Full wwPDB/EMDataBank EM Map/Model Validation Report (i)

Jan 5, 2017 – 02:04 PM EST

PDB ID	:	5ME1
EMDB ID:	:	EMD-3495
Title	:	Structure of the 30S Pre-Initiation Complex 2 (30S IC-2) Stalled by GE81112
Authors	:	Lopez-Alonso, J.P.; Fabbretti, A.; Kaminishi, T.; Iturrioz, I.; Brandi, L.; Gil Carton, D.; Gualerzi, C.; Fucini, P.; Connell, S.
Deposited on	:	2016-11-14
Resolution	:	13.50 Å(reported)
Based on PDB ID	:	2IFE, 4YBB, 3JCN, 1HR0, 1TIF

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

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

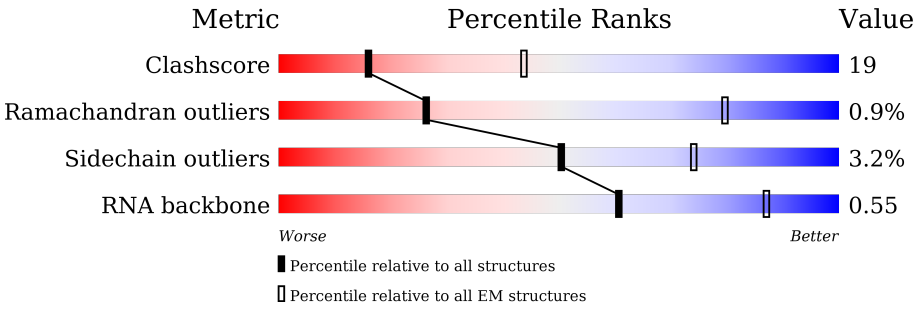
MolProbity	:	4.02b-467
Mogul	:	1.7.1 (RC1), CSD as537be (2016)
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20028442

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 13.50 Å.

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



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

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

Mol	Chain	Length	Quality of chain
1	A	1534	70% 24% 6%
2	B	241	71% 20% • 7%
3	C	233	73% 15% • 12%
4	D	206	87% 12%
5	E	167	66% 25% • 7%
6	F	131	69% 11% 19%
7	G	156	73% 22% • •
8	H	130	78% 20% • •

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Mol	Chain	Length	Quality of chain
9	I	130	72% 26%
10	J	103	53% 39%
11	K	129	71% 20% 9%
12	L	123	86% 14%
13	M	118	65% 31%
14	N	101	71% 27%
15	O	89	88% 10%
16	P	102	75% 20%
17	Q	84	76% 19% 5%
18	R	75	63% 11% 27%
19	S	92	67% 16% 14%
20	T	87	80% 18%
21	U	71	61% 17% 21%
22	V	72	17% 67% 15%
23	W	890	36% 19% 44%
24	Y	171	32% 11% 56%
25	Z	144	31% 25% 7% 37%
26	X	77	13% 57% 26%

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
1	2MG	A	966	-	-	X	-
26	4SU	X	8	-	-	X	-
27	FME	X	101	-	-	X	-

2 Entry composition

There are 27 unique types of molecules in this entry. The entry contains 59063 atoms, of which 1 is hydrogen 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 ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
1	A	1534	32930	14694	6041	10661	1534	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	224	1753	1109	315	321	8	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	C	206	1624	1028	305	288	3	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	D	205	1643	1026	315	298	4	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	E	155	1144	711	216	211	6	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	F	106	862	545	156	154	7	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	151	Total	C	N	O	S	0	0
			1181	735	227	215	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	129	Total	C	N	O	S	0	0
			979	616	173	184	6		

- 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
			1022	634	206	179	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	99	Total	C	N	O	S	0	0
			795	498	152	144	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
11	K	117	Total	C	N	O	S	0	0
			877	540	174	160	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
12	L	123	Total	C	N	O	S	0	0
			957	591	196	165	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
13	M	114	Total	C	N	O	S	0	0
			883	546	178	156	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
14	N	100	Total	C	N	O	S	0	0
			805	499	164	139	3		

- 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
			714	439	144	130	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
16	P	82	Total	C	N	O	S	0	0
			649	406	128	114	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
17	Q	80	Total	C	N	O	S	0	0
			648	411	121	113	3		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
18	R	55	Total	C	N	O	0	0
			455	288	86	81		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
19	S	79	Total	C	N	O	S	0	0
			637	408	120	107	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
20	T	86	Total	C	N	O	S	0	0
			670	414	138	115	3		

- Molecule 21 is a protein called 30S ribosomal protein S21.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	U	56	Total	C	N	O	S	0	0
			465	290	96	78	1		

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

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

- Molecule 23 is a protein called Translation initiation factor IF-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	W	501	Total	C	N	O	S	0	0
			3781	2368	663	735	15		

- Molecule 24 is a protein called Translation initiation factor IF-3.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	Y	76	Total	C	N	O	S	0	0
			623	390	119	112	2		

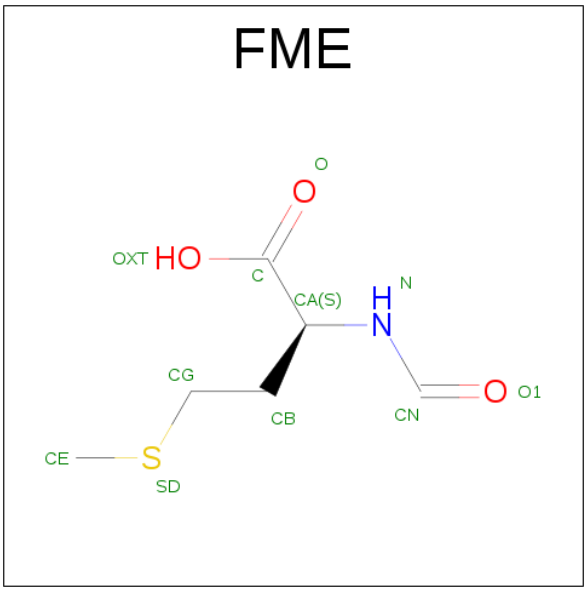
- Molecule 25 is a protein called Translation initiation factor IF-3.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	Z	91	Total	C	N	O	S	0	0
			743	470	135	134	4		

- Molecule 26 is a RNA chain called fMet-tRNA.

Mol	Chain	Residues	Atoms						AltConf	Trace
26	X	77	Total	C	N	O	P	S	0	0
			1643	733	297	535	77	1		

- Molecule 27 is N-FORMYLMETHIONINE (three-letter code: FME) (formula: $C_6H_{11}NO_3S$).



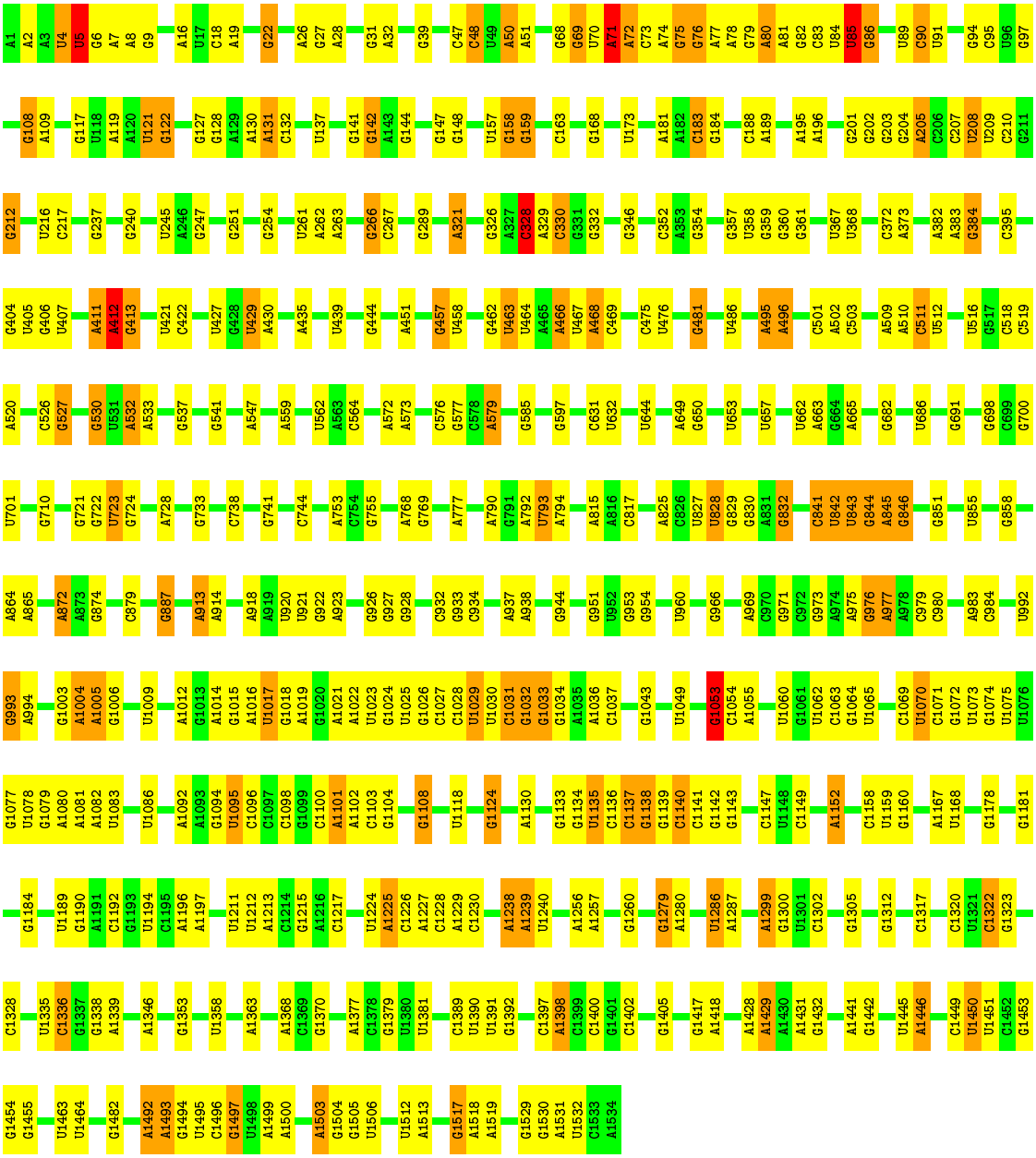
Mol	Chain	Residues	Atoms						AltConf
27	X	1	Total	C	H	N	O	S	0
			10	6	1	1	1	1	

3 Residue-property plots (i)

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

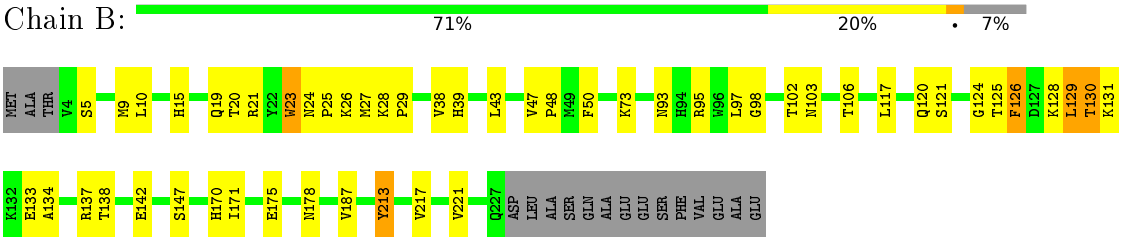
- Molecule 1: 16S ribosomal RNA

Chain A: 70% 24% 6%



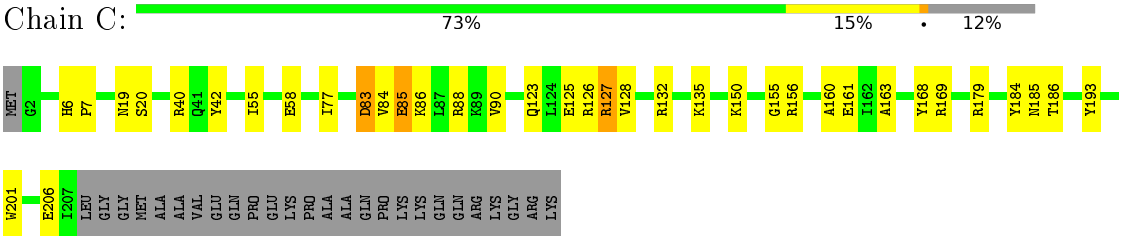
- Molecule 2: 30S ribosomal protein S2

Chain B:



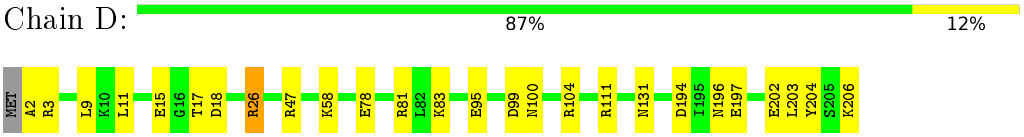
- Molecule 3: 30S ribosomal protein S3

Chain C:



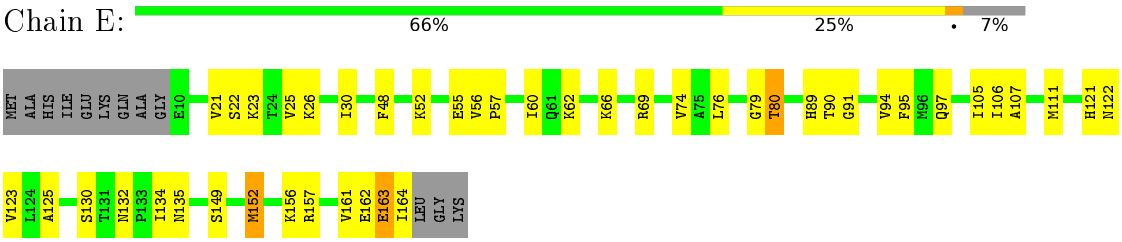
- Molecule 4: 30S ribosomal protein S4

Chain D:



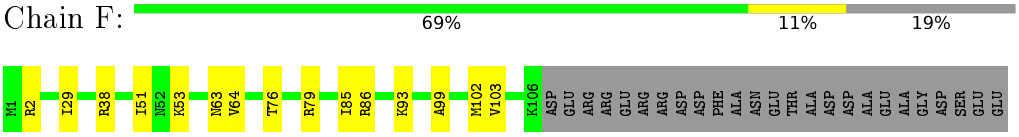
- Molecule 5: 30S ribosomal protein S5

Chain E:



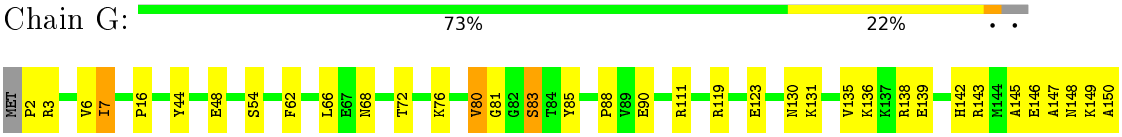
- Molecule 6: 30S ribosomal protein S6

Chain F:



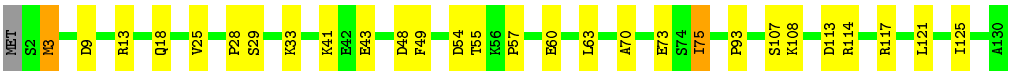
- Molecule 7: 30S ribosomal protein S7

Chain G:



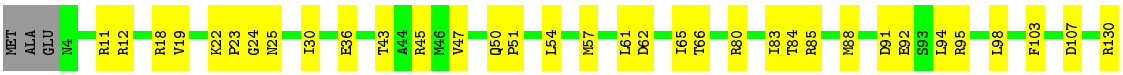
- Molecule 8: 30S ribosomal protein S8

Chain H:



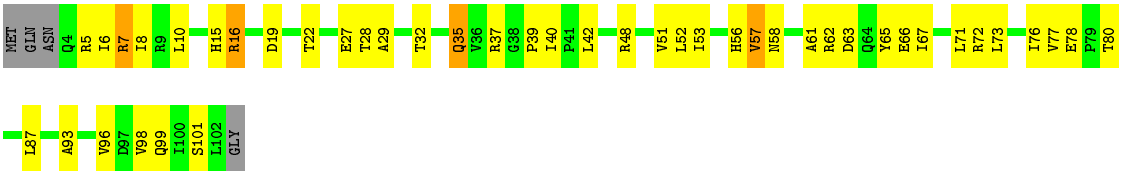
- Molecule 9: 30S ribosomal protein S9

Chain I:



- Molecule 10: 30S ribosomal protein S10

Chain J:



- Molecule 11: 30S ribosomal protein S11

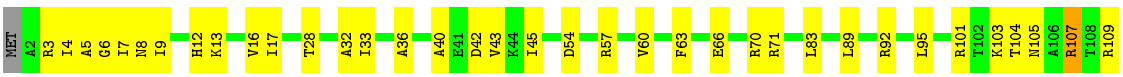
Chain K:

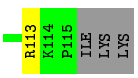
- Molecule 12: 30S ribosomal protein S12

Chain L:

- Molecule 13: 30S ribosomal protein S13

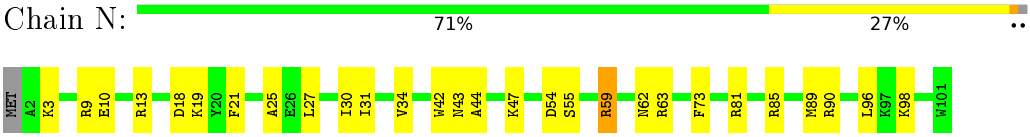
Chain M:





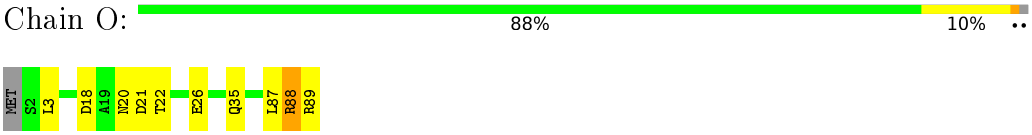
- Molecule 14: 30S ribosomal protein S14

Chain N:



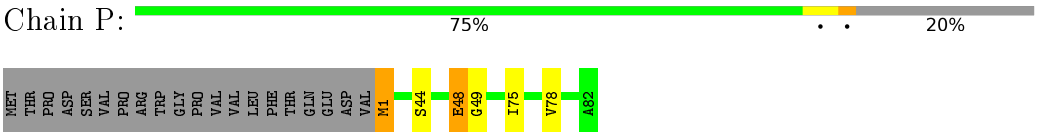
- Molecule 15: 30S ribosomal protein S15

Chain O:



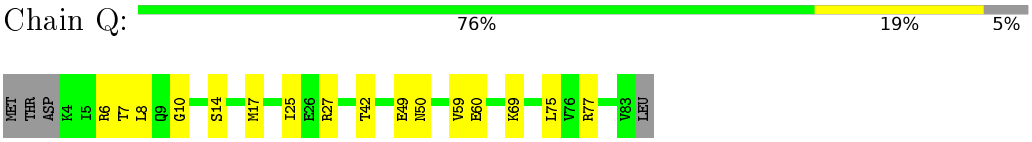
- Molecule 16: 30S ribosomal protein S16

Chain P:



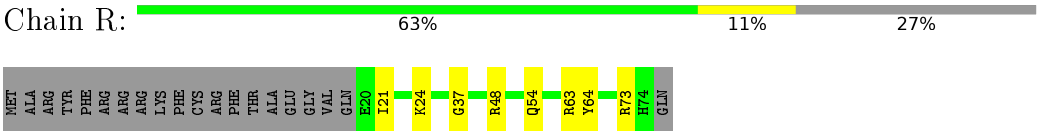
- Molecule 17: 30S ribosomal protein S17

Chain Q:



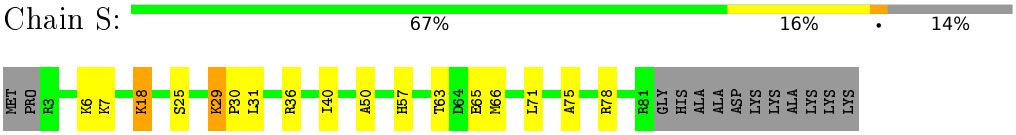
- Molecule 18: 30S ribosomal protein S18

Chain R:



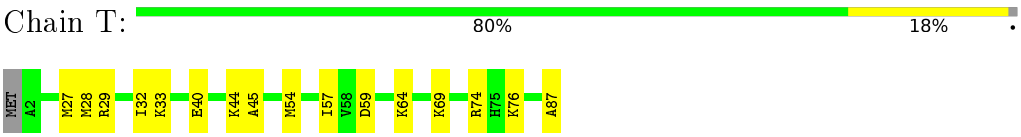
- Molecule 19: 30S ribosomal protein S19

Chain S:



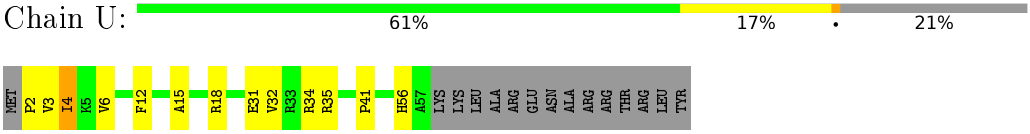
- Molecule 20: 30S ribosomal protein S20

Chain T:



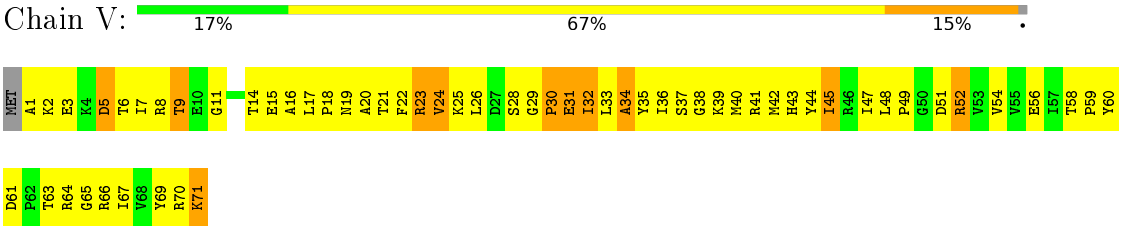
- Molecule 21: 30S ribosomal protein S21

Chain U:



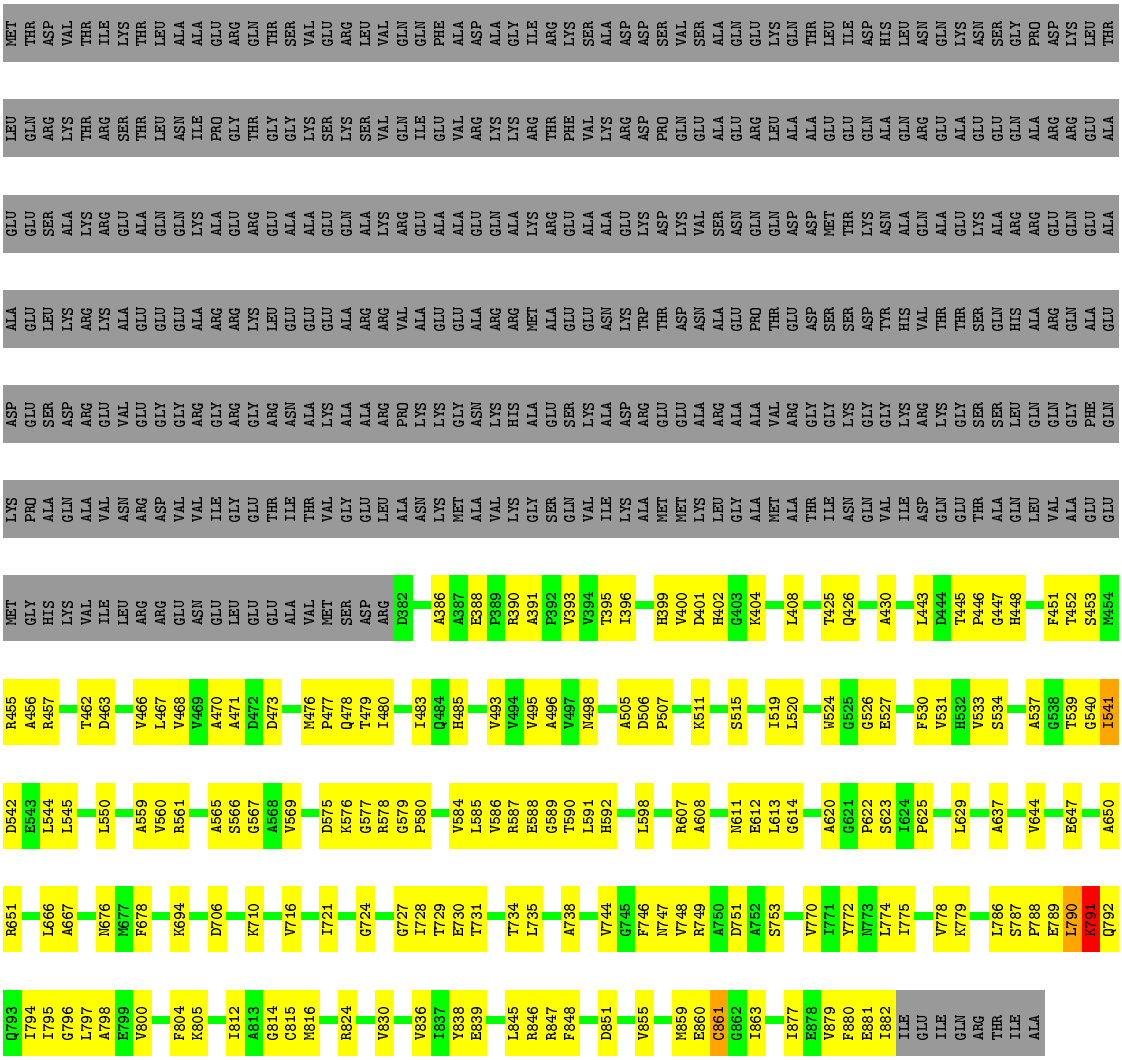
• Molecule 22: Translation initiation factor IF-1

Chain V:



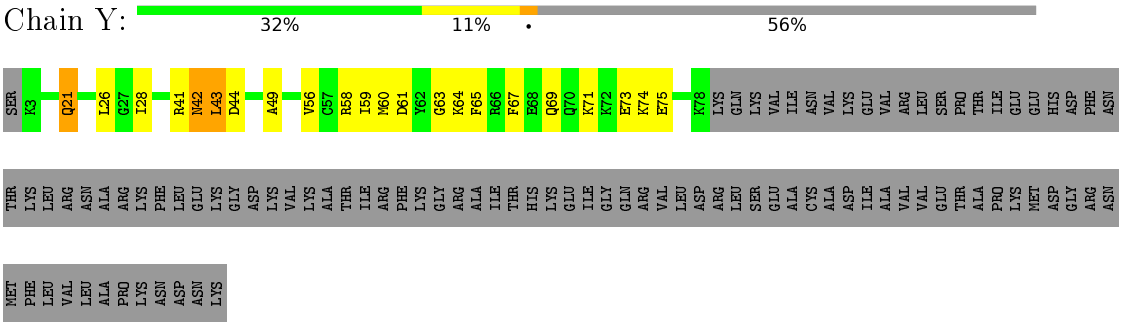
• Molecule 23: Translation initiation factor IF-2

Chain W:



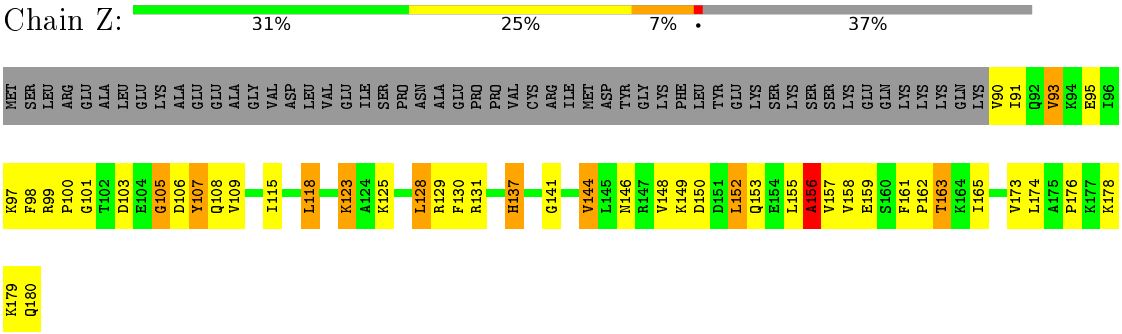
• Molecule 24: Translation initiation factor IF-3

Chain Y:



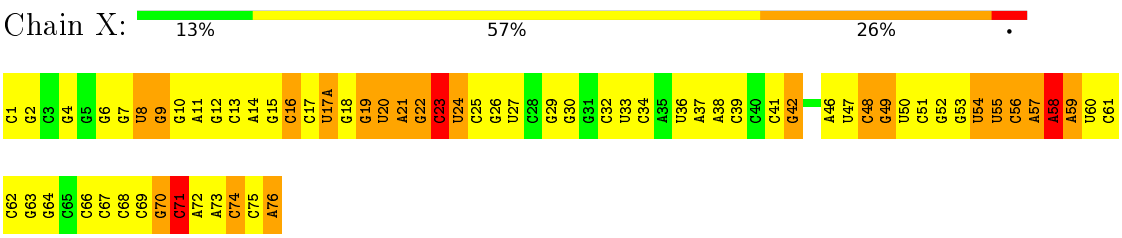
• Molecule 25: Translation initiation factor IF-3

Chain Z:



• Molecule 26: fMet-tRNA

Chain X:



4 Experimental information (i)

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of particles used	26776	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	Not provided	Depositor
Microscope	JEOL 2200FSC	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/Å^2$)	Not provided	Depositor
Minimum defocus (nm)	Not provided	Depositor
Maximum defocus (nm)	Not provided	Depositor
Magnification	74183	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, FME, MA6, G7M, D2T, H2U, 2MG, 5MC, UR3, 4OC, 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	0.58	0/36591	0.98	33/57073 (0.1%)
10	J	0.57	0/805	0.68	0/1089
11	K	0.39	0/893	0.54	0/1205
12	L	0.49	0/960	0.65	0/1286
13	M	0.38	0/892	0.63	0/1193
14	N	0.40	0/817	0.60	0/1088
15	O	0.42	0/722	0.52	0/964
16	P	0.40	0/659	0.59	0/884
17	Q	0.44	0/657	0.61	0/881
18	R	0.41	0/462	0.55	0/621
19	S	0.38	0/652	0.56	0/877
2	B	0.36	0/1784	0.55	0/2403
20	T	0.40	0/676	0.53	0/895
21	U	0.53	0/472	0.57	0/627
22	V	0.39	0/580	0.70	0/782
23	W	0.25	0/3829	0.46	1/5176 (0.0%)
24	Y	0.32	0/629	0.62	0/838
25	Z	1.18	0/751	1.61	13/999 (1.3%)
26	X	0.22	0/1746	0.81	5/2721 (0.2%)
3	C	0.39	0/1651	0.55	0/2225
4	D	0.37	0/1665	0.53	0/2227
5	E	0.48	0/1157	0.61	0/1557
6	F	0.43	0/881	0.56	0/1189
7	G	0.35	0/1195	0.51	0/1602
8	H	0.43	0/989	0.58	0/1326
9	I	0.37	0/1034	0.60	0/1375
All	All	0.52	0/63149	0.86	52/93103 (0.1%)

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
25	Z	0	6

There are no bond length outliers.

All (52) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	117	G	O5'-P-OP2	-9.51	97.14	105.70
25	Z	107	TYR	CB-CG-CD2	-8.11	116.13	121.00
26	X	71	C	N1-C1'-C2'	-7.46	103.80	112.00
25	Z	144	VAL	CA-CB-CG2	-7.42	99.77	110.90
25	Z	156	ALA	CB-CA-C	-6.93	99.71	110.10
1	A	4	U	C2-N1-C1'	6.91	125.99	117.70
1	A	1279	G	C4-N9-C1'	6.86	135.41	126.50
1	A	887	G	O5'-P-OP2	-6.75	99.62	105.70
1	A	330	C	C2-N3-C4	6.73	123.27	119.90
1	A	330	C	C5-C6-N1	6.56	124.28	121.00
1	A	1053	G	OP2-P-O3'	6.32	119.10	105.20
1	A	579	A	O5'-P-OP2	-6.22	100.10	105.70
1	A	330	C	C6-N1-C2	-6.14	117.85	120.30
25	Z	152	LEU	CB-CA-C	-6.13	98.55	110.20
26	X	71	C	C4'-C3'-O3'	6.12	125.23	113.00
1	A	328	C	N1-C2-O2	6.10	122.56	118.90
1	A	321	A	O5'-P-OP2	-6.05	100.26	105.70
1	A	844	G	C2-N3-C4	6.04	114.92	111.90
1	A	971	G	O4'-C1'-N9	6.02	113.02	108.20
1	A	330	C	C2-N1-C1'	6.00	125.40	118.80
1	A	872	A	O4'-C1'-N9	5.98	112.99	108.20
25	Z	163	THR	N-CA-CB	-5.88	99.13	110.30
1	A	328	C	N3-C2-O2	-5.87	117.79	121.90
25	Z	162	PRO	C-N-CA	5.77	136.13	121.70
1	A	412	A	N9-C1'-C2'	5.70	121.41	114.00
1	A	330	C	N1-C2-O2	5.70	122.32	118.90
25	Z	156	ALA	N-CA-CB	5.67	118.03	110.10
1	A	1279	G	C8-N9-C1'	-5.65	119.66	127.00
1	A	1279	G	N7-C8-N9	5.61	115.90	113.10
1	A	85	U	C2-N1-C1'	5.58	124.40	117.70
1	A	183	C	C6-N1-C2	-5.51	118.10	120.30
1	A	412	A	O4'-C1'-N9	5.40	112.52	108.20
23	W	787	SER	C-N-CD	5.40	139.73	128.40
1	A	22	G	O5'-P-OP2	-5.39	100.85	105.70
1	A	1418	A	C8-N9-C4	-5.39	103.64	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	71	A	N1-C6-N6	5.38	121.83	118.60
26	X	23	C	C2'-C3'-O3'	-5.33	97.78	109.50
26	X	23	C	N1-C1'-C2'	-5.32	106.15	112.00
25	Z	146	ASN	CA-CB-CG	5.20	124.84	113.40
26	X	58	A	C2'-C3'-O3'	-5.19	98.08	109.50
1	A	792	A	O4'-C1'-N9	5.17	112.34	108.20
1	A	328	C	C2-N1-C1'	5.14	124.45	118.80
1	A	1286	U	C2-N1-C1'	5.13	123.86	117.70
25	Z	115	ILE	CB-CA-C	-5.13	101.35	111.60
1	A	858	G	N3-C4-N9	5.12	129.07	126.00
25	Z	93	VAL	CG1-CB-CG2	-5.10	102.74	110.90
25	Z	152	LEU	C-N-CA	5.08	134.41	121.70
1	A	5	U	C5-C6-N1	5.08	125.24	122.70
1	A	1279	G	C6-C5-N7	-5.03	127.38	130.40
25	Z	157	VAL	CB-CA-C	-5.03	101.85	111.40
25	Z	107	TYR	CA-CB-CG	5.02	122.94	113.40
1	A	1108	G	C5-C6-O6	-5.00	125.60	128.60

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
25	Z	103	ASP	Peptide
25	Z	107	TYR	Sidechain
25	Z	137	HIS	Peptide
25	Z	156	ALA	Peptide
25	Z	161	PHE	Sidechain,Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	32930	0	16565	918	0
2	B	1753	0	1775	134	0
3	C	1624	0	1696	37	0
4	D	1643	0	1707	21	0
5	E	1144	0	1182	118	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	F	862	0	864	10	0
7	G	1181	0	1236	110	0
8	H	979	0	1031	18	0
9	I	1022	0	1068	36	0
10	J	795	0	836	39	0
11	K	877	0	887	103	0
12	L	957	0	1016	53	0
13	M	883	0	941	32	0
14	N	805	0	844	27	0
15	O	714	0	734	5	0
16	P	649	0	666	3	0
17	Q	648	0	691	11	0
18	R	455	0	478	7	0
19	S	637	0	665	16	0
20	T	670	0	719	12	0
21	U	465	0	491	8	0
22	V	570	0	592	201	0
23	W	3781	0	3836	318	0
24	Y	623	0	651	52	0
25	Z	743	0	773	185	0
26	X	1643	0	831	380	0
27	X	9	1	10	14	0
All	All	59062	1	42785	1894	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 19.

All (1894) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:790:A:C8	26:X:38:A:H4'	1.24	1.71
1:A:790:A:C8	26:X:38:A:C4'	1.77	1.68
12:L:51:LYS:HE3	22:V:60:TYR:CD2	1.28	1.67
1:A:828:U:C2	2:B:25:PRO:CD	1.78	1.66
25:Z:91:ILE:HB	26:X:13:C:C4'	1.23	1.66
1:A:928:G:C2	1:A:1391:U:H1'	1.23	1.64
7:G:143:ARG:HA	11:K:61:PHE:CZ	1.32	1.60
25:Z:91:ILE:CB	26:X:13:C:H4'	1.17	1.58
1:A:18:C:C2	1:A:1080:A:C2	1.91	1.55
1:A:19:A:C5'	1:A:1078:U:H3	0.94	1.54
25:Z:91:ILE:HB	26:X:13:C:C5'	1.32	1.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1072:G:C5'	5:E:62:LYS:NZ	1.68	1.51
1:A:927:G:H4'	1:A:1503:A:C2'	1.35	1.51
7:G:149:LYS:HG2	11:K:95:SER:CB	1.32	1.51
1:A:1101:A:C8	2:B:171:ILE:CD1	1.94	1.51
7:G:149:LYS:CD	11:K:95:SER:HB2	1.41	1.50
1:A:1339:A:C2	26:X:30:G:H1'	1.41	1.50
1:A:1100:C:N4	2:B:95:ARG:CD	1.74	1.49
7:G:147:ALA:HA	11:K:62:ALA:N	1.24	1.48
1:A:790:A:C8	26:X:38:A:C3'	1.94	1.47
7:G:143:ARG:O	11:K:61:PHE:CD2	1.66	1.47
1:A:790:A:N9	26:X:38:A:H4'	1.19	1.46
1:A:1100:C:N4	2:B:95:ARG:HD3	1.22	1.46
1:A:927:G:C4'	1:A:1503:A:H2'	1.40	1.46
1:A:1493:A:C8	22:V:18:PRO:O	1.66	1.46
1:A:1400:C:C5	26:X:34:C:H1'	1.48	1.46
1:A:1492:A:C2	22:V:35:TYR:HB3	1.51	1.45
1:A:1400:C:C6	26:X:34:C:C2	2.02	1.45
7:G:149:LYS:CG	11:K:95:SER:HB2	1.45	1.44
1:A:966:2MG:C4	26:X:34:C:O2'	1.69	1.43
1:A:864:A:C4'	1:A:1078:U:C5	2.00	1.43
1:A:1230:C:C5'	26:X:30:G:OP1	1.63	1.43
12:L:51:LYS:CE	22:V:60:TYR:CD2	2.00	1.42
1:A:864:A:C5'	1:A:1078:U:C5	2.03	1.42
1:A:966:2MG:C5	1:A:1400:C:N4	1.76	1.41
7:G:148:ASN:CA	11:K:59:THR:HB	1.50	1.41
1:A:700:G:C2	24:Y:63:GLY:HA3	1.55	1.41
9:I:130:ARG:NH2	26:X:32:C:H41	1.11	1.41
1:A:927:G:O2'	1:A:1531:A:C1'	1.66	1.40
1:A:928:G:C2	1:A:1391:U:C1'	2.04	1.40
1:A:828:U:C2	2:B:25:PRO:HD2	0.88	1.40
1:A:1494:G:C8	22:V:18:PRO:N	1.88	1.38
1:A:828:U:O2	2:B:25:PRO:HD2	1.22	1.38
25:Z:91:ILE:CA	26:X:13:C:H4'	1.42	1.38
25:Z:125:LYS:CD	26:X:25:C:O2'	1.69	1.38
1:A:928:G:N1	1:A:1391:U:H1'	1.33	1.38
1:A:532:A:H61	3:C:160:ALA:CA	1.34	1.37
1:A:829:G:OP1	2:B:23:TRP:CH2	1.76	1.37
1:A:1494:G:C8	22:V:18:PRO:CD	2.08	1.37
1:A:1101:A:N9	2:B:171:ILE:HD12	1.37	1.36
1:A:927:G:N3	1:A:1531:A:H4'	1.32	1.36
1:A:1079:G:H5'	5:E:135:ASN:CG	1.40	1.35

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:966:2MG:C6	1:A:1400:C:N4	1.90	1.35
1:A:1078:U:C2	5:E:91:GLY:N	1.94	1.35
25:Z:123:LYS:CD	26:X:12:G:H1'	1.53	1.35
1:A:1400:C:C5	26:X:34:C:C1'	2.10	1.35
7:G:149:LYS:CG	11:K:95:SER:CB	2.00	1.34
1:A:1389:C:N4	1:A:1391:U:C4	1.94	1.34
1:A:1497:G:OP1	25:Z:99:ARG:CD	1.74	1.34
1:A:19:A:H5'	1:A:1078:U:N3	1.03	1.33
25:Z:93:VAL:CB	26:X:24:U:O2	1.74	1.33
1:A:1389:C:C4	1:A:1391:U:C5	2.16	1.33
1:A:1517:G:C5	25:Z:106:ASP:OD1	1.80	1.33
25:Z:123:LYS:HD2	26:X:12:G:C1'	1.59	1.33
1:A:1101:A:C8	2:B:171:ILE:HD12	1.56	1.31
1:A:1517:G:N7	25:Z:106:ASP:OD1	1.63	1.31
23:W:848:PHE:H	27:X:101:FME:CN	1.41	1.30
9:I:130:ARG:NH2	26:X:32:C:N4	1.79	1.30
12:L:51:LYS:HE3	22:V:60:TYR:CG	1.65	1.29
1:A:790:A:C8	26:X:38:A:O2'	1.83	1.29
1:A:700:G:N1	24:Y:63:GLY:HA2	1.46	1.28
25:Z:93:VAL:HB	26:X:24:U:O2	1.11	1.28
1:A:1400:C:C4	26:X:34:C:H1'	1.68	1.28
1:A:18:C:O2	1:A:1079:G:N2	1.67	1.27
1:A:1072:G:H5"	5:E:62:LYS:CE	1.61	1.27
1:A:1230:C:C4'	26:X:30:G:OP1	1.81	1.27
1:A:1338:G:N2	26:X:29:G:N2	1.83	1.27
9:I:130:ARG:HH22	26:X:32:C:N4	1.32	1.27
1:A:927:G:H2'	1:A:1531:A:O2'	1.11	1.26
1:A:828:U:N3	2:B:25:PRO:HD2	1.50	1.26
1:A:790:A:H8	26:X:38:A:C3'	1.36	1.26
1:A:1100:C:C4	2:B:95:ARG:CD	2.19	1.26
1:A:1100:C:C4	2:B:95:ARG:HD2	1.71	1.25
23:W:812:ILE:HG12	26:X:76:A:N9	1.50	1.25
1:A:1494:G:N7	22:V:18:PRO:HB3	1.47	1.25
1:A:1072:G:H5'	5:E:62:LYS:NZ	1.31	1.24
1:A:698:G:OP1	24:Y:74:LYS:HG2	1.32	1.24
1:A:1230:C:H5"	26:X:30:G:OP1	1.21	1.24
1:A:790:A:C8	26:X:38:A:C2'	2.20	1.24
1:A:1339:A:H1'	26:X:41:C:O2	1.38	1.24
1:A:1494:G:H8	22:V:18:PRO:N	1.23	1.24
7:G:147:ALA:C	11:K:59:THR:OG1	1.76	1.23
1:A:700:G:C2	24:Y:63:GLY:CA	2.21	1.23

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:W:812:ILE:HG12	26:X:76:A:C1'	1.67	1.23
1:A:829:G:OP1	2:B:23:TRP:HH2	0.91	1.23
1:A:829:G:O4'	2:B:25:PRO:HG3	1.33	1.22
1:A:966:2MG:N7	1:A:1400:C:N4	1.84	1.22
7:G:143:ARG:O	11:K:61:PHE:CE2	1.91	1.21
25:Z:95:GLU:OE1	26:X:25:C:O3'	1.57	1.21
1:A:1494:G:C8	22:V:18:PRO:HD3	1.72	1.21
1:A:1338:G:N3	26:X:42:G:O2'	1.66	1.21
1:A:1495:U:O2'	25:Z:101:GLY:CA	1.88	1.21
1:A:1074:G:OP2	5:E:66:LYS:HE3	1.40	1.20
1:A:530:G:H1'	22:V:39:LYS:CD	1.72	1.20
1:A:1492:A:N3	22:V:35:TYR:HB3	1.56	1.20
7:G:143:ARG:CA	11:K:61:PHE:CZ	2.24	1.19
7:G:149:LYS:CE	11:K:95:SER:HB2	1.72	1.19
1:A:532:A:N6	3:C:160:ALA:CA	2.01	1.19
1:A:927:G:C2	1:A:1392:G:O4'	1.96	1.19
1:A:368:U:O5'	23:W:607:ARG:HG2	1.03	1.19
1:A:1230:C:H5"	26:X:30:G:P	1.82	1.19
1:A:1339:A:H2	26:X:30:G:C1'	1.55	1.19
1:A:966:2MG:C5	26:X:34:C:O2'	1.95	1.19
1:A:686:U:H2'	24:Y:42:ASN:OD1	1.38	1.19
7:G:148:ASN:N	11:K:59:THR:HB	1.58	1.18
23:W:804:PHE:HB2	23:W:812:ILE:CG2	1.73	1.18
1:A:359:G:H1'	23:W:576:LYS:HG3	1.24	1.18
23:W:531:VAL:HG11	23:W:544:LEU:HB2	1.20	1.18
1:A:1072:G:C5'	5:E:62:LYS:CE	2.16	1.18
1:A:18:C:C2	1:A:1079:G:N2	2.11	1.17
1:A:1492:A:H2'	22:V:19:ASN:O	1.43	1.17
1:A:928:G:N1	1:A:1391:U:C1'	2.01	1.17
12:L:41:THR:HG23	22:V:64:ARG:NH1	1.61	1.16
1:A:361:G:OP1	23:W:730:GLU:N	1.78	1.16
1:A:1101:A:C8	2:B:171:ILE:HD13	1.69	1.16
1:A:700:G:N1	24:Y:63:GLY:CA	2.09	1.15
1:A:864:A:H4'	1:A:1078:U:C5	1.33	1.15
1:A:790:A:C4	26:X:38:A:H4'	1.82	1.15
1:A:368:U:P	23:W:607:ARG:HG2	1.85	1.15
26:X:8:4SU:S4	26:X:14:A:N7	2.19	1.15
25:Z:125:LYS:HD2	26:X:25:C:O2'	0.99	1.15
1:A:368:U:O5'	23:W:607:ARG:CG	1.96	1.14
23:W:812:ILE:CD1	26:X:76:A:C4	2.30	1.14
1:A:1338:G:H21	26:X:42:G:H1'	0.98	1.14

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1400:C:C5	26:X:34:C:C2	2.36	1.14
26:X:71:C:O2'	26:X:72:A:H5'	1.43	1.14
7:G:147:ALA:C	11:K:59:THR:CB	2.16	1.14
1:A:928:G:N2	1:A:1391:U:O4'	1.81	1.14
23:W:540:GLY:HA2	23:W:541:ILE:HG22	1.25	1.14
1:A:1389:C:C4	1:A:1391:U:C4	2.34	1.13
1:A:920:U:H4'	1:A:1082:A:H5'	1.25	1.13
1:A:1492:A:N3	22:V:35:TYR:CB	2.11	1.13
1:A:1230:C:H4'	26:X:30:G:OP1	1.42	1.13
1:A:1338:G:N2	26:X:29:G:H21	1.40	1.13
1:A:698:G:OP1	24:Y:74:LYS:CG	1.95	1.13
25:Z:93:VAL:HG23	26:X:12:G:N3	1.63	1.13
23:W:846:ARG:HB3	26:X:76:A:C2	1.85	1.12
1:A:1102:A:O2'	2:B:98:GLY:N	1.81	1.12
1:A:1400:C:C5	26:X:34:C:N1	2.18	1.12
1:A:358:U:C1'	23:W:577:GLY:O	1.98	1.12
25:Z:95:GLU:OE1	26:X:25:C:H4'	1.49	1.11
1:A:829:G:O4'	2:B:25:PRO:CG	1.96	1.11
7:G:148:ASN:HA	11:K:59:THR:HB	1.24	1.11
25:Z:90:VAL:HG21	26:X:14:A:C8	1.85	1.11
26:X:21:A:N6	26:X:48:C:OP1	1.84	1.11
1:A:1496:C:O2'	25:Z:99:ARG:NH2	1.82	1.11
1:A:918:A:H2	1:A:1080:A:C2	1.68	1.10
1:A:828:U:O2'	2:B:25:PRO:C	1.76	1.10
1:A:927:G:H4'	1:A:1503:A:C3'	1.69	1.10
1:A:1079:G:H5'	5:E:135:ASN:OD1	1.38	1.10
1:A:1072:G:P	5:E:62:LYS:NZ	2.24	1.10
1:A:395:C:H5'	23:W:647:GLU:OE2	1.50	1.10
3:C:168:TYR:CD1	5:E:55:GLU:OE1	2.03	1.10
1:A:700:G:N7	24:Y:67:PHE:HB2	1.66	1.10
25:Z:180:GLN:HA	26:X:69:C:C2	1.86	1.10
1:A:358:U:O4'	23:W:577:GLY:O	1.68	1.09
1:A:530:G:H1'	22:V:39:LYS:CE	1.81	1.09
1:A:790:A:N7	26:X:38:A:O2'	1.75	1.09
25:Z:125:LYS:HD2	26:X:25:C:C2'	1.81	1.09
1:A:790:A:H8	26:X:38:A:O3'	1.36	1.09
1:A:532:A:N6	3:C:160:ALA:HA	1.65	1.09
7:G:143:ARG:HD3	11:K:61:PHE:HZ	1.16	1.09
1:A:1073:U:O2	2:B:103:ASN:ND2	1.87	1.08
1:A:966:2MG:O6	1:A:1400:C:N4	1.83	1.08
7:G:147:ALA:C	11:K:61:PHE:H	1.54	1.08

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:W:534:SER:CB	23:W:537:ALA:HB3	1.84	1.08
1:A:519:C:O2	22:V:2:LYS:HE2	1.54	1.08
1:A:1339:A:C2	26:X:30:G:C1'	2.31	1.08
1:A:358:U:O3'	23:W:579:GLY:HA2	1.54	1.08
1:A:532:A:H8	3:C:193:TYR:CZ	1.72	1.07
3:C:168:TYR:CE1	5:E:55:GLU:CD	2.28	1.07
1:A:1493:A:H3'	22:V:18:PRO:C	1.68	1.07
1:A:927:G:H1	1:A:1391:U:H2'	1.10	1.07
1:A:18:C:O2	1:A:1080:A:C2	2.08	1.07
23:W:848:PHE:H	27:X:101:FME:HCN	1.18	1.07
23:W:812:ILE:HD13	26:X:76:A:C5	1.89	1.06
7:G:147:ALA:CA	11:K:62:ALA:N	2.18	1.06
1:A:927:G:H21	1:A:1531:A:H5"	1.15	1.06
25:Z:129:ARG:NE	26:X:37:A:O3'	1.86	1.06
25:Z:180:GLN:OE1	26:X:71:C:N4	1.88	1.06
1:A:927:G:C2'	1:A:1531:A:O2'	2.02	1.06
1:A:1494:G:N7	22:V:18:PRO:CB	2.19	1.06
25:Z:95:GLU:OE1	26:X:25:C:C4'	2.03	1.06
26:X:71:C:H2'	26:X:72:A:H8	1.14	1.06
1:A:1497:G:OP1	25:Z:99:ARG:HD3	1.53	1.05
1:A:1230:C:C5'	26:X:30:G:P	2.43	1.05
1:A:830:G:H5'	2:B:23:TRP:H	1.15	1.05
1:A:927:G:C6	1:A:1392:G:N9	2.25	1.05
25:Z:123:LYS:HD2	26:X:12:G:H1'	1.12	1.05
25:Z:159:GLU:OE2	26:X:11:A:O3'	1.72	1.05
1:A:1389:C:N4	1:A:1391:U:N3	2.04	1.05
7:G:147:ALA:C	11:K:61:PHE:N	2.09	1.05
25:Z:91:ILE:CB	26:X:13:C:C5'	2.24	1.05
1:A:1339:A:C1'	26:X:41:C:O2	2.03	1.05
1:A:927:G:N2	1:A:1391:U:O2'	1.90	1.04
23:W:804:PHE:HB2	23:W:812:ILE:HG23	1.37	1.04
7:G:148:ASN:HA	11:K:59:THR:CB	1.86	1.04
25:Z:180:GLN:OXT	26:X:69:C:N3	1.89	1.04
1:A:829:G:P	2:B:23:TRP:CH2	2.47	1.04
1:A:1492:A:C2	22:V:35:TYR:CB	2.38	1.04
1:A:920:U:H4'	1:A:1082:A:C5'	1.86	1.04
1:A:927:G:C5'	1:A:1503:A:H2'	1.87	1.04
1:A:19:A:H5'	1:A:1078:U:C4	1.93	1.03
23:W:540:GLY:HA2	23:W:541:ILE:CG2	1.88	1.03
7:G:148:ASN:ND2	11:K:59:THR:HG22	1.71	1.03
25:Z:91:ILE:C	26:X:13:C:O2'	1.75	1.03

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1400:C:OP2	26:X:34:C:C5	2.11	1.03
1:A:790:A:C8	26:X:38:A:O3'	2.07	1.03
7:G:148:ASN:ND2	11:K:59:THR:CG2	2.20	1.03
23:W:591:LEU:HD12	23:W:620:ALA:HB3	1.36	1.03
12:L:47:SER:OG	22:V:35:TYR:CE1	2.11	1.03
1:A:1072:G:OP1	5:E:52:LYS:O	1.75	1.03
25:Z:125:LYS:CE	26:X:25:C:H1'	1.88	1.02
1:A:1102:A:O2'	2:B:98:GLY:CA	2.06	1.02
1:A:19:A:OP1	1:A:1078:U:O2	1.76	1.02
1:A:358:U:O2'	23:W:576:LYS:O	1.76	1.02
1:A:1493:A:C2	22:V:22:PHE:N	2.26	1.02
1:A:1338:G:N2	26:X:42:G:H1'	1.74	1.02
1:A:532:A:H8	3:C:193:TYR:CE1	1.76	1.02
25:Z:123:LYS:CD	26:X:12:G:C1'	2.24	1.02
1:A:1101:A:OP1	2:B:170:HIS:HE1	1.41	1.02
1:A:1389:C:C5	1:A:1391:U:C5	2.48	1.02
22:V:14:THR:HB	22:V:23:ARG:HB3	1.40	1.01
1:A:1400:C:H5'	26:X:34:C:N4	1.75	1.01
7:G:149:LYS:HE2	11:K:95:SER:CA	1.90	1.01
25:Z:90:VAL:CG2	26:X:13:C:H2'	1.90	1.01
23:W:812:ILE:HD13	26:X:76:A:C4	1.92	1.01
1:A:530:G:C1'	22:V:39:LYS:HE2	1.87	1.01
9:I:130:ARG:CZ	26:X:32:C:H41	1.74	1.01
12:L:71:GLY:HA2	22:V:60:TYR:OH	1.60	1.00
1:A:1497:G:OP1	25:Z:99:ARG:HD2	1.37	1.00
25:Z:123:LYS:HD3	26:X:12:G:H1'	1.40	1.00
1:A:1389:C:N3	1:A:1391:U:C6	2.30	1.00
1:A:927:G:C2'	1:A:1531:A:H1'	1.90	1.00
25:Z:93:VAL:HB	26:X:24:U:C2	1.96	1.00
1:A:828:U:C2	2:B:25:PRO:CG	2.45	1.00
1:A:864:A:H5'	1:A:1078:U:C5	1.89	1.00
1:A:358:U:O2'	23:W:576:LYS:C	2.00	1.00
1:A:1494:G:H8	22:V:18:PRO:CA	1.75	1.00
25:Z:95:GLU:OE1	26:X:25:C:C3'	2.09	0.99
26:X:71:C:H2'	26:X:72:A:C8	1.97	0.99
1:A:19:A:H5"	1:A:1078:U:H3	1.25	0.99
1:A:1338:G:H22	26:X:29:G:N2	1.51	0.99
7:G:147:ALA:HA	11:K:61:PHE:C	1.68	0.99
1:A:1494:G:O2'	22:V:15:GLU:OE2	1.77	0.99
1:A:698:G:P	24:Y:74:LYS:HD3	2.03	0.99
1:A:1078:U:O5'	5:E:90:THR:OG1	1.79	0.99

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:W:848:PHE:N	27:X:101:FME:CN	2.25	0.99
1:A:1079:G:C5'	5:E:135:ASN:OD1	2.11	0.99
1:A:1078:U:C3'	5:E:90:THR:OG1	1.95	0.98
1:A:1517:G:C8	25:Z:106:ASP:HA	1.98	0.98
1:A:358:U:C2'	23:W:576:LYS:O	2.11	0.98
1:A:1072:G:H5"	5:E:62:LYS:CD	1.92	0.98
7:G:148:ASN:CA	11:K:59:THR:CB	2.41	0.98
23:W:805:LYS:HD2	26:X:74:C:N3	1.76	0.98
23:W:812:ILE:HG21	26:X:76:A:O4'	1.64	0.98
1:A:1074:G:OP2	5:E:66:LYS:CE	2.11	0.98
1:A:530:G:N7	22:V:38:GLY:HA3	1.80	0.97
1:A:700:G:N2	24:Y:63:GLY:HA3	1.79	0.97
7:G:149:LYS:CD	11:K:95:SER:CB	2.33	0.97
1:A:1517:G:H5"	25:Z:109:VAL:HG21	1.42	0.97
1:A:1078:U:H1'	5:E:91:GLY:N	1.75	0.97
23:W:848:PHE:N	27:X:101:FME:HCN	1.80	0.97
26:X:22:G:C4	26:X:23:C:C5	2.51	0.97
1:A:532:A:H61	3:C:160:ALA:HA	0.81	0.97
1:A:966:2MG:C5	1:A:1400:C:H41	1.20	0.97
1:A:927:G:C4'	1:A:1503:A:C2'	2.16	0.97
7:G:147:ALA:HB2	11:K:61:PHE:HD2	1.27	0.97
1:A:1079:G:H5'	5:E:135:ASN:ND2	1.80	0.97
1:A:828:U:C6	2:B:25:PRO:HG2	1.99	0.97
7:G:149:LYS:HG2	11:K:95:SER:HB3	0.97	0.97
1:A:1492:A:C2'	22:V:19:ASN:O	2.13	0.96
1:A:1078:U:H1'	5:E:89:HIS:O	1.64	0.96
1:A:698:G:OP1	24:Y:74:LYS:CD	2.12	0.96
25:Z:90:VAL:HG21	26:X:14:A:H8	1.22	0.96
1:A:1101:A:O4'	2:B:171:ILE:CD1	2.12	0.96
1:A:1339:A:H1'	26:X:41:C:C2	2.01	0.96
7:G:149:LYS:H	11:K:61:PHE:N	1.57	0.96
1:A:1494:G:C8	22:V:18:PRO:CA	2.47	0.96
1:A:1493:A:H2	22:V:22:PHE:H	1.10	0.96
1:A:1100:C:N4	2:B:95:ARG:NE	2.12	0.96
1:A:927:G:H1	1:A:1391:U:C2'	1.76	0.96
1:A:1074:G:H5'	2:B:102:THR:O	1.65	0.96
1:A:1400:C:H5	26:X:34:C:C1'	1.75	0.96
1:A:864:A:O3'	1:A:1079:G:O6	1.84	0.96
1:A:701:U:H5'	24:Y:64:LYS:CB	1.95	0.96
7:G:143:ARG:HA	11:K:61:PHE:CE2	2.01	0.95
1:A:701:U:H2'	24:Y:64:LYS:CB	1.96	0.95

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:928:G:N2	1:A:1391:U:C1'	2.28	0.95
1:A:1517:G:O4'	25:Z:105:GLY:O	1.84	0.95
1:A:927:G:C6	1:A:1392:G:C4	2.55	0.95
1:A:359:G:C1'	23:W:576:LYS:HG3	1.95	0.95
1:A:918:A:C2	1:A:1080:A:C2	2.55	0.95
25:Z:91:ILE:HB	26:X:13:C:H5'	1.45	0.95
1:A:1079:G:O4'	5:E:135:ASN:ND2	2.00	0.95
1:A:361:G:OP1	23:W:729:THR:HB	1.66	0.95
1:A:864:A:H5"	1:A:1078:U:C5	2.02	0.95
1:A:790:A:N9	26:X:38:A:C4'	2.08	0.95
7:G:149:LYS:HE2	11:K:95:SER:HA	1.49	0.94
7:G:149:LYS:HE2	11:K:95:SER:CB	1.98	0.94
25:Z:91:ILE:CA	26:X:13:C:C4'	2.25	0.94
1:A:530:G:H1'	22:V:39:LYS:HE2	1.41	0.94
1:A:927:G:N3	1:A:1531:A:C4'	2.29	0.94
1:A:1073:U:C2	2:B:103:ASN:ND2	2.25	0.94
7:G:147:ALA:O	11:K:59:THR:OG1	1.70	0.94
9:I:130:ARG:NH2	26:X:32:C:C5	2.34	0.94
1:A:18:C:C2	1:A:1080:A:H2	1.70	0.94
1:A:358:U:H1'	23:W:577:GLY:O	1.66	0.94
23:W:727:GLY:HA2	23:W:748:VAL:HG23	1.49	0.94
25:Z:91:ILE:C	26:X:13:C:H4'	1.83	0.94
1:A:927:G:C3'	1:A:1503:A:H2'	1.97	0.94
26:X:76:A:O2'	27:X:101:FME:O1	1.86	0.94
1:A:966:2MG:N9	26:X:34:C:O2'	2.01	0.93
26:X:22:G:HO2'	26:X:23:C:H6	0.94	0.93
1:A:1073:U:OP2	5:E:66:LYS:NZ	2.00	0.93
1:A:1518:MA6:H103	1:A:1519:MA6:H102	1.50	0.93
1:A:701:U:H5'	24:Y:64:LYS:HB2	1.50	0.93
1:A:530:G:H1'	22:V:39:LYS:HD3	1.51	0.93
1:A:927:G:C5	1:A:1392:G:H1'	2.04	0.93
1:A:1079:G:C5'	5:E:135:ASN:CG	2.35	0.93
1:A:830:G:OP1	2:B:20:THR:O	1.85	0.93
1:A:1072:G:H5'	5:E:62:LYS:HZ1	1.16	0.93
1:A:700:G:H1	24:Y:63:GLY:HA2	1.28	0.93
7:G:149:LYS:HE2	11:K:95:SER:HB2	1.47	0.93
1:A:1400:C:O4'	26:X:34:C:N3	2.02	0.93
1:A:832:G:OP2	2:B:21:ARG:NH2	1.68	0.92
1:A:1389:C:C4	1:A:1391:U:C6	2.57	0.92
1:A:358:U:H4'	23:W:578:ARG:C	1.90	0.92
1:A:532:A:C8	3:C:193:TYR:CE1	2.56	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:41:THR:CG2	22:V:64:ARG:HH11	1.82	0.92
3:C:168:TYR:CD1	5:E:55:GLU:CD	2.42	0.92
1:A:368:U:C5	23:W:608:ALA:HB2	2.04	0.92
1:A:790:A:H8	26:X:38:A:C2'	1.67	0.92
1:A:829:G:O4'	2:B:25:PRO:CD	2.17	0.92
1:A:1078:U:H3'	5:E:90:THR:OG1	1.68	0.92
1:A:361:G:H5"	23:W:730:GLU:HB2	1.50	0.92
25:Z:123:LYS:HD2	26:X:12:G:O4'	1.69	0.92
7:G:146:GLU:OE2	11:K:61:PHE:HE1	1.51	0.92
7:G:143:ARG:HA	11:K:61:PHE:CE1	2.04	0.91
1:A:1078:U:C1'	5:E:89:HIS:O	2.15	0.91
1:A:530:G:C8	22:V:39:LYS:N	2.37	0.91
7:G:148:ASN:HA	11:K:59:THR:CA	2.01	0.91
1:A:927:G:C4	1:A:1392:G:H1'	2.06	0.91
1:A:927:G:O6	1:A:1392:G:C4	2.24	0.91
7:G:147:ALA:CA	11:K:62:ALA:H	1.81	0.91
23:W:812:ILE:CG1	26:X:76:A:N9	2.33	0.91
1:A:19:A:C5'	1:A:1078:U:N3	1.80	0.91
12:L:51:LYS:HE2	22:V:60:TYR:CD2	2.04	0.91
7:G:149:LYS:CB	11:K:60:PRO:C	2.38	0.91
1:A:1495:U:O2'	25:Z:101:GLY:HA3	1.70	0.91
1:A:1494:G:C8	22:V:18:PRO:CB	2.54	0.91
1:A:361:G:P	23:W:729:THR:HB	2.11	0.90
1:A:1104:G:OP1	2:B:147:SER:OG	1.90	0.90
1:A:828:U:N3	2:B:25:PRO:CD	2.18	0.90
25:Z:156:ALA:HB1	25:Z:174:LEU:HD11	1.54	0.90
1:A:1495:U:O2'	25:Z:101:GLY:HA2	1.71	0.90
1:A:18:C:N1	1:A:1080:A:C2	2.38	0.90
7:G:143:ARG:CA	11:K:61:PHE:CE2	2.55	0.90
1:A:829:G:P	2:B:25:PRO:HB3	2.08	0.90
12:L:41:THR:CG2	22:V:64:ARG:NH1	2.33	0.90
1:A:1494:G:C8	22:V:17:LEU:C	2.45	0.90
1:A:357:G:H4'	23:W:607:ARG:CD	2.02	0.90
23:W:812:ILE:HD12	23:W:863:ILE:O	1.72	0.90
1:A:927:G:P	1:A:1503:A:O2'	2.22	0.90
25:Z:91:ILE:C	26:X:13:C:C4'	2.40	0.89
1:A:1101:A:O4'	2:B:171:ILE:HD11	1.69	0.89
1:A:519:C:C2	22:V:2:LYS:HE2	2.06	0.89
1:A:1390:U:C6	1:A:1391:U:O5'	2.10	0.89
1:A:530:G:C1'	22:V:39:LYS:CE	2.44	0.89
7:G:147:ALA:HA	11:K:62:ALA:H	1.09	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:927:G:O2'	1:A:1531:A:H1'	0.72	0.89
23:W:565:ALA:HB2	23:W:590:THR:CG2	2.02	0.89
1:A:829:G:O5'	2:B:25:PRO:HB3	1.71	0.89
1:A:829:G:C4'	2:B:25:PRO:HG3	2.02	0.89
1:A:1081:A:OP1	5:E:21:VAL:HB	1.72	0.89
1:A:1400:C:OP2	26:X:34:C:H5	1.49	0.89
1:A:864:A:C4'	1:A:1078:U:H5	1.60	0.88
1:A:1101:A:N9	2:B:171:ILE:CD1	2.21	0.88
1:A:1338:G:H21	26:X:42:G:C1'	1.86	0.88
1:A:1101:A:H8	2:B:171:ILE:CD1	1.84	0.88
11:K:94:GLU:OE2	11:K:98:ARG:NH2	2.06	0.88
1:A:395:C:C5'	23:W:647:GLU:OE2	2.20	0.88
1:A:701:U:H5'	24:Y:64:LYS:CG	1.98	0.88
1:A:1130:A:OP1	9:I:18:ARG:NH1	2.07	0.88
7:G:147:ALA:C	11:K:59:THR:HB	1.88	0.88
1:A:829:G:O5'	2:B:25:PRO:CB	2.20	0.88
1:A:1102:A:O2'	2:B:98:GLY:HA3	1.73	0.88
22:V:45:ILE:HD13	22:V:70:ARG:HD3	1.55	0.88
1:A:1101:A:C1'	2:B:171:ILE:HD12	2.02	0.88
1:A:1400:C:N4	26:X:34:C:H1'	1.87	0.88
25:Z:93:VAL:HG23	26:X:12:G:C2	2.08	0.88
1:A:359:G:C4'	23:W:576:LYS:HA	2.03	0.88
11:K:13:ARG:NH2	11:K:77:TYR:OH	2.07	0.88
1:A:1078:U:O2	5:E:91:GLY:N	1.93	0.87
1:A:828:U:O2	2:B:25:PRO:CD	1.94	0.87
25:Z:180:GLN:CD	26:X:71:C:H41	1.77	0.87
7:G:143:ARG:HD3	11:K:61:PHE:CZ	2.08	0.87
23:W:531:VAL:HG21	23:W:544:LEU:HA	1.54	0.87
23:W:812:ILE:HD11	26:X:76:A:N3	1.88	0.87
1:A:927:G:O5'	1:A:1503:A:C2'	2.22	0.87
1:A:1072:G:C5'	5:E:62:LYS:HE2	2.02	0.87
23:W:540:GLY:HA2	23:W:541:ILE:CB	2.05	0.87
1:A:358:U:H1'	23:W:577:GLY:HA2	1.55	0.87
23:W:812:ILE:HG12	26:X:76:A:H1'	1.56	0.87
1:A:1072:G:H5'	5:E:62:LYS:CE	1.93	0.86
7:G:149:LYS:HB3	11:K:60:PRO:C	1.95	0.86
12:L:41:THR:HG23	22:V:64:ARG:HH11	1.35	0.86
23:W:728:ILE:HG13	23:W:748:VAL:HG21	1.56	0.86
25:Z:123:LYS:HG3	26:X:12:G:C4'	2.05	0.86
25:Z:178:LYS:HB3	26:X:69:C:H1'	1.55	0.86
1:A:701:U:C2'	24:Y:61:ASP:HB3	2.05	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:Z:159:GLU:OE2	26:X:12:G:H5'	1.74	0.86
23:W:812:ILE:HG12	26:X:76:A:C4	2.11	0.86
1:A:1070:U:H5'	5:E:23:LYS:HE3	1.56	0.86
1:A:532:A:C8	3:C:193:TYR:CZ	2.63	0.86
1:A:828:U:N1	2:B:25:PRO:CG	2.35	0.86
1:A:358:U:H4'	23:W:579:GLY:N	1.90	0.86
1:A:359:G:OP1	23:W:580:PRO:HD3	1.76	0.86
1:A:361:G:H5"	23:W:730:GLU:CB	2.06	0.86
7:G:148:ASN:N	11:K:59:THR:CB	2.38	0.86
1:A:19:A:H5'	1:A:1078:U:C2	2.11	0.85
3:C:168:TYR:CZ	5:E:55:GLU:OE2	2.29	0.85
1:A:701:U:H2'	24:Y:64:LYS:HB3	1.56	0.85
1:A:830:G:H5'	2:B:23:TRP:N	1.89	0.85
1:A:790:A:N7	26:X:38:A:C4'	2.38	0.85
26:X:11:A:N6	26:X:24:U:O4	2.08	0.85
1:A:1073:U:H5"	5:E:69:ARG:NH2	1.92	0.85
12:L:51:LYS:CE	22:V:60:TYR:HD2	1.82	0.85
1:A:1493:A:H8	22:V:18:PRO:O	1.57	0.85
1:A:18:C:O2	1:A:1080:A:N1	2.08	0.85
23:W:534:SER:OG	23:W:537:ALA:CB	2.25	0.85
1:A:927:G:O6	1:A:1392:G:C5	2.30	0.85
1:A:1102:A:C2'	2:B:98:GLY:H	1.90	0.85
22:V:48:LEU:HA	25:Z:131:ARG:HH12	1.42	0.85
1:A:1072:G:H5"	5:E:62:LYS:NZ	1.70	0.84
1:A:18:C:N1	1:A:1080:A:N3	2.24	0.84
25:Z:125:LYS:CD	26:X:25:C:C2'	2.46	0.84
1:A:966:2MG:C6	26:X:34:C:H1'	2.11	0.84
1:A:1338:G:H22	26:X:29:G:H21	1.02	0.84
1:A:50:A:N6	23:W:753:SER:CB	2.40	0.84
12:L:56:ARG:HH12	23:W:738:ALA:CA	1.91	0.84
1:A:1400:C:N1	26:X:34:C:C2	2.45	0.84
12:L:41:THR:HG23	22:V:64:ARG:CZ	2.08	0.84
1:A:701:U:C2'	24:Y:61:ASP:CB	2.54	0.84
1:A:1517:G:C6	25:Z:106:ASP:OD1	2.31	0.84
1:A:358:U:H1'	23:W:577:GLY:CA	2.08	0.84
1:A:865:A:OP1	1:A:1077:G:O3'	1.93	0.84
1:A:1492:A:N3	22:V:35:TYR:HB2	1.93	0.84
1:A:1072:G:O5'	5:E:62:LYS:NZ	2.11	0.84
7:G:143:ARG:C	11:K:61:PHE:CE2	2.50	0.84
1:A:1400:C:C2	26:X:34:C:O2	2.31	0.84
23:W:812:ILE:CG1	26:X:76:A:C4	2.61	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1493:A:H2	22:V:22:PHE:N	1.67	0.83
1:A:1070:U:C5'	5:E:23:LYS:HE3	2.07	0.83
25:Z:123:LYS:HG3	26:X:12:G:H4'	1.61	0.83
1:A:927:G:N2	1:A:1531:A:H5"	1.93	0.83
7:G:146:GLU:OE2	11:K:61:PHE:CE1	2.31	0.83
1:A:357:G:H4'	23:W:607:ARG:HD2	1.60	0.83
1:A:790:A:C5	26:X:38:A:H4'	2.13	0.83
1:A:1101:A:H8	2:B:171:ILE:HD13	1.39	0.83
22:V:17:LEU:HB3	22:V:18:PRO:HD2	1.60	0.83
26:X:22:G:N3	26:X:23:C:C6	2.47	0.83
1:A:1400:C:C6	26:X:34:C:N1	2.39	0.83
1:A:828:U:O2'	2:B:25:PRO:O	1.96	0.82
7:G:149:LYS:H	11:K:61:PHE:H	1.25	0.82
1:A:18:C:C2	1:A:1080:A:N3	2.45	0.82
22:V:25:LYS:HA	22:V:31:GLU:HB3	1.61	0.82
23:W:795:ILE:HG22	23:W:879:VAL:HG13	1.61	0.82
1:A:966:2MG:C6	26:X:34:C:C1'	2.61	0.82
12:L:41:THR:CG2	22:V:64:ARG:HD2	2.10	0.82
23:W:790:LEU:C	23:W:791:LYS:HZ1	1.83	0.82
23:W:531:VAL:HG11	23:W:544:LEU:CB	2.06	0.82
23:W:534:SER:HB3	23:W:537:ALA:HB3	1.61	0.82
25:Z:125:LYS:HD3	26:X:25:C:O2'	1.76	0.82
25:Z:91:ILE:CB	26:X:13:C:C4'	1.97	0.82
12:L:47:SER:OG	22:V:35:TYR:CZ	2.32	0.82
22:V:52:ARG:HH11	22:V:52:ARG:HB2	1.43	0.82
1:A:927:G:N1	1:A:1392:G:O4'	2.12	0.82
1:A:1494:G:H8	22:V:17:LEU:C	1.80	0.81
1:A:828:U:N1	2:B:25:PRO:HG2	1.94	0.81
1:A:927:G:H21	1:A:1531:A:C5'	1.93	0.81
1:A:1400:C:C6	26:X:34:C:O2	2.31	0.81
1:A:1493:A:N9	22:V:18:PRO:O	2.13	0.81
1:A:1101:A:OP1	2:B:170:HIS:CE1	2.31	0.81
23:W:426:GLN:HE22	23:W:770:VAL:HB	1.44	0.81
1:A:966:2MG:O6	1:A:1400:C:C4	2.33	0.81
7:G:148:ASN:CG	11:K:59:THR:CG2	2.48	0.81
22:V:15:GLU:HB3	22:V:23:ARG:HB2	1.62	0.81
23:W:795:ILE:CG2	23:W:879:VAL:HG13	2.11	0.81
7:G:147:ALA:HB1	11:K:59:THR:OG1	1.81	0.81
1:A:918:A:C2	1:A:1080:A:H2	1.99	0.81
1:A:1100:C:C5	2:B:95:ARG:HD2	2.15	0.81
7:G:148:ASN:N	11:K:61:PHE:H	1.77	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:X:8:4SU:H6	26:X:21:A:H2	1.45	0.81
1:A:1072:G:H5"	5:E:62:LYS:HD3	1.61	0.80
3:C:168:TYR:CE1	5:E:55:GLU:OE2	2.33	0.80
1:A:927:G:C6	1:A:1392:G:C1'	2.64	0.80
1:A:829:G:C5'	2:B:25:PRO:HG3	2.11	0.80
1:A:1079:G:C5'	5:E:135:ASN:ND2	2.45	0.80
12:L:56:ARG:NH1	23:W:738:ALA:HA	1.96	0.80
1:A:1493:A:H61	22:V:33:LEU:HD12	1.46	0.80
23:W:589:GLY:HA3	23:W:622:PRO:N	1.97	0.80
22:V:15:GLU:H	22:V:23:ARG:HB2	1.47	0.80
1:A:530:G:C1'	22:V:39:LYS:CD	2.58	0.80
1:A:1492:A:H2	22:V:35:TYR:HB3	1.40	0.80
1:A:50:A:H61	23:W:753:SER:CB	1.95	0.80
25:Z:125:LYS:HD2	26:X:25:C:HO2'	0.97	0.80
1:A:358:U:H2'	23:W:576:LYS:O	1.80	0.79
1:A:1072:G:P	5:E:62:LYS:HZ2	2.02	0.79
1:A:18:C:O2	1:A:1079:G:C2	2.35	0.79
1:A:1070:U:OP1	5:E:23:LYS:CD	2.27	0.79
1:A:1494:G:C8	22:V:18:PRO:HB3	2.17	0.79
1:A:927:G:N2	1:A:1391:U:HO2'	1.80	0.79
1:A:790:A:N7	26:X:38:A:H4'	1.92	0.79
1:A:1100:C:H41	2:B:95:ARG:HD3	0.85	0.79
1:A:127:G:O2'	17:Q:6:ARG:NH1	2.15	0.79
1:A:829:G:O4'	2:B:25:PRO:HD3	1.82	0.79
1:A:1390:U:H6	1:A:1391:U:O5'	1.64	0.79
7:G:149:LYS:CG	11:K:95:SER:HB3	1.90	0.79
26:X:71:C:O2'	26:X:72:A:C5'	2.29	0.79
1:A:1517:G:H5"	25:Z:109:VAL:CG2	2.12	0.79
1:A:1103:C:O4'	2:B:98:GLY:N	2.00	0.79
1:A:1517:G:C5	25:Z:106:ASP:CG	2.56	0.79
4:D:100:ASN:OD1	4:D:111:ARG:NH1	2.16	0.79
1:A:530:G:C1'	22:V:39:LYS:HD3	2.13	0.79
25:Z:180:GLN:CD	26:X:71:C:N4	2.35	0.79
1:A:1400:C:C5'	26:X:34:C:N4	2.44	0.78
25:Z:125:LYS:CE	26:X:25:C:C1'	2.61	0.78
1:A:358:U:O3'	23:W:579:GLY:CA	2.31	0.78
1:A:1073:U:P	5:E:66:LYS:NZ	2.56	0.78
1:A:966:2MG:C8	26:X:34:C:O2'	2.35	0.78
23:W:537:ALA:HB3	23:W:539:THR:HG23	1.65	0.78
1:A:358:U:H1'	23:W:577:GLY:C	2.03	0.78
23:W:791:LYS:O	23:W:791:LYS:HD2	1.81	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1078:U:C1'	5:E:91:GLY:H	1.88	0.78
1:A:1494:G:N7	22:V:18:PRO:CD	2.46	0.78
1:A:927:G:C2	1:A:1531:A:H4'	2.18	0.78
1:A:829:G:C1'	2:B:25:PRO:HD3	2.14	0.78
23:W:565:ALA:HB2	23:W:590:THR:HG23	1.66	0.78
1:A:928:G:H5'	1:A:1531:A:N3	1.97	0.78
22:V:34:ALA:HA	22:V:65:GLY:O	1.84	0.78
1:A:920:U:O2'	1:A:1082:A:OP1	2.00	0.78
7:G:148:ASN:ND2	11:K:59:THR:HG21	1.97	0.78
23:W:848:PHE:N	27:X:101:FME:O1	2.14	0.78
25:Z:90:VAL:CG2	26:X:13:C:C2'	2.62	0.78
12:L:56:ARG:NH1	23:W:738:ALA:CA	2.46	0.78
1:A:530:G:N7	22:V:38:GLY:CA	2.48	0.77
23:W:790:LEU:O	23:W:791:LYS:HB3	1.83	0.77
1:A:1495:U:O2'	25:Z:101:GLY:N	2.17	0.77
1:A:1073:U:O3'	5:E:69:ARG:NH1	2.17	0.77
7:G:68:ASN:O	7:G:138:ARG:NH1	2.17	0.77
25:Z:180:GLN:CA	26:X:69:C:C2	2.67	0.77
25:Z:178:LYS:HB3	26:X:69:C:C1'	2.14	0.77
23:W:613:LEU:HD12	23:W:614:GLY:N	1.99	0.77
1:A:927:G:C2'	1:A:1531:A:C1'	2.54	0.77
1:A:966:2MG:C6	1:A:1400:C:C4	2.73	0.77
7:G:147:ALA:CB	11:K:59:THR:OG1	2.33	0.77
1:A:1074:G:H5'	2:B:102:THR:C	2.05	0.77
25:Z:125:LYS:HD2	26:X:25:C:C1'	2.14	0.77
1:A:18:C:N3	1:A:1080:A:C2	2.53	0.76
1:A:1147:C:O2	9:I:18:ARG:NH2	2.18	0.76
26:X:18:G:O2'	26:X:19:G:H5'	1.85	0.76
25:Z:91:ILE:CG1	26:X:13:C:H5'	2.15	0.76
1:A:1339:A:O3'	26:X:41:C:H4'	1.84	0.76
1:A:701:U:H2'	24:Y:61:ASP:HB3	1.67	0.76
1:A:1101:A:C5	2:B:171:ILE:HG23	2.20	0.76
1:A:830:G:C5'	2:B:23:TRP:H	1.98	0.76
7:G:147:ALA:CA	11:K:59:THR:OG1	2.33	0.76
1:A:368:U:P	23:W:607:ARG:CG	2.71	0.76
25:Z:93:VAL:HG21	26:X:11:A:H2	1.51	0.76
1:A:701:U:O2'	24:Y:61:ASP:CB	2.33	0.76
25:Z:93:VAL:CG1	26:X:24:U:O2	2.33	0.76
23:W:790:LEU:HB3	23:W:791:LYS:NZ	2.01	0.76
1:A:701:U:O2'	24:Y:61:ASP:HB3	1.85	0.76
1:A:1078:U:O2	5:E:91:GLY:CA	2.34	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1493:A:H8	22:V:19:ASN:HB2	1.49	0.75
1:A:864:A:C5'	1:A:1078:U:C4	2.54	0.75
7:G:111:ARG:NH1	7:G:123:GLU:OE2	2.19	0.75
25:Z:91:ILE:CB	26:X:13:C:H5'	2.08	0.75
23:W:860:GLU:HG3	27:X:101:FME:HE2	1.68	0.75
1:A:701:U:H2'	24:Y:64:LYS:HB2	1.67	0.75
25:Z:129:ARG:CZ	26:X:37:A:O3'	2.35	0.75
22:V:54:VAL:HB	22:V:69:TYR:HB2	1.69	0.75
22:V:49:PRO:HD3	25:Z:131:ARG:NH1	2.02	0.75
1:A:1494:G:N7	22:V:18:PRO:HD3	2.02	0.75
12:L:51:LYS:HE2	22:V:60:TYR:CE2	2.22	0.75
1:A:1400:C:C5	26:X:34:C:O2	2.38	0.75
1:A:701:U:C5'	24:Y:64:LYS:CG	2.65	0.75
1:A:927:G:O5'	1:A:1503:A:H2'	1.84	0.75
25:Z:93:VAL:CG2	26:X:12:G:N3	2.48	0.75
1:A:701:U:O4	24:Y:44:ASP:OD2	2.04	0.75
1:A:1134:G:N2	1:A:1140:C:N3	2.34	0.75
7:G:147:ALA:HB2	11:K:61:PHE:CD2	2.18	0.75
1:A:1339:A:O3'	26:X:41:C:C4'	2.35	0.74
1:A:1101:A:C1'	2:B:171:ILE:CD1	2.63	0.74
26:X:20:H2U:H4'	26:X:21:A:OP2	1.87	0.74
1:A:927:G:O2'	1:A:1503:A:C8	2.39	0.74
23:W:790:LEU:HB3	23:W:791:LYS:HZ3	1.51	0.74
1:A:1100:C:C4	2:B:95:ARG:HD3	2.01	0.74
1:A:1400:C:C4	26:X:34:C:O2	2.39	0.74
1:A:1493:A:C3'	22:V:18:PRO:C	2.47	0.74
7:G:143:ARG:HA	11:K:61:PHE:HZ	1.41	0.74
1:A:918:A:H2	1:A:1080:A:N1	1.85	0.74
1:A:927:G:C4'	1:A:1503:A:C3'	2.58	0.74
1:A:927:G:C5	1:A:1392:G:C1'	2.70	0.74
1:A:1079:G:H5"	5:E:134:ILE:HG23	1.70	0.73
1:A:921:U:H5'	1:A:1082:A:OP1	1.88	0.73
1:A:1400:C:C6	26:X:34:C:N3	2.56	0.73
1:A:1339:A:N3	26:X:41:C:O2	2.21	0.73
1:A:927:G:C6	1:A:1392:G:C8	2.76	0.73
3:C:40:ARG:NH1	3:C:55:ILE:O	2.21	0.73
1:A:927:G:N1	1:A:1391:U:H2'	1.96	0.73
1:A:1229:A:H4'	26:X:29:G:OP1	1.88	0.73
23:W:540:GLY:CA	23:W:541:ILE:HG22	2.13	0.73
23:W:790:LEU:C	23:W:791:LYS:NZ	2.41	0.73
25:Z:179:LYS:CB	26:X:4:G:H21	2.01	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:Z:90:VAL:HG23	26:X:13:C:H2'	1.69	0.73
26:X:8:4SU:H1'	26:X:21:A:C2	2.22	0.73
25:Z:180:GLN:HG3	26:X:69:C:C5	2.24	0.73
22:V:52:ARG:HB2	22:V:52:ARG:NH1	2.02	0.73
1:A:790:A:N7	26:X:38:A:C2'	2.43	0.73
23:W:534:SER:OG	23:W:537:ALA:HB3	1.85	0.73
1:A:700:G:C6	24:Y:63:GLY:O	2.42	0.73
1:A:519:C:O2	22:V:2:LYS:CE	2.33	0.73
1:A:698:G:P	24:Y:74:LYS:CD	2.76	0.73
1:A:927:G:H2'	1:A:1531:A:C2'	2.18	0.73
1:A:1390:U:H3'	1:A:1392:G:OP2	1.88	0.72
25:Z:90:VAL:HG23	26:X:13:C:C2'	2.19	0.72
26:X:58:A:O2'	26:X:60:U:H5	1.72	0.72
26:X:8:4SU:H6	26:X:21:A:C2	2.23	0.72
1:A:19:A:C5'	1:A:1078:U:C2	2.70	0.72
1:A:864:A:C5'	1:A:1078:U:H5	1.67	0.72
26:X:71:C:HO2'	26:X:72:A:H5'	1.52	0.72
1:A:1101:A:C4	2:B:171:ILE:HG23	2.24	0.72
1:A:1100:C:H42	2:B:95:ARG:NE	1.85	0.72
1:A:1389:C:C2	1:A:1391:U:C6	2.76	0.72
1:A:864:A:H5'	1:A:1078:U:C4	2.21	0.72
26:X:58:A:HO2'	26:X:60:U:H5	1.36	0.72
25:Z:90:VAL:HG21	26:X:13:C:H2'	1.72	0.72
7:G:145:ALA:C	11:K:61:PHE:HB2	1.94	0.72
22:V:25:LYS:HE3	22:V:29:GLY:O	1.89	0.72
23:W:812:ILE:CD1	26:X:76:A:N3	2.49	0.72
1:A:18:C:N3	1:A:1080:A:H2	1.87	0.72
1:A:828:U:O2	2:B:25:PRO:N	2.23	0.72
1:A:1102:A:C2'	2:B:98:GLY:HA3	2.20	0.72
22:V:48:LEU:HD23	25:Z:131:ARG:NH1	2.05	0.72
1:A:1073:U:H5"	5:E:69:ARG:HH22	1.52	0.71
1:A:18:C:C6	1:A:1080:A:N3	2.58	0.71
1:A:361:G:OP1	23:W:729:THR:CB	2.37	0.71
25:Z:125:LYS:CD	26:X:25:C:H1'	2.19	0.71
1:A:1073:U:C4'	5:E:69:ARG:HH22	2.03	0.71
1:A:1073:U:P	5:E:66:LYS:HZ2	2.13	0.71
25:Z:91:ILE:HB	26:X:13:C:O5'	1.89	0.71
1:A:18:C:H1'	1:A:1080:A:C6	2.26	0.71
1:A:790:A:C1'	26:X:38:A:H5"	2.19	0.71
26:X:41:C:H3'	26:X:42:G:H5"	1.71	0.71
1:A:1517:G:C4	25:Z:106:ASP:HB2	2.25	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:Z:179:LYS:HB2	26:X:4:G:H21	1.56	0.71
1:A:1390:U:C3'	1:A:1392:G:OP2	2.30	0.71
1:A:1230:C:H5'	26:X:30:G:P	2.30	0.71
25:Z:125:LYS:HE3	26:X:25:C:H1'	1.70	0.71
1:A:790:A:N7	26:X:38:A:C1'	2.54	0.71
22:V:49:PRO:CD	25:Z:131:ARG:NH1	2.53	0.71
1:A:1078:U:N1	5:E:91:GLY:N	2.12	0.71
23:W:716:VAL:HG21	23:W:786:LEU:HD21	1.73	0.71
1:A:358:U:H4'	23:W:579:GLY:CA	2.20	0.70
22:V:15:GLU:H	22:V:23:ARG:CB	2.04	0.70
1:A:928:G:C6	1:A:1391:U:H1'	2.23	0.70
1:A:359:G:H5'	23:W:575:ASP:O	1.91	0.70
24:Y:71:LYS:O	24:Y:75:GLU:HG2	1.91	0.70
1:A:530:G:C2'	22:V:39:LYS:HD3	2.21	0.70
1:A:1230:C:H5"	26:X:29:G:O3'	1.91	0.70
1:A:1078:U:O2	5:E:91:GLY:HA3	1.92	0.70
1:A:1074:G:C5'	2:B:102:THR:O	2.38	0.70
1:A:359:G:O4'	23:W:576:LYS:HA	1.90	0.70
23:W:804:PHE:CB	23:W:812:ILE:CG2	2.64	0.70
1:A:1494:G:N9	22:V:18:PRO:HD3	2.07	0.70
1:A:966:2MG:C4	26:X:34:C:C2'	2.74	0.70
1:A:19:A:H5"	1:A:1078:U:N3	1.92	0.70
26:X:58:A:H1'	26:X:60:U:O4	1.92	0.70
12:L:51:LYS:HE3	22:V:60:TYR:CB	2.22	0.70
7:G:143:ARG:O	11:K:61:PHE:CG	2.40	0.70
22:V:52:ARG:CB	22:V:52:ARG:HH11	2.05	0.70
25:Z:173:VAL:HG11	26:X:11:A:O2'	1.90	0.70
1:A:864:A:H5"	1:A:1078:U:H5	1.45	0.69
9:I:12:ARG:NH2	9:I:107:ASP:OD2	2.24	0.69
26:X:70:G:H2'	26:X:71:C:C6	2.27	0.69
26:X:17:C:H2'	26:X:17(A):U:H5	1.55	0.69
1:A:530:G:H1'	22:V:39:LYS:CG	2.22	0.69
7:G:148:ASN:CB	11:K:59:THR:HB	2.21	0.69
7:G:147:ALA:CA	11:K:61:PHE:N	2.46	0.69
1:A:520:A:OP1	22:V:58:THR:OG1	2.09	0.69
23:W:792:GLN:HB3	23:W:881:GLU:O	1.91	0.69
25:Z:90:VAL:HB	26:X:13:C:C2'	2.04	0.69
22:V:45:ILE:CD1	22:V:70:ARG:HD3	2.22	0.69
1:A:845:A:O3'	18:R:48:ARG:NH2	2.25	0.69
1:A:1101:A:C4	2:B:171:ILE:HD12	2.23	0.69
13:M:4:ILE:O	13:M:7:ILE:N	2.26	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1518:MA6:H103	1:A:1519:MA6:C10	2.21	0.69
1:A:360:G:H4'	23:W:751:ASP:OD2	1.93	0.69
1:A:532:A:N6	3:C:160:ALA:C	2.46	0.69
23:W:796:GLY:O	23:W:879:VAL:HG12	1.93	0.69
1:A:1072:G:OP1	5:E:62:LYS:NZ	2.26	0.68
7:G:148:ASN:CG	11:K:59:THR:HG21	2.14	0.68
21:U:31:GLU:OE2	21:U:34:ARG:NH2	2.25	0.68
1:A:518:C:OP2	22:V:39:LYS:HE2	1.93	0.68
23:W:790:LEU:HD23	23:W:790:LEU:O	1.94	0.68
9:I:130:ARG:NH2	26:X:32:C:H5	1.89	0.68
25:Z:179:LYS:C	26:X:69:C:H2'	2.13	0.68
23:W:533:VAL:HG12	23:W:541:ILE:H	1.57	0.68
1:A:1496:C:H5'	25:Z:101:GLY:HA3	1.76	0.68
7:G:149:LYS:HB2	11:K:60:PRO:C	2.13	0.68
1:A:359:G:H4'	23:W:576:LYS:HA	1.76	0.68
1:A:1338:G:H21	26:X:29:G:N2	1.90	0.68
1:A:1400:C:O4'	26:X:34:C:C4	2.47	0.68
1:A:738:C:OP1	6:F:2:ARG:NH2	2.27	0.68
23:W:426:GLN:HE22	23:W:770:VAL:CB	2.06	0.68
25:Z:93:VAL:HG21	26:X:11:A:C2	2.29	0.68
1:A:927:G:O5'	1:A:1503:A:O2'	2.08	0.68
12:L:51:LYS:HE3	22:V:60:TYR:HD2	1.31	0.68
23:W:550:LEU:C	23:W:550:LEU:HD23	2.14	0.68
1:A:1100:C:C5	2:B:95:ARG:CD	2.76	0.68
23:W:797:LEU:HD23	23:W:798:ALA:N	2.08	0.68
26:X:20:H2U:O5'	26:X:21:A:OP2	2.12	0.68
24:Y:21:GLN:H	24:Y:21:GLN:HE21	1.40	0.68
1:A:828:U:O2	2:B:24:ASN:OD1	2.11	0.67
1:A:927:G:H4'	1:A:1503:A:C1'	2.22	0.67
1:A:1338:G:C4	26:X:42:G:O2'	2.44	0.67
1:A:1230:C:C5'	26:X:29:G:O3'	2.41	0.67
1:A:1073:U:C5'	5:E:69:ARG:HH22	2.08	0.67
1:A:980:C:O3'	14:N:13:ARG:NH2	2.28	0.67
1:A:50:A:N6	23:W:753:SER:HB3	2.08	0.67
1:A:359:G:H1'	23:W:576:LYS:CG	2.15	0.67
7:G:149:LYS:HD3	11:K:95:SER:HB2	1.66	0.67
23:W:396:ILE:HG22	23:W:404:LYS:HG3	1.77	0.67
23:W:540:GLY:CA	23:W:542:ASP:H	2.08	0.67
25:Z:129:ARG:CD	26:X:38:A:OP1	2.43	0.67
1:A:927:G:O6	1:A:1391:U:O2	2.13	0.67
1:A:1400:C:N1	26:X:34:C:O2	2.26	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:412:A:H1'	1:A:413:G:H5'	1.76	0.67
1:A:1494:G:N7	22:V:18:PRO:CG	2.58	0.67
26:X:22:G:C4	26:X:23:C:C6	2.82	0.67
25:Z:180:GLN:HA	26:X:69:C:N1	2.09	0.67
1:A:1078:U:C2	5:E:91:GLY:CA	2.78	0.67
22:V:66:ARG:HB3	22:V:66:ARG:NH1	2.10	0.67
7:G:138:ARG:NH2	7:G:139:GLU:OE2	2.29	0.67
1:A:19:A:H4'	1:A:1078:U:O4	1.93	0.66
13:M:4:ILE:O	13:M:6:GLY:N	2.28	0.66
23:W:396:ILE:CG2	23:W:404:LYS:HG3	2.25	0.66
1:A:793:U:O4	25:Z:109:VAL:HG21	1.94	0.66
1:A:920:U:H4'	1:A:1082:A:H5"	1.77	0.66
16:P:1:MET:N	16:P:1:MET:SD	2.64	0.66
23:W:812:ILE:HD12	23:W:863:ILE:C	2.15	0.66
25:Z:125:LYS:HD2	26:X:25:C:H1'	1.76	0.66
23:W:812:ILE:HD11	26:X:76:A:C2	2.31	0.66
1:A:927:G:C2	1:A:1391:U:O2'	2.49	0.66
1:A:865:A:H5'	1:A:1077:G:O2'	1.96	0.66
12:L:56:ARG:HH12	23:W:738:ALA:N	1.94	0.66
22:V:48:LEU:CD2	25:Z:131:ARG:NH1	2.58	0.66
1:A:1517:G:O4'	25:Z:105:GLY:C	2.33	0.66
23:W:565:ALA:HB2	23:W:590:THR:HG22	1.77	0.66
1:A:1081:A:OP1	5:E:21:VAL:CB	2.44	0.66
3:C:19:ASN:ND2	14:N:90:ARG:O	2.28	0.66
23:W:589:GLY:HA3	23:W:622:PRO:CD	2.25	0.66
22:V:15:GLU:CB	22:V:23:ARG:HB2	2.25	0.66
25:Z:180:GLN:N	26:X:69:C:H2'	2.10	0.66
1:A:1074:G:H5"	2:B:102:THR:HB	1.76	0.65
1:A:1390:U:H6	1:A:1391:U:P	2.19	0.65
1:A:518:C:O2'	22:V:38:GLY:HA3	1.96	0.65
3:C:179:ARG:NH1	3:C:206:GLU:OE1	2.29	0.65
1:A:790:A:C1'	26:X:38:A:H4'	2.23	0.65
1:A:7:A:N6	5:E:97:GLN:OE1	2.30	0.65
25:Z:156:ALA:CB	25:Z:174:LEU:HD11	2.26	0.65
25:Z:93:VAL:CG2	26:X:24:U:O2	2.42	0.65
1:A:1497:G:OP1	25:Z:99:ARG:NH1	2.25	0.65
1:A:928:G:C8	1:A:1531:A:O2'	2.50	0.65
7:G:147:ALA:CA	11:K:61:PHE:C	2.41	0.65
1:A:1074:G:OP2	5:E:66:LYS:CD	2.45	0.65
1:A:519:C:N3	22:V:2:LYS:HE2	2.11	0.65
1:A:1339:A:C2'	26:X:41:C:O2	2.43	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:W:468:VAL:HB	23:W:498:ASN:HD21	1.62	0.64
25:Z:93:VAL:N	26:X:12:G:H21	1.95	0.64
26:X:66:C:H2'	26:X:67:C:C6	2.32	0.64
1:A:263:A:OP2	20:T:74:ARG:NH1	2.29	0.64
1:A:829:G:O5'	2:B:25:PRO:HG3	1.98	0.64
1:A:1073:U:O2	2:B:103:ASN:CG	2.33	0.64
3:C:168:TYR:CG	5:E:55:GLU:OE1	2.49	0.64
8:H:54:ASP:OD1	8:H:55:THR:N	2.30	0.64
1:A:845:A:O2'	18:R:48:ARG:NH2	2.31	0.64
23:W:855:VAL:HG11	23:W:861:CYS:CB	2.27	0.64
26:X:22:G:O2'	26:X:23:C:O5'	2.15	0.64
25:Z:123:LYS:CG	26:X:12:G:C1'	2.76	0.64
1:A:530:G:N7	22:V:38:GLY:C	2.51	0.64
23:W:569:VAL:HG22	23:W:584:VAL:HG22	1.78	0.64
25:Z:90:VAL:CB	26:X:13:C:C2'	2.73	0.64
23:W:393:VAL:HG12	23:W:462:THR:HG22	1.79	0.64
12:L:51:LYS:CE	22:V:60:TYR:CE2	2.73	0.64
23:W:544:LEU:C	23:W:544:LEU:HD23	2.17	0.64
26:X:54:5MU:H72	26:X:55:PSU:O2	1.98	0.64
1:A:1496:C:C2'	25:Z:99:ARG:NH2	2.61	0.64
1:A:1071:C:O3'	5:E:62:LYS:NZ	2.31	0.64
1:A:1070:U:OP1	5:E:23:LYS:HD3	1.98	0.63
9:I:22:LYS:O	9:I:62:ASP:N	2.29	0.63
26:X:73:A:H8	26:X:73:A:O5'	1.80	0.63
11:K:119:ASN:OD1	21:U:35:ARG:NH1	2.31	0.63
26:X:67:C:H2'	26:X:68:C:C6	2.33	0.63
26:X:8:4SU:H5"	26:X:8:4SU:O2	1.98	0.63
1:A:927:G:C5'	1:A:1503:A:C2'	2.63	0.63
1:A:8:A:C6	4:D:206:LYS:HB3	2.33	0.63
1:A:1074:G:P	5:E:69:ARG:HH12	2.21	0.63
5:E:79:GLY:O	5:E:121:HIS:N	2.28	0.63
1:A:927:G:N1	1:A:1391:U:C2'	2.58	0.63
1:A:927:G:C2	1:A:1392:G:C1'	2.82	0.63
23:W:533:VAL:HG12	23:W:541:ILE:N	2.12	0.63
1:A:1073:U:O2	2:B:103:ASN:CB	2.47	0.63
25:Z:128:LEU:HD11	25:Z:141:GLY:HA2	1.81	0.63
1:A:829:G:O5'	2:B:25:PRO:CG	2.46	0.63
19:S:36:ARG:NH2	19:S:75:ALA:O	2.32	0.63
23:W:830:VAL:HG22	23:W:877:ILE:HG12	1.81	0.63
1:A:1400:C:P	26:X:34:C:C5	2.92	0.63
22:V:5:ASP:O	22:V:59:PRO:HD3	1.99	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:W:540:GLY:HA3	23:W:542:ASP:H	1.63	0.63
1:A:790:A:O2'	25:Z:97:LYS:HG3	1.98	0.63
1:A:829:G:H1'	2:B:25:PRO:HD3	1.79	0.63
26:X:41:C:C3'	26:X:42:G:H5"	2.29	0.63
1:A:700:G:C6	24:Y:63:GLY:HA2	2.32	0.63
1:A:927:G:C4	1:A:1392:G:C1'	2.81	0.63
1:A:1079:G:C4'	5:E:135:ASN:ND2	2.61	0.62
23:W:847:ARG:HA	27:X:101:FME:CN	2.29	0.62
1:A:1493:A:H3'	22:V:18:PRO:CA	2.29	0.62
23:W:537:ALA:CB	23:W:539:THR:HG23	2.29	0.62
26:X:22:G:C5	26:X:23:C:C5	2.86	0.62
26:X:22:G:N3	26:X:23:C:C5	2.66	0.62
1:A:518:C:O2'	22:V:38:GLY:CA	2.48	0.62
1:A:1075:U:H5"	2:B:178:ASN:ND2	2.15	0.62
12:L:56:ARG:HH12	23:W:738:ALA:CB	2.13	0.62
26:X:51:C:H2'	26:X:52:G:C8	2.34	0.62
1:A:1072:G:H5"	5:E:62:LYS:HE2	1.63	0.62
1:A:928:G:N1	1:A:1391:U:N1	2.22	0.62
1:A:1073:U:P	5:E:66:LYS:HZ3	2.22	0.62
7:G:147:ALA:C	11:K:59:THR:HG1	1.79	0.62
1:A:790:A:C8	26:X:38:A:C1'	2.82	0.62
22:V:36:ILE:O	22:V:41:ARG:HD2	1.98	0.62
23:W:534:SER:OG	23:W:537:ALA:HB2	1.99	0.62
26:X:8:4SU:H1'	26:X:21:A:N1	2.14	0.62
1:A:18:C:C1'	1:A:1080:A:C4	2.83	0.62
1:A:405:U:OP2	4:D:3:ARG:NH1	2.32	0.62
7:G:149:LYS:HB3	11:K:95:SER:OG	2.00	0.62
17:Q:60:GLU:OE1	17:Q:77:ARG:NE	2.33	0.62
23:W:716:VAL:CG2	23:W:786:LEU:HD21	2.29	0.62
1:A:1194:U:O4'	5:E:26:LYS:O	2.18	0.62
22:V:66:ARG:HH11	22:V:66:ARG:HB3	1.65	0.62
23:W:531:VAL:CG1	23:W:544:LEU:HB2	2.14	0.61
26:X:56:C:O2'	26:X:57:A:H5'	2.00	0.61
23:W:812:ILE:CG2	26:X:76:A:O4'	2.44	0.61
1:A:966:2MG:O6	1:A:1400:C:C5	2.53	0.61
1:A:828:U:O2'	2:B:26:LYS:N	2.31	0.61
1:A:1074:G:C5'	2:B:102:THR:C	2.69	0.61
23:W:611:ASN:O	23:W:612:GLU:HG2	2.00	0.61
1:A:927:G:N1	1:A:1392:G:C1'	2.63	0.61
1:A:927:G:O6	1:A:1392:G:C8	2.53	0.61
22:V:36:ILE:HG22	22:V:41:ARG:HG3	1.80	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:X:19:G:O2'	26:X:20:H2U:OP2	2.17	0.61
25:Z:91:ILE:CG2	26:X:13:C:H4'	2.21	0.61
1:A:922:G:OP1	1:A:1069:C:OP1	2.18	0.61
22:V:45:ILE:HG23	22:V:71:LYS:HE3	1.82	0.61
23:W:483:ILE:HD12	23:W:519:ILE:HG21	1.82	0.61
23:W:855:VAL:HG11	23:W:861:CYS:HB3	1.82	0.61
11:K:112:ASP:HB3	21:U:2:PRO:HG2	1.83	0.61
1:A:530:G:O4'	22:V:39:LYS:HE2	2.01	0.61
26:X:8:4SU:H3'	26:X:8:4SU:O2	1.99	0.61
25:Z:180:GLN:OXT	26:X:69:C:C4	2.53	0.61
23:W:814:GLY:HA3	27:X:101:FME:SD	2.41	0.61
25:Z:93:VAL:O	26:X:24:U:O2'	2.13	0.61
1:A:1225:A:H2'	1:A:1226:C:C5	2.35	0.61
1:A:1338:G:H1'	26:X:42:G:O2'	2.01	0.61
2:B:120:GLN:O	2:B:125:THR:N	2.34	0.61
7:G:90:GLU:N	7:G:90:GLU:OE2	2.34	0.61
1:A:19:A:C4'	1:A:1078:U:O4	2.48	0.61
1:A:1495:U:C2'	25:Z:101:GLY:HA3	2.30	0.60
1:A:1339:A:H2	26:X:30:G:H1'	0.63	0.60
1:A:530:G:H8	22:V:39:LYS:H	1.47	0.60
1:A:790:A:OP1	26:X:39:C:H6	1.84	0.60
13:M:3:ARG:O	13:M:57:ARG:NH2	2.33	0.60
1:A:358:U:C1'	23:W:577:GLY:C	2.64	0.60
22:V:5:ASP:HB2	22:V:59:PRO:HG3	1.82	0.60
1:A:1517:G:C1'	25:Z:105:GLY:C	2.70	0.60
1:A:411:A:OP2	4:D:26:ARG:NH2	2.33	0.60
1:A:790:A:C1'	26:X:38:A:C4'	2.79	0.60
1:A:19:A:H5'	1:A:1078:U:H3	0.45	0.60
1:A:927:G:C2'	1:A:1531:A:C2'	2.78	0.60
22:V:40:MET:HE2	22:V:47:ILE:HD11	1.81	0.60
1:A:701:U:H5'	24:Y:64:LYS:HG3	1.83	0.60
1:A:1103:C:O2'	2:B:97:LEU:HD12	2.01	0.60
9:I:88:MET:SD	9:I:95:ARG:HG2	2.42	0.60
1:A:701:U:O2	24:Y:43:LEU:HD12	2.01	0.60
23:W:855:VAL:HG13	23:W:859:MET:CE	2.32	0.60
26:X:6:G:O2'	26:X:7:G:H5'	2.02	0.60
25:Z:125:LYS:NZ	26:X:25:C:C2'	2.53	0.60
1:A:1074:G:OP1	5:E:69:ARG:NH1	2.35	0.60
12:L:110:ARG:NH1	12:L:112:GLN:O	2.34	0.60
1:A:1494:G:C8	22:V:18:PRO:CG	2.84	0.59
1:A:8:A:N6	4:D:202:GLU:O	2.34	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:56:ARG:HH12	23:W:738:ALA:HB2	1.66	0.59
1:A:790:A:H1'	26:X:38:A:H5"	1.84	0.59
9:I:95:ARG:O	9:I:98:LEU:N	2.35	0.59
12:L:41:THR:HG23	22:V:64:ARG:HD2	1.83	0.59
14:N:31:ILE:HA	14:N:34:VAL:HG23	1.84	0.59
23:W:448:HIS:HD2	23:W:772:TYR:OH	1.86	0.59
25:Z:125:LYS:CD	26:X:25:C:C1'	2.75	0.59
1:A:920:U:O2'	1:A:1082:A:P	2.59	0.59
1:A:1102:A:C2'	2:B:98:GLY:N	2.57	0.59
1:A:966:2MG:C6	1:A:1400:C:C5	2.89	0.59
12:L:41:THR:HG23	22:V:64:ARG:CD	2.32	0.59
22:V:70:ARG:C	22:V:71:LYS:HD2	2.23	0.59
1:A:844:G:H2'	1:A:844:G:N3	2.16	0.59
5:E:161:VAL:HG12	5:E:162:GLU:H	1.67	0.59
10:J:63:ASP:HB3	10:J:65:TYR:CE1	2.36	0.59
19:S:29:LYS:HB3	19:S:30:PRO:HD2	1.85	0.59
22:V:20:ALA:HB1	22:V:36:ILE:HD12	1.84	0.59
22:V:45:ILE:HG12	22:V:70:ARG:HH11	1.68	0.59
26:X:33:U:N3	26:X:36:U:OP2	2.34	0.59
25:Z:129:ARG:HD2	26:X:38:A:OP1	2.02	0.59
1:A:1228:C:P	13:M:107:ARG:HH22	2.26	0.59
1:A:701:U:C2'	24:Y:64:LYS:HB2	2.29	0.59
23:W:797:LEU:C	23:W:797:LEU:HD23	2.22	0.59
1:A:701:U:C5'	24:Y:64:LYS:HB2	2.27	0.59
1:A:1178:G:N2	1:A:1181:G:OP2	2.34	0.59
1:A:700:G:N2	24:Y:63:GLY:CA	2.51	0.59
1:A:1079:G:C5'	5:E:134:ILE:HG23	2.31	0.59
1:A:1493:A:C8	22:V:19:ASN:HB2	2.35	0.59
1:A:359:G:O4'	23:W:576:LYS:O	2.21	0.59
26:X:17:C:H2'	26:X:17(A):U:C5	2.37	0.59
1:A:1400:C:H5'	26:X:34:C:H41	1.61	0.59
24:Y:21:GLN:H	24:Y:21:GLN:NE2	2.01	0.59
1:A:1517:G:C5'	25:Z:109:VAL:HG21	2.25	0.58
25:Z:91:ILE:N	26:X:13:C:O2'	2.35	0.58
1:A:1102:A:C2'	2:B:98:GLY:CA	2.79	0.58
1:A:825:A:O2'	8:H:13:ARG:NH1	2.37	0.58
23:W:399:HIS:CB	23:W:402:HIS:HE1	2.17	0.58
1:A:1494:G:O2'	22:V:16:ALA:C	2.32	0.58
7:G:149:LYS:CB	11:K:95:SER:CB	2.79	0.58
14:N:21:PHE:HA	14:N:25:ALA:HB3	1.85	0.58
26:X:8:4SU:C6	26:X:21:A:H2	2.13	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:18:C:O4'	1:A:1080:A:C4	2.57	0.58
1:A:1496:C:H5'	25:Z:101:GLY:CA	2.33	0.58
8:H:113:ASP:OD1	8:H:117:ARG:NH2	2.37	0.58
26:X:20:H2U:C4'	26:X:21:A:OP2	2.51	0.58
1:A:80:A:C2	1:A:90:C:N3	2.71	0.58
7:G:148:ASN:CG	11:K:59:THR:HB	2.23	0.58
1:A:966:2MG:N7	26:X:34:C:O2'	2.35	0.58
10:J:48:ARG:NH1	10:J:66:GLU:OE1	2.37	0.58
23:W:589:GLY:HA3	23:W:622:PRO:HD3	1.86	0.58
1:A:1075:U:H5"	2:B:178:ASN:HD21	1.69	0.58
23:W:471:ALA:HB3	23:W:505:ALA:HB1	1.84	0.58
1:A:1060:U:OP1	14:N:85:ARG:NH2	2.37	0.57
1:A:207:C:N4	1:A:212:G:O6	2.37	0.57
1:A:1073:U:C5'	5:E:69:ARG:NH2	2.65	0.57
12:L:41:THR:CG2	22:V:64:ARG:CD	2.82	0.57
25:Z:90:VAL:HG13	26:X:14:A:H3'	1.85	0.57
26:X:56:C:H2'	26:X:57:A:C8	2.38	0.57
23:W:721:ILE:HG22	23:W:735:LEU:HD21	1.86	0.57
23:W:812:ILE:CG1	26:X:76:A:C1'	2.62	0.57
25:Z:90:VAL:HG23	26:X:13:C:O2'	2.03	0.57
7:G:146:GLU:N	11:K:61:PHE:CG	2.56	0.57
12:L:56:ARG:HH11	23:W:738:ALA:HA	1.67	0.57
1:A:1400:C:N3	26:X:34:C:O2	2.38	0.57
1:A:790:A:OP1	26:X:39:C:C6	2.58	0.57
1:A:1101:A:H5"	2:B:171:ILE:HD11	1.86	0.57
1:A:1102:A:H2'	2:B:98:GLY:H	1.68	0.57
12:L:56:ARG:NH1	23:W:738:ALA:HB2	2.19	0.57
18:R:37:GLY:O	18:R:63:ARG:NH2	2.35	0.57
23:W:812:ILE:HD13	26:X:76:A:C6	2.38	0.57
1:A:518:C:OP2	22:V:39:LYS:CE	2.52	0.57
22:V:25:LYS:HA	22:V:31:GLU:CB	2.34	0.57
22:V:25:LYS:CA	22:V:31:GLU:HB3	2.31	0.57
25:Z:129:ARG:NE	26:X:38:A:P	2.77	0.57
1:A:1400:C:C4	26:X:34:C:C1'	2.60	0.57
1:A:701:U:O2'	24:Y:61:ASP:HB2	2.03	0.57
1:A:1229:A:C4'	26:X:29:G:OP1	2.53	0.57
1:A:927:G:O3'	1:A:1503:A:H2'	2.01	0.57
1:A:427:U:O2'	1:A:541:G:OP1	2.21	0.57
23:W:746:PHE:O	23:W:747:ASN:OD1	2.22	0.57
3:C:126:ARG:O	3:C:127:ARG:HB2	2.05	0.57
4:D:78:GLU:OE2	4:D:81:ARG:NH2	2.36	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1079:G:O2'	5:E:132:ASN:ND2	2.38	0.57
23:W:399:HIS:CD2	23:W:476:MET:CB	2.88	0.57
23:W:586:VAL:HG23	23:W:622:PRO:HA	1.86	0.57
1:A:686:U:C2'	24:Y:42:ASN:OD1	2.32	0.57
1:A:516:PSU:O3'	22:V:2:LYS:HE3	2.04	0.56
9:I:84:THR:HG21	9:I:103:PHE:HB3	1.87	0.56
10:J:7:ARG:HG2	10:J:101:SER:HB2	1.87	0.56
12:L:49:LEU:HD12	22:V:58:THR:OG1	2.05	0.56
1:A:368:U:H5"	23:W:607:ARG:HA	1.87	0.56
23:W:748:VAL:HG22	23:W:749:ARG:N	2.21	0.56
22:V:49:PRO:HD2	25:Z:131:ARG:NH1	2.20	0.56
1:A:1079:G:H5"	5:E:134:ILE:CG2	2.34	0.56
7:G:147:ALA:CB	11:K:61:PHE:HD2	2.08	0.56
1:A:1338:G:C2	26:X:42:G:H1'	2.38	0.56
1:A:1074:G:O3'	2:B:102:THR:CB	2.53	0.56
1:A:1102:A:H1'	2:B:98:GLY:HA3	1.88	0.56
23:W:727:GLY:O	23:W:728:ILE:HG13	2.05	0.56
3:C:132:ARG:HH12	4:D:47:ARG:NH2	2.04	0.56
23:W:591:LEU:HD12	23:W:620:ALA:CB	2.24	0.56
1:A:1189:U:OP1	14:N:98:LYS:NZ	2.39	0.56
8:H:3:MET:N	8:H:3:MET:SD	2.73	0.56
10:J:57:VAL:HG22	10:J:58:ASN:H	1.70	0.56
1:A:1217:C:P	14:N:9:ARG:HH21	2.29	0.56
7:G:150:ALA:HA	11:K:92:GLY:H	1.70	0.56
23:W:396:ILE:HG12	23:W:466:VAL:HB	1.86	0.56
1:A:368:U:OP2	23:W:607:ARG:CG	2.54	0.56
25:Z:90:VAL:CB	26:X:13:C:H2'	2.35	0.56
22:V:49:PRO:CD	25:Z:131:ARG:HH11	2.17	0.56
23:W:846:ARG:CB	26:X:76:A:C2	2.76	0.56
1:A:1496:C:OP1	25:Z:100:PRO:HG2	2.06	0.56
1:A:1103:C:O2'	2:B:97:LEU:CD1	2.53	0.56
1:A:261:U:OP2	20:T:74:ARG:NH2	2.38	0.56
23:W:467:LEU:HB2	23:W:495:VAL:HG12	1.88	0.56
25:Z:178:LYS:CB	26:X:69:C:C1'	2.82	0.56
1:A:1389:C:C5	1:A:1391:U:C4	2.85	0.55
7:G:145:ALA:O	11:K:61:PHE:HB2	2.05	0.55
23:W:399:HIS:HB3	23:W:402:HIS:CE1	2.41	0.55
1:A:1338:G:N2	26:X:42:G:N3	2.53	0.55
23:W:847:ARG:HA	27:X:101:FME:HCN	1.88	0.55
1:A:790:A:C1'	26:X:38:A:C5'	2.85	0.55
1:A:1492:A:O2'	22:V:19:ASN:O	2.24	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:16:VAL:HG23	11:K:17:SER:H	1.72	0.55
12:L:49:LEU:HD12	22:V:58:THR:CB	2.36	0.55
12:L:41:THR:HG21	22:V:64:ARG:HH11	1.68	0.55
1:A:1229:A:H4'	26:X:29:G:P	2.47	0.55
1:A:928:G:H1	1:A:1391:U:C1'	2.07	0.55
1:A:407:U:OP1	4:D:3:ARG:NH2	2.40	0.55
22:V:48:LEU:HD23	25:Z:131:ARG:HH12	1.69	0.55
23:W:457:ARG:HH12	23:W:637:ALA:HB3	1.71	0.55
23:W:544:LEU:HD23	23:W:544:LEU:O	2.05	0.55
23:W:860:GLU:HG3	27:X:101:FME:CE	2.36	0.55
25:Z:159:GLU:OE2	26:X:12:G:P	2.64	0.55
1:A:1226:C:N4	13:M:103:LYS:HE3	2.22	0.55
3:C:7:PRO:HG2	3:C:184:TYR:CG	2.42	0.55
22:V:58:THR:CG2	22:V:60:TYR:HB2	2.37	0.55
1:A:1389:C:N4	1:A:1391:U:C2	2.75	0.55
10:J:40:ILE:CG1	10:J:73:LEU:HB3	2.37	0.55
7:G:149:LYS:HB3	11:K:60:PRO:O	2.07	0.55
1:A:1492:A:C3'	22:V:19:ASN:CB	2.78	0.55
1:A:50:A:N6	23:W:753:SER:HB2	2.20	0.55
23:W:791:LYS:HZ2	23:W:791:LYS:N	2.05	0.55
1:A:203:G:N2	1:A:204:G:O6	2.39	0.55
7:G:147:ALA:O	11:K:61:PHE:N	2.40	0.55
23:W:694:LYS:HG2	23:W:724:GLY:HA3	1.88	0.55
23:W:805:LYS:HD2	26:X:74:C:C2	2.41	0.55
1:A:927:G:O3'	1:A:1503:A:C2'	2.48	0.54
23:W:812:ILE:HG12	26:X:76:A:C8	2.38	0.54
1:A:976:G:OP2	1:A:1358:U:O2'	2.25	0.54
1:A:1072:G:N3	2:B:106:THR:HG21	2.22	0.54
22:V:61:ASP:OD1	22:V:63:THR:HB	2.06	0.54
23:W:567:GLY:HA2	23:W:587:ARG:HG3	1.88	0.54
23:W:589:GLY:N	23:W:622:PRO:HB3	2.22	0.54
25:Z:91:ILE:CA	26:X:13:C:O2'	2.53	0.54
1:A:368:U:H5	23:W:608:ALA:HB2	1.65	0.54
7:G:148:ASN:HA	11:K:59:THR:HA	1.86	0.54
1:A:1135:U:N3	1:A:1137:C:O2	2.39	0.54
25:Z:118:LEU:HD22	25:Z:156:ALA:HB2	1.89	0.54
1:A:1101:A:H61	2:B:175:GLU:HG2	1.72	0.54
1:A:927:G:C5	1:A:1392:G:C4	2.95	0.54
1:A:691:G:O6	11:K:57:LYS:NZ	2.33	0.54
10:J:40:ILE:HG12	10:J:73:LEU:HB3	1.89	0.54
26:X:23:C:O2'	26:X:24:U:O5'	2.24	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1229:A:O3'	26:X:29:G:H4'	2.08	0.54
25:Z:93:VAL:HG22	25:Z:123:LYS:HD3	1.89	0.54
1:A:700:G:C6	24:Y:63:GLY:CA	2.90	0.54
1:A:1339:A:C1'	26:X:41:C:C2	2.77	0.54
1:A:1101:A:C5'	2:B:171:ILE:HD11	2.38	0.54
1:A:404:G:N7	4:D:2:ALA:HB3	2.23	0.54
12:L:71:GLY:HA2	22:V:60:TYR:HH	1.71	0.54
1:A:1517:G:C4	25:Z:106:ASP:CB	2.89	0.54
1:A:358:U:H4'	23:W:578:ARG:O	2.07	0.54
23:W:882:ILE:O	23:W:882:ILE:HG13	2.07	0.54
12:L:56:ARG:NH1	23:W:738:ALA:CB	2.71	0.54
1:A:1390:U:N3	1:A:1392:G:N7	2.56	0.53
1:A:843:U:OP1	1:A:846:G:N2	2.42	0.53
1:A:951:G:OP2	13:M:101:ARG:NH2	2.41	0.53
10:J:65:TYR:HB3	14:N:96:LEU:HD11	1.90	0.53
22:V:58:THR:HG22	22:V:60:TYR:HB2	1.90	0.53
23:W:812:ILE:O	23:W:812:ILE:HG23	2.08	0.53
1:A:927:G:C6	1:A:1391:U:O2	2.61	0.53
1:A:19:A:C5'	1:A:1078:U:C4	2.70	0.53
12:L:41:THR:HG22	22:V:64:ARG:HD2	1.89	0.53
1:A:842:U:H3'	1:A:843:U:C5'	2.37	0.53
23:W:534:SER:CB	23:W:537:ALA:CB	2.70	0.53
26:X:58:A:O2'	26:X:60:U:C5	2.51	0.53
1:A:1517:G:N9	25:Z:106:ASP:HA	2.24	0.53
25:Z:180:GLN:O	26:X:4:G:C2	2.56	0.53
25:Z:90:VAL:HB	26:X:13:C:H2'	1.85	0.53
1:A:1124:G:H5'	10:J:37:ARG:HH11	1.73	0.53
2:B:27:MET:HE1	2:B:187:VAL:HG12	1.91	0.53
1:A:938:A:H5'	7:G:76:LYS:NZ	2.23	0.53
23:W:566:SER:HB3	23:W:588:GLU:OE1	2.08	0.53
23:W:795:ILE:HG23	23:W:796:GLY:N	2.23	0.53
1:A:793:U:O4	25:Z:109:VAL:CG2	2.33	0.53
26:X:57:A:O2'	26:X:58:A:O5'	2.20	0.53
1:A:920:U:O2'	1:A:1081:A:O3'	2.23	0.53
1:A:1492:A:C2	22:V:35:TYR:CA	2.92	0.53
13:M:6:GLY:CA	13:M:66:GLU:HG3	2.37	0.53
23:W:395:THR:HB	23:W:462:THR:HG21	1.90	0.53
23:W:585:LEU:HD23	23:W:625:PRO:HB3	1.90	0.53
23:W:830:VAL:O	23:W:836:VAL:HG23	2.08	0.53
5:E:149:SER:HB3	5:E:152:MET:CG	2.39	0.53
1:A:1494:G:C5	22:V:18:PRO:HD3	2.43	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:W:612:GLU:HG3	23:W:613:LEU:N	2.24	0.53
23:W:727:GLY:CA	23:W:748:VAL:HG23	2.33	0.53
26:X:18:G:O2'	26:X:19:G:C5'	2.57	0.53
26:X:6:G:N2	26:X:67:C:O2	2.34	0.53
1:A:1081:A:OP1	5:E:21:VAL:CG1	2.57	0.53
1:A:927:G:O6	1:A:1391:U:C2	2.61	0.53
1:A:790:A:C4	26:X:38:A:C4'	2.74	0.53
22:V:15:GLU:N	22:V:23:ARG:HB2	2.19	0.53
24:Y:49:ALA:HB3	24:Y:56:VAL:HB	1.90	0.53
1:A:1074:G:O3'	2:B:102:THR:HB	2.07	0.53
1:A:769:G:H4'	1:A:1513:A:H4'	1.90	0.53
1:A:790:A:C8	26:X:38:A:O4'	2.59	0.53
12:L:31:ARG:HH12	23:W:731:THR:CB	2.22	0.53
22:V:44:TYR:O	22:V:45:ILE:HB	2.07	0.53
1:A:526:C:C2'	1:A:527:G7M:H5'	2.39	0.53
1:A:530:G:N7	22:V:39:LYS:N	2.57	0.53
15:O:20:ASN:O	15:O:22:THR:N	2.41	0.53
22:V:15:GLU:HG3	22:V:17:LEU:HG	1.90	0.53
23:W:399:HIS:CD2	23:W:476:MET:HB3	2.44	0.53
1:A:361:G:H5"	23:W:730:GLU:HB3	1.85	0.53
26:X:14:A:H2'	26:X:15:G:O4'	2.09	0.53
1:A:928:G:N3	1:A:1391:U:H1'	2.03	0.52
1:A:828:U:N3	2:B:25:PRO:HD3	2.19	0.52
1:A:1379:G:N7	7:G:2:PRO:HB2	2.24	0.52
8:H:48:ASP:OD1	8:H:49:PHE:N	2.38	0.52
10:J:6:ILE:HG13	10:J:76:ILE:HB	1.91	0.52
13:M:12:HIS:ND1	13:M:45:ILE:HG13	2.24	0.52
1:A:1032:G:H2'	1:A:1033:G:H4'	1.90	0.52
1:A:1496:C:O2'	25:Z:99:ARG:CZ	2.56	0.52
1:A:927:G:O2'	1:A:1503:A:O4'	2.27	0.52
7:G:149:LYS:CE	11:K:95:SER:CB	2.54	0.52
26:X:26:G:H2'	26:X:27:U:H5'	1.91	0.52
25:Z:180:GLN:HA	26:X:69:C:N3	2.22	0.52
1:A:1078:U:C5'	5:E:90:THR:OG1	2.13	0.52
1:A:1390:U:H6	1:A:1391:U:OP2	1.92	0.52
1:A:1400:C:C4'	26:X:34:C:N4	2.73	0.52
1:A:1428:A:H2'	1:A:1429:A:O4'	2.10	0.52
13:M:12:HIS:HA	13:M:45:ILE:CG1	2.39	0.52
23:W:847:ARG:O	23:W:847:ARG:HG3	2.09	0.52
1:A:18:C:C1'	1:A:1080:A:C5	2.93	0.52
13:M:8:ASN:OD1	13:M:9:ILE:N	2.42	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:W:800:VAL:HG12	23:W:815:CYS:HB3	1.91	0.52
1:A:1400:C:C5'	26:X:34:C:C4	2.92	0.52
1:A:1031:C:O2'	1:A:1032:G:OP2	2.26	0.52
26:X:10:G:N2	26:X:26:G:H1'	2.25	0.52
26:X:51:C:H1'	26:X:64:G:N2	2.24	0.52
1:A:157:U:C2'	1:A:158:G:H5'	2.40	0.52
26:X:59:A:H2'	26:X:60:U:O4'	2.10	0.52
1:A:829:G:O5'	2:B:25:PRO:CA	2.57	0.52
7:G:147:ALA:CB	11:K:61:PHE:CD2	2.89	0.52
23:W:855:VAL:HG13	23:W:859:MET:HE3	1.89	0.52
23:W:855:VAL:HG11	23:W:861:CYS:HB2	1.91	0.52
26:X:56:C:H2'	26:X:57:A:H8	1.74	0.52
9:I:85:ARG:HA	9:I:88:MET:CE	2.39	0.52
12:L:49:LEU:HD12	22:V:58:THR:HB	1.91	0.52
23:W:816:MET:SD	23:W:860:GLU:HA	2.50	0.52
23:W:391:ALA:HB3	23:W:623:SER:HB2	1.91	0.52
1:A:1060:U:H4'	10:J:53:ILE:HG23	1.91	0.51
1:A:181:A:N6	1:A:195:A:OP2	2.43	0.51
7:G:148:ASN:CG	11:K:59:THR:CB	2.78	0.51
1:A:537:G:OP1	12:L:110:ARG:NH2	2.43	0.51
1:A:741:G:OP1	15:O:35:GLN:NE2	2.43	0.51
22:V:32:ILE:H	22:V:32:ILE:HD13	1.75	0.51
23:W:792:GLN:HG3	23:W:882:ILE:HG22	1.91	0.51
23:W:804:PHE:HB2	23:W:812:ILE:HG22	1.80	0.51
1:A:532:A:N1	3:C:161:GLU:N	2.59	0.51
26:X:49:G:N2	26:X:66:C:H1'	2.26	0.51
2:B:130:THR:O	2:B:131:LYS:HB2	2.10	0.51
22:V:17:LEU:HB3	22:V:18:PRO:CD	2.37	0.51
22:V:7:ILE:HG22	22:V:8:ARG:N	2.25	0.51
23:W:791:LYS:HD2	23:W:791:LYS:C	2.30	0.51
1:A:1016:A:N3	1:A:1016:A:H2'	2.26	0.51
1:A:722:G:N3	1:A:722:G:H3'	2.25	0.51
2:B:126:PHE:C	2:B:128:LYS:H	2.13	0.51
7:G:148:ASN:HD22	11:K:59:THR:HG22	1.72	0.51
1:A:121:U:H5"	1:A:122:G:OP2	2.11	0.51
1:A:357:G:H4'	23:W:607:ARG:HD3	1.91	0.51
1:A:1074:G:O3'	2:B:102:THR:HG21	2.11	0.51
6:F:38:ARG:HB3	6:F:63:ASN:HB2	1.92	0.51
22:V:49:PRO:HD2	25:Z:131:ARG:HH11	1.76	0.51
23:W:744:VAL:HG21	23:W:774:LEU:HD13	1.92	0.51
26:X:22:G:C2	26:X:23:C:C5	2.99	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:W:812:ILE:HB	26:X:76:A:C8	2.46	0.51
23:W:812:ILE:CG1	26:X:76:A:H1'	2.35	0.51
25:Z:98:PHE:HB3	25:Z:144:VAL:HG11	1.91	0.51
1:A:18:C:N1	1:A:1080:A:C4	2.79	0.51
1:A:411:A:P	4:D:26:ARG:HH22	2.33	0.51
7:G:149:LYS:HZ2	11:K:64:GLN:HG3	1.76	0.51
26:X:71:C:C2'	26:X:72:A:O5'	2.59	0.51
6:F:29:ILE:HD13	6:F:64:VAL:HG11	1.93	0.51
1:A:1492:A:H2	22:V:35:TYR:CA	2.24	0.51
23:W:815:CYS:SG	23:W:861:CYS:C	2.89	0.51
1:A:1339:A:O4'	26:X:42:G:H4'	2.11	0.51
1:A:19:A:H4'	1:A:1078:U:C4	2.45	0.51
23:W:447:GLY:HA2	23:W:455:ARG:HD3	1.93	0.51
26:X:22:G:C2	26:X:23:C:C4	2.98	0.51
1:A:1449:C:C2'	1:A:1450:U:H5'	2.40	0.51
7:G:88:PRO:HG2	7:G:152:ALA:HB2	1.93	0.51
23:W:795:ILE:CG2	23:W:796:GLY:N	2.74	0.51
26:X:66:C:H2'	26:X:67:C:H6	1.76	0.51
1:A:927:G:N7	1:A:1392:G:N3	2.59	0.51
14:N:42:TRP:HD1	14:N:44:ALA:N	2.09	0.51
22:V:1:ALA:O	22:V:2:LYS:HB2	2.10	0.51
23:W:812:ILE:CG1	26:X:76:A:C8	2.94	0.51
2:B:117:LEU:HA	2:B:120:GLN:HG2	1.93	0.50
7:G:147:ALA:C	11:K:62:ALA:H	2.14	0.50
15:O:26:GLU:OE1	15:O:26:GLU:N	2.34	0.50
1:A:530:G:H1'	22:V:39:LYS:HG2	1.91	0.50
23:W:727:GLY:O	23:W:748:VAL:HG21	2.11	0.50
23:W:790:LEU:O	23:W:791:LYS:CB	2.58	0.50
25:Z:178:LYS:HB2	26:X:69:C:C4'	2.39	0.50
26:X:68:C:H2'	26:X:69:C:C6	2.46	0.50
25:Z:178:LYS:HB2	26:X:69:C:H4'	1.91	0.50
1:A:1078:U:H1'	5:E:91:GLY:H	1.44	0.50
1:A:18:C:H1'	1:A:1080:A:C5	2.45	0.50
13:M:95:LEU:C	13:M:109:ARG:HG2	2.32	0.50
19:S:29:LYS:HB3	19:S:30:PRO:CD	2.41	0.50
1:A:361:G:OP1	23:W:729:THR:CA	2.60	0.50
23:W:814:GLY:CA	27:X:101:FME:SD	2.99	0.50
1:A:1074:G:P	5:E:69:ARG:NH1	2.84	0.50
1:A:790:A:C5	26:X:38:A:C4'	2.86	0.50
12:L:51:LYS:CE	22:V:60:TYR:CG	2.59	0.50
23:W:612:GLU:HG3	23:W:613:LEU:H	1.76	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:Y:21:GLN:HE22	24:Y:41:ARG:HH11	1.59	0.50
1:A:928:G:H8	1:A:1531:A:O2'	1.94	0.50
23:W:613:LEU:C	23:W:613:LEU:HD12	2.32	0.50
23:W:778:VAL:HG23	23:W:779:LYS:N	2.27	0.50
23:W:860:GLU:OE2	27:X:101:FME:HE1	2.11	0.50
26:X:8:4SU:O2'	26:X:9:G:O5'	2.28	0.50
1:A:216:U:H2'	1:A:217:C:C6	2.46	0.50
1:A:412:A:H1'	1:A:413:G:C5'	2.39	0.50
26:X:71:C:C2'	26:X:72:A:H5'	2.40	0.50
1:A:204:G:C3'	1:A:205:A:H5"	2.42	0.50
1:A:457:G:N2	1:A:476:U:O2	2.45	0.50
1:A:368:U:C5'	23:W:607:ARG:HG2	2.26	0.50
23:W:540:GLY:HA2	23:W:541:ILE:HB	1.88	0.50
23:W:847:ARG:CA	27:X:101:FME:HCN	2.41	0.50
1:A:1299:A:H2'	1:A:1299:A:N3	2.26	0.50
1:A:1102:A:N3	2:B:98:GLY:O	2.44	0.50
8:H:9:ASP:OD2	8:H:13:ARG:HD2	2.12	0.50
14:N:27:LEU:O	14:N:31:ILE:HG12	2.11	0.50
22:V:2:LYS:HB3	22:V:2:LYS:NZ	2.26	0.50
1:A:526:C:H2'	1:A:527:G7M:H5'	1.94	0.50
1:A:532:A:H61	3:C:160:ALA:C	2.04	0.50
1:A:841:C:C5	1:A:843:U:H5'	2.47	0.50
10:J:15:HIS:CE1	10:J:16:ARG:HD3	2.46	0.50
10:J:76:ILE:CD1	10:J:87:LEU:HD11	2.42	0.50
13:M:12:HIS:HA	13:M:45:ILE:HG12	1.93	0.50
20:T:44:LYS:HG3	20:T:45:ALA:N	2.27	0.50
23:W:789:GLU:HG3	23:W:789:GLU:O	2.12	0.50
23:W:792:GLN:CD	23:W:882:ILE:HA	2.32	0.50
26:X:53:G:N1	26:X:61:C:N3	2.50	0.50
1:A:1005:A:H3'	1:A:1006:G:C8	2.47	0.49
2:B:133:GLU:OE2	2:B:137:ARG:NH1	2.39	0.49
1:A:1390:U:C6	1:A:1391:U:P	3.01	0.49
1:A:109:A:C6	1:A:326:G:C6	3.00	0.49
1:A:928:G:H4'	1:A:1532:U:C6	2.47	0.49
22:V:7:ILE:HG22	22:V:9:THR:H	1.78	0.49
23:W:812:ILE:CD1	23:W:863:ILE:O	2.54	0.49
1:A:532:A:C8	3:C:193:TYR:CD1	3.00	0.49
8:H:18:GLN:CG	8:H:70:ALA:HB1	2.42	0.49
5:E:156:LYS:NZ	8:H:73:GLU:OE1	2.45	0.49
10:J:53:ILE:HG13	14:N:85:ARG:CZ	2.42	0.49
1:A:147:G:H2'	1:A:148:G:C8	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1517:G:H1'	25:Z:105:GLY:C	2.31	0.49
1:A:1074:G:OP2	5:E:66:LYS:HD2	2.12	0.49
23:W:792:GLN:HG3	23:W:882:ILE:HA	1.94	0.49
1:A:966:2MG:C5	26:X:34:C:C2'	2.95	0.49
22:V:31:GLU:H	22:V:31:GLU:CD	2.16	0.49
23:W:399:HIS:CD2	23:W:476:MET:HB2	2.48	0.49
23:W:611:ASN:C	23:W:612:GLU:HG2	2.33	0.49
23:W:812:ILE:CD1	26:X:76:A:C2	2.94	0.49
26:X:1:C:OP2	26:X:2:G:H3'	2.11	0.49
1:A:1238:A:H5'	1:A:1336:C:H41	1.77	0.49
1:A:184:G:O2'	20:T:69:LYS:NZ	2.36	0.49
1:A:918:A:C2	1:A:1080:A:N1	2.72	0.49
1:A:266:G:H3'	17:Q:69:LYS:HB2	1.95	0.49
19:S:50:ALA:HB1	19:S:57:HIS:HB3	1.93	0.49
23:W:452:THR:HG23	23:W:453:SER:N	2.27	0.49
1:A:359:G:C5'	23:W:575:ASP:O	2.60	0.49
23:W:791:LYS:NZ	23:W:791:LYS:N	2.60	0.49
25:Z:90:VAL:CG2	26:X:14:A:H8	2.11	0.49
26:X:8:4SU:H1'	26:X:21:A:H2	1.74	0.49
1:A:16:A:O2'	1:A:1081:A:OP1	2.30	0.49
5:E:56:VAL:N	5:E:57:PRO:HD2	2.28	0.49
12:L:31:ARG:HH12	23:W:731:THR:HB	1.77	0.49
13:M:40:ALA:HB3	13:M:43:VAL:CG2	2.43	0.49
26:X:71:C:C2'	26:X:72:A:C5'	2.90	0.49
1:A:1496:C:C5'	25:Z:101:GLY:HA3	2.42	0.49
3:C:185:ASN:OD1	3:C:186:THR:N	2.45	0.49
4:D:99:ASP:OD1	4:D:100:ASN:N	2.45	0.49
1:A:1072:G:H5'	5:E:62:LYS:HE2	1.79	0.48
1:A:1517:G:C6	25:Z:106:ASP:CG	2.83	0.48
18:R:21:ILE:HG21	18:R:54:GLN:HB3	1.95	0.48
1:A:1494:G:O3'	22:V:16:ALA:CB	2.61	0.48
26:X:51:C:H42	26:X:62:C:H42	1.60	0.48
26:X:54:5MU:C5	26:X:55:PSU:C2	3.01	0.48
26:X:58:A:C6	26:X:61:C:H1'	2.47	0.48
1:A:937:A:O2'	7:G:76:LYS:NZ	2.38	0.48
13:M:16:VAL:HG12	13:M:17:ILE:HD12	1.93	0.48
22:V:44:TYR:CD1	22:V:44:TYR:N	2.81	0.48
1:A:26:A:H2'	1:A:27:G:H5'	1.95	0.48
1:A:383:A:C5	1:A:384:G:H1'	2.49	0.48
6:F:76:THR:O	6:F:79:ARG:N	2.44	0.48
11:K:16:VAL:HG23	11:K:17:SER:N	2.28	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:518:C:O2'	22:V:38:GLY:N	2.46	0.48
23:W:836:VAL:HG13	23:W:836:VAL:O	2.12	0.48
1:A:1230:C:OP1	26:X:29:G:O3'	2.31	0.48
1:A:1072:G:OP1	5:E:62:LYS:CD	2.61	0.48
1:A:864:A:C3'	1:A:1079:G:O6	2.43	0.48
1:A:927:G:N1	1:A:1392:G:C8	2.81	0.48
1:A:1072:G:H21	2:B:106:THR:CG2	2.27	0.48
10:J:53:ILE:CG2	10:J:61:ALA:HB1	2.44	0.48
23:W:539:THR:O	23:W:541:ILE:HB	2.13	0.48
1:A:1003:G:N2	1:A:1004:A:O2'	2.46	0.48
1:A:1062:U:H2'	1:A:1063:C:C6	2.48	0.48
1:A:1078:U:O3'	5:E:89:HIS:CE1	2.66	0.48
1:A:966:2MG:C5	26:X:34:C:C1'	2.96	0.48
1:A:830:G:H5'	2:B:23:TRP:HD1	1.79	0.48
1:A:1102:A:C1'	2:B:98:GLY:HA3	2.43	0.48
4:D:17:THR:HG22	4:D:18:ASP:N	2.29	0.48
9:I:130:ARG:NH2	26:X:32:C:C4	2.34	0.48
1:A:1137:C:H1'	1:A:1138:G:N2	2.28	0.48
1:A:1192:C:O2'	5:E:30:ILE:HD11	2.14	0.48
1:A:830:G:C5'	2:B:23:TRP:HD1	2.27	0.48
1:A:1073:U:C3'	5:E:69:ARG:HH22	2.26	0.48
14:N:10:GLU:HG3	14:N:63:ARG:HD2	1.96	0.48
23:W:728:ILE:HG22	23:W:729:THR:N	2.27	0.48
1:A:1390:U:HO3'	1:A:1392:G:P	2.37	0.48
2:B:15:HIS:HB3	2:B:43:LEU:HD11	1.95	0.48
5:E:162:GLU:HG3	5:E:163:GLU:N	2.28	0.48
22:V:36:ILE:CG2	22:V:41:ARG:HG3	2.44	0.48
1:A:700:G:C8	24:Y:67:PHE:HB2	2.43	0.48
22:V:48:LEU:HD23	25:Z:131:ARG:CZ	2.44	0.48
1:A:973:G:H1'	10:J:56:HIS:HD2	1.78	0.48
23:W:519:ILE:HG12	23:W:520:LEU:HD12	1.95	0.48
1:A:1016:A:C2	1:A:1017:U:H4'	2.48	0.48
1:A:701:U:C2'	24:Y:64:LYS:CB	2.72	0.48
10:J:7:ARG:CG	10:J:101:SER:HB2	2.44	0.48
10:J:51:VAL:HB	14:N:81:ARG:HB2	1.96	0.48
22:V:45:ILE:O	22:V:45:ILE:HG22	2.14	0.48
1:A:700:G:C5	24:Y:63:GLY:O	2.67	0.48
1:A:1079:G:C5'	5:E:135:ASN:HD21	2.26	0.47
1:A:131:A:H2'	1:A:132:C:C6	2.49	0.47
1:A:207:C:H2'	1:A:208:U:C2	2.49	0.47
1:A:790:A:N7	26:X:38:A:O4'	2.46	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:94:VAL:HG22	5:E:111:MET:CE	2.44	0.47
7:G:150:ALA:C	11:K:91:PRO:HB3	2.13	0.47
13:M:107:ARG:HH21	13:M:113:ARG:HB3	1.79	0.47
6:F:86:ARG:NH1	18:R:64:TYR:O	2.46	0.47
1:A:159:G:H5"	1:A:159:G:H8	1.79	0.47
23:W:399:HIS:HB3	23:W:402:HIS:HE1	1.78	0.47
1:A:368:U:OP2	23:W:607:ARG:HG3	2.14	0.47
24:Y:28:ILE:HD12	24:Y:28:ILE:N	2.29	0.47
1:A:701:U:N3	24:Y:61:ASP:HA	2.29	0.47
1:A:75:G:C2	1:A:76:G:H1'	2.50	0.47
10:J:8:ILE:HA	10:J:99:GLN:O	2.14	0.47
23:W:611:ASN:O	23:W:612:GLU:CG	2.62	0.47
23:W:812:ILE:CB	26:X:76:A:C8	2.97	0.47
1:A:1073:U:O3'	5:E:69:ARG:NH2	2.47	0.47
25:Z:130:PHE:CE1	25:Z:137:HIS:CD2	3.03	0.47
1:A:1389:C:N3	1:A:1391:U:N1	2.60	0.47
1:A:358:U:H4'	23:W:579:GLY:HA3	1.94	0.47
7:G:130:ASN:HA	7:G:135:VAL:HG11	1.96	0.47
13:M:33:ILE:HD11	13:M:63:PHE:CE2	2.50	0.47
26:X:22:G:C6	26:X:23:C:N4	2.82	0.47
1:A:1079:G:H4'	5:E:134:ILE:HG23	1.96	0.47
1:A:927:G:N1	1:A:1391:U:O2'	2.47	0.47
1:A:237:G:OP1	17:Q:42:THR:OG1	2.30	0.47
1:A:429:U:H5'	4:D:9:LEU:HD12	1.95	0.47
1:A:532:A:C2	3:C:161:GLU:HB2	2.48	0.47
26:X:53:G:O2'	26:X:54:5MU:O5'	2.26	0.47
1:A:1517:G:C5	25:Z:106:ASP:CB	2.97	0.47
25:Z:118:LEU:HD21	25:Z:176:PRO:HA	1.96	0.47
1:A:19:A:O4'	1:A:1079:G:N2	2.47	0.47
7:G:149:LYS:HD3	11:K:95:SER:CB	2.34	0.47
1:A:1230:C:H5'	26:X:29:G:O3'	2.15	0.47
1:A:790:A:O4'	26:X:38:A:C3'	2.44	0.47
26:X:8:4SU:H3'	26:X:8:4SU:C2	2.44	0.47
26:X:8:4SU:S4	26:X:14:A:C8	3.02	0.47
25:Z:159:GLU:OE2	26:X:12:G:C5'	2.56	0.47
1:A:19:A:H5"	1:A:1078:U:C2	2.46	0.47
1:A:76:G:N3	1:A:76:G:H2'	2.29	0.47
2:B:20:THR:HG22	2:B:39:HIS:CE1	2.50	0.47
9:I:23:PRO:HA	9:I:61:LEU:HA	1.95	0.47
10:J:42:LEU:HB2	10:J:71:LEU:HB3	1.96	0.47
6:F:102:MET:CE	18:R:24:LYS:HB3	2.45	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:V:20:ALA:HB1	22:V:36:ILE:CG1	2.45	0.47
23:W:540:GLY:CA	23:W:541:ILE:CB	2.85	0.47
25:Z:159:GLU:OE1	26:X:11:A:O2'	2.31	0.47
2:B:120:GLN:HG3	2:B:121:SER:N	2.28	0.47
19:S:7:LYS:H	19:S:7:LYS:HD2	1.79	0.47
23:W:772:TYR:HA	23:W:775:ILE:HG22	1.96	0.47
1:A:1229:A:H4'	26:X:29:G:O5'	2.15	0.47
1:A:468:A:C8	1:A:469:C:C6	3.03	0.47
10:J:35:GLN:HG3	10:J:78:GLU:HG2	1.97	0.47
14:N:21:PHE:HA	14:N:25:ALA:CB	2.45	0.47
22:V:48:LEU:HD22	25:Z:131:ARG:NH1	2.30	0.47
1:A:1339:A:C2	26:X:30:G:O2'	2.60	0.46
3:C:123:GLN:HG2	3:C:128:VAL:HG21	1.97	0.46
5:E:80:THR:OG1	5:E:122:ASN:O	2.32	0.46
14:N:42:TRP:CD1	14:N:43:ASN:N	2.83	0.46
12:L:51:LYS:NZ	22:V:60:TYR:HD2	2.11	0.46
23:W:591:LEU:O	23:W:592:HIS:CG	2.68	0.46
1:A:1517:G:C8	25:Z:106:ASP:OD1	2.55	0.46
1:A:1101:A:O4'	2:B:171:ILE:HD12	1.94	0.46
1:A:1228:C:P	13:M:107:ARG:NH2	2.88	0.46
1:A:872:A:C8	1:A:874:G:C8	3.03	0.46
1:A:913:A:OP1	12:L:88:LYS:NZ	2.47	0.46
22:V:37:SER:HB3	22:V:67:ILE:O	2.15	0.46
12:L:39:THR:CG2	22:V:60:TYR:HB3	2.46	0.46
23:W:396:ILE:HG21	23:W:404:LYS:HG3	1.96	0.46
25:Z:159:GLU:OE2	26:X:11:A:O2'	2.32	0.46
1:A:1072:G:H21	2:B:106:THR:HG21	1.80	0.46
1:A:944:G:N1	1:A:1338:G:OP2	2.41	0.46
22:V:20:ALA:HB1	22:V:36:ILE:CD1	2.44	0.46
23:W:534:SER:CB	23:W:539:THR:HG23	2.46	0.46
23:W:590:THR:O	23:W:591:LEU:HG	2.15	0.46
23:W:786:LEU:N	23:W:786:LEU:HD23	2.30	0.46
1:A:109:A:H2'	1:A:326:G:N2	2.31	0.46
1:A:451:A:H61	1:A:481:G:H5'	1.80	0.46
1:A:1492:A:H4'	12:L:44:LYS:HE2	1.97	0.46
23:W:526:GLY:O	23:W:527:GLU:HG2	2.15	0.46
25:Z:123:LYS:HG3	26:X:12:G:C1'	2.43	0.46
25:Z:125:LYS:NZ	26:X:25:C:H2'	2.28	0.46
1:A:1229:A:OP2	13:M:113:ARG:NH1	2.48	0.46
1:A:927:G:N2	1:A:1392:G:H5'	2.30	0.46
13:M:6:GLY:HA3	13:M:66:GLU:HG3	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:V:40:MET:HE3	22:V:70:ARG:HB3	1.97	0.46
1:A:966:2MG:C5	26:X:34:C:H1'	2.49	0.46
8:H:108:LYS:HG3	8:H:121:LEU:HD11	1.97	0.46
13:M:54:ASP:HA	13:M:57:ARG:HD2	1.98	0.46
1:A:1339:A:C4	26:X:41:C:O2	2.68	0.46
22:V:17:LEU:HD11	22:V:23:ARG:NH1	2.31	0.46
22:V:66:ARG:NH1	22:V:66:ARG:CB	2.77	0.46
25:Z:95:GLU:CD	26:X:25:C:O3'	2.47	0.46
1:A:358:U:O2'	23:W:577:GLY:N	2.47	0.46
1:A:790:A:N9	26:X:38:A:C5'	2.77	0.46
2:B:129:LEU:HD22	2:B:134:ALA:HB2	1.98	0.46
9:I:130:ARG:CZ	26:X:32:C:N4	2.54	0.46
20:T:44:LYS:HB3	20:T:87:ALA:HB3	1.98	0.46
22:V:32:ILE:N	22:V:32:ILE:HD13	2.29	0.46
1:A:927:G:N2	1:A:1392:G:O4'	2.44	0.46
9:I:19:VAL:HG13	9:I:65:ILE:HG22	1.97	0.46
10:J:22:THR:CG2	10:J:39:PRO:HB3	2.46	0.46
22:V:25:LYS:HD2	22:V:30:PRO:O	2.16	0.46
23:W:792:GLN:CG	23:W:882:ILE:HA	2.46	0.46
1:A:18:C:C1'	1:A:1080:A:C2	2.99	0.46
1:A:1152:A:H5"	10:J:15:HIS:HB2	1.98	0.46
1:A:5:U:H6	1:A:5:U:H3'	1.81	0.46
1:A:71:A:O2'	1:A:72:A:OP2	2.27	0.46
2:B:10:LEU:HD12	2:B:15:HIS:ND1	2.31	0.46
8:H:28:PRO:O	8:H:33:LYS:NZ	2.38	0.46
10:J:15:HIS:CG	10:J:16:ARG:N	2.84	0.46
11:K:111:THR:HG23	21:U:3:VAL:HG22	1.98	0.46
7:G:150:ALA:CA	11:K:92:GLY:H	2.28	0.46
7:G:147:ALA:CA	11:K:61:PHE:CD2	2.98	0.45
7:G:62:PHE:HE1	7:G:66:LEU:HD22	1.81	0.45
9:I:19:VAL:HG11	9:I:83:ILE:HA	1.98	0.45
14:N:18:ASP:OD1	14:N:19:LYS:N	2.49	0.45
22:V:54:VAL:CB	22:V:69:TYR:HB2	2.43	0.45
23:W:404:LYS:NZ	23:W:445:THR:O	2.46	0.45
1:A:1339:A:C2	26:X:30:G:C2'	2.99	0.45
1:A:19:A:C4'	1:A:1078:U:C4	2.98	0.45
4:D:58:LYS:HD2	4:D:204:TYR:OH	2.16	0.45
1:A:1194:U:C4'	5:E:26:LYS:O	2.63	0.45
23:W:396:ILE:HD12	23:W:408:LEU:HD11	1.98	0.45
1:A:1339:A:C5'	26:X:41:C:O3'	2.62	0.45
1:A:657:U:O2	15:O:22:THR:HG23	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:52:LEU:HD23	10:J:62:ARG:HD3	1.97	0.45
14:N:21:PHE:HB2	14:N:55:SER:O	2.16	0.45
23:W:456:ALA:HA	23:W:485:HIS:HD2	1.82	0.45
23:W:795:ILE:CG2	23:W:879:VAL:CG1	2.88	0.45
23:W:795:ILE:HG23	23:W:879:VAL:HG13	1.94	0.45
24:Y:43:LEU:HD23	24:Y:59:ILE:HG22	1.98	0.45
1:A:254:G:H4'	17:Q:17:MET:HE2	1.98	0.45
2:B:217:VAL:O	2:B:221:VAL:HG23	2.17	0.45
7:G:83:SER:HB2	7:G:85:TYR:CE2	2.51	0.45
10:J:6:ILE:CG1	10:J:76:ILE:HB	2.46	0.45
10:J:67:ILE:HG13	14:N:96:LEU:HD13	1.99	0.45
25:Z:90:VAL:CG1	26:X:14:A:H3'	2.47	0.45
26:X:22:G:N1	26:X:23:C:C4	2.84	0.45
26:X:22:G:C6	26:X:23:C:C4	3.05	0.45
25:Z:128:LEU:CD1	25:Z:141:GLY:HA2	2.45	0.45
1:A:1134:G:H2'	1:A:1135:U:C6	2.51	0.45
1:A:2:A:O2'	4:D:83:LYS:NZ	2.43	0.45
1:A:1073:U:H4'	5:E:69:ARG:HH22	1.81	0.45
23:W:496:ALA:HB2	23:W:544:LEU:HD12	1.97	0.45
1:A:1312:G:C5'	19:S:6:LYS:HE2	2.47	0.45
1:A:405:U:O4	4:D:2:ALA:N	2.50	0.45
5:E:74:VAL:HG22	5:E:76:LEU:HD23	1.99	0.45
1:A:1018:G:H2'	1:A:1018:G:N3	2.30	0.45
1:A:85:U:H6	1:A:86:G:N1	2.15	0.45
22:V:31:GLU:CD	22:V:31:GLU:N	2.70	0.45
1:A:357:G:O3'	23:W:607:ARG:CZ	2.65	0.45
12:L:56:ARG:NH2	23:W:734:THR:HG23	2.32	0.45
26:X:18:G:H4'	26:X:60:U:O2	2.17	0.45
25:Z:95:GLU:HB2	26:X:25:C:H4'	1.99	0.45
1:A:31:G:O2'	1:A:48:C:N4	2.50	0.45
14:N:21:PHE:CD1	14:N:55:SER:HB3	2.52	0.45
1:A:1493:A:N6	22:V:33:LEU:HD12	2.23	0.45
23:W:797:LEU:C	23:W:797:LEU:CD2	2.86	0.45
25:Z:129:ARG:CZ	26:X:38:A:P	3.04	0.45
1:A:1494:G:O2'	22:V:16:ALA:HB3	2.16	0.45
1:A:495:A:C2	1:A:496:A:C6	3.05	0.45
1:A:7:A:O2'	5:E:106:ILE:HD11	2.16	0.45
1:A:358:U:C4'	23:W:579:GLY:CA	2.93	0.45
26:X:16:C:H4'	26:X:60:U:O2'	2.17	0.45
26:X:54:5MU:C4	26:X:55:PSU:O2	2.70	0.45
1:A:1517:G:C8	25:Z:106:ASP:CA	2.87	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:150:LYS:HB3	3:C:169:ARG:CG	2.46	0.45
3:C:77:ILE:HA	3:C:84:VAL:CG2	2.47	0.45
7:G:111:ARG:O	7:G:119:ARG:NH2	2.48	0.45
1:A:1494:G:C4	22:V:18:PRO:HD3	2.51	0.45
23:W:506:ASP:HA	23:W:507:PRO:HD3	1.83	0.45
26:X:56:C:C6	26:X:56:C:OP1	2.70	0.45
1:A:1031:C:H4'	1:A:1032:G:O5'	2.17	0.44
19:S:29:LYS:CB	19:S:30:PRO:HD2	2.46	0.44
1:A:1322:C:P	19:S:78:ARG:HH22	2.40	0.44
22:V:6:THR:HG22	22:V:7:ILE:N	2.32	0.44
26:X:62:C:H2'	26:X:63:G:O4'	2.16	0.44
1:A:1073:U:H4'	5:E:69:ARG:NH2	2.32	0.44
1:A:1101:A:N6	2:B:175:GLU:HG2	2.32	0.44
1:A:828:U:C5	2:B:25:PRO:HG2	2.47	0.44
22:V:40:MET:SD	22:V:67:ILE:HG22	2.57	0.44
23:W:399:HIS:HB2	23:W:479:THR:HG23	1.99	0.44
1:A:920:U:O3'	1:A:1082:A:H5"	2.17	0.44
1:A:1217:C:OP2	14:N:9:ARG:NH2	2.44	0.44
2:B:213:TYR:O	2:B:217:VAL:HG23	2.18	0.44
3:C:156:ARG:H	3:C:163:ALA:HA	1.83	0.44
12:L:110:ARG:HB2	12:L:119:VAL:HG21	1.98	0.44
12:L:39:THR:HG21	22:V:60:TYR:HB3	1.99	0.44
14:N:30:ILE:O	14:N:34:VAL:HG23	2.17	0.44
23:W:586:VAL:O	23:W:586:VAL:HG23	2.17	0.44
23:W:812:ILE:CD1	23:W:863:ILE:C	2.85	0.44
23:W:794:ILE:HA	23:W:880:PHE:HB3	2.00	0.44
25:Z:159:GLU:CD	26:X:11:A:O2'	2.56	0.44
7:G:149:LYS:N	11:K:61:PHE:H	2.04	0.44
23:W:430:ALA:HB2	23:W:443:LEU:HD13	1.98	0.44
23:W:855:VAL:HG13	23:W:859:MET:HE2	1.99	0.44
26:X:21:A:O2'	26:X:22:G:C8	2.70	0.44
26:X:22:G:C2	26:X:23:C:C6	3.04	0.44
1:A:1339:A:C2	26:X:29:G:N2	2.85	0.44
25:Z:93:VAL:HG23	26:X:12:G:N2	2.32	0.44
2:B:28:LYS:N	2:B:29:PRO:CD	2.81	0.44
3:C:155:GLY:HA2	3:C:163:ALA:HB1	2.00	0.44
5:E:105:ILE:HG23	5:E:123:VAL:HG23	1.99	0.44
17:Q:8:LEU:HD13	17:Q:25:ILE:HG13	1.99	0.44
20:T:27:MET:CE	20:T:57:ILE:HG12	2.48	0.44
26:X:71:C:H2'	26:X:72:A:O5'	2.17	0.44
25:Z:180:GLN:HB2	26:X:70:G:OP2	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1016:A:N1	1:A:1017:U:O2'	2.44	0.44
1:A:1029:U:O2'	1:A:1032:G:N1	2.49	0.44
1:A:1100:C:H42	2:B:95:ARG:HE	1.65	0.44
1:A:1074:G:O2'	1:A:1101:A:N1	2.50	0.44
2:B:9:MET:CE	2:B:50:PHE:HD2	2.31	0.44
22:V:58:THR:HG22	22:V:60:TYR:H	1.82	0.44
23:W:794:ILE:HA	23:W:880:PHE:CB	2.48	0.44
25:Z:178:LYS:HB2	26:X:69:C:C2'	2.31	0.44
7:G:16:PRO:HB3	9:I:43:THR:HG23	1.98	0.44
9:I:36:GLU:HA	9:I:45:ARG:HE	1.83	0.44
10:J:29:ALA:HA	10:J:32:THR:HG22	2.00	0.44
21:U:6:VAL:HG22	21:U:15:ALA:HB1	1.99	0.44
7:G:72:THR:HG22	7:G:142:HIS:NE2	2.33	0.44
17:Q:7:THR:HG21	17:Q:60:GLU:CG	2.48	0.44
26:X:24:U:H2'	26:X:25:C:H6	1.83	0.44
25:Z:125:LYS:CD	26:X:25:C:HO2'	1.87	0.44
1:A:790:A:O4'	26:X:38:A:H5"	2.17	0.44
1:A:75:G:C4	1:A:76:G:C8	3.06	0.44
2:B:121:SER:HA	2:B:126:PHE:CE1	2.53	0.44
8:H:93:PRO:HG3	8:H:125:ILE:HD13	2.00	0.44
8:H:41:LYS:HD2	8:H:48:ASP:HA	2.00	0.44
10:J:10:LEU:CD2	10:J:98:VAL:HG12	2.48	0.44
13:M:107:ARG:HH11	13:M:107:ARG:HG2	1.83	0.44
13:M:4:ILE:CG2	13:M:60:VAL:HG11	2.48	0.44
23:W:791:LYS:NZ	23:W:791:LYS:HB3	2.33	0.44
23:W:796:GLY:H	23:W:879:VAL:HG13	1.83	0.44
26:X:29:G:H1	26:X:41:C:H42	1.66	0.44
1:A:1389:C:C5	1:A:1391:U:H5	2.27	0.43
1:A:1463:U:H2'	1:A:1464:U:C6	2.53	0.43
3:C:42:TYR:CZ	3:C:90:VAL:HG21	2.52	0.43
23:W:791:LYS:HZ1	23:W:791:LYS:HB3	1.83	0.43
1:A:701:U:C5'	24:Y:64:LYS:HG3	2.44	0.43
1:A:158:G:H2'	1:A:159:G:H5"	1.99	0.43
1:A:359:G:O4'	23:W:576:LYS:CA	2.61	0.43
1:A:502:A:H2'	1:A:503:C:O4'	2.18	0.43
3:C:6:HIS:CG	14:N:89:MET:HB3	2.52	0.43
7:G:135:VAL:HG23	7:G:136:LYS:N	2.33	0.43
7:G:80:VAL:HG12	7:G:81:GLY:N	2.33	0.43
10:J:53:ILE:HG22	10:J:61:ALA:O	2.18	0.43
23:W:544:LEU:CD2	23:W:544:LEU:C	2.85	0.43
1:A:358:U:C4'	23:W:577:GLY:O	2.65	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:W:666:LEU:HD12	23:W:667:ALA:N	2.32	0.43
25:Z:158:VAL:HA	25:Z:174:LEU:HA	1.99	0.43
3:C:83:ASP:HA	3:C:86:LYS:HG2	1.99	0.43
11:K:34:ILE:HG12	11:K:70:CYS:SG	2.58	0.43
13:M:89:LEU:HD23	13:M:92:ARG:HH21	1.84	0.43
6:F:102:MET:HE1	18:R:24:LYS:HB3	2.00	0.43
22:V:23:ARG:O	22:V:24:VAL:C	2.57	0.43
23:W:727:GLY:C	23:W:728:ILE:HG13	2.38	0.43
26:X:51:C:H1'	26:X:64:G:H22	1.84	0.43
24:Y:58:ARG:HD2	24:Y:60:MET:CE	2.49	0.43
3:C:135:LYS:HE2	5:E:57:PRO:HG3	2.00	0.43
8:H:25:VAL:HG22	8:H:63:LEU:HD21	1.99	0.43
9:I:50:GLN:N	9:I:51:PRO:HD2	2.33	0.43
9:I:85:ARG:HA	9:I:88:MET:HE2	2.00	0.43
10:J:5:ARG:HG2	10:J:77:VAL:HA	1.99	0.43
17:Q:49:GLU:O	17:Q:50:ASN:HB2	2.18	0.43
22:V:33:LEU:O	22:V:34:ALA:O	2.37	0.43
23:W:727:GLY:C	23:W:748:VAL:HG21	2.38	0.43
23:W:838:TYR:CZ	23:W:839:GLU:O	2.71	0.43
25:Z:91:ILE:HG12	26:X:13:C:H5'	1.96	0.43
25:Z:93:VAL:HG11	26:X:25:C:C1'	2.48	0.43
25:Z:128:LEU:HD22	25:Z:130:PHE:CE1	2.53	0.43
1:A:1014:A:OP1	19:S:18:LYS:NZ	2.51	0.43
1:A:1073:U:C4'	5:E:69:ARG:NH2	2.76	0.43
1:A:927:G:H21	1:A:1531:A:C4'	2.30	0.43
1:A:928:G:O5'	1:A:1531:A:O2'	2.37	0.43
5:E:95:PHE:CZ	5:E:97:GLN:HG3	2.54	0.43
1:A:1494:G:O3'	22:V:16:ALA:HB1	2.17	0.43
1:A:464:U:C2	1:A:466:A:H5"	2.53	0.43
2:B:19:GLN:HA	2:B:38:VAL:HA	2.01	0.43
9:I:24:GLY:H	9:I:61:LEU:HA	1.84	0.43
11:K:107:ILE:HG13	21:U:12:PHE:CE1	2.54	0.43
23:W:578:ARG:HB3	23:W:629:LEU:HD11	2.01	0.43
26:X:20:H2U:O2	26:X:20:H2U:H2'	2.19	0.43
26:X:22:G:O2'	26:X:23:C:P	2.77	0.43
25:Z:93:VAL:HG11	26:X:24:U:O2	2.15	0.43
25:Z:144:VAL:O	25:Z:148:VAL:HG23	2.19	0.43
1:A:1073:U:O2	2:B:103:ASN:HB2	2.17	0.43
1:A:1074:G:O3'	2:B:102:THR:CG2	2.67	0.43
3:C:168:TYR:CE1	5:E:55:GLU:CG	3.02	0.43
23:W:390:ARG:NH1	23:W:463:ASP:OD2	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:W:477:PRO:HA	23:W:480:ILE:HG22	2.01	0.43
23:W:515:SER:OG	23:W:524:TRP:CZ3	2.70	0.43
23:W:846:ARG:HA	23:W:851:ASP:HA	1.99	0.43
25:Z:179:LYS:HB3	26:X:70:G:H1'	1.49	0.43
1:A:1495:U:H2'	25:Z:101:GLY:HA3	2.01	0.43
10:J:28:THR:O	10:J:32:THR:HG22	2.18	0.43
10:J:56:HIS:O	10:J:57:VAL:HG12	2.19	0.43
12:L:31:ARG:NH1	23:W:731:THR:CB	2.82	0.43
1:A:1328:C:H5"	13:M:28:THR:HG21	1.99	0.43
13:M:32:ALA:O	13:M:36:ALA:N	2.47	0.43
23:W:390:ARG:HD3	23:W:559:ALA:HB2	2.01	0.43
23:W:451:PHE:CD1	23:W:451:PHE:N	2.86	0.43
23:W:386:ALA:HB3	23:W:560:VAL:HG23	2.01	0.43
23:W:575:ASP:OD1	23:W:576:LYS:N	2.52	0.43
26:X:51:C:H42	26:X:62:C:N4	2.16	0.43
1:A:927:G:N1	1:A:1392:G:N9	2.65	0.43
1:A:475:C:H2'	1:A:476:U:O4'	2.19	0.43
4:D:95:GLU:OE2	4:D:104:ARG:CZ	2.67	0.43
7:G:149:LYS:HB2	11:K:61:PHE:N	2.33	0.43
8:H:29:SER:HB3	8:H:57:PRO:HB2	2.00	0.43
22:V:15:GLU:CD	22:V:16:ALA:H	2.21	0.43
23:W:493:VAL:HG11	23:W:519:ILE:HD11	2.01	0.43
23:W:716:VAL:HG21	23:W:786:LEU:CD2	2.46	0.43
25:Z:93:VAL:H	26:X:12:G:H21	1.63	0.43
26:X:46:A:O2'	26:X:47:U:H5"	2.19	0.43
1:A:1152:A:H5"	10:J:15:HIS:CD2	2.54	0.43
10:J:22:THR:HG21	10:J:39:PRO:CB	2.49	0.43
16:P:75:ILE:HA	16:P:78:VAL:HG12	2.01	0.43
22:V:22:PHE:HE1	22:V:36:ILE:HD11	1.84	0.43
25:Z:123:LYS:CD	26:X:12:G:O4'	2.54	0.43
26:X:2:G:N3	26:X:2:G:H2'	2.33	0.43
26:X:38:A:H2'	26:X:39:C:O4'	2.19	0.43
1:A:1078:U:C2	5:E:90:THR:C	2.74	0.42
4:D:58:LYS:HD3	4:D:203:LEU:HD23	2.00	0.42
7:G:149:LYS:HD3	11:K:64:GLN:HB2	2.01	0.42
13:M:103:LYS:HG2	13:M:104:THR:HG23	2.01	0.42
22:V:17:LEU:HB2	22:V:21:THR:HB	2.00	0.42
22:V:7:ILE:O	22:V:56:GLU:HA	2.19	0.42
23:W:396:ILE:HA	23:W:466:VAL:O	2.19	0.42
23:W:647:GLU:O	23:W:651:ARG:HG3	2.18	0.42
24:Y:65:PHE:O	24:Y:69:GLN:HG2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:141:G:H2'	1:A:142:G:H5"	2.01	0.42
1:A:927:G:C3'	1:A:1503:A:C2'	2.76	0.42
10:J:35:GLN:HB2	10:J:77:VAL:HB	2.01	0.42
10:J:93:ALA:HB3	10:J:96:VAL:HG23	2.01	0.42
20:T:44:LYS:HG3	20:T:45:ALA:H	1.83	0.42
23:W:495:VAL:HG11	23:W:520:LEU:HD11	2.01	0.42
25:Z:149:LYS:HE3	25:Z:158:VAL:HG21	1.99	0.42
25:Z:91:ILE:CB	26:X:13:C:O5'	2.60	0.42
1:A:157:U:H2'	1:A:158:G:H5'	2.01	0.42
1:A:768:A:N3	1:A:1512:U:O2'	2.49	0.42
1:A:933:G:O6	7:G:3:ARG:NH1	2.49	0.42
23:W:511:LYS:HG3	23:W:530:PHE:HE2	1.83	0.42
23:W:748:VAL:CG2	23:W:749:ARG:N	2.81	0.42
2:B:47:VAL:N	2:B:48:PRO:HD2	2.34	0.42
1:A:1069:C:O3'	5:E:25:VAL:HG11	2.20	0.42
9:I:24:GLY:N	9:I:61:LEU:HA	2.34	0.42
12:L:74:LEU:HD21	12:L:104:CYS:SG	2.60	0.42
22:V:43:HIS:O	22:V:45:ILE:HG13	2.20	0.42
25:Z:93:VAL:HG11	26:X:25:C:H1'	2.01	0.42
1:A:1082:A:H2'	1:A:1083:U:O4'	2.20	0.42
1:A:1101:A:C4'	2:B:171:ILE:HD11	2.46	0.42
5:E:157:ARG:HD2	8:H:43:GLU:O	2.19	0.42
1:A:1078:U:P	5:E:90:THR:HG1	2.39	0.42
9:I:91:ASP:O	9:I:92:GLU:CB	2.67	0.42
20:T:28:MET:HE2	20:T:32:ILE:HD11	2.02	0.42
22:V:23:ARG:HH21	22:V:33:LEU:CD2	2.33	0.42
23:W:445:THR:OG1	23:W:446:PRO:HD2	2.19	0.42
2:B:124:GLY:O	2:B:125:THR:HG22	2.19	0.42
2:B:138:THR:O	2:B:142:GLU:N	2.42	0.42
7:G:131:LYS:HA	7:G:135:VAL:HG21	2.02	0.42
8:H:75:ILE:O	8:H:75:ILE:HG23	2.19	0.42
23:W:778:VAL:CG2	23:W:779:LYS:N	2.82	0.42
1:A:1397:C:O2'	1:A:1398:A:OP1	2.34	0.42
1:A:1431:A:C6	1:A:1432:G:C6	3.08	0.42
1:A:68:G:C5	1:A:69:G:H1'	2.55	0.42
5:E:94:VAL:HG13	5:E:111:MET:CE	2.49	0.42
5:E:132:ASN:OD1	5:E:134:ILE:HG22	2.18	0.42
1:A:1377:A:N3	7:G:2:PRO:HG3	2.35	0.42
22:V:66:ARG:CZ	22:V:66:ARG:CB	2.98	0.42
1:A:1064:G:H1'	1:A:1190:G:N2	2.35	0.42
1:A:516:PSU:H1'	22:V:2:LYS:HD2	1.69	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:585:G:N3	1:A:879:C:H4'	2.34	0.42
5:E:94:VAL:HG22	5:E:111:MET:HE1	2.01	0.42
14:N:54:ASP:HA	14:N:59:ARG:HD3	2.02	0.42
22:V:38:GLY:O	22:V:39:LYS:C	2.58	0.42
23:W:388:GLU:HG3	23:W:561:ARG:HG2	2.02	0.42
1:A:928:G:C4	1:A:1391:U:H1'	2.52	0.42
1:A:828:U:C2	2:B:25:PRO:HG2	2.39	0.42
2:B:129:LEU:O	2:B:130:THR:CB	2.67	0.42
5:E:161:VAL:O	5:E:164:ILE:N	2.47	0.42
12:L:49:LEU:O	12:L:51:LYS:NZ	2.48	0.42
10:J:65:TYR:CB	14:N:96:LEU:HD11	2.50	0.42
16:P:48:GLU:HG2	16:P:49:GLY:H	1.85	0.42
23:W:566:SER:O	23:W:587:ARG:N	2.50	0.42
23:W:598:LEU:HD12	23:W:650:ALA:HB1	2.01	0.42
23:W:838:TYR:CG	23:W:839:GLU:N	2.87	0.42
1:A:1449:C:C2	1:A:1455:G:C2	3.08	0.42
4:D:11:LEU:O	4:D:15:GLU:HG2	2.20	0.42
10:J:5:ARG:HH21	10:J:77:VAL:HG22	1.85	0.42
13:M:107:ARG:NH2	13:M:113:ARG:HB3	2.35	0.42
23:W:399:HIS:CD2	23:W:478:GLN:HB3	2.55	0.42
26:X:2:G:N3	26:X:2:G:C2'	2.83	0.42
24:Y:28:ILE:HD12	24:Y:28:ILE:H	1.84	0.42
1:A:1417:G:C6	1:A:1482:G:C6	3.08	0.41
1:A:842:U:H3'	1:A:843:U:H4'	2.02	0.41
1:A:966:2MG:C4	26:X:34:C:C3'	3.02	0.41
6:F:99:ALA:HB1	6:F:103:VAL:HB	2.01	0.41
9:I:30:ILE:HA	9:I:65:ILE:HG13	2.02	0.41
9:I:19:VAL:HA	9:I:65:ILE:HG22	2.02	0.41
1:A:501:C:OP1	12:L:114:ARG:NH2	2.52	0.41
19:S:63:THR:HG22	19:S:65:GLU:H	1.84	0.41
23:W:545:LEU:HD12	23:W:545:LEU:HA	1.83	0.41
23:W:644:VAL:HG21	23:W:650:ALA:HB2	2.01	0.41
23:W:774:LEU:O	23:W:778:VAL:HG13	2.20	0.41
23:W:796:GLY:O	23:W:879:VAL:CG1	2.65	0.41
1:A:108:G:N3	1:A:108:G:H5'	2.36	0.41
1:A:501:C:H2'	1:A:502:A:C8	2.55	0.41
3:C:85:GLU:HB2	3:C:88:ARG:NH2	2.36	0.41
1:A:1152:A:H5'	10:J:72:ARG:HH22	1.85	0.41
13:M:66:GLU:OE1	13:M:70:ARG:NH2	2.48	0.41
11:K:89:PRO:HG3	21:U:32:VAL:HG11	2.02	0.41
22:V:70:ARG:O	22:V:71:LYS:HD2	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:W:470:ALA:HB3	23:W:473:ASP:HB2	2.01	0.41
23:W:676:ASN:ND2	23:W:678:PHE:O	2.53	0.41
1:A:1405:G:O4'	1:A:1519:MA6:H4'	2.20	0.41
1:A:1493:A:H61	22:V:33:LEU:CD1	2.26	0.41
1:A:196:A:OP1	20:T:64:LYS:NZ	2.47	0.41
1:A:202:G:HO2'	1:A:468:A:H8	1.66	0.41
1:A:7:A:H3'	5:E:106:ILE:HD13	2.02	0.41
23:W:804:PHE:C	23:W:812:ILE:HG22	2.40	0.41
26:X:53:G:H2'	26:X:54:5MU:O4'	2.20	0.41
1:A:662:U:H2'	1:A:663:A:C8	2.56	0.41
1:A:927:G:O2'	1:A:1531:A:C2'	2.54	0.41
9:I:80:ARG:O	9:I:84:THR:HG23	2.20	0.41
9:I:85:ARG:HA	9:I:88:MET:HE3	2.00	0.41
13:M:83:LEU:HD11	19:S:66:MET:HG2	2.02	0.41
14:N:47:LYS:HD3	14:N:47:LYS:HA	1.92	0.41
19:S:31:LEU:N	19:S:31:LEU:HD12	2.36	0.41
19:S:6:LYS:HA	19:S:6:LYS:HD3	1.88	0.41
20:T:29:ARG:O	20:T:33:LYS:HG3	2.20	0.41
22:V:26:LEU:N	22:V:30:PRO:O	2.53	0.41
1:A:358:U:H5"	23:W:607:ARG:NH1	2.35	0.41
1:A:1402:4OC:HM42	1:A:1500:A:H61	1.85	0.41
1:A:537:G:H1'	22:V:1:ALA:N	2.35	0.41
1:A:993:G:O2'	1:A:994:A:N7	2.54	0.41
22:V:40:MET:CE	22:V:70:ARG:HB3	2.51	0.41
1:A:510:A:H5"	1:A:511:C:P	2.61	0.41
11:K:28:ASN:O	11:K:57:LYS:HD3	2.20	0.41
13:M:12:HIS:HA	13:M:45:ILE:HG13	2.02	0.41
1:A:1494:G:O5'	22:V:18:PRO:HA	2.20	0.41
9:I:130:ARG:CZ	26:X:32:C:C5	3.01	0.41
1:A:148:G:N3	1:A:1446:A:H2	2.19	0.41
1:A:841:C:C6	1:A:843:U:H5'	2.55	0.41
21:U:4:ILE:HG23	21:U:18:ARG:NH1	2.36	0.41
23:W:838:TYR:CE2	23:W:839:GLU:O	2.74	0.41
26:X:23:C:O2'	26:X:24:U:P	2.78	0.41
26:X:41:C:C2'	26:X:42:G:H5"	2.49	0.41
1:A:1239:A:H62	1:A:1299:A:N6	2.19	0.41
1:A:1492:A:C3'	22:V:19:ASN:HB2	2.50	0.41
4:D:95:GLU:OE2	4:D:104:ARG:NH1	2.53	0.41
9:I:30:ILE:HB	9:I:65:ILE:HD11	2.03	0.41
23:W:399:HIS:CB	23:W:402:HIS:CE1	3.00	0.41
1:A:358:U:C5'	23:W:607:ARG:NH1	2.84	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:W:728:ILE:C	23:W:729:THR:CG2	2.89	0.41
23:W:804:PHE:HB2	23:W:812:ILE:HG21	1.89	0.41
1:A:108:G:C5'	1:A:108:G:N3	2.84	0.41
1:A:1095:U:H2'	1:A:1096:C:C6	2.56	0.41
5:E:107:ALA:HB2	5:E:125:ALA:HB3	2.02	0.41
5:E:162:GLU:HG2	8:H:114:ARG:NH2	2.36	0.41
7:G:6:VAL:HG12	7:G:7:ILE:N	2.36	0.41
9:I:54:LEU:N	9:I:54:LEU:HD12	2.36	0.41
12:L:39:THR:HG23	22:V:60:TYR:O	2.20	0.41
15:O:87:LEU:O	15:O:88:ARG:CB	2.68	0.41
22:V:6:THR:HG21	22:V:56:GLU:HG2	2.03	0.41
23:W:706:ASP:O	23:W:710:LYS:HG3	2.21	0.41
23:W:716:VAL:CG2	23:W:786:LEU:CD2	2.98	0.41
1:A:1103:C:H5"	2:B:97:LEU:HD23	2.02	0.41
1:A:188:C:H2'	1:A:189:A:O4'	2.21	0.41
1:A:923:A:OP1	5:E:26:LYS:HG2	2.20	0.41
14:N:62:ASN:HB3	14:N:73:PHE:CD2	2.56	0.41
17:Q:10:GLY:HA3	17:Q:25:ILE:HD13	2.03	0.41
1:A:263:A:P	20:T:74:ARG:HH11	2.43	0.41
1:A:1095:U:H2'	1:A:1096:C:O4'	2.21	0.41
1:A:1312:G:H5'	19:S:6:LYS:CE	2.51	0.41
1:A:1335:U:O2'	1:A:1336:C:OP2	2.35	0.41
1:A:1493:A:H3'	22:V:18:PRO:HA	2.02	0.41
1:A:1074:G:O2'	2:B:102:THR:OG1	2.13	0.41
1:A:1149:C:OP2	9:I:11:ARG:NH2	2.54	0.41
19:S:40:ILE:HD11	19:S:71:LEU:HD23	2.03	0.41
23:W:425:THR:O	23:W:446:PRO:HB3	2.21	0.41
23:W:590:THR:O	23:W:591:LEU:HD23	2.21	0.41
23:W:824:ARG:HE	23:W:845:LEU:HB3	1.86	0.41
26:X:22:G:O2'	26:X:23:C:C5'	2.69	0.41
1:A:361:G:OP1	23:W:729:THR:C	2.52	0.40
1:A:462:G:N7	1:A:463:U:C5	2.89	0.40
1:A:597:G:C2	1:A:644:U:C2	3.09	0.40
13:M:6:GLY:HA2	13:M:66:GLU:HG3	2.01	0.40
17:Q:59:VAL:HG21	17:Q:75:LEU:HD13	2.03	0.40
20:T:59:ASP:OD1	20:T:76:LYS:NZ	2.47	0.40
22:V:20:ALA:CB	22:V:36:ILE:HD12	2.49	0.40
23:W:728:ILE:CG2	23:W:729:THR:N	2.84	0.40
25:Z:125:LYS:CE	26:X:25:C:C2'	2.97	0.40
1:A:1400:C:C1'	26:X:34:C:N3	2.84	0.40
26:X:47:U:C4	26:X:50:U:H5"	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1049:U:H2'	14:N:3:LYS:HE3	2.03	0.40
1:A:1103:C:C1'	2:B:98:GLY:O	2.69	0.40
1:A:1118:U:OP1	9:I:11:ARG:HD2	2.22	0.40
1:A:927:G:OP1	1:A:1504:G:O4'	2.39	0.40
1:A:744:C:O2'	1:A:851:G:N2	2.48	0.40
1:A:1100:C:C5	2:B:95:ARG:HD3	2.51	0.40
5:E:149:SER:H	5:E:152:MET:HG3	1.86	0.40
7:G:44:TYR:O	7:G:48:GLU:N	2.40	0.40
8:H:18:GLN:HG3	8:H:70:ALA:CB	2.51	0.40
11:K:52:PHE:O	11:K:53:ARG:HD2	2.21	0.40
23:W:515:SER:OG	23:W:524:TRP:CH2	2.71	0.40
26:X:73:A:H2'	26:X:74:C:H5"	2.02	0.40
1:A:953:G:H2'	1:A:954:G:O4'	2.22	0.40
1:A:983:A:H5"	1:A:984:C:OP2	2.22	0.40
22:V:25:LYS:HD2	22:V:26:LEU:N	2.37	0.40
22:V:11:GLY:HA3	22:V:26:LEU:HA	2.03	0.40
26:X:41:C:H2'	26:X:42:G:H5"	2.03	0.40
1:A:1070:U:OP1	5:E:23:LYS:CG	2.69	0.40
1:A:328:C:O2	1:A:328:C:H2'	2.21	0.40
1:A:701:U:O5'	24:Y:64:LYS:CD	2.63	0.40
1:A:977:A:O2'	1:A:979:C:OP2	2.39	0.40
6:F:51:ILE:HD11	6:F:85:ILE:CD1	2.52	0.40
9:I:57:MET:HG3	9:I:61:LEU:H	1.85	0.40
13:M:42:ASP:OD1	13:M:42:ASP:N	2.54	0.40
17:Q:7:THR:CG2	17:Q:8:LEU:N	2.85	0.40
19:S:29:LYS:CB	19:S:30:PRO:CD	2.99	0.40
23:W:400:VAL:O	23:W:401:ASP:CB	2.70	0.40
1:A:1053:G:H5"	1:A:1055:A:OP1	2.21	0.40
1:A:1073:U:O3'	5:E:69:ARG:CZ	2.68	0.40
1:A:1224:U:H3'	1:A:1225:A:H5'	2.03	0.40
1:A:1390:U:OP2	1:A:1391:U:OP2	2.24	0.40
1:A:411:A:P	4:D:26:ARG:NH2	2.95	0.40
1:A:723:U:H2'	1:A:855:U:H4'	2.03	0.40
1:A:579:A:H5'	1:A:728:A:H1'	2.02	0.40
5:E:57:PRO:HA	5:E:60:ILE:CG1	2.51	0.40
1:A:710:G:OP1	6:F:53:LYS:HE3	2.21	0.40
11:K:16:VAL:HG22	11:K:77:TYR:CB	2.52	0.40
23:W:794:ILE:HA	23:W:880:PHE:HA	2.03	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	222/241 (92%)	209 (94%)	11 (5%)	2 (1%)	21 67
3	C	204/233 (88%)	193 (95%)	10 (5%)	1 (0%)	34 77
4	D	203/206 (98%)	199 (98%)	4 (2%)	0	100 100
5	E	153/167 (92%)	145 (95%)	8 (5%)	0	100 100
6	F	104/131 (79%)	96 (92%)	8 (8%)	0	100 100
7	G	149/156 (96%)	138 (93%)	10 (7%)	1 (1%)	26 71
8	H	127/130 (98%)	119 (94%)	8 (6%)	0	100 100
9	I	125/130 (96%)	111 (89%)	13 (10%)	1 (1%)	24 69
10	J	97/103 (94%)	88 (91%)	8 (8%)	1 (1%)	19 65
11	K	115/129 (89%)	104 (90%)	11 (10%)	0	100 100
12	L	120/123 (98%)	111 (92%)	9 (8%)	0	100 100
13	M	112/118 (95%)	101 (90%)	8 (7%)	3 (3%)	6 45
14	N	98/101 (97%)	91 (93%)	7 (7%)	0	100 100
15	O	86/89 (97%)	80 (93%)	3 (4%)	3 (4%)	4 39
16	P	80/102 (78%)	73 (91%)	6 (8%)	1 (1%)	15 60
17	Q	78/84 (93%)	73 (94%)	5 (6%)	0	100 100
18	R	53/75 (71%)	51 (96%)	1 (2%)	1 (2%)	10 52
19	S	77/92 (84%)	69 (90%)	7 (9%)	1 (1%)	15 60
20	T	84/87 (97%)	83 (99%)	1 (1%)	0	100 100
21	U	54/71 (76%)	53 (98%)	1 (2%)	0	100 100
22	V	69/72 (96%)	47 (68%)	15 (22%)	7 (10%)	1 14
23	W	499/890 (56%)	480 (96%)	17 (3%)	2 (0%)	39 80
24	Y	74/171 (43%)	73 (99%)	1 (1%)	0	100 100
25	Z	89/144 (62%)	76 (85%)	10 (11%)	3 (3%)	5 40
All	All	3072/3845 (80%)	2863 (93%)	182 (6%)	27 (1%)	26 67

All (27) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	130	THR
3	C	127	ARG
9	I	25	ASN
10	J	57	VAL
13	M	5	ALA
22	V	24	VAL
22	V	28	SER
22	V	34	ALA
23	W	791	LYS
25	Z	153	GLN
25	Z	163	THR
13	M	13	LYS
15	O	88	ARG
22	V	9	THR
25	Z	105	GLY
2	B	126	PHE
16	P	48	GLU
18	R	73	ARG
22	V	30	PRO
7	G	80	VAL
15	O	18	ASP
15	O	21	ASP
22	V	3	GLU
13	M	105	ASN
23	W	788	PRO
19	S	29	LYS
22	V	45	ILE

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	B	186/199 (94%)	180 (97%)	6 (3%)	46	76
3	C	170/190 (90%)	164 (96%)	6 (4%)	43	74
4	D	172/173 (99%)	167 (97%)	5 (3%)	50	78

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
5	E	118/126 (94%)	112 (95%)	6 (5%)	29 66
6	F	92/112 (82%)	91 (99%)	1 (1%)	80 91
7	G	124/129 (96%)	121 (98%)	3 (2%)	57 82
8	H	104/105 (99%)	100 (96%)	4 (4%)	40 73
9	I	105/107 (98%)	102 (97%)	3 (3%)	50 78
10	J	87/90 (97%)	81 (93%)	6 (7%)	19 56
11	K	90/99 (91%)	89 (99%)	1 (1%)	80 91
12	L	102/102 (100%)	101 (99%)	1 (1%)	82 92
13	M	92/96 (96%)	90 (98%)	2 (2%)	60 83
14	N	83/84 (99%)	82 (99%)	1 (1%)	78 90
15	O	76/77 (99%)	74 (97%)	2 (3%)	54 80
16	P	65/84 (77%)	63 (97%)	2 (3%)	47 77
17	Q	74/78 (95%)	72 (97%)	2 (3%)	52 79
18	R	48/65 (74%)	48 (100%)	0	100 100
19	S	70/79 (89%)	68 (97%)	2 (3%)	50 78
20	T	65/66 (98%)	63 (97%)	2 (3%)	47 77
21	U	48/61 (79%)	45 (94%)	3 (6%)	22 59
22	V	62/63 (98%)	54 (87%)	8 (13%)	5 28
23	W	402/713 (56%)	398 (99%)	4 (1%)	82 92
24	Y	66/149 (44%)	61 (92%)	5 (8%)	16 53
25	Z	81/128 (63%)	73 (90%)	8 (10%)	10 39
All	All	2582/3175 (81%)	2499 (97%)	83 (3%)	50 76

All (83) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	5	SER
2	B	23	TRP
2	B	73	LYS
2	B	93	ASN
2	B	129	LEU
2	B	213	TYR
3	C	20	SER
3	C	58	GLU
3	C	83	ASP

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Mol	Chain	Res	Type
3	C	85	GLU
3	C	125	GLU
3	C	201	TRP
4	D	26	ARG
4	D	131	ASN
4	D	194	ASP
4	D	196	ASN
4	D	197	GLU
5	E	22	SER
5	E	48	PHE
5	E	80	THR
5	E	130	SER
5	E	152	MET
5	E	163	GLU
6	F	93	LYS
7	G	7	ILE
7	G	54	SER
7	G	83	SER
8	H	3	MET
8	H	60	GLU
8	H	75	ILE
8	H	107	SER
9	I	47	VAL
9	I	66	THR
9	I	94	LEU
10	J	7	ARG
10	J	16	ARG
10	J	19	ASP
10	J	27	GLU
10	J	35	GLN
10	J	80	THR
11	K	33	THR
12	L	15	LYS
13	M	71	ARG
13	M	107	ARG
14	N	59	ARG
15	O	3	LEU
15	O	89	ARG
16	P	1	MET
16	P	44	SER
17	Q	14	SER
17	Q	27	ARG

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Mol	Chain	Res	Type
19	S	18	LYS
19	S	25	SER
20	T	40	GLU
20	T	54	MET
21	U	4	ILE
21	U	41	PRO
21	U	56	HIS
22	V	5	ASP
22	V	23	ARG
22	V	31	GLU
22	V	32	ILE
22	V	42	MET
22	V	51	ASP
22	V	52	ARG
22	V	71	LYS
23	W	541	ILE
23	W	790	LEU
23	W	791	LYS
23	W	861	CYS
24	Y	21	GLN
24	Y	26	LEU
24	Y	42	ASN
24	Y	43	LEU
24	Y	73	GLU
25	Z	108	GLN
25	Z	118	LEU
25	Z	123	LYS
25	Z	128	LEU
25	Z	150	ASP
25	Z	152	LEU
25	Z	155	LEU
25	Z	165	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	103	ASN
2	B	170	HIS
2	B	178	ASN
3	C	123	GLN
7	G	52	GLN
7	G	148	ASN

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Mol	Chain	Res	Type
23	W	399	HIS
23	W	402	HIS
23	W	426	GLN
23	W	437	ASN
23	W	448	HIS
23	W	484	GLN
23	W	498	ASN
24	Y	21	GLN
25	Z	92	GLN
25	Z	108	GLN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	1528/1534 (99%)	257 (16%)	9 (0%)
26	X	76/77 (98%)	24 (31%)	11 (14%)
All	All	1604/1611 (99%)	281 (17%)	20 (1%)

All (281) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	5	U
1	A	6	G
1	A	9	G
1	A	22	G
1	A	28	A
1	A	32	A
1	A	39	G
1	A	47	C
1	A	48	C
1	A	50	A
1	A	51	A
1	A	69	G
1	A	70	U
1	A	71	A
1	A	72	A
1	A	73	C
1	A	74	A
1	A	75	G
1	A	76	G
1	A	77	A

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Mol	Chain	Res	Type
1	A	78	A
1	A	79	G
1	A	80	A
1	A	81	A
1	A	82	G
1	A	83	C
1	A	84	U
1	A	85	U
1	A	86	G
1	A	89	U
1	A	90	C
1	A	91	U
1	A	94	G
1	A	95	C
1	A	97	G
1	A	108	G
1	A	119	A
1	A	121	U
1	A	122	G
1	A	128	G
1	A	130	A
1	A	131	A
1	A	137	U
1	A	142	G
1	A	144	G
1	A	158	G
1	A	159	G
1	A	163	C
1	A	168	G
1	A	173	U
1	A	183	C
1	A	201	G
1	A	205	A
1	A	208	U
1	A	209	U
1	A	210	C
1	A	212	G
1	A	240	G
1	A	245	U
1	A	247	G
1	A	251	G
1	A	262	A

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Mol	Chain	Res	Type
1	A	266	G
1	A	267	C
1	A	289	G
1	A	321	A
1	A	328	C
1	A	329	A
1	A	330	C
1	A	332	G
1	A	346	G
1	A	352	C
1	A	354	G
1	A	367	U
1	A	372	C
1	A	373	A
1	A	382	A
1	A	384	G
1	A	406	G
1	A	411	A
1	A	412	A
1	A	413	G
1	A	421	U
1	A	422	C
1	A	429	U
1	A	430	A
1	A	435	A
1	A	439	U
1	A	444	G
1	A	457	G
1	A	458	U
1	A	463	U
1	A	466	A
1	A	467	U
1	A	468	A
1	A	481	G
1	A	486	U
1	A	495	A
1	A	496	A
1	A	509	A
1	A	511	C
1	A	512	U
1	A	527	G7M
1	A	530	G

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Mol	Chain	Res	Type
1	A	532	A
1	A	533	A
1	A	547	A
1	A	559	A
1	A	562	U
1	A	564	C
1	A	572	A
1	A	573	A
1	A	576	C
1	A	577	G
1	A	631	C
1	A	632	U
1	A	649	A
1	A	650	G
1	A	653	U
1	A	665	A
1	A	682	G
1	A	721	G
1	A	723	U
1	A	724	G
1	A	733	G
1	A	753	A
1	A	755	G
1	A	777	A
1	A	793	U
1	A	794	A
1	A	815	A
1	A	817	C
1	A	827	U
1	A	828	U
1	A	832	G
1	A	841	C
1	A	842	U
1	A	843	U
1	A	845	A
1	A	846	G
1	A	887	G
1	A	913	A
1	A	914	A
1	A	926	G
1	A	932	C
1	A	934	C

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Mol	Chain	Res	Type
1	A	960	U
1	A	969	A
1	A	975	A
1	A	976	G
1	A	977	A
1	A	992	U
1	A	993	G
1	A	1004	A
1	A	1005	A
1	A	1009	U
1	A	1012	A
1	A	1015	G
1	A	1017	U
1	A	1019	A
1	A	1021	A
1	A	1022	A
1	A	1023	U
1	A	1025	U
1	A	1026	G
1	A	1027	C
1	A	1028	C
1	A	1029	U
1	A	1030	U
1	A	1031	C
1	A	1032	G
1	A	1033	G
1	A	1034	G
1	A	1036	A
1	A	1037	C
1	A	1043	G
1	A	1053	G
1	A	1054	C
1	A	1065	U
1	A	1070	U
1	A	1086	U
1	A	1092	A
1	A	1094	G
1	A	1095	U
1	A	1098	C
1	A	1101	A
1	A	1108	G
1	A	1124	G

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Mol	Chain	Res	Type
1	A	1133	G
1	A	1135	U
1	A	1136	C
1	A	1137	C
1	A	1138	G
1	A	1139	G
1	A	1140	C
1	A	1141	C
1	A	1142	G
1	A	1143	G
1	A	1152	A
1	A	1158	C
1	A	1159	U
1	A	1160	G
1	A	1167	A
1	A	1168	U
1	A	1184	G
1	A	1196	A
1	A	1197	A
1	A	1212	U
1	A	1213	A
1	A	1215	G
1	A	1225	A
1	A	1227	A
1	A	1238	A
1	A	1239	A
1	A	1240	U
1	A	1256	A
1	A	1257	A
1	A	1260	G
1	A	1279	G
1	A	1280	A
1	A	1286	U
1	A	1287	A
1	A	1299	A
1	A	1300	G
1	A	1302	C
1	A	1305	G
1	A	1317	C
1	A	1320	C
1	A	1322	C
1	A	1323	G

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Mol	Chain	Res	Type
1	A	1336	C
1	A	1346	A
1	A	1353	G
1	A	1363	A
1	A	1368	A
1	A	1370	G
1	A	1381	U
1	A	1398	A
1	A	1429	A
1	A	1441	A
1	A	1442	G
1	A	1445	U
1	A	1446	A
1	A	1450	U
1	A	1451	U
1	A	1453	G
1	A	1454	G
1	A	1492	A
1	A	1493	A
1	A	1497	G
1	A	1499	A
1	A	1503	A
1	A	1505	G
1	A	1506	U
1	A	1517	G
1	A	1529	G
1	A	1530	G
26	X	8	4SU
26	X	9	G
26	X	16	C
26	X	17(A)	U
26	X	19	G
26	X	20	H2U
26	X	21	A
26	X	22	G
26	X	23	C
26	X	24	U
26	X	42	G
26	X	48	C
26	X	49	G
26	X	54	5MU
26	X	55	PSU

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Mol	Chain	Res	Type
26	X	56	C
26	X	57	A
26	X	58	A
26	X	59	A
26	X	70	G
26	X	71	C
26	X	74	C
26	X	75	C
26	X	76	A

All (20) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	4	U
1	A	209	U
1	A	412	A
1	A	429	U
1	A	653	U
1	A	793	U
1	A	1024	G
1	A	1031	C
1	A	1211	U
26	X	8	4SU
26	X	19	G
26	X	20	H2U
26	X	21	A
26	X	22	G
26	X	23	C
26	X	55	PSU
26	X	56	C
26	X	57	A
26	X	58	A
26	X	70	G

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

16 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	$\#\|Z\| > 2$
1	2MG	A	1207	1	18,26,27	1.14	2 (11%)	21,38,41	2.37	7 (33%)
1	4OC	A	1402	1	15,23,24	0.64	0	21,32,35	1.91	3 (14%)
1	5MC	A	1407	1	14,22,23	1.49	1 (7%)	17,32,35	1.03	1 (5%)
1	UR3	A	1498	1	13,22,23	0.60	0	18,32,35	0.71	0
1	2MG	A	1516	1	18,26,27	1.04	2 (11%)	21,38,41	2.12	7 (33%)
1	MA6	A	1518	1	18,26,27	0.93	1 (5%)	15,38,41	2.00	2 (13%)
1	MA6	A	1519	1	18,26,27	0.90	1 (5%)	15,38,41	2.54	3 (20%)
1	PSU	A	516	1,22	15,21,22	1.11	1 (6%)	16,30,33	1.64	3 (18%)
1	G7M	A	527	1	18,26,27	1.07	1 (5%)	21,39,42	2.26	5 (23%)
1	2MG	A	966	1,26	18,26,27	1.25	2 (11%)	21,38,41	2.27	6 (28%)
1	5MC	A	967	1	14,22,23	1.22	1 (7%)	17,32,35	1.19	1 (5%)
12	D2T	L	89	12	4,9,10	0.56	0	4,11,13	1.16	0
26	H2U	X	20	26	17,21,22	0.81	0	23,30,33	1.33	5 (21%)
26	5MU	X	54	26	13,22,23	0.77	0	16,32,35	2.62	2 (12%)
26	PSU	X	55	26	15,21,22	1.40	1 (6%)	16,30,33	2.39	5 (31%)
26	4SU	X	8	26	12,21,22	1.13	2 (16%)	15,30,33	1.88	6 (40%)

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
1	2MG	A	1207	1	-	0/5/27/28	0/3/3/3
1	4OC	A	1402	1	-	0/7/29/30	0/2/2/2
1	5MC	A	1407	1	-	0/3/25/26	0/2/2/2
1	UR3	A	1498	1	-	0/3/25/26	0/2/2/2
1	2MG	A	1516	1	-	0/5/27/28	0/3/3/3
1	MA6	A	1518	1	-	0/7/29/30	0/3/3/3
1	MA6	A	1519	1	-	0/7/29/30	0/3/3/3
1	PSU	A	516	1,22	-	0/7/25/26	0/2/2/2
1	G7M	A	527	1	-	0/3/25/26	0/3/3/3
1	2MG	A	966	1,26	-	0/5/27/28	0/3/3/3
1	5MC	A	967	1	-	0/3/25/26	0/2/2/2
12	D2T	L	89	12	-	0/2/12/14	0/0/0/0
26	H2U	X	20	26	-	0/7/38/39	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	5MU	X	54	26	-	0/3/25/26	0/2/2/2
26	PSU	X	55	26	-	0/7/25/26	0/2/2/2
26	4SU	X	8	26	-	0/3/25/26	0/2/2/2

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	X	55	PSU	C5-C1'	-4.40	1.48	1.52
26	X	8	4SU	C2-N3	-2.17	1.33	1.38
1	A	1519	MA6	C5-C4	2.52	1.46	1.40
26	X	8	4SU	O4'-C1'	2.55	1.44	1.41
1	A	1516	2MG	C5-C4	2.77	1.46	1.40
1	A	1516	2MG	C6-C5	2.90	1.47	1.41
1	A	1518	MA6	C5-C4	2.91	1.47	1.40
1	A	1207	2MG	C5-C4	2.95	1.47	1.40
1	A	1207	2MG	C6-C5	3.14	1.47	1.41
1	A	516	PSU	C4-N3	3.17	1.38	1.33
1	A	966	2MG	C5-C4	3.18	1.47	1.40
1	A	966	2MG	C6-C5	3.43	1.48	1.41
1	A	527	G7M	C6-C5	3.75	1.48	1.41
1	A	967	5MC	C5-C4	4.25	1.48	1.41
1	A	1407	5MC	C5-C4	5.16	1.49	1.41

All (56) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	X	54	5MU	C5-C4-N3	-7.49	119.06	125.35
1	A	1519	MA6	N3-C2-N1	-7.34	123.11	128.87
1	A	1402	4OC	CM4-N4-C4	-6.29	117.57	122.87
1	A	1518	MA6	N3-C2-N1	-5.95	124.20	128.87
1	A	527	G7M	C1'-N9-C4	-4.84	121.40	126.81
1	A	527	G7M	C5-C6-N1	-4.83	117.21	123.52
1	A	966	2MG	C5-C6-N1	-4.70	117.38	123.52
1	A	1207	2MG	C5-C6-N1	-4.31	117.89	123.52
1	A	966	2MG	CM2-N2-C2	-3.98	118.56	123.03
1	A	1519	MA6	C1'-N9-C4	-3.88	122.47	126.81
1	A	1207	2MG	CM2-N2-C2	-3.86	118.69	123.03
26	X	55	PSU	C5-C6-N1	-3.76	119.13	124.38
1	A	1516	2MG	C5-C6-N1	-3.61	118.81	123.52
26	X	8	4SU	C5-C4-N3	-3.44	119.92	123.56
1	A	1207	2MG	C6-C5-C4	-3.32	117.06	120.86
1	A	527	G7M	N3-C2-N1	-3.27	123.11	127.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	1516	2MG	C6-C5-C4	-3.24	117.16	120.86
26	X	55	PSU	C5-C1'-C2'	-3.20	110.00	115.44
1	A	1516	2MG	CM2-N2-C2	-3.04	119.61	123.03
1	A	966	2MG	C6-C5-C4	-2.85	117.60	120.86
26	X	8	4SU	O4'-C4'-C3'	-2.62	99.84	105.16
26	X	20	H2U	C4-N3-C2	-2.59	123.42	125.77
1	A	1207	2MG	N3-C2-N1	-2.55	122.37	126.19
1	A	516	PSU	C5-C6-N1	-2.47	120.94	124.38
1	A	527	G7M	C6-C5-C4	-2.41	118.10	120.86
1	A	1516	2MG	C1'-N9-C4	-2.40	124.13	126.81
26	X	20	H2U	C5-C6-N1	-2.27	108.28	110.76
26	X	8	4SU	C2'-C1'-N1	-2.12	107.76	113.46
1	A	966	2MG	N3-C2-N1	-2.10	123.05	126.19
1	A	1516	2MG	C2'-C1'-N9	-2.01	108.08	113.47
26	X	20	H2U	C6-N1-C2	2.24	125.61	122.16
26	X	20	H2U	C3'-C2'-C1'	2.24	105.93	101.44
26	X	55	PSU	O4'-C1'-C2'	2.26	107.14	104.69
1	A	1207	2MG	N2-C2-N1	2.33	119.64	116.94
1	A	516	PSU	O4'-C1'-C2'	2.36	107.24	104.69
1	A	1407	5MC	N4-C4-N3	2.54	120.64	116.92
26	X	20	H2U	C1'-N1-C2	2.57	121.79	118.19
26	X	8	4SU	O4'-C1'-N1	2.58	113.01	108.10
26	X	8	4SU	O3'-C3'-C2'	2.71	120.61	111.86
1	A	1402	4OC	C6-C5-C4	2.99	118.59	117.42
26	X	8	4SU	O3'-C3'-C4'	3.17	120.48	111.01
26	X	55	PSU	C3'-C2'-C1'	3.46	105.81	101.71
1	A	967	5MC	N4-C4-N3	3.47	122.00	116.92
1	A	1518	MA6	C2-N1-C6	4.13	121.37	111.64
1	A	1516	2MG	C6-N1-C2	4.17	121.22	115.24
1	A	1519	MA6	C2-N1-C6	4.36	121.92	111.64
1	A	1402	4OC	C2-N3-C4	4.47	121.12	115.43
1	A	1516	2MG	C2-N3-C4	4.73	120.17	114.99
1	A	966	2MG	C2-N3-C4	4.83	120.28	114.99
1	A	516	PSU	C4-N3-C2	4.93	119.27	115.16
1	A	966	2MG	C6-N1-C2	4.98	122.37	115.24
1	A	1207	2MG	C2-N3-C4	5.05	120.53	114.99
1	A	527	G7M	C6-N1-C2	5.06	121.82	115.88
1	A	1207	2MG	C6-N1-C2	5.17	122.65	115.24
26	X	54	5MU	C4-N3-C2	6.57	120.64	115.16
26	X	55	PSU	C4-N3-C2	6.58	120.65	115.16

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

10 monomers are involved in 51 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	1402	4OC	1	0
1	A	1518	MA6	2	0
1	A	1519	MA6	3	0
1	A	516	PSU	2	0
1	A	527	G7M	2	0
1	A	966	2MG	21	0
26	X	20	H2U	5	0
26	X	54	5MU	5	0
26	X	55	PSU	3	0
26	X	8	4SU	12	0

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

1 ligand is modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
27	FME	X	101	26	8,8,10	0.40	0	8,8,11	1.47	2 (25%)

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
27	FME	X	101	26	-	0/7/7/11	0/0/0/0

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
27	X	101	FME	O1-CN-N	-2.65	120.75	124.80
27	X	101	FME	CA-N-CN	-2.64	120.70	124.12

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
27	X	101	FME	14	0

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	2

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	926:G	O3'	927:G	P	5.84
1	A	1390:U	O3'	1391:U	P	4.62