



wwPDB EM Map/Model Validation Report ⓘ

Sep 27, 2016 – 03:39 PM EDT

PDB ID : 5LMR
EMDB ID: : EMD-4077
Title : Structure of bacterial 30S-IF1-IF3-mRNA-tRNA translation pre-initiation complex(state-2B)
Authors : Hussain, T.; Llacer, J.L.; Wimberly, B.T.; Ramakrishnan, V.
Deposited on : 2016-08-01
Resolution : 4.45 Å(reported)

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

MolProbity : 4.02b-467
Mogul : 1.7.1 (RC1), CSD as537be (2016)
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20027939

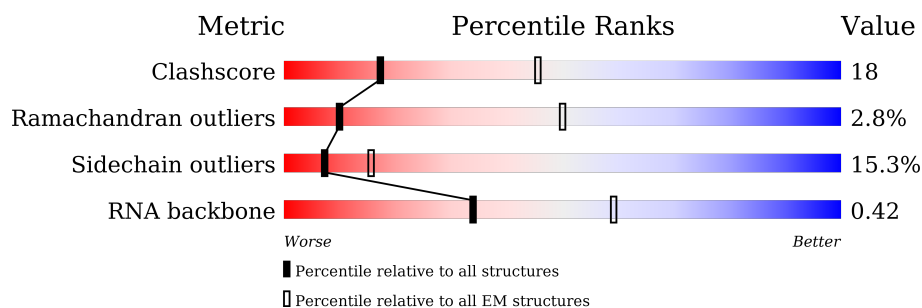
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.45 Å.

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














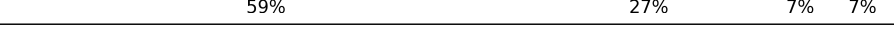





Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	114402	924
Ramachandran outliers	111179	726
Sidechain outliers	111093	686
RNA backbone	3027	244

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

Mol	Chain	Length	Quality of chain
1	A	1522	27% 55% 17% .
2	B	256	56% 30% 5% . 9%
3	C	239	46% 33% 7% 14%
4	D	209	57% 38% .
5	E	162	59% 27% 6% . 7%
6	F	101	66% 31% ..
7	G	156	73% 26% .
8	H	138	63% 31% 6%

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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
26	ZN	D	300	-	-	X	-

2 Entry composition

There are 27 unique types of molecules in this entry. The entry contains 55662 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	1515	Total	C	N	O	P	0	0
			32542	14490	6022	10519	1511		

- 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	S	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	119	Total	C	N	O	S	0	0
			885	549	168	165	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	121	Total	C	N	O	S	0	0
			964	597	199	166	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	17	Total	C	N	O	P	0	0
			373	166	74	116	17		

- Molecule 25 is a RNA chain called tRNAi.

Mol	Chain	Residues	Atoms						AltConf	Trace
25	Z	77	Total	C	N	O	P	S	0	0
			1646	735	297	536	77	1		

- Molecule 26 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

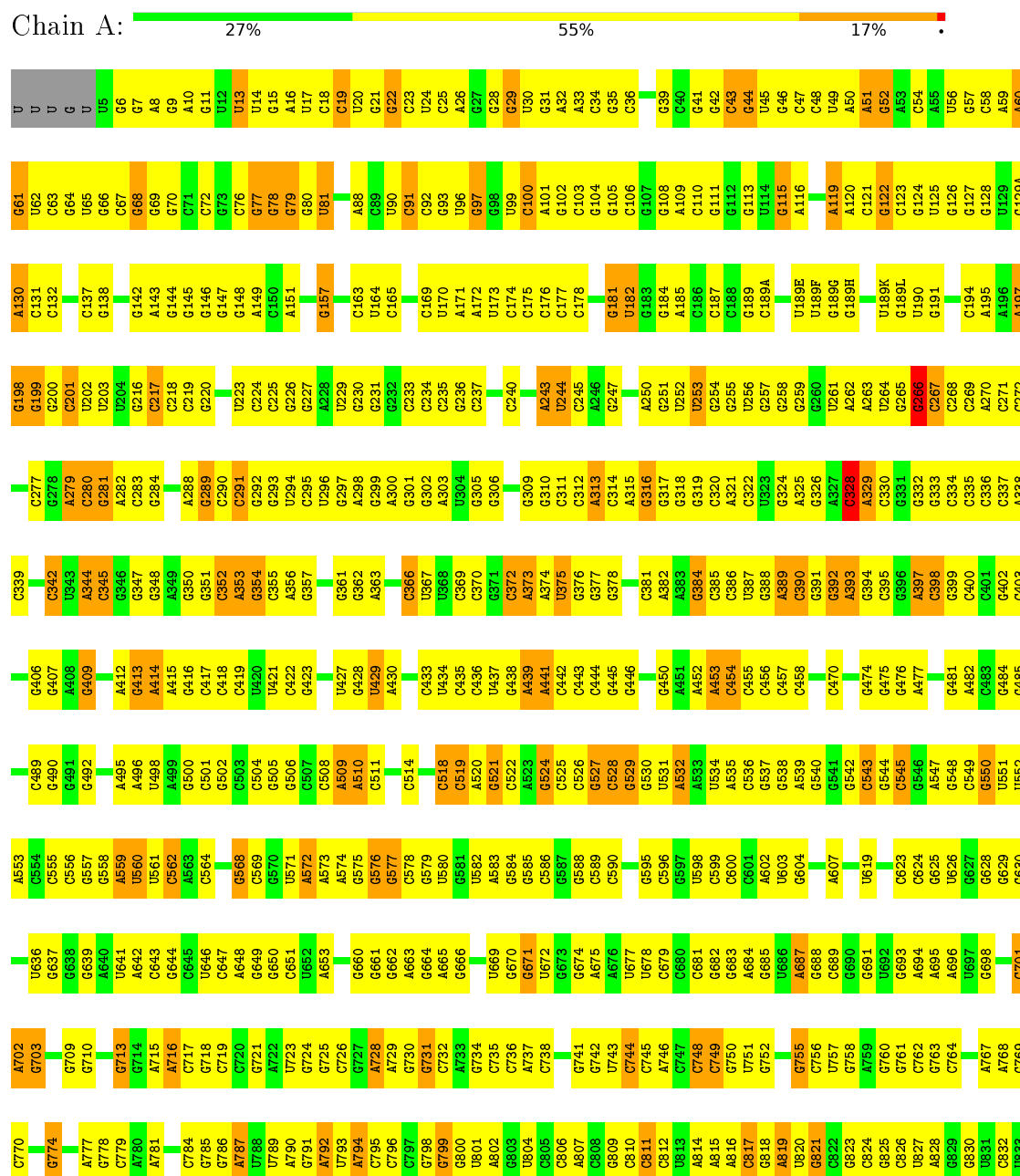
- Molecule 27 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
27	W	1	Total	Mg	0
			1	1	
27	Z	1	Total	Mg	0
			1	1	

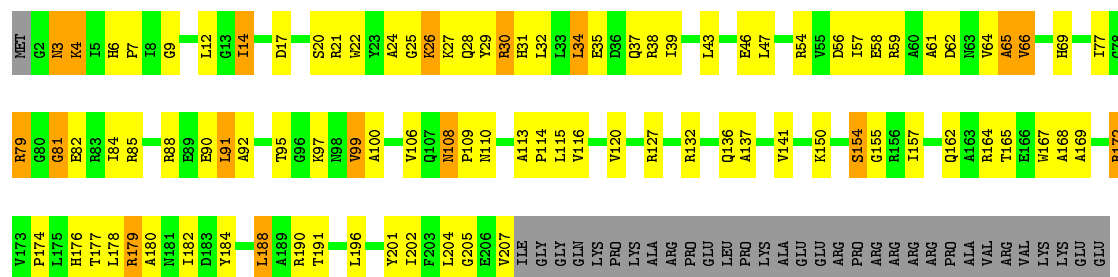
3 Residue-property plots

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

• Molecule 1: 16S rRNA

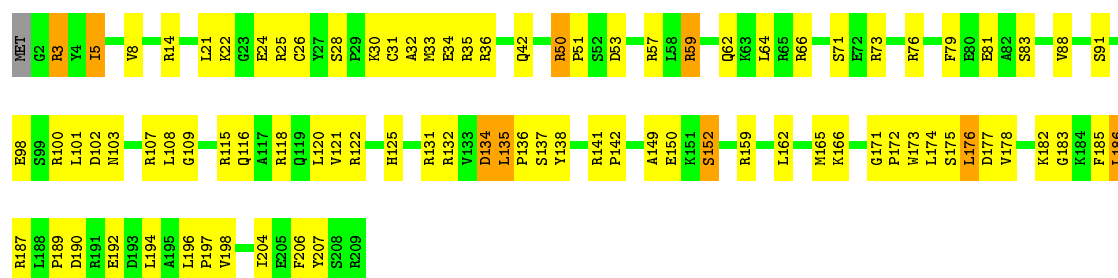


Chain C: 



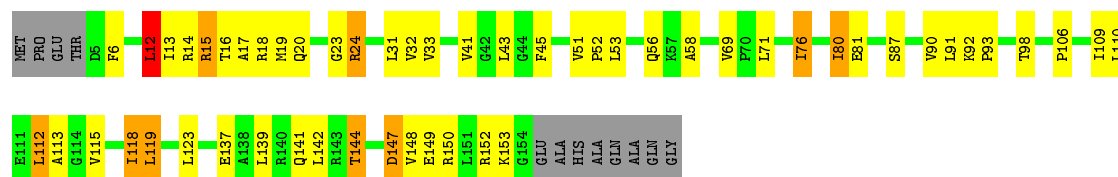
- Molecule 4: 30S ribosomal protein S4

Chain D: 



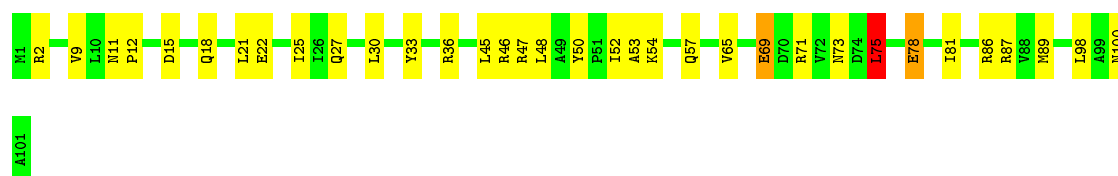
- Molecule 5: 30S ribosomal protein S5

Chain E: 



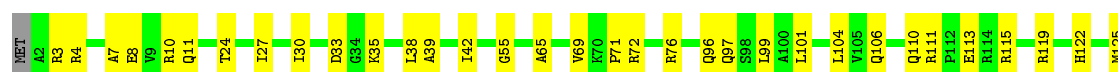
- Molecule 6: 30S ribosomal protein S6

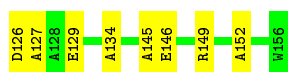
Chain F: 



- Molecule 7: 30S ribosomal protein S7

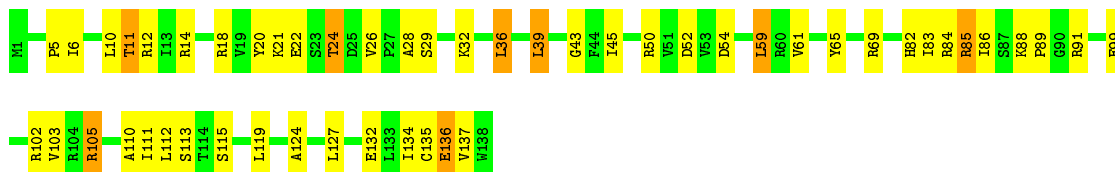
Chain G: 





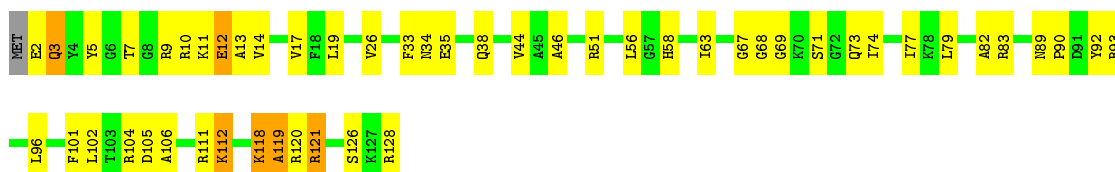
• Molecule 8: 30S ribosomal protein S8

Chain H: 63% 31% 6%



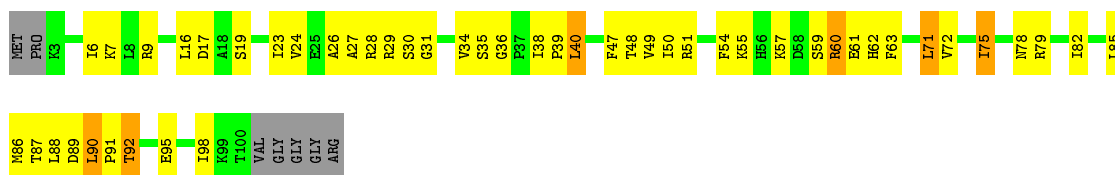
• Molecule 9: 30S ribosomal protein S9

Chain I: 59% 35% 5%



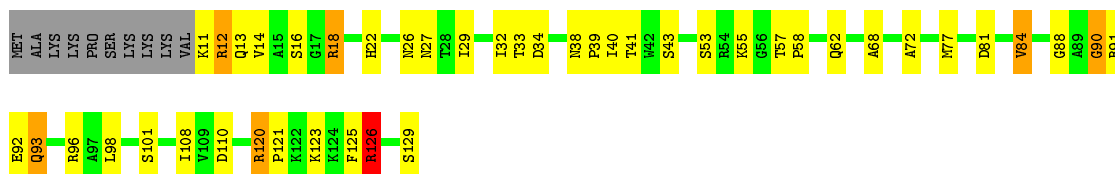
• Molecule 10: 30S ribosomal protein S10

Chain J: 47% 41% 6% 7%



• Molecule 11: 30S ribosomal protein S11

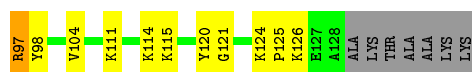
Chain K: 58% 29% 5% 8%



• Molecule 12: 30S ribosomal protein S12

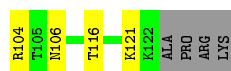
Chain L: 56% 33% 5% 6%





- Molecule 13: 30S ribosomal protein S13

Chain M: 63% 29%



- Molecule 14: 30S ribosomal protein S14 type Z

Chain N: 51% 44%



- Molecule 15: 30S ribosomal protein S15

Chain O: 63% 31%



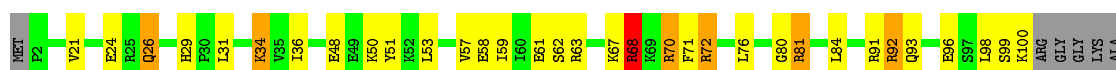
- Molecule 16: 30S ribosomal protein S16

Chain P: 59% 34% 6%



- Molecule 17: 30S ribosomal protein S17

Chain Q: 63% 25% 6% 6%



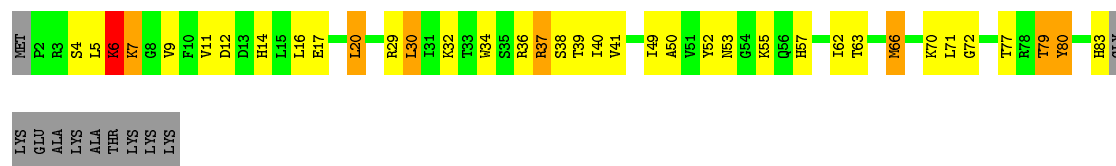
- Molecule 18: 30S ribosomal protein S18

Chain R: 50% 31% 17%



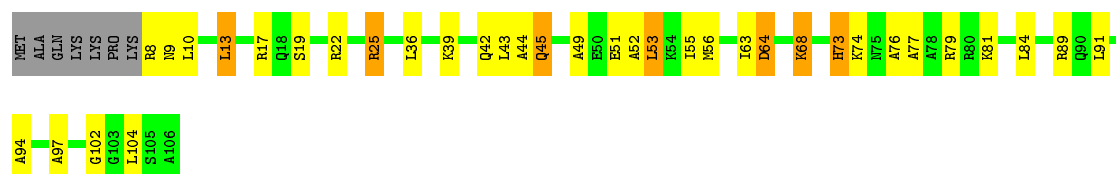
- Molecule 19: 30S ribosomal protein S19

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: 



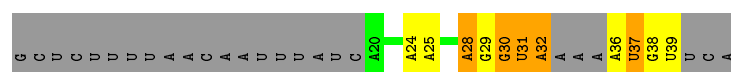
- Molecule 23: Translation initiation factor IF-3

Chain X: 




- Molecule 24: mRNA

Chain Y: 



- Molecule 25: tRNAi

Chain Z: 



4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of particles used	17176	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	Not provided	Depositor
Microscope	FEI POLARA 300	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	Not provided	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	3500	Depositor
Magnification	78000	Depositor
Image detector	Not provided	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	0.33	0/36416	0.73	13/56813 (0.0%)
10	J	0.48	0/805	0.80	2/1082 (0.2%)
11	K	0.47	0/900	0.82	0/1213
12	L	0.38	0/986	0.75	0/1320
13	M	0.45	0/974	0.78	1/1303 (0.1%)
14	N	0.41	0/501	0.82	1/664 (0.2%)
15	O	0.44	0/745	0.82	0/992
16	P	0.42	0/716	0.77	0/963
17	Q	0.40	0/836	0.75	0/1117
18	R	0.45	0/604	0.81	0/801
19	S	0.48	0/670	0.80	1/903 (0.1%)
2	B	0.51	0/1935	0.82	2/2609 (0.1%)
20	T	0.45	0/765	0.88	0/1007
21	V	0.48	0/212	0.75	0/277
22	W	0.53	0/580	0.90	1/782 (0.1%)
23	X	0.48	0/1375	0.78	0/1844
24	Y	0.43	0/418	0.69	0/649
25	Z	0.43	0/1719	0.86	2/2674 (0.1%)
3	C	0.44	0/1636	0.88	6/2205 (0.3%)
4	D	0.42	0/1733	0.78	0/2318
5	E	0.43	0/1162	0.89	3/1564 (0.2%)
6	F	0.43	0/856	0.78	1/1154 (0.1%)
7	G	0.44	0/1276	0.77	0/1709
8	H	0.40	0/1136	0.78	0/1527
9	I	0.42	0/1029	0.72	0/1379
All	All	0.38	0/59985	0.76	33/88869 (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
2	B	0	1
23	X	0	1
All	All	0	2

There are no bond length outliers.

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	65	ALA	CB-CA-C	-14.85	87.83	110.10
5	E	15	ARG	CB-CA-C	-12.38	85.65	110.40
22	W	23	ARG	N-CA-C	-11.78	79.19	111.00
5	E	15	ARG	N-CA-C	-8.75	87.37	111.00
3	C	66	VAL	N-CA-C	-8.72	87.46	111.00
10	J	61	GLU	N-CA-CB	-8.33	95.61	110.60
13	M	81	LEU	CA-CB-CG	8.13	134.00	115.30
1	A	1145	C	C2'-C3'-O3'	7.83	126.74	109.50
1	A	266	G	C2'-C3'-O3'	7.73	126.51	109.50
3	C	65	ALA	N-CA-C	-7.49	90.77	111.00
14	N	44	LEU	CA-CB-CG	7.28	132.05	115.30
1	A	1498	U	C2'-C3'-O3'	7.08	125.08	109.50
1	A	1190	G	C2'-C3'-O3'	7.04	125.00	109.50
3	C	34	LEU	CA-CB-CG	6.55	130.38	115.30
5	E	12	LEU	CA-CB-CG	6.50	130.25	115.30
25	Z	47	U	C2'-C3'-O3'	6.45	124.01	113.70
3	C	91	LEU	CA-CB-CG	6.43	130.10	115.30
1	A	1301	U	C2'-C3'-O3'	6.43	123.99	113.70
2	B	221	LEU	CA-CB-CG	6.25	129.68	115.30
1	A	687	A	C2'-C3'-O3'	6.17	123.57	113.70
6	F	75	LEU	CA-CB-CG	6.09	129.31	115.30
1	A	1346	A	C2'-C3'-O3'	5.90	123.14	113.70
1	A	1000	U	C2'-C3'-O3'	5.83	123.02	113.70
1	A	792	A	C2'-C3'-O3'	5.82	123.01	113.70
25	Z	36	U	C2'-C3'-O3'	5.69	122.80	113.70
1	A	328	C	C2'-C3'-O3'	5.63	122.70	113.70
1	A	281	G	C2'-C3'-O3'	5.60	122.66	113.70
10	J	88	LEU	CA-CB-CG	5.52	127.99	115.30
3	C	178	LEU	CA-CB-CG	5.45	127.84	115.30
1	A	965	A	C2'-C3'-O3'	5.44	122.41	113.70
2	B	187	LEU	CA-CB-CG	5.34	127.58	115.30
19	S	20	LEU	CA-CB-CG	5.31	127.52	115.30
1	A	1531	A	C2'-C3'-O3'	5.19	122.00	113.70

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	16	HIS	Peptide
23	X	53	ASP	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	32542	0	16447	1122	0
2	B	1900	0	1951	39	0
3	C	1612	0	1674	77	0
4	D	1703	0	1766	42	0
5	E	1146	0	1207	46	0
6	F	843	0	857	15	0
7	G	1257	0	1296	24	0
8	H	1116	0	1177	40	0
9	I	1010	0	1037	32	0
10	J	792	0	835	48	0
11	K	885	0	904	20	0
12	L	970	0	1057	32	0
13	M	964	0	1034	25	0
14	N	492	0	529	28	0
15	O	734	0	771	13	0
16	P	700	0	720	19	0
17	Q	823	0	891	20	0
18	R	598	0	670	17	0
19	S	655	0	672	35	0
20	T	763	0	861	17	0
21	V	208	0	221	3	0
22	W	570	0	599	25	0
23	X	1356	0	1401	15	0
24	Y	373	0	186	17	0
25	Z	1646	0	845	109	0
26	D	1	0	0	4	0
26	N	1	0	0	0	0
27	W	1	0	0	0	0
27	Z	1	0	0	0	0
All	All	55662	0	39608	1691	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 18.

All (1691) 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)
22:W:21:THR:CG2	22:W:33:LEU:HD11	1.53	1.36
10:J:7:LYS:HG3	10:J:71:LEU:CD2	1.55	1.33
1:A:1358:U:H3	1:A:1363(A):A:N6	1.36	1.24
1:A:1345:U:N3	1:A:1375:A:N6	1.87	1.21
5:E:93:PRO:HG3	8:H:105:ARG:NH2	1.53	1.20
9:I:5:TYR:CE2	9:I:7:THR:OG1	1.95	1.19
1:A:1358:U:O4	1:A:1363(A):A:N1	1.75	1.19
5:E:93:PRO:CG	8:H:105:ARG:NH2	2.05	1.18
22:W:21:THR:HG22	22:W:33:LEU:CD1	1.79	1.12
22:W:21:THR:HG21	22:W:33:LEU:HD11	1.24	1.11
10:J:7:LYS:HG3	10:J:71:LEU:HD21	1.18	1.11
1:A:92:C:H2'	1:A:93:G:C8	1.85	1.11
1:A:918:A:H2	1:A:1079:G:N2	1.46	1.11
1:A:1256:A:H3'	3:C:27:LYS:NZ	1.66	1.11
3:C:29:TYR:OH	14:N:54:PRO:HG2	1.50	1.09
1:A:92:C:H2'	1:A:93:G:H8	0.99	1.09
22:W:21:THR:CG2	22:W:33:LEU:CD1	2.31	1.07
10:J:7:LYS:CG	10:J:71:LEU:HD21	1.84	1.07
25:Z:1:C:H2'	25:Z:2:G:H8	1.14	1.06
5:E:93:PRO:CG	8:H:105:ARG:HH22	1.63	1.04
1:A:827:U:O4	1:A:872:A:N1	1.91	1.04
1:A:1532:U:H5''	1:A:1533:C:OP2	1.58	1.04
10:J:7:LYS:HG3	10:J:71:LEU:HD23	1.37	1.02
1:A:1256:A:H5''	3:C:27:LYS:CE	1.90	1.01
1:A:827:U:H3	1:A:872:A:N6	1.57	1.01
1:A:80:G:H3'	1:A:81:U:H5''	1.39	1.01
10:J:7:LYS:CG	10:J:71:LEU:CD2	2.39	1.00
1:A:1219:U:H2'	1:A:1220:G:C8	1.97	0.97
4:D:31:CYS:SG	26:D:300:ZN:ZN	1.54	0.97
10:J:40:LEU:HD11	10:J:71:LEU:HG	1.44	0.97
1:A:1074:G:H1'	2:B:104:ASN:HD21	1.27	0.95
16:P:59:TRP:O	16:P:62:VAL:CG2	2.14	0.94
1:A:864:A:H2'	1:A:865:A:C8	2.03	0.93
1:A:918:A:C2	1:A:1079:G:N2	2.33	0.93
1:A:827:U:N3	1:A:872:A:N6	2.13	0.93
3:C:28:GLN:HA	3:C:31:HIS:CD2	2.04	0.93
9:I:5:TYR:HE2	9:I:7:THR:OG1	1.40	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:918:A:H2	1:A:1079:G:H22	1.05	0.92
10:J:50:ILE:HG13	10:J:60:ARG:HD2	1.51	0.92
1:A:1492:A:H8	22:W:19:ASN:HB3	1.34	0.92
1:A:1227:A:C2	19:S:83:HIS:HB3	2.04	0.92
1:A:958:A:N1	19:S:55:LYS:HB2	1.85	0.92
3:C:92:ALA:O	3:C:95:THR:O	1.87	0.91
16:P:59:TRP:O	16:P:62:VAL:HG22	1.71	0.90
5:E:93:PRO:HG2	8:H:105:ARG:CZ	2.01	0.90
1:A:1358:U:N3	1:A:1363(A):A:N6	2.05	0.90
1:A:13:U:H5'	1:A:14:U:H5	1.38	0.89
1:A:1061:G:H5'	10:J:59:SER:OG	1.71	0.89
1:A:664:G:H22	1:A:741:G:H1	1.19	0.88
1:A:745:C:H2'	1:A:746:A:C8	2.08	0.88
1:A:1256:A:H5''	3:C:27:LYS:HE2	1.54	0.88
1:A:1071:C:H2'	1:A:1072:G:H8	1.38	0.88
1:A:1345:U:C2	1:A:1375:A:N6	2.41	0.88
1:A:1535:C:N3	1:A:1536:C:C5	2.42	0.88
25:Z:50:U:H2'	25:Z:51:C:C6	2.09	0.88
1:A:1000:U:H2'	1:A:1001:A:H1'	1.56	0.87
1:A:67:C:H2'	1:A:68:G:C8	2.09	0.87
10:J:62:HIS:HB3	14:N:59:ALA:HB3	1.56	0.87
3:C:30:ARG:NH1	14:N:35:ARG:O	2.06	0.87
9:I:82:ALA:HB1	9:I:96:LEU:HD21	1.57	0.87
1:A:1073:U:H3	1:A:1102:A:H61	1.24	0.86
1:A:1227:A:N1	19:S:83:HIS:HB3	1.89	0.86
1:A:966:G:C2	25:Z:34:C:H5'	2.10	0.86
25:Z:1:C:H2'	25:Z:2:G:C8	2.06	0.86
1:A:1530:G:H2'	1:A:1531:A:O4'	1.76	0.86
5:E:93:PRO:CB	8:H:105:ARG:HH22	1.89	0.85
1:A:1256:A:C3'	3:C:27:LYS:NZ	2.38	0.85
1:A:1227:A:C2	19:S:83:HIS:CB	2.59	0.85
1:A:1345:U:H3	1:A:1375:A:N6	1.72	0.85
1:A:1061:G:C5'	10:J:59:SER:OG	2.25	0.85
1:A:1077:G:N2	1:A:1079:G:H3'	1.92	0.85
5:E:93:PRO:CG	8:H:105:ARG:CZ	2.56	0.84
1:A:1101:A:H4'	1:A:1102:A:O5'	1.76	0.84
10:J:7:LYS:HA	10:J:71:LEU:HD22	1.60	0.84
9:I:5:TYR:CZ	9:I:7:THR:OG1	2.26	0.83
1:A:501:C:H2'	1:A:502:G:C8	2.14	0.83
1:A:920:U:H2'	1:A:921:U:C6	2.13	0.83
9:I:112:LYS:HG2	9:I:119:ALA:H	1.41	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:33:ARG:HD3	12:L:62:SER:HB3	1.59	0.83
1:A:1070:U:H2'	1:A:1071:C:C6	2.14	0.83
1:A:67:C:H2'	1:A:68:G:H8	1.43	0.82
1:A:1535:C:C4	1:A:1536:C:C5	2.68	0.82
1:A:1531:A:H2'	1:A:1532:U:O4'	1.79	0.82
1:A:1000:U:H2'	1:A:1001:A:C1'	2.09	0.82
1:A:17:U:H2'	1:A:18:C:C6	2.15	0.81
1:A:19:C:H2'	1:A:20:U:C6	2.15	0.81
1:A:1071:C:H2'	1:A:1072:G:C8	2.14	0.81
22:W:32:ILE:HB	22:W:63:THR:C	2.01	0.81
1:A:501:C:H2'	1:A:502:G:H8	1.43	0.80
1:A:674:G:H2'	1:A:675:A:H8	1.44	0.80
5:E:93:PRO:HG3	8:H:105:ARG:HH22	1.23	0.80
1:A:123:C:H2'	1:A:124:G:H8	1.46	0.80
1:A:958:A:C2	19:S:55:LYS:HB2	2.17	0.80
1:A:13:U:H5'	1:A:14:U:C5	2.16	0.80
25:Z:55:PSU:H3'	25:Z:56:C:H5''	1.63	0.80
1:A:1014:A:H4'	19:S:14:HIS:HB3	1.62	0.79
5:E:93:PRO:HB2	8:H:105:ARG:HH12	1.47	0.79
1:A:78:G:H2'	1:A:79:G:O4'	1.82	0.79
4:D:26:CYS:HG	26:D:300:ZN:ZN	0.94	0.79
25:Z:34:C:H2'	25:Z:35:A:C8	2.18	0.79
3:C:29:TYR:HD1	14:N:36:PHE:CE2	2.02	0.78
1:A:1492:A:C8	22:W:19:ASN:HB3	2.19	0.78
25:Z:3:C:H2'	25:Z:4:G:C8	2.18	0.78
2:B:72:GLY:HA3	2:B:81:VAL:HG21	1.66	0.78
25:Z:66:C:H2'	25:Z:67:C:O4'	1.82	0.78
1:A:24:U:H2'	1:A:25:C:C6	2.18	0.77
1:A:917:G:H2'	1:A:918:A:C8	2.18	0.77
3:C:9:GLY:HA2	3:C:12:LEU:HG	1.66	0.77
1:A:662:G:H2'	1:A:663:A:C8	2.19	0.77
25:Z:56:C:H2'	25:Z:57:A:C8	2.20	0.77
3:C:29:TYR:OH	14:N:54:PRO:CG	2.33	0.77
25:Z:39:C:H2'	25:Z:40:C:C6	2.20	0.77
1:A:1535:C:C2	1:A:1536:C:C6	2.73	0.76
1:A:745:C:H2'	1:A:746:A:H8	1.49	0.76
1:A:299:G:H2'	1:A:300:A:C8	2.21	0.76
4:D:26:CYS:SG	26:D:300:ZN:ZN	1.75	0.76
19:S:34:TRP:HA	19:S:52:TYR:HB2	1.68	0.76
5:E:93:PRO:HG2	8:H:105:ARG:NH1	2.01	0.76
10:J:40:LEU:HD11	10:J:71:LEU:CG	2.16	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:80:G:H3'	1:A:81:U:C5'	2.16	0.76
1:A:21:G:H2'	1:A:22:G:C8	2.21	0.75
1:A:1123:A:H4'	10:J:36:GLY:HA3	1.67	0.75
19:S:11:VAL:HA	19:S:38:SER:HB2	1.68	0.75
1:A:1296:C:H5'	13:M:14:ARG:HD2	1.69	0.75
1:A:316:G:H1	1:A:337:C:H42	1.33	0.74
1:A:1536:C:H1'	24:Y:30:G:H22	1.50	0.74
3:C:30:ARG:HB2	3:C:30:ARG:HH21	1.51	0.74
9:I:44:VAL:HG12	9:I:51:ARG:HH12	1.52	0.74
16:P:59:TRP:O	16:P:62:VAL:HG23	1.85	0.74
1:A:170:U:H2'	1:A:171:A:H8	1.52	0.74
1:A:543:C:H2'	1:A:544:G:H8	1.52	0.74
10:J:16:LEU:HA	10:J:19:SER:HB3	1.69	0.74
1:A:90:U:H2'	1:A:91:C:C6	2.23	0.73
1:A:977:A:N7	1:A:1223:C:H2'	2.03	0.73
1:A:966:G:N3	25:Z:34:C:H5'	2.03	0.73
1:A:1080:A:H5''	5:E:16:THR:HB	1.70	0.73
1:A:1218:C:H2'	1:A:1219:U:C6	2.22	0.73
1:A:524:G:C6	1:A:525:C:N4	2.57	0.73
1:A:1386:G:H2'	1:A:1387:G:H8	1.54	0.72
1:A:45:U:H2'	1:A:46:G:H8	1.53	0.72
1:A:1219:U:H2'	1:A:1220:G:H8	1.54	0.72
3:C:28:GLN:HA	3:C:31:HIS:NE2	2.04	0.72
11:K:58:PRO:HB2	11:K:93:GLN:HG3	1.71	0.72
1:A:1270:C:H2'	1:A:1271:G:H8	1.53	0.72
1:A:729:A:H2'	1:A:730:G:H8	1.55	0.72
10:J:6:ILE:HG22	10:J:98:ILE:HG12	1.71	0.72
4:D:25:ARG:HA	4:D:28:SER:HB3	1.70	0.72
18:R:86:VAL:O	18:R:87:ARG:HB2	1.88	0.72
1:A:1103:C:H2'	1:A:1104:G:O4'	1.89	0.71
1:A:69:G:H1	1:A:100:C:H42	1.38	0.71
3:C:174:PRO:HB2	3:C:177:THR:HG22	1.72	0.71
22:W:21:THR:HG22	22:W:33:LEU:HD12	1.71	0.71
1:A:584:G:H2'	1:A:585:G:H8	1.56	0.71
3:C:29:TYR:CZ	14:N:54:PRO:HG2	2.24	0.71
1:A:45:U:H2'	1:A:46:G:C8	2.25	0.71
1:A:19:C:H2'	1:A:20:U:H6	1.53	0.71
1:A:78:G:O2'	1:A:79:G:O4'	2.07	0.71
3:C:77:ILE:HA	3:C:84:ILE:HB	1.73	0.71
23:X:90:PHE:HB2	23:X:120:ILE:HG12	1.72	0.71
1:A:584:G:H2'	1:A:585:G:C8	2.24	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:R:40:LEU:HB3	18:R:79:LEU:HD11	1.73	0.71
1:A:1000:U:H6	1:A:1000:U:H3'	1.55	0.71
1:A:1098:C:H1'	1:A:1168:A:H2	1.55	0.71
1:A:1359:C:H3'	14:N:35:ARG:NH2	2.05	0.70
1:A:1475:G:H2'	1:A:1476:G:H8	1.55	0.70
1:A:123:C:H2'	1:A:124:G:C8	2.26	0.70
1:A:1360:A:H8	1:A:1360:A:OP1	1.74	0.70
1:A:743:U:H2'	1:A:744:C:C6	2.26	0.70
2:B:130:ARG:HB3	2:B:131:PRO:HD2	1.73	0.70
1:A:1036:G:H2'	1:A:1037:C:O4'	1.92	0.70
1:A:1342:C:H2'	1:A:1343:G:C8	2.26	0.70
17:Q:81:ARG:HE	17:Q:84:LEU:HD12	1.55	0.70
24:Y:24:A:H2'	24:Y:25:A:H8	1.57	0.69
25:Z:48:C:H2'	25:Z:59:A:H4'	1.74	0.69
1:A:78:G:C2'	1:A:79:G:O4'	2.40	0.69
1:A:398:C:H2'	1:A:399:G:H8	1.56	0.69
1:A:1099:G:H5''	2:B:96:ARG:HE	1.58	0.69
4:D:101:LEU:HB2	4:D:138:TYR:HB3	1.74	0.69
1:A:1064:G:N2	1:A:1190:G:H2'	2.08	0.69
1:A:1280:A:H3'	1:A:1281:U:H5''	1.74	0.69
1:A:181:G:H4'	1:A:182:U:H5'	1.74	0.69
12:L:87:GLY:HA2	12:L:98:TYR:HA	1.75	0.69
1:A:1081:G:H5''	1:A:1081:G:C8	2.27	0.69
10:J:7:LYS:HA	10:J:71:LEU:CD2	2.23	0.69
1:A:536:C:H2'	1:A:537:G:C8	2.28	0.69
1:A:1264:C:H2'	1:A:1265:G:H8	1.58	0.68
25:Z:36:U:H2'	25:Z:37:A:H8	1.58	0.68
1:A:671:G:C2	1:A:736:C:N3	2.62	0.68
10:J:7:LYS:CB	10:J:71:LEU:HD21	2.22	0.68
1:A:10:A:H2'	1:A:11:G:C8	2.29	0.68
1:A:1234:C:H2'	1:A:1235:U:C6	2.28	0.68
1:A:718:G:H21	18:R:49:LYS:HE3	1.59	0.68
25:Z:50:U:N3	25:Z:51:C:N4	2.42	0.68
1:A:736:C:H2'	1:A:737:A:C8	2.27	0.68
3:C:62:ASP:HA	3:C:97:LYS:HD3	1.76	0.68
1:A:1346:A:H2'	7:G:10:ARG:HH22	1.59	0.68
1:A:662:G:H2'	1:A:663:A:H8	1.56	0.68
3:C:28:GLN:O	3:C:32:LEU:HG	1.94	0.68
3:C:29:TYR:CD1	14:N:36:PHE:CE2	2.82	0.68
1:A:398:C:H2'	1:A:399:G:C8	2.29	0.68
2:B:69:LEU:HB3	2:B:162:ILE:HG12	1.76	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:Z:35:A:H2'	25:Z:36:U:C6	2.28	0.68
1:A:1073:U:H3	1:A:1102:A:N6	1.91	0.67
1:A:16:A:C2	1:A:1080:A:H1'	2.29	0.67
1:A:1218:C:H2'	1:A:1219:U:H6	1.59	0.67
1:A:579:G:H5'	1:A:728:A:H1'	1.76	0.67
1:A:1103:C:H5''	2:B:98:LEU:HD23	1.76	0.67
1:A:701:C:H1'	1:A:703:G:C5	2.30	0.67
5:E:12:LEU:HG	5:E:31:LEU:HD12	1.77	0.67
1:A:1342:C:H2'	1:A:1343:G:H8	1.59	0.67
1:A:1264:C:H2'	1:A:1265:G:C8	2.30	0.67
3:C:30:ARG:NH2	14:N:35:ARG:O	2.26	0.67
1:A:1356:G:H2'	1:A:1357:A:C8	2.30	0.67
1:A:302:G:H2'	1:A:303:A:C8	2.30	0.67
1:A:524:G:C2	1:A:525:C:N3	2.62	0.67
1:A:1536:C:H1'	24:Y:30:G:N2	2.10	0.67
1:A:1384:C:H2'	1:A:1385:G:C8	2.29	0.67
15:O:75:PRO:O	15:O:79:ARG:HG3	1.95	0.67
1:A:457:C:H2'	1:A:458:C:C6	2.29	0.67
10:J:47:PHE:HB2	10:J:63:PHE:HB2	1.76	0.67
1:A:674:G:H2'	1:A:675:A:C8	2.30	0.66
1:A:1227:A:C2	19:S:83:HIS:HB2	2.30	0.66
22:W:15:GLU:HB3	22:W:23:ARG:HB2	1.76	0.66
1:A:956:U:O2'	19:S:80:TYR:HB3	1.95	0.66
1:A:1280:A:OP1	1:A:1281:U:H5	1.78	0.66
1:A:17:U:O2	1:A:1079:G:N2	2.29	0.66
1:A:6:G:H2'	5:E:119:LEU:HD21	1.76	0.66
7:G:39:ALA:HA	7:G:42:ILE:HD12	1.78	0.66
1:A:562:C:H41	1:A:884:U:H2'	1.61	0.66
1:A:1016:A:H2'	1:A:1017:G:O4'	1.95	0.65
3:C:20:SER:HB3	3:C:22:TRP:HE1	1.61	0.65
24:Y:28:A:H3'	24:Y:29:G:C8	2.32	0.65
1:A:101:A:H2'	1:A:102:G:H8	1.61	0.65
3:C:21:ARG:HG3	3:C:58:GLU:HG2	1.78	0.65
1:A:1438:G:N2	1:A:1439:C:C2	2.64	0.65
5:E:149:GLU:O	5:E:153:LYS:HB2	1.97	0.65
6:F:9:VAL:HB	6:F:87:ARG:HB2	1.78	0.65
1:A:1345:U:N3	1:A:1375:A:C6	2.63	0.65
8:H:105:ARG:HG2	8:H:105:ARG:NH2	2.10	0.65
12:L:27:LEU:HG	12:L:28:LYS:HG3	1.79	0.65
1:A:543:C:H2'	1:A:544:G:C8	2.31	0.65
1:A:671:G:N2	1:A:736:C:C2	2.64	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1442(A):G:H5''	1:A:1442(B):A:H5'	1.79	0.65
1:A:279:A:H5''	1:A:280:C:H3'	1.77	0.65
1:A:701:C:H4'	1:A:702:A:O5'	1.97	0.65
17:Q:67:LYS:O	17:Q:68:ARG:HB3	1.97	0.65
1:A:189(K):U:H2'	1:A:189(L):G:C8	2.32	0.65
1:A:814:A:H2'	1:A:816:A:H5''	1.78	0.65
1:A:1354:C:H2'	1:A:1355:G:H8	1.62	0.65
1:A:943:U:H2'	1:A:944:G:H8	1.62	0.65
1:A:998:G:N2	1:A:999:C:C2	2.65	0.65
22:W:32:ILE:HD11	22:W:55:VAL:HG11	1.79	0.65
1:A:1004:A:H5''	1:A:1025:U:C5	2.32	0.64
2:B:34:ALA:HB3	2:B:41:ILE:HD12	1.79	0.64
5:E:93:PRO:CB	8:H:105:ARG:HH12	2.09	0.64
6:F:52:ILE:HD11	18:R:77:GLY:HA3	1.78	0.64
1:A:1125:U:H5'	1:A:1126:U:H5	1.62	0.64
3:C:58:GLU:HB3	10:J:92:THR:HG21	1.78	0.64
10:J:50:ILE:CG1	10:J:60:ARG:HD2	2.26	0.64
1:A:1099:G:C6	1:A:1100:C:N3	2.65	0.64
1:A:1443:G:C6	1:A:1444:C:N4	2.66	0.64
1:A:79:G:H2'	1:A:80:G:H8	1.62	0.64
10:J:7:LYS:CB	10:J:71:LEU:CD2	2.76	0.64
25:Z:36:U:H2'	25:Z:37:A:C8	2.32	0.64
1:A:1105:A:H2'	1:A:1106:G:H8	1.62	0.64
1:A:266:G:C8	1:A:266:G:H5''	2.33	0.64
1:A:525:C:H2'	1:A:526:C:C6	2.33	0.64
1:A:61:G:H2'	1:A:62:U:O4'	1.98	0.64
1:A:1081:G:H2'	1:A:1082:G:C8	2.33	0.64
1:A:1392:G:N2	1:A:1502:A:H8	1.95	0.64
1:A:518:C:O2'	12:L:50:SER:HB3	1.97	0.64
4:D:176:LEU:HA	4:D:183:GLY:HA2	1.79	0.64
1:A:1074:G:C1'	2:B:104:ASN:HD21	2.06	0.64
19:S:6:LYS:HB2	19:S:7:LYS:HE3	1.80	0.64
1:A:988:G:N1	1:A:989:C:C2	2.67	0.63
1:A:1070:U:H2'	1:A:1071:C:H6	1.64	0.63
24:Y:28:A:H3'	24:Y:29:G:H8	1.62	0.63
1:A:1358:U:C4	1:A:1363(A):A:N1	2.62	0.63
1:A:880:C:H2'	1:A:881:G:H8	1.63	0.63
2:B:184:VAL:H	2:B:198:ASP:HB2	1.63	0.63
1:A:1081:G:H2'	1:A:1082:G:H8	1.64	0.63
1:A:1475:G:H2'	1:A:1476:G:C8	2.33	0.63
1:A:335:C:H2'	1:A:336:C:C6	2.33	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1128:C:H2'	1:A:1139:G:N7	2.13	0.63
1:A:926:G:H3'	1:A:1505:G:H21	1.63	0.63
13:M:10:PRO:HB2	13:M:18:ALA:HB1	1.80	0.63
1:A:919:A:C2	1:A:1080:A:H2	2.16	0.63
25:Z:51:C:H2'	25:Z:52:G:O4'	1.99	0.63
1:A:1391:U:H2'	1:A:1392:G:C8	2.33	0.63
1:A:1445:C:C2	1:A:1458:G:C2	2.87	0.63
1:A:1048:G:H5''	14:N:3:ARG:HG2	1.79	0.63
25:Z:52:G:C2	25:Z:63:G:C2	2.86	0.63
1:A:316:G:H1	1:A:337:C:N4	1.97	0.62
3:C:154:SER:HA	3:C:165:THR:HG23	1.79	0.62
1:A:1061:G:H5''	10:J:59:SER:OG	1.99	0.62
1:A:1125:U:H5'	1:A:1126:U:C5	2.34	0.62
1:A:920:U:H2'	1:A:921:U:H6	1.63	0.62
25:Z:49:G:C6	25:Z:50:U:C2	2.87	0.62
1:A:1535:C:N3	1:A:1536:C:C6	2.67	0.62
2:B:204:ASN:HB3	2:B:210:SER:OG	2.00	0.62
1:A:1354:C:H2'	1:A:1355:G:C8	2.34	0.62
12:L:25:PRO:C	12:L:27:LEU:H	2.01	0.62
1:A:877:C:H2'	1:A:878:G:H8	1.64	0.62
1:A:973:G:H3'	1:A:974:A:H5''	1.80	0.62
23:X:4:GLU:HA	23:X:66:ARG:HH12	1.64	0.62
1:A:1014:A:C2	19:S:34:TRP:CG	2.88	0.62
1:A:69:G:H1	1:A:100:C:N4	1.97	0.62
25:Z:33:U:O2	25:Z:36:U:H5	1.82	0.62
1:A:1256:A:N6	1:A:1278:U:C2	2.68	0.62
1:A:234:C:H2'	1:A:235:C:C6	2.34	0.62
10:J:7:LYS:CA	10:J:71:LEU:HD22	2.30	0.62
23:X:64:LYS:O	23:X:68:GLU:HG2	2.00	0.62
1:A:17:U:O2	1:A:1079:G:N3	2.32	0.62
1:A:1102:A:H2'	1:A:1103:C:C6	2.35	0.62
1:A:313:A:H2'	1:A:314:C:C6	2.34	0.62
3:C:108:ASN:HD21	3:C:110:ASN:HB2	1.65	0.62
1:A:1014:A:C2	19:S:34:TRP:CD2	2.87	0.62
23:X:157:LEU:HB2	23:X:160:ASP:HB2	1.82	0.62
25:Z:55:PSU:H5'	25:Z:55:PSU:H6	1.65	0.62
1:A:868:C:H2'	1:A:869:G:O4'	2.00	0.62
1:A:1127:G:H21	1:A:1147:C:H41	1.47	0.62
8:H:105:ARG:HG2	8:H:105:ARG:HH21	1.65	0.62
1:A:24:U:H2'	1:A:25:C:H6	1.64	0.61
1:A:694:A:H5'	11:K:53:SER:HB2	1.81	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:695:A:H2'	1:A:696:A:C8	2.35	0.61
10:J:57:LYS:O	10:J:60:ARG:HD3	2.00	0.61
1:A:939:G:H1'	1:A:1375:A:C2	2.35	0.61
8:H:11:THR:HA	8:H:14:ARG:NH1	2.15	0.61
1:A:1164:G:N2	1:A:1165:C:C2	2.69	0.61
1:A:582:U:H2'	1:A:583:A:C8	2.35	0.61
10:J:27:ALA:HB2	10:J:85:LEU:HD21	1.81	0.61
1:A:1386:G:H2'	1:A:1387:G:C8	2.35	0.61
10:J:38:ILE:HD12	10:J:71:LEU:O	1.99	0.61
1:A:588:G:N2	1:A:589:C:C2	2.68	0.61
1:A:302:G:H2'	1:A:303:A:H8	1.64	0.61
23:X:90:PHE:HE2	23:X:118:VAL:HG12	1.66	0.61
24:Y:24:A:H2'	24:Y:25:A:C8	2.35	0.61
1:A:1256:A:H5''	3:C:27:LYS:NZ	2.14	0.61
1:A:1366:C:O2'	10:J:60:ARG:NH2	2.33	0.61
1:A:509:A:H4'	1:A:510:A:OP1	2.00	0.61
1:A:960:U:H4'	1:A:961:U:H5''	1.82	0.61
1:A:312:C:H2'	1:A:313:A:C8	2.36	0.61
1:A:1349:A:H5''	9:I:121:ARG:HB2	1.83	0.61
9:I:118:LYS:O	9:I:120:ARG:N	2.33	0.61
9:I:17:VAL:HG22	9:I:63:ILE:HG12	1.82	0.61
13:M:87:TYR:HA	13:M:90:LEU:HD12	1.83	0.61
1:A:376:G:H2'	1:A:377:G:H8	1.65	0.60
1:A:568:G:N2	1:A:883:C:C2	2.69	0.60
25:Z:47:U:H4'	25:Z:48:C:H5'	1.83	0.60
3:C:28:GLN:CA	3:C:31:HIS:CD2	2.82	0.60
16:P:59:TRP:C	16:P:62:VAL:HG22	2.21	0.60
1:A:623:C:H2'	1:A:624:C:O4'	2.01	0.60
14:N:24:CYS:HB3	14:N:28:GLY:H	1.67	0.60
1:A:1132:C:H2'	1:A:1133:G:C8	2.35	0.60
1:A:1384:C:H2'	1:A:1385:G:H8	1.65	0.60
1:A:1000:U:C6	1:A:1000:U:H3'	2.35	0.60
1:A:370:C:C2	1:A:392:G:N2	2.69	0.60
1:A:1464:G:N2	1:A:1465:C:C2	2.70	0.60
1:A:677:U:H2'	1:A:678:U:C6	2.37	0.60
1:A:960:U:H4'	1:A:961:U:C5'	2.31	0.60
1:A:96:U:H2'	1:A:97:G:H8	1.66	0.60
18:R:52:PRO:HG2	18:R:54:ARG:CZ	2.31	0.60
1:A:399:G:H2'	1:A:400:C:C6	2.37	0.60
1:A:999:C:O2	1:A:1043:C:O2	2.18	0.60
3:C:7:PRO:HG2	3:C:184:TYR:HB2	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:5:ILE:H	4:D:115:ARG:HH22	1.48	0.60
1:A:932:C:H5'	7:G:3:ARG:HB3	1.84	0.60
3:C:30:ARG:CZ	14:N:35:ARG:O	2.49	0.60
20:T:44:ALA:HB1	20:T:91:LEU:HB2	1.84	0.60
1:A:1532:U:H2'	1:A:1533:C:H1'	1.83	0.60
1:A:884:U:H4'	1:A:885:G:H5''	1.84	0.60
23:X:157:LEU:HD11	23:X:162:ASN:HB3	1.84	0.60
1:A:1513:A:H2'	1:A:1514:C:C6	2.37	0.59
1:A:390:C:H2'	1:A:391:G:H8	1.67	0.59
1:A:1411:C:H5'	22:W:64:ARG:HH22	1.66	0.59
10:J:9:ARG:HG3	10:J:95:GLU:HB3	1.82	0.59
14:N:12:ARG:O	14:N:14:PRO:HD3	2.02	0.59
19:S:40:ILE:HG21	19:S:62:ILE:HD11	1.84	0.59
1:A:921:U:H5'	1:A:1081:G:O2'	2.02	0.59
1:A:170:U:H2'	1:A:171:A:C8	2.35	0.59
25:Z:37:A:H2'	25:Z:38:A:C8	2.37	0.59
25:Z:40:C:H2'	25:Z:41:C:C6	2.37	0.59
1:A:189(L):G:H2'	1:A:190:U:C6	2.38	0.59
1:A:1005:A:O4'	1:A:1036:G:N2	2.35	0.59
1:A:1430:C:C2	1:A:1471:G:N2	2.71	0.59
1:A:735:C:H5'	18:R:71:LYS:HD3	1.84	0.59
1:A:556:C:H2'	1:A:557:G:O4'	2.02	0.59
25:Z:64:G:H2'	25:Z:65:C:O4'	2.03	0.59
1:A:521:G:N2	1:A:522:C:C2	2.71	0.59
1:A:59:A:H5''	1:A:387:U:H5''	1.83	0.59
5:E:33:VAL:HG21	5:E:109:ILE:HG12	1.84	0.59
1:A:1081:G:H5''	1:A:1081:G:H8	1.66	0.59
1:A:1074:G:O2'	1:A:1101:A:N1	2.35	0.59
1:A:691:G:H3'	11:K:26:ASN:HD21	1.66	0.59
25:Z:53:G:C2	25:Z:62:C:C2	2.90	0.59
1:A:1435:G:H2'	1:A:1436:U:C6	2.38	0.59
5:E:18:ARG:HD3	5:E:20:GLN:HE21	1.67	0.59
1:A:17:U:H2'	1:A:18:C:C5	2.38	0.58
1:A:1310:G:N2	1:A:1328:C:C2	2.71	0.58
2:B:17:PHE:HD1	2:B:18:GLY:H	1.51	0.58
8:H:105:ARG:CG	8:H:105:ARG:HH21	2.14	0.58
1:A:1493:A:C2	22:W:46:ARG:HA	2.38	0.58
1:A:258:G:N2	1:A:269:C:C2	2.71	0.58
3:C:26:LYS:HE3	3:C:26:LYS:H	1.68	0.58
1:A:1022:G:H2'	1:A:1023:G:C8	2.39	0.58
1:A:1025:U:H2'	1:A:1026:G:C8	2.39	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:216:G:C6	1:A:217:C:N4	2.71	0.58
1:A:757:U:H2'	1:A:758:G:O4'	2.03	0.58
3:C:20:SER:HB3	3:C:22:TRP:NE1	2.18	0.58
13:M:87:TYR:O	13:M:91:ARG:HG2	2.03	0.58
1:A:1162:C:C2	1:A:1175:G:C2	2.92	0.58
1:A:820:U:H3'	1:A:821:G:C5'	2.34	0.58
2:B:135:GLN:HA	2:B:138:LEU:HD12	1.84	0.58
4:D:196:LEU:HB3	4:D:198:VAL:HG12	1.84	0.58
25:Z:50:U:H3	25:Z:51:C:N4	2.01	0.58
10:J:57:LYS:HB2	10:J:60:ARG:NH1	2.19	0.58
1:A:1216:G:H5''	14:N:5:ALA:HB2	1.86	0.58
1:A:576:G:H3'	1:A:577:G:H5''	1.85	0.58
1:A:824:C:H2'	1:A:825:G:C8	2.39	0.58
1:A:109:A:H2'	1:A:326:G:N2	2.18	0.58
25:Z:3:C:H2'	25:Z:4:G:H8	1.69	0.58
1:A:1456:G:C2	1:A:1457:G:C8	2.92	0.58
2:B:122:PHE:HA	2:B:127:ILE:HG12	1.85	0.58
1:A:1241:G:N2	1:A:1242:C:C2	2.71	0.58
1:A:725:G:N2	1:A:726:C:C2	2.72	0.58
25:Z:17:C:OP1	25:Z:18:G:H5'	2.04	0.58
1:A:243:A:H4'	1:A:244:U:O5'	2.04	0.57
1:A:928:G:H1	1:A:1389:C:H42	1.51	0.57
5:E:93:PRO:CG	8:H:105:ARG:NH1	2.66	0.57
1:A:1515:C:H2'	1:A:1516:G:C8	2.39	0.57
1:A:911:U:H2'	1:A:912:C:C6	2.40	0.57
9:I:10:ARG:HE	9:I:11:LYS:HB2	1.69	0.57
10:J:50:ILE:HA	10:J:59:SER:O	2.04	0.57
1:A:1106:G:N2	1:A:1107:C:C2	2.73	0.57
25:Z:64:G:C5	25:Z:65:C:C4	2.92	0.57
1:A:354:G:N2	1:A:355:C:C2	2.72	0.57
4:D:166:LYS:HG3	4:D:178:VAL:HG11	1.87	0.57
9:I:96:LEU:HG	9:I:101:PHE:HB2	1.86	0.57
9:I:26:VAL:HB	9:I:33:PHE:HB2	1.86	0.57
15:O:24:SER:HB3	15:O:27:VAL:HG23	1.87	0.57
1:A:1347:G:N2	1:A:1373:G:H2'	2.20	0.57
1:A:769:G:N2	1:A:770:C:C2	2.73	0.57
8:H:12:ARG:HB3	8:H:24:THR:HG21	1.87	0.57
10:J:6:ILE:HG13	10:J:72:VAL:O	2.05	0.57
1:A:1391:U:H2'	1:A:1392:G:H8	1.68	0.57
1:A:524:G:C2	1:A:525:C:C4	2.93	0.57
1:A:551:U:H2'	1:A:552:U:C6	2.39	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:558:G:H3'	1:A:559:A:H5''	1.86	0.57
1:A:958:A:O5'	1:A:958:A:H8	1.88	0.57
4:D:26:CYS:HA	4:D:31:CYS:HB2	1.87	0.57
1:A:1095:U:H2'	1:A:1096:C:C6	2.40	0.57
1:A:1530:G:C2'	1:A:1531:A:O4'	2.50	0.57
1:A:18:C:H4'	1:A:1078:U:H1'	1.87	0.57
1:A:384:G:H2'	1:A:385:C:C6	2.40	0.57
5:E:14:ARG:HE	5:E:45:PHE:HZ	1.53	0.57
25:Z:50:U:C2	25:Z:51:C:C5	2.93	0.57
1:A:1106:G:C6	1:A:1107:C:N4	2.73	0.57
3:C:106:VAL:HG21	3:C:115:LEU:HD11	1.86	0.57
25:Z:1:C:H42	25:Z:72:A:H61	1.50	0.57
25:Z:39:C:H2'	25:Z:40:C:H6	1.66	0.57
1:A:1464:G:N1	1:A:1465:C:C4	2.73	0.57
1:A:874:G:N2	1:A:875:C:C2	2.73	0.57
1:A:943:U:H2'	1:A:944:G:C8	2.40	0.57
2:B:130:ARG:HH22	3:C:207:VAL:HG22	1.70	0.57
1:A:1076:C:H2'	1:A:1077:G:C8	2.40	0.56
1:A:1270:C:H2'	1:A:1271:G:C8	2.37	0.56
1:A:128:G:N2	1:A:234:C:C2	2.73	0.56
1:A:590:C:C2	1:A:650:G:C2	2.93	0.56
5:E:33:VAL:HG12	5:E:112:LEU:HD12	1.86	0.56
10:J:23:ILE:HG23	10:J:85:LEU:HD22	1.87	0.56
23:X:122:PHE:HE2	23:X:161:MET:HB2	1.69	0.56
25:Z:37:A:H3'	25:Z:38:A:H8	1.70	0.56
25:Z:55:PSU:C3'	25:Z:56:C:H5''	2.34	0.56
1:A:763:G:H2'	1:A:764:C:C6	2.40	0.56
1:A:1314:C:H2'	1:A:1315:U:C6	2.40	0.56
1:A:1438:G:N1	1:A:1439:C:C4	2.73	0.56
1:A:974:A:H8	1:A:974:A:OP1	1.88	0.56
17:Q:51:TYR:HE1	17:Q:76:LEU:HB2	1.70	0.56
1:A:1222:G:C6	1:A:1223:C:N4	2.73	0.56
1:A:1404:C:H42	1:A:1497:G:H1	1.51	0.56
1:A:253:U:H2'	1:A:254:G:H8	1.70	0.56
1:A:598:U:H2'	1:A:599:C:C6	2.40	0.56
1:A:589:C:O2	1:A:651:C:O2	2.24	0.56
1:A:810:C:H2'	1:A:811:C:O4'	2.05	0.56
1:A:90:U:O2'	1:A:91:C:H5'	2.05	0.56
1:A:975:A:H4'	1:A:976:G:O5'	2.05	0.56
5:E:106:PRO:HA	5:E:109:ILE:HD12	1.87	0.56
16:P:54:GLU:HA	16:P:57:ARG:HD2	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1164:G:N1	1:A:1165:C:C4	2.74	0.56
1:A:1323:G:H2'	1:A:1324:A:C8	2.41	0.56
1:A:1500:A:H5''	1:A:1508:G:H5''	1.88	0.56
1:A:755:G:N2	1:A:756:C:C2	2.73	0.56
20:T:43:LEU:HD22	20:T:51:GLU:HG3	1.88	0.56
22:W:32:ILE:HB	22:W:63:THR:O	2.05	0.56
25:Z:41:C:H2'	25:Z:42:G:C8	2.40	0.56
1:A:417:C:N4	1:A:418:C:N4	2.54	0.56
6:F:22:GLU:HA	6:F:25:ILE:HD12	1.88	0.56
1:A:930:C:H2'	1:A:931:C:O4'	2.05	0.56
1:A:96:U:H2'	1:A:97:G:C8	2.39	0.56
7:G:115:ARG:O	7:G:119:ARG:HG3	2.05	0.56
1:A:255:G:H2'	1:A:256:U:C6	2.41	0.56
1:A:678:U:H2'	1:A:679:C:C6	2.41	0.56
1:A:914:A:H2'	1:A:915:A:H8	1.69	0.56
1:A:998:G:N1	1:A:999:C:C4	2.74	0.56
2:B:84:GLU:HB3	2:B:219:VAL:HG21	1.87	0.56
1:A:1537:U:H3	24:Y:28:A:H61	1.52	0.56
1:A:999:C:C2'	1:A:1000:U:H5'	2.36	0.56
1:A:1233:G:C6	1:A:1234:C:N4	2.73	0.56
1:A:538:G:H2'	1:A:539:A:H8	1.71	0.56
1:A:790:A:H2'	1:A:791:G:C8	2.40	0.56
1:A:78:G:HO2'	1:A:79:G:C4'	2.19	0.56
1:A:939:G:H1'	1:A:1375:A:H2	1.71	0.56
1:A:377:G:H1	1:A:386:C:H42	1.53	0.56
1:A:891:U:H2'	1:A:892:A:H8	1.71	0.56
25:Z:4:G:H2'	25:Z:5:G:C8	2.41	0.56
1:A:1005:A:OP1	1:A:1006:C:C5	2.58	0.55
1:A:1353:G:N2	1:A:1354:C:C2	2.74	0.55
13:M:10:PRO:CB	13:M:18:ALA:HB1	2.35	0.55
25:Z:54:5MU:H73	25:Z:55:PSU:C2	2.42	0.55
1:A:1098:C:H1'	1:A:1168:A:C2	2.39	0.55
1:A:1515:C:H2'	1:A:1516:G:H8	1.70	0.55
1:A:60:A:H4'	1:A:61:G:O5'	2.06	0.55
8:H:113:SER:HB3	8:H:132:GLU:HB3	1.87	0.55
18:R:47:THR:HA	18:R:83:GLU:HB2	1.87	0.55
25:Z:63:G:N1	25:Z:64:G:C5	2.75	0.55
2:B:97:TRP:HZ2	2:B:102:LEU:HD13	1.70	0.55
1:A:128:G:C2	1:A:234:C:C2	2.95	0.55
1:A:910:C:H4'	1:A:1413:A:H4'	1.88	0.55
1:A:1227:A:N1	19:S:83:HIS:CB	2.67	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1540:U:H3	24:Y:25:A:H61	1.53	0.55
1:A:189(K):U:H2'	1:A:189(L):G:H8	1.72	0.55
1:A:279:A:H4'	1:A:280:C:OP2	2.06	0.55
19:S:50:ALA:HB1	19:S:57:HIS:HB3	1.87	0.55
1:A:1127:G:H21	1:A:1147:C:N4	2.05	0.55
1:A:1485:U:H2'	1:A:1486:G:H8	1.72	0.55
1:A:233:C:H2'	1:A:234:C:H6	1.72	0.55
1:A:390:C:H2'	1:A:391:G:C8	2.42	0.55
1:A:457:C:H2'	1:A:458:C:H6	1.71	0.55
2:B:54:THR:HG21	2:B:201:ILE:HD11	1.89	0.55
5:E:93:PRO:HB2	8:H:105:ARG:NH1	2.21	0.55
8:H:85:ARG:HH21	8:H:134:ILE:HG23	1.72	0.55
1:A:1223:C:H5''	1:A:1224:G:H5''	1.89	0.55
1:A:774:G:N2	1:A:806:C:C2	2.74	0.55
1:A:530:G:O2'	22:W:39:LYS:HG2	2.07	0.55
1:A:1166:G:N2	1:A:1170:A:OP2	2.30	0.55
1:A:939:G:C6	1:A:940:C:N4	2.74	0.55
7:G:24:THR:HA	7:G:27:ILE:HD12	1.89	0.55
13:M:88:ARG:HG3	13:M:98:VAL:CG1	2.37	0.55
1:A:1000:U:H2'	1:A:1001:A:O4'	2.06	0.54
1:A:397:A:N3	1:A:397:A:H3'	2.21	0.54
1:A:695:A:H2'	1:A:696:A:H8	1.71	0.54
3:C:30:ARG:CB	3:C:30:ARG:HH21	2.20	0.54
10:J:7:LYS:CA	10:J:71:LEU:CD2	2.86	0.54
25:Z:56:C:H2'	25:Z:57:A:H8	1.66	0.54
1:A:1005:A:OP1	1:A:1006:C:H5	1.91	0.54
1:A:1010:G:H2'	1:A:1011:G:C8	2.42	0.54
1:A:1134:G:N2	1:A:1141:C:C2	2.75	0.54
1:A:683:G:H2'	1:A:684:A:C8	2.42	0.54
8:H:88:LYS:HB2	8:H:91:ARG:HB3	1.89	0.54
1:A:1491:G:H5''	12:L:47:LYS:HE2	1.89	0.54
22:W:10:GLU:HG2	22:W:54:VAL:HG22	1.88	0.54
24:Y:36:A:C2	24:Y:37:U:C2	2.95	0.54
1:A:1368:G:N2	1:A:1369:C:C2	2.76	0.54
1:A:691:G:H8	11:K:26:ASN:HD22	1.53	0.54
25:Z:48:C:H2'	25:Z:59:A:C4'	2.38	0.54
1:A:1359:C:H3'	14:N:35:ARG:HH22	1.71	0.54
1:A:729:A:H2'	1:A:730:G:C8	2.38	0.54
1:A:946:A:H2'	1:A:947:G:C8	2.42	0.54
1:A:1079:G:H5''	5:E:14:ARG:NH2	2.22	0.54
5:E:81:GLU:HG2	5:E:90:VAL:HG22	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:878:G:H5'	8:H:89:PRO:HG2	1.89	0.54
25:Z:17:C:O2	25:Z:17:C:C2'	2.55	0.54
1:A:1169:A:H2'	1:A:1170:A:O4'	2.07	0.54
1:A:33:A:H2'	1:A:34:C:C6	2.43	0.54
1:A:35:G:H2'	1:A:36:C:C6	2.42	0.54
1:A:999:C:N3	1:A:1043:C:N3	2.55	0.54
8:H:111:ILE:HG22	8:H:134:ILE:HD12	1.89	0.54
8:H:28:ALA:HA	8:H:59:LEU:HD12	1.90	0.54
1:A:1370:G:H4'	9:I:12:GLU:OE2	2.07	0.54
1:A:1098:C:C1'	1:A:1168:A:H2	2.20	0.54
1:A:1112:C:H1'	3:C:179:ARG:HH21	1.72	0.54
1:A:1244:C:H2'	1:A:1245:A:C8	2.43	0.54
1:A:34:C:H2'	1:A:35:G:C8	2.43	0.54
1:A:761:G:C2	1:A:762:C:C2	2.96	0.54
3:C:113:ALA:HA	3:C:202:ILE:HD12	1.89	0.54
4:D:102:ASP:HB3	4:D:136:PRO:HB3	1.88	0.54
1:A:1378:C:N3	7:G:76:ARG:NH2	2.56	0.54
17:Q:68:ARG:HG3	17:Q:68:ARG:O	2.08	0.54
1:A:235:C:H5'	17:Q:70:ARG:HG2	1.90	0.54
1:A:1230:C:C5'	25:Z:30:G:H5''	2.38	0.54
9:I:46:ALA:HB2	9:I:74:ILE:HG23	1.89	0.54
1:A:530:G:H8	22:W:38:GLY:HA3	1.73	0.54
1:A:1262:C:H2'	1:A:1263:C:C6	2.43	0.54
1:A:1325:C:H2'	1:A:1326:C:C6	2.43	0.54
1:A:434:U:H2'	1:A:435:C:C6	2.43	0.54
1:A:582:U:H2'	1:A:583:A:H8	1.72	0.54
3:C:113:ALA:N	3:C:114:PRO:CD	2.71	0.54
8:H:91:ARG:HD3	12:L:7:ILE:HG21	1.90	0.54
12:L:37:CYS:SG	12:L:58:VAL:HG22	2.48	0.54
1:A:1312:G:C2	1:A:1326:C:C2	2.95	0.53
1:A:504:C:N3	1:A:542:G:C2	2.76	0.53
1:A:555:C:H2'	1:A:556:C:C6	2.43	0.53
1:A:827:U:C4	1:A:872:A:N1	2.72	0.53
1:A:500:G:C6	1:A:501:C:N4	2.76	0.53
9:I:104:ARG:HH11	9:I:106:ALA:HA	1.73	0.53
1:A:522:C:H5''	12:L:120:TYR:OH	2.08	0.53
23:X:110:LEU:HD13	23:X:148:ALA:HB2	1.89	0.53
25:Z:70:G:H2'	25:Z:71:C:O4'	2.08	0.53
1:A:1133:G:H1	1:A:1141:C:H42	1.55	0.53
1:A:948:C:H2'	1:A:949:A:H8	1.74	0.53
1:A:532:A:N6	3:C:127:ARG:HB3	2.23	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:79:G:H2'	1:A:80:G:C8	2.42	0.53
12:L:58:VAL:HG21	12:L:85:ILE:HD11	1.91	0.53
25:Z:37:A:H2'	25:Z:38:A:O4'	2.09	0.53
1:A:1027:C:H2'	1:A:1028:C:H5'	1.89	0.53
1:A:521:G:N1	1:A:522:C:C4	2.77	0.53
1:A:975:A:H5''	1:A:975:A:C8	2.44	0.53
8:H:36:LEU:HD21	8:H:61:VAL:HG22	1.91	0.53
1:A:910:C:H5''	12:L:97:ARG:NH2	2.24	0.53
1:A:1314:C:H42	19:S:4:SER:HB2	1.74	0.53
1:A:975:A:H4'	1:A:976:G:C5'	2.39	0.53
4:D:109:GLY:HA3	4:D:165:MET:HG3	1.91	0.53
7:G:33:ASP:HB2	7:G:35:LYS:HG3	1.90	0.53
1:A:1414:U:H2'	1:A:1415:G:C8	2.43	0.53
1:A:1437:C:H2'	1:A:1438:G:H8	1.74	0.53
1:A:1418:A:N6	1:A:1482:G:O2'	2.40	0.53
1:A:216:G:C2	1:A:217:C:N3	2.77	0.53
1:A:138:G:H1	1:A:225:C:H42	1.57	0.53
25:Z:48:C:H5''	25:Z:50:U:OP2	2.09	0.53
1:A:1510:U:H2'	1:A:1511:G:C8	2.44	0.53
1:A:974:A:H4'	1:A:975:A:H3'	1.90	0.53
2:B:10:LEU:HG	2:B:48:MET:HG3	1.89	0.53
1:A:598:U:H2'	1:A:599:C:H6	1.74	0.53
1:A:376:G:H5''	16:P:5:ARG:HD2	1.90	0.53
1:A:662:G:C2	1:A:744:C:O2	2.62	0.53
1:A:928:G:H1	1:A:1389:C:N4	2.07	0.53
5:E:20:GLN:HB2	5:E:23:GLY:O	2.09	0.53
23:X:112:GLU:HB3	23:X:114:HIS:CD2	2.43	0.53
1:A:1105:A:H2'	1:A:1106:G:C8	2.44	0.52
1:A:46:G:H2'	1:A:366:C:C5	2.43	0.52
10:J:90:LEU:H	10:J:91:PRO:HD2	1.74	0.52
1:A:1050:G:C6	1:A:1051:C:N4	2.77	0.52
1:A:1106:G:C2	1:A:1107:C:C4	2.98	0.52
1:A:1456:G:N2	1:A:1457:G:N7	2.57	0.52
1:A:266:G:O2'	1:A:267:C:OP2	2.22	0.52
1:A:317:G:P	1:A:353:A:H61	2.33	0.52
1:A:369:C:H2'	1:A:370:C:C6	2.44	0.52
1:A:529:G:H5'	1:A:530:G:OP2	2.09	0.52
2:B:80:ILE:O	2:B:84:GLU:HG2	2.09	0.52
1:A:1114:C:H2'	1:A:1115:C:C6	2.45	0.52
1:A:1125:U:C5'	1:A:1126:U:H5	2.20	0.52
1:A:122:G:C2	1:A:123:C:C2	2.96	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1525:G:H2'	1:A:1526:G:H8	1.75	0.52
1:A:148:G:C2	1:A:175:C:C2	2.98	0.52
1:A:312:C:H2'	1:A:313:A:H8	1.75	0.52
1:A:392:G:H2'	1:A:393:A:C8	2.44	0.52
1:A:1251:A:H2'	1:A:1252:A:O4'	2.09	0.52
1:A:1534:A:C4	1:A:1535:C:C5	2.98	0.52
1:A:568:G:C2	1:A:883:C:C2	2.98	0.52
1:A:890:G:O2'	1:A:906:G:O6	2.24	0.52
13:M:94:ARG:HB3	13:M:96:LEU:HD12	1.92	0.52
15:O:82:ILE:HA	15:O:87:ILE:HD12	1.90	0.52
1:A:1124:G:H1	1:A:1149:C:H42	1.57	0.52
1:A:1162:C:C2	1:A:1175:G:N2	2.77	0.52
1:A:437:U:H2'	1:A:438:G:O4'	2.09	0.52
4:D:108:LEU:HD21	4:D:174:LEU:HD22	1.91	0.52
25:Z:52:G:C4	25:Z:53:G:C8	2.97	0.52
25:Z:64:G:C2	25:Z:65:C:C2	2.98	0.52
1:A:1096:C:H2'	1:A:1097:C:C6	2.44	0.52
1:A:145:G:N2	1:A:178:C:C2	2.78	0.52
1:A:876:G:C6	1:A:877:C:N4	2.77	0.52
8:H:6:ILE:O	8:H:10:LEU:HG	2.09	0.52
1:A:1229:A:H2'	1:A:1230:C:H6	1.75	0.52
1:A:333:G:N2	1:A:334:C:C2	2.77	0.52
1:A:505:G:H2'	1:A:506:G:H8	1.74	0.52
1:A:674:G:O5'	1:A:674:G:H8	1.93	0.52
3:C:26:LYS:N	3:C:26:LYS:CE	2.73	0.52
1:A:1001(A):G:N1	1:A:1002:G:C6	2.78	0.52
1:A:1365:G:C2	1:A:1366:C:C2	2.98	0.52
1:A:1365:G:C6	1:A:1366:C:C4	2.98	0.52
1:A:1424:C:H42	1:A:1476:G:H1	1.56	0.52
1:A:99:U:H2'	1:A:100:C:C6	2.45	0.52
25:Z:17(A):U:C3'	25:Z:18:G:H5''	2.40	0.52
1:A:1129:C:O5'	1:A:1130:A:H5'	2.10	0.52
1:A:130:A:H8	1:A:130:A:OP1	1.93	0.52
1:A:200:G:C2	1:A:218:C:C2	2.98	0.52
1:A:269:C:H2'	1:A:270:A:C8	2.44	0.52
1:A:413:G:N2	1:A:429:U:OP2	2.38	0.52
5:E:139:LEU:HA	5:E:142:LEU:HD12	1.91	0.52
9:I:10:ARG:CD	9:I:105:ASP:HB3	2.40	0.52
1:A:100:C:H2'	1:A:101:A:C8	2.45	0.52
1:A:1010:G:H2'	1:A:1011:G:H8	1.74	0.52
1:A:124:G:H2'	1:A:125:U:O4'	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1434:A:H2'	1:A:1435:G:O4'	2.10	0.52
8:H:11:THR:HA	8:H:14:ARG:HH12	1.75	0.52
13:M:33:ALA:HB2	13:M:64:TRP:HH2	1.74	0.52
19:S:6:LYS:HD2	19:S:7:LYS:H	1.75	0.52
1:A:70:G:C2	1:A:100:C:C2	2.98	0.51
10:J:57:LYS:HB2	10:J:60:ARG:HH12	1.74	0.51
19:S:17:GLU:HA	19:S:20:LEU:HG	1.91	0.51
1:A:1029:C:H2'	1:A:1030:C:C6	2.45	0.51
1:A:1137:C:H4'	1:A:1138:G:C2	2.45	0.51
1:A:1392:G:H21	1:A:1502:A:H8	1.59	0.51
1:A:560:U:H2'	5:E:123:LEU:HD22	1.91	0.51
5:E:92:LYS:HG2	5:E:93:PRO:HD2	1.91	0.51
15:O:30:ALA:HA	15:O:85:LEU:HD11	1.92	0.51
17:Q:34:LYS:HG3	17:Q:36:ILE:HG23	1.91	0.51
25:Z:68:C:H2'	25:Z:69:C:C6	2.45	0.51
1:A:1280:A:OP1	1:A:1281:U:C5	2.62	0.51
1:A:967:C:H2'	1:A:968:A:C8	2.45	0.51
23:X:67:TYR:O	23:X:71:MET:HG2	2.11	0.51
1:A:1068:G:N2	1:A:1069:C:C2	2.78	0.51
1:A:1369:C:H2'	1:A:1370:G:O4'	2.10	0.51
1:A:1389:C:H2'	1:A:1390:U:O4'	2.11	0.51
1:A:476:G:H2'	1:A:477:A:C8	2.45	0.51
1:A:681:C:H42	1:A:709:G:H1	1.58	0.51
3:C:30:ARG:NH2	3:C:30:ARG:CB	2.73	0.51
7:G:111:ARG:CZ	7:G:122:HIS:HB3	2.41	0.51
1:A:277:C:H5'	17:Q:68:ARG:NH1	2.25	0.51
1:A:223:U:H5'	20:T:68:LYS:HZ1	1.76	0.51
1:A:1126:U:H2'	1:A:1126:U:O2	2.09	0.51
1:A:1431:C:C2	1:A:1470:G:N2	2.79	0.51
1:A:1443:G:N2	1:A:1444:C:C2	2.79	0.51
1:A:1493:A:H2'	22:W:20:ALA:H	1.75	0.51
1:A:184:G:H2'	1:A:185:A:H8	1.75	0.51
1:A:737:A:H2'	1:A:738:C:C6	2.46	0.51
1:A:838:G:C2	1:A:849:C:C2	2.99	0.51
5:E:19:MET:SD	5:E:24:ARG:HB3	2.51	0.51
1:A:522:C:H41	12:L:53:ARG:HH21	1.59	0.51
1:A:1244:C:H2'	1:A:1245:A:H8	1.75	0.51
1:A:1464:G:C2	1:A:1465:C:C4	2.98	0.51
3:C:26:LYS:CD	3:C:26:LYS:N	2.73	0.51
6:F:78:GLU:HA	6:F:81:ILE:HD12	1.92	0.51
1:A:1367:C:H4'	10:J:48:THR:HG21	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:90:LEU:HA	13:M:93:ARG:HD2	1.91	0.51
22:W:13:VAL:HB	22:W:50:GLY:H	1.75	0.51
1:A:1405:G:H2'	1:A:1406:U:H6	1.75	0.51
1:A:880:C:H2'	1:A:881:G:C8	2.46	0.51
20:T:45:GLN:HG2	20:T:91:LEU:HD22	1.93	0.51
1:A:1048:G:H1	1:A:1209:C:H42	1.59	0.51
1:A:1283:G:N2	1:A:1284:C:C2	2.79	0.51
1:A:264:U:H2'	1:A:265:G:O4'	2.11	0.51
1:A:70:G:C2	1:A:100:C:O2	2.64	0.51
4:D:30:LYS:C	4:D:32:ALA:H	2.14	0.51
1:A:1230:C:H5''	25:Z:30:G:H5''	1.92	0.51
1:A:1027:C:C2'	1:A:1028:C:H5'	2.40	0.51
1:A:1064:G:H21	1:A:1190:G:H2'	1.75	0.51
1:A:1079:G:H2'	1:A:1080:A:C8	2.46	0.51
1:A:1325:C:H2'	1:A:1326:C:H6	1.75	0.51
1:A:1363(A):A:H1'	1:A:1365:G:C5	2.45	0.51
1:A:173:U:H5'	1:A:197:A:O4'	2.11	0.51
1:A:824:C:H2'	1:A:825:G:H8	1.74	0.51
1:A:864:A:C2	1:A:865:A:C2	2.99	0.51
25:Z:70:G:C6	25:Z:71:C:C4	2.99	0.51
1:A:1201:A:H4'	1:A:1202:G:O5'	2.11	0.51
1:A:1534:A:C4	1:A:1535:C:C6	2.99	0.51
1:A:504:C:C2	1:A:542:G:N2	2.79	0.51
25:Z:31:G:H2'	25:Z:32:OMC:H6	1.76	0.51
1:A:1360:A:OP2	14:N:35:ARG:NH2	2.44	0.50
17:Q:93:GLN:O	17:Q:96:GLU:HB2	2.12	0.50
25:Z:29:G:H2'	25:Z:30:G:O4'	2.11	0.50
1:A:17:U:O2	1:A:1079:G:C2	2.64	0.50
1:A:1130:A:H2'	1:A:1131:G:C8	2.46	0.50
1:A:1229:A:H2'	1:A:1230:C:C6	2.46	0.50
1:A:876:G:H2'	1:A:877:C:C6	2.45	0.50
1:A:10:A:H2'	1:A:11:G:H8	1.72	0.50
1:A:1507:A:H2'	1:A:1508:G:C8	2.45	0.50
1:A:967:C:H4'	9:I:128:ARG:NE	2.26	0.50
5:E:152:ARG:HB3	8:H:43:GLY:HA3	1.94	0.50
7:G:65:ALA:O	7:G:69:VAL:HG23	2.12	0.50
25:Z:69:C:H2'	25:Z:70:G:O4'	2.11	0.50
1:A:132:C:C2	1:A:231:G:N2	2.80	0.50
1:A:309:G:H2'	1:A:310:G:H8	1.76	0.50
1:A:558:G:H3'	1:A:559:A:C5'	2.42	0.50
1:A:914:A:H2'	1:A:915:A:C8	2.46	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:149:ALA:HB3	4:D:152:SER:HB2	1.93	0.50
7:G:97:GLN:O	7:G:101:LEU:HG	2.11	0.50
24:Y:36:A:H2'	24:Y:37:U:O4'	2.12	0.50
1:A:1128:C:H1'	1:A:1146:A:H61	1.77	0.50
1:A:236:G:C2	1:A:237:C:C2	3.00	0.50
1:A:381:C:H2'	1:A:382:A:O4'	2.12	0.50
1:A:56:U:H2'	1:A:57:G:C8	2.45	0.50
1:A:1106:G:H5''	3:C:172:ARG:HD2	1.92	0.50
3:C:188:LEU:HD12	3:C:190:ARG:HG3	1.92	0.50
4:D:79:PHE:CZ	4:D:204:ILE:HA	2.47	0.50
1:A:1255:G:H2'	1:A:1279:A:N6	2.26	0.50
1:A:1361:G:C6	1:A:1362:C:N3	2.80	0.50
1:A:777:A:H2'	1:A:778:G:C8	2.46	0.50
1:A:966:G:C4	25:Z:34:C:H5'	2.46	0.50
2:B:51:LEU:HG	2:B:201:ILE:HG23	1.93	0.50
4:D:121:VAL:O	4:D:134:ASP:HA	2.12	0.50
10:J:51:ARG:N	10:J:59:SER:O	2.37	0.50
1:A:16:A:N3	1:A:1080:A:H1'	2.27	0.50
1:A:1081:G:O5'	5:E:18:ARG:HB2	2.12	0.50
1:A:229:U:H2'	1:A:230:G:C8	2.47	0.50
1:A:648:A:H2'	1:A:649:G:H8	1.77	0.50
14:N:24:CYS:HB2	14:N:40:CYS:HB3	1.93	0.50
25:Z:53:G:N2	25:Z:62:C:C2	2.80	0.50
1:A:1028:C:H2'	1:A:1029:C:O4'	2.12	0.50
1:A:1132:C:H2'	1:A:1133:G:H8	1.76	0.50
1:A:142:G:H2'	1:A:143:A:C8	2.47	0.50
1:A:1532:U:H5''	1:A:1533:C:P	2.51	0.50
1:A:22:G:C6	1:A:23:C:C4	2.99	0.50
1:A:474:G:H2'	1:A:475:G:C8	2.47	0.50
6:F:27:GLN:HA	6:F:30:LEU:HD12	1.93	0.50
1:A:1000:U:C3'	1:A:1000:U:C6	2.95	0.50
1:A:1017:G:C2	1:A:1018:C:C2	2.99	0.50
1:A:1280:A:C3'	1:A:1281:U:H5''	2.41	0.50
1:A:1518:A:H2'	1:A:1519:A:C8	2.47	0.50
1:A:399:G:C6	1:A:400:C:N4	2.80	0.50
1:A:784:C:C2	1:A:799:G:N2	2.80	0.50
1:A:939:G:H2'	1:A:940:C:C6	2.47	0.50
7:G:145:ALA:O	7:G:146:GLU:HB2	2.11	0.50
1:A:1135:U:H4'	1:A:1136:U:C5	2.47	0.49
14:N:7:ILE:HG22	14:N:10:ALA:HB2	1.93	0.49
10:J:62:HIS:CB	14:N:59:ALA:HB3	2.37	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:P:22:THR:HA	16:P:33:ILE:HD12	1.93	0.49
25:Z:22:G:N2	25:Z:23:C:C2	2.79	0.49
1:A:1172:C:H2'	1:A:1173:G:H8	1.77	0.49
1:A:1220:G:H2'	1:A:1221:G:C8	2.47	0.49
1:A:1385:G:H2'	1:A:1386:G:H8	1.77	0.49
1:A:1525:G:H2'	1:A:1526:G:C8	2.47	0.49
1:A:416:G:C6	1:A:417:C:C4	3.00	0.49
1:A:538:G:H2'	1:A:539:A:C8	2.46	0.49
2:B:174:VAL:HG13	2:B:184:VAL:HG11	1.94	0.49
8:H:12:ARG:HD3	8:H:26:VAL:HG12	1.94	0.49
10:J:57:LYS:HA	10:J:60:ARG:HH11	1.77	0.49
1:A:1059:C:O3'	14:N:45:ARG:NH2	2.45	0.49
1:A:105:G:H2'	1:A:106:C:C6	2.46	0.49
1:A:1405:G:H2'	1:A:1406:U:C6	2.46	0.49
1:A:115:G:O2'	1:A:289:G:H5''	2.13	0.49
1:A:384:G:C6	1:A:385:C:N4	2.80	0.49
25:Z:52:G:H2'	25:Z:53:G:O4'	2.13	0.49
1:A:919:A:C2	1:A:1080:A:C2	2.99	0.49
1:A:1114:C:C2	1:A:1187:G:C2	3.00	0.49
1:A:1256:A:H1'	1:A:1258:G:C4	2.48	0.49
1:A:1493:A:H4'	1:A:1494:G:OP1	2.13	0.49
1:A:293:G:C6	1:A:294:U:C4	3.00	0.49
1:A:41:G:H2'	1:A:42:G:H8	1.78	0.49
3:C:25:GLY:O	3:C:29:TYR:HB2	2.12	0.49
15:O:39:LEU:HD22	15:O:56:LEU:HB2	1.94	0.49
1:A:1222:G:OP1	19:S:77:THR:HG23	2.12	0.49
25:Z:37:A:H3'	25:Z:38:A:C8	2.47	0.49
1:A:1262:C:H42	1:A:1273:G:H1	1.60	0.49
1:A:1345:U:H4'	1:A:1346:A:O5'	2.12	0.49
1:A:1416:G:H2'	1:A:1417:G:O4'	2.12	0.49
1:A:1428:A:H2'	1:A:1429:C:C6	2.48	0.49
1:A:270:A:H2'	1:A:271:C:C6	2.47	0.49
1:A:416:G:C2	1:A:417:C:C2	3.01	0.49
1:A:544:G:OP1	4:D:62:GLN:HG3	2.12	0.49
5:E:139:LEU:O	5:E:142:LEU:HB2	2.12	0.49
12:L:37:CYS:SG	12:L:56:ALA:HB1	2.52	0.49
20:T:22:ARG:HG2	20:T:25:ARG:HH22	1.76	0.49
1:A:122:G:C6	1:A:123:C:C4	3.00	0.49
1:A:132:C:N3	1:A:231:G:C2	2.81	0.49
1:A:1409:C:H2'	1:A:1410:G:H8	1.77	0.49
1:A:1443:G:C2	1:A:1444:C:C4	3.00	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:22:G:C2	1:A:23:C:C2	3.01	0.49
1:A:744:C:H2'	1:A:745:C:C6	2.48	0.49
11:K:33:THR:HA	11:K:39:PRO:HA	1.94	0.49
20:T:43:LEU:HB3	20:T:52:ALA:HB2	1.94	0.49
22:W:56:GLU:HB3	22:W:66:ARG:HH11	1.76	0.49
23:X:141:THR:HG22	23:X:165:LEU:HD11	1.93	0.49
1:A:940:C:H2'	1:A:941:G:C8	2.48	0.49
1:A:125:U:H2'	1:A:126:G:C8	2.47	0.49
1:A:1456:G:N2	1:A:1457:G:C8	2.81	0.49
1:A:20:U:H2'	1:A:21:G:O4'	2.13	0.49
1:A:552:U:H2'	1:A:553:A:C8	2.48	0.49
1:A:864:A:O2'	1:A:865:A:O4'	2.31	0.49
1:A:148:G:H2'	1:A:149:A:C8	2.47	0.49
1:A:15:G:H2'	1:A:16:A:H8	1.78	0.49
1:A:28:G:O2'	1:A:296:U:OP1	2.31	0.49
1:A:940:C:H2'	1:A:941:G:H8	1.78	0.49
5:E:51:VAL:HG13	5:E:52:PRO:HD3	1.95	0.49
13:M:94:ARG:HH22	19:S:80:TYR:HA	1.77	0.49
25:Z:64:G:C6	25:Z:65:C:C4	3.00	0.49
1:A:1217:C:N4	1:A:1218:C:N4	2.61	0.49
1:A:1484:C:H2'	1:A:1485:U:O4'	2.13	0.49
1:A:189:G:C2	1:A:189(A):C:C2	3.00	0.49
1:A:224:C:H2'	1:A:225:C:C6	2.48	0.49
1:A:1030:C:C2	1:A:1032:G:N2	2.81	0.48
1:A:1357:A:N6	1:A:1363(A):A:C2	2.80	0.48
1:A:977:A:H2'	1:A:978:A:H5''	1.95	0.48
18:R:69:THR:HA	18:R:72:ARG:HD2	1.94	0.48
25:Z:36:U:H2'	25:Z:37:A:O4'	2.12	0.48
25:Z:64:G:H2'	25:Z:65:C:C6	2.48	0.48
1:A:1266:G:N2	1:A:1270:C:C2	2.81	0.48
1:A:427:U:OP2	4:D:36:ARG:NH2	2.46	0.48
1:A:568:G:C6	1:A:569:C:N4	2.81	0.48
1:A:648:A:H2'	1:A:649:G:C8	2.48	0.48
10:J:7:LYS:CG	10:J:71:LEU:HD23	2.24	0.48
12:L:32:PHE:HB3	12:L:84:LEU:HD11	1.95	0.48
25:Z:70:G:C2	25:Z:71:C:C2	3.01	0.48
1:A:198:G:H2'	1:A:199:G:C8	2.48	0.48
1:A:229:U:H2'	1:A:230:G:H8	1.78	0.48
1:A:261:U:N3	1:A:264:U:OP2	2.39	0.48
1:A:442:C:H2'	1:A:443:C:C6	2.49	0.48
1:A:778:G:C6	1:A:779:C:C4	3.01	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:130:A:H5'	17:Q:63:ARG:HE	1.79	0.48
1:A:1147:C:HO2'	9:I:5:TYR:HH	1.61	0.48
1:A:1226:C:H2'	13:M:103:THR:HB	1.94	0.48
1:A:778:G:C2	1:A:779:C:C2	3.02	0.48
1:A:823:G:N2	1:A:824:C:C2	2.81	0.48
3:C:29:TYR:CE2	14:N:54:PRO:HG2	2.48	0.48
5:E:71:LEU:HD21	5:E:115:VAL:HG22	1.96	0.48
12:L:57:LYS:HG2	12:L:67:THR:HG22	1.96	0.48
1:A:588:G:N1	1:A:589:C:C4	2.81	0.48
1:A:719:C:H1'	18:R:49:LYS:HG2	1.94	0.48
1:A:877:C:H2'	1:A:878:G:C8	2.46	0.48
1:A:947:G:H2'	1:A:948:C:O4'	2.13	0.48
1:A:951:G:C6	1:A:1231:G:C6	3.02	0.48
2:B:21:ARG:HD3	2:B:21:ARG:H	1.79	0.48
1:A:1345:U:O4	1:A:1375:A:N1	2.47	0.48
1:A:253:U:H2'	1:A:254:G:C8	2.48	0.48
1:A:361:G:H2'	1:A:362:G:O4'	2.13	0.48
10:J:26:ALA:HA	10:J:29:ARG:HH21	1.78	0.48
1:A:35:G:O2'	12:L:121:GLY:HA2	2.12	0.48
19:S:32:LYS:HA	19:S:50:ALA:HB3	1.95	0.48
25:Z:1:C:N4	25:Z:72:A:H61	2.12	0.48
1:A:1385:G:H2'	1:A:1386:G:C8	2.49	0.48
1:A:1443:G:C2	1:A:1444:C:N3	2.81	0.48
25:Z:50:U:H2'	25:Z:51:C:H6	1.71	0.48
1:A:1216:G:N2	1:A:1217:C:C2	2.81	0.48
1:A:434:U:H2'	1:A:435:C:H6	1.79	0.48
1:A:518:C:O2'	1:A:519:C:OP2	2.25	0.48
1:A:602:A:H2'	1:A:603:U:O4'	2.13	0.48
1:A:600:C:C2	1:A:639:G:C2	3.01	0.48
1:A:750:G:N3	15:O:23:GLY:HA3	2.28	0.48
1:A:988:G:C6	1:A:989:C:N3	2.82	0.48
3:C:132:ARG:HG2	3:C:136:GLN:HE21	1.79	0.48
3:C:54:ARG:H	3:C:69:HIS:HB2	1.79	0.48
4:D:57:ARG:HB3	4:D:206:PHE:HB2	1.94	0.48
5:E:33:VAL:HG11	5:E:109:ILE:HA	1.94	0.48
10:J:24:VAL:HG22	10:J:72:VAL:HG21	1.95	0.48
15:O:9:GLN:HA	15:O:12:ILE:HD12	1.95	0.48
1:A:1077:G:H22	1:A:1079:G:H3'	1.78	0.48
1:A:169:C:H2'	1:A:170:U:C6	2.49	0.48
1:A:603:U:H2'	1:A:604:G:H8	1.78	0.48
1:A:568:G:C2	1:A:883:C:N3	2.82	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:Z:62:C:H2'	25:Z:63:G:C8	2.48	0.48
1:A:1038:C:H2'	1:A:1039:C:H6	1.79	0.48
1:A:110:C:H4'	16:P:25:ARG:HB3	1.96	0.48
1:A:296:U:H2'	1:A:297:G:C8	2.49	0.48
1:A:715:A:H2'	1:A:716:A:O4'	2.14	0.48
3:C:57:ILE:HA	3:C:65:ALA:O	2.13	0.48
4:D:22:LYS:HB2	4:D:26:CYS:SG	2.54	0.48
21:V:14:TRP:HZ3	21:V:15:ARG:HE	1.62	0.48
25:Z:63:G:C2	25:Z:64:G:C5	3.01	0.48
1:A:1508:G:C2	1:A:1509:C:C2	3.02	0.47
1:A:761:G:C6	1:A:762:C:C4	3.01	0.47
7:G:125:MET:O	7:G:129:GLU:HG2	2.14	0.47
1:A:1301:U:H1'	1:A:1302:U:OP1	2.13	0.47
1:A:403:C:H5''	4:D:136:PRO:HD2	1.96	0.47
1:A:577:G:C2	1:A:578:C:C2	3.01	0.47
1:A:784:C:H42	1:A:798:G:H1	1.60	0.47
12:L:114:LYS:HE2	12:L:125:PRO:HB3	1.96	0.47
25:Z:16:C:O4'	25:Z:59:A:C2	2.67	0.47
1:A:538:G:OP2	12:L:115:LYS:HB2	2.14	0.47
1:A:636:U:H2'	1:A:637:G:C8	2.49	0.47
1:A:975:A:H4'	1:A:976:G:H5'	1.95	0.47
3:C:116:VAL:O	3:C:120:VAL:HG23	2.13	0.47
3:C:155:GLY:O	3:C:196:LEU:HG	2.13	0.47
5:E:32:VAL:HB	5:E:58:ALA:HB1	1.95	0.47
1:A:263:A:OP1	20:T:79:ARG:HD3	2.14	0.47
1:A:1305:G:HO2'	1:A:1306:A:H8	1.62	0.47
1:A:669:U:H2'	1:A:670:G:H8	1.79	0.47
1:A:988:G:H2'	1:A:989:C:O4'	2.14	0.47
3:C:77:ILE:HG22	3:C:81:GLY:HA2	1.96	0.47
4:D:31:CYS:HG	26:D:300:ZN:ZN	1.24	0.47
8:H:86:ILE:HD11	8:H:136:GLU:HB3	1.96	0.47
1:A:1444:C:O5'	1:A:1444:C:H6	1.97	0.47
1:A:377:G:H1	1:A:386:C:N4	2.12	0.47
1:A:669:U:H2'	1:A:670:G:C8	2.49	0.47
1:A:681:C:C2	1:A:710:G:N2	2.82	0.47
1:A:875:C:O2'	8:H:14:ARG:HD2	2.14	0.47
1:A:881:G:C2	1:A:882:C:C2	3.02	0.47
3:C:64:VAL:O	3:C:99:VAL:HG23	2.14	0.47
8:H:20:TYR:HA	8:H:65:TYR:CZ	2.49	0.47
25:Z:12:G:N1	25:Z:13:C:C2	2.83	0.47
25:Z:53:G:H3'	25:Z:54:5MU:H71	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1084:G:H1'	1:A:1103:C:H41	1.78	0.47
1:A:1188:A:H2'	1:A:1189:C:O4'	2.15	0.47
1:A:1283:G:C6	1:A:1284:C:N4	2.82	0.47
1:A:172:A:H2'	1:A:174:C:H5	1.78	0.47
1:A:189:G:C6	1:A:189(A):C:C4	3.03	0.47
1:A:883:C:H2'	1:A:884:U:C6	2.50	0.47
1:A:945:G:H2'	1:A:945:G:N3	2.30	0.47
1:A:949:A:OP2	13:M:106:ASN:HB2	2.13	0.47
1:A:1346:A:H2'	7:G:10:ARG:NH2	2.26	0.47
11:K:72:ALA:HB1	11:K:77:MET:HG3	1.95	0.47
25:Z:31:G:C2	25:Z:40:C:C2	3.02	0.47
25:Z:52:G:C5	25:Z:53:G:N7	2.82	0.47
1:A:1119:C:H2'	1:A:1120:G:H8	1.78	0.47
25:Z:4:G:H2'	25:Z:5:G:H8	1.80	0.47
1:A:1228:C:H4'	13:M:116:THR:HA	1.96	0.47
1:A:333:G:C6	1:A:334:C:N4	2.82	0.47
1:A:590:C:N3	1:A:650:G:C2	2.83	0.47
1:A:960:U:H4'	1:A:961:U:O5'	2.13	0.47
2:B:187:LEU:HA	2:B:201:ILE:HB	1.97	0.47
3:C:54:ARG:HB3	3:C:69:HIS:CD2	2.50	0.47
8:H:103:VAL:HG21	8:H:110:ALA:HB2	1.95	0.47
24:Y:28:A:H5'	24:Y:29:G:OP2	2.15	0.47
1:A:1050:G:N2	1:A:1051:C:C2	2.83	0.47
1:A:362:G:H5''	12:L:61:THR:HB	1.97	0.47
3:C:99:VAL:CG2	3:C:100:ALA:N	2.78	0.47
4:D:120:LEU:HA	4:D:125:HIS:HD2	1.79	0.47
15:O:15:PHE:HE2	15:O:84:LYS:HB3	1.79	0.47
16:P:49:LEU:HD13	16:P:73:LEU:HD22	1.97	0.47
1:A:1030:C:H42	1:A:1031:G:H1	1.62	0.47
1:A:1038:C:H2'	1:A:1039:C:C6	2.49	0.47
1:A:236:G:C6	1:A:237:C:C4	3.03	0.47
1:A:628:G:H2'	1:A:629:G:C8	2.50	0.47
1:A:643:C:H2'	1:A:644:G:H8	1.80	0.47
1:A:823:G:H2'	1:A:824:C:C6	2.50	0.47
1:A:928:G:H2'	1:A:929:G:C8	2.49	0.47
2:B:177:ALA:HA	2:B:182:ILE:HD12	1.96	0.47
3:C:34:LEU:O	3:C:38:ARG:HG2	2.15	0.47
1:A:957:U:H4'	19:S:79:THR:HG23	1.96	0.47
1:A:1533:C:H2'	1:A:1534:A:N1	2.30	0.47
1:A:988:G:C6	1:A:989:C:C2	3.03	0.47
6:F:53:ALA:HB3	6:F:86:ARG:HH11	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:S:36:ARG:HD3	19:S:72:GLY:HA3	1.97	0.47
22:W:32:ILE:HG22	22:W:63:THR:HA	1.97	0.47
1:A:14:U:H1'	1:A:17:U:H5	1.80	0.46
1:A:199:G:N2	1:A:219:C:C2	2.83	0.46
2:B:80:ILE:HG21	2:B:212:GLN:HA	1.96	0.46
13:M:11:ARG:HG3	13:M:12:ASN:HB2	1.97	0.46
1:A:1119:C:OP2	9:I:9:ARG:NH2	2.44	0.46
1:A:1171:G:N2	1:A:1172:C:C2	2.82	0.46
1:A:201:C:H42	1:A:216:G:H1	1.63	0.46
1:A:199:G:C2	1:A:219:C:N3	2.83	0.46
1:A:269:C:H2'	1:A:270:A:H8	1.79	0.46
17:Q:61:GLU:HA	17:Q:71:PHE:CE1	2.50	0.46
1:A:1320:C:OP1	19:S:70:LYS:HE3	2.15	0.46
1:A:1084:G:H2'	1:A:1085:U:C5	2.51	0.46
1:A:1127:G:N2	1:A:1145:C:C2	2.83	0.46
1:A:290:C:H2'	1:A:291:C:O4'	2.16	0.46
1:A:585:G:C2	1:A:586:C:C2	3.04	0.46
1:A:908:A:H2'	1:A:909:A:H8	1.80	0.46
3:C:137:ALA:O	3:C:141:VAL:HG23	2.15	0.46
5:E:110:LEU:HD13	5:E:118:ILE:HD12	1.97	0.46
9:I:7:THR:O	9:I:83:ARG:CD	2.64	0.46
1:A:1535:C:C4	1:A:1536:C:H5	2.29	0.46
1:A:23:C:C4	1:A:24:U:C4	3.03	0.46
1:A:277:C:H5'	17:Q:68:ARG:HH12	1.79	0.46
1:A:35:G:C6	1:A:36:C:N4	2.84	0.46
1:A:725:G:N1	1:A:726:C:C4	2.83	0.46
1:A:806:C:H2'	1:A:807:A:C8	2.51	0.46
1:A:834:C:C2	1:A:853:G:C2	3.02	0.46
6:F:100:ASN:HB3	18:R:28:GLU:HA	1.96	0.46
10:J:31:GLY:HA2	10:J:78:ASN:HD22	1.81	0.46
13:M:88:ARG:HG3	13:M:98:VAL:HG11	1.97	0.46
16:P:7:ALA:O	16:P:17:TYR:HA	2.15	0.46
25:Z:49:G:C8	25:Z:49:G:O5'	2.68	0.46
1:A:1431:C:H3'	1:A:1432:G:H8	1.81	0.46
1:A:194:C:H4'	20:T:64:ASP:HB3	1.96	0.46
1:A:376:G:H5''	16:P:5:ARG:HB2	1.96	0.46
1:A:895:G:H1	1:A:904:C:H42	1.63	0.46
2:B:213:LEU:O	2:B:217:ARG:HG2	2.15	0.46
11:K:22:HIS:HB3	11:K:29:ILE:HG23	1.98	0.46
1:A:1077:G:N2	1:A:1080:A:OP2	2.41	0.46
1:A:259:G:C2	1:A:268:C:C2	3.04	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:663:A:H2'	1:A:664:G:O4'	2.16	0.46
1:A:838:G:N2	1:A:849:C:C2	2.83	0.46
1:A:977:A:O2'	1:A:979:C:OP2	2.21	0.46
14:N:44:LEU:HD22	14:N:53:LEU:HD11	1.98	0.46
1:A:1050:G:C2	1:A:1209:C:C2	3.04	0.46
1:A:289:G:N2	1:A:290:C:C2	2.84	0.46
1:A:931:C:H3'	1:A:932:C:H5''	1.98	0.46
17:Q:92:ARG:HH11	17:Q:92:ARG:HB3	1.81	0.46
1:A:1078:U:H5	1:A:1079:G:N1	2.14	0.46
1:A:1419:G:C2	1:A:1420:C:C2	3.04	0.46
1:A:1533:C:H4'	24:Y:32:A:H61	1.80	0.46
1:A:127:G:N2	1:A:235:C:C2	2.84	0.46
1:A:389:A:H3'	1:A:390:C:C6	2.51	0.46
1:A:392:G:H5'	16:P:12:LYS:HG3	1.98	0.46
5:E:93:PRO:CB	8:H:105:ARG:NH1	2.78	0.46
22:W:26:LEU:HD12	22:W:30:PRO:HD2	1.98	0.46
25:Z:58:A:O2'	25:Z:60:U:OP2	2.34	0.46
1:A:919:A:N3	1:A:1080:A:H2	2.13	0.46
1:A:1119:C:H42	1:A:1154:G:H1	1.63	0.46
1:A:1440:C:H42	1:A:1461:G:H1	1.63	0.46
1:A:1508:G:C6	1:A:1509:C:C4	3.04	0.46
1:A:971:G:OP1	1:A:972:C:H5''	2.16	0.46
1:A:986:A:H2'	1:A:987:G:C8	2.50	0.46
3:C:26:LYS:H	3:C:26:LYS:CE	2.28	0.46
11:K:88:GLY:O	11:K:90:GLY:N	2.47	0.46
1:A:1074:G:C6	1:A:1075:C:C4	3.03	0.46
1:A:1430:C:C2	1:A:1471:G:C2	3.03	0.46
1:A:200:G:N2	1:A:218:C:C2	2.84	0.46
1:A:917:G:H2'	1:A:918:A:H8	1.79	0.46
1:A:928:G:H2'	1:A:929:G:H8	1.80	0.46
4:D:59:ARG:HH12	4:D:62:GLN:HG3	1.81	0.46
12:L:41:ARG:HD2	12:L:43:VAL:HG22	1.98	0.46
1:A:18:C:H2'	1:A:19:C:C6	2.51	0.45
1:A:21:G:H21	1:A:914:A:H62	1.62	0.45
1:A:113:G:H1'	1:A:354:G:H5'	1.98	0.45
1:A:763:G:C2	1:A:764:C:C2	3.04	0.45
1:A:908:A:H2'	1:A:909:A:C8	2.50	0.45
1:A:988:G:C6	1:A:989:C:C4	3.04	0.45
3:C:157:ILE:HD12	3:C:164:ARG:HB2	1.97	0.45
4:D:116:GLN:O	4:D:120:LEU:HG	2.16	0.45
7:G:101:LEU:HA	7:G:104:LEU:HD12	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:932:C:O5'	7:G:4:ARG:HG2	2.15	0.45
1:A:579:G:H2'	1:A:580:U:C6	2.51	0.45
1:A:781:A:N6	1:A:802:A:H1'	2.31	0.45
1:A:1256:A:C5'	3:C:27:LYS:CE	2.81	0.45
5:E:144:THR:HB	5:E:147:ASP:H	1.81	0.45
14:N:37:PHE:HB3	14:N:39:LEU:HD12	1.97	0.45
17:Q:48:GLU:HB2	17:Q:50:LYS:HB2	1.97	0.45
25:Z:70:G:N1	25:Z:71:C:C2	2.85	0.45
1:A:1033:G:H2'	1:A:1034:G:C8	2.52	0.45
1:A:291:C:H2'	1:A:292:G:H8	1.81	0.45
1:A:548:G:C2	1:A:549:C:C2	3.04	0.45
2:B:87:ARG:HE	2:B:219:VAL:CG1	2.29	0.45
11:K:32:ILE:HG22	11:K:40:ILE:HD12	1.98	0.45
16:P:6:LEU:HD11	16:P:73:LEU:HD12	1.98	0.45
1:A:184:G:H2'	1:A:185:A:C8	2.51	0.45
1:A:233:C:H2'	1:A:234:C:C6	2.52	0.45
1:A:399:G:C2	1:A:400:C:C2	3.04	0.45
1:A:662:G:N1	1:A:744:C:C2	2.84	0.45
1:A:671:G:C2	1:A:736:C:C2	3.04	0.45
1:A:774:G:C2	1:A:806:C:N3	2.84	0.45
11:K:84:VAL:HG23	11:K:110:ASP:HA	1.98	0.45
1:A:1081:G:H8	1:A:1081:G:OP2	2.00	0.45
1:A:122:G:N1	1:A:123:C:C2	2.85	0.45
1:A:1401:G:H2'	1:A:1402:C:O4'	2.16	0.45
1:A:1459:C:H2'	1:A:1460:A:H8	1.82	0.45
1:A:439:A:C6	1:A:441:A:H1'	2.51	0.45
1:A:865:A:H2'	1:A:866:C:C6	2.51	0.45
1:A:872:A:C4	1:A:874:G:N7	2.84	0.45
13:M:68:GLY:HA2	13:M:71:ARG:HD2	1.98	0.45
1:A:1536:C:C2	24:Y:30:G:N1	2.85	0.45
1:A:1106:G:N1	1:A:1107:C:C4	2.85	0.45
1:A:19:C:O2	1:A:917:G:C2	2.69	0.45
1:A:226:G:H2'	1:A:227:G:O4'	2.17	0.45
1:A:500:G:C2	1:A:501:C:N3	2.84	0.45
1:A:968:A:OP1	1:A:968:A:H8	1.99	0.45
1:A:991:U:C4	1:A:1212:U:H1'	2.51	0.45
11:K:43:SER:HB3	11:K:68:ALA:HB2	1.98	0.45
12:L:25:PRO:C	12:L:27:LEU:N	2.69	0.45
3:C:30:ARG:NH2	14:N:38:GLY:N	2.65	0.45
20:T:63:ILE:HG21	20:T:81:LYS:HG3	1.99	0.45
25:Z:17:C:OP1	25:Z:60:U:O2'	2.26	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:Z:10:G:N2	25:Z:26:G:H1'	2.32	0.45
1:A:1017:G:C6	1:A:1018:C:C4	3.04	0.45
1:A:63:C:H42	1:A:104:G:H1	1.65	0.45
1:A:1305:G:OP2	21:V:5:ASP:HB2	2.17	0.45
1:A:1478:C:H2'	1:A:1479:C:C6	2.52	0.45
1:A:1508:G:H2'	1:A:1509:C:O4'	2.16	0.45
1:A:571:U:H3'	1:A:572:A:H5''	1.98	0.45
1:A:767:A:H2'	1:A:768:A:O4'	2.17	0.45
1:A:880:C:H5''	12:L:12:ARG:HH21	1.81	0.45
1:A:977:A:H3'	1:A:977:A:N3	2.32	0.45
20:T:63:ILE:HG23	20:T:77:ALA:HB1	1.97	0.45
1:A:1390:U:H2'	1:A:1391:U:C6	2.52	0.45
1:A:187:C:N3	1:A:191:G:C2	2.84	0.45
1:A:571:U:C3'	1:A:572:A:H5''	2.47	0.45
1:A:929:G:C2	1:A:930:C:C2	3.04	0.45
1:A:939:G:C2	1:A:940:C:N3	2.85	0.45
3:C:174:PRO:HD2	3:C:182:ILE:HD11	1.99	0.45
1:A:1120:G:H2'	1:A:1121:U:C6	2.51	0.45
1:A:1488:G:H2'	1:A:1489:G:H8	1.81	0.45
1:A:15:G:C5	1:A:16:A:N7	2.85	0.45
1:A:370:C:N3	1:A:392:G:C2	2.85	0.45
1:A:886:G:C2	1:A:912:C:O2	2.70	0.45
1:A:15:G:N2	5:E:17:ALA:O	2.47	0.45
6:F:48:LEU:HD13	6:F:52:ILE:HB	1.99	0.45
7:G:65:ALA:HB1	7:G:127:ALA:HB3	1.99	0.45
25:Z:70:G:C6	25:Z:71:C:N3	2.85	0.45
1:A:1171:G:C2	1:A:1172:C:C2	3.05	0.45
1:A:1343:G:C6	1:A:1344:C:N3	2.85	0.45
1:A:145:G:C2	1:A:178:C:N3	2.86	0.45
1:A:743:U:H2'	1:A:744:C:H6	1.81	0.45
4:D:88:VAL:HG12	4:D:91:SER:H	1.82	0.45
17:Q:29:HIS:CE1	17:Q:31:LEU:HB3	2.52	0.45
1:A:105:G:C2	1:A:106:C:C2	3.05	0.44
1:A:1086:U:O5'	1:A:1086:U:H6	2.00	0.44
1:A:127:G:C2	1:A:235:C:N3	2.85	0.44
1:A:1327:C:H2'	1:A:1328:C:C6	2.52	0.44
1:A:1526:G:H2'	1:A:1527:C:C6	2.51	0.44
1:A:252:U:H2'	1:A:253:U:C6	2.52	0.44
1:A:443:C:C2	1:A:492:G:N2	2.85	0.44
1:A:864:A:C2'	1:A:865:A:C8	2.88	0.44
3:C:57:ILE:HG12	3:C:66:VAL:HG22	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:93:PRO:CB	8:H:105:ARG:NH2	2.64	0.44
1:A:101:A:C4	1:A:102:G:C8	3.05	0.44
1:A:1222:G:C2	1:A:1223:C:N3	2.85	0.44
1:A:1225:A:N3	1:A:1225:A:H2'	2.31	0.44
1:A:1252:A:H2'	1:A:1253:G:O4'	2.17	0.44
1:A:1371:G:H2'	1:A:1372:U:C6	2.52	0.44
1:A:1478:C:H2'	1:A:1479:C:H6	1.81	0.44
1:A:823:G:C2	1:A:824:C:C2	3.05	0.44
9:I:89:ASN:HB3	9:I:92:TYR:CE2	2.52	0.44
13:M:88:ARG:O	13:M:92:HIS:HD2	2.00	0.44
1:A:1134:G:C2	1:A:1141:C:N3	2.85	0.44
1:A:518:C:H2'	1:A:530:G:C8	2.52	0.44
1:A:514:C:H42	1:A:537:G:H1	1.65	0.44
1:A:914:A:C4	1:A:915:A:N7	2.86	0.44
4:D:57:ARG:HG3	4:D:57:ARG:HH11	1.82	0.44
17:Q:21:VAL:HG11	17:Q:59:ILE:HG13	1.99	0.44
25:Z:37:A:C5	25:Z:38:A:C5	3.06	0.44
1:A:1014:A:N1	19:S:34:TRP:CE2	2.86	0.44
1:A:1133:G:H1	1:A:1141:C:N4	2.15	0.44
1:A:1537:U:H3	24:Y:28:A:N6	2.15	0.44
1:A:262:A:H5''	20:T:76:ALA:HB2	2.00	0.44
1:A:255:G:C2	1:A:272:C:C2	3.06	0.44
1:A:748:C:H1'	1:A:749:C:H5	1.82	0.44
1:A:982:U:H4'	1:A:983:A:O4'	2.18	0.44
2:B:126:GLU:HA	2:B:129:GLU:HG3	1.99	0.44
3:C:24:ALA:HB3	3:C:29:TYR:CD2	2.53	0.44
5:E:18:ARG:HD3	5:E:20:GLN:NE2	2.32	0.44
23:X:4:GLU:HA	23:X:66:ARG:NH1	2.32	0.44
1:A:1220:G:H2'	1:A:1221:G:O4'	2.17	0.44
1:A:138:G:H1	1:A:225:C:N4	2.15	0.44
1:A:1464:G:C2	1:A:1465:C:N3	2.86	0.44
1:A:256:U:H2'	1:A:257:G:C8	2.52	0.44
1:A:109:A:C6	1:A:326:G:C6	3.06	0.44
1:A:354:G:N1	1:A:355:C:C4	2.86	0.44
1:A:577:G:C6	1:A:578:C:C4	3.05	0.44
1:A:590:C:C2	1:A:650:G:N2	2.85	0.44
1:A:932:C:C2	1:A:1386:G:N2	2.85	0.44
7:G:27:ILE:HA	7:G:30:ILE:HD12	1.98	0.44
9:I:3:GLN:HA	9:I:19:LEU:O	2.18	0.44
15:O:85:LEU:HD12	15:O:87:ILE:HD11	1.98	0.44
1:A:1129:C:O5'	1:A:1130:A:H8	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:76:ILE:HD12	5:E:118:ILE:HG21	2.00	0.44
1:A:1380:U:C5	7:G:3:ARG:HG3	2.53	0.44
1:A:1004:A:H5''	1:A:1025:U:C4	2.52	0.44
1:A:1353:G:N1	1:A:1354:C:C4	2.86	0.44
1:A:1419:G:C6	1:A:1420:C:C4	3.05	0.44
1:A:230:G:H2'	1:A:231:G:O4'	2.18	0.44
1:A:372:C:H4'	1:A:373:A:O5'	2.17	0.44
1:A:806:C:H2'	1:A:807:A:H8	1.83	0.44
1:A:929:G:C6	1:A:930:C:C4	3.06	0.44
1:A:975:A:C5'	1:A:975:A:H8	2.31	0.44
3:C:150:LYS:HG3	3:C:169:ALA:HB2	1.99	0.44
3:C:79:ARG:HG3	3:C:82:GLU:HG2	1.99	0.44
4:D:107:ARG:HD3	4:D:173:TRP:HZ2	1.82	0.44
1:A:701:C:H3'	23:X:67:TYR:OH	2.17	0.44
25:Z:49:G:H8	25:Z:49:G:O5'	2.00	0.44
1:A:585:G:C6	1:A:586:C:C4	3.05	0.44
1:A:769:G:H4'	1:A:1513:A:H4'	2.00	0.44
1:A:823:G:C6	1:A:824:C:N4	2.85	0.44
1:A:90:U:H2'	1:A:91:C:C5	2.52	0.44
1:A:947:G:C2	1:A:948:C:C2	3.06	0.44
1:A:956:U:O2	1:A:956:U:C2'	2.66	0.44
19:S:34:TRP:HA	19:S:52:TYR:CB	2.43	0.44
25:Z:16:C:H2'	25:Z:17:C:C5	2.53	0.44
25:Z:18:G:H21	25:Z:57:A:H2'	1.83	0.44
1:A:105:G:C5	1:A:106:C:C4	3.05	0.44
1:A:1408:A:H2'	1:A:1409:C:C6	2.53	0.44
1:A:1437:C:H2'	1:A:1438:G:C8	2.53	0.44
1:A:1464:G:C6	1:A:1465:C:N4	2.86	0.44
1:A:1422:G:H1	1:A:1478:C:H42	1.66	0.44
1:A:223:U:H5'	20:T:68:LYS:NZ	2.33	0.44
1:A:524:G:N2	1:A:525:C:N3	2.66	0.44
1:A:874:G:N1	1:A:875:C:C4	2.85	0.44
6:F:50:TYR:CE1	18:R:77:GLY:HA2	2.52	0.44
25:Z:37:A:C3'	25:Z:38:A:H8	2.31	0.44
25:Z:40:C:H2'	25:Z:41:C:H6	1.80	0.44
25:Z:60:U:H2'	25:Z:61:C:C5	2.53	0.44
25:Z:65:C:H2'	25:Z:66:C:O4'	2.18	0.44
1:A:1257:U:H4'	1:A:1258:G:O5'	2.18	0.43
1:A:1422:G:H1	1:A:1478:C:N4	2.16	0.43
1:A:1504:G:H4'	1:A:1505:G:O5'	2.17	0.43
1:A:1507:A:C2	1:A:1508:G:C4	3.06	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:819:A:H5'	1:A:820:U:H5	1.82	0.43
4:D:100:ARG:CZ	4:D:137:SER:HA	2.48	0.43
6:F:33:TYR:HB2	6:F:75:LEU:HD23	1.99	0.43
1:A:1534:A:N1	24:Y:31:U:O4	2.51	0.43
25:Z:19:G:H5''	25:Z:60:U:O4	2.18	0.43
1:A:1119:C:H2'	1:A:1120:G:C8	2.53	0.43
1:A:1233:G:C2	1:A:1234:C:N3	2.87	0.43
1:A:130:A:C8	1:A:130:A:OP1	2.71	0.43
1:A:1526:G:C2	1:A:1527:C:C2	3.06	0.43
1:A:51:A:H4'	1:A:52:G:C5'	2.48	0.43
1:A:825:G:C2	1:A:826:C:C2	3.06	0.43
4:D:31:CYS:C	4:D:33:MET:H	2.21	0.43
7:G:69:VAL:HG11	7:G:134:ALA:HB1	2.00	0.43
12:L:64:TYR:HB3	12:L:66:VAL:HG13	2.00	0.43
16:P:59:TRP:HA	16:P:62:VAL:HG22	2.00	0.43
22:W:15:GLU:HB3	22:W:23:ARG:CB	2.45	0.43
22:W:70:ARG:HB2	22:W:71:LYS:HD2	2.00	0.43
25:Z:52:G:N2	25:Z:63:G:N3	2.65	0.43
1:A:1096:C:H2'	1:A:1097:C:H6	1.81	0.43
1:A:1425:U:H2'	1:A:1426:C:C6	2.53	0.43
1:A:320:C:H2'	1:A:321:A:C8	2.52	0.43
1:A:389:A:H3'	1:A:390:C:H6	1.82	0.43
1:A:774:G:C2	1:A:806:C:C2	3.05	0.43
1:A:861:G:C2	1:A:862:C:C2	3.06	0.43
2:B:172:ILE:H	2:B:172:ILE:HG13	1.43	0.43
1:A:1014:A:C2	19:S:34:TRP:CD1	3.06	0.43
1:A:1050:G:C2	1:A:1209:C:O2	2.71	0.43
1:A:1356:G:C2	1:A:1367:C:C2	3.07	0.43
1:A:198:G:H1	1:A:219:C:N4	2.16	0.43
1:A:25:C:H2'	1:A:26:A:C8	2.53	0.43
1:A:352:C:H4'	1:A:354:G:OP1	2.17	0.43
1:A:769:G:N1	1:A:770:C:C4	2.86	0.43
6:F:11:ASN:HB2	6:F:86:ARG:HH21	1.83	0.43
9:I:104:ARG:NH1	9:I:106:ALA:HA	2.33	0.43
25:Z:67:C:H2'	25:Z:68:C:C6	2.54	0.43
1:A:1063:C:H42	1:A:1193:G:H1	1.65	0.43
1:A:1241:G:N1	1:A:1242:C:C4	2.86	0.43
1:A:394:G:C2	1:A:395:C:C2	3.06	0.43
1:A:926:G:N2	24:Y:37:U:OP2	2.52	0.43
10:J:71:LEU:HA	10:J:71:LEU:HD22	1.71	0.43
16:P:9:PHE:CD1	16:P:18:ARG:HG3	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:T:43:LEU:HD13	20:T:52:ALA:HA	1.99	0.43
25:Z:50:U:C2	25:Z:51:C:C4	3.07	0.43
1:A:1022:G:H2'	1:A:1023:G:H8	1.79	0.43
1:A:1053:G:N7	1:A:1200:C:H5''	2.34	0.43
1:A:1249:C:H4'	9:I:73:GLN:HE22	1.83	0.43
1:A:1286:A:H2'	1:A:1287:A:H4'	2.01	0.43
1:A:1365:G:C5	1:A:1366:C:C4	3.07	0.43
1:A:34:C:H2'	1:A:35:G:H8	1.83	0.43
1:A:456:C:C4	1:A:457:C:N4	2.87	0.43
4:D:177:ASP:HB3	4:D:182:LYS:HB2	2.01	0.43
1:A:1149:C:H2'	1:A:1150:U:O4'	2.19	0.43
1:A:1431:C:H2'	1:A:1432:G:O4'	2.18	0.43
1:A:1505:G:H4'	1:A:1506:U:H5''	2.01	0.43
1:A:384:G:C2	1:A:385:C:C2	3.07	0.43
2:B:142:LEU:O	2:B:146:GLN:HB2	2.18	0.43
15:O:3:ILE:HA	15:O:38:ARG:HH22	1.84	0.43
25:Z:37:A:C2'	25:Z:38:A:C8	3.02	0.43
1:A:1074:G:C2	1:A:1075:C:C2	3.07	0.43
1:A:1207:G:C6	1:A:1208:C:C4	3.07	0.43
1:A:504:C:C2	1:A:542:G:C2	3.07	0.43
1:A:70:G:C6	1:A:100:C:N3	2.87	0.43
1:A:881:G:C6	1:A:882:C:C4	3.06	0.43
1:A:955:U:H1'	1:A:1227:A:H61	1.84	0.43
3:C:32:LEU:HG	3:C:32:LEU:H	1.70	0.43
9:I:89:ASN:HA	9:I:90:PRO:HD2	1.79	0.43
15:O:87:ILE:HG22	15:O:88:ARG:H	1.82	0.43
19:S:11:VAL:HB	19:S:16:LEU:HD22	2.00	0.43
23:X:20:GLY:HA2	23:X:59:ILE:HD12	2.00	0.43
1:A:235:C:OP1	17:Q:70:ARG:NH1	2.51	0.43
1:A:524:G:N2	1:A:525:C:C2	2.87	0.43
2:B:124:SER:O	2:B:127:ILE:HG13	2.19	0.43
1:A:1250:A:H4'	9:I:67:GLY:HA2	2.00	0.43
13:M:18:ALA:O	13:M:21:TYR:HB2	2.19	0.43
25:Z:52:G:C6	25:Z:53:G:C5	3.07	0.43
1:A:101:A:H2'	1:A:102:G:C8	2.48	0.43
1:A:17:U:O2'	1:A:1079:G:H1'	2.18	0.43
1:A:1077:G:C2	1:A:1079:G:H3'	2.50	0.43
1:A:1135:U:H4'	1:A:1136:U:H5	1.84	0.43
1:A:385:C:H2'	1:A:386:C:O4'	2.19	0.43
1:A:500:G:H1	1:A:545:C:H42	1.67	0.43
1:A:876:G:C2	1:A:877:C:N3	2.87	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:966:G:C2	1:A:967:C:C2	3.07	0.43
8:H:39:LEU:HB3	8:H:45:ILE:HG12	2.00	0.43
13:M:23:TYR:HB3	13:M:67:GLU:HA	2.00	0.43
14:N:9:LYS:HG3	14:N:21:TYR:O	2.19	0.43
25:Z:17:C:O2	25:Z:17:C:H2'	2.18	0.43
1:A:102:G:C2	1:A:103:C:C2	3.07	0.42
1:A:1163:C:C2	1:A:1174:G:N2	2.87	0.42
1:A:1524:C:H5''	11:K:120:ARG:NH2	2.34	0.42
1:A:216:G:H2'	1:A:217:C:C6	2.53	0.42
1:A:685:G:H5'	11:K:12:ARG:HH12	1.84	0.42
1:A:79:G:C2'	1:A:80:G:H8	2.32	0.42
2:B:18:GLY:HA3	2:B:41:ILE:HA	2.00	0.42
17:Q:26:GLN:HB2	17:Q:26:GLN:HE21	1.74	0.42
1:A:1179:A:OP2	9:I:93:ARG:NH2	2.51	0.42
1:A:1207:G:C2	1:A:1208:C:C2	3.07	0.42
1:A:1489:G:C2	1:A:1490:C:C2	3.06	0.42
1:A:164:U:H2'	1:A:165:C:C6	2.53	0.42
1:A:374:A:C6	1:A:375:U:C4	3.08	0.42
1:A:402:G:C2	1:A:403:C:C2	3.07	0.42
1:A:550:G:H2'	1:A:551:U:C6	2.54	0.42
1:A:855:G:C6	1:A:856:C:C4	3.07	0.42
1:A:867:G:N2	1:A:868:C:C2	2.87	0.42
1:A:903:G:C2	1:A:904:C:C2	3.07	0.42
1:A:91:C:C6	1:A:91:C:H3'	2.54	0.42
3:C:35:GLU:HB3	3:C:59:ARG:HH22	1.83	0.42
10:J:50:ILE:N	10:J:60:ARG:HG3	2.34	0.42
19:S:5:LEU:HD13	19:S:9:VAL:HA	2.01	0.42
25:Z:18:G:O5'	25:Z:18:G:H8	2.01	0.42
25:Z:55:PSU:H2'	25:Z:56:C:H3'	2.00	0.42
1:A:110:C:H2'	1:A:111:G:O4'	2.20	0.42
1:A:1151:A:O2'	1:A:1152:A:H8	2.02	0.42
1:A:1231:G:H4'	9:I:126:SER:HB3	2.01	0.42
1:A:728:A:H2'	1:A:729:A:C8	2.54	0.42
1:A:926:G:C6	1:A:1505:G:C6	3.08	0.42
3:C:150:LYS:HB3	3:C:201:TYR:HB2	2.01	0.42
1:A:1050:G:C2	1:A:1051:C:C2	3.07	0.42
1:A:1078:U:O2'	1:A:1079:G:O4'	2.36	0.42
1:A:1097:C:H2'	1:A:1098:C:C6	2.55	0.42
1:A:1165:C:H42	1:A:1171:G:H1	1.68	0.42
1:A:1363(A):A:H1'	1:A:1365:G:N7	2.34	0.42
1:A:342:C:C2	1:A:348:G:N2	2.87	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:500:G:N2	1:A:501:C:C2	2.88	0.42
1:A:562:C:H1'	12:L:15:ARG:HG3	2.01	0.42
1:A:64:G:H4'	1:A:65:U:H5''	2.01	0.42
1:A:682:G:H2'	1:A:683:G:O4'	2.19	0.42
1:A:872:A:H2'	1:A:872:A:N3	2.35	0.42
1:A:918:A:H2	1:A:1079:G:H21	1.50	0.42
12:L:93:LEU:HA	12:L:94:PRO:HD3	1.91	0.42
1:A:1088:G:H2'	1:A:1089:G:O4'	2.20	0.42
1:A:1220:G:H2'	1:A:1221:G:H8	1.84	0.42
1:A:1353:G:C6	1:A:1354:C:N4	2.88	0.42
1:A:1540:U:H3	24:Y:25:A:N6	2.17	0.42
1:A:245:C:C2	1:A:284:G:C2	3.07	0.42
1:A:309:G:H2'	1:A:310:G:C8	2.53	0.42
1:A:318:G:N2	1:A:336:C:C2	2.88	0.42
1:A:500:G:C2	1:A:501:C:C2	3.08	0.42
1:A:734:G:C2	1:A:735:C:C2	3.07	0.42
1:A:917:G:C6	1:A:918:A:C6	3.08	0.42
3:C:177:THR:HG23	3:C:180:ALA:HB2	2.01	0.42
22:W:40:MET:HA	22:W:45:ILE:HD12	2.01	0.42
1:A:1230:C:H5'	25:Z:30:G:H5''	2.01	0.42
25:Z:41:C:H2'	25:Z:42:G:H8	1.82	0.42
1:A:1253:G:C2	1:A:1254:C:C2	3.08	0.42
1:A:1310:G:C2	1:A:1328:C:N3	2.88	0.42
10:J:24:VAL:HG12	10:J:28:ARG:HE	1.83	0.42
1:A:1116:C:H2'	1:A:1117:G:O4'	2.20	0.42
1:A:1305:G:N2	1:A:1331:G:H1'	2.34	0.42
1:A:1445:C:O2	1:A:1458:G:C2	2.72	0.42
1:A:1526:G:C6	1:A:1527:C:N4	2.88	0.42
1:A:198:G:OP2	1:A:198:G:C8	2.72	0.42
1:A:444:C:H42	1:A:490:G:H1	1.67	0.42
1:A:742:G:H2'	1:A:743:U:O4'	2.20	0.42
1:A:786:G:H2'	1:A:787:A:O4'	2.20	0.42
1:A:975:A:C5'	1:A:975:A:C8	3.02	0.42
2:B:233:SER:HA	2:B:234:PRO:HD3	1.77	0.42
9:I:13:ALA:HB2	9:I:68:GLY:HA3	2.00	0.42
13:M:102:ARG:NH1	13:M:104:ARG:HB3	2.34	0.42
18:R:47:THR:HG22	18:R:83:GLU:H	1.84	0.42
1:A:1074:G:N1	1:A:1075:C:C2	2.88	0.42
1:A:1084:G:H2'	1:A:1085:U:C6	2.54	0.42
1:A:1144:G:N2	1:A:1146:A:H62	2.17	0.42
1:A:147:G:C2	1:A:176:C:C2	3.07	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:321:A:H2'	1:A:322:C:H6	1.85	0.42
1:A:416:G:C6	1:A:417:C:N3	2.88	0.42
1:A:42:G:C6	1:A:43:C:C4	3.07	0.42
1:A:736:C:H2'	1:A:737:A:H8	1.83	0.42
1:A:800:G:H2'	1:A:801:U:C6	2.54	0.42
1:A:855:G:C2	1:A:856:C:C2	3.08	0.42
12:L:124:LYS:HA	12:L:125:PRO:HD2	1.82	0.42
1:A:553:A:H1'	12:L:31:PRO:HG3	2.02	0.42
1:A:1080:A:H5''	5:E:16:THR:CB	2.46	0.42
1:A:1538:C:C5	18:R:16:PRO:HA	2.55	0.42
1:A:409:G:OP1	4:D:24:GLU:HB3	2.20	0.42
1:A:445:G:H2'	1:A:446:G:O4'	2.19	0.42
1:A:370:C:O2	1:A:482:A:O2'	2.38	0.42
1:A:689:C:H42	1:A:698:G:H1	1.67	0.42
1:A:784:C:N3	1:A:799:G:C2	2.88	0.42
1:A:79:G:N1	1:A:91:C:C2	2.87	0.42
1:A:817:C:C2	1:A:819:A:O4'	2.73	0.42
1:A:895:G:C2	1:A:896:C:C2	3.07	0.42
1:A:918:A:H2'	1:A:919:A:O4'	2.20	0.42
2:B:28:PHE:HA	2:B:194:PRO:HG3	2.02	0.42
3:C:46:GLU:HB2	3:C:47:LEU:HD12	2.02	0.42
4:D:185:PHE:HZ	4:D:189:PRO:HD3	1.84	0.42
1:A:1371:G:OP1	9:I:68:GLY:HA2	2.20	0.42
12:L:24:VAL:HG13	12:L:98:TYR:HE1	1.85	0.42
20:T:73:HIS:HB3	20:T:74:LYS:HG3	2.01	0.42
1:A:1064:G:N2	1:A:1190:G:C2'	2.79	0.42
1:A:1106:G:C2	1:A:1107:C:N3	2.88	0.42
1:A:354:G:C6	1:A:355:C:N4	2.88	0.42
1:A:356:A:H2'	1:A:357:G:O4'	2.20	0.42
1:A:376:G:H2'	1:A:377:G:C8	2.50	0.42
1:A:505:G:H2'	1:A:506:G:C8	2.53	0.42
10:J:75:ILE:HG13	10:J:75:ILE:H	1.55	0.42
15:O:35:ARG:HB3	15:O:59:MET:SD	2.60	0.42
17:Q:29:HIS:HE1	17:Q:31:LEU:HB3	1.85	0.42
25:Z:60:U:H2'	25:Z:61:C:H5	1.85	0.42
1:A:104:G:C2	1:A:105:G:C5	3.08	0.41
1:A:1116:C:H3'	1:A:1117:G:H5''	2.02	0.41
1:A:1241:G:C6	1:A:1242:C:N4	2.88	0.41
1:A:1314:C:OP2	19:S:6:LYS:HB3	2.19	0.41
1:A:1387:G:C2	1:A:1388:C:C2	3.08	0.41
1:A:1423:G:C2	1:A:1424:C:C2	3.08	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1488:G:H2'	1:A:1489:G:C8	2.54	0.41
1:A:319:G:C2	1:A:320:C:C2	3.07	0.41
1:A:338:A:H2'	1:A:339:C:O4'	2.20	0.41
1:A:402:G:C6	1:A:403:C:C4	3.07	0.41
1:A:407:G:C2	1:A:436:C:C2	3.08	0.41
1:A:43:C:H2'	1:A:44:G:C8	2.55	0.41
1:A:524:G:N1	1:A:525:C:N4	2.68	0.41
1:A:81:U:H1'	1:A:88:A:H62	1.86	0.41
1:A:903:G:C6	1:A:904:C:C4	3.08	0.41
1:A:949:A:O2'	1:A:971:G:O6	2.25	0.41
1:A:959:A:H1'	1:A:985:C:H1'	2.01	0.41
6:F:15:ASP:OD1	6:F:18:GLN:HB2	2.20	0.41
11:K:27:ASN:HB2	11:K:55:LYS:HB3	2.01	0.41
13:M:84:ILE:HG22	19:S:66:MET:HE3	2.02	0.41
19:S:12:ASP:OD1	19:S:37:ARG:HB2	2.20	0.41
25:Z:18:G:O5'	25:Z:18:G:C8	2.73	0.41
1:A:1040:U:H2'	1:A:1041:A:C8	2.55	0.41
1:A:258:G:C2	1:A:269:C:C2	3.09	0.41
1:A:28:G:H2'	1:A:29:G:O4'	2.20	0.41
1:A:295:C:C4	1:A:296:U:C4	3.08	0.41
1:A:333:G:C2	1:A:334:C:C2	3.08	0.41
1:A:344:A:H5''	1:A:345:C:H5	1.85	0.41
1:A:662:G:C6	1:A:744:C:N3	2.88	0.41
1:A:681:C:N4	1:A:709:G:H1	2.18	0.41
1:A:825:G:C6	1:A:826:C:C4	3.08	0.41
2:B:19:HIS:CD2	2:B:20:GLU:HG2	2.55	0.41
3:C:30:ARG:NH2	3:C:30:ARG:HB2	2.23	0.41
18:R:19:LYS:HB3	18:R:20:ALA:H	1.69	0.41
25:Z:22:G:C2	25:Z:23:C:C2	3.08	0.41
1:A:1078:U:H5	1:A:1079:G:C6	2.39	0.41
1:A:1074:G:H1	1:A:1083:U:H3	1.69	0.41
1:A:1166:G:N2	1:A:1169:A:H3'	2.35	0.41
1:A:1375:A:N3	1:A:1375:A:H2'	2.34	0.41
1:A:310:G:H5'	16:P:31:LYS:HB2	2.01	0.41
1:A:321:A:H2'	1:A:322:C:C6	2.54	0.41
1:A:414:A:H2'	1:A:415:A:O4'	2.19	0.41
1:A:453:A:H2'	1:A:454:C:C6	2.55	0.41
1:A:576:G:H3'	1:A:577:G:C5'	2.49	0.41
1:A:646:U:H2'	1:A:647:C:C6	2.55	0.41
1:A:794:A:H2'	1:A:795:C:C6	2.55	0.41
1:A:981:U:O4	1:A:1223:C:N4	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1190:G:H5'	3:C:176:HIS:HE1	1.84	0.41
3:C:3:ASN:HB2	3:C:4:LYS:H	1.72	0.41
4:D:3:ARG:HH21	4:D:71:SER:HB2	1.85	0.41
6:F:12:PRO:HG3	6:F:57:GLN:O	2.20	0.41
8:H:82:HIS:CE1	8:H:84:ARG:HB2	2.55	0.41
1:A:1371:G:O3'	9:I:69:GLY:HA3	2.21	0.41
25:Z:36:U:C2	25:Z:37:A:C8	3.09	0.41
1:A:1424:C:N4	1:A:1476:G:H1	2.18	0.41
1:A:157:G:C6	1:A:165:C:N3	2.89	0.41
1:A:446:G:N2	1:A:489:C:C2	2.88	0.41
1:A:519:C:H2'	1:A:520:A:C8	2.54	0.41
1:A:660:G:H2'	1:A:661:G:O4'	2.20	0.41
1:A:77:G:C8	1:A:77:G:H3'	2.56	0.41
1:A:876:G:C2	1:A:877:C:C2	3.08	0.41
2:B:54:THR:HG23	2:B:199:TYR:HB3	2.02	0.41
4:D:8:VAL:HG11	4:D:21:LEU:HB2	2.03	0.41
13:M:84:ILE:HG22	19:S:66:MET:CE	2.50	0.41
16:P:59:TRP:CA	16:P:62:VAL:HG22	2.50	0.41
11:K:110:ASP:HB3	18:R:85:LEU:HB3	2.02	0.41
20:T:36:LEU:HA	20:T:36:LEU:HD23	1.90	0.41
25:Z:22:G:N1	25:Z:23:C:C4	2.89	0.41
1:A:1157:A:H4'	1:A:1158:C:O5'	2.19	0.41
1:A:15:G:O4'	1:A:1396:A:O2'	2.39	0.41
1:A:317:G:H2'	1:A:318:G:O4'	2.20	0.41
1:A:518:C:H4'	1:A:519:C:O5'	2.21	0.41
1:A:830:G:N2	1:A:857:C:C2	2.89	0.41
1:A:947:G:C6	1:A:948:C:C4	3.08	0.41
4:D:175:SER:HB3	4:D:186:LEU:HD11	2.02	0.41
8:H:119:LEU:HD13	8:H:124:ALA:HB2	2.03	0.41
1:A:1171:G:N1	1:A:1172:C:C4	2.89	0.41
1:A:289:G:C2	1:A:290:C:C2	3.08	0.41
1:A:363:A:C6	12:L:31:PRO:HD2	2.56	0.41
1:A:41:G:H2'	1:A:42:G:C8	2.56	0.41
1:A:42:G:C2	1:A:43:C:C2	3.08	0.41
1:A:551:U:H2'	1:A:552:U:H6	1.82	0.41
1:A:832:C:O2	1:A:855:G:C2	2.74	0.41
1:A:910:C:H5''	12:L:97:ARG:HH21	1.86	0.41
2:B:184:VAL:N	2:B:198:ASP:HB2	2.30	0.41
3:C:108:ASN:HA	3:C:109:PRO:HD2	1.77	0.41
8:H:29:SER:HB3	8:H:32:LYS:HB2	2.02	0.41
17:Q:62:SER:OG	17:Q:72:ARG:HG3	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:V:10:ARG:HA	21:V:13:ILE:HD12	2.03	0.41
23:X:100:GLN:HA	23:X:103:LEU:HD23	2.02	0.41
1:A:1292:U:H2'	1:A:1293:G:C8	2.56	0.41
1:A:1368:G:N1	1:A:1369:C:C4	2.88	0.41
1:A:299:G:C6	1:A:300:A:C6	3.09	0.41
1:A:336:C:H2'	1:A:337:C:C6	2.56	0.41
1:A:456:C:C2	1:A:476:G:C2	3.09	0.41
1:A:671:G:C6	1:A:736:C:N4	2.88	0.41
1:A:763:G:C6	1:A:764:C:C4	3.09	0.41
1:A:872:A:C8	1:A:874:G:C8	3.09	0.41
8:H:83:ILE:HG13	8:H:137:VAL:HG22	2.03	0.41
9:I:74:ILE:HA	9:I:77:ILE:HD12	2.02	0.41
3:C:6:HIS:CG	14:N:49:HIS:HB3	2.56	0.41
1:A:1068:G:C2	1:A:1069:C:C2	3.09	0.41
1:A:1235:U:H2'	1:A:1236:A:O4'	2.20	0.41
1:A:1253:G:C6	1:A:1254:C:C4	3.08	0.41
1:A:146:G:C2	1:A:177:C:C2	3.09	0.41
1:A:217:C:H2'	1:A:218:C:H6	1.85	0.41
1:A:319:G:C6	1:A:320:C:C4	3.09	0.41
1:A:741:G:H2'	1:A:742:G:O4'	2.21	0.41
1:A:863:U:H2'	1:A:865:A:OP2	2.21	0.41
2:B:167:PRO:HG2	2:B:192:SER:OG	2.20	0.41
4:D:135:LEU:HA	4:D:136:PRO:HD3	1.92	0.41
4:D:196:LEU:HA	4:D:197:PRO:HD3	1.89	0.41
4:D:50:ARG:HA	4:D:51:PRO:HD3	1.87	0.41
5:E:69:VAL:HG21	5:E:113:ALA:HB1	2.02	0.41
10:J:50:ILE:HG13	10:J:60:ARG:CD	2.35	0.41
11:K:18:ARG:HA	11:K:81:ASP:H	1.84	0.41
15:O:39:LEU:HD13	15:O:56:LEU:HA	2.03	0.41
25:Z:60:U:H3'	25:Z:61:C:C5	2.55	0.41
1:A:1000:U:C5	1:A:1001:A:C8	3.08	0.41
1:A:1075:C:H5'	1:A:1101:A:N6	2.36	0.41
1:A:1076:C:H2'	1:A:1077:G:H8	1.83	0.41
1:A:119:A:H2'	1:A:240:C:H41	1.85	0.41
1:A:1292:U:H2'	1:A:1293:G:H8	1.86	0.41
1:A:1307:U:H2'	1:A:1308:U:C6	2.55	0.41
1:A:1369:C:OP1	14:N:61:TRP:NE1	2.51	0.41
1:A:643:C:H2'	1:A:644:G:C8	2.55	0.41
1:A:691:G:H3'	11:K:26:ASN:ND2	2.35	0.41
1:A:77:G:C8	1:A:77:G:C3'	3.04	0.41
1:A:832:C:C2	1:A:855:G:C2	3.09	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:862:C:H2'	1:A:863:U:O4'	2.20	0.41
1:A:895:G:C6	1:A:896:C:C4	3.09	0.41
6:F:69:GLU:HG3	6:F:69:GLU:H	1.57	0.41
7:G:149:ARG:HG2	7:G:152:ALA:HB2	2.03	0.41
7:G:69:VAL:O	7:G:71:PRO:HD3	2.21	0.41
1:A:392:G:P	16:P:8:ARG:HH22	2.44	0.41
18:R:44:LEU:HD12	18:R:79:LEU:HD22	2.03	0.41
20:T:53:LEU:HD22	20:T:102:GLY:HA3	2.01	0.41
1:A:999:C:H2'	1:A:1000:U:H5'	2.03	0.41
1:A:1028:C:H2'	1:A:1029:C:C4'	2.51	0.41
1:A:1255:G:O2'	1:A:1258:G:H1'	2.21	0.41
1:A:433:C:H2'	1:A:434:U:C6	2.56	0.41
1:A:542:G:C6	1:A:543:C:N4	2.89	0.41
1:A:544:G:C2	1:A:545:C:C2	3.09	0.41
1:A:579:G:H1	1:A:762:C:H42	1.68	0.41
1:A:725:G:C2	1:A:726:C:C2	3.09	0.41
1:A:837:G:H2'	1:A:838:G:O4'	2.21	0.41
1:A:918:A:C6	1:A:919:A:C6	3.09	0.41
2:B:12:GLU:HG3	2:B:15:VAL:HB	2.02	0.41
4:D:98:GLU:HG3	4:D:103:ASN:ND2	2.36	0.41
1:A:1080:A:P	5:E:14:ARG:HH22	2.43	0.41
11:K:121:PRO:HB2	11:K:125:PHE:HB2	2.02	0.41
17:Q:61:GLU:HA	17:Q:71:PHE:CD1	2.56	0.41
20:T:89:ARG:HD2	20:T:104:LEU:HD22	2.03	0.41
1:A:1348:U:H2'	1:A:1349:A:H8	1.86	0.41
1:A:13:U:H3'	1:A:14:U:H6	1.86	0.41
1:A:324:G:N2	1:A:326:G:H3'	2.36	0.41
1:A:625:G:H2'	1:A:626:U:C6	2.56	0.41
1:A:896:C:H2'	1:A:897:C:O4'	2.21	0.41
1:A:919:A:N3	1:A:1080:A:C2	2.89	0.41
1:A:975:A:H5''	1:A:975:A:H8	1.85	0.41
7:G:113:GLU:HG2	7:G:119:ARG:HG2	2.03	0.41
1:A:1492:A:H2'	22:W:19:ASN:HA	2.02	0.41
25:Z:51:C:H42	25:Z:63:G:H1	1.68	0.41
1:A:1050:G:N1	1:A:1051:C:C4	2.89	0.40
1:A:942:G:C6	1:A:1342:C:N3	2.89	0.40
1:A:1345:U:C4	1:A:1375:A:N6	2.60	0.40
1:A:1411:C:H4'	12:L:43:VAL:HG11	2.03	0.40
1:A:1423:G:C6	1:A:1424:C:C4	3.10	0.40
1:A:44:G:OP2	16:P:12:LYS:HE3	2.20	0.40
1:A:527:G:N2	1:A:528:C:C2	2.89	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:956:U:H2'	1:A:957:U:O4'	2.22	0.40
13:M:96:LEU:HD23	13:M:97:PRO:HD2	2.03	0.40
1:A:1314:C:N4	19:S:4:SER:HB2	2.35	0.40
1:A:1060:C:P	14:N:45:ARG:HH22	2.44	0.40
1:A:1077:G:N1	1:A:1080:A:OP2	2.51	0.40
1:A:1312:G:N2	1:A:1326:C:C2	2.89	0.40
1:A:1371:G:H2'	1:A:1372:U:H6	1.85	0.40
1:A:1528:U:H1'	1:A:1530:G:H5'	2.03	0.40
1:A:289:G:C6	1:A:290:C:C4	3.09	0.40
1:A:373:A:H2'	1:A:374:A:H8	1.86	0.40
1:A:552:U:H2'	1:A:553:A:H8	1.86	0.40
1:A:751:U:H2'	1:A:752:G:O4'	2.21	0.40
1:A:861:G:C6	1:A:862:C:C4	3.09	0.40
1:A:921:U:H2'	1:A:922:G:O4'	2.20	0.40
1:A:986:A:H2'	1:A:987:G:O4'	2.20	0.40
1:A:988:G:C2	1:A:989:C:C2	3.08	0.40
7:G:106:GLN:O	7:G:110:GLN:HG2	2.21	0.40
11:K:34:ASP:OD2	11:K:38:ASN:HB2	2.20	0.40
12:L:60:LEU:HD21	12:L:66:VAL:HG22	2.02	0.40
1:A:1129:C:H1'	1:A:1132:C:H5	1.86	0.40
1:A:1409:C:H2'	1:A:1410:G:C8	2.55	0.40
1:A:1431:C:H42	1:A:1469:G:H1	1.69	0.40
1:A:1512:U:H2'	1:A:1513:A:C8	2.57	0.40
1:A:174:C:H2'	1:A:175:C:C6	2.56	0.40
1:A:394:G:C6	1:A:395:C:C4	3.09	0.40
1:A:677:U:H3	1:A:713:G:H1	1.68	0.40
1:A:678:U:H2'	1:A:679:C:H6	1.82	0.40
1:A:731:G:C6	1:A:732:C:C4	3.10	0.40
6:F:50:TYR:HE1	18:R:77:GLY:HA2	1.86	0.40
25:Z:31:G:H2'	25:Z:32:OMC:C6	2.55	0.40
25:Z:2:G:C2	25:Z:3:C:C2	3.10	0.40
1:A:105:G:C6	1:A:106:C:C4	3.09	0.40
1:A:1351:U:H2'	1:A:1352:C:H6	1.85	0.40
1:A:1361:G:C2	1:A:1362:C:O2	2.74	0.40
1:A:1440:C:N4	1:A:1461:G:H1	2.19	0.40
1:A:1461:G:H2'	1:A:1462:G:C8	2.56	0.40
1:A:671:G:H2'	1:A:672:U:O4'	2.21	0.40
3:C:39:ILE:O	3:C:43:LEU:HG	2.21	0.40
3:C:82:GLU:O	3:C:85:ARG:HB3	2.20	0.40
4:D:171:GLY:C	4:D:173:TRP:H	2.25	0.40
5:E:80:ILE:HD12	5:E:91:LEU:HB2	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:22:ILE:HG22	13:M:24:GLY:H	1.86	0.40
25:Z:18:G:C4	25:Z:57:A:C6	3.09	0.40
1:A:137:C:C2	1:A:227:G:C2	3.09	0.40
1:A:16:A:C2	1:A:17:U:C6	3.09	0.40
1:A:200:G:C6	1:A:201:C:N3	2.90	0.40
1:A:123:C:H5''	1:A:311:C:O2'	2.21	0.40
1:A:328:C:H4'	1:A:329:A:H5'	2.03	0.40
1:A:542:G:C2	1:A:543:C:C2	3.10	0.40
1:A:629:G:H2'	1:A:630:G:O4'	2.21	0.40
1:A:902:G:H2'	1:A:903:G:H8	1.86	0.40
1:A:968:A:C8	1:A:1062:U:H4'	2.56	0.40
7:G:96:GLN:HA	7:G:99:LEU:HD12	2.03	0.40
11:K:123:LYS:HA	11:K:126:ARG:HG3	2.03	0.40
13:M:45:VAL:HA	13:M:48:LEU:HD12	2.04	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%)	195 (84%)	24 (10%)	13 (6%)	2	29
3	C	204/239 (85%)	177 (87%)	18 (9%)	9 (4%)	3	34
4	D	206/209 (99%)	191 (93%)	12 (6%)	3 (2%)	13	58
5	E	148/162 (91%)	140 (95%)	8 (5%)	0	100	100
6	F	99/101 (98%)	94 (95%)	5 (5%)	0	100	100
7	G	153/156 (98%)	144 (94%)	7 (5%)	2 (1%)	15	60
8	H	136/138 (99%)	129 (95%)	6 (4%)	1 (1%)	26	71
9	I	125/128 (98%)	107 (86%)	15 (12%)	3 (2%)	7	49
10	J	96/105 (91%)	72 (75%)	16 (17%)	8 (8%)	1	18

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
11	K	117/129 (91%)	99 (85%)	13 (11%)	5 (4%)	3	35
12	L	122/132 (92%)	101 (83%)	17 (14%)	4 (3%)	5	42
13	M	119/126 (94%)	102 (86%)	16 (13%)	1 (1%)	24	70
14	N	58/61 (95%)	51 (88%)	5 (9%)	2 (3%)	5	42
15	O	86/89 (97%)	84 (98%)	1 (1%)	1 (1%)	16	62
16	P	81/88 (92%)	73 (90%)	7 (9%)	1 (1%)	16	62
17	Q	97/105 (92%)	88 (91%)	6 (6%)	3 (3%)	5	44
18	R	71/88 (81%)	66 (93%)	4 (6%)	1 (1%)	14	59
19	S	80/93 (86%)	66 (82%)	11 (14%)	3 (4%)	4	38
20	T	97/106 (92%)	80 (82%)	12 (12%)	5 (5%)	2	30
21	V	22/27 (82%)	21 (96%)	1 (4%)	0	100	100
22	W	69/72 (96%)	58 (84%)	7 (10%)	4 (6%)	2	28
23	X	166/171 (97%)	150 (90%)	13 (8%)	3 (2%)	11	55
All	All	2584/2781 (93%)	2288 (88%)	224 (9%)	72 (3%)	10	46

All (72) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	21	ARG
2	B	24	TRP
9	I	119	ALA
11	K	101	SER
12	L	79	GLU
18	R	87	ARG
20	T	94	ALA
23	X	8	ASN
23	X	54	PRO
2	B	17	PHE
2	B	207	ALA
3	C	61	ALA
3	C	154	SER
3	C	179	ARG
7	G	7	ALA
9	I	56	LEU
10	J	55	LYS
16	P	81	ARG
19	S	30	LEU

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Mol	Chain	Res	Type
20	T	13	LEU
20	T	49	ALA
2	B	20	GLU
2	B	99	GLY
2	B	204	ASN
2	B	228	GLY
3	C	14	ILE
10	J	30	SER
10	J	34	VAL
10	J	35	SER
10	J	90	LEU
11	K	126	ARG
12	L	27	LEU
14	N	31	ARG
15	O	88	ARG
17	Q	68	ARG
19	S	6	LYS
22	W	2	LYS
2	B	95	GLN
3	C	4	LYS
3	C	81	GLY
3	C	108	ASN
3	C	168	ALA
4	D	5	ILE
4	D	172	PRO
9	I	58	HIS
14	N	23	ARG
17	Q	99	SER
19	S	71	LEU
20	T	97	ALA
22	W	44	TYR
2	B	229	VAL
10	J	39	PRO
10	J	54	PHE
11	K	12	ARG
11	K	13	GLN
12	L	45	PRO
17	Q	80	GLY
20	T	9	ASN
23	X	73	GLU
2	B	130	ARG
7	G	55	GLY

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Mol	Chain	Res	Type
10	J	40	LEU
12	L	51	ALA
13	M	6	GLY
22	W	45	ILE
3	C	205	GLY
4	D	142	PRO
8	H	5	PRO
11	K	90	GLY
2	B	125	PRO
2	B	208	ILE
22	W	50	GLY

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	B	202/220 (92%)	166 (82%)	36 (18%)	2	17
3	C	160/188 (85%)	142 (89%)	18 (11%)	7	36
4	D	180/181 (99%)	148 (82%)	32 (18%)	2	17
5	E	115/123 (94%)	93 (81%)	22 (19%)	2	14
6	F	90/90 (100%)	75 (83%)	15 (17%)	3	20
7	G	126/127 (99%)	121 (96%)	5 (4%)	38	72
8	H	119/119 (100%)	98 (82%)	21 (18%)	2	18
9	I	98/99 (99%)	84 (86%)	14 (14%)	4	27
10	J	87/92 (95%)	76 (87%)	11 (13%)	5	31
11	K	90/99 (91%)	73 (81%)	17 (19%)	2	14
12	L	104/109 (95%)	89 (86%)	15 (14%)	4	27
13	M	97/101 (96%)	84 (87%)	13 (13%)	5	29
14	N	49/50 (98%)	43 (88%)	6 (12%)	6	33
15	O	79/80 (99%)	64 (81%)	15 (19%)	2	14
16	P	72/74 (97%)	59 (82%)	13 (18%)	2	16

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
17	Q	94/97 (97%)	80 (85%)	14 (15%)	4	25
18	R	64/77 (83%)	52 (81%)	12 (19%)	2	15
19	S	71/80 (89%)	58 (82%)	13 (18%)	2	15
20	T	76/82 (93%)	60 (79%)	16 (21%)	1	11
21	V	19/22 (86%)	19 (100%)	0	100	100
22	W	62/63 (98%)	52 (84%)	10 (16%)	3	22
23	X	145/150 (97%)	126 (87%)	19 (13%)	5	30
All	All	2199/2323 (95%)	1862 (85%)	337 (15%)	7	24

All (337) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	11	LEU
2	B	21	ARG
2	B	23	ARG
2	B	24	TRP
2	B	25	ASN
2	B	44	LEU
2	B	48	MET
2	B	51	LEU
2	B	59	GLU
2	B	61	LEU
2	B	67	THR
2	B	96	ARG
2	B	97	TRP
2	B	103	THR
2	B	107	THR
2	B	108	ILE
2	B	111	ARG
2	B	136	VAL
2	B	137	ARG
2	B	144	ARG
2	B	154	LEU
2	B	163	PHE
2	B	165	VAL
2	B	172	ILE
2	B	178	ARG
2	B	179	LYS
2	B	187	LEU
2	B	198	ASP

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Mol	Chain	Res	Type
2	B	204	ASN
2	B	208	ILE
2	B	213	LEU
2	B	215	LEU
2	B	216	SER
2	B	236	TYR
2	B	238	LEU
2	B	240	GLN
3	C	3	ASN
3	C	14	ILE
3	C	17	ASP
3	C	26	LYS
3	C	30	ARG
3	C	37	GLN
3	C	56	ASP
3	C	79	ARG
3	C	88	ARG
3	C	90	GLU
3	C	91	LEU
3	C	99	VAL
3	C	162	GLN
3	C	167	TRP
3	C	172	ARG
3	C	188	LEU
3	C	191	THR
3	C	204	LEU
4	D	3	ARG
4	D	14	ARG
4	D	34	GLU
4	D	35	ARG
4	D	42	GLN
4	D	50	ARG
4	D	53	ASP
4	D	59	ARG
4	D	64	LEU
4	D	66	ARG
4	D	73	ARG
4	D	76	ARG
4	D	81	GLU
4	D	83	SER
4	D	118	ARG
4	D	122	ARG

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Mol	Chain	Res	Type
4	D	131	ARG
4	D	132	ARG
4	D	134	ASP
4	D	135	LEU
4	D	141	ARG
4	D	150	GLU
4	D	152	SER
4	D	159	ARG
4	D	162	LEU
4	D	176	LEU
4	D	186	LEU
4	D	187	ARG
4	D	190	ASP
4	D	192	GLU
4	D	194	LEU
4	D	207	TYR
5	E	6	PHE
5	E	12	LEU
5	E	13	ILE
5	E	15	ARG
5	E	24	ARG
5	E	41	VAL
5	E	43	LEU
5	E	53	LEU
5	E	56	GLN
5	E	76	ILE
5	E	80	ILE
5	E	87	SER
5	E	98	THR
5	E	112	LEU
5	E	118	ILE
5	E	119	LEU
5	E	137	GLU
5	E	141	GLN
5	E	144	THR
5	E	147	ASP
5	E	148	VAL
5	E	150	ARG
6	F	2	ARG
6	F	21	LEU
6	F	36	ARG
6	F	45	LEU

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Mol	Chain	Res	Type
6	F	46	ARG
6	F	47	ARG
6	F	54	LYS
6	F	65	VAL
6	F	69	GLU
6	F	71	ARG
6	F	73	ASN
6	F	75	LEU
6	F	78	GLU
6	F	89	MET
6	F	98	LEU
7	G	8	GLU
7	G	11	GLN
7	G	38	LEU
7	G	72	ARG
7	G	126	ASP
8	H	11	THR
8	H	18	ARG
8	H	21	LYS
8	H	22	GLU
8	H	24	THR
8	H	36	LEU
8	H	39	LEU
8	H	50	ARG
8	H	52	ASP
8	H	54	ASP
8	H	59	LEU
8	H	69	ARG
8	H	85	ARG
8	H	99	GLU
8	H	102	ARG
8	H	105	ARG
8	H	112	LEU
8	H	115	SER
8	H	127	LEU
8	H	135	CYS
8	H	136	GLU
9	I	2	GLU
9	I	3	GLN
9	I	12	GLU
9	I	14	VAL
9	I	34	ASN

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Mol	Chain	Res	Type
9	I	35	GLU
9	I	38	GLN
9	I	71	SER
9	I	79	LEU
9	I	102	LEU
9	I	111	ARG
9	I	112	LYS
9	I	118	LYS
9	I	121	ARG
10	J	17	ASP
10	J	49	VAL
10	J	60	ARG
10	J	71	LEU
10	J	75	ILE
10	J	79	ARG
10	J	82	ILE
10	J	86	MET
10	J	87	THR
10	J	89	ASP
10	J	92	THR
11	K	11	LYS
11	K	14	VAL
11	K	16	SER
11	K	18	ARG
11	K	41	THR
11	K	57	THR
11	K	62	GLN
11	K	84	VAL
11	K	91	ARG
11	K	92	GLU
11	K	93	GLN
11	K	96	ARG
11	K	98	LEU
11	K	108	ILE
11	K	120	ARG
11	K	126	ARG
11	K	129	SER
12	L	6	THR
12	L	13	LYS
12	L	15	ARG
12	L	33	ARG
12	L	37	CYS

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Mol	Chain	Res	Type
12	L	41	ARG
12	L	42	THR
12	L	53	ARG
12	L	59	ARG
12	L	77	LEU
12	L	78	GLN
12	L	97	ARG
12	L	104	VAL
12	L	111	LYS
12	L	126	LYS
13	M	12	ASN
13	M	16	ASP
13	M	31	LYS
13	M	32	GLU
13	M	35	GLU
13	M	44	ARG
13	M	56	LEU
13	M	80	ARG
13	M	81	LEU
13	M	84	ILE
13	M	96	LEU
13	M	102	ARG
13	M	121	LYS
14	N	16	PHE
14	N	17	LYS
14	N	22	THR
14	N	41	ARG
14	N	44	LEU
14	N	61	TRP
15	O	3	ILE
15	O	5	LYS
15	O	8	LYS
15	O	25	THR
15	O	31	LEU
15	O	39	LEU
15	O	41	GLU
15	O	43	LEU
15	O	52	SER
15	O	54	ARG
15	O	56	LEU
15	O	63	ARG
15	O	64	ARG

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Mol	Chain	Res	Type
15	O	70	LEU
15	O	81	LEU
16	P	8	ARG
16	P	26	ARG
16	P	28	ARG
16	P	44	THR
16	P	53	VAL
16	P	60	LEU
16	P	67	THR
16	P	68	ASP
16	P	69	THR
16	P	71	ARG
16	P	72	ARG
16	P	79	VAL
16	P	83	GLU
17	Q	24	GLU
17	Q	26	GLN
17	Q	34	LYS
17	Q	53	LEU
17	Q	57	VAL
17	Q	58	GLU
17	Q	68	ARG
17	Q	70	ARG
17	Q	72	ARG
17	Q	81	ARG
17	Q	91	ARG
17	Q	92	ARG
17	Q	98	LEU
17	Q	100	LYS
18	R	17	SER
18	R	21	LYS
18	R	23	LYS
18	R	25	THR
18	R	39	VAL
18	R	47	THR
18	R	53	ARG
18	R	55	ARG
18	R	75	ILE
18	R	81	PHE
18	R	82	THR
18	R	87	ARG
19	S	6	LYS

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Mol	Chain	Res	Type
19	S	7	LYS
19	S	29	ARG
19	S	30	LEU
19	S	37	ARG
19	S	39	THR
19	S	41	VAL
19	S	49	ILE
19	S	53	ASN
19	S	63	THR
19	S	66	MET
19	S	79	THR
19	S	80	TYR
20	T	8	ARG
20	T	10	LEU
20	T	13	LEU
20	T	17	ARG
20	T	19	SER
20	T	25	ARG
20	T	39	LYS
20	T	42	GLN
20	T	45	GLN
20	T	53	LEU
20	T	55	ILE
20	T	56	MET
20	T	64	ASP
20	T	68	LYS
20	T	73	HIS
20	T	84	LEU
22	W	2	LYS
22	W	6	THR
22	W	14	THR
22	W	21	THR
22	W	32	ILE
22	W	33	LEU
22	W	46	ARG
22	W	58	THR
22	W	63	THR
22	W	71	LYS
23	X	7	THR
23	X	12	ARG
23	X	31	THR
23	X	35	LEU

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Mol	Chain	Res	Type
23	X	64	LYS
23	X	67	TYR
23	X	87	SER
23	X	91	ARG
23	X	92	VAL
23	X	95	ASP
23	X	98	ASP
23	X	103	LEU
23	X	118	VAL
23	X	125	ARG
23	X	147	LEU
23	X	151	GLU
23	X	162	ASN
23	X	164	LEU
23	X	168	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	19	HIS
2	B	104	ASN
3	C	6	HIS
3	C	69	HIS
3	C	108	ASN
3	C	136	GLN
3	C	176	HIS
4	D	45	GLN
4	D	62	GLN
4	D	161	ASN
5	E	20	GLN
7	G	28	ASN
7	G	37	ASN
9	I	73	GLN
9	I	124	GLN
10	J	76	ASN
10	J	78	ASN
11	K	26	ASN
11	K	38	ASN
12	L	75	HIS
13	M	92	HIS
17	Q	26	GLN
19	S	53	ASN

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Mol	Chain	Res	Type
19	S	56	GLN
19	S	83	HIS
23	X	100	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	1505/1522 (98%)	420 (27%)	103 (6%)
24	Y	15/42 (35%)	7 (46%)	0
25	Z	74/77 (96%)	33 (44%)	9 (12%)
All	All	1594/1641 (97%)	460 (28%)	112 (7%)

All (460) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	8	A
1	A	9	G
1	A	13	U
1	A	19	C
1	A	22	G
1	A	29	G
1	A	31	G
1	A	32	A
1	A	39	G
1	A	43	C
1	A	44	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	58	C
1	A	60	A
1	A	61	G
1	A	66	G
1	A	68	G
1	A	72	C
1	A	76	C
1	A	77	G

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Mol	Chain	Res	Type
1	A	78	G
1	A	79	G
1	A	81	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	129(A)	G
1	A	130	A
1	A	131	C
1	A	144	G
1	A	151	A
1	A	157	G
1	A	163	C
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	217	C
1	A	220	G
1	A	244	U
1	A	247	G
1	A	251	G
1	A	253	U
1	A	266	G
1	A	267	C
1	A	280	C
1	A	281	G
1	A	282	A

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Mol	Chain	Res	Type
1	A	283	C
1	A	288	A
1	A	289	G
1	A	291	C
1	A	298	A
1	A	301	G
1	A	306	G
1	A	313	A
1	A	315	A
1	A	316	G
1	A	325	A
1	A	328	C
1	A	329	A
1	A	330	C
1	A	332	G
1	A	342	C
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	354	G
1	A	366	C
1	A	367	U
1	A	372	C
1	A	373	A
1	A	375	U
1	A	378	G
1	A	384	G
1	A	388	G
1	A	390	C
1	A	392	G
1	A	393	A
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	414	A

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Mol	Chain	Res	Type
1	A	419	C
1	A	421	U
1	A	422	C
1	A	423	G
1	A	428	G
1	A	429	U
1	A	430	A
1	A	439	A
1	A	441	A
1	A	450	G
1	A	452	A
1	A	453	A
1	A	454	C
1	A	455	C
1	A	470	C
1	A	481	G
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	527	G
1	A	528	C
1	A	529	G
1	A	531	U
1	A	532	A
1	A	534	U
1	A	535	A
1	A	540	G
1	A	543	C
1	A	545	C
1	A	547	A
1	A	550	G
1	A	559	A
1	A	560	U

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Mol	Chain	Res	Type
1	A	561	U
1	A	562	C
1	A	564	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	596	C
1	A	607	A
1	A	619	U
1	A	641	U
1	A	642	A
1	A	653	A
1	A	665	A
1	A	666	G
1	A	671	G
1	A	687	A
1	A	688	G
1	A	693	G
1	A	701	C
1	A	702	A
1	A	703	G
1	A	713	G
1	A	716	A
1	A	717	C
1	A	721	G
1	A	723	U
1	A	724	G
1	A	728	A
1	A	731	G
1	A	744	C
1	A	748	C
1	A	749	C
1	A	755	G
1	A	760	G
1	A	774	G
1	A	785	G
1	A	787	A
1	A	789	U

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Mol	Chain	Res	Type
1	A	792	A
1	A	793	U
1	A	794	A
1	A	796	C
1	A	799	G
1	A	804	U
1	A	809	G
1	A	811	C
1	A	812	C
1	A	815	A
1	A	817	C
1	A	818	G
1	A	819	A
1	A	821	G
1	A	828	A
1	A	839	U
1	A	841	U
1	A	853	G
1	A	855	G
1	A	864	A
1	A	870	U
1	A	871	U
1	A	873	A
1	A	876	G
1	A	882	C
1	A	885	G
1	A	900	A
1	A	902	G
1	A	919	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	938	A
1	A	945	G
1	A	951	G
1	A	955	U
1	A	956	U

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Mol	Chain	Res	Type
1	A	957	U
1	A	958	A
1	A	959	A
1	A	961	U
1	A	965	A
1	A	966	G
1	A	969	A
1	A	971	G
1	A	974	A
1	A	975	A
1	A	976	G
1	A	977	A
1	A	985	C
1	A	986	A
1	A	991	U
1	A	992	U
1	A	993	G
1	A	994	A
1	A	998	G
1	A	1000	U
1	A	1001	A
1	A	1002	G
1	A	1005	A
1	A	1014	A
1	A	1015	A
1	A	1016	A
1	A	1017	G
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	1036	G
1	A	1045	C
1	A	1050	G
1	A	1051	C
1	A	1053	G
1	A	1054	C
1	A	1056	U
1	A	1060	C

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Mol	Chain	Res	Type
1	A	1064	G
1	A	1065	U
1	A	1066	C
1	A	1067	A
1	A	1075	C
1	A	1076	C
1	A	1078	U
1	A	1079	G
1	A	1085	U
1	A	1086	U
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	1124	G
1	A	1125	U
1	A	1127	G
1	A	1128	C
1	A	1129	C
1	A	1130	A
1	A	1131	G
1	A	1134	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	1171	G
1	A	1183	A
1	A	1184	G
1	A	1187	G
1	A	1190	G
1	A	1191	A

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Mol	Chain	Res	Type
1	A	1195	C
1	A	1196	U
1	A	1197	G
1	A	1200	C
1	A	1201	A
1	A	1202	G
1	A	1210	C
1	A	1212	U
1	A	1213	A
1	A	1215	G
1	A	1222	G
1	A	1223	C
1	A	1224	G
1	A	1225	A
1	A	1226	C
1	A	1227	A
1	A	1236	A
1	A	1238	A
1	A	1250	A
1	A	1253	G
1	A	1256	A
1	A	1257	U
1	A	1258	G
1	A	1260	C
1	A	1270	C
1	A	1278	U
1	A	1279	A
1	A	1280	A
1	A	1281	U
1	A	1282	C
1	A	1285	A
1	A	1286	A
1	A	1287	A
1	A	1290	G
1	A	1299	A
1	A	1300	G
1	A	1301	U
1	A	1302	U
1	A	1303	C
1	A	1305	G
1	A	1312	G
1	A	1315	U

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Mol	Chain	Res	Type
1	A	1317	C
1	A	1318	A
1	A	1319	A
1	A	1320	C
1	A	1322	C
1	A	1323	G
1	A	1328	C
1	A	1336	C
1	A	1346	A
1	A	1347	G
1	A	1353	G
1	A	1357	A
1	A	1363	C
1	A	1363(A)	A
1	A	1364	U
1	A	1367	C
1	A	1370	G
1	A	1379	G
1	A	1380	U
1	A	1381	U
1	A	1394	A
1	A	1398	A
1	A	1412	C
1	A	1419	G
1	A	1423	G
1	A	1440	C
1	A	1442	G
1	A	1443	G
1	A	1447	A
1	A	1452	C
1	A	1456	G
1	A	1457	G
1	A	1488	G
1	A	1492	A
1	A	1493	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

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Mol	Chain	Res	Type
1	A	1507	A
1	A	1517	G
1	A	1520	G
1	A	1528	U
1	A	1529	G
1	A	1530	G
1	A	1531	A
1	A	1532	U
1	A	1533	C
1	A	1534	A
1	A	1535	C
1	A	1536	C
1	A	1537	U
1	A	1539	C
1	A	1540	U
1	A	1541	U
24	Y	28	A
24	Y	30	G
24	Y	31	U
24	Y	32	A
24	Y	37	U
24	Y	38	G
24	Y	39	U
25	Z	3	C
25	Z	6	G
25	Z	7	G
25	Z	8	4SU
25	Z	9	G
25	Z	13	C
25	Z	16	C
25	Z	17	C
25	Z	17(A)	U
25	Z	18	G
25	Z	19	G
25	Z	20	U
25	Z	26	G
25	Z	34	C
25	Z	36	U
25	Z	37	A
25	Z	40	C
25	Z	42	G
25	Z	43	A

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Mol	Chain	Res	Type
25	Z	47	U
25	Z	48	C
25	Z	50	U
25	Z	51	C
25	Z	53	G
25	Z	55	PSU
25	Z	56	C
25	Z	59	A
25	Z	66	C
25	Z	67	C
25	Z	68	C
25	Z	69	C
25	Z	70	G
25	Z	76	A

All (112) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	7	G
1	A	30	U
1	A	31	G
1	A	48	C
1	A	49	U
1	A	51	A
1	A	60	A
1	A	115	G
1	A	119	A
1	A	129(A)	G
1	A	181	G
1	A	189(F)	U
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	305	G
1	A	315	A
1	A	328	C
1	A	329	A
1	A	344	A

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Mol	Chain	Res	Type
1	A	351	G
1	A	372	C
1	A	389	A
1	A	428	G
1	A	429	U
1	A	484	G
1	A	495	A
1	A	496	A
1	A	508	C
1	A	509	A
1	A	518	C
1	A	531	U
1	A	535	A
1	A	559	A
1	A	560	U
1	A	561	U
1	A	575	G
1	A	576	G
1	A	595	G
1	A	641	U
1	A	687	A
1	A	701	C
1	A	703	G
1	A	717	C
1	A	748	C
1	A	792	A
1	A	864	A
1	A	872	A
1	A	884	U
1	A	931	C
1	A	933	G
1	A	934	C
1	A	956	U
1	A	958	A
1	A	960	U
1	A	965	A
1	A	968	A
1	A	975	A
1	A	992	U
1	A	993	G
1	A	1000	U
1	A	1065	U

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Mol	Chain	Res	Type
1	A	1078	U
1	A	1101	A
1	A	1139	G
1	A	1145	C
1	A	1182	G
1	A	1190	G
1	A	1196	U
1	A	1201	A
1	A	1212	U
1	A	1214	C
1	A	1222	G
1	A	1224	G
1	A	1225	A
1	A	1226	C
1	A	1239	A
1	A	1257	U
1	A	1278	U
1	A	1279	A
1	A	1285	A
1	A	1299	A
1	A	1300	G
1	A	1301	U
1	A	1318	A
1	A	1331	G
1	A	1346	A
1	A	1363(A)	A
1	A	1380	U
1	A	1415	G
1	A	1442(B)	A
1	A	1447	A
1	A	1493	A
1	A	1498	U
1	A	1504	G
1	A	1531	A
1	A	1533	C
1	A	1534	A
1	A	1536	C
25	Z	17	C
25	Z	36	U
25	Z	47	U
25	Z	50	U
25	Z	51	C

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Mol	Chain	Res	Type
25	Z	55	PSU
25	Z	58	A
25	Z	60	U
25	Z	71	C

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	0.76	1 (6%)	20,31,34	1.76	4 (20%)
25	G7M	Z	46	25	18,26,27	2.79	4 (22%)	21,39,42	2.77	7 (33%)
25	5MU	Z	54	25	13,22,23	0.85	0	16,32,35	3.41	3 (18%)
25	PSU	Z	55	25	15,21,22	1.16	1 (6%)	16,30,33	2.36	2 (12%)
25	4SU	Z	8	25	12,21,22	0.97	1 (8%)	15,30,33	1.52	3 (20%)

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	55	PSU	C5-C1'	-2.74	1.49	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	Z	46	G7M	O4'-C1'	2.02	1.44	1.41
25	Z	8	4SU	O4'-C1'	2.14	1.44	1.41
25	Z	32	OMC	O4'-C1'	2.24	1.44	1.41
25	Z	46	G7M	C6-C5	3.66	1.48	1.41
25	Z	46	G7M	C8-N7	7.24	1.46	1.33
25	Z	46	G7M	C8-N9	8.02	1.48	1.33

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	Z	54	5MU	C5-C4-N3	-9.60	117.29	125.35
25	Z	46	G7M	N7-C8-N9	-7.71	97.28	108.67
25	Z	46	G7M	C5-C6-N1	-5.36	116.52	123.52
25	Z	8	4SU	C5-C4-N3	-4.05	119.27	123.56
25	Z	46	G7M	N3-C2-N1	-3.23	123.16	127.56
25	Z	55	PSU	O2'-C2'-C1'	-2.61	106.26	111.93
25	Z	46	G7M	CN7-N7-C8	-2.37	112.94	125.31
25	Z	8	4SU	C6-N1-C2	-2.22	117.70	121.33
25	Z	32	OMC	C6-N1-C2	-2.06	117.97	121.33
25	Z	8	4SU	O4'-C1'-N1	2.00	111.91	108.10
25	Z	32	OMC	O3'-C3'-C2'	2.02	116.96	111.13
25	Z	46	G7M	C2'-C1'-N9	2.10	119.10	113.47
25	Z	54	5MU	O4'-C1'-N1	2.23	112.34	108.10
25	Z	46	G7M	O4'-C1'-N9	2.23	112.33	108.11
25	Z	32	OMC	O4'-C1'-N1	3.01	113.83	108.10
25	Z	32	OMC	C6-C5-C4	5.42	119.56	117.44
25	Z	46	G7M	C6-N1-C2	5.83	122.71	115.88
25	Z	55	PSU	C4-N3-C2	8.15	121.96	115.16
25	Z	54	5MU	C4-N3-C2	8.92	122.60	115.16

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
25	Z	32	OMC	2	0
25	Z	54	5MU	2	0
25	Z	55	PSU	5	0

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 4 ligands modelled in this entry, 4 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	7
25	Z	2

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	841:U	O3'	848:C	P	5.77
1	A	84:U	O3'	88:A	P	5.45
1	A	93:G	O3'	96:U	P	5.02
1	A	204:U	O3'	216:G	P	3.93
1	A	1442(A):G	O3'	1442(B):A	P	3.82
1	Z	21:A	O3'	22:G	P	3.81
1	A	1389:C	O3'	1390:U	P	3.33
1	Z	14:A	O3'	15:G	P	3.31
1	A	927:G	O3'	928:G	P	3.06