.84	0.48
7:G:71:PRO:HG3	7:G:103:TRP:CH2	2.48	0.48
15:O:87:ILE:C	15:O:89:GLY:H	2.16	0.48
1:A:1119:C:H2'	1:A:1120:G:H8	1.79	0.48
1:A:1133:G:H1	1:A:1141:C:H42	1.61	0.48
1:A:1233:G:N2	1:A:1234:C:C2	2.82	0.48
1:A:1352:C:H2'	1:A:1353:G:C8	2.49	0.48
2:B:93:VAL:HG11	2:B:97:TRP:CD1	2.47	0.48
3:C:91:LEU:HD22	3:C:101:LEU:HD12	1.96	0.48
3:C:153:VAL:HG13	3:C:198:VAL:HG22	1.96	0.48
1:A:755:G:OP2	15:O:65:ARG:HG2	2.14	0.48
19:S:42:PRO:HA	19:S:45:VAL:HG23	1.95	0.48
20:T:73:HIS:HB3	20:T:74:LYS:HZ1	1.79	0.48
1:A:588:G:N1	1:A:589:C:C4	2.82	0.48
1:A:734:G:C6	1:A:735:C:C4	3.02	0.48
1:A:90:U:H2'	1:A:91:C:H6	1.76	0.48
2:B:167:PRO:HB3	2:B:174:VAL:HG21	1.95	0.48
2:B:76:GLN:HG2	2:B:76:GLN:H	1.51	0.48
19:S:32:LYS:HA	19:S:50:ALA:O	2.14	0.48
1:A:1050:G:N1	1:A:1051:C:C4	2.82	0.47
1:A:1135:U:H4'	1:A:1136:U:C5	2.49	0.47
1:A:1298:C:C4	7:G:114:ARG:HD3	2.49	0.47
2:B:80:ILE:HG21	2:B:212:GLN:HA	1.95	0.47
4:D:157:LEU:HA	4:D:160:GLN:HE21	1.78	0.47
10:J:12:ASP:HB3	10:J:15:THR:HG22	1.95	0.47
1:A:1237:C:H3'	1:A:1336:C:H41	1.79	0.47
11:K:72:ALA:O	11:K:77:MET:HB2	2.13	0.47
15:O:21:ASP:OD1	15:O:24:SER:HB2	2.14	0.47
15:O:3:ILE:HG21	15:O:34:LEU:HD11	1.95	0.47
15:O:87:ILE:O	15:O:88:ARG:HG3	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:127:G:C2	1:A:235:C:N3	2.82	0.47
1:A:189:G:C2	1:A:189(A):C:C2	3.02	0.47
1:A:533:A:O2'	1:A:535:A:OP2	2.28	0.47
1:A:551:U:H2'	1:A:552:U:C6	2.50	0.47
1:A:688:G:H1	1:A:699:C:H42	1.63	0.47
1:A:96:U:H2'	1:A:97:G:C8	2.50	0.47
14:N:9:LYS:O	14:N:12:ARG:NH2	2.46	0.47
1:A:1371:G:H2'	1:A:1372:U:C6	2.50	0.47
1:A:439:A:P	1:A:493:G:N1	2.77	0.47
1:A:443:C:C2	1:A:492:G:N2	2.82	0.47
1:A:502:G:H2'	1:A:503:C:O4'	2.14	0.47
1:A:827:U:N3	1:A:872:A:C6	2.69	0.47
1:A:922:G:H3'	1:A:923:A:C8	2.49	0.47
6:F:67:MET:HB2	6:F:68:PRO:CD	2.44	0.47
9:I:71:SER:HA	9:I:74:ILE:HD12	1.97	0.47
17:Q:64:PRO:HB3	17:Q:70:ARG:HG3	1.95	0.47
1:A:1515:C:H2'	1:A:1516:G:C8	2.50	0.47
1:A:643:C:H2'	1:A:644:G:H8	1.79	0.47
9:I:5:TYR:OH	9:I:7:THR:HG23	2.14	0.47
13:M:45:VAL:HA	13:M:48:LEU:HD12	1.95	0.47
13:M:51:ALA:O	13:M:55:ARG:HG3	2.13	0.47
1:A:1355:G:H2'	1:A:1356:G:H8	1.79	0.47
1:A:13:U:H3	1:A:915:A:H62	1.59	0.47
5:E:10:MET:HA	5:E:32:VAL:HG23	1.95	0.47
7:G:146:GLU:C	7:G:148:ASN:H	2.16	0.47
1:A:1114:C:C2	1:A:1187:G:C2	3.02	0.47
1:A:1117:G:H5'	1:A:1118:C:OP2	2.15	0.47
1:A:1366:C:O2'	10:J:60:ARG:NH2	2.48	0.47
1:A:1412:C:H2'	1:A:1413:A:O4'	2.14	0.47
1:A:1430:C:C2	1:A:1471:G:N2	2.82	0.47
1:A:42:G:C6	1:A:43:C:C4	3.03	0.47
1:A:803:G:H2'	1:A:804:U:O4'	2.14	0.47
4:D:24:GLU:O	4:D:25:ARG:HB3	2.14	0.47
23:X:18:VAL:HB	23:X:29:MET:HG2	1.96	0.47
25:Z:2:G:H1	25:Z:71:C:H42	1.62	0.47
1:A:132:C:N4	1:A:231:G:C6	2.83	0.47
1:A:585:G:C2	1:A:586:C:C2	3.03	0.47
1:A:778:G:C6	1:A:779:C:C4	3.02	0.47
1:A:860:A:H2'	1:A:861:G:O4'	2.15	0.47
23:X:33:GLU:HA	23:X:36:ARG:HD2	1.97	0.47
1:A:1171:G:N2	1:A:1172:C:C2	2.83	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1305:G:N2	1:A:1331:G:H1'	2.30	0.47
1:A:131:C:H2'	1:A:132:C:C6	2.50	0.47
1:A:1367:C:H5'	10:J:60:ARG:HH12	1.78	0.47
1:A:1472:U:H2'	1:A:1473:A:C8	2.50	0.47
1:A:1506:U:N3	1:A:1522:U:OP1	2.43	0.47
1:A:123:C:H5''	1:A:311:C:O2'	2.15	0.47
1:A:646:U:H2'	1:A:647:C:C6	2.50	0.47
1:A:731:G:OP1	1:A:766:A:H1'	2.15	0.47
4:D:97:LEU:O	4:D:100:ARG:HG3	2.14	0.47
6:F:43:LEU:HB3	6:F:46:ARG:HD2	1.95	0.47
22:W:32:ILE:HD13	22:W:32:ILE:O	2.14	0.47
1:A:1033:G:H2'	1:A:1034:G:C8	2.50	0.47
1:A:1312:G:N2	1:A:1326:C:C2	2.83	0.47
1:A:81:U:H4'	1:A:81:U:OP1	2.15	0.47
1:A:836:G:H1	1:A:850:U:H3	1.63	0.47
4:D:176:LEU:HA	4:D:183:GLY:HA2	1.97	0.47
5:E:15:ARG:HG2	5:E:28:PHE:CE1	2.39	0.47
8:H:11:THR:HA	8:H:14:ARG:NH1	2.30	0.47
1:A:1095:U:H2'	1:A:1096:C:C6	2.49	0.47
1:A:765:G:N1	1:A:812:C:H2'	2.30	0.47
1:A:920:U:H2'	1:A:921:U:H6	1.70	0.47
8:H:48:TYR:HD2	8:H:59:LEU:HD21	1.81	0.47
8:H:79:VAL:HG13	8:H:80:ILE:HG13	1.97	0.47
1:A:1508:G:C2	1:A:1509:C:C2	3.03	0.46
1:A:128:G:C2	1:A:234:C:C2	3.03	0.46
1:A:399:G:H2'	1:A:400:C:C6	2.50	0.46
1:A:524:G:H2'	1:A:525:C:C6	2.50	0.46
1:A:615:C:H2'	1:A:616:G:C8	2.50	0.46
1:A:680:C:C2	1:A:711:G:N2	2.83	0.46
1:A:769:G:N1	1:A:770:C:C4	2.82	0.46
1:A:943:U:H2'	1:A:944:G:H8	1.80	0.46
5:E:80:ILE:HD13	5:E:138:ALA:HB1	1.97	0.46
7:G:113:GLU:HG2	7:G:119:ARG:HG2	1.97	0.46
25:Z:22:G:N2	25:Z:23:C:C2	2.83	0.46
25:Z:2:G:C4	25:Z:3:C:C5	3.03	0.46
25:Z:55:PSU:O2'	25:Z:57:A:N7	2.30	0.46
1:A:1116:C:H2'	1:A:1117:G:O4'	2.15	0.46
1:A:1242:C:H2'	1:A:1243:C:C6	2.50	0.46
1:A:1347:G:HO2'	1:A:1373:G:H1	1.61	0.46
1:A:1511:G:H2'	1:A:1512:U:O4'	2.15	0.46
1:A:308:C:H2'	1:A:309:G:H8	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:519:C:H2'	1:A:520:A:C8	2.50	0.46
1:A:70:G:C2	1:A:100:C:C2	3.04	0.46
2:B:98:LEU:O	2:B:101:MET:HG3	2.15	0.46
2:B:97:TRP:CZ2	2:B:102:LEU:HD13	2.50	0.46
3:C:113:ALA:N	3:C:114:PRO:CD	2.78	0.46
10:J:76:ASN:HA	10:J:77:PRO:HD3	1.72	0.46
1:A:1060:C:H5'	10:J:51:ARG:HB3	1.97	0.46
1:A:590:C:C2	1:A:650:G:N2	2.84	0.46
1:A:601:C:H2'	1:A:602:A:C8	2.50	0.46
1:A:786:G:N2	1:A:797:C:C2	2.83	0.46
2:B:93:VAL:HG11	2:B:97:TRP:HD1	1.80	0.46
3:C:108:ASN:HA	3:C:109:PRO:HD2	1.83	0.46
10:J:70:ARG:HA	10:J:70:ARG:HD3	1.35	0.46
25:Z:35:A:O2'	25:Z:36:U:H5'	2.16	0.46
25:Z:2:G:C6	25:Z:3:C:C4	3.04	0.46
1:A:1176:A:H2'	1:A:1177:G:C8	2.51	0.46
1:A:1238:A:H5'	1:A:1336:C:H41	1.79	0.46
1:A:184:G:H2'	1:A:185:A:H8	1.79	0.46
1:A:219:C:H2'	1:A:220:G:O4'	2.14	0.46
1:A:310:G:C2	1:A:311:C:C2	3.03	0.46
1:A:406:G:H2'	1:A:407:G:H8	1.81	0.46
1:A:41:G:H2'	1:A:42:G:H8	1.80	0.46
1:A:589:C:O2	1:A:651:C:O2	2.33	0.46
1:A:935:A:H2'	1:A:936:C:H6	1.80	0.46
5:E:81:GLU:HG2	5:E:90:VAL:HG22	1.96	0.46
5:E:94:ALA:HB2	5:E:119:LEU:HD12	1.97	0.46
1:A:135:C:O2	16:P:1:MET:HB2	2.15	0.46
1:A:13:U:H5'	1:A:14:U:C5	2.51	0.46
1:A:437:U:H3'	1:A:438:G:C8	2.49	0.46
1:A:54:C:H41	1:A:352:C:H2'	1.81	0.46
5:E:15:ARG:HH22	5:E:26:PHE:HB3	1.75	0.46
1:A:948:C:P	13:M:108:ARG:H	2.38	0.46
1:A:1321:C:H5'	13:M:87:TYR:CE2	2.50	0.46
25:Z:47:U:C6	25:Z:50:U:OP1	2.69	0.46
1:A:1373:G:H5'	7:G:36:LYS:HB2	1.97	0.46
1:A:974:A:H1'	14:N:31:ARG:NH2	2.31	0.46
1:A:738:C:H5''	6:F:69:GLU:HB3	1.96	0.46
22:W:16:ALA:HA	22:W:22:PHE:CD1	2.49	0.46
22:W:32:ILE:CD1	22:W:32:ILE:H	2.27	0.46
23:X:19:VAL:HG21	25:Z:56:C:H41	1.80	0.46
1:A:1017:G:C2	1:A:1018:C:C2	3.03	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1537:U:H2'	1:A:1537:U:O2	2.16	0.46
1:A:236:G:C6	1:A:237:C:C4	3.03	0.46
1:A:245:C:C2	1:A:284:G:C2	3.03	0.46
1:A:276:G:C2	1:A:277:C:C2	3.04	0.46
1:A:333:G:C2	1:A:334:C:C4	3.03	0.46
1:A:13:U:N3	1:A:915:A:N6	2.61	0.46
1:A:98:G:H2'	1:A:99:U:O4'	2.16	0.46
2:B:204:ASN:HD22	2:B:204:ASN:C	2.19	0.46
10:J:26:ALA:HB1	10:J:84:GLN:HB3	1.98	0.46
1:A:1367:C:H4'	10:J:48:THR:HG21	1.98	0.46
1:A:1368:G:H5''	14:N:61:TRP:HZ2	1.80	0.46
1:A:1102:A:H2'	1:A:1103:C:H6	1.77	0.46
1:A:1350:A:P	9:I:121:ARG:HG3	2.55	0.46
1:A:59:A:H3'	1:A:331:G:H22	1.80	0.46
1:A:786:G:H2'	1:A:787:A:O4'	2.16	0.46
2:B:97:TRP:CH2	2:B:101:MET:HB2	2.51	0.46
4:D:67:ILE:HD11	4:D:197:PRO:HG2	1.98	0.46
23:X:17:ARG:HB2	23:X:56:VAL:HG22	1.97	0.46
25:Z:49:G:C2	25:Z:66:C:C4	3.04	0.46
1:A:1080:A:O3'	5:E:16:THR:CG2	2.60	0.46
1:A:1307:U:H2'	1:A:1308:U:C6	2.51	0.46
1:A:1304:G:H21	1:A:1333:A:H62	1.63	0.46
1:A:1504:G:H5''	1:A:1505:G:O4'	2.16	0.46
1:A:855:G:C6	1:A:856:C:C4	3.04	0.46
1:A:862:C:H2'	1:A:863:U:O4'	2.15	0.46
10:J:8:LEU:HB2	10:J:70:ARG:HB3	1.97	0.46
12:L:25:PRO:C	12:L:27:LEU:N	2.69	0.46
14:N:37:PHE:HB3	14:N:39:LEU:HB2	1.96	0.46
3:C:6:HIS:HB3	14:N:49:HIS:HB3	1.97	0.46
1:A:102:G:C2	1:A:103:C:C2	3.04	0.46
1:A:1057:G:H2'	1:A:1058:G:C8	2.50	0.46
1:A:1097:C:H2'	1:A:1098:C:C6	2.51	0.46
1:A:1117:G:O3'	9:I:104:ARG:NE	2.49	0.46
1:A:1446:U:O2'	1:A:1456:G:O6	2.32	0.46
1:A:127:G:N2	1:A:235:C:C2	2.83	0.46
1:A:399:G:C2	1:A:400:C:C2	3.05	0.46
1:A:427:U:O2'	1:A:541:G:OP1	2.28	0.46
1:A:548:G:C2	1:A:549:C:C2	3.03	0.46
1:A:584:G:C4	1:A:585:G:C8	3.04	0.46
1:A:585:G:C6	1:A:586:C:C4	3.04	0.46
1:A:562:C:H41	1:A:884:U:H2'	1.81	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:187:LEU:HD21	2:B:214:ILE:HD13	1.98	0.46
6:F:19:LEU:HD21	6:F:59:TYR:CZ	2.51	0.46
7:G:101:LEU:HA	7:G:104:LEU:HD12	1.98	0.46
25:Z:2:G:H3'	25:Z:3:C:C6	2.51	0.46
1:A:1046:A:H3'	1:A:1047:G:H8	1.81	0.45
1:A:1361:G:C2	1:A:1362:C:O2	2.69	0.45
1:A:17:U:C2	1:A:1079:G:N2	2.83	0.45
1:A:356:A:H2'	1:A:357:G:C8	2.50	0.45
1:A:477:A:H2'	1:A:479:C:C6	2.51	0.45
1:A:527:G:N2	1:A:528:C:C2	2.84	0.45
1:A:542:G:N1	1:A:543:C:C4	2.84	0.45
1:A:883:C:H2'	1:A:884:U:C6	2.51	0.45
4:D:35:ARG:HB3	4:D:35:ARG:CZ	2.45	0.45
4:D:6:GLY:O	4:D:8:VAL:HG23	2.16	0.45
20:T:32:ALA:O	20:T:36:LEU:HB2	2.16	0.45
25:Z:44:A:H2'	25:Z:45:G:C8	2.51	0.45
25:Z:64:G:C2	25:Z:65:C:H1'	2.50	0.45
25:Z:9:G:C2'	25:Z:10:G:N7	2.79	0.45
1:A:1007:C:N3	1:A:1022:G:N2	2.64	0.45
1:A:865:A:H8	1:A:865:A:O5'	1.98	0.45
18:R:73:ALA:HA	18:R:76:LEU:HD12	1.98	0.45
25:Z:49:G:N1	25:Z:66:C:C4	2.84	0.45
1:A:1464:G:C2	1:A:1465:C:C4	3.04	0.45
1:A:269:C:H2'	1:A:270:A:H8	1.76	0.45
1:A:289:G:C6	1:A:290:C:N4	2.84	0.45
1:A:344:A:H5''	1:A:345:C:H5	1.81	0.45
1:A:688:G:C6	1:A:689:C:N4	2.85	0.45
1:A:1186:G:H4'	9:I:110:GLU:CD	2.37	0.45
1:A:1027:C:C2'	1:A:1028:C:H5'	2.45	0.45
1:A:1074:G:C2	1:A:1075:C:C2	3.05	0.45
1:A:1135:U:H4'	1:A:1136:U:H5	1.81	0.45
1:A:1164:G:N1	1:A:1165:C:C4	2.84	0.45
1:A:1382:C:H2'	1:A:1383:C:H6	1.81	0.45
1:A:1419:G:C2	1:A:1420:C:C2	3.05	0.45
1:A:1436:U:H2'	1:A:1437:C:O4'	2.16	0.45
1:A:247:G:N1	1:A:248:C:C4	2.84	0.45
1:A:254:G:H1	1:A:272:C:N4	2.12	0.45
1:A:434:U:H2'	1:A:435:C:H6	1.79	0.45
1:A:537:G:H5''	12:L:113:ARG:NH1	2.28	0.45
1:A:568:G:N2	1:A:569:C:C2	2.85	0.45
1:A:571:U:H3'	1:A:572:A:C5'	2.47	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:632:A:H2'	1:A:633:G:O4'	2.16	0.45
1:A:91:C:N4	1:A:92:C:N4	2.64	0.45
3:C:28:GLN:OE1	3:C:28:GLN:N	2.49	0.45
7:G:152:ALA:HB1	7:G:155:ARG:NH2	2.31	0.45
3:C:33:LEU:HD11	14:N:53:LEU:CD2	2.47	0.45
20:T:43:LEU:HB3	20:T:52:ALA:HB2	1.98	0.45
1:A:1077:G:N2	1:A:1079:G:H3'	2.31	0.45
1:A:1127:G:N2	1:A:1145:C:C2	2.71	0.45
1:A:115:G:H1'	1:A:116:A:N7	2.31	0.45
1:A:1241:G:C6	1:A:1242:C:N4	2.85	0.45
1:A:125:U:H2'	1:A:126:G:C8	2.52	0.45
1:A:1328:C:H2'	1:A:1329:A:H8	1.81	0.45
1:A:437:U:H2'	1:A:438:G:O4'	2.17	0.45
1:A:678:U:H2'	1:A:679:C:C6	2.51	0.45
1:A:941:G:H2'	1:A:942:G:O4'	2.17	0.45
3:C:11:ARG:NH1	3:C:177:THR:O	2.49	0.45
4:D:196:LEU:C	4:D:198:VAL:H	2.20	0.45
4:D:36:ARG:HD3	4:D:38:TYR:OH	2.15	0.45
1:A:1207:G:C2	1:A:1208:C:C2	3.05	0.45
1:A:1253:G:C2	1:A:1254:C:C2	3.04	0.45
1:A:1368:G:N2	1:A:1369:C:C2	2.84	0.45
1:A:1512:U:H2'	1:A:1513:A:C8	2.52	0.45
1:A:293:G:C6	1:A:294:U:C4	3.05	0.45
1:A:823:G:C2	1:A:824:C:C2	3.05	0.45
1:A:961:U:O4	1:A:974:A:C6	2.62	0.45
6:F:78:GLU:HA	6:F:81:ILE:HD12	1.97	0.45
10:J:45:ARG:O	10:J:64:GLU:HA	2.16	0.45
1:A:834:C:H5''	18:R:60:ALA:HB2	1.97	0.45
20:T:73:HIS:HB3	20:T:74:LYS:NZ	2.31	0.45
1:A:120:A:C5	1:A:122:G:C5	3.05	0.45
1:A:1366:C:H2'	1:A:1367:C:H6	1.80	0.45
1:A:1464:G:N2	1:A:1465:C:C2	2.84	0.45
1:A:259:G:C2	1:A:268:C:C2	3.05	0.45
1:A:271:C:H2'	1:A:272:C:C6	2.52	0.45
1:A:583:A:O2'	17:Q:91:ARG:HG3	2.17	0.45
2:B:146:GLN:HG2	2:B:153:ARG:HH21	1.81	0.45
9:I:13:ALA:HB2	9:I:68:GLY:HA3	1.98	0.45
20:T:45:GLN:HA	20:T:91:LEU:HD22	1.99	0.45
1:A:1127:G:H1	1:A:1145:C:N4	2.15	0.45
1:A:1408:A:H2'	1:A:1409:C:C6	2.52	0.45
1:A:1484:C:O5'	1:A:1484:C:H6	2.00	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:314:C:H2'	1:A:315:A:C8	2.52	0.45
1:A:59:A:H5''	1:A:387:U:H5''	1.97	0.45
4:D:25:ARG:C	4:D:27:TYR:N	2.69	0.45
10:J:65:LEU:HD23	14:N:56:VAL:HG22	1.98	0.45
17:Q:61:GLU:HA	17:Q:71:PHE:CD1	2.52	0.45
22:W:17:LEU:HB3	22:W:18:PRO:CD	2.46	0.45
1:A:104:G:H4'	1:A:174:C:H5'	1.98	0.45
1:A:1079:G:C6	1:A:1080:A:N6	2.85	0.45
1:A:1355:G:H2'	1:A:1356:G:C8	2.51	0.45
1:A:577:G:C2	1:A:578:C:C2	3.05	0.45
2:B:54:THR:CG2	2:B:185:ILE:HG23	2.46	0.45
4:D:26:CYS:HA	4:D:31:CYS:HB2	1.99	0.45
12:L:87:GLY:HA2	12:L:98:TYR:HA	1.98	0.45
25:Z:10:G:N3	25:Z:10:G:H2'	2.32	0.45
1:A:1129:C:OP1	1:A:1130:A:H5'	2.17	0.45
1:A:249:U:O2'	1:A:252:U:H4'	2.17	0.45
1:A:333:G:N1	1:A:334:C:C4	2.85	0.45
1:A:377:G:H2'	1:A:378:G:C8	2.52	0.45
1:A:416:G:C6	1:A:417:C:C4	3.06	0.45
1:A:684:A:H4'	11:K:12:ARG:NH2	2.32	0.45
1:A:874:G:N1	1:A:875:C:C4	2.85	0.45
4:D:173:TRP:O	4:D:186:LEU:HB2	2.16	0.45
5:E:148:VAL:O	5:E:152:ARG:HG2	2.17	0.45
6:F:69:GLU:CD	6:F:69:GLU:H	2.19	0.45
9:I:118:LYS:O	9:I:119:ALA:HB3	2.17	0.45
1:A:1244:C:H2'	1:A:1245:A:C8	2.52	0.44
1:A:229:U:H2'	1:A:230:G:H8	1.82	0.44
1:A:539:A:H2'	1:A:540:G:C8	2.52	0.44
1:A:689:C:H2'	1:A:690:G:O4'	2.17	0.44
1:A:755:G:N1	1:A:756:C:C4	2.85	0.44
1:A:761:G:H2'	1:A:762:C:C6	2.52	0.44
1:A:823:G:C6	1:A:824:C:N4	2.84	0.44
2:B:212:GLN:HG3	2:B:239:VAL:CG2	2.47	0.44
5:E:87:SER:HA	5:E:125:SER:HB3	1.99	0.44
16:P:57:ARG:CZ	16:P:79:VAL:O	2.66	0.44
23:X:11:ILE:HG23	23:X:47:LEU:HD22	1.98	0.44
25:Z:37:A:C4	25:Z:38:A:C8	3.05	0.44
25:Z:6:G:C2	25:Z:7:G:C5	3.05	0.44
1:A:1401:G:C6	1:A:1402:C:C2	3.05	0.44
1:A:189:G:C6	1:A:189(A):C:C4	3.05	0.44
1:A:266:G:O2'	1:A:267:C:OP2	2.21	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:310:G:C6	1:A:311:C:C4	3.05	0.44
1:A:584:G:C5	1:A:585:G:N7	2.85	0.44
1:A:891:U:H2'	1:A:892:A:H8	1.83	0.44
4:D:31:CYS:C	4:D:33:MET:H	2.20	0.44
1:A:552:U:H1'	12:L:32:PHE:CE1	2.52	0.44
1:A:1115:C:C2	1:A:1186:G:C2	3.05	0.44
1:A:372:C:H1'	1:A:373:A:OP2	2.17	0.44
1:A:674:G:H2'	1:A:675:A:C8	2.51	0.44
1:A:778:G:C2	1:A:779:C:C2	3.06	0.44
1:A:824:C:H2'	1:A:825:G:C8	2.51	0.44
4:D:162:LEU:HD12	4:D:178:VAL:HG23	1.98	0.44
5:E:15:ARG:NH2	5:E:15:ARG:CG	2.73	0.44
13:M:22:ILE:HG22	13:M:24:GLY:H	1.82	0.44
18:R:37:VAL:HG13	18:R:78:LEU:HB3	2.00	0.44
22:W:51:ASP:OD2	23:X:125:ARG:HD3	2.18	0.44
1:A:1207:G:C6	1:A:1208:C:C4	3.06	0.44
1:A:1277:C:HO2'	1:A:1279:A:H8	1.64	0.44
1:A:407:G:H2'	1:A:408:A:C8	2.52	0.44
1:A:502:G:C2	1:A:503:C:C2	3.05	0.44
1:A:681:C:C2	1:A:710:G:N2	2.84	0.44
1:A:834:C:H5''	18:R:60:ALA:HB3	1.99	0.44
1:A:407:G:H5''	4:D:115:ARG:HB2	2.00	0.44
16:P:67:THR:HG22	16:P:68:ASP:H	1.82	0.44
19:S:6:LYS:HE3	19:S:7:LYS:HE3	2.00	0.44
25:Z:38:A:H2'	25:Z:39:C:O4'	2.18	0.44
1:A:1064:G:H8	1:A:1064:G:OP1	2.01	0.44
1:A:1133:G:H1	1:A:1141:C:N4	2.16	0.44
1:A:1351:U:H2'	1:A:1352:C:H6	1.81	0.44
1:A:1390:U:H2'	1:A:1391:U:C6	2.51	0.44
1:A:1504:G:H4'	1:A:1505:G:O5'	2.17	0.44
1:A:861:G:C2	1:A:862:C:C2	3.05	0.44
6:F:11:ASN:HD21	6:F:13:ASN:HD22	1.65	0.44
6:F:74:ASP:HA	6:F:77:ARG:HD2	2.00	0.44
9:I:36:TYR:HE2	9:I:73:GLN:OE1	2.00	0.44
1:A:1148:U:C5'	9:I:7:THR:HG21	2.47	0.44
18:R:31:LEU:O	18:R:69:THR:HG21	2.18	0.44
1:A:1305:G:H5''	21:V:5:ASP:HB2	2.00	0.44
25:Z:17:C:H4'	25:Z:17(A):U:OP2	2.17	0.44
1:A:1004:A:H5''	1:A:1025:U:C5	2.53	0.44
1:A:1048:G:H5''	14:N:3:ARG:HG3	1.99	0.44
1:A:43:C:H2'	1:A:44:G:O4'	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:98:SER:HA	7:G:101:LEU:HD12	2.00	0.44
13:M:125:ARG:NH2	25:Z:30:G:OP2	2.50	0.44
20:T:74:LYS:HB2	20:T:75:ASN:H	1.31	0.44
25:Z:27:U:H2'	25:Z:28:C:H6	1.83	0.44
25:Z:49:G:C6	25:Z:66:C:N4	2.86	0.44
1:A:1048:G:H2'	1:A:1050:G:H8	1.83	0.44
1:A:1189:C:OP1	10:J:51:ARG:NH2	2.50	0.44
1:A:1226:C:H2'	13:M:103:THR:CB	2.43	0.44
1:A:1237:C:H5''	1:A:1238:A:O4'	2.18	0.44
1:A:1411:C:H5''	22:W:64:ARG:HH22	1.82	0.44
1:A:223:U:H2'	1:A:224:C:C6	2.53	0.44
1:A:382:A:H2'	1:A:383:A:H8	1.81	0.44
1:A:399:G:C6	1:A:400:C:N4	2.86	0.44
1:A:41:G:H2'	1:A:42:G:C8	2.53	0.44
1:A:568:G:C2	1:A:569:C:N3	2.86	0.44
1:A:807:A:H2'	1:A:808:C:C6	2.53	0.44
8:H:101:PRO:HB2	8:H:103:VAL:HG23	1.98	0.44
9:I:27:THR:HB	9:I:62:TYR:HD1	1.82	0.44
20:T:10:LEU:HD12	20:T:11:SER:N	2.32	0.44
22:W:33:LEU:HD22	22:W:33:LEU:H	1.83	0.44
25:Z:23:C:H2'	25:Z:24:U:C6	2.53	0.44
1:A:108:G:H5'	1:A:109:A:H5''	2.00	0.44
1:A:1171:G:C6	1:A:1172:C:N4	2.86	0.44
1:A:1280:A:H3'	1:A:1281:U:C5'	2.41	0.44
1:A:1305:G:H22	1:A:1331:G:H1'	1.83	0.44
1:A:1446:U:H1'	1:A:1457:G:C2	2.53	0.44
1:A:1392:G:N2	1:A:1502:A:H8	2.16	0.44
1:A:296:U:H2'	1:A:297:G:C8	2.53	0.44
1:A:317:G:C2	1:A:337:C:C2	3.05	0.44
1:A:579:G:H1	1:A:762:C:H42	1.65	0.44
1:A:778:G:C6	1:A:779:C:N3	2.86	0.44
1:A:881:G:C2	1:A:882:C:C2	3.05	0.44
4:D:104:VAL:O	4:D:108:LEU:HD12	2.18	0.44
13:M:18:ALA:O	13:M:21:TYR:HB2	2.18	0.44
17:Q:74:LEU:HG	17:Q:75:ARG:HG2	2.00	0.44
25:Z:64:G:C6	25:Z:65:C:C2	3.05	0.44
1:A:1040:U:H2'	1:A:1041:A:C8	2.53	0.44
1:A:1145:C:H1'	1:A:1146:A:C8	2.53	0.44
1:A:1387:G:C2	1:A:1388:C:C2	3.06	0.44
1:A:129(A):G:O2'	1:A:189(F):U:H2'	2.18	0.44
1:A:255:G:C2	1:A:272:C:C2	3.06	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:721:G:H4'	1:A:722:A:O4'	2.18	0.44
1:A:867:G:N2	1:A:868:C:C2	2.85	0.44
1:A:947:G:C6	1:A:948:C:C4	3.06	0.44
13:M:65:LYS:NZ	13:M:73:GLU:HB2	2.32	0.44
1:A:1041:A:H2'	1:A:1042:G:C8	2.52	0.43
1:A:625:G:H2'	1:A:626:U:C6	2.52	0.43
1:A:741:G:H2'	1:A:742:G:O4'	2.18	0.43
1:A:758:G:O2'	1:A:759:A:H5'	2.17	0.43
1:A:763:G:C2	1:A:764:C:C2	3.06	0.43
1:A:966:G:C6	25:Z:34:C:H5'	2.52	0.43
1:A:985:C:C2	1:A:1221:G:N2	2.86	0.43
1:A:998:G:N2	1:A:999:C:C2	2.86	0.43
4:D:30:LYS:C	4:D:32:ALA:H	2.20	0.43
12:L:30:ALA:HA	12:L:31:PRO:HD3	1.85	0.43
13:M:11:ARG:HH11	13:M:45:VAL:HG12	1.82	0.43
14:N:43:CYS:O	14:N:47:LEU:HG	2.18	0.43
1:A:1508:G:C6	1:A:1509:C:C4	3.07	0.43
1:A:174:C:H2'	1:A:175:C:C6	2.53	0.43
1:A:243:A:H4'	1:A:244:U:C5'	2.47	0.43
1:A:322:C:H2'	1:A:323:U:C6	2.53	0.43
5:E:16:THR:HB	5:E:27:ARG:O	2.19	0.43
19:S:22:LEU:HA	19:S:25:LYS:HB3	2.00	0.43
1:A:1328:C:H2'	1:A:1329:A:C8	2.54	0.43
1:A:1445:C:O2	1:A:1458:G:C2	2.70	0.43
1:A:1525:G:H2'	1:A:1526:G:C8	2.53	0.43
1:A:295:C:H2'	1:A:296:U:O4'	2.18	0.43
1:A:355:C:C4	1:A:356:A:N7	2.86	0.43
1:A:403:C:H2'	1:A:404:U:C6	2.53	0.43
1:A:856:C:N4	1:A:857:C:N4	2.66	0.43
5:E:12:LEU:HB3	5:E:31:LEU:HB3	2.00	0.43
10:J:40:LEU:HD23	10:J:41:PRO:HD2	2.00	0.43
3:C:29:TYR:CZ	14:N:54:PRO:CG	2.90	0.43
19:S:20:LEU:HD12	19:S:21:GLU:HG3	2.00	0.43
1:A:966:G:C5	25:Z:34:C:H5'	2.53	0.43
1:A:1001:A:C6	1:A:1001(A):G:C6	3.07	0.43
1:A:1081:G:H2'	1:A:1082:G:O4'	2.18	0.43
1:A:10:A:H2'	1:A:11:G:H8	1.80	0.43
1:A:120:A:C5	1:A:122:G:C6	3.06	0.43
1:A:189:G:H2'	1:A:189(A):C:C6	2.54	0.43
1:A:132:C:C4	1:A:231:G:N1	2.86	0.43
1:A:289:G:C2	1:A:290:C:C2	3.07	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:451:A:N6	1:A:480:U:H2'	2.34	0.43
1:A:683:G:N2	1:A:708:C:C2	2.86	0.43
1:A:878:G:H2'	1:A:879:C:C6	2.54	0.43
13:M:80:ARG:O	13:M:84:ILE:HG12	2.19	0.43
23:X:152:MET:HG2	23:X:164:LEU:HB3	2.01	0.43
1:A:1429:C:H2'	1:A:1430:C:C6	2.52	0.43
1:A:179:A:C2	1:A:180:U:C2	3.07	0.43
1:A:407:G:H2'	1:A:408:A:H8	1.83	0.43
1:A:577:G:C6	1:A:578:C:C4	3.06	0.43
1:A:682:G:H2'	1:A:683:G:O4'	2.19	0.43
1:A:872:A:H2'	1:A:872:A:N3	2.32	0.43
2:B:188:ALA:HB3	2:B:200:ILE:HG23	2.00	0.43
4:D:109:GLY:HA3	4:D:165:MET:HG3	2.00	0.43
4:D:35:ARG:CB	4:D:35:ARG:CZ	2.97	0.43
5:E:127:ASN:HD21	5:E:129:ILE:HD12	1.83	0.43
6:F:55:ASP:HA	6:F:56:PRO:HD2	1.85	0.43
13:M:91:ARG:HH21	13:M:96:LEU:HB3	1.84	0.43
23:X:8:ASN:HD21	23:X:44:ASP:HA	1.82	0.43
25:Z:39:C:O2'	25:Z:40:C:H5'	2.19	0.43
1:A:1048:G:C2	1:A:1210:C:N3	2.87	0.43
1:A:1061:G:H2'	1:A:1062:U:O4'	2.18	0.43
1:A:1279:A:H5'	10:J:7:LYS:HE2	2.00	0.43
1:A:1360:A:H2'	1:A:1361:G:C8	2.53	0.43
1:A:812:C:HO2'	1:A:813:U:P	2.41	0.43
1:A:916:G:H2'	1:A:917:G:H8	1.83	0.43
2:B:61:LEU:HD11	2:B:160:ASP:HB2	2.01	0.43
11:K:48:ILE:HG13	11:K:48:ILE:H	1.48	0.43
15:O:41:GLU:HA	15:O:44:LYS:HD2	2.00	0.43
23:X:132:LEU:O	23:X:136:ILE:HG13	2.18	0.43
25:Z:22:G:N1	25:Z:23:C:C4	2.86	0.43
1:A:1088:G:H2'	1:A:1089:G:O4'	2.18	0.43
1:A:1133:G:H2'	1:A:1134:G:C8	2.53	0.43
1:A:448:A:H62	1:A:486:U:H3	1.67	0.43
1:A:29:G:N2	1:A:555:C:C2	2.87	0.43
1:A:903:G:C2	1:A:904:C:C2	3.06	0.43
2:B:96:ARG:HB3	2:B:148:TYR:HE2	1.83	0.43
4:D:18:LYS:HE3	4:D:31:CYS:HB3	2.01	0.43
10:J:8:LEU:HA	10:J:95:GLU:O	2.19	0.43
17:Q:6:LEU:HD23	17:Q:23:VAL:HG11	1.99	0.43
1:A:1114:C:H2'	1:A:1115:C:H6	1.83	0.43
1:A:1114:C:H2'	1:A:1115:C:C6	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1162:C:C2	1:A:1175:G:N2	2.87	0.43
1:A:1244:C:H42	1:A:1293:G:H1	1.65	0.43
1:A:1253:G:C6	1:A:1254:C:C4	3.07	0.43
1:A:134:A:H2'	1:A:135:C:O4'	2.19	0.43
1:A:1369:C:H2'	1:A:1370:G:O4'	2.19	0.43
1:A:184:G:H2'	1:A:185:A:C8	2.54	0.43
1:A:280:C:N4	17:Q:91:ARG:NH2	2.67	0.43
1:A:426:G:H2'	1:A:427:U:O4'	2.18	0.43
9:I:116:LYS:HA	9:I:123:PRO:HD3	1.99	0.43
13:M:25:ILE:HG12	13:M:29:ARG:HB3	2.00	0.43
25:Z:67:C:H2'	25:Z:68:C:H6	1.83	0.43
1:A:109:A:H5'	1:A:110:C:H5	1.84	0.43
1:A:1292:U:H2'	1:A:1293:G:C8	2.54	0.43
1:A:1371:G:H2'	1:A:1372:U:H6	1.83	0.43
1:A:193:C:H2'	1:A:194:C:C6	2.54	0.43
1:A:23:C:C4	1:A:24:U:C4	3.07	0.43
1:A:384:G:C2	1:A:385:C:C2	3.07	0.43
1:A:439:A:C6	1:A:496:A:C4	3.07	0.43
1:A:444:C:N4	1:A:490:G:H1	2.17	0.43
1:A:617:G:C2	1:A:618:C:C4	3.06	0.43
1:A:698:G:C2	1:A:699:C:C2	3.06	0.43
1:A:725:G:C2	1:A:726:C:C4	3.07	0.43
1:A:769:G:H4'	1:A:1513:A:H4'	2.01	0.43
1:A:855:G:C2	1:A:856:C:C2	3.07	0.43
1:A:874:G:C2	1:A:875:C:C2	3.07	0.43
1:A:1081:G:P	5:E:27:ARG:NE	2.80	0.43
7:G:27:ILE:HA	7:G:30:ILE:HD12	2.00	0.43
7:G:79:ARG:NH2	7:G:82:GLY:H	2.17	0.43
13:M:44:ARG:H	13:M:47:ASP:HB2	1.84	0.43
18:R:16:PRO:HB2	18:R:18:ARG:HB2	2.00	0.43
1:A:1068:G:N1	1:A:1069:C:C4	2.87	0.43
1:A:1333:A:H3'	1:A:1334:G:H8	1.83	0.43
1:A:280:C:O2	17:Q:38:ARG:HA	2.19	0.43
1:A:392:G:H5'	16:P:12:LYS:HG2	2.01	0.43
1:A:714:G:H2'	1:A:715:A:H8	1.75	0.43
1:A:975:A:H4'	1:A:976:G:O5'	2.19	0.43
2:B:84:GLU:HB2	2:B:215:LEU:HD22	2.01	0.43
9:I:92:TYR:O	9:I:96:LEU:HB2	2.19	0.43
12:L:8:ASN:O	12:L:12:ARG:HG3	2.19	0.43
1:A:137:C:H1'	16:P:62:VAL:O	2.19	0.43
25:Z:53:G:N2	25:Z:61:C:C2	2.87	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1347:G:O2'	1:A:1348:U:P	2.77	0.42
1:A:1419:G:C6	1:A:1420:C:C4	3.06	0.42
1:A:1481:U:H2'	1:A:1482:G:C8	2.53	0.42
1:A:258:G:C2	1:A:269:C:C2	3.07	0.42
1:A:584:G:H2'	1:A:585:G:C8	2.53	0.42
4:D:36:ARG:CG	4:D:38:TYR:CZ	3.02	0.42
5:E:11:ILE:HG22	5:E:12:LEU:HB2	2.01	0.42
8:H:127:LEU:HB3	8:H:129:VAL:HG12	2.01	0.42
8:H:29:SER:O	8:H:33:GLU:HB2	2.19	0.42
25:Z:22:G:C2	25:Z:23:C:C2	3.07	0.42
25:Z:31:G:C2	25:Z:40:C:N3	2.87	0.42
1:A:1002:G:N1	1:A:1039:C:C2	2.81	0.42
1:A:1189:C:H5'	14:N:58:LYS:NZ	2.34	0.42
1:A:35:G:C6	1:A:36:C:N4	2.87	0.42
1:A:416:G:C2	1:A:417:C:C2	3.08	0.42
1:A:823:G:N1	1:A:824:C:C4	2.87	0.42
2:B:172:ILE:H	2:B:172:ILE:HG13	1.56	0.42
4:D:33:MET:CA	4:D:36:ARG:O	2.67	0.42
1:A:247:G:P	17:Q:100:LYS:HD2	2.59	0.42
1:A:1352:C:P	21:V:3:LYS:HZ1	2.42	0.42
22:W:32:ILE:N	22:W:32:ILE:CD1	2.82	0.42
22:W:35:TYR:CZ	22:W:66:ARG:HG3	2.54	0.42
25:Z:71:C:C2'	25:Z:72:A:O4'	2.66	0.42
1:A:102:G:C6	1:A:103:C:C4	3.07	0.42
1:A:279:A:OP2	17:Q:95:TYR:OH	2.35	0.42
1:A:505:G:H2'	1:A:506:G:H8	1.84	0.42
1:A:542:G:C2	1:A:543:C:C2	3.07	0.42
1:A:741:G:H5''	15:O:39:LEU:HD11	2.01	0.42
18:R:52:PRO:HB2	18:R:54:ARG:HG3	2.01	0.42
19:S:49:ILE:HG22	19:S:51:VAL:HG23	2.01	0.42
1:A:1353:G:C6	1:A:1354:C:N4	2.87	0.42
1:A:1511:G:H2'	1:A:1512:U:C6	2.54	0.42
1:A:241:C:C2	1:A:286:G:C2	3.07	0.42
1:A:544:G:H2'	1:A:545:C:O4'	2.19	0.42
3:C:13:GLY:HA3	14:N:57:ARG:HE	1.84	0.42
4:D:185:PHE:HZ	4:D:189:PRO:HD3	1.84	0.42
11:K:21:ILE:HD11	11:K:98:LEU:HD12	2.00	0.42
14:N:23:ARG:NH1	14:N:30:ALA:HB2	2.34	0.42
23:X:85:VAL:HA	23:X:115:LYS:O	2.20	0.42
25:Z:12:G:C6	25:Z:13:C:C4	3.07	0.42
1:A:1233:G:C2	1:A:1234:C:C2	3.07	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1387:G:C6	1:A:1388:C:C4	3.07	0.42
1:A:1514:C:H2'	1:A:1515:C:H6	1.82	0.42
1:A:1526:G:C2	1:A:1527:C:C2	3.07	0.42
1:A:276:G:C6	1:A:277:C:C4	3.07	0.42
1:A:687:A:H4'	1:A:688:G:O5'	2.19	0.42
1:A:79:G:H2'	1:A:80:G:C8	2.46	0.42
11:K:18:ARG:HD3	11:K:35:PRO:HA	2.00	0.42
20:T:23:ARG:HG3	20:T:24:LEU:N	2.35	0.42
1:A:1152:A:H2'	1:A:1153:C:C6	2.54	0.42
1:A:1154:G:H2'	1:A:1155:G:H8	1.83	0.42
1:A:1198:G:H2'	1:A:1199:U:C6	2.54	0.42
1:A:1270:C:H2'	1:A:1271:G:H8	1.85	0.42
1:A:1353:G:OP2	21:V:3:LYS:NZ	2.51	0.42
1:A:164:U:H2'	1:A:165:C:C6	2.54	0.42
1:A:329:A:H4'	1:A:330:C:OP1	2.18	0.42
1:A:333:G:C2	1:A:334:C:C2	3.07	0.42
1:A:51:A:H4'	1:A:52:G:C5'	2.50	0.42
1:A:556:C:H2'	1:A:557:G:O4'	2.20	0.42
1:A:670:G:H1	1:A:736:C:N4	2.16	0.42
2:B:118:LEU:O	2:B:122:PHE:HB2	2.18	0.42
2:B:122:PHE:HA	2:B:127:ILE:HG12	2.00	0.42
2:B:34:ALA:HB3	2:B:36:ARG:NH1	2.35	0.42
12:L:59:ARG:HB2	12:L:59:ARG:NH1	2.35	0.42
25:Z:21:A:N6	25:Z:46:G7M:C2'	2.76	0.42
25:Z:31:G:C2	25:Z:40:C:C2	3.07	0.42
1:A:1106:G:C2	1:A:1107:C:C4	3.08	0.42
1:A:1106:G:C2	1:A:1107:C:C2	3.07	0.42
1:A:1459:C:H2'	1:A:1460:A:H8	1.84	0.42
1:A:1502:A:H2'	1:A:1504:G:C8	2.54	0.42
1:A:325:A:H2'	1:A:326:G:O4'	2.20	0.42
1:A:36:C:H2'	1:A:37:U:O4'	2.20	0.42
1:A:559:A:H4'	1:A:560:U:C5'	2.49	0.42
1:A:929:G:C2	1:A:930:C:C2	3.07	0.42
1:A:932:C:H5'	7:G:3:ARG:HB2	2.02	0.42
1:A:939:G:C2	1:A:940:C:C2	3.07	0.42
5:E:15:ARG:NH2	5:E:26:PHE:HB3	2.35	0.42
25:Z:31:G:N2	25:Z:40:C:C2	2.88	0.42
25:Z:7:G:C5	25:Z:49:G:C8	3.08	0.42
1:A:1115:C:C2	1:A:1186:G:N2	2.87	0.42
1:A:11:G:H2'	1:A:12:U:O4'	2.19	0.42
1:A:338:A:C6	1:A:339:C:C4	3.08	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:501:C:OP1	12:L:117:ARG:NH2	2.52	0.42
1:A:650:G:N2	1:A:651:C:C2	2.88	0.42
1:A:661:G:C2	1:A:745:C:N3	2.88	0.42
1:A:806:C:H2'	1:A:807:A:H8	1.84	0.42
1:A:825:G:H1	1:A:875:C:H42	1.68	0.42
2:B:77:ALA:C	2:B:79:ASP:H	2.23	0.42
5:E:11:ILE:HD13	5:E:33:VAL:HG23	2.02	0.42
14:N:17:LYS:H	14:N:17:LYS:HG3	1.64	0.42
1:A:1002:G:O6	1:A:1039:C:N3	2.53	0.42
1:A:1050:G:C2	1:A:1051:C:C4	3.08	0.42
1:A:155:C:H2'	1:A:156:G:H8	1.85	0.42
1:A:394:G:C2	1:A:395:C:C2	3.07	0.42
1:A:447:G:C3'	1:A:485:G:H22	2.33	0.42
3:C:62:ASP:HA	3:C:97:LYS:CE	2.50	0.42
4:D:129:ASN:ND2	4:D:145:GLU:H	2.16	0.42
23:X:152:MET:HB3	23:X:155:GLU:OE1	2.20	0.42
25:Z:70:G:C6	25:Z:71:C:N3	2.88	0.42
1:A:1001(A):G:N1	1:A:1002:G:C6	2.88	0.42
1:A:1029:C:H2'	1:A:1030:C:C6	2.55	0.42
1:A:1283:G:C6	1:A:1284:C:N4	2.87	0.42
1:A:252:U:H2'	1:A:253:U:C6	2.55	0.42
1:A:319:G:C2	1:A:320:C:C2	3.08	0.42
1:A:774:G:C2	1:A:806:C:C2	3.07	0.42
1:A:903:G:C6	1:A:904:C:C4	3.08	0.42
2:B:25:ASN:HA	2:B:26:PRO:HD3	1.83	0.42
3:C:6:HIS:HA	3:C:7:PRO:HD3	1.88	0.42
5:E:76:ILE:HG23	5:E:78:HIS:H	1.85	0.42
1:A:169:C:H2'	1:A:170:U:C6	2.55	0.41
1:A:436:C:O2'	4:D:155:LEU:HD21	2.19	0.41
1:A:590:C:OP1	8:H:30:ARG:N	2.49	0.41
1:A:718:G:H5'	11:K:117:ASN:HB2	2.01	0.41
1:A:731:G:C6	1:A:732:C:C4	3.08	0.41
1:A:836:G:H2'	1:A:837:G:C8	2.54	0.41
5:E:15:ARG:NH2	5:E:26:PHE:CB	2.76	0.41
9:I:111:ARG:NH1	14:N:61:TRP:OXT	2.52	0.41
20:T:44:ALA:HB1	20:T:91:LEU:HB2	2.02	0.41
25:Z:38:A:C8	25:Z:39:C:C5	3.08	0.41
1:A:1068:G:C2	1:A:1069:C:C2	3.09	0.41
1:A:1095:U:OP1	1:A:1108:G:N1	2.53	0.41
1:A:1116:C:C2	1:A:1185:G:C2	3.07	0.41
1:A:1241:G:N1	1:A:1242:C:C4	2.89	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1347:G:C8	9:I:107:ARG:HB3	2.55	0.41
1:A:442:C:H2'	1:A:443:C:C6	2.55	0.41
1:A:450:G:N7	1:A:481:G:C6	2.88	0.41
1:A:481:G:O2'	1:A:483:C:N4	2.53	0.41
1:A:977:A:H1'	1:A:982:U:O4	2.20	0.41
2:B:97:TRP:CZ2	2:B:101:MET:HB2	2.54	0.41
3:C:29:TYR:CD1	3:C:33:LEU:HB2	2.55	0.41
5:E:31:LEU:HD23	5:E:45:PHE:HD1	1.84	0.41
19:S:5:LEU:HB3	19:S:6:LYS:H	1.46	0.41
23:X:19:VAL:HG21	25:Z:56:C:C4	2.55	0.41
1:A:142:G:H2'	1:A:143:A:H8	1.85	0.41
1:A:1459:C:H2'	1:A:1460:A:O4'	2.20	0.41
1:A:1502:A:H2	1:A:1505:G:N1	2.18	0.41
1:A:1541:U:H3	24:Y:24:A:N6	2.18	0.41
1:A:183:G:H2'	1:A:184:G:O4'	2.21	0.41
1:A:189(L):G:H2'	1:A:190:U:C6	2.55	0.41
1:A:321:A:H2'	1:A:322:C:H6	1.85	0.41
1:A:542:G:C6	1:A:543:C:N4	2.89	0.41
1:A:881:G:C6	1:A:882:C:C4	3.08	0.41
7:G:111:ARG:HA	7:G:112:PRO:HD3	1.80	0.41
13:M:82:MET:HA	13:M:89:GLY:HA3	2.02	0.41
14:N:12:ARG:H	14:N:12:ARG:HG2	1.71	0.41
16:P:9:PHE:CD2	16:P:18:ARG:HG3	2.55	0.41
16:P:73:LEU:HA	16:P:73:LEU:HD23	1.97	0.41
23:X:45:LEU:HG	23:X:57:ALA:HB1	2.02	0.41
1:A:1226:C:H5''	13:M:96:LEU:HD13	2.01	0.41
1:A:1478:C:H2'	1:A:1479:C:C6	2.55	0.41
1:A:778:G:N1	1:A:779:C:C2	2.88	0.41
1:A:861:G:C6	1:A:862:C:C4	3.09	0.41
1:A:914:A:C5	1:A:915:A:N7	2.89	0.41
12:L:93:LEU:HA	12:L:94:PRO:HD3	1.78	0.41
1:A:986:A:H1'	19:S:54:GLY:O	2.21	0.41
1:A:1050:G:C2	1:A:1209:C:C2	3.08	0.41
1:A:1258:G:H2'	1:A:1259:C:C6	2.55	0.41
1:A:1283:G:C2	1:A:1284:C:C4	3.08	0.41
1:A:1452:C:H4'	1:A:1456:G:O4'	2.21	0.41
1:A:489:C:H2'	1:A:490:G:H8	1.85	0.41
1:A:916:G:C2	1:A:917:G:N7	2.88	0.41
1:A:921:U:H2'	1:A:922:G:O4'	2.20	0.41
4:D:3:ARG:HB3	4:D:4:TYR:H	1.69	0.41
4:D:90:GLY:O	4:D:93:PHE:HB3	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:85:ILE:HG22	12:L:87:GLY:H	1.85	0.41
14:N:21:TYR:O	14:N:23:ARG:N	2.53	0.41
1:A:1106:G:C2	1:A:1107:C:N3	2.89	0.41
1:A:113:G:H1'	1:A:354:G:H5'	2.02	0.41
1:A:1171:G:N1	1:A:1172:C:C4	2.88	0.41
1:A:1171:G:C2	1:A:1172:C:C2	3.08	0.41
1:A:502:G:C6	1:A:503:C:C4	3.09	0.41
2:B:33:TYR:HB3	2:B:41:ILE:HG22	2.02	0.41
2:B:84:GLU:HA	2:B:87:ARG:HB2	2.01	0.41
7:G:18:TYR:CE1	7:G:59:LEU:HB2	2.55	0.41
10:J:34:VAL:HG13	10:J:72:VAL:CG1	2.50	0.41
20:T:63:ILE:HG21	20:T:81:LYS:HG3	2.01	0.41
23:X:46:VAL:O	23:X:48:VAL:HG22	2.20	0.41
1:A:1126:U:H2'	1:A:1126:U:O2	2.20	0.41
1:A:1128:C:O2'	1:A:1130:A:N7	2.42	0.41
1:A:365:U:O2	1:A:365:U:H2'	2.20	0.41
1:A:399:G:N2	1:A:400:C:C2	2.89	0.41
1:A:626:U:H2'	1:A:627:G:C8	2.56	0.41
1:A:785:G:H1	1:A:797:C:N4	2.19	0.41
1:A:790:A:H4'	23:X:87:SER:OG	2.20	0.41
7:G:9:VAL:HB	7:G:11:GLN:HE22	1.86	0.41
8:H:79:VAL:HG13	8:H:80:ILE:N	2.35	0.41
1:A:1329:A:H5''	13:M:25:ILE:HA	2.02	0.41
15:O:41:GLU:O	15:O:44:LYS:HB2	2.20	0.41
17:Q:19:VAL:HG23	17:Q:44:ALA:HB3	2.03	0.41
21:V:3:LYS:HD3	21:V:14:TRP:CD1	2.56	0.41
1:A:1292:U:H2'	1:A:1293:G:H8	1.86	0.41
1:A:1302:U:H3'	1:A:1303:C:C5'	2.51	0.41
1:A:1443:G:C2	1:A:1444:C:N3	2.89	0.41
1:A:1458:G:H5''	20:T:31:SER:HB3	2.02	0.41
1:A:1507:A:C8	1:A:1530:G:N2	2.88	0.41
1:A:284:G:C2	1:A:285:G:C5	3.08	0.41
1:A:354:G:C2	1:A:355:C:C4	3.09	0.41
1:A:402:G:C2	1:A:403:C:C2	3.09	0.41
1:A:767:A:H2'	1:A:768:A:C8	2.56	0.41
10:J:4:ILE:HD12	10:J:74:ILE:HD13	2.01	0.41
1:A:291:C:O2	1:A:310:G:C2	2.74	0.41
1:A:662:G:C2	1:A:744:C:O2	2.74	0.41
1:A:542:G:O3'	4:D:14:ARG:NH2	2.53	0.41
4:D:185:PHE:CZ	4:D:189:PRO:HD3	2.56	0.41
14:N:24:CYS:HB3	14:N:29:ARG:N	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:472:A:OP1	16:P:75:ARG:NH1	2.54	0.41
25:Z:53:G:H2'	25:Z:54:5MU:C6	2.56	0.41
25:Z:2:G:H1	25:Z:71:C:N4	2.19	0.41
1:A:1017:G:C6	1:A:1018:C:C4	3.09	0.41
1:A:1069:C:H2'	1:A:1070:U:O4'	2.21	0.41
1:A:1217:C:N4	1:A:1218:C:N4	2.68	0.41
1:A:1286:A:H3'	1:A:1286:A:C8	2.56	0.41
1:A:1396:A:O3'	1:A:1397:C:H5''	2.21	0.41
1:A:146:G:N2	1:A:177:C:C2	2.89	0.41
1:A:310:G:OP1	16:P:27:LYS:HD2	2.21	0.41
1:A:76:C:O2'	1:A:77:G:H5'	2.21	0.41
5:E:37:ARG:HH12	5:E:111:GLU:HB3	1.86	0.41
1:A:1371:G:O3'	9:I:69:GLY:HA3	2.20	0.41
9:I:89:ASN:ND2	9:I:91:ASP:HB2	2.35	0.41
10:J:49:VAL:HG11	14:N:44:LEU:HD12	2.03	0.41
3:C:33:LEU:HD11	14:N:53:LEU:HD22	2.02	0.41
18:R:72:ARG:O	18:R:75:ILE:HG22	2.20	0.41
1:A:1096:C:H2'	1:A:1097:C:C6	2.56	0.41
1:A:1162:C:C2	1:A:1175:G:C2	3.09	0.41
1:A:333:G:H2'	1:A:334:C:C6	2.56	0.41
1:A:399:G:C6	1:A:400:C:C4	3.08	0.41
1:A:701:C:H1'	1:A:703:G:C5	2.56	0.41
1:A:786:G:C2	1:A:797:C:N3	2.89	0.41
1:A:895:G:C2	1:A:896:C:C2	3.09	0.41
2:B:16:HIS:HB3	2:B:17:PHE:H	1.76	0.41
3:C:83:ARG:O	3:C:87:LEU:HG	2.21	0.41
5:E:95:ALA:O	5:E:98:THR:OG1	2.39	0.41
11:K:10:VAL:C	11:K:12:ARG:H	2.23	0.41
11:K:31:THR:HG23	11:K:42:TRP:HB3	2.02	0.41
14:N:27:CYS:SG	14:N:28:GLY:N	2.94	0.41
22:W:37:SER:HB2	22:W:67:ILE:O	2.20	0.41
23:X:123:ARG:HB3	23:X:124:GLY:H	1.69	0.41
25:Z:2:G:N3	25:Z:3:C:C6	2.89	0.41
1:A:1243:C:C2	1:A:1295:G:C2	3.09	0.40
1:A:1247:U:H1'	1:A:1291:G:N2	2.36	0.40
1:A:13:U:H5'	1:A:14:U:H5	1.85	0.40
1:A:865:A:H2'	1:A:866:C:C6	2.56	0.40
3:C:29:TYR:CE1	3:C:33:LEU:HD13	2.51	0.40
4:D:117:ALA:O	4:D:121:VAL:HG23	2.22	0.40
1:A:1291:G:H4'	9:I:38:GLN:O	2.21	0.40
9:I:33:PHE:CZ	9:I:47:LEU:HG	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1119:C:H2'	1:A:1120:G:C8	2.56	0.40
1:A:1431:C:N3	1:A:1470:G:C2	2.90	0.40
1:A:146:G:C2	1:A:177:C:C2	3.10	0.40
1:A:37:U:O2'	1:A:500:G:H4'	2.20	0.40
1:A:599:C:H2'	1:A:600:C:C6	2.56	0.40
1:A:943:U:H2'	1:A:944:G:C8	2.56	0.40
2:B:212:GLN:HG3	2:B:239:VAL:HG23	2.03	0.40
4:D:33:MET:O	4:D:36:ARG:O	2.37	0.40
12:L:82:VAL:HG12	12:L:105:TYR:HB3	2.02	0.40
16:P:33:ILE:H	16:P:33:ILE:HG13	1.76	0.40
18:R:42:ARG:NH1	18:R:42:ARG:HB3	2.36	0.40
19:S:5:LEU:HD13	19:S:10:PHE:H	1.85	0.40
25:Z:58:A:H2	25:Z:60:U:H2'	1.85	0.40
1:A:1000:U:C3'	1:A:1000:U:C6	3.04	0.40
1:A:1145:C:HO2'	1:A:1146:A:C5'	2.34	0.40
1:A:931:C:O2	1:A:1387:G:C2	2.75	0.40
1:A:1518:A:H2'	1:A:1519:A:H8	1.83	0.40
1:A:1526:G:C6	1:A:1527:C:C4	3.09	0.40
1:A:148:G:C2	1:A:175:C:C2	3.09	0.40
1:A:482:A:C2	1:A:483:C:H1'	2.56	0.40
1:A:548:G:C6	1:A:549:C:C4	3.10	0.40
1:A:922:G:C2	1:A:923:A:C4	3.09	0.40
1:A:929:G:C6	1:A:930:C:C4	3.10	0.40
1:A:939:G:C2	1:A:940:C:N3	2.89	0.40
3:C:20:SER:HB3	3:C:22:TRP:NE1	2.36	0.40
3:C:54:ARG:HB2	3:C:69:HIS:HB2	2.02	0.40
4:D:196:LEU:HA	4:D:197:PRO:HD2	1.84	0.40
10:J:61:GLU:OE2	14:N:58:LYS:HG2	2.20	0.40
23:X:11:ILE:HG12	23:X:47:LEU:CB	2.51	0.40
1:A:1023:G:N3	1:A:1023:G:H2'	2.35	0.40
1:A:1121:U:H2'	1:A:1122:U:C6	2.57	0.40
1:A:112:G:P	16:P:27:LYS:HG2	2.62	0.40
1:A:1242:C:H4'	1:A:1304:G:OP1	2.22	0.40
1:A:1317:C:H42	19:S:37:ARG:HH22	1.69	0.40
1:A:1489:G:C2	1:A:1490:C:C2	3.10	0.40
1:A:489:C:H2'	1:A:490:G:C8	2.56	0.40
1:A:778:G:H2'	1:A:779:C:O4'	2.20	0.40
1:A:76:C:C3'	1:A:77:G:H5'	2.51	0.40
1:A:966:G:C6	1:A:967:C:N3	2.89	0.40
5:E:127:ASN:O	5:E:128:PRO:C	2.59	0.40
8:H:10:LEU:HD12	8:H:85:ARG:HB2	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:51:ARG:CD	10:J:59:SER:HB3	2.48	0.40
10:J:8:LEU:HG	10:J:96:ILE:HG23	2.03	0.40
16:P:49:LEU:HD13	16:P:73:LEU:HD22	2.04	0.40
18:R:21:LYS:HG2	18:R:57:GLY:HA3	2.04	0.40
25:Z:7:G:C6	25:Z:49:G:C8	3.09	0.40
1:A:1184:G:H2'	1:A:1185:G:H8	1.87	0.40
1:A:1276:G:H2'	1:A:1277:C:O4'	2.22	0.40
1:A:1389:C:H2'	1:A:1390:U:O4'	2.21	0.40
1:A:1461:G:H2'	1:A:1462:G:C8	2.57	0.40
1:A:230:G:H2'	1:A:231:G:O4'	2.21	0.40
1:A:306:G:N2	1:A:307:C:C2	2.89	0.40
1:A:369:C:C2	1:A:393:A:C2	3.10	0.40
1:A:577:G:N1	1:A:578:C:C4	2.89	0.40
1:A:761:G:C5	1:A:762:C:C4	3.09	0.40
1:A:914:A:H2'	1:A:915:A:C8	2.55	0.40
2:B:208:ILE:HG13	2:B:208:ILE:H	1.45	0.40
13:M:94:ARG:HB3	13:M:96:LEU:HD12	2.04	0.40
1:A:1539:C:N4	24:Y:26:G:H1	2.15	0.40
1:A:1536:C:H42	24:Y:29:G:H1	1.69	0.40
25:Z:53:G:H2'	25:Z:54:5MU:H6	1.86	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	
2	B	232/256 (91%)	187 (81%)	33 (14%)	12 (5%)	2	27
3	C	204/239 (85%)	176 (86%)	20 (10%)	8 (4%)	3	33
4	D	206/209 (99%)	185 (90%)	14 (7%)	7 (3%)	4	37
5	E	148/162 (91%)	134 (90%)	12 (8%)	2 (1%)	13	54

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
6	F	99/101 (98%)	90 (91%)	7 (7%)	2 (2%)	9	48
7	G	153/156 (98%)	134 (88%)	15 (10%)	4 (3%)	6	42
8	H	136/138 (99%)	122 (90%)	11 (8%)	3 (2%)	8	46
9	I	125/128 (98%)	106 (85%)	16 (13%)	3 (2%)	7	44
10	J	96/105 (91%)	74 (77%)	14 (15%)	8 (8%)	1	16
11	K	120/129 (93%)	100 (83%)	14 (12%)	6 (5%)	2	28
12	L	122/132 (92%)	99 (81%)	19 (16%)	4 (3%)	4	37
13	M	123/126 (98%)	105 (85%)	15 (12%)	3 (2%)	7	44
14	N	58/61 (95%)	49 (84%)	6 (10%)	3 (5%)	2	27
15	O	86/89 (97%)	79 (92%)	6 (7%)	1 (1%)	15	57
16	P	81/88 (92%)	73 (90%)	8 (10%)	0	100	100
17	Q	97/105 (92%)	87 (90%)	9 (9%)	1 (1%)	18	61
18	R	71/88 (81%)	64 (90%)	4 (6%)	3 (4%)	3	31
19	S	80/93 (86%)	59 (74%)	17 (21%)	4 (5%)	2	28
20	T	97/106 (92%)	84 (87%)	8 (8%)	5 (5%)	2	27
21	V	22/27 (82%)	19 (86%)	3 (14%)	0	100	100
22	W	69/72 (96%)	61 (88%)	6 (9%)	2 (3%)	5	40
23	X	166/171 (97%)	143 (86%)	15 (9%)	8 (5%)	2	29
All	All	2591/2781 (93%)	2230 (86%)	272 (10%)	89 (3%)	7	37

All (89) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	21	ARG
2	B	24	TRP
4	D	37	PRO
9	I	56	LEU
13	M	113	PRO
14	N	22	THR
20	T	49	ALA
22	W	70	ARG
23	X	8	ASN
23	X	54	PRO
23	X	94	ILE
4	D	5	ILE
4	D	26	CYS

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Mol	Chain	Res	Type
5	E	37	ARG
6	F	15	ASP
6	F	93	SER
10	J	39	PRO
10	J	55	LYS
11	K	11	LYS
11	K	12	ARG
13	M	124	PRO
14	N	14	PRO
18	R	76	LEU
19	S	5	LEU
22	W	2	LYS
23	X	47	LEU
23	X	82	ARG
23	X	83	THR
3	C	12	LEU
3	C	16	ARG
3	C	108	ASN
7	G	7	ALA
8	H	5	PRO
10	J	31	GLY
10	J	34	VAL
10	J	57	LYS
12	L	27	LEU
13	M	5	ALA
15	O	88	ARG
19	S	71	LEU
20	T	9	ASN
20	T	95	ALA
2	B	8	LYS
2	B	65	GLY
3	C	4	LYS
4	D	3	ARG
4	D	39	PRO
4	D	208	SER
7	G	149	ARG
8	H	55	GLY
9	I	54	ASP
10	J	40	LEU
10	J	54	PHE
10	J	82	ILE
11	K	14	VAL

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Mol	Chain	Res	Type
11	K	27	ASN
11	K	101	SER
12	L	28	LYS
12	L	51	ALA
17	Q	30	PRO
20	T	97	ALA
23	X	55	PRO
2	B	16	HIS
2	B	37	ASN
2	B	130	ARG
2	B	229	VAL
3	C	127	ARG
3	C	168	ALA
3	C	175	LEU
8	H	54	ASP
9	I	55	ALA
18	R	48	GLY
18	R	77	GLY
19	S	30	LEU
20	T	73	HIS
2	B	78	GLN
7	G	55	GLY
7	G	81	GLY
12	L	25	PRO
19	S	80	TYR
2	B	194	PRO
5	E	49	PRO
23	X	127	VAL
2	B	232	PRO
3	C	155	GLY
14	N	7	ILE
2	B	131	PRO
4	D	197	PRO
11	K	48	ILE

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	B	202/220 (92%)	148 (73%)	54 (27%)	0	5
3	C	160/188 (85%)	143 (89%)	17 (11%)	8	35
4	D	180/181 (99%)	141 (78%)	39 (22%)	1	8
5	E	115/123 (94%)	85 (74%)	30 (26%)	0	5
6	F	90/90 (100%)	71 (79%)	19 (21%)	1	9
7	G	126/127 (99%)	109 (86%)	17 (14%)	4	26
8	H	119/119 (100%)	90 (76%)	29 (24%)	1	6
9	I	98/99 (99%)	81 (83%)	17 (17%)	2	16
10	J	87/92 (95%)	65 (75%)	22 (25%)	0	6
11	K	92/99 (93%)	75 (82%)	17 (18%)	2	14
12	L	104/109 (95%)	85 (82%)	19 (18%)	2	14
13	M	100/101 (99%)	89 (89%)	11 (11%)	7	33
14	N	49/50 (98%)	37 (76%)	12 (24%)	1	6
15	O	79/80 (99%)	58 (73%)	21 (27%)	0	5
16	P	72/74 (97%)	56 (78%)	16 (22%)	1	8
17	Q	94/97 (97%)	84 (89%)	10 (11%)	8	35
18	R	64/77 (83%)	50 (78%)	14 (22%)	1	8
19	S	71/80 (89%)	56 (79%)	15 (21%)	1	9
20	T	76/82 (93%)	61 (80%)	15 (20%)	1	12
21	V	19/22 (86%)	16 (84%)	3 (16%)	3	21
22	W	62/63 (98%)	51 (82%)	11 (18%)	2	16
23	X	145/150 (97%)	122 (84%)	23 (16%)	3	20
All	All	2204/2323 (95%)	1773 (80%)	431 (20%)	4	12

All (431) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	8	LYS
2	B	10	LEU
2	B	16	HIS
2	B	21	ARG
2	B	23	ARG
2	B	24	TRP
2	B	30	ARG
2	B	32	ILE

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Mol	Chain	Res	Type
2	B	39	ILE
2	B	51	LEU
2	B	52	GLU
2	B	60	ASP
2	B	61	LEU
2	B	63	MET
2	B	67	THR
2	B	75	LYS
2	B	76	GLN
2	B	83	MET
2	B	95	GLN
2	B	96	ARG
2	B	98	LEU
2	B	103	THR
2	B	107	THR
2	B	114	ARG
2	B	121	LEU
2	B	122	PHE
2	B	124	SER
2	B	130	ARG
2	B	137	ARG
2	B	140	HIS
2	B	142	LEU
2	B	144	ARG
2	B	150	SER
2	B	152	PHE
2	B	153	ARG
2	B	156	LYS
2	B	165	VAL
2	B	168	THR
2	B	172	ILE
2	B	178	ARG
2	B	180	LEU
2	B	187	LEU
2	B	190	THR
2	B	195	ASP
2	B	198	ASP
2	B	204	ASN
2	B	205	ASP
2	B	208	ILE
2	B	211	ILE
2	B	215	LEU

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Mol	Chain	Res	Type
2	B	220	ASP
2	B	221	LEU
2	B	233	SER
2	B	235	SER
3	C	3	ASN
3	C	14	ILE
3	C	21	ARG
3	C	29	TYR
3	C	45	LYS
3	C	79	ARG
3	C	90	GLU
3	C	94	LEU
3	C	97	LYS
3	C	104	GLN
3	C	111	LEU
3	C	142	MET
3	C	167	TRP
3	C	188	LEU
3	C	190	ARG
3	C	191	THR
3	C	195	VAL
4	D	10	ARG
4	D	12	CYS
4	D	13	ARG
4	D	19	LEU
4	D	25	ARG
4	D	27	TYR
4	D	35	ARG
4	D	36	ARG
4	D	49	ARG
4	D	50	ARG
4	D	52	SER
4	D	53	ASP
4	D	59	ARG
4	D	61	LYS
4	D	66	ARG
4	D	70	ILE
4	D	72	GLU
4	D	74	GLN
4	D	76	ARG
4	D	78	LEU
4	D	85	LYS

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Mol	Chain	Res	Type
4	D	92	VAL
4	D	94	LEU
4	D	97	LEU
4	D	103	ASN
4	D	104	VAL
4	D	118	ARG
4	D	120	LEU
4	D	122	ARG
4	D	131	ARG
4	D	132	ARG
4	D	141	ARG
4	D	152	SER
4	D	159	ARG
4	D	162	LEU
4	D	165	MET
4	D	174	LEU
4	D	176	LEU
4	D	191	ARG
5	E	5	ASP
5	E	12	LEU
5	E	14	ARG
5	E	18	ARG
5	E	19	MET
5	E	24	ARG
5	E	27	ARG
5	E	32	VAL
5	E	34	VAL
5	E	36	ASP
5	E	41	VAL
5	E	63	ARG
5	E	64	ARG
5	E	68	GLU
5	E	71	LEU
5	E	73	ASN
5	E	76	ILE
5	E	80	ILE
5	E	98	THR
5	E	105	VAL
5	E	112	LEU
5	E	118	ILE
5	E	119	LEU
5	E	126	ARG

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Mol	Chain	Res	Type
5	E	135	THR
5	E	136	MET
5	E	140	ARG
5	E	142	LEU
5	E	147	ASP
5	E	150	ARG
6	F	9	VAL
6	F	10	LEU
6	F	15	ASP
6	F	19	LEU
6	F	28	ARG
6	F	31	GLU
6	F	36	ARG
6	F	38	GLU
6	F	39	LYS
6	F	40	VAL
6	F	42	GLU
6	F	54	LYS
6	F	61	LEU
6	F	75	LEU
6	F	77	ARG
6	F	78	GLU
6	F	83	ASP
6	F	86	ARG
6	F	95	GLU
7	G	8	GLU
7	G	10	ARG
7	G	16	LEU
7	G	22	LEU
7	G	37	ASN
7	G	62	PHE
7	G	67	GLU
7	G	72	ARG
7	G	74	GLU
7	G	79	ARG
7	G	80	VAL
7	G	94	ARG
7	G	99	LEU
7	G	106	GLN
7	G	136	LYS
7	G	146	GLU
7	G	156	TRP

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Mol	Chain	Res	Type
8	H	2	LEU
8	H	14	ARG
8	H	18	ARG
8	H	23	SER
8	H	29	SER
8	H	31	PHE
8	H	39	LEU
8	H	41	ARG
8	H	50	ARG
8	H	53	VAL
8	H	56	LYS
8	H	59	LEU
8	H	63	LEU
8	H	69	ARG
8	H	70	GLN
8	H	75	ARG
8	H	84	ARG
8	H	85	ARG
8	H	92	ARG
8	H	104	ARG
8	H	105	ARG
8	H	112	LEU
8	H	115	SER
8	H	120	THR
8	H	121	ASP
8	H	122	ARG
8	H	123	GLU
8	H	127	LEU
8	H	134	ILE
9	I	14	VAL
9	I	32	ASP
9	I	38	GLN
9	I	42	ARG
9	I	48	GLU
9	I	56	LEU
9	I	60	ASP
9	I	64	THR
9	I	78	LYS
9	I	85	LEU
9	I	87	GLN
9	I	102	LEU
9	I	104	ARG

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Mol	Chain	Res	Type
9	I	109	VAL
9	I	111	ARG
9	I	121	ARG
9	I	127	LYS
10	J	4	ILE
10	J	8	LEU
10	J	16	LEU
10	J	17	ASP
10	J	19	SER
10	J	35	SER
10	J	40	LEU
10	J	42	THR
10	J	48	THR
10	J	49	VAL
10	J	51	ARG
10	J	57	LYS
10	J	60	ARG
10	J	61	GLU
10	J	66	ARG
10	J	70	ARG
10	J	73	ASP
10	J	74	ILE
10	J	82	ILE
10	J	87	THR
10	J	96	ILE
10	J	99	LYS
11	K	13	GLN
11	K	18	ARG
11	K	25	TYR
11	K	34	ASP
11	K	40	ILE
11	K	41	THR
11	K	48	ILE
11	K	53	SER
11	K	63	LEU
11	K	77	MET
11	K	78	GLN
11	K	84	VAL
11	K	91	ARG
11	K	93	GLN
11	K	96	ARG
11	K	116	HIS

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Mol	Chain	Res	Type
11	K	117	ASN
12	L	6	THR
12	L	10	LEU
12	L	17	LYS
12	L	19	ARG
12	L	34	ARG
12	L	42	THR
12	L	46	LYS
12	L	50	SER
12	L	53	ARG
12	L	59	ARG
12	L	60	LEU
12	L	62	SER
12	L	65	GLU
12	L	79	GLU
12	L	92	ASP
12	L	100	ILE
12	L	112	ASP
12	L	116	SER
12	L	117	ARG
13	M	9	ILE
13	M	12	ASN
13	M	15	VAL
13	M	39	ILE
13	M	44	ARG
13	M	46	LYS
13	M	66	LEU
13	M	83	ASP
13	M	102	ARG
13	M	110	ARG
13	M	115	LYS
14	N	9	LYS
14	N	12	ARG
14	N	15	LYS
14	N	17	LYS
14	N	29	ARG
14	N	31	ARG
14	N	32	SER
14	N	33	VAL
14	N	40	CYS
14	N	44	LEU
14	N	46	GLU

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Mol	Chain	Res	Type
14	N	58	LYS
15	O	3	ILE
15	O	4	THR
15	O	9	GLN
15	O	13	GLN
15	O	17	ARG
15	O	21	ASP
15	O	34	LEU
15	O	37	ASN
15	O	43	LEU
15	O	52	SER
15	O	56	LEU
15	O	59	MET
15	O	60	VAL
15	O	63	ARG
15	O	65	ARG
15	O	70	LEU
15	O	71	GLN
15	O	77	ARG
15	O	85	LEU
15	O	87	ILE
15	O	88	ARG
16	P	5	ARG
16	P	28	ARG
16	P	36	ILE
16	P	40	ASP
16	P	44	THR
16	P	45	THR
16	P	51	VAL
16	P	54	GLU
16	P	57	ARG
16	P	60	LEU
16	P	71	ARG
16	P	72	ARG
16	P	76	GLN
16	P	79	VAL
16	P	81	ARG
16	P	82	GLN
17	Q	6	LEU
17	Q	36	ILE
17	Q	55	ASP
17	Q	60	ILE

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Mol	Chain	Res	Type
17	Q	61	GLU
17	Q	63	ARG
17	Q	70	ARG
17	Q	92	ARG
17	Q	98	LEU
17	Q	100	LYS
18	R	18	ARG
18	R	21	LYS
18	R	28	GLU
18	R	36	ASN
18	R	37	VAL
18	R	38	GLU
18	R	41	LYS
18	R	42	ARG
18	R	44	LEU
18	R	53	ARG
18	R	55	ARG
18	R	75	ILE
18	R	86	VAL
18	R	87	ARG
19	S	5	LEU
19	S	7	LYS
19	S	12	ASP
19	S	15	LEU
19	S	17	GLU
19	S	19	VAL
19	S	22	LEU
19	S	29	ARG
19	S	38	SER
19	S	41	VAL
19	S	53	ASN
19	S	62	ILE
19	S	63	THR
19	S	77	THR
19	S	80	TYR
20	T	10	LEU
20	T	19	SER
20	T	23	ARG
20	T	24	LEU
20	T	27	LYS
20	T	31	SER
20	T	45	GLN

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Mol	Chain	Res	Type
20	T	53	LEU
20	T	57	ARG
20	T	62	LEU
20	T	63	ILE
20	T	68	LYS
20	T	73	HIS
20	T	74	LYS
20	T	84	LEU
21	V	6	ARG
21	V	8	THR
21	V	9	ARG
22	W	12	VAL
22	W	19	ASN
22	W	28	SER
22	W	32	ILE
22	W	41	ARG
22	W	52	ARG
22	W	54	VAL
22	W	58	THR
22	W	64	ARG
22	W	69	TYR
22	W	71	LYS
23	X	6	LEU
23	X	17	ARG
23	X	18	VAL
23	X	28	ILE
23	X	30	ASP
23	X	32	ARG
23	X	35	LEU
23	X	39	GLN
23	X	44	ASP
23	X	48	VAL
23	X	51	ASN
23	X	53	ASP
23	X	66	ARG
23	X	67	TYR
23	X	87	SER
23	X	92	VAL
23	X	98	ASP
23	X	118	VAL
23	X	125	ARG
23	X	127	VAL

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Mol	Chain	Res	Type
23	X	143	ASP
23	X	144	LEU
23	X	162	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (27) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	204	ASN
2	B	212	GLN
3	C	6	HIS
3	C	31	HIS
3	C	108	ASN
4	D	45	GLN
4	D	74	GLN
4	D	129	ASN
4	D	160	GLN
4	D	161	ASN
4	D	201	GLN
6	F	13	ASN
6	F	73	ASN
7	G	11	GLN
7	G	84	ASN
7	G	86	GLN
7	G	97	GLN
8	H	82	HIS
9	I	58	HIS
10	J	56	HIS
10	J	78	ASN
11	K	13	GLN
11	K	117	ASN
13	M	62	ASN
19	S	53	ASN
19	S	69	HIS
19	S	83	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	1506/1522 (98%)	394 (26%)	107 (7%)
24	Y	20/42 (47%)	8 (40%)	2 (10%)

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
25	Z	76/77 (98%)	51 (67%)	9 (11%)
All	All	1602/1641 (97%)	453 (28%)	118 (7%)

All (453) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	6	G
1	A	7	G
1	A	8	A
1	A	9	G
1	A	13	U
1	A	16	A
1	A	18	C
1	A	22	G
1	A	26	A
1	A	31	G
1	A	32	A
1	A	39	G
1	A	47	C
1	A	48	C
1	A	49	U
1	A	50	A
1	A	51	A
1	A	52	G
1	A	54	C
1	A	60	A
1	A	61	G
1	A	76	C
1	A	77	G
1	A	79	G
1	A	81	U
1	A	82	U
1	A	91	C
1	A	97	G
1	A	100	C
1	A	108	G
1	A	115	G
1	A	116	A
1	A	120	A
1	A	121	C
1	A	122	G
1	A	127	G

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Mol	Chain	Res	Type
1	A	129(A)	G
1	A	130	A
1	A	131	C
1	A	142	G
1	A	144	G
1	A	151	A
1	A	155	C
1	A	163	C
1	A	171	A
1	A	181	G
1	A	182	U
1	A	189(E)	U
1	A	189(F)	U
1	A	189(G)	G
1	A	189(H)	G
1	A	195	A
1	A	197	A
1	A	198	G
1	A	199	G
1	A	201	C
1	A	203	U
1	A	204	U
1	A	217	C
1	A	243	A
1	A	244	U
1	A	245	C
1	A	247	G
1	A	251	G
1	A	253	U
1	A	266	G
1	A	267	C
1	A	279	A
1	A	280	C
1	A	281	G
1	A	282	A
1	A	283	C
1	A	288	A
1	A	289	G
1	A	298	A
1	A	301	G
1	A	306	G
1	A	307	C

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Mol	Chain	Res	Type
1	A	315	A
1	A	316	G
1	A	321	A
1	A	324	G
1	A	328	C
1	A	329	A
1	A	330	C
1	A	332	G
1	A	344	A
1	A	345	C
1	A	347	G
1	A	350	G
1	A	351	G
1	A	352	C
1	A	353	A
1	A	366	C
1	A	367	U
1	A	371	G
1	A	372	C
1	A	373	A
1	A	378	G
1	A	384	G
1	A	386	C
1	A	392	G
1	A	397	A
1	A	398	C
1	A	406	G
1	A	409	G
1	A	412	A
1	A	413	G
1	A	415	A
1	A	421	U
1	A	422	C
1	A	423	G
1	A	424	G
1	A	428	G
1	A	429	U
1	A	430	A
1	A	439	A
1	A	442	C
1	A	448	A
1	A	450	G

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Mol	Chain	Res	Type
1	A	452	A
1	A	470	C
1	A	473	G
1	A	481	G
1	A	482	A
1	A	484	G
1	A	485	G
1	A	495	A
1	A	496	A
1	A	498	U
1	A	509	A
1	A	510	A
1	A	511	C
1	A	518	C
1	A	519	C
1	A	521	G
1	A	524	G
1	A	525	C
1	A	527	G
1	A	528	C
1	A	529	G
1	A	531	U
1	A	532	A
1	A	534	U
1	A	545	C
1	A	547	A
1	A	550	G
1	A	559	A
1	A	560	U
1	A	561	U
1	A	562	C
1	A	568	G
1	A	572	A
1	A	573	A
1	A	574	A
1	A	575	G
1	A	576	G
1	A	577	G
1	A	587	G
1	A	588	G
1	A	596	C
1	A	639	G

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Mol	Chain	Res	Type
1	A	642	A
1	A	653	A
1	A	661	G
1	A	665	A
1	A	671	G
1	A	672	U
1	A	686	U
1	A	687	A
1	A	688	G
1	A	693	G
1	A	694	A
1	A	701	C
1	A	702	A
1	A	703	G
1	A	717	C
1	A	721	G
1	A	723	U
1	A	731	G
1	A	733	A
1	A	734	G
1	A	748	C
1	A	749	C
1	A	755	G
1	A	759	A
1	A	774	G
1	A	777	A
1	A	785	G
1	A	789	U
1	A	792	A
1	A	793	U
1	A	794	A
1	A	804	U
1	A	812	C
1	A	813	U
1	A	815	A
1	A	817	C
1	A	820	U
1	A	821	G
1	A	828	A
1	A	839	U
1	A	840	C
1	A	841	U

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Mol	Chain	Res	Type
1	A	853	G
1	A	855	G
1	A	864	A
1	A	865	A
1	A	873	A
1	A	874	G
1	A	876	G
1	A	882	C
1	A	884	U
1	A	885	G
1	A	889	A
1	A	891	U
1	A	900	A
1	A	902	G
1	A	911	U
1	A	913	A
1	A	922	G
1	A	926	G
1	A	927	G
1	A	931	C
1	A	932	C
1	A	933	G
1	A	934	C
1	A	935	A
1	A	950	U
1	A	951	G
1	A	954	G
1	A	960	U
1	A	961	U
1	A	965	A
1	A	966	G
1	A	968	A
1	A	969	A
1	A	971	G
1	A	972	C
1	A	974	A
1	A	975	A
1	A	976	G
1	A	977	A
1	A	982	U
1	A	986	A
1	A	991	U

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Mol	Chain	Res	Type
1	A	992	U
1	A	993	G
1	A	994	A
1	A	1001	A
1	A	1014	A
1	A	1023	G
1	A	1025	U
1	A	1026	G
1	A	1028	C
1	A	1029	C
1	A	1030	C
1	A	1031	G
1	A	1045	C
1	A	1046	A
1	A	1050	G
1	A	1053	G
1	A	1054	C
1	A	1056	U
1	A	1060	C
1	A	1065	U
1	A	1066	C
1	A	1067	A
1	A	1068	G
1	A	1070	U
1	A	1076	C
1	A	1078	U
1	A	1084	G
1	A	1085	U
1	A	1089	G
1	A	1094	G
1	A	1095	U
1	A	1101	A
1	A	1102	A
1	A	1104	G
1	A	1117	G
1	A	1118	C
1	A	1124	G
1	A	1125	U
1	A	1126	U
1	A	1127	G
1	A	1128	C
1	A	1129	C

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Mol	Chain	Res	Type
1	A	1130	A
1	A	1131	G
1	A	1135	U
1	A	1136	U
1	A	1137	C
1	A	1138	G
1	A	1139	G
1	A	1140	C
1	A	1145	C
1	A	1146	A
1	A	1152	A
1	A	1157	A
1	A	1159	U
1	A	1160	G
1	A	1183	A
1	A	1184	G
1	A	1190	G
1	A	1191	A
1	A	1196	U
1	A	1197	G
1	A	1200	C
1	A	1201	A
1	A	1202	G
1	A	1211	U
1	A	1212	U
1	A	1213	A
1	A	1214	C
1	A	1215	G
1	A	1218	C
1	A	1225	A
1	A	1226	C
1	A	1227	A
1	A	1228	C
1	A	1236	A
1	A	1238	A
1	A	1248	A
1	A	1249	C
1	A	1250	A
1	A	1253	G
1	A	1257	U
1	A	1258	G
1	A	1260	C

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Mol	Chain	Res	Type
1	A	1270	C
1	A	1277	C
1	A	1279	A
1	A	1280	A
1	A	1281	U
1	A	1285	A
1	A	1286	A
1	A	1287	A
1	A	1300	G
1	A	1301	U
1	A	1302	U
1	A	1303	C
1	A	1304	G
1	A	1305	G
1	A	1316	G
1	A	1317	C
1	A	1318	A
1	A	1319	A
1	A	1321	C
1	A	1322	C
1	A	1324	A
1	A	1332	A
1	A	1335	C
1	A	1336	C
1	A	1340	A
1	A	1345	U
1	A	1346	A
1	A	1347	G
1	A	1348	U
1	A	1353	G
1	A	1360	A
1	A	1362	C
1	A	1363	C
1	A	1363(A)	A
1	A	1364	U
1	A	1370	G
1	A	1379	G
1	A	1381	U
1	A	1394	A
1	A	1398	A
1	A	1402	C
1	A	1433	A

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Mol	Chain	Res	Type
1	A	1442	G
1	A	1442(A)	G
1	A	1443	G
1	A	1447	A
1	A	1452	C
1	A	1456	G
1	A	1475	G
1	A	1477	C
1	A	1492	A
1	A	1494	G
1	A	1499	A
1	A	1502	A
1	A	1503	A
1	A	1504	G
1	A	1505	G
1	A	1506	U
1	A	1507	A
1	A	1517	G
1	A	1520	G
1	A	1529	G
1	A	1530	G
1	A	1535	C
24	Y	28	A
24	Y	30	G
24	Y	31	U
24	Y	33	A
24	Y	34	A
24	Y	36	A
24	Y	38	G
24	Y	39	U
25	Z	4	G
25	Z	5	G
25	Z	6	G
25	Z	9	G
25	Z	10	G
25	Z	13	C
25	Z	14	A
25	Z	15	G
25	Z	16	C
25	Z	17	C
25	Z	17(A)	U
25	Z	18	G

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Mol	Chain	Res	Type
25	Z	19	G
25	Z	20	U
25	Z	21	A
25	Z	22	G
25	Z	27	U
25	Z	31	G
25	Z	33	U
25	Z	34	C
25	Z	35	A
25	Z	36	U
25	Z	37	A
25	Z	38	A
25	Z	39	C
25	Z	40	C
25	Z	41	C
25	Z	42	G
25	Z	43	A
25	Z	44	A
25	Z	45	G
25	Z	46	G7M
25	Z	47	U
25	Z	48	C
25	Z	49	G
25	Z	53	G
25	Z	55	PSU
25	Z	56	C
25	Z	58	A
25	Z	59	A
25	Z	60	U
25	Z	61	C
25	Z	63	G
25	Z	65	C
25	Z	66	C
25	Z	67	C
25	Z	68	C
25	Z	70	G
25	Z	73	A
25	Z	75	C
25	Z	76	A

All (118) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	7	G
1	A	30	U
1	A	48	C
1	A	49	U
1	A	51	A
1	A	60	A
1	A	73	G
1	A	81	U
1	A	115	G
1	A	119	A
1	A	129(A)	G
1	A	157	G
1	A	181	G
1	A	197	A
1	A	202	U
1	A	243	A
1	A	250	A
1	A	266	G
1	A	279	A
1	A	281	G
1	A	328	C
1	A	329	A
1	A	344	A
1	A	351	G
1	A	366	C
1	A	372	C
1	A	421	U
1	A	422	C
1	A	428	G
1	A	429	U
1	A	481	G
1	A	484	G
1	A	495	A
1	A	496	A
1	A	509	A
1	A	518	C
1	A	532	A
1	A	559	A
1	A	560	U
1	A	575	G
1	A	576	G
1	A	587	G
1	A	641	U

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Mol	Chain	Res	Type
1	A	687	A
1	A	701	C
1	A	702	A
1	A	703	G
1	A	717	C
1	A	748	C
1	A	792	A
1	A	809	G
1	A	812	C
1	A	840	C
1	A	864	A
1	A	872	A
1	A	884	U
1	A	960	U
1	A	965	A
1	A	974	A
1	A	975	A
1	A	982	U
1	A	988	G
1	A	992	U
1	A	993	G
1	A	1000	U
1	A	1001	A
1	A	1032	G
1	A	1049	U
1	A	1065	U
1	A	1067	A
1	A	1101	A
1	A	1139	G
1	A	1145	C
1	A	1151	A
1	A	1182	G
1	A	1183	A
1	A	1190	G
1	A	1196	U
1	A	1201	A
1	A	1212	U
1	A	1213	A
1	A	1214	C
1	A	1226	C
1	A	1227	A
1	A	1239	A

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Mol	Chain	Res	Type
1	A	1257	U
1	A	1279	A
1	A	1280	A
1	A	1285	A
1	A	1300	G
1	A	1301	U
1	A	1331	G
1	A	1335	C
1	A	1345	U
1	A	1346	A
1	A	1347	G
1	A	1380	U
1	A	1397	C
1	A	1442(B)	A
1	A	1447	A
1	A	1493	A
1	A	1498	U
1	A	1503	A
1	A	1504	G
1	A	1520	G
1	A	1529	G
1	A	1534	A
24	Y	34	A
24	Y	38	G
25	Z	26	G
25	Z	35	A
25	Z	36	U
25	Z	37	A
25	Z	39	C
25	Z	40	C
25	Z	44	A
25	Z	58	A
25	Z	60	U

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

5 non-standard protein/DNA/RNA residues are 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$
25	OMC	Z	32	25	15,22,23	0.88	1 (6%)	19,31,34	1.15	1 (5%)
25	G7M	Z	46	25	19,26,27	2.79	3 (15%)	19,39,42	2.44	6 (31%)
25	5MU	Z	54	25	14,22,23	0.97	1 (7%)	16,32,35	3.10	4 (25%)
25	PSU	Z	55	25	16,21,22	0.85	0	20,30,33	3.70	8 (40%)
25	4SU	Z	8	25	14,21,22	1.36	2 (14%)	15,30,33	2.08	5 (33%)

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
25	OMC	Z	32	25	-	0/5/27/28	0/2/2/2
25	G7M	Z	46	25	-	0/3/25/26	0/3/3/3
25	5MU	Z	54	25	-	0/3/25/26	0/2/2/2
25	PSU	Z	55	25	-	0/7/25/26	0/2/2/2
25	4SU	Z	8	25	-	0/3/25/26	0/2/2/2

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	Z	8	4SU	C4-S4	-3.58	1.60	1.67
25	Z	8	4SU	O4'-C1'	2.23	1.44	1.41
25	Z	32	OMC	O4'-C1'	2.43	1.44	1.41
25	Z	54	5MU	O4'-C1'	2.78	1.45	1.41
25	Z	46	G7M	C6-C5	4.43	1.49	1.41
25	Z	46	G7M	C8-N7	6.95	1.45	1.33
25	Z	46	G7M	C8-N9	8.28	1.48	1.33

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	Z	55	PSU	N1-C2-N3	-9.79	121.36	128.40
25	Z	55	PSU	C5-C4-N3	-8.50	118.45	125.43
25	Z	54	5MU	C5-C4-N3	-6.39	118.20	125.24
25	Z	46	G7M	C5-C6-N1	-5.65	115.44	123.48
25	Z	8	4SU	C5-C4-N3	-3.78	118.95	123.73
25	Z	8	4SU	C6-N1-C2	-3.41	115.75	121.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	Z	46	G7M	N3-C2-N1	-2.94	123.16	127.46
25	Z	46	G7M	CN7-N7-C8	-2.78	112.25	125.45
25	Z	55	PSU	C5-C1'-C2'	-2.66	110.97	115.55
25	Z	55	PSU	C5-C6-N1	-2.29	121.42	124.39
25	Z	54	5MU	O4'-C4'-C5'	2.03	116.24	109.40
25	Z	46	G7M	O4'-C4'-C3'	2.04	109.22	105.17
25	Z	8	4SU	C4'-O4'-C1'	2.04	111.94	109.77
25	Z	55	PSU	O4'-C1'-C5	2.27	113.44	109.93
25	Z	8	4SU	O4'-C1'-N1	2.30	112.69	108.08
25	Z	54	5MU	O4'-C1'-N1	2.34	112.77	108.08
25	Z	55	PSU	C3'-C2'-C1'	2.73	105.08	101.93
25	Z	32	OMC	O4'-C1'-N1	2.79	113.67	108.08
25	Z	55	PSU	C6-N1-C2	3.81	121.45	115.36
25	Z	46	G7M	C2-N3-C4	4.44	120.34	115.16
25	Z	8	4SU	C2-N3-C4	4.85	122.26	115.11
25	Z	46	G7M	C6-N1-C2	5.23	123.59	116.06
25	Z	55	PSU	C4-N3-C2	7.33	121.57	115.16
25	Z	54	5MU	C4-N3-C2	9.46	123.44	115.16

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
25	Z	46	G7M	4	0
25	Z	54	5MU	2	0
25	Z	55	PSU	1	0
25	Z	8	4SU	1	0

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 66 ligands modelled in this entry, 66 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	6

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	84:U	O3'	88:A	P	4.82
1	A	93:G	O3'	96:U	P	4.82
1	A	841:U	O3'	848:C	P	4.25
1	A	204:U	O3'	216:G	P	3.81
1	A	1442(A):G	O3'	1442(B):A	P	3.32
1	A	927:G	O3'	928:G	P	3.10