



Full wwPDB/EMDatabank EM Map/Model Validation Report ⓘ

Jan 5, 2017 – 02:49 PM EST

PDB ID : 5ME0
EMDB ID: : EMD-3494
Title : Structure of the 30S Pre-Initiation Complex 1 (30S IC-1) 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 ⓘ 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

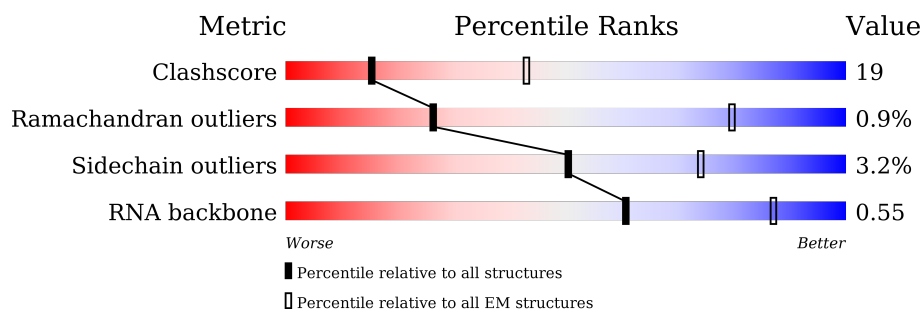
1 Overall quality at a glance

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.

















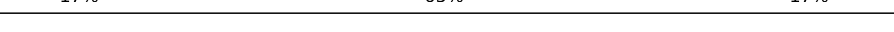
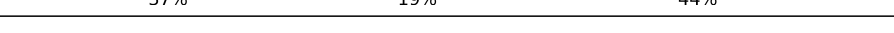
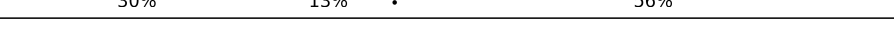
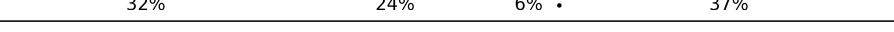
Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	114402	924
Ramachandran outliers	111179	726
Sidechain outliers	111093	686
RNA backbone	3027	244

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 $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	A	1534	71% 23% 6%
2	B	241	71% 21% 7%
3	C	233	73% 14% 12%
4	D	206	86% 13%
5	E	167	58% 33% 7%
6	F	131	71% 10% 19%
7	G	156	78% 17% ..
8	H	130	70% 28% ..

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
9	I	130	
10	J	103	
11	K	129	
12	L	123	
13	M	118	
14	N	101	
15	O	89	
16	P	102	
17	Q	84	
18	R	75	
19	S	92	
20	T	87	
21	U	71	
22	V	72	
23	W	890	
24	Y	171	
25	Z	144	
26	X	77	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
26	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
1	A	1534	Total	C	N	O	P	0	0
			32930	14694	6041	10661	1534		

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

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

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

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

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

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

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

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

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

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

- 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		

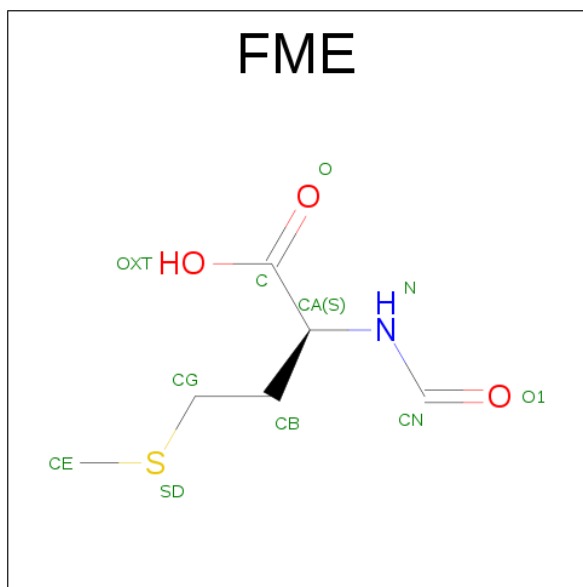
There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Z	37	MET	-	initiating methionine	UNP P0A707

- 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: C₆H₁₁NO₃S).

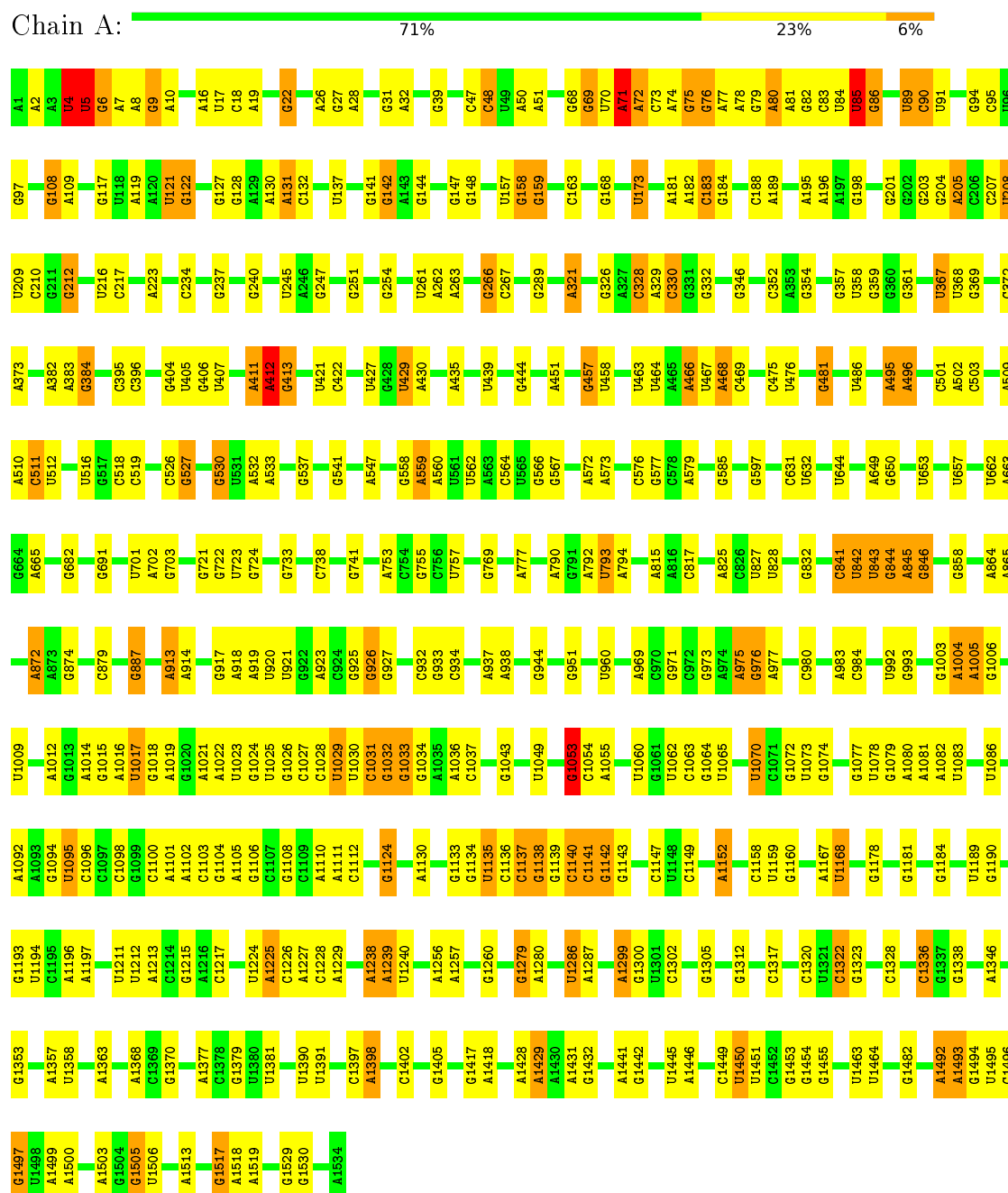


Mol	Chain	Residues	Atoms						AltConf
			Total	C	H	N	O	S	
27	X	1	10	6	1	1	1	1	0

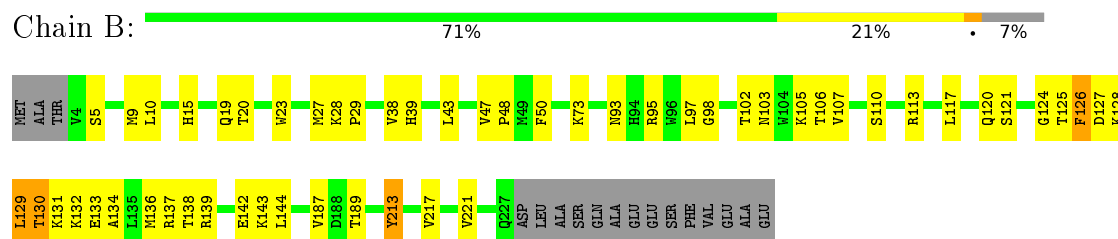
3 Residue-property plots

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

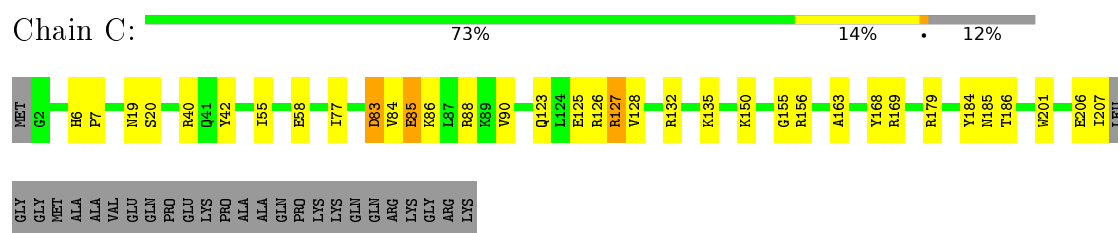
- Molecule 1: 16S ribosomal RNA



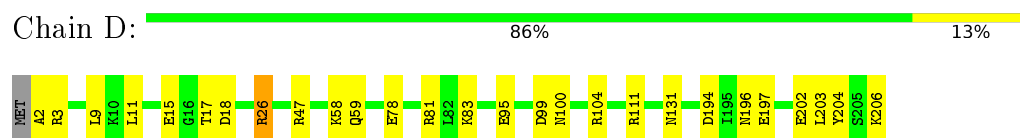
- Molecule 2: 30S ribosomal protein S2



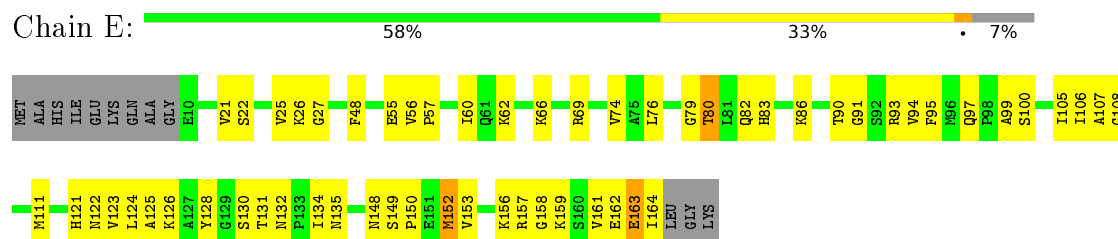
- Molecule 3: 30S ribosomal protein S3



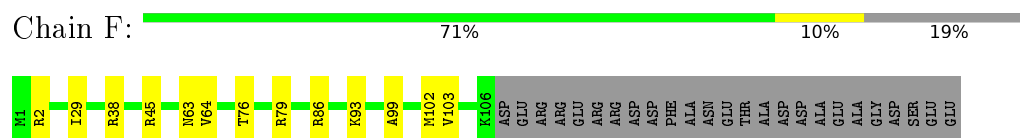
- Molecule 4: 30S ribosomal protein S4



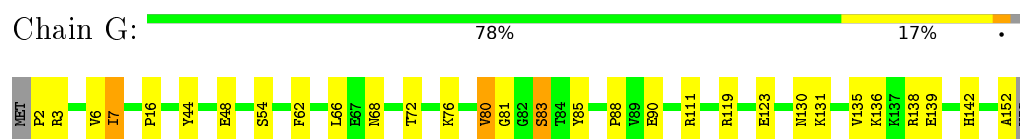
- Molecule 5: 30S ribosomal protein S5



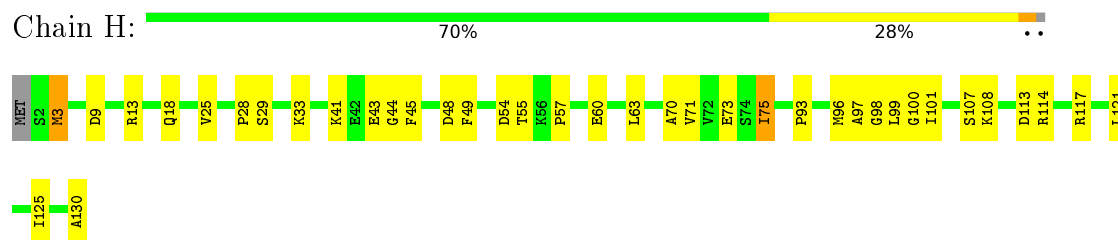
- Molecule 6: 30S ribosomal protein S6



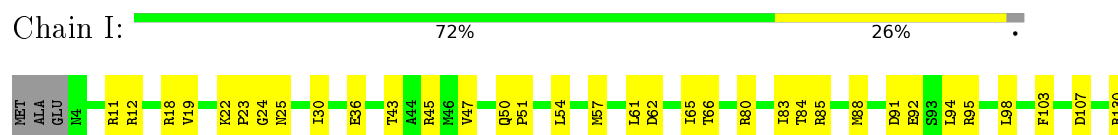
- Molecule 7: 30S ribosomal protein S7



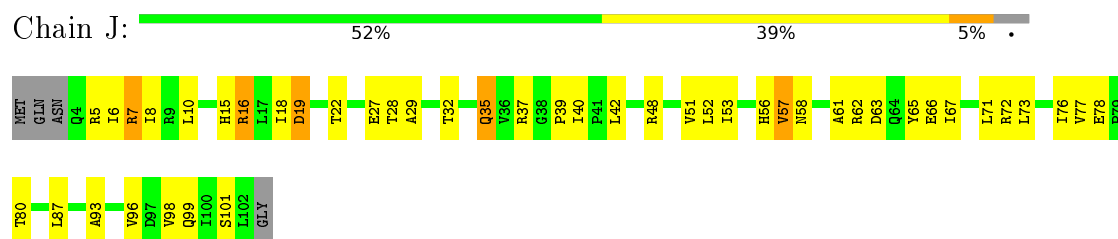
- Molecule 8: 30S ribosomal protein S8



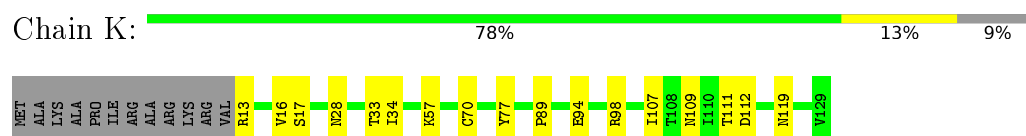
- Molecule 9: 30S ribosomal protein S9



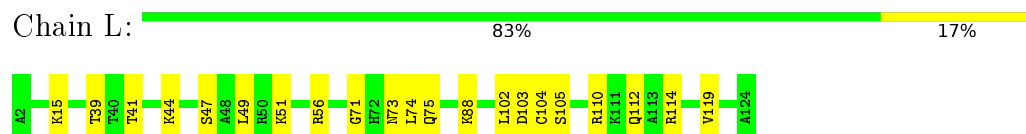
- Molecule 10: 30S ribosomal protein S10



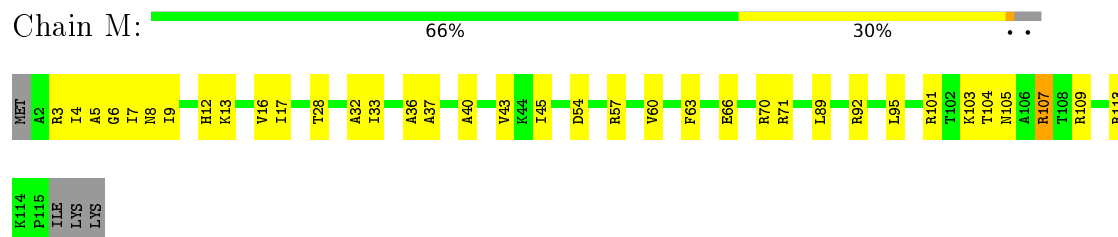
- Molecule 11: 30S ribosomal protein S11



- Molecule 12: 30S ribosomal protein S12

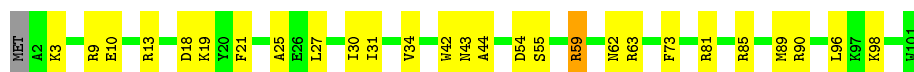


- Molecule 13: 30S ribosomal protein S13




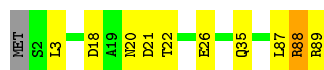
- Molecule 14: 30S ribosomal protein S14

Chain N:  72% 26% ..



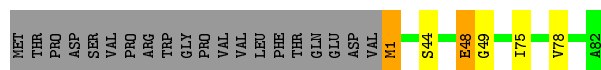
- Molecule 15: 30S ribosomal protein S15

Chain O:  88% 10% ..




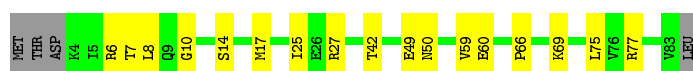
- Molecule 16: 30S ribosomal protein S16

Chain P:  75% 20% ..



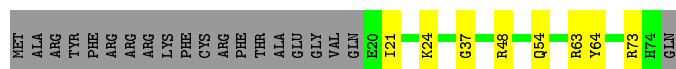
- Molecule 17: 30S ribosomal protein S17

Chain Q:  75% 20% 5%



- Molecule 18: 30S ribosomal protein S18

Chain R:  63% 11% 27%




- Molecule 19: 30S ribosomal protein S19

Chain S:  68% 15% 14%



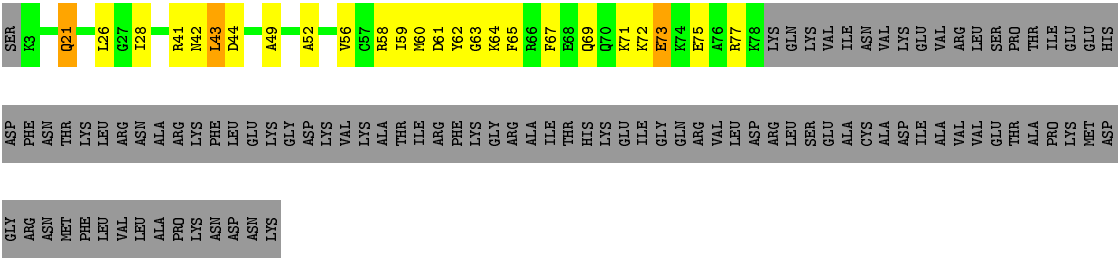
- Molecule 20: 30S ribosomal protein S20

Chain T:  83% 16% .

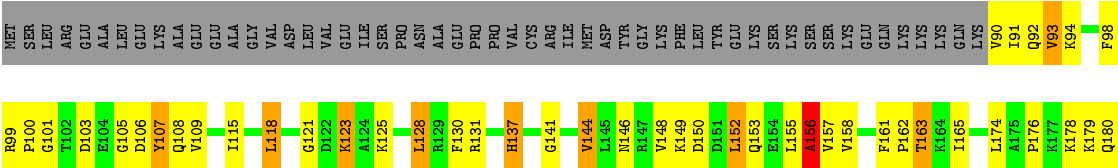
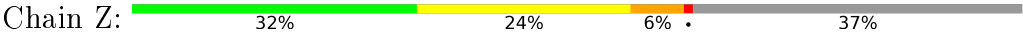


- Molecule 21: 30S ribosomal protein S21

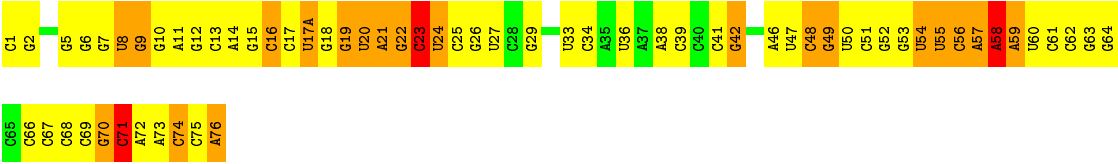
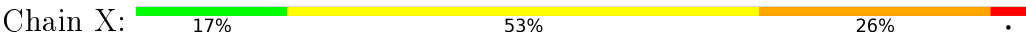
Chain U:  59% 18% 21%



● Molecule 25: Translation initiation factor IF-3



● Molecule 26: fMet-tRNA



4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of particles used	23112	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 ($e^-/\text{\AA}^2$)	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	0.41	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	0/3828	0.46	1/5173 (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	0.23	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	0/63148	0.86	52/93100 (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(°)	Ideal(°)
1	A	117	G	O5'-P-OP2	-9.51	97.14	105.70
25	Z	107	TYR	CB-CG-CD2	-8.06	116.17	121.00
26	X	71	C	N1-C1'-C2'	-7.48	103.77	112.00
25	Z	144	VAL	CA-CB-CG2	-7.43	99.75	110.90
25	Z	156	ALA	CB-CA-C	-6.97	99.65	110.10
1	A	4	U	C2-N1-C1'	6.88	125.95	117.70
1	A	1279	G	C4-N9-C1'	6.85	135.40	126.50
1	A	330	C	C2-N3-C4	6.84	123.32	119.90
1	A	887	G	O5'-P-OP2	-6.78	99.60	105.70
1	A	330	C	C5-C6-N1	6.61	124.31	121.00
1	A	1053	G	OP2-P-O3'	6.33	119.12	105.20
1	A	579	A	O5'-P-OP2	-6.22	100.10	105.70
25	Z	152	LEU	CB-CA-C	-6.14	98.54	110.20
1	A	330	C	C6-N1-C2	-6.09	117.86	120.30
26	X	71	C	C4'-C3'-O3'	6.09	125.18	113.00
1	A	971	G	O4'-C1'-N9	6.09	113.07	108.20
1	A	321	A	O5'-P-OP2	-6.08	100.23	105.70
1	A	328	C	N1-C2-O2	6.05	122.53	118.90
1	A	330	C	C2-N1-C1'	6.00	125.39	118.80
1	A	872	A	O4'-C1'-N9	5.98	112.99	108.20
1	A	844	G	C2-N3-C4	5.98	114.89	111.90
25	Z	163	THR	N-CA-CB	-5.88	99.14	110.30
1	A	328	C	N3-C2-O2	-5.79	117.85	121.90
25	Z	162	PRO	C-N-CA	5.78	136.14	121.70
1	A	412	A	N9-C1'-C2'	5.71	121.43	114.00
25	Z	156	ALA	N-CA-CB	5.70	118.08	110.10
1	A	330	C	N1-C2-O2	5.69	122.31	118.90
1	A	1279	G	C8-N9-C1'	-5.64	119.67	127.00
1	A	1279	G	N7-C8-N9	5.61	115.91	113.10
1	A	85	U	C2-N1-C1'	5.60	124.42	117.70
1	A	183	C	C6-N1-C2	-5.46	118.11	120.30
1	A	71	A	N1-C6-N6	5.44	121.86	118.60
1	A	412	A	O4'-C1'-N9	5.41	112.53	108.20
1	A	1418	A	C8-N9-C4	-5.40	103.64	105.80
23	W	787	SER	C-N-CD	5.39	139.72	128.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	22	G	O5'-P-OP2	-5.38	100.86	105.70
26	X	23	C	N1-C1'-C2'	-5.36	106.10	112.00
26	X	23	C	C2'-C3'-O3'	-5.33	97.76	109.50
1	A	792	A	O4'-C1'-N9	5.23	112.38	108.20
26	X	58	A	C2'-C3'-O3'	-5.19	98.08	109.50
25	Z	146	ASN	CA-CB-CG	5.16	124.76	113.40
1	A	5	U	C5-C6-N1	5.16	125.28	122.70
1	A	328	C	C2-N1-C1'	5.16	124.47	118.80
25	Z	115	ILE	CB-CA-C	-5.13	101.34	111.60
1	A	1286	U	C2-N1-C1'	5.12	123.84	117.70
1	A	858	G	N3-C4-N9	5.11	129.07	126.00
25	Z	93	VAL	CG1-CB-CG2	-5.09	102.76	110.90
25	Z	152	LEU	C-N-CA	5.08	134.39	121.70
25	Z	107	TYR	CA-CB-CG	5.06	123.02	113.40
1	A	330	C	N3-C4-C5	-5.04	119.89	121.90
1	A	1168	U	C2-N1-C1'	5.00	123.71	117.70
25	Z	157	VAL	CB-CA-C	-5.00	101.90	111.40

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 ⓘ

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	16574	826	0
2	B	1753	0	1771	174	0
3	C	1624	0	1696	63	0
4	D	1643	0	1707	26	0
5	E	1144	0	1173	224	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	F	862	0	864	8	0
7	G	1181	0	1238	21	0
8	H	979	0	1029	93	0
9	I	1022	0	1070	27	0
10	J	795	0	836	39	0
11	K	877	0	887	13	0
12	L	957	0	1015	78	0
13	M	883	0	941	31	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	6	0
19	S	637	0	665	14	0
20	T	670	0	719	11	0
21	U	465	0	491	9	0
22	V	570	0	594	195	0
23	W	3781	0	3831	362	0
24	Y	623	0	649	95	0
25	Z	743	0	779	209	0
26	X	1643	0	828	356	0
27	X	9	1	9	19	0
All	All	59062	1	42779	1945	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 (1945) 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:1112:C:P	2:B:131:LYS:HB2	1.24	1.65
1:A:919:A:C2	1:A:1080:A:C2	1.85	1.64
1:A:864:A:H1'	1:A:1078:U:C5	1.32	1.60
26:X:71:C:H2'	26:X:72:A:C8	1.32	1.59
1:A:1390:U:C6	1:A:1391:U:C5	1.84	1.59
25:Z:176:PRO:CD	26:X:12:G:H4'	1.17	1.57
1:A:864:A:C1'	1:A:1078:U:C5	1.84	1.56
24:Y:49:ALA:HB2	26:X:19:G:C6	1.39	1.55
25:Z:125:LYS:NZ	26:X:26:G:C4'	1.68	1.54
12:L:105:SER:HB3	23:W:666:LEU:CD2	1.31	1.54
5:E:157:ARG:HG2	8:H:45:PHE:CE2	1.35	1.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:Z:176:PRO:HG2	26:X:12:G:C3'	1.34	1.52
1:A:1492:A:C2	22:V:35:TYR:HB3	1.39	1.52
24:Y:77:ARG:NH2	26:X:16:C:C5	1.77	1.52
1:A:7:A:C3'	5:E:106:ILE:HD11	1.37	1.52
24:Y:49:ALA:CB	26:X:19:G:C6	1.88	1.51
1:A:17:U:C2'	1:A:1079:G:H2'	1.04	1.50
1:A:1493:A:C8	22:V:18:PRO:O	1.64	1.50
25:Z:176:PRO:HD2	26:X:12:G:C4'	1.38	1.49
1:A:7:A:H3'	5:E:106:ILE:CD1	1.05	1.48
1:A:1110:A:C2	2:B:136:MET:HG3	1.44	1.47
1:A:7:A:C3'	5:E:106:ILE:CD1	1.90	1.46
1:A:17:U:C2'	1:A:1079:G:C2'	1.90	1.46
1:A:1106:G:OP1	2:B:113:ARG:CZ	1.64	1.46
1:A:864:A:O2'	1:A:1078:U:C5	1.67	1.46
1:A:519:C:H5'	22:V:66:ARG:NH2	1.22	1.45
1:A:7:A:C8	5:E:124:LEU:HD13	1.51	1.45
5:E:161:VAL:HB	8:H:114:ARG:NH1	1.27	1.45
1:A:18:C:H2'	1:A:1078:U:C2	1.51	1.44
1:A:864:A:C2'	1:A:1078:U:H5	1.31	1.44
5:E:153:VAL:CG1	8:H:99:LEU:HB3	1.47	1.43
1:A:925:G:C6	1:A:927:G:C6	2.06	1.43
24:Y:49:ALA:HB1	26:X:19:G:N1	1.28	1.43
25:Z:179:LYS:CB	26:X:68:C:O2	1.67	1.43
1:A:358:U:H5''	23:W:607:ARG:NH1	1.13	1.43
1:A:1390:U:C2	1:A:1391:U:C4	2.06	1.42
24:Y:72:LYS:CE	26:X:17(A):U:H1'	1.49	1.42
24:Y:77:ARG:NH1	26:X:16:C:H41	0.95	1.41
1:A:1110:A:N3	2:B:136:MET:HG3	1.11	1.41
1:A:519:C:C5'	22:V:66:ARG:NH2	1.81	1.40
25:Z:94:LYS:CD	26:X:24:U:O2'	1.68	1.40
1:A:918:A:C2	1:A:1079:G:N1	1.87	1.40
25:Z:125:LYS:NZ	26:X:26:G:H4'	1.08	1.39
1:A:701:U:C3'	24:Y:64:LYS:H	1.35	1.38
24:Y:77:ARG:NH1	26:X:16:C:N4	1.69	1.38
1:A:1078:U:O2'	5:E:135:ASN:ND2	1.56	1.38
24:Y:49:ALA:HB2	26:X:19:G:O6	1.23	1.37
25:Z:92:GLN:HG2	26:X:12:G:N2	1.33	1.37
5:E:157:ARG:HG2	8:H:45:PHE:CZ	1.60	1.36
1:A:1493:A:C2'	22:V:21:THR:N	1.75	1.36
1:A:16:A:N3	1:A:1080:A:H2'	1.40	1.36
25:Z:179:LYS:HD3	26:X:5:G:N2	1.40	1.36

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:Z:90:VAL:N	26:X:22:G:N1	1.67	1.36
5:E:153:VAL:CG1	8:H:99:LEU:CB	2.03	1.36
1:A:358:U:O3'	23:W:579:GLY:CA	1.71	1.35
1:A:16:A:C4	1:A:1080:A:O2'	1.75	1.35
1:A:530:G:H1'	22:V:39:LYS:CD	1.54	1.35
1:A:395:C:C4'	23:W:647:GLU:OE2	1.75	1.34
5:E:156:LYS:CD	8:H:130:ALA:OXT	1.76	1.34
1:A:919:A:C2	1:A:1080:A:N1	1.95	1.34
1:A:530:G:H1'	22:V:39:LYS:CE	1.56	1.34
1:A:358:U:C5'	23:W:607:ARG:NH1	1.90	1.34
1:A:1494:G:C8	22:V:18:PRO:CA	2.10	1.33
5:E:156:LYS:HD2	8:H:130:ALA:OXT	1.24	1.33
1:A:18:C:C6	1:A:1079:G:H1'	1.09	1.33
1:A:925:G:C6	1:A:927:G:C5	2.16	1.33
25:Z:90:VAL:N	26:X:22:G:H1	0.85	1.33
1:A:6:G:C6	5:E:99:ALA:HB1	1.64	1.32
1:A:701:U:H3'	24:Y:64:LYS:N	1.01	1.32
26:X:71:C:C2'	26:X:72:A:H8	1.40	1.32
23:W:812:ILE:HG12	26:X:76:A:C1'	1.59	1.32
1:A:1494:G:N7	22:V:18:PRO:CB	1.91	1.32
1:A:919:A:N3	1:A:1080:A:N1	1.78	1.32
1:A:18:C:C6	1:A:1079:G:C1'	1.93	1.31
12:L:104:CYS:O	23:W:662:ARG:NH1	1.62	1.31
25:Z:91:ILE:HD13	26:X:13:C:O4'	1.26	1.31
1:A:1112:C:P	2:B:131:LYS:CB	2.17	1.31
5:E:157:ARG:CG	8:H:45:PHE:CE2	2.14	1.31
1:A:1494:G:H8	22:V:18:PRO:CA	1.41	1.30
1:A:7:A:C2'	5:E:106:ILE:HD11	1.59	1.30
1:A:1494:G:N7	22:V:18:PRO:HB3	0.99	1.30
1:A:1390:U:C2	1:A:1391:U:N3	1.99	1.30
1:A:1493:A:C2'	22:V:21:THR:H	1.34	1.30
25:Z:125:LYS:NZ	26:X:26:G:C5'	1.96	1.29
1:A:1493:A:C8	22:V:19:ASN:HB2	1.67	1.29
1:A:925:G:C2'	1:A:927:G:H5''	1.61	1.28
1:A:519:C:C5'	22:V:66:ARG:HH21	1.40	1.28
1:A:16:A:H2'	1:A:1080:A:O2'	1.27	1.28
1:A:1494:G:C8	22:V:18:PRO:CB	2.15	1.28
2:B:129:LEU:CA	3:C:179:ARG:HE	1.46	1.27
1:A:358:U:H4'	23:W:578:ARG:O	1.12	1.27
23:W:814:GLY:HA3	27:X:101:FME:SD	1.73	1.27
1:A:1078:U:C4'	5:E:90:THR:OG1	1.82	1.27

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:7:A:C8	5:E:124:LEU:CD1	2.17	1.27
25:Z:90:VAL:HG13	26:X:22:G:O6	1.19	1.26
1:A:1105:A:OP1	2:B:144:LEU:CD2	1.83	1.26
25:Z:91:ILE:CD1	26:X:12:G:H2'	1.63	1.26
1:A:1492:A:C2	22:V:35:TYR:CB	2.18	1.26
1:A:16:A:N3	1:A:1080:A:C2'	1.96	1.26
25:Z:125:LYS:HZ2	26:X:26:G:C4'	1.33	1.26
1:A:1495:U:O2'	25:Z:101:GLY:HA3	1.31	1.26
1:A:358:U:O3'	23:W:579:GLY:HA3	1.26	1.26
25:Z:176:PRO:HG2	26:X:12:G:O3'	1.12	1.25
1:A:1494:G:C8	22:V:18:PRO:N	2.03	1.25
1:A:1494:G:C8	22:V:18:PRO:HB3	1.69	1.25
24:Y:72:LYS:HD2	26:X:17(A):U:N1	1.50	1.25
12:L:75:GLN:HE21	23:W:669:GLN:CD	1.19	1.25
2:B:129:LEU:HA	3:C:179:ARG:NE	1.50	1.25
1:A:918:A:C2	1:A:1079:G:C2	2.24	1.24
1:A:18:C:H6	1:A:1079:G:C1'	1.38	1.24
1:A:864:A:O2'	1:A:1078:U:H5	1.03	1.24
25:Z:176:PRO:CG	26:X:12:G:O3'	1.85	1.24
25:Z:94:LYS:HD3	26:X:24:U:O2'	1.08	1.24
1:A:917:G:N2	1:A:1078:U:O4	1.71	1.24
12:L:51:LYS:HE3	22:V:60:TYR:CD2	1.72	1.23
23:W:791:LYS:O	23:W:880:PHE:CE1	1.92	1.23
1:A:358:U:H4'	23:W:578:ARG:C	1.58	1.23
25:Z:179:LYS:HB3	26:X:68:C:O2	1.09	1.23
1:A:16:A:C2'	1:A:1080:A:O2'	1.86	1.23
1:A:920:U:C1'	1:A:1081:A:O2'	1.86	1.23
23:W:846:ARG:HB3	26:X:76:A:C2	1.74	1.22
5:E:159:LYS:CE	8:H:43:GLU:OE1	1.73	1.22
1:A:560:A:O2'	5:E:128:TYR:HB3	1.37	1.22
25:Z:90:VAL:CG1	26:X:22:G:O6	1.85	1.22
1:A:921:U:H5'	1:A:1082:A:OP1	1.36	1.22
1:A:864:A:H1'	1:A:1078:U:C4	1.75	1.21
22:V:49:PRO:CD	25:Z:131:ARG:NH1	2.03	1.21
1:A:17:U:H2'	1:A:1079:G:C2'	1.53	1.21
12:L:102:LEU:O	23:W:662:ARG:CD	1.87	1.21
1:A:1390:U:O2	1:A:1391:U:C2	1.94	1.21
1:A:1110:A:C2	2:B:136:MET:CG	2.24	1.21
1:A:1105:A:OP1	2:B:144:LEU:HD21	1.05	1.20
1:A:925:G:O6	1:A:927:G:O6	1.57	1.20
1:A:7:A:H8	5:E:124:LEU:CD1	1.54	1.20

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:W:531:VAL:HG11	23:W:544:LEU:HB2	1.20	1.20
1:A:18:C:O2'	1:A:1078:U:C6	1.94	1.20
1:A:701:U:C3'	24:Y:64:LYS:N	1.97	1.19
12:L:105:SER:CB	23:W:666:LEU:HD22	1.73	1.19
25:Z:91:ILE:CD1	26:X:13:C:O4'	1.90	1.19
1:A:567:G:H4'	5:E:93:ARG:NH1	1.56	1.19
1:A:921:U:C5'	1:A:1082:A:OP1	1.91	1.19
1:A:925:G:O6	1:A:927:G:C6	1.96	1.19
5:E:163:GLU:HB3	8:H:114:ARG:CZ	1.51	1.18
1:A:1096:C:H4'	2:B:139:ARG:HH21	1.05	1.18
1:A:920:U:O2'	1:A:1081:A:O3'	1.59	1.18
1:A:1112:C:H5''	2:B:131:LYS:HG2	1.22	1.18
5:E:153:VAL:HG11	8:H:99:LEU:CB	1.67	1.18
23:W:804:PHE:HB2	23:W:812:ILE:CG2	1.73	1.18
23:W:814:GLY:CA	27:X:101:FME:SD	2.32	1.18
1:A:1110:A:N3	2:B:136:MET:CG	2.06	1.17
1:A:18:C:C2'	1:A:1078:U:C2	2.27	1.17
1:A:793:U:O4	25:Z:109:VAL:HG11	1.43	1.17
12:L:75:GLN:CD	23:W:669:GLN:CG	2.05	1.17
22:V:48:LEU:HA	25:Z:131:ARG:HH12	1.01	1.17
1:A:530:G:C1'	22:V:39:LYS:HE2	1.74	1.17
1:A:1111:A:O3'	2:B:131:LYS:CB	1.92	1.16
5:E:153:VAL:HG13	8:H:99:LEU:CB	1.71	1.16
24:Y:72:LYS:CE	26:X:17(A):U:C1'	2.23	1.16
25:Z:176:PRO:CG	26:X:12:G:H4'	1.74	1.16
2:B:128:LYS:CB	3:C:207:ILE:HD12	1.74	1.16
26:X:8:4SU:S4	26:X:14:A:N7	2.19	1.16
25:Z:91:ILE:HD12	26:X:12:G:C2'	1.74	1.16
1:A:1492:A:H2'	22:V:19:ASN:O	1.44	1.16
12:L:105:SER:CB	23:W:666:LEU:CD2	2.21	1.16
25:Z:92:GLN:CG	26:X:12:G:N2	2.06	1.16
24:Y:72:LYS:HE2	26:X:17(A):U:C1'	1.77	1.16
25:Z:179:LYS:CD	26:X:5:G:H21	1.58	1.16
1:A:1106:G:OP1	2:B:113:ARG:NH2	1.80	1.15
1:A:864:A:H4'	1:A:1078:U:H6	1.02	1.15
1:A:1390:U:C2	1:A:1391:U:C2	2.33	1.15
5:E:159:LYS:HD2	8:H:43:GLU:HA	1.29	1.15
1:A:6:G:H2'	5:E:124:LEU:CD2	1.75	1.15
1:A:926:G:C8	1:A:927:G:OP1	2.00	1.14
1:A:1096:C:H4'	2:B:139:ARG:NH2	1.61	1.14
5:E:157:ARG:HD3	8:H:45:PHE:HE2	1.10	1.14

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:6:G:C1'	5:E:124:LEU:HD11	1.76	1.14
25:Z:125:LYS:HZ2	26:X:26:G:C5'	1.57	1.14
1:A:790:A:OP2	26:X:39:C:H4'	1.47	1.14
12:L:104:CYS:N	23:W:662:ARG:HH22	1.45	1.13
1:A:519:C:O2	22:V:2:LYS:HE2	1.48	1.13
1:A:918:A:C2	1:A:1079:G:N2	2.16	1.13
25:Z:176:PRO:CG	26:X:12:G:C3'	2.25	1.13
1:A:920:U:O3'	1:A:1082:A:C5'	1.96	1.13
5:E:159:LYS:HE3	8:H:43:GLU:OE1	1.41	1.13
25:Z:92:GLN:CG	26:X:12:G:H22	1.56	1.12
12:L:105:SER:HB3	23:W:666:LEU:HD21	1.32	1.12
24:Y:49:ALA:CB	26:X:19:G:O6	1.85	1.12
1:A:6:G:H2'	5:E:124:LEU:HD21	1.25	1.12
1:A:357:G:O3'	23:W:607:ARG:NE	1.81	1.12
1:A:8:A:H1'	5:E:108:GLY:HA2	1.26	1.12
23:W:812:ILE:HG12	26:X:76:A:N9	1.63	1.11
24:Y:72:LYS:NZ	26:X:17(A):U:H1'	1.65	1.11
24:Y:77:ARG:NH2	26:X:16:C:H5	1.21	1.11
25:Z:90:VAL:HG22	26:X:22:G:C6	1.84	1.11
1:A:864:A:C4'	1:A:1078:U:C6	2.33	1.11
24:Y:72:LYS:HD2	26:X:17(A):U:C6	1.86	1.11
24:Y:77:ARG:CZ	26:X:16:C:C5	2.32	1.11
1:A:701:U:O2'	24:Y:62:TYR:N	1.81	1.11
1:A:1390:U:N1	1:A:1391:U:C5	1.79	1.11
1:A:1111:A:OP2	2:B:132:LYS:NZ	1.83	1.11
1:A:1495:U:O2'	25:Z:101:GLY:CA	1.97	1.10
22:V:49:PRO:HD2	25:Z:131:ARG:HH11	1.16	1.10
1:A:1110:A:H2	2:B:136:MET:CB	1.64	1.10
1:A:793:U:C4	25:Z:109:VAL:HG11	1.86	1.10
1:A:702:A:C5'	24:Y:64:LYS:HD3	1.80	1.10
1:A:917:G:H1	1:A:1079:G:N2	1.50	1.10
1:A:918:A:C2	1:A:1080:A:N1	2.20	1.10
23:W:791:LYS:HB3	23:W:792:GLN:O	1.34	1.10
24:Y:49:ALA:HB1	26:X:19:G:C6	1.69	1.10
1:A:357:G:O3'	23:W:607:ARG:CD	2.00	1.10
25:Z:121:GLY:HA3	26:X:13:C:H4'	1.33	1.10
1:A:18:C:H2'	1:A:1078:U:N3	1.66	1.09
1:A:6:G:C5	5:E:99:ALA:HA	1.87	1.09
23:W:540:GLY:HA2	23:W:541:ILE:HG22	1.25	1.09
26:X:21:A:N6	26:X:48:C:OP1	1.84	1.09
25:Z:90:VAL:HB	26:X:12:G:O6	1.51	1.09

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1110:A:H3'	2:B:132:LYS:HZ1	1.17	1.09
1:A:864:A:H4'	1:A:1078:U:C6	1.87	1.09
1:A:6:G:N7	5:E:99:ALA:HA	1.67	1.08
1:A:1493:A:H8	22:V:19:ASN:CB	1.67	1.08
1:A:1096:C:C4'	2:B:139:ARG:HH21	1.66	1.08
24:Y:72:LYS:HE2	26:X:17(A):U:H1'	1.09	1.08
1:A:925:G:C5	1:A:927:G:N7	2.21	1.08
1:A:919:A:N3	1:A:1080:A:C6	2.21	1.08
25:Z:180:GLN:OXT	26:X:67:C:H2'	1.54	1.08
1:A:16:A:N9	1:A:1080:A:O2'	1.87	1.08
1:A:920:U:O3'	1:A:1082:A:H5''	1.54	1.08
1:A:1494:G:H8	22:V:18:PRO:HA	1.18	1.08
12:L:102:LEU:O	23:W:662:ARG:HD2	0.92	1.07
1:A:790:A:OP2	26:X:39:C:C4'	2.01	1.07
22:V:49:PRO:HD3	25:Z:131:ARG:NH1	1.66	1.07
1:A:1111:A:H1'	2:B:133:GLU:N	1.47	1.07
1:A:6:G:C2'	5:E:124:LEU:HD11	1.85	1.07
22:V:49:PRO:HD2	25:Z:131:ARG:NH1	1.65	1.07
1:A:357:G:C4'	23:W:607:ARG:HD2	1.82	1.07
1:A:1078:U:C5'	5:E:90:THR:OG1	2.03	1.06
25:Z:176:PRO:CD	26:X:12:G:C4'	2.07	1.06
1:A:16:A:C2	1:A:1080:A:H2'	1.88	1.06
23:W:534:SER:CB	23:W:537:ALA:HB3	1.84	1.06
23:W:812:ILE:HG12	26:X:76:A:H1'	1.38	1.06
22:V:49:PRO:CD	25:Z:131:ARG:HH11	1.66	1.06
1:A:17:U:C3'	1:A:1079:G:C2'	2.20	1.06
1:A:530:G:H1'	22:V:39:LYS:HE2	1.28	1.06
1:A:923:A:OP1	5:E:26:LYS:HE2	1.56	1.06
23:W:804:PHE:HB2	23:W:812:ILE:HG23	1.37	1.06
1:A:17:U:O2'	1:A:1079:G:H2'	1.54	1.06
1:A:1390:U:C2	1:A:1391:U:C5	2.36	1.06
2:B:129:LEU:CA	3:C:179:ARG:NE	2.14	1.05
1:A:864:A:C2'	1:A:1078:U:C5	2.15	1.05
1:A:1106:G:OP1	2:B:113:ARG:NE	1.87	1.05
1:A:7:A:C8	5:E:124:LEU:HB3	1.92	1.05
1:A:7:A:H3'	5:E:106:ILE:HD13	1.06	1.05
26:X:71:C:C2'	26:X:72:A:C8	2.22	1.05
25:Z:176:PRO:CG	26:X:12:G:C4'	2.34	1.05
1:A:920:U:H1'	1:A:1081:A:O2'	1.55	1.05
12:L:105:SER:HB3	23:W:666:LEU:HD22	1.13	1.05
1:A:1493:A:C1'	22:V:21:THR:N	2.07	1.05

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:702:A:C8	24:Y:64:LYS:CG	2.40	1.05
23:W:789:GLU:C	23:W:792:GLN:NE2	2.10	1.05
1:A:530:G:H1'	22:V:39:LYS:HD3	1.36	1.04
1:A:567:G:H4'	5:E:93:ARG:HH12	0.90	1.04
1:A:6:G:C6	5:E:99:ALA:CB	2.21	1.04
24:Y:77:ARG:CZ	26:X:16:C:H41	1.70	1.04
1:A:864:A:C4'	1:A:1078:U:H6	1.69	1.04
1:A:701:U:O2'	24:Y:61:ASP:C	1.96	1.04
1:A:7:A:O2'	5:E:125:ALA:N	1.87	1.04
1:A:567:G:C4'	5:E:93:ARG:HH12	1.70	1.04
25:Z:179:LYS:HD2	26:X:6:G:H1'	1.33	1.04
2:B:129:LEU:C	3:C:179:ARG:HE	1.59	1.04
2:B:128:LYS:HB2	3:C:207:ILE:HD12	1.40	1.04
23:W:591:LEU:HD12	23:W:620:ALA:HB3	1.36	1.04
1:A:925:G:O3'	1:A:927:G:C5'	2.04	1.04
25:Z:179:LYS:CD	26:X:6:G:H1'	1.88	1.04
5:E:148:ASN:ND2	8:H:96:MET:HE1	1.40	1.04
12:L:75:GLN:NE2	23:W:669:GLN:CB	2.19	1.04
1:A:1390:U:C5	1:A:1391:U:C5	2.42	1.03
1:A:1493:A:H2'	22:V:21:THR:H	0.87	1.03
1:A:6:G:C5	5:E:99:ALA:HB1	1.93	1.03
1:A:925:G:C2	1:A:927:G:C4	2.45	1.03
1:A:7:A:H3'	5:E:106:ILE:HD12	1.40	1.03
1:A:559:A:OP2	5:E:126:LYS:NZ	1.92	1.03
5:E:159:LYS:NZ	8:H:43:GLU:OE1	1.91	1.03
1:A:918:A:N1	1:A:1080:A:C2	2.27	1.03
2:B:129:LEU:O	3:C:179:ARG:NH2	1.92	1.03
1:A:918:A:N1	1:A:1080:A:N1	2.06	1.02
1:A:358:U:C4'	23:W:578:ARG:O	2.05	1.02
1:A:702:A:OP2	24:Y:61:ASP:CB	2.03	1.02
23:W:540:GLY:HA2	23:W:541:ILE:CG2	1.88	1.02
25:Z:93:VAL:N	26:X:25:C:C6	2.14	1.02
1:A:1492:A:N3	22:V:35:TYR:CB	2.21	1.02
1:A:1112:C:OP1	2:B:131:LYS:HB2	1.57	1.02
12:L:39:THR:OG1	22:V:61:ASP:CB	2.07	1.02
12:L:41:THR:HG23	22:V:64:ARG:NH1	1.75	1.02
12:L:104:CYS:C	23:W:662:ARG:HH12	1.61	1.02
1:A:7:A:C8	5:E:124:LEU:CB	2.43	1.01
1:A:6:G:C5	5:E:99:ALA:CB	2.42	1.01
1:A:925:G:C3'	1:A:927:G:H5''	1.88	1.01
1:A:701:U:H5'	24:Y:63:GLY:HA3	1.40	1.01

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:918:A:N1	1:A:1079:G:N2	2.08	1.01
1:A:1078:U:H4'	5:E:90:THR:OG1	1.23	1.01
1:A:6:G:C5	5:E:99:ALA:CA	2.39	1.01
1:A:357:G:H4'	23:W:607:ARG:HD2	1.01	1.01
1:A:1112:C:OP1	2:B:131:LYS:CB	2.08	1.01
5:E:163:GLU:CB	8:H:114:ARG:CZ	2.32	1.00
1:A:358:U:O3'	23:W:579:GLY:HA2	1.55	1.00
1:A:1111:A:O3'	2:B:131:LYS:HB2	1.53	1.00
5:E:148:ASN:ND2	8:H:96:MET:HE2	1.67	1.00
1:A:790:A:OP2	26:X:39:C:C5'	2.09	1.00
5:E:153:VAL:HG11	8:H:99:LEU:HB2	1.43	1.00
2:B:129:LEU:O	3:C:179:ARG:CZ	2.09	1.00
25:Z:94:LYS:HZ2	26:X:24:U:H1'	1.25	1.00
23:W:848:PHE:H	27:X:101:FME:CN	1.73	1.00
24:Y:77:ARG:HH11	26:X:16:C:H41	1.06	1.00
1:A:1390:U:C6	1:A:1391:U:C4	2.50	1.00
1:A:702:A:C8	24:Y:64:LYS:HG3	1.96	1.00
1:A:918:A:H2	1:A:1079:G:N1	1.36	1.00
5:E:157:ARG:HB3	8:H:43:GLU:HB3	1.38	1.00
1:A:1492:A:N3	22:V:35:TYR:HB2	1.76	1.00
3:C:168:TYR:CE1	5:E:55:GLU:CD	2.34	0.99
1:A:395:C:H4'	23:W:647:GLU:OE2	0.83	0.99
2:B:128:LYS:HB3	3:C:207:ILE:HD12	1.40	0.99
5:E:161:VAL:CB	8:H:114:ARG:NH1	2.24	0.99
5:E:161:VAL:HB	8:H:114:ARG:HH12	1.25	0.99
1:A:16:A:N3	1:A:1080:A:O2'	1.88	0.99
1:A:925:G:N1	1:A:927:G:C5	2.30	0.99
5:E:148:ASN:ND2	8:H:96:MET:CE	0.84	0.99
5:E:157:ARG:CD	8:H:45:PHE:HE2	1.75	0.99
22:V:14:THR:HB	22:V:23:ARG:HB3	1.40	0.99
24:Y:49:ALA:CB	26:X:19:G:N1	2.11	0.99
1:A:1096:C:C5'	2:B:139:ARG:HH21	1.75	0.99
1:A:1112:C:H5''	2:B:131:LYS:CG	1.81	0.99
1:A:359:G:H5'	23:W:579:GLY:HA2	1.38	0.99
2:B:105:LYS:HE2	5:E:66:LYS:HD3	1.45	0.99
1:A:18:C:O2'	1:A:1078:U:N1	1.94	0.98
26:X:22:G:C4	26:X:23:C:C5	2.51	0.98
1:A:6:G:N9	5:E:124:LEU:HD11	1.76	0.98
1:A:530:G:C1'	22:V:39:LYS:CE	2.23	0.98
5:E:82:GLN:O	8:H:97:ALA:HB2	1.64	0.98
24:Y:77:ARG:NH1	26:X:16:C:C4	2.32	0.98

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:Z:176:PRO:HG2	26:X:12:G:C4'	1.92	0.98
1:A:702:A:H8	24:Y:64:LYS:CG	1.77	0.97
1:A:6:G:C2'	5:E:124:LEU:CD1	2.42	0.97
5:E:157:ARG:CG	8:H:45:PHE:CZ	2.36	0.97
1:A:925:G:C5	1:A:927:G:C5	2.51	0.97
1:A:702:A:H8	24:Y:64:LYS:CD	1.76	0.97
1:A:925:G:C2'	1:A:927:G:C5'	2.42	0.97
1:A:6:G:N1	5:E:99:ALA:HB1	1.78	0.97
12:L:104:CYS:N	23:W:662:ARG:NH2	2.10	0.97
1:A:702:A:H8	24:Y:64:LYS:HD2	1.28	0.97
25:Z:176:PRO:HG2	26:X:12:G:C2'	1.93	0.97
1:A:8:A:H1'	5:E:108:GLY:CA	1.83	0.97
5:E:157:ARG:HD3	8:H:45:PHE:CE2	1.99	0.97
5:E:157:ARG:CD	8:H:45:PHE:CE2	2.47	0.96
25:Z:176:PRO:CG	26:X:12:G:O2'	2.13	0.96
2:B:128:LYS:CB	3:C:207:ILE:CD1	2.44	0.96
1:A:357:G:H4'	23:W:607:ARG:CD	1.93	0.96
1:A:16:A:C1'	1:A:1080:A:O2'	2.13	0.96
1:A:1103:C:H5'	2:B:98:GLY:N	1.80	0.96
12:L:103:ASP:C	23:W:662:ARG:NH2	2.18	0.96
2:B:128:LYS:O	3:C:179:ARG:HD3	1.63	0.96
26:X:76:A:O2'	27:X:101:FME:O1	1.82	0.96
23:W:812:ILE:CD1	26:X:76:A:C4	2.48	0.95
1:A:358:U:C5'	23:W:607:ARG:HH11	1.63	0.95
2:B:129:LEU:HA	3:C:179:ARG:CZ	1.96	0.95
1:A:368:U:H5''	23:W:593:LYS:HE3	1.48	0.95
1:A:7:A:H2'	5:E:106:ILE:HD11	1.49	0.95
1:A:530:G:C1'	22:V:39:LYS:CD	2.43	0.95
24:Y:72:LYS:CD	26:X:17(A):U:N1	2.30	0.95
5:E:156:LYS:O	8:H:44:GLY:O	1.84	0.95
1:A:1494:G:O2'	22:V:16:ALA:O	1.69	0.95
25:Z:179:LYS:HD3	26:X:5:G:H21	0.96	0.95
1:A:1111:A:O5'	2:B:132:LYS:HE3	1.67	0.94
12:L:75:GLN:CD	23:W:669:GLN:HG2	1.72	0.94
1:A:1111:A:H2'	2:B:130:THR:C	1.86	0.94
1:A:1103:C:H5'	2:B:98:GLY:H	1.32	0.94
2:B:129:LEU:O	3:C:179:ARG:NE	2.00	0.94
1:A:925:G:C4	1:A:927:G:C8	2.55	0.94
5:E:148:ASN:ND2	8:H:96:MET:HE3	1.29	0.94
1:A:1494:G:C8	22:V:18:PRO:CD	2.49	0.94
1:A:1518:MA6:H103	1:A:1519:MA6:H102	1.50	0.94

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:925:G:N1	1:A:927:G:C6	2.35	0.94
1:A:518:C:O2'	22:V:38:GLY:HA3	1.66	0.94
1:A:701:U:H5'	24:Y:63:GLY:CA	1.97	0.94
12:L:51:LYS:CE	22:V:60:TYR:CD2	2.50	0.94
24:Y:77:ARG:CZ	26:X:16:C:H5	1.77	0.93
1:A:1105:A:H5''	2:B:113:ARG:HG2	1.49	0.93
1:A:1110:A:H3'	2:B:132:LYS:NZ	1.84	0.93
23:W:727:GLY:HA2	23:W:748:VAL:HG23	1.49	0.93
24:Y:49:ALA:HB1	26:X:19:G:H1	1.22	0.93
1:A:530:G:C1'	22:V:39:LYS:HD3	1.99	0.93
1:A:7:A:H8	5:E:124:LEU:HD13	0.76	0.93
24:Y:77:ARG:CZ	26:X:16:C:N4	2.28	0.93
1:A:16:A:H2'	1:A:1080:A:C2'	1.87	0.92
1:A:1110:A:C2	2:B:136:MET:CB	2.52	0.92
3:C:168:TYR:CD1	5:E:55:GLU:OE1	2.23	0.92
1:A:702:A:C8	24:Y:64:LYS:HD2	2.04	0.92
5:E:157:ARG:NH2	8:H:100:GLY:O	2.02	0.92
1:A:359:G:C5'	23:W:579:GLY:HA2	2.00	0.92
25:Z:94:LYS:HZ2	26:X:24:U:C1'	1.82	0.92
12:L:39:THR:OG1	22:V:61:ASP:HB2	1.67	0.92
25:Z:94:LYS:CE	26:X:24:U:O2'	2.17	0.92
1:A:926:G:P	1:A:927:G:C5'	2.57	0.92
1:A:8:A:H5''	5:E:125:ALA:O	1.68	0.92
24:Y:77:ARG:NH1	26:X:16:C:C5	2.38	0.92
1:A:1078:U:H5'	5:E:90:THR:OG1	1.71	0.91
1:A:1073:U:O2'	2:B:105:LYS:HG2	1.70	0.91
1:A:925:G:O2'	1:A:927:G:H5''	1.69	0.91
1:A:1105:A:P	2:B:144:LEU:HD21	2.09	0.91
1:A:359:G:O4'	23:W:576:LYS:O	1.86	0.91
25:Z:179:LYS:HA	26:X:69:C:C1'	2.01	0.91
1:A:6:G:H2'	5:E:124:LEU:CD1	2.01	0.91
1:A:358:U:O2'	23:W:579:GLY:N	2.03	0.91
23:W:812:ILE:HD13	26:X:76:A:C4	2.05	0.91
1:A:519:C:C2	22:V:2:LYS:HE2	2.05	0.91
12:L:105:SER:HA	23:W:662:ARG:NH1	1.86	0.90
1:A:1110:A:H2'	2:B:132:LYS:HE3	1.54	0.90
12:L:75:GLN:NE2	23:W:669:GLN:CG	0.79	0.90
1:A:864:A:O4'	1:A:1078:U:C6	2.24	0.90
1:A:864:A:C1'	1:A:1078:U:C6	2.54	0.90
26:X:22:G:HO2'	26:X:23:C:H6	0.95	0.90
1:A:790:A:OP2	26:X:39:C:H5'	1.69	0.90

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:361:G:OP1	23:W:729:THR:HB	1.71	0.90
1:A:701:U:H3'	24:Y:63:GLY:C	1.87	0.90
12:L:75:GLN:HE21	23:W:669:GLN:CG	0.43	0.90
1:A:919:A:H2	1:A:1080:A:C2	1.60	0.89
23:W:565:ALA:HB2	23:W:590:THR:CG2	2.03	0.89
23:W:812:ILE:HD12	23:W:863:ILE:O	1.72	0.89
25:Z:156:ALA:HB1	25:Z:174:LEU:HD11	1.54	0.89
25:Z:179:LYS:HB3	26:X:68:C:C2	2.07	0.89
22:V:48:LEU:HA	25:Z:131:ARG:NH1	1.86	0.89
11:K:94:GLU:OE2	11:K:98:ARG:NH2	2.06	0.89
1:A:1492:A:H2	22:V:35:TYR:HB3	1.07	0.89
24:Y:72:LYS:HD2	26:X:17(A):U:C2	2.08	0.89
25:Z:93:VAL:O	26:X:24:U:H2'	1.72	0.89
1:A:10:A:OP2	5:E:131:THR:OG1	1.90	0.89
1:A:790:A:H5''	26:X:39:C:H5'	1.52	0.89
23:W:531:VAL:HG21	23:W:544:LEU:HA	1.54	0.89
25:Z:180:GLN:NE2	26:X:69:C:OP2	2.05	0.89
22:V:48:LEU:CA	25:Z:131:ARG:HH12	1.84	0.88
1:A:925:G:O3'	1:A:927:G:H5''	1.69	0.88
1:A:927:G:N1	1:A:1391:U:O2	2.05	0.88
23:W:812:ILE:HG21	26:X:76:A:O4'	1.73	0.88
1:A:1493:A:H8	22:V:19:ASN:HB2	0.77	0.88
22:V:45:ILE:HD13	22:V:70:ARG:HD3	1.55	0.88
25:Z:90:VAL:HG22	26:X:22:G:N1	1.87	0.88
1:A:1390:U:C6	1:A:1391:U:H5	1.60	0.88
25:Z:125:LYS:HZ3	26:X:26:G:C5'	1.81	0.88
1:A:1130:A:OP1	9:I:18:ARG:NH1	2.07	0.88
25:Z:94:LYS:NZ	26:X:24:U:O2'	2.07	0.88
1:A:1493:A:N9	22:V:18:PRO:O	2.07	0.88
1:A:357:G:O3'	23:W:607:ARG:CZ	2.22	0.88
1:A:917:G:N1	1:A:1079:G:N2	2.20	0.87
25:Z:179:LYS:C	26:X:68:C:O2	2.12	0.87
1:A:925:G:C3'	1:A:927:G:C5'	2.51	0.87
3:C:168:TYR:CE1	5:E:55:GLU:OE2	2.27	0.87
1:A:519:C:C4'	22:V:66:ARG:NH2	2.37	0.87
1:A:1074:G:O4'	2:B:103:ASN:CG	2.13	0.87
1:A:368:U:H5''	23:W:593:LYS:CE	2.05	0.87
26:X:71:C:C4	26:X:72:A:C5	2.63	0.87
2:B:128:LYS:HB2	3:C:207:ILE:CD1	2.02	0.87
11:K:13:ARG:NH2	11:K:77:TYR:OH	2.07	0.87
12:L:39:THR:OG1	22:V:61:ASP:OD2	1.92	0.87

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:702:A:O5'	24:Y:64:LYS:HD3	1.74	0.87
5:E:156:LYS:NZ	8:H:73:GLU:HB2	1.89	0.86
23:W:540:GLY:HA2	23:W:541:ILE:CB	2.05	0.86
2:B:133:GLU:CB	3:C:179:ARG:HH22	1.88	0.86
3:C:168:TYR:CZ	5:E:55:GLU:OE2	2.28	0.86
25:Z:91:ILE:O	26:X:11:A:N1	2.08	0.86
1:A:8:A:C5'	5:E:125:ALA:O	2.22	0.86
1:A:519:C:C5'	22:V:66:ARG:CZ	2.52	0.86
1:A:927:G:C2	1:A:1391:U:O2	2.29	0.86
12:L:104:CYS:O	23:W:662:ARG:CZ	2.23	0.86
1:A:701:U:C5'	24:Y:63:GLY:HA3	2.05	0.86
1:A:358:U:H5"	23:W:607:ARG:HH12	1.33	0.86
25:Z:179:LYS:HD3	26:X:5:G:C2	2.10	0.86
1:A:1493:A:H2'	22:V:21:THR:N	1.60	0.86
26:X:11:A:N6	26:X:24:U:O4	2.08	0.86
1:A:19:A:C8	1:A:1078:U:N3	2.37	0.85
1:A:1390:U:N3	1:A:1391:U:N3	2.09	0.85
25:Z:125:LYS:NZ	26:X:26:G:O5'	2.09	0.85
3:C:132:ARG:HH12	4:D:47:ARG:NH2	1.73	0.85
22:V:48:LEU:HD23	25:Z:131:ARG:CZ	2.06	0.85
1:A:1111:A:O5'	2:B:132:LYS:CE	2.25	0.85
25:Z:92:GLN:HG2	26:X:12:G:H21	1.34	0.85
23:W:534:SER:OG	23:W:537:ALA:CB	2.25	0.85
24:Y:77:ARG:CZ	26:X:16:C:C4	2.59	0.85
1:A:358:U:H5"	23:W:607:ARG:HH11	1.02	0.85
1:A:920:U:O4'	1:A:1081:A:O2'	1.95	0.85
25:Z:91:ILE:HD11	26:X:13:C:C5'	2.06	0.84
25:Z:94:LYS:NZ	26:X:24:U:C1'	2.39	0.84
1:A:919:A:H1'	1:A:1080:A:H61	1.41	0.84
1:A:1074:G:O4'	2:B:103:ASN:CB	2.25	0.84
23:W:728:ILE:HG13	23:W:748:VAL:HG21	1.56	0.84
24:Y:72:LYS:CD	26:X:17(A):U:C2	2.61	0.84
23:W:789:GLU:CA	23:W:792:GLN:HE21	1.90	0.84
1:A:530:G:C8	22:V:39:LYS:N	2.46	0.84
1:A:918:A:H2	1:A:1079:G:C2	1.74	0.83
1:A:368:U:H3'	23:W:593:LYS:NZ	1.93	0.83
23:W:531:VAL:HG11	23:W:544:LEU:CB	2.06	0.83
2:B:129:LEU:C	3:C:179:ARG:HH21	1.80	0.83
5:E:157:ARG:HH21	8:H:100:GLY:C	1.82	0.83
22:V:17:LEU:HB3	22:V:18:PRO:HD2	1.60	0.83
26:X:71:C:C6	26:X:72:A:N7	2.47	0.83

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:6:G:H2'	5:E:124:LEU:HD11	1.59	0.83
1:A:8:A:C4	5:E:107:ALA:O	2.31	0.83
1:A:920:U:O3'	1:A:1082:A:H5'	1.78	0.83
2:B:133:GLU:HB2	3:C:179:ARG:NH2	1.94	0.83
5:E:156:LYS:CE	8:H:130:ALA:OXT	2.27	0.83
1:A:1111:A:H1'	2:B:133:GLU:H	1.41	0.83
22:V:25:LYS:HA	22:V:31:GLU:HB3	1.61	0.83
5:E:163:GLU:HG3	8:H:98:GLY:O	1.79	0.82
2:B:128:LYS:HB3	3:C:207:ILE:CD1	2.08	0.82
1:A:702:A:OP2	24:Y:61:ASP:HB3	1.77	0.82
1:A:1072:G:OP1	5:E:62:LYS:NZ	2.07	0.82
1:A:518:C:OP2	22:V:39:LYS:HE2	1.78	0.82
25:Z:176:PRO:CB	26:X:12:G:O3'	2.26	0.82
23:W:534:SER:HB3	23:W:537:ALA:HB3	1.61	0.82
12:L:75:GLN:HE21	23:W:669:GLN:CB	1.82	0.82
26:X:22:G:N3	26:X:23:C:C6	2.47	0.82
12:L:56:ARG:NH1	23:W:738:ALA:HB2	1.95	0.82
1:A:920:U:C3'	1:A:1082:A:H5'	2.09	0.82
1:A:925:G:H2'	1:A:927:G:C5'	2.10	0.82
25:Z:94:LYS:NZ	26:X:24:U:H1'	1.95	0.82
26:X:71:C:C2	26:X:72:A:C8	2.67	0.82
12:L:73:ASN:HB3	23:W:670:GLN:HG3	1.62	0.82
23:W:789:GLU:HB2	23:W:792:GLN:NE2	1.93	0.82
24:Y:73:GLU:OE1	26:X:17(A):U:O2	1.98	0.82
1:A:1390:U:C2	1:A:1391:U:C6	2.58	0.81
1:A:1492:A:H2	22:V:35:TYR:CB	1.76	0.81
12:L:104:CYS:C	23:W:662:ARG:HH22	1.83	0.81
5:E:156:LYS:NZ	8:H:130:ALA:OXT	2.13	0.81
23:W:426:GLN:HE22	23:W:770:VAL:HB	1.44	0.81
23:W:790:LEU:N	23:W:792:GLN:NE2	2.28	0.81
23:W:795:ILE:HG22	23:W:879:VAL:HG13	1.61	0.81
1:A:926:G:OP2	1:A:927:G:H5'	1.79	0.81
5:E:153:VAL:HG13	8:H:99:LEU:HB3	0.82	0.81
22:V:15:GLU:HB3	22:V:23:ARG:HB2	1.62	0.81
1:A:359:G:P	23:W:579:GLY:HA2	2.19	0.81
25:Z:92:GLN:HG2	26:X:12:G:H22	1.01	0.81
25:Z:179:LYS:CG	26:X:5:G:H21	1.93	0.81
1:A:1194:U:H5'	5:E:27:GLY:HA2	1.62	0.81
12:L:105:SER:HB3	23:W:666:LEU:HD23	1.59	0.81
1:A:702:A:H5'	24:Y:64:LYS:HD3	1.62	0.81
1:A:1074:G:O4'	2:B:103:ASN:HB2	1.80	0.81

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:358:U:O2'	23:W:577:GLY:C	2.19	0.81
26:X:8:4SU:H6	26:X:21:A:H2	1.45	0.80
1:A:358:U:C4'	23:W:578:ARG:C	2.47	0.80
23:W:812:ILE:HD11	26:X:76:A:N3	1.96	0.80
23:W:795:ILE:CG2	23:W:879:VAL:HG13	2.11	0.80
1:A:1496:C:H5'	25:Z:100:PRO:O	1.82	0.80
22:V:52:ARG:HH11	22:V:52:ARG:HB2	1.44	0.80
25:Z:91:ILE:HD13	26:X:13:C:C1'	2.12	0.80
1:A:927:G:N2	1:A:1391:U:O2	2.15	0.80
1:A:7:A:N9	5:E:124:LEU:HB3	1.97	0.80
12:L:71:GLY:HA2	22:V:60:TYR:OH	1.80	0.80
1:A:357:G:O3'	23:W:607:ARG:HD3	1.79	0.80
23:W:589:GLY:HA3	23:W:622:PRO:N	1.97	0.80
1:A:1111:A:C2'	2:B:130:THR:C	2.50	0.80
22:V:48:LEU:HD23	25:Z:131:ARG:NH2	1.97	0.80
1:A:1110:A:H3'	2:B:132:LYS:CE	2.12	0.79
1:A:926:G:H8	1:A:927:G:OP1	1.60	0.79
26:X:69:C:C2'	26:X:70:G:H5'	2.12	0.79
1:A:865:A:C4'	1:A:1077:G:O2'	2.29	0.79
1:A:368:U:H3'	23:W:593:LYS:HZ1	1.47	0.79
22:V:15:GLU:H	22:V:23:ARG:HB2	1.47	0.79
12:L:104:CYS:CA	23:W:662:ARG:HH22	1.96	0.79
1:A:518:C:O2'	22:V:38:GLY:CA	2.30	0.79
1:A:920:U:O2'	1:A:1081:A:O2'	2.00	0.79
12:L:103:ASP:C	23:W:662:ARG:HH22	1.83	0.79
25:Z:179:LYS:HB2	26:X:68:C:O2	1.79	0.79
1:A:925:G:N1	1:A:927:G:C4	2.50	0.79
2:B:128:LYS:HG2	3:C:207:ILE:HG13	1.64	0.79
12:L:73:ASN:HB3	23:W:670:GLN:CG	2.12	0.79
25:Z:176:PRO:HG3	26:X:12:G:O2'	1.81	0.79
1:A:864:A:O2'	1:A:1078:U:C6	2.35	0.79
4:D:100:ASN:OD1	4:D:111:ARG:NH1	2.16	0.79
1:A:926:G:C8	1:A:927:G:P	2.77	0.78
1:A:1111:A:C1'	2:B:133:GLU:N	2.38	0.78
1:A:358:U:C5'	23:W:607:ARG:CZ	2.62	0.78
1:A:519:C:O2	22:V:2:LYS:CE	2.30	0.78
1:A:127:G:O2'	17:Q:6:ARG:NH1	2.15	0.78
5:E:156:LYS:HZ3	8:H:73:GLU:HB2	1.45	0.78
1:A:7:A:C2'	5:E:124:LEU:HB3	2.14	0.78
1:A:1110:A:H2	2:B:136:MET:CG	1.80	0.78
1:A:926:G:P	1:A:927:G:H5'	2.24	0.78

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:47:SER:OG	22:V:35:TYR:CE1	2.35	0.78
22:V:34:ALA:HA	22:V:65:GLY:O	1.84	0.78
7:G:68:ASN:O	7:G:138:ARG:NH1	2.17	0.77
12:L:51:LYS:HE3	22:V:60:TYR:CG	2.19	0.77
23:W:565:ALA:HB2	23:W:590:THR:HG23	1.66	0.77
1:A:359:G:C5'	23:W:575:ASP:O	2.32	0.77
25:Z:180:GLN:OXT	26:X:67:C:C2'	2.30	0.77
25:Z:91:ILE:HD11	26:X:13:C:O5'	1.83	0.77
23:W:812:ILE:CG1	26:X:76:A:N9	2.46	0.77
5:E:82:GLN:O	8:H:97:ALA:CB	2.31	0.77
25:Z:90:VAL:CG2	26:X:22:G:C6	2.66	0.77
1:A:1105:A:OP1	2:B:144:LEU:CG	2.32	0.77
1:A:18:C:C2'	1:A:1078:U:N1	2.46	0.77
1:A:1110:A:C2'	2:B:132:LYS:HE3	2.15	0.77
1:A:1111:A:P	2:B:132:LYS:NZ	2.57	0.77
1:A:864:A:O4'	1:A:1078:U:C5	2.35	0.77
1:A:1147:C:O2	9:I:18:ARG:NH2	2.18	0.77
23:W:537:ALA:HB3	23:W:539:THR:HG23	1.65	0.77
23:W:789:GLU:CB	23:W:792:GLN:NE2	2.47	0.77
24:Y:72:LYS:NZ	26:X:17(A):U:C1'	2.41	0.77
1:A:920:U:C2'	1:A:1081:A:O2'	2.33	0.77
26:X:71:C:N1	26:X:72:A:C8	2.53	0.77
1:A:1111:A:O3'	2:B:131:LYS:CA	2.33	0.76
1:A:1100:C:N4	2:B:95:ARG:NE	2.34	0.76
1:A:920:U:O2'	1:A:1081:A:C3'	2.33	0.76
1:A:1493:A:N7	22:V:18:PRO:O	2.18	0.76
23:W:613:LEU:HD12	23:W:614:GLY:N	1.99	0.76
26:X:18:G:O2'	26:X:19:G:H5'	1.85	0.76
25:Z:179:LYS:CA	26:X:68:C:O2	2.32	0.76
1:A:919:A:H1'	1:A:1080:A:N6	1.99	0.76
12:L:39:THR:OG1	22:V:61:ASP:CG	2.24	0.76
1:A:357:G:C4'	23:W:607:ARG:CD	2.59	0.76
7:G:111:ARG:NH1	7:G:123:GLU:OE2	2.19	0.76
23:W:791:LYS:O	23:W:880:PHE:CZ	2.39	0.76
23:W:534:SER:OG	23:W:537:ALA:HB3	1.85	0.76
1:A:1134:G:N2	1:A:1140:C:N3	2.34	0.75
23:W:812:ILE:CG1	26:X:76:A:C1'	2.54	0.75
1:A:790:A:C5'	26:X:38:A:O3'	2.33	0.75
1:A:919:A:N1	1:A:1080:A:C2	2.51	0.75
1:A:7:A:C8	5:E:124:LEU:CG	2.70	0.75
1:A:1103:C:C5'	2:B:98:GLY:N	2.49	0.75

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:560:A:H2'	5:E:128:TYR:CD1	2.21	0.75
1:A:920:U:O2'	1:A:1082:A:H5'	1.85	0.75
23:W:791:LYS:CB	23:W:792:GLN:O	2.04	0.75
23:W:814:GLY:HA2	27:X:101:FME:CB	2.16	0.75
23:W:540:GLY:CA	23:W:541:ILE:HG22	2.13	0.75
1:A:530:G:O4'	22:V:39:LYS:HE2	1.85	0.75
26:X:8:4SU:H1'	26:X:21:A:C2	2.22	0.75
1:A:359:G:P	23:W:579:GLY:CA	2.75	0.75
1:A:925:G:C4	1:A:927:G:N7	2.54	0.75
22:V:54:VAL:HB	22:V:69:TYR:HB2	1.69	0.75
2:B:128:LYS:O	3:C:179:ARG:CD	2.35	0.74
1:A:368:U:P	23:W:607:ARG:HA	2.26	0.74
12:L:41:THR:HG23	22:V:64:ARG:HH11	1.52	0.74
25:Z:94:LYS:HA	26:X:25:C:C4'	2.17	0.74
1:A:518:C:OP2	22:V:39:LYS:CE	2.35	0.74
25:Z:92:GLN:NE2	26:X:12:G:H22	1.85	0.74
1:A:1494:G:O2'	22:V:16:ALA:C	2.25	0.74
25:Z:180:GLN:CB	26:X:69:C:OP2	2.27	0.74
1:A:8:A:C5'	5:E:107:ALA:HA	2.15	0.74
1:A:17:U:H2'	1:A:1079:G:H2'	0.76	0.74
3:C:40:ARG:NH1	3:C:55:ILE:O	2.21	0.74
22:V:52:ARG:HB2	22:V:52:ARG:NH1	2.02	0.74
1:A:1493:A:C8	22:V:19:ASN:CB	2.54	0.74
23:W:812:ILE:CG1	26:X:76:A:H1'	2.14	0.74
1:A:8:A:N9	5:E:107:ALA:O	2.14	0.73
24:Y:72:LYS:CD	26:X:17(A):U:C1'	2.65	0.73
1:A:1492:A:N3	22:V:35:TYR:HB3	1.87	0.73
1:A:701:U:H5'	24:Y:63:GLY:C	2.09	0.73
1:A:925:G:H2'	1:A:927:G:O4'	1.89	0.73
25:Z:90:VAL:CB	26:X:12:G:O6	2.34	0.73
25:Z:179:LYS:HA	26:X:69:C:H1'	1.69	0.73
2:B:129:LEU:C	3:C:179:ARG:NE	2.31	0.73
26:X:58:A:O2'	26:X:60:U:H5	1.72	0.73
1:A:519:C:H5'	22:V:66:ARG:HH21	0.60	0.73
26:X:41:C:H3'	26:X:42:G:H5''	1.71	0.73
25:Z:180:GLN:CD	26:X:69:C:OP2	2.27	0.73
22:V:25:LYS:HE3	22:V:29:GLY:O	1.89	0.73
25:Z:94:LYS:CG	26:X:24:U:O2'	2.36	0.73
1:A:6:G:C1'	5:E:124:LEU:CD1	2.61	0.73
1:A:7:A:H2'	5:E:124:LEU:HB3	1.71	0.73
25:Z:90:VAL:CA	26:X:22:G:H1	1.99	0.73

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:702:A:C8	24:Y:64:LYS:CD	2.61	0.72
1:A:1110:A:H2	2:B:136:MET:HB3	1.53	0.72
5:E:156:LYS:HD3	8:H:130:ALA:OXT	1.87	0.72
12:L:105:SER:OG	23:W:666:LEU:HD22	1.86	0.72
26:X:71:C:C5	26:X:72:A:C5	2.77	0.72
1:A:18:C:C6	1:A:1079:G:C2'	2.72	0.72
22:V:48:LEU:CD2	25:Z:131:ARG:CZ	2.68	0.72
26:X:8:4SU:H6	26:X:21:A:C2	2.23	0.72
23:W:789:GLU:CA	23:W:792:GLN:NE2	2.52	0.72
26:X:17:C:H2'	26:X:17(A):U:H5	1.55	0.72
1:A:8:A:C1'	5:E:108:GLY:CA	2.59	0.71
1:A:1390:U:C2	1:A:1391:U:N1	2.58	0.71
5:E:161:VAL:HB	8:H:114:ARG:HH11	1.50	0.71
1:A:519:C:H4'	22:V:66:ARG:NH2	2.04	0.71
1:A:1070:U:OP1	5:E:25:VAL:HG11	1.91	0.71
12:L:75:GLN:CD	23:W:669:GLN:HG3	1.87	0.71
25:Z:91:ILE:O	26:X:11:A:C6	2.43	0.71
1:A:7:A:N7	5:E:124:LEU:CD1	2.53	0.71
25:Z:94:LYS:CA	26:X:25:C:C4'	2.69	0.71
24:Y:71:LYS:O	24:Y:75:GLU:HG2	1.91	0.71
1:A:1518:MA6:H103	1:A:1519:MA6:C10	2.21	0.71
1:A:920:U:H4'	1:A:1082:A:H5'	1.73	0.71
1:A:396:C:OP1	23:W:648:LYS:HB2	1.90	0.70
23:W:716:VAL:HG21	23:W:786:LEU:HD21	1.73	0.70
23:W:804:PHE:CB	23:W:812:ILE:CG2	2.64	0.70
23:W:812:ILE:HD13	26:X:76:A:C5	2.26	0.70
25:Z:91:ILE:CD1	26:X:13:C:O5'	2.38	0.70
25:Z:179:LYS:CD	26:X:5:G:N2	2.27	0.70
1:A:920:U:C1'	1:A:1081:A:HO2'	1.99	0.70
25:Z:94:LYS:CA	26:X:25:C:H4'	2.21	0.70
1:A:927:G:OP1	1:A:1505:G:N2	2.24	0.70
22:V:15:GLU:H	22:V:23:ARG:CB	2.04	0.70
25:Z:90:VAL:N	26:X:22:G:C2	2.57	0.70
25:Z:92:GLN:O	26:X:11:A:H2	1.73	0.70
1:A:359:G:H5'	23:W:575:ASP:O	1.91	0.70
1:A:6:G:H2'	5:E:124:LEU:CG	2.22	0.70
1:A:790:A:C5'	26:X:39:C:H5'	2.21	0.70
9:I:12:ARG:NH2	9:I:107:ASP:OD2	2.24	0.70
1:A:5:U:O2'	5:E:100:SER:HB3	1.90	0.70
1:A:6:G:C2'	5:E:124:LEU:HD21	2.14	0.70
25:Z:92:GLN:CD	26:X:12:G:H22	1.95	0.70

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:X:58:A:H1'	26:X:60:U:O4	1.92	0.70
1:A:16:A:C2	1:A:1080:A:C2'	2.60	0.70
1:A:1492:A:C2'	22:V:19:ASN:O	2.32	0.70
23:W:848:PHE:H	27:X:101:FME:HCN	1.54	0.70
1:A:1073:U:P	5:E:66:LYS:NZ	2.65	0.70
3:C:168:TYR:CE1	5:E:55:GLU:OE1	2.44	0.70
3:C:132:ARG:NH1	4:D:47:ARG:NH2	2.39	0.70
25:Z:91:ILE:HD12	26:X:12:G:H2'	0.78	0.70
5:E:83:HIS:CG	8:H:96:MET:HA	2.27	0.69
23:W:812:ILE:CD1	26:X:76:A:N3	2.55	0.69
22:V:45:ILE:CD1	22:V:70:ARG:HD3	2.22	0.69
1:A:17:U:HO2'	1:A:1080:A:P	2.15	0.69
22:V:52:ARG:CB	22:V:52:ARG:HH11	2.05	0.69
1:A:845:A:O3'	18:R:48:ARG:NH2	2.25	0.69
23:W:846:ARG:CB	26:X:76:A:C2	2.65	0.69
1:A:921:U:H5'	1:A:1082:A:P	2.31	0.69
23:W:533:VAL:HG12	23:W:541:ILE:H	1.57	0.69
26:X:20:H2U:H4'	26:X:21:A:OP2	1.87	0.69
1:A:8:A:H5'	5:E:107:ALA:HA	1.74	0.69
26:X:70:G:H2'	26:X:71:C:C6	2.27	0.69
1:A:702:A:O4'	24:Y:64:LYS:CD	2.40	0.69
23:W:797:LEU:HD23	23:W:798:ALA:N	2.08	0.69
22:V:48:LEU:CD2	25:Z:131:ARG:NH1	2.56	0.69
1:A:1111:A:O3'	2:B:131:LYS:HB3	1.90	0.69
25:Z:121:GLY:CA	26:X:13:C:H4'	2.18	0.68
21:U:31:GLU:OE2	21:U:34:ARG:NH2	2.25	0.68
26:X:20:H2U:O5'	26:X:21:A:OP2	2.12	0.68
1:A:1494:G:H8	22:V:18:PRO:N	1.63	0.68
24:Y:72:LYS:HD2	26:X:17(A):U:C1'	2.24	0.68
1:A:921:U:P	1:A:1082:A:H5''	2.32	0.68
1:A:1074:G:C1'	2:B:103:ASN:HB2	2.23	0.68
1:A:738:C:OP1	6:F:2:ARG:NH2	2.27	0.68
1:A:1110:A:H2'	2:B:132:LYS:CE	2.23	0.68
1:A:701:U:C4'	24:Y:63:GLY:HA3	2.24	0.68
1:A:357:G:C3'	23:W:607:ARG:CD	2.71	0.68
25:Z:94:LYS:HA	26:X:25:C:C5'	2.23	0.68
1:A:1112:C:OP1	2:B:131:LYS:CG	2.41	0.68
1:A:1111:A:C2'	2:B:131:LYS:N	2.54	0.68
23:W:848:PHE:N	27:X:101:FME:CN	2.55	0.68
1:A:925:G:H2'	1:A:927:G:H5''	1.62	0.67
1:A:980:C:O3'	14:N:13:ARG:NH2	2.27	0.67

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:8:A:C8	5:E:107:ALA:N	2.62	0.67
5:E:163:GLU:HB3	8:H:114:ARG:NH1	2.08	0.67
23:W:426:GLN:HE22	23:W:770:VAL:CB	2.06	0.67
23:W:550:LEU:C	23:W:550:LEU:HD23	2.14	0.67
25:Z:178:LYS:O	26:X:69:C:O4'	2.12	0.67
26:X:22:G:C4	26:X:23:C:C6	2.82	0.67
25:Z:180:GLN:NE2	26:X:69:C:P	2.67	0.67
1:A:412:A:H1'	1:A:413:G:H5'	1.76	0.67
1:A:919:A:H2	1:A:1080:A:N3	1.93	0.67
23:W:790:LEU:HD23	23:W:790:LEU:O	1.94	0.67
23:W:796:GLY:O	23:W:879:VAL:HG12	1.94	0.67
1:A:1110:A:C3'	2:B:132:LYS:CE	2.72	0.67
1:A:18:C:H6	1:A:1079:G:C2'	2.03	0.67
5:E:161:VAL:HB	8:H:114:ARG:CZ	2.18	0.67
5:E:156:LYS:NZ	8:H:130:ALA:C	2.48	0.67
23:W:789:GLU:CB	23:W:792:GLN:HE21	2.06	0.67
23:W:812:ILE:HG12	26:X:76:A:C4	2.30	0.67
24:Y:77:ARG:HH12	26:X:16:C:N4	1.82	0.67
24:Y:21:GLN:H	24:Y:21:GLN:HE21	1.40	0.67
25:Z:94:LYS:HZ1	26:X:24:U:C4'	2.07	0.67
1:A:6:G:C2	5:E:99:ALA:HB1	2.29	0.67
1:A:530:G:C2'	22:V:39:LYS:HD3	2.25	0.67
23:W:396:ILE:CG2	23:W:404:LYS:HG3	2.25	0.67
23:W:396:ILE:HG22	23:W:404:LYS:HG3	1.77	0.67
23:W:789:GLU:C	23:W:792:GLN:HE21	1.92	0.67
1:A:920:U:C4'	1:A:1082:A:H5'	2.25	0.67
23:W:789:GLU:HB2	23:W:792:GLN:HE21	1.60	0.67
1:A:6:G:C2'	5:E:124:LEU:CD2	2.66	0.66
23:W:812:ILE:HD12	23:W:863:ILE:C	2.15	0.66
25:Z:94:LYS:HA	26:X:25:C:H5'	1.77	0.66
1:A:1073:U:C2	2:B:106:THR:HG21	2.30	0.66
1:A:1111:A:P	2:B:132:LYS:HZ2	2.18	0.66
22:V:66:ARG:HB3	22:V:66:ARG:NH1	2.10	0.66
23:W:589:GLY:HA3	23:W:622:PRO:CD	2.25	0.66
23:W:847:ARG:HA	27:X:101:FME:CN	2.26	0.66
1:A:920:U:C4'	1:A:1081:A:O2'	2.44	0.66
2:B:105:LYS:CE	5:E:66:LYS:HD3	2.22	0.66
7:G:138:ARG:NH2	7:G:139:GLU:OE2	2.29	0.66
13:M:4:ILE:O	13:M:6:GLY:N	2.28	0.66
22:V:48:LEU:HD23	25:Z:131:ARG:NH1	2.09	0.66
1:A:1111:A:O3'	2:B:131:LYS:C	2.31	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:Z:123:LYS:HB2	26:X:12:G:C1'	2.26	0.66
25:Z:90:VAL:HG21	26:X:9:G:N7	2.11	0.66
22:V:15:GLU:CB	22:V:23:ARG:HB2	2.25	0.66
1:A:1112:C:OP1	2:B:131:LYS:HG3	1.95	0.66
23:W:540:GLY:CA	23:W:542:ASP:H	2.08	0.66
25:Z:156:ALA:CB	25:Z:174:LEU:HD11	2.26	0.66
13:M:4:ILE:O	13:M:7:ILE:N	2.26	0.66
12:L:105:SER:CA	23:W:662:ARG:HH12	2.08	0.66
3:C:179:ARG:NH1	3:C:206:GLU:OE1	2.29	0.65
12:L:102:LEU:O	23:W:662:ARG:NH2	2.29	0.65
25:Z:91:ILE:HG13	26:X:12:G:H3'	1.78	0.65
1:A:1110:A:C3'	2:B:132:LYS:HE3	2.27	0.65
1:A:368:U:O5'	23:W:607:ARG:HA	1.95	0.65
1:A:793:U:N3	25:Z:109:VAL:HG11	2.11	0.65
1:A:263:A:OP2	20:T:74:ARG:NH1	2.29	0.65
1:A:17:U:O2'	1:A:1079:G:C2'	2.25	0.65
3:C:19:ASN:ND2	14:N:90:ARG:O	2.29	0.65
23:W:393:VAL:HG12	23:W:462:THR:HG22	1.79	0.65
23:W:569:VAL:HG22	23:W:584:VAL:HG22	1.78	0.65
25:Z:91:ILE:CG1	26:X:12:G:H2'	2.27	0.65
26:X:58:A:HO2'	26:X:60:U:H5	1.36	0.65
26:X:69:C:O2'	26:X:70:G:H5'	1.96	0.65
2:B:133:GLU:CB	3:C:179:ARG:NH2	2.53	0.65
2:B:133:GLU:HG3	3:C:179:ARG:NH2	2.11	0.65
1:A:1073:U:O5'	5:E:66:LYS:NZ	2.28	0.65
5:E:158:GLY:HA3	8:H:44:GLY:HA3	1.78	0.65
12:L:75:GLN:NE2	23:W:669:GLN:CD	1.90	0.65
1:A:1494:G:C8	22:V:18:PRO:HA	2.05	0.65
23:W:544:LEU:C	23:W:544:LEU:HD23	2.17	0.65
23:W:565:ALA:HB2	23:W:590:THR:HG22	1.77	0.65
23:W:855:VAL:HG11	23:W:861:CYS:CB	2.27	0.65
9:I:22:LYS:O	9:I:62:ASP:N	2.29	0.65
1:A:8:A:H5'	5:E:125:ALA:O	1.97	0.64
23:W:468:VAL:HB	23:W:498:ASN:HD21	1.63	0.64
1:A:1096:C:C5'	2:B:139:ARG:NH2	2.55	0.64
2:B:133:GLU:CG	3:C:179:ARG:HH22	2.09	0.64
23:W:533:VAL:HG12	23:W:541:ILE:N	2.11	0.64
1:A:358:U:C3'	23:W:579:GLY:CA	2.76	0.64
25:Z:94:LYS:HA	26:X:25:C:H4'	1.79	0.64
25:Z:91:ILE:CD1	26:X:12:G:C2'	2.52	0.64
1:A:368:U:C5'	23:W:593:LYS:CE	2.75	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:530:G:H1'	22:V:39:LYS:CG	2.26	0.64
5:E:79:GLY:O	5:E:121:HIS:N	2.28	0.64
1:A:845:A:O2'	18:R:48:ARG:NH2	2.31	0.64
25:Z:94:LYS:HD3	26:X:24:U:C2'	2.24	0.64
8:H:54:ASP:OD1	8:H:55:THR:N	2.30	0.64
25:Z:90:VAL:CB	26:X:22:G:O6	2.45	0.64
26:X:54:5MU:H72	26:X:55:PSU:O2	1.97	0.64
1:A:701:U:O2	24:Y:44:ASP:OD2	2.16	0.64
1:A:919:A:C4	1:A:1080:A:N1	2.64	0.64
1:A:8:A:C6	4:D:206:LYS:HB3	2.33	0.64
26:X:66:C:H2'	26:X:67:C:C6	2.32	0.64
1:A:6:G:C8	5:E:124:LEU:HD11	2.32	0.64
11:K:119:ASN:OD1	21:U:35:ARG:NH1	2.31	0.64
24:Y:52:ALA:HB2	26:X:19:G:H1	1.62	0.64
26:X:22:G:O2'	26:X:23:C:O5'	2.15	0.64
1:A:702:A:O4'	24:Y:64:LYS:HD3	1.98	0.63
1:A:7:A:O2'	5:E:124:LEU:C	2.35	0.63
1:A:1494:G:C8	22:V:18:PRO:HD3	2.33	0.63
1:A:918:A:C2	1:A:1080:A:C6	2.87	0.63
23:W:848:PHE:N	27:X:101:FME:O1	2.27	0.63
25:Z:176:PRO:HD2	26:X:12:G:H4'	0.63	0.63
26:X:67:C:H2'	26:X:68:C:C6	2.33	0.63
23:W:814:GLY:HA2	27:X:101:FME:HB2	1.79	0.63
1:A:7:A:N7	5:E:124:LEU:HD12	2.14	0.63
12:L:104:CYS:C	23:W:662:ARG:NH2	2.51	0.63
23:W:812:ILE:CG1	26:X:76:A:C4	2.81	0.63
26:X:8:4SU:H5''	26:X:8:4SU:O2	1.98	0.63
25:Z:128:LEU:HD11	25:Z:141:GLY:HA2	1.81	0.63
1:A:919:A:C2	1:A:1080:A:H2	1.99	0.63
1:A:925:G:H2'	1:A:927:G:C8	2.33	0.63
1:A:1096:C:H5''	2:B:139:ARG:HH21	1.62	0.63
19:S:36:ARG:NH2	19:S:75:ALA:O	2.32	0.63
25:Z:92:GLN:HE21	26:X:12:G:H22	1.44	0.63
1:A:1110:A:H2	2:B:136:MET:HB2	1.63	0.63
1:A:1112:C:O5'	2:B:131:LYS:HB2	1.69	0.63
26:X:51:C:H2'	26:X:52:G:C8	2.34	0.63
26:X:71:C:C5	26:X:72:A:N7	2.66	0.63
23:W:716:VAL:CG2	23:W:786:LEU:HD21	2.29	0.63
26:X:22:G:N3	26:X:23:C:C5	2.66	0.63
26:X:41:C:C3'	26:X:42:G:H5''	2.28	0.63
26:X:8:4SU:H1'	26:X:21:A:N1	2.14	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1492:A:H2	22:V:35:TYR:CA	2.11	0.63
26:X:22:G:C5	26:X:23:C:C5	2.86	0.63
1:A:6:G:C4	5:E:99:ALA:HB1	2.33	0.63
23:W:814:GLY:HA2	27:X:101:FME:SD	2.36	0.63
23:W:847:ARG:HA	27:X:101:FME:HCN	1.79	0.63
5:E:157:ARG:HD3	8:H:101:ILE:HG12	1.81	0.62
22:V:5:ASP:O	22:V:59:PRO:HD3	1.99	0.62
1:A:921:U:C4'	1:A:1082:A:OP1	2.47	0.62
22:V:36:ILE:O	22:V:41:ARG:HD2	1.98	0.62
23:W:830:VAL:HG22	23:W:877:ILE:HG12	1.81	0.62
25:Z:125:LYS:HZ3	26:X:26:G:H5'	1.59	0.62
2:B:129:LEU:C	3:C:179:ARG:NH2	2.45	0.62
12:L:41:THR:CG2	22:V:64:ARG:HH11	2.12	0.62
1:A:359:G:C4'	23:W:576:LYS:HA	2.29	0.62
1:A:925:G:C2	1:A:927:G:C5	2.83	0.62
23:W:540:GLY:HA3	23:W:542:ASP:H	1.63	0.62
1:A:17:U:O3'	1:A:1080:A:C5'	2.21	0.62
2:B:128:LYS:HB3	3:C:207:ILE:CG1	2.29	0.62
1:A:1073:U:P	5:E:66:LYS:HZ2	2.23	0.62
23:W:537:ALA:CB	23:W:539:THR:HG23	2.29	0.62
26:X:8:4SU:O2	26:X:8:4SU:H3'	1.99	0.62
25:Z:176:PRO:HD2	26:X:12:G:C5'	2.23	0.62
1:A:702:A:C4'	24:Y:64:LYS:HD3	2.30	0.62
12:L:105:SER:CB	23:W:666:LEU:HD21	2.07	0.62
23:W:483:ILE:HD12	23:W:519:ILE:HG21	1.82	0.62
23:W:534:SER:OG	23:W:537:ALA:HB2	1.99	0.62
1:A:1105:A:H5''	2:B:113:ARG:CG	2.25	0.62
22:V:36:ILE:HG22	22:V:41:ARG:HG3	1.80	0.62
1:A:921:U:H5''	1:A:1082:A:OP1	1.94	0.62
1:A:359:G:H1'	23:W:576:LYS:HG3	1.81	0.62
26:X:71:C:C4	26:X:72:A:C6	2.88	0.62
17:Q:60:GLU:OE1	17:Q:77:ARG:NE	2.33	0.61
22:V:66:ARG:HH11	22:V:66:ARG:HB3	1.65	0.61
26:X:56:C:O2'	26:X:57:A:H5'	2.00	0.61
1:A:7:A:C8	5:E:124:LEU:HD12	2.32	0.61
1:A:918:A:N3	1:A:1079:G:N1	2.19	0.61
1:A:919:A:C2	1:A:1080:A:C6	2.78	0.61
25:Z:91:ILE:CG1	26:X:12:G:C2'	2.77	0.61
25:Z:123:LYS:HB2	26:X:12:G:H1'	1.81	0.61
25:Z:90:VAL:N	26:X:22:G:C6	2.65	0.61
5:E:153:VAL:CG1	8:H:99:LEU:HB2	2.07	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:V:5:ASP:HB2	22:V:59:PRO:HG3	1.82	0.61
23:W:611:ASN:O	23:W:612:GLU:HG2	2.00	0.61
26:X:8:4SU:C6	26:X:21:A:H2	2.13	0.61
1:A:1073:U:O2	2:B:106:THR:HB	2.01	0.61
1:A:1112:C:H6	2:B:130:THR:O	1.81	0.61
1:A:1225:A:H2'	1:A:1226:C:C5	2.35	0.61
1:A:405:U:OP2	4:D:3:ARG:NH1	2.32	0.61
1:A:925:G:O3'	1:A:927:G:O5'	2.14	0.61
1:A:17:U:O3'	1:A:1080:A:H5'	1.68	0.61
1:A:1494:G:C8	22:V:17:LEU:C	2.72	0.61
1:A:411:A:OP2	4:D:26:ARG:NH2	2.33	0.61
11:K:112:ASP:HB3	21:U:2:PRO:HG2	1.83	0.61
13:M:3:ARG:O	13:M:57:ARG:NH2	2.33	0.61
5:E:157:ARG:C	8:H:44:GLY:HA3	2.21	0.61
2:B:120:GLN:O	2:B:125:THR:N	2.34	0.61
12:L:41:THR:CG2	22:V:64:ARG:NH1	2.58	0.61
25:Z:178:LYS:C	26:X:68:C:O2'	2.39	0.61
25:Z:91:ILE:CD1	26:X:13:C:C5'	2.78	0.61
1:A:359:G:H5''	23:W:574:LEU:HD11	1.83	0.61
1:A:358:U:H5'	23:W:607:ARG:NH1	2.07	0.61
1:A:519:C:N3	22:V:2:LYS:HE2	2.14	0.60
1:A:920:U:O2'	1:A:1081:A:C2'	2.47	0.60
1:A:1103:C:O2'	2:B:97:LEU:HD12	2.01	0.60
18:R:37:GLY:O	18:R:63:ARG:NH2	2.34	0.60
1:A:368:U:OP2	23:W:607:ARG:HG2	2.01	0.60
1:A:1111:A:H3'	2:B:132:LYS:HD2	1.82	0.60
1:A:1193:G:O2'	5:E:27:GLY:HA3	2.01	0.60
10:J:63:ASP:HB3	10:J:65:TYR:CE1	2.36	0.60
12:L:103:ASP:C	23:W:662:ARG:HH21	2.02	0.60
26:X:33:U:N3	26:X:36:U:OP2	2.34	0.60
22:V:45:ILE:HG23	22:V:71:LYS:HE3	1.82	0.60
1:A:844:G:H2'	1:A:844:G:N3	2.16	0.60
12:L:110:ARG:NH1	12:L:112:GLN:O	2.34	0.60
16:P:1:MET:N	16:P:1:MET:SD	2.64	0.60
1:A:359:G:C1'	23:W:576:LYS:O	2.48	0.60
1:A:1110:A:C2'	2:B:132:LYS:CE	2.79	0.60
2:B:128:LYS:C	3:C:179:ARG:HD3	2.21	0.60
23:W:531:VAL:CG1	23:W:544:LEU:HB2	2.14	0.60
23:W:814:GLY:C	27:X:101:FME:SD	2.79	0.60
26:X:6:G:O2'	26:X:7:G:H5'	2.02	0.60
1:A:6:G:O2'	5:E:124:LEU:HD13	2.01	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:128:LYS:CG	3:C:207:ILE:HG13	2.31	0.60
9:I:88:MET:SD	9:I:95:ARG:HG2	2.42	0.60
9:I:95:ARG:O	9:I:98:LEU:N	2.35	0.60
1:A:560:A:H2'	5:E:128:TYR:HD1	1.65	0.60
23:W:855:VAL:HG11	23:W:861:CYS:HB3	1.82	0.60
25:Z:91:ILE:HD13	26:X:13:C:C6	2.36	0.60
1:A:1178:G:N2	1:A:1181:G:OP2	2.34	0.60
1:A:17:U:O2'	1:A:1079:G:C3'	2.49	0.60
1:A:10:A:OP2	5:E:131:THR:CB	2.50	0.60
25:Z:178:LYS:O	26:X:68:C:O2'	2.19	0.60
25:Z:90:VAL:HG13	26:X:22:G:C6	2.25	0.60
1:A:19:A:H1'	1:A:1078:U:O4	1.90	0.60
1:A:17:U:O2'	1:A:1080:A:P	2.60	0.60
25:Z:179:LYS:HA	26:X:69:C:O4'	2.02	0.60
7:G:90:GLU:N	7:G:90:GLU:OE2	2.34	0.59
23:W:855:VAL:HG13	23:W:859:MET:CE	2.32	0.59
1:A:359:G:H5'	23:W:579:GLY:CA	2.25	0.59
1:A:530:G:N7	22:V:38:GLY:HA3	2.16	0.59
5:E:159:LYS:HD2	8:H:43:GLU:CA	2.18	0.59
22:V:70:ARG:C	22:V:71:LYS:HD2	2.23	0.59
23:W:797:LEU:HD23	23:W:797:LEU:C	2.23	0.59
22:V:45:ILE:HG12	22:V:70:ARG:HH11	1.68	0.59
23:W:471:ALA:HB3	23:W:505:ALA:HB1	1.84	0.59
26:X:71:C:C2	26:X:72:A:N9	2.70	0.59
1:A:8:A:N6	4:D:202:GLU:O	2.34	0.59
5:E:157:ARG:C	8:H:44:GLY:CA	2.71	0.59
1:A:567:G:C4'	5:E:93:ARG:NH1	2.45	0.59
19:S:29:LYS:HB3	19:S:30:PRO:HD2	1.85	0.59
1:A:703:G:N7	24:Y:61:ASP:OD2	2.35	0.59
2:B:137:ARG:HH22	3:C:206:GLU:CD	2.06	0.59
14:N:31:ILE:HA	14:N:34:VAL:HG23	1.84	0.59
1:A:925:G:N1	1:A:927:G:N1	2.51	0.59
5:E:157:ARG:HB3	8:H:43:GLU:CB	2.24	0.59
5:E:161:VAL:HG12	5:E:162:GLU:H	1.67	0.59
24:Y:73:GLU:OE1	26:X:17(A):U:C2	2.56	0.59
25:Z:91:ILE:O	26:X:24:U:C4	2.56	0.59
1:A:368:U:C5'	23:W:593:LYS:HE2	2.32	0.59
4:D:78:GLU:OE2	4:D:81:ARG:NH2	2.36	0.58
1:A:7:A:H2'	5:E:124:LEU:CB	2.32	0.58
23:W:399:HIS:CB	23:W:402:HIS:HE1	2.17	0.58
23:W:586:VAL:HG23	23:W:622:PRO:HA	1.86	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1496:C:H4'	25:Z:99:ARG:NE	2.18	0.58
5:E:156:LYS:NZ	8:H:73:GLU:CB	2.63	0.58
10:J:48:ARG:NH1	10:J:66:GLU:OE1	2.37	0.58
12:L:39:THR:CG2	22:V:61:ASP:HB2	2.33	0.58
24:Y:21:GLN:H	24:Y:21:GLN:NE2	2.01	0.58
1:A:1228:C:P	13:M:107:ARG:HH22	2.26	0.58
8:H:113:ASP:OD1	8:H:117:ARG:NH2	2.37	0.58
1:A:359:G:H4'	23:W:575:ASP:O	2.04	0.58
1:A:359:G:O4'	23:W:576:LYS:HA	2.03	0.58
1:A:358:U:H5'	23:W:607:ARG:HH11	1.61	0.58
25:Z:90:VAL:CG2	26:X:22:G:O6	2.51	0.58
26:X:73:A:C2	26:X:74:C:N3	2.72	0.58
1:A:1073:U:O3'	2:B:105:LYS:HD3	2.03	0.58
1:A:80:A:C2	1:A:90:C:N3	2.71	0.58
5:E:156:LYS:HZ3	8:H:130:ALA:C	2.06	0.58
23:W:848:PHE:N	27:X:101:FME:HCN	2.18	0.58
1:A:1493:A:C8	22:V:18:PRO:C	2.67	0.58
1:A:1096:C:H5''	2:B:139:ARG:NH2	2.19	0.58
23:W:448:HIS:HD2	23:W:772:TYR:OH	1.85	0.58
25:Z:179:LYS:HB3	26:X:5:G:N2	2.18	0.58
1:A:865:A:H4'	1:A:1077:G:O2'	2.02	0.58
14:N:21:PHE:HA	14:N:25:ALA:HB3	1.85	0.58
22:V:25:LYS:HA	22:V:31:GLU:CB	2.34	0.58
22:V:20:ALA:HB1	22:V:36:ILE:HD12	1.84	0.58
23:W:396:ILE:HG12	23:W:466:VAL:HB	1.86	0.58
26:X:71:C:C2'	26:X:72:A:O5'	2.51	0.58
1:A:395:C:C3'	23:W:647:GLU:OE2	2.51	0.58
26:X:20:H2U:C4'	26:X:21:A:OP2	2.51	0.58
25:Z:180:GLN:HE21	26:X:69:C:P	2.26	0.58
12:L:51:LYS:HE3	22:V:60:TYR:HD2	1.56	0.58
26:X:56:C:H2'	26:X:57:A:C8	2.38	0.57
1:A:16:A:C4	1:A:1080:A:C2'	2.61	0.57
1:A:825:A:O2'	8:H:13:ARG:NH1	2.37	0.57
1:A:1060:U:OP1	14:N:85:ARG:NH2	2.37	0.57
1:A:567:G:C5'	5:E:93:ARG:HH12	2.17	0.57
10:J:57:VAL:HG22	10:J:58:ASN:H	1.70	0.57
23:W:746:PHE:O	23:W:747:ASN:OD1	2.22	0.57
1:A:207:C:N4	1:A:212:G:O6	2.37	0.57
1:A:701:U:HO2'	24:Y:62:TYR:N	1.98	0.57
3:C:135:LYS:HE2	5:E:57:PRO:HG3	1.87	0.57
3:C:132:ARG:HH12	4:D:47:ARG:HH21	1.50	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:104:CYS:O	23:W:662:ARG:NH2	2.37	0.57
2:B:129:LEU:CA	3:C:179:ARG:NH2	2.68	0.57
26:X:17:C:H2'	26:X:17(A):U:C5	2.37	0.57
26:X:19:G:O2'	26:X:20:H2U:OP2	2.17	0.57
25:Z:91:ILE:CD1	26:X:13:C:C4'	2.83	0.57
1:A:1517:G:C5	25:Z:106:ASP:OD1	2.58	0.57
2:B:133:GLU:HG3	3:C:179:ARG:HH22	1.69	0.57
22:V:25:LYS:CA	22:V:31:GLU:HB3	2.31	0.57
23:W:544:LEU:HD23	23:W:544:LEU:O	2.05	0.57
26:X:69:C:H2'	26:X:70:G:H5'	1.84	0.57
1:A:865:A:OP1	1:A:1077:G:C5'	2.53	0.57
5:E:161:VAL:C	8:H:114:ARG:NH2	2.58	0.57
23:W:399:HIS:CD2	23:W:476:MET:CB	2.88	0.57
1:A:18:C:O2	1:A:1078:U:C4	2.58	0.56
5:E:157:ARG:HD2	8:H:43:GLU:HB3	1.85	0.56
12:L:56:ARG:NH1	23:W:738:ALA:CB	2.66	0.56
2:B:129:LEU:CA	3:C:179:ARG:HH21	2.18	0.56
1:A:558:G:H5''	5:E:126:LYS:HE3	1.87	0.56
1:A:261:U:OP2	20:T:74:ARG:NH2	2.38	0.56
25:Z:94:LYS:NZ	26:X:24:U:O4'	2.38	0.56
1:A:1189:U:OP1	14:N:98:LYS:NZ	2.39	0.56
1:A:925:G:C4	1:A:927:G:C5	2.93	0.56
26:X:57:A:O2'	26:X:58:A:O5'	2.20	0.56
1:A:559:A:P	5:E:126:LYS:NZ	2.78	0.56
12:L:103:ASP:CA	23:W:662:ARG:HH21	2.18	0.56
12:L:105:SER:N	23:W:662:ARG:HH12	2.03	0.56
23:W:727:GLY:O	23:W:728:ILE:HG13	2.05	0.56
23:W:791:LYS:O	23:W:880:PHE:CD1	2.54	0.56
1:A:1217:C:P	14:N:9:ARG:HH21	2.29	0.56
1:A:427:U:O2'	1:A:541:G:OP1	2.21	0.56
1:A:925:G:C2	1:A:927:G:N3	2.74	0.56
1:A:1104:G:H4'	2:B:110:SER:CB	2.35	0.56
1:A:7:A:HO2'	5:E:125:ALA:N	2.02	0.56
10:J:7:ARG:HG2	10:J:101:SER:HB2	1.87	0.56
25:Z:178:LYS:C	26:X:68:C:HO2'	2.09	0.56
26:X:71:C:C6	26:X:72:A:C8	2.94	0.56
25:Z:176:PRO:CG	26:X:12:G:C2'	2.66	0.56
23:W:721:ILE:HG22	23:W:735:LEU:HD21	1.86	0.56
23:W:748:VAL:HG22	23:W:749:ARG:N	2.21	0.56
24:Y:72:LYS:CE	26:X:17(A):U:N1	2.60	0.56
1:A:1494:G:N9	22:V:18:PRO:HD3	2.21	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:W:457:ARG:HH12	23:W:637:ALA:HB3	1.71	0.56
23:W:589:GLY:HA3	23:W:622:PRO:HD3	1.86	0.56
2:B:27:MET:HE1	2:B:187:VAL:HG12	1.88	0.56
1:A:1100:C:H41	2:B:95:ARG:NE	2.02	0.56
3:C:126:ARG:O	3:C:127:ARG:HB2	2.05	0.56
26:X:23:C:O2'	26:X:24:U:O5'	2.24	0.56
8:H:48:ASP:OD1	8:H:49:PHE:N	2.38	0.55
1:A:1135:U:N3	1:A:1137:C:O2	2.39	0.55
1:A:203:G:N2	1:A:204:G:O6	2.39	0.55
9:I:84:THR:HG21	9:I:103:PHE:HB3	1.87	0.55
23:W:399:HIS:HB3	23:W:402:HIS:CE1	2.41	0.55
25:Z:179:LYS:CE	26:X:6:G:H1'	2.36	0.55
22:V:40:MET:HE2	22:V:47:ILE:HD11	1.88	0.55
25:Z:91:ILE:O	26:X:24:U:O4	2.23	0.55
25:Z:93:VAL:O	26:X:24:U:C2'	2.50	0.55
1:A:925:G:C3'	1:A:927:G:H5'	2.36	0.55
1:A:925:G:H2'	1:A:927:G:H8	1.71	0.55
11:K:16:VAL:HG23	11:K:17:SER:H	1.72	0.55
22:V:40:MET:HE3	22:V:70:ARG:HB3	1.88	0.55
1:A:357:G:C3'	23:W:607:ARG:HD2	2.33	0.55
23:W:694:LYS:HG2	23:W:724:GLY:HA3	1.88	0.55
1:A:519:C:H4'	22:V:66:ARG:CZ	2.36	0.55
3:C:7:PRO:HG2	3:C:184:TYR:CG	2.42	0.55
1:A:358:U:C3'	23:W:579:GLY:HA3	2.31	0.55
1:A:1226:C:N4	13:M:103:LYS:HE3	2.22	0.55
1:A:407:U:OP1	4:D:3:ARG:NH2	2.40	0.55
12:L:104:CYS:C	23:W:662:ARG:NH1	2.36	0.55
1:A:1111:A:C1'	2:B:133:GLU:H	2.12	0.55
1:A:1110:A:C2	2:B:136:MET:HB3	2.33	0.55
10:J:40:ILE:CG1	10:J:73:LEU:HB3	2.37	0.55
13:M:6:GLY:CA	13:M:66:GLU:HG3	2.37	0.55
1:A:18:C:HO2'	1:A:1078:U:N1	1.45	0.55
2:B:105:LYS:HB3	5:E:69:ARG:CZ	2.36	0.55
22:V:58:THR:CG2	22:V:60:TYR:HB2	2.37	0.55
23:W:467:LEU:HB2	23:W:495:VAL:HG12	1.88	0.55
1:A:1495:U:HO2'	25:Z:101:GLY:CA	2.18	0.55
1:A:1074:G:H5'	2:B:103:ASN:HA	1.88	0.54
1:A:530:G:N7	22:V:39:LYS:N	2.56	0.54
1:A:7:A:C3'	5:E:106:ILE:HD13	1.98	0.54
5:E:157:ARG:HG2	8:H:45:PHE:CD2	2.24	0.54
10:J:40:ILE:HG12	10:J:73:LEU:HB3	1.89	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:18:C:O2	1:A:1078:U:O4	2.25	0.54
1:A:842:U:H3'	1:A:843:U:C5'	2.37	0.54
1:A:925:G:N1	1:A:927:G:C2	2.75	0.54
1:A:951:G:OP2	13:M:101:ARG:NH2	2.41	0.54
23:W:567:GLY:HA2	23:W:587:ARG:HG3	1.88	0.54
1:A:865:A:C5'	1:A:1077:G:O2'	2.55	0.54
1:A:359:G:C4'	23:W:575:ASP:O	2.56	0.54
25:Z:94:LYS:C	26:X:25:C:H4'	2.27	0.54
1:A:359:G:H4'	23:W:576:LYS:HA	1.90	0.54
25:Z:118:LEU:HD22	25:Z:156:ALA:HB2	1.89	0.54
1:A:530:G:H8	22:V:39:LYS:HG2	1.72	0.54
22:V:61:ASP:OD1	22:V:63:THR:HB	2.06	0.54
23:W:830:VAL:O	23:W:836:VAL:HG23	2.08	0.54
1:A:923:A:OP1	5:E:26:LYS:CE	2.43	0.54
5:E:156:LYS:HB3	8:H:45:PHE:CE1	2.41	0.54
25:Z:93:VAL:O	26:X:25:C:C6	2.60	0.54
23:W:795:ILE:HG23	23:W:796:GLY:N	2.23	0.54
23:W:882:ILE:O	23:W:882:ILE:HG13	2.07	0.54
25:Z:93:VAL:HG22	25:Z:123:LYS:HD3	1.89	0.54
12:L:75:GLN:HE22	23:W:669:GLN:CB	2.00	0.54
23:W:589:GLY:N	23:W:622:PRO:HB3	2.22	0.54
23:W:789:GLU:C	23:W:792:GLN:HE22	2.08	0.54
23:W:812:ILE:HG23	23:W:812:ILE:O	2.08	0.54
1:A:404:G:N7	4:D:2:ALA:HB3	2.23	0.54
5:E:156:LYS:HZ1	8:H:73:GLU:HB2	1.70	0.54
15:O:20:ASN:O	15:O:22:THR:N	2.41	0.54
26:X:56:C:H2'	26:X:57:A:H8	1.74	0.54
25:Z:94:LYS:HZ2	26:X:24:U:C2'	2.20	0.54
2:B:129:LEU:HA	3:C:179:ARG:NH2	2.22	0.53
26:X:71:C:N3	26:X:72:A:C4	2.76	0.53
1:A:1096:C:H5''	2:B:139:ARG:HE	1.72	0.53
1:A:1494:G:C8	22:V:18:PRO:CG	2.87	0.53
1:A:1495:U:O2'	25:Z:101:GLY:HA2	2.04	0.53
1:A:7:A:O5'	5:E:124:LEU:HD22	2.08	0.53
24:Y:72:LYS:HE2	26:X:17(A):U:O4'	2.08	0.53
25:Z:180:GLN:OE1	26:X:68:C:P	2.66	0.53
1:A:369:G:C5'	23:W:593:LYS:HZ1	2.21	0.53
22:V:15:GLU:HG3	22:V:17:LEU:HG	1.90	0.53
1:A:367:U:H4'	23:W:605:ARG:HD2	1.91	0.53
1:A:1032:G:H2'	1:A:1033:G:H4'	1.90	0.53
1:A:1124:G:H5'	10:J:37:ARG:HH11	1.73	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:976:G:OP2	1:A:1358:U:O2'	2.25	0.53
1:A:843:U:OP1	1:A:846:G:N2	2.42	0.53
1:A:19:A:OP1	5:E:135:ASN:ND2	2.40	0.53
1:A:1379:G:N7	7:G:2:PRO:HB2	2.24	0.53
23:W:846:ARG:HB3	26:X:76:A:N3	2.18	0.53
1:A:1060:U:H4'	10:J:53:ILE:HG23	1.91	0.53
2:B:133:GLU:OE2	2:B:137:ARG:NH1	2.39	0.53
13:M:12:HIS:ND1	13:M:45:ILE:HG13	2.24	0.53
22:V:58:THR:HG22	22:V:60:TYR:HB2	1.90	0.53
23:W:540:GLY:HA2	23:W:541:ILE:HB	1.88	0.53
1:A:530:G:N7	22:V:38:GLY:C	2.62	0.53
1:A:6:G:C8	5:E:124:LEU:CD1	2.92	0.53
13:M:8:ASN:OD1	13:M:9:ILE:N	2.42	0.53
1:A:526:C:C2'	1:A:527:G7M:H5'	2.39	0.53
1:A:702:A:C8	24:Y:64:LYS:HG2	2.39	0.53
1:A:702:A:O4'	24:Y:64:LYS:HD2	2.07	0.53
1:A:938:A:H5'	7:G:76:LYS:NZ	2.23	0.53
10:J:6:ILE:HG13	10:J:76:ILE:HB	1.91	0.53
23:W:395:THR:HB	23:W:462:THR:HG21	1.90	0.53
26:X:26:G:H2'	26:X:27:U:H5'	1.91	0.53
1:A:790:A:H5''	26:X:38:A:O3'	2.07	0.53
22:V:49:PRO:CD	25:Z:131:ARG:HH12	1.99	0.53
1:A:769:G:H4'	1:A:1513:A:H4'	1.90	0.53
5:E:149:SER:HB3	5:E:152:MET:CG	2.39	0.53
22:V:15:GLU:N	22:V:23:ARG:HB2	2.19	0.53
26:X:51:C:H1'	26:X:64:G:N2	2.24	0.53
1:A:920:U:C2'	1:A:1082:A:H5'	2.38	0.53
1:A:926:G:H8	1:A:927:G:P	2.26	0.53
5:E:156:LYS:HD3	8:H:71:VAL:O	2.09	0.53
22:V:44:TYR:O	22:V:45:ILE:HB	2.07	0.53
23:W:566:SER:HB3	23:W:588:GLU:OE1	2.08	0.53
26:X:22:G:O2'	26:X:23:C:H6	1.76	0.53
1:A:790:A:OP1	26:X:38:A:O2'	2.27	0.53
1:A:19:A:C8	1:A:1078:U:C2	2.96	0.52
8:H:3:MET:N	8:H:3:MET:SD	2.73	0.52
24:Y:49:ALA:HB3	24:Y:56:VAL:HB	1.90	0.52
25:Z:91:ILE:HD11	26:X:13:C:H5''	1.89	0.52
1:A:701:U:OP2	24:Y:67:PHE:HB2	2.09	0.52
9:I:85:ARG:HA	9:I:88:MET:CE	2.39	0.52
15:O:26:GLU:N	15:O:26:GLU:OE1	2.34	0.52
26:X:14:A:H2'	26:X:15:G:O4'	2.09	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:Z:94:LYS:HE3	26:X:24:U:H4'	1.90	0.52
1:A:691:G:O6	11:K:57:LYS:NZ	2.33	0.52
23:W:847:ARG:O	23:W:847:ARG:HG3	2.09	0.52
25:Z:93:VAL:O	26:X:25:C:H6	1.93	0.52
1:A:181:A:N6	1:A:195:A:OP2	2.43	0.52
9:I:130:ARG:HH22	26:X:34:C:H4'	1.73	0.52
10:J:65:TYR:HB3	14:N:96:LEU:HD11	1.91	0.52
13:M:12:HIS:HA	13:M:45:ILE:CG1	2.39	0.52
23:W:399:HIS:CD2	23:W:476:MET:HB3	2.44	0.52
2:B:126:PHE:C	2:B:128:LYS:H	2.13	0.52
5:E:157:ARG:NH2	8:H:100:GLY:C	2.55	0.52
12:L:75:GLN:NE2	23:W:669:GLN:HG3	0.85	0.52
23:W:391:ALA:HB3	23:W:623:SER:HB2	1.91	0.52
12:L:75:GLN:HE22	23:W:669:GLN:CG	1.17	0.52
1:A:1111:A:C2'	2:B:130:THR:O	2.57	0.52
1:A:702:A:O5'	24:Y:64:LYS:CD	2.38	0.52
1:A:741:G:OP1	15:O:35:GLN:NE2	2.43	0.52
23:W:585:LEU:HD23	23:W:625:PRO:HB3	1.90	0.52
23:W:800:VAL:HG12	23:W:815:CYS:HB3	1.91	0.52
26:X:59:A:H2'	26:X:60:U:O4'	2.10	0.52
1:A:722:G:N3	1:A:722:G:H3'	2.25	0.52
1:A:537:G:OP1	12:L:110:ARG:NH2	2.43	0.52
23:W:855:VAL:HG11	23:W:861:CYS:HB2	1.91	0.52
25:Z:92:GLN:O	26:X:11:A:C2	2.60	0.52
25:Z:98:PHE:HB3	25:Z:144:VAL:HG11	1.91	0.52
1:A:1428:A:H2'	1:A:1429:A:O4'	2.10	0.52
1:A:558:G:C5'	5:E:126:LYS:HE3	2.40	0.52
3:C:132:ARG:HH22	4:D:47:ARG:HH21	1.57	0.52
1:A:1103:C:O2'	2:B:107:VAL:HG13	2.09	0.52
1:A:1449:C:C2'	1:A:1450:U:H5'	2.40	0.52
1:A:157:U:C2'	1:A:158:G:H5'	2.40	0.52
1:A:411:A:P	4:D:26:ARG:HH22	2.33	0.52
23:W:612:GLU:HG3	23:W:613:LEU:N	2.24	0.52
26:X:53:G:N1	26:X:61:C:N3	2.51	0.52
26:X:10:G:N2	26:X:26:G:H1'	2.25	0.51
22:V:32:ILE:H	22:V:32:ILE:HD13	1.75	0.51
23:W:744:VAL:HG21	23:W:774:LEU:HD13	1.92	0.51
23:W:815:CYS:SG	23:W:861:CYS:C	2.89	0.51
26:X:22:G:C2	26:X:23:C:C4	2.98	0.51
25:Z:94:LYS:NZ	26:X:24:U:C4'	2.73	0.51
25:Z:94:LYS:HZ1	26:X:24:U:H4'	1.75	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:816:MET:SD	23:W:860:GLU:HA	2.49	0.51
1:A:1299:A:H2'	1:A:1299:A:N3	2.26	0.51
1:A:1493:A:C8	22:V:19:ASN:CA	2.93	0.51
1:A:368:U:H5'	23:W:593:LYS:HE2	1.91	0.51
23:W:804:PHE:HB2	23:W:812:ILE:HG22	1.80	0.51
26:X:1:C:OP2	26:X:2:G:H3'	2.11	0.51
7:G:88:PRO:HG2	7:G:152:ALA:HB2	1.93	0.51
14:N:27:LEU:O	14:N:31:ILE:HG12	2.11	0.51
26:X:22:G:C2	26:X:23:C:C5	2.99	0.51
1:A:9:G:H5'	5:E:108:GLY:HA3	1.93	0.51
10:J:15:HIS:CE1	10:J:16:ARG:HD3	2.46	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
26:X:49:G:N2	26:X:66:C:H1'	2.26	0.51
6:F:29:ILE:HD13	6:F:64:VAL:HG11	1.93	0.51
13:M:12:HIS:HA	13:M:45:ILE:HG12	1.93	0.51
23:W:812:ILE:CD1	23:W:863:ILE:O	2.54	0.51
23:W:447:GLY:HA2	23:W:455:ARG:HD3	1.93	0.51
25:Z:176:PRO:HG3	26:X:12:G:HO2'	1.75	0.51
1:A:121:U:H5''	1:A:122:G:OP2	2.11	0.51
1:A:1073:U:C2'	2:B:105:LYS:HG2	2.41	0.51
25:Z:91:ILE:CD1	26:X:13:C:C6	2.94	0.51
1:A:216:U:H2'	1:A:217:C:C6	2.46	0.51
1:A:395:C:C5'	23:W:647:GLU:OE2	2.55	0.51
23:W:795:ILE:CG2	23:W:796:GLY:N	2.74	0.51
1:A:1111:A:P	2:B:132:LYS:CE	2.99	0.50
1:A:5:U:O2'	5:E:100:SER:CB	2.59	0.50
1:A:918:A:N1	1:A:1080:A:H2	2.04	0.50
6:F:38:ARG:HB3	6:F:63:ASN:HB2	1.91	0.50
19:S:29:LYS:HB3	19:S:30:PRO:CD	2.41	0.50
22:V:2:LYS:HB3	22:V:2:LYS:NZ	2.26	0.50
1:A:865:A:O4'	1:A:1077:G:O2'	2.26	0.50
1:A:516:PSU:O3'	22:V:2:LYS:HE3	2.09	0.50
1:A:920:U:H4'	1:A:1082:A:C5'	2.40	0.50
5:E:162:GLU:N	8:H:114:ARG:NH2	2.59	0.50
1:A:17:U:H2'	1:A:1079:G:C1'	2.36	0.50
1:A:7:A:C1'	5:E:124:LEU:HB3	2.41	0.50
13:M:95:LEU:C	13:M:109:ARG:HG2	2.32	0.50
23:W:727:GLY:O	23:W:748:VAL:HG21	2.11	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:X:8:4SU:O2'	26:X:9:G:O5'	2.28	0.50
24:Y:72:LYS:HG2	26:X:17(A):U:C2	2.47	0.50
1:A:18:C:C2'	1:A:1078:U:N3	2.56	0.50
1:A:412:A:H1'	1:A:413:G:C5'	2.39	0.50
19:S:50:ALA:HB1	19:S:57:HIS:HB3	1.93	0.50
1:A:7:A:H2'	5:E:124:LEU:HD22	1.93	0.50
1:A:358:U:C5'	23:W:578:ARG:O	2.59	0.50
1:A:1105:A:OP2	2:B:143:LYS:NZ	2.33	0.50
1:A:457:G:N2	1:A:476:U:O2	2.45	0.50
2:B:117:LEU:HA	2:B:120:GLN:HG2	1.93	0.50
8:H:9:ASP:OD2	8:H:13:ARG:HD2	2.12	0.50
23:W:814:GLY:HA2	27:X:101:FME:HB3	1.94	0.50
1:A:530:G:H8	22:V:39:LYS:H	1.58	0.50
23:W:795:ILE:HG23	23:W:879:VAL:HG13	1.94	0.50
1:A:204:G:C3'	1:A:205:A:H5''	2.42	0.50
4:D:99:ASP:OD1	4:D:100:ASN:N	2.45	0.50
26:X:71:C:C4	26:X:72:A:C4	2.99	0.50
1:A:1016:A:N3	1:A:1016:A:H2'	2.26	0.50
1:A:559:A:P	5:E:126:LYS:HZ1	2.35	0.50
6:F:76:THR:O	6:F:79:ARG:N	2.44	0.50
1:A:841:C:C5	1:A:843:U:H5'	2.47	0.49
26:X:58:A:O2'	26:X:60:U:C5	2.51	0.49
22:V:48:LEU:HD22	25:Z:131:ARG:NH1	2.27	0.49
1:A:1096:C:H5''	2:B:139:ARG:NE	2.27	0.49
1:A:701:U:C2	24:Y:44:ASP:OD2	2.65	0.49
1:A:920:U:O2'	1:A:1082:A:P	2.68	0.49
2:B:128:LYS:CB	3:C:207:ILE:CG1	2.89	0.49
1:A:1111:A:C3'	2:B:132:LYS:HD2	2.42	0.49
5:E:83:HIS:HB3	8:H:97:ALA:N	2.27	0.49
13:M:16:VAL:HG12	13:M:17:ILE:HD12	1.93	0.49
20:T:44:LYS:HG3	20:T:45:ALA:N	2.27	0.49
23:W:452:THR:HG23	23:W:453:SER:N	2.27	0.49
23:W:591:LEU:HD12	23:W:620:ALA:CB	2.24	0.49
23:W:612:GLU:HG3	23:W:613:LEU:H	1.76	0.49
23:W:613:LEU:C	23:W:613:LEU:HD12	2.32	0.49
23:W:728:ILE:HG22	23:W:729:THR:N	2.27	0.49
23:W:855:VAL:HG13	23:W:859:MET:HE3	1.94	0.49
1:A:1005:A:H3'	1:A:1006:G:C8	2.47	0.49
1:A:1073:U:P	5:E:66:LYS:HZ3	2.35	0.49
26:X:18:G:O2'	26:X:19:G:C5'	2.57	0.49
26:X:51:C:H42	26:X:62:C:H42	1.60	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:53:ILE:HG13	14:N:85:ARG:CZ	2.42	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
1:A:793:U:O4	25:Z:109:VAL:CG1	2.36	0.49
22:V:31:GLU:H	22:V:31:GLU:CD	2.16	0.49
12:L:39:THR:CB	22:V:61:ASP:HB2	2.42	0.49
23:W:789:GLU:HG3	23:W:789:GLU:O	2.12	0.49
2:B:15:HIS:HB3	2:B:43:LEU:HD11	1.95	0.49
5:E:163:GLU:CB	8:H:114:ARG:NE	2.75	0.49
5:E:158:GLY:CA	8:H:44:GLY:HA3	2.43	0.49
22:V:7:ILE:HG22	22:V:9:THR:H	1.78	0.49
23:W:855:VAL:HG13	23:W:859:MET:HE2	1.94	0.49
1:A:1390:U:O2	1:A:1391:U:N1	2.39	0.49
1:A:147:G:H2'	1:A:148:G:C8	2.47	0.49
1:A:973:G:H1'	10:J:56:HIS:HD2	1.78	0.49
23:W:519:ILE:HG12	23:W:520:LEU:HD12	1.95	0.49
23:W:539:THR:O	23:W:541:ILE:HB	2.13	0.49
23:W:795:ILE:CG2	23:W:879:VAL:CG1	2.88	0.49
1:A:526:C:H2'	1:A:527:G7M:H5'	1.93	0.49
1:A:702:A:OP2	24:Y:64:LYS:HE2	2.13	0.49
1:A:975:A:H8	1:A:1357:A:HO2'	1.61	0.49
8:H:18:GLN:CG	8:H:70:ALA:HB1	2.42	0.49
11:K:16:VAL:HG23	11:K:17:SER:N	2.28	0.49
6:F:86:ARG:NH1	18:R:64:TYR:O	2.46	0.49
23:W:778:VAL:HG23	23:W:779:LYS:N	2.27	0.49
23:W:836:VAL:O	23:W:836:VAL:HG13	2.12	0.49
2:B:129:LEU:N	3:C:179:ARG:HE	2.08	0.49
1:A:567:G:C5'	5:E:93:ARG:NH1	2.75	0.49
13:M:40:ALA:HB3	13:M:43:VAL:CG2	2.43	0.49
1:A:18:C:H2'	1:A:1078:U:C4	2.45	0.49
1:A:109:A:C6	1:A:326:G:C6	3.00	0.49
1:A:1194:U:C5'	5:E:27:GLY:HA2	2.38	0.49
5:E:56:VAL:N	5:E:57:PRO:HD2	2.28	0.49
24:Y:21:GLN:HE22	24:Y:41:ARG:HH11	1.59	0.49
25:Z:123:LYS:HB2	26:X:12:G:O4'	2.12	0.49
1:A:16:A:H2'	1:A:1080:A:C4'	2.35	0.48
1:A:920:U:H4'	1:A:1082:A:C4'	2.43	0.48
1:A:369:G:H5'	23:W:593:LYS:HZ1	1.77	0.48
1:A:429:U:H5'	4:D:9:LEU:HD12	1.95	0.48
18:R:21:ILE:HG21	18:R:54:GLN:HB3	1.95	0.48
3:C:185:ASN:OD1	3:C:186:THR:N	2.45	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:76:ILE:CD1	10:J:87:LEU:HD11	2.42	0.48
26:X:58:A:C6	26:X:61:C:H1'	2.47	0.48
1:A:1016:A:C2	1:A:1017:U:H4'	2.48	0.48
1:A:1062:U:H2'	1:A:1063:C:C6	2.48	0.48
22:V:44:TYR:CD1	22:V:44:TYR:N	2.82	0.48
1:A:1102:A:H2	2:B:103:ASN:HD22	1.61	0.48
1:A:383:A:C5	1:A:384:G:H1'	2.49	0.48
2:B:120:GLN:HG3	2:B:121:SER:N	2.28	0.48
1:A:1111:A:H2'	2:B:130:THR:CB	2.44	0.48
1:A:1100:C:N4	2:B:95:ARG:CZ	2.77	0.48
1:A:1137:C:H1'	1:A:1138:G:N2	2.28	0.48
3:C:132:ARG:NH1	4:D:47:ARG:HH21	2.08	0.48
1:A:1238:A:H5'	1:A:1336:C:H41	1.77	0.48
1:A:925:G:N2	1:A:927:G:N3	2.61	0.48
5:E:156:LYS:HZ1	8:H:73:GLU:CD	2.16	0.48
13:M:107:ARG:HH21	13:M:113:ARG:HB3	1.79	0.48
12:L:75:GLN:NE2	23:W:669:GLN:HG2	0.81	0.48
25:Z:91:ILE:HG13	26:X:12:G:C3'	2.42	0.48
1:A:1003:G:N2	1:A:1004:A:O2'	2.46	0.48
1:A:19:A:H8	1:A:1078:U:C2	2.32	0.48
1:A:71:A:O2'	1:A:72:A:OP2	2.27	0.48
1:A:7:A:C3'	5:E:106:ILE:HD12	2.14	0.48
4:D:17:THR:HG22	4:D:18:ASP:N	2.29	0.48
10:J:8:ILE:HA	10:J:99:GLN:O	2.14	0.48
1:A:266:G:H3'	17:Q:69:LYS:HB2	1.95	0.48
1:A:518:C:O2'	22:V:38:GLY:N	2.47	0.48
22:V:45:ILE:O	22:V:45:ILE:HG22	2.14	0.48
23:W:812:ILE:CG2	26:X:76:A:O4'	2.52	0.48
1:A:26:A:H2'	1:A:27:G:H5'	1.95	0.48
1:A:530:G:C8	22:V:39:LYS:HG2	2.48	0.48
1:A:1111:A:P	2:B:132:LYS:HE3	2.53	0.48
1:A:1100:C:H41	2:B:95:ARG:CD	2.27	0.48
23:W:772:TYR:HA	23:W:775:ILE:HG22	1.96	0.48
26:X:53:G:O2'	26:X:54:5MU:O5'	2.26	0.48
26:X:6:G:N2	26:X:67:C:O2	2.34	0.48
25:Z:91:ILE:HG22	26:X:11:A:C2	2.49	0.48
1:A:207:C:H2'	1:A:208:U:C2	2.49	0.48
5:E:162:GLU:HG3	5:E:163:GLU:N	2.28	0.48
10:J:53:ILE:CG2	10:J:61:ALA:HB1	2.44	0.48
26:X:54:5MU:C5	26:X:55:PSU:C2	3.01	0.48
25:Z:179:LYS:HE2	26:X:6:G:O4'	2.14	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:76:G:N3	1:A:76:G:H2'	2.29	0.47
1:A:7:A:C8	5:E:124:LEU:HB2	2.43	0.47
10:J:7:ARG:CG	10:J:101:SER:HB2	2.44	0.47
25:Z:118:LEU:HD21	25:Z:176:PRO:HA	1.96	0.47
25:Z:178:LYS:O	26:X:69:C:C4'	2.61	0.47
14:N:10:GLU:HG3	14:N:63:ARG:HD2	1.96	0.47
12:L:56:ARG:NH2	23:W:734:THR:HG22	2.29	0.47
1:A:1016:A:N1	1:A:1017:U:O2'	2.44	0.47
1:A:560:A:C8	5:E:128:TYR:CE1	3.03	0.47
1:A:75:G:C2	1:A:76:G:H1'	2.50	0.47
1:A:8:A:O3'	5:E:108:GLY:CA	2.63	0.47
5:E:94:VAL:HG22	5:E:111:MET:CE	2.45	0.47
9:I:23:PRO:HA	9:I:61:LEU:HA	1.95	0.47
1:A:1493:A:H3'	22:V:18:PRO:C	1.98	0.47
23:W:591:LEU:O	23:W:592:HIS:CG	2.68	0.47
26:X:8:4SU:S4	26:X:14:A:C8	3.02	0.47
23:W:611:ASN:O	23:W:612:GLU:CG	2.62	0.47
23:W:847:ARG:CA	27:X:101:FME:HCN	2.45	0.47
24:Y:28:ILE:HD12	24:Y:28:ILE:N	2.29	0.47
1:A:1074:G:O4'	2:B:103:ASN:OD1	2.31	0.47
1:A:19:A:H8	1:A:1078:U:O2	1.97	0.47
1:A:367:U:O5'	23:W:605:ARG:NH2	2.47	0.47
8:H:28:PRO:O	8:H:33:LYS:NZ	2.38	0.47
9:I:19:VAL:HG13	9:I:65:ILE:HG22	1.97	0.47
22:V:36:ILE:CG2	22:V:41:ARG:HG3	2.44	0.47
26:X:8:4SU:C2	26:X:8:4SU:H3'	2.44	0.47
25:Z:130:PHE:CE1	25:Z:137:HIS:CD2	3.03	0.47
13:M:6:GLY:HA3	13:M:66:GLU:HG3	1.97	0.47
19:S:7:LYS:H	19:S:7:LYS:HD2	1.79	0.47
22:V:20:ALA:HB1	22:V:36:ILE:CG1	2.45	0.47
1:A:159:G:H5"	1:A:159:G:H8	1.79	0.47
12:L:75:GLN:HE22	23:W:669:GLN:CA	2.27	0.47
14:N:42:TRP:CD1	14:N:43:ASN:N	2.83	0.47
1:A:1073:U:O2	2:B:106:THR:CB	2.60	0.47
10:J:42:LEU:HB2	10:J:71:LEU:HB3	1.96	0.47
10:J:51:VAL:HB	14:N:81:ARG:HB2	1.96	0.47
22:V:20:ALA:HB1	22:V:36:ILE:CD1	2.44	0.47
23:W:590:THR:O	23:W:591:LEU:HG	2.15	0.47
1:A:369:G:C5'	23:W:593:LYS:NZ	2.78	0.47
25:Z:92:GLN:C	26:X:11:A:C2	2.88	0.47
1:A:131:A:H2'	1:A:132:C:C6	2.49	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:793:U:N3	25:Z:109:VAL:CG1	2.77	0.47
6:F:102:MET:CE	18:R:24:LYS:HB3	2.45	0.47
1:A:1096:C:C4'	2:B:139:ARG:NH2	2.41	0.46
1:A:1103:C:O2'	2:B:107:VAL:CG1	2.64	0.46
3:C:123:GLN:HG2	3:C:128:VAL:HG21	1.97	0.46
13:M:32:ALA:O	13:M:36:ALA:N	2.47	0.46
1:A:1111:A:H2'	2:B:130:THR:O	2.12	0.46
1:A:701:U:O2'	24:Y:61:ASP:CA	2.61	0.46
1:A:913:A:OP1	12:L:88:LYS:NZ	2.47	0.46
1:A:937:A:O2'	7:G:76:LYS:NZ	2.38	0.46
1:A:1492:A:H4'	12:L:44:LYS:HE2	1.97	0.46
26:X:66:C:H2'	26:X:67:C:H6	1.76	0.46
24:Y:43:LEU:HD23	24:Y:59:ILE:HG22	1.98	0.46
1:A:701:U:C5'	24:Y:63:GLY:C	2.81	0.46
1:A:872:A:C8	1:A:874:G:C8	3.04	0.46
1:A:925:G:H2'	1:A:927:G:C4'	2.45	0.46
2:B:27:MET:HE2	2:B:189:THR:HA	1.96	0.46
5:E:80:THR:OG1	5:E:122:ASN:O	2.32	0.46
22:V:17:LEU:HD11	22:V:23:ARG:NH1	2.31	0.46
23:W:526:GLY:O	23:W:527:GLU:HG2	2.15	0.46
26:X:71:C:N4	26:X:72:A:C6	2.83	0.46
25:Z:92:GLN:HE21	26:X:12:G:N2	2.13	0.46
1:A:109:A:H2'	1:A:326:G:N2	2.31	0.46
1:A:237:G:OP1	17:Q:42:THR:OG1	2.30	0.46
7:G:130:ASN:HA	7:G:135:VAL:HG11	1.96	0.46
5:E:156:LYS:HZ1	8:H:73:GLU:CB	2.27	0.46
13:M:33:ILE:HD11	13:M:63:PHE:CE2	2.50	0.46
1:A:368:U:C3'	23:W:593:LYS:HZ1	2.24	0.46
26:X:62:C:H2'	26:X:63:G:O4'	2.16	0.46
1:A:361:G:OP1	23:W:729:THR:CB	2.54	0.46
1:A:451:A:H61	1:A:481:G:H5'	1.80	0.46
8:H:108:LYS:HG3	8:H:121:LEU:HD11	1.97	0.46
12:L:104:CYS:C	23:W:662:ARG:CZ	2.81	0.46
22:V:66:ARG:NH1	22:V:66:ARG:CB	2.77	0.46
2:B:20:THR:HG22	2:B:39:HIS:CE1	2.50	0.46
4:D:58:LYS:HD2	4:D:204:TYR:OH	2.16	0.46
22:V:37:SER:HB3	22:V:67:ILE:O	2.15	0.46
12:L:75:GLN:HE22	23:W:669:GLN:HG3	0.86	0.46
26:X:71:C:C5	26:X:72:A:C6	3.03	0.46
1:A:1072:G:H4'	5:E:62:LYS:HE2	1.84	0.46
1:A:359:G:O4'	23:W:576:LYS:C	2.53	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:468:A:C8	1:A:469:C:C6	3.03	0.46
26:X:71:C:C1'	26:X:72:A:C8	2.97	0.46
25:Z:94:LYS:CE	26:X:24:U:H4'	2.45	0.46
1:A:1111:A:H2'	2:B:130:THR:HG22	1.98	0.46
1:A:1228:C:P	13:M:107:ARG:NH2	2.88	0.46
1:A:1492:A:C2	22:V:35:TYR:CA	2.89	0.46
1:A:2:A:O2'	4:D:83:LYS:NZ	2.43	0.46
2:B:129:LEU:HD22	2:B:134:ALA:HB2	1.97	0.46
1:A:1112:C:C5'	2:B:131:LYS:HG2	2.14	0.46
14:N:21:PHE:HA	14:N:25:ALA:CB	2.45	0.46
1:A:1493:A:C4	22:V:18:PRO:O	2.69	0.46
22:V:32:ILE:N	22:V:32:ILE:HD13	2.29	0.46
23:W:430:ALA:HB2	23:W:443:LEU:HD13	1.98	0.46
23:W:727:GLY:CA	23:W:748:VAL:HG23	2.33	0.46
25:Z:90:VAL:CG2	26:X:12:G:O6	2.63	0.46
26:X:71:C:H2'	26:X:72:A:O5'	2.16	0.46
26:X:73:A:N3	26:X:74:C:N3	2.64	0.46
1:A:864:A:C4'	1:A:1078:U:C5	2.84	0.46
1:A:254:G:H4'	17:Q:17:MET:HE2	1.98	0.46
11:K:111:THR:HG23	21:U:3:VAL:HG22	1.98	0.46
22:V:54:VAL:CB	22:V:69:TYR:HB2	2.43	0.46
23:W:786:LEU:N	23:W:786:LEU:HD23	2.30	0.46
25:Z:93:VAL:N	26:X:25:C:C2	2.67	0.46
1:A:184:G:O2'	20:T:69:LYS:NZ	2.36	0.46
1:A:702:A:OP2	24:Y:61:ASP:HB2	2.06	0.46
2:B:10:LEU:HD12	2:B:15:HIS:ND1	2.31	0.46
20:T:44:LYS:HB3	20:T:87:ALA:HB3	1.98	0.46
12:L:73:ASN:CB	23:W:670:GLN:CG	2.86	0.46
26:X:22:G:C6	26:X:23:C:N4	2.82	0.46
5:E:153:VAL:HG11	8:H:100:GLY:N	2.10	0.45
25:Z:91:ILE:HD12	26:X:13:C:O5'	2.15	0.45
1:A:405:U:O4	4:D:2:ALA:N	2.50	0.45
1:A:1074:G:H1'	2:B:103:ASN:HB2	1.99	0.45
1:A:1081:A:OP1	5:E:21:VAL:HB	2.15	0.45
9:I:19:VAL:HG11	9:I:83:ILE:HA	1.98	0.45
7:G:16:PRO:HB3	9:I:43:THR:HG23	1.99	0.45
10:J:15:HIS:CG	10:J:16:ARG:N	2.84	0.45
10:J:35:GLN:HG3	10:J:78:GLU:HG2	1.98	0.45
14:N:21:PHE:HB2	14:N:55:SER:O	2.16	0.45
1:A:1018:G:H2'	1:A:1018:G:N3	2.30	0.45
1:A:1074:G:H4'	2:B:102:THR:O	2.17	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1152:A:H5''	10:J:15:HIS:HB2	1.98	0.45
1:A:1229:A:OP2	13:M:113:ARG:NH1	2.48	0.45
1:A:1390:U:C6	1:A:1391:U:C6	2.62	0.45
1:A:5:U:H6	1:A:5:U:H3'	1.81	0.45
1:A:8:A:O3'	5:E:108:GLY:HA3	2.16	0.45
7:G:83:SER:HB2	7:G:85:TYR:CE2	2.51	0.45
22:V:25:LYS:HD2	22:V:30:PRO:O	2.16	0.45
23:W:456:ALA:HA	23:W:485:HIS:HD2	1.82	0.45
23:W:534:SER:CB	23:W:539:THR:HG23	2.46	0.45
24:Y:72:LYS:CG	26:X:17(A):U:C2	2.98	0.45
26:X:22:G:N1	26:X:23:C:C4	2.84	0.45
25:Z:94:LYS:HG2	26:X:24:U:O2'	2.14	0.45
1:A:1074:G:C4'	2:B:103:ASN:HB2	2.45	0.45
5:E:159:LYS:NZ	8:H:43:GLU:CD	2.64	0.45
10:J:6:ILE:CG1	10:J:76:ILE:HB	2.46	0.45
14:N:18:ASP:OD1	14:N:19:LYS:N	2.49	0.45
1:A:369:G:H5''	23:W:593:LYS:NZ	2.31	0.45
23:W:812:ILE:CD1	23:W:863:ILE:C	2.85	0.45
1:A:1134:G:H2'	1:A:1135:U:C6	2.51	0.45
1:A:1494:G:O2'	22:V:16:ALA:HB3	2.17	0.45
1:A:657:U:O2	15:O:22:THR:HG23	2.16	0.45
5:E:74:VAL:HG22	5:E:76:LEU:HD23	1.99	0.45
12:L:110:ARG:HB2	12:L:119:VAL:HG21	1.98	0.45
1:A:1322:C:P	19:S:78:ARG:HH22	2.40	0.45
23:W:396:ILE:HG21	23:W:404:LYS:HG3	1.96	0.45
23:W:666:LEU:HD12	23:W:667:ALA:N	2.32	0.45
1:A:790:A:P	26:X:39:C:H5'	2.54	0.45
1:A:864:A:H4'	1:A:1078:U:O5'	2.17	0.45
7:G:62:PHE:HE1	7:G:66:LEU:HD22	1.81	0.45
22:V:31:GLU:CD	22:V:31:GLU:N	2.70	0.45
23:W:496:ALA:HB2	23:W:544:LEU:HD12	1.97	0.45
1:A:1029:U:O2'	1:A:1032:G:N1	2.49	0.45
1:A:31:G:O2'	1:A:48:C:N4	2.50	0.45
1:A:85:U:H6	1:A:86:G:N1	2.15	0.45
10:J:52:LEU:HD23	10:J:62:ARG:HD3	1.97	0.45
1:A:1328:C:H5''	13:M:28:THR:HG21	1.99	0.45
13:M:54:ASP:HA	13:M:57:ARG:HD2	1.98	0.45
1:A:495:A:C2	1:A:496:A:C6	3.05	0.45
10:J:67:ILE:HG13	14:N:96:LEU:HD13	1.99	0.45
22:V:6:THR:HG22	22:V:7:ILE:N	2.32	0.45
23:W:544:LEU:CD2	23:W:544:LEU:C	2.85	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:X:16:C:H4'	26:X:60:U:O2'	2.17	0.45
24:Y:77:ARG:HG3	26:X:16:C:N4	2.32	0.45
26:X:18:G:H4'	26:X:60:U:O2	2.17	0.45
26:X:22:G:C2	26:X:23:C:C6	3.04	0.45
1:A:1031:C:O2'	1:A:1032:G:OP2	2.26	0.45
1:A:865:A:C4'	1:A:1077:G:HO2'	2.29	0.45
1:A:757:U:O2'	1:A:879:C:O2	2.34	0.45
3:C:150:LYS:HB3	3:C:169:ARG:CG	2.46	0.45
9:I:85:ARG:HA	9:I:88:MET:HE2	1.98	0.45
10:J:22:THR:CG2	10:J:39:PRO:HB3	2.46	0.45
19:S:29:LYS:CB	19:S:30:PRO:HD2	2.46	0.45
23:W:399:HIS:HB2	23:W:479:THR:HG23	1.99	0.45
23:W:396:ILE:HD12	23:W:408:LEU:HD11	1.98	0.45
23:W:481:GLU:O	23:W:485:HIS:ND1	2.45	0.45
26:X:8:4SU:H1'	26:X:21:A:H2	1.74	0.45
26:X:22:G:C6	26:X:23:C:C4	3.05	0.45
1:A:1111:A:C2'	2:B:133:GLU:H	2.30	0.45
3:C:132:ARG:NH2	4:D:47:ARG:HH21	2.14	0.45
3:C:77:ILE:HA	3:C:84:VAL:CG2	2.47	0.45
22:V:58:THR:HG22	22:V:60:TYR:H	1.82	0.45
25:Z:123:LYS:N	26:X:12:G:H1'	2.32	0.45
2:B:121:SER:HA	2:B:126:PHE:CE1	2.53	0.44
3:C:42:TYR:CZ	3:C:90:VAL:HG21	2.53	0.44
3:C:6:HIS:CG	14:N:89:MET:HB3	2.52	0.44
3:C:83:ASP:HA	3:C:86:LYS:HG2	1.99	0.44
1:A:6:G:H1'	5:E:124:LEU:CD1	2.45	0.44
23:W:586:VAL:O	23:W:586:VAL:HG23	2.17	0.44
23:W:797:LEU:CD2	23:W:797:LEU:C	2.86	0.44
5:E:156:LYS:HZ3	8:H:73:GLU:CB	2.21	0.44
26:X:21:A:O2'	26:X:22:G:C8	2.70	0.44
1:A:1312:G:C5'	19:S:6:LYS:HE2	2.47	0.44
26:X:54:5MU:C4	26:X:55:PSU:O2	2.70	0.44
25:Z:128:LEU:CD1	25:Z:141:GLY:HA2	2.45	0.44
2:B:133:GLU:CG	3:C:179:ARG:NH2	2.72	0.44
5:E:153:VAL:HG11	8:H:99:LEU:CA	2.02	0.44
10:J:28:THR:O	10:J:32:THR:HG22	2.18	0.44
10:J:10:LEU:CD2	10:J:98:VAL:HG12	2.48	0.44
22:V:40:MET:SD	22:V:67:ILE:HG22	2.57	0.44
23:W:791:LYS:CG	23:W:792:GLN:O	2.52	0.44
1:A:944:G:N1	1:A:1338:G:OP2	2.41	0.44
1:A:927:G:N1	1:A:1391:U:C2	2.72	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:865:A:P	1:A:1077:G:H5''	2.57	0.44
2:B:9:MET:CE	2:B:50:PHE:HD2	2.31	0.44
13:M:66:GLU:OE1	13:M:70:ARG:NH2	2.48	0.44
14:N:21:PHE:CD1	14:N:55:SER:HB3	2.52	0.44
26:X:24:U:H2'	26:X:25:C:H6	1.83	0.44
1:A:158:G:H2'	1:A:159:G:H5''	1.99	0.44
1:A:530:G:N7	22:V:38:GLY:CA	2.78	0.44
2:B:213:TYR:O	2:B:217:VAL:HG23	2.18	0.44
5:E:156:LYS:HZ2	8:H:130:ALA:C	2.20	0.44
11:K:34:ILE:HG12	11:K:70:CYS:SG	2.58	0.44
20:T:44:LYS:HG3	20:T:45:ALA:H	1.83	0.44
23:W:511:LYS:HG3	23:W:530:PHE:HE2	1.83	0.44
1:A:1111:A:O2'	2:B:133:GLU:N	2.49	0.44
1:A:502:A:H2'	1:A:503:C:O4'	2.18	0.44
2:B:129:LEU:O	2:B:130:THR:OG1	2.33	0.44
2:B:217:VAL:O	2:B:221:VAL:HG23	2.17	0.44
12:L:73:ASN:HB2	23:W:666:LEU:HB2	2.00	0.44
20:T:27:MET:CE	20:T:57:ILE:HG12	2.48	0.44
23:W:515:SER:OG	23:W:524:TRP:CZ3	2.70	0.44
23:W:716:VAL:HG21	23:W:786:LEU:CD2	2.46	0.44
23:W:727:GLY:C	23:W:728:ILE:HG13	2.38	0.44
26:X:56:C:C6	26:X:56:C:OP1	2.70	0.44
25:Z:179:LYS:HE2	26:X:6:G:C1'	2.48	0.44
1:A:1517:G:N7	25:Z:106:ASP:OD1	2.50	0.44
1:A:18:C:O2'	1:A:1078:U:C2'	2.66	0.44
5:E:105:ILE:HG23	5:E:123:VAL:HG23	2.00	0.44
5:E:149:SER:O	8:H:99:LEU:HB3	2.17	0.44
13:M:107:ARG:HG2	13:M:107:ARG:HH11	1.83	0.44
13:M:4:ILE:CG2	13:M:60:VAL:HG11	2.48	0.44
14:N:30:ILE:O	14:N:34:VAL:HG23	2.17	0.44
23:W:846:ARG:HA	23:W:851:ASP:HA	2.00	0.44
25:Z:94:LYS:NZ	26:X:24:U:H4'	2.33	0.44
1:A:1463:U:H2'	1:A:1464:U:C6	2.53	0.44
1:A:75:G:C4	1:A:76:G:C8	3.06	0.44
1:A:560:A:C2'	5:E:128:TYR:HB3	2.39	0.44
7:G:135:VAL:HG23	7:G:136:LYS:N	2.33	0.44
8:H:25:VAL:HG22	8:H:63:LEU:HD21	1.99	0.44
17:Q:8:LEU:HD13	17:Q:25:ILE:HG13	1.99	0.44
17:Q:7:THR:HG21	17:Q:60:GLU:CG	2.48	0.44
12:L:105:SER:HG	23:W:666:LEU:HD22	1.82	0.44
23:W:838:TYR:CZ	23:W:839:GLU:O	2.71	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:Z:176:PRO:HB2	26:X:12:G:O3'	2.14	0.44
1:A:1014:A:OP1	19:S:18:LYS:NZ	2.51	0.43
1:A:1031:C:H4'	1:A:1032:G:O5'	2.17	0.43
1:A:918:A:H2	1:A:1080:A:C6	2.35	0.43
1:A:702:A:OP2	24:Y:61:ASP:OD2	2.31	0.43
25:Z:128:LEU:HD22	25:Z:130:PHE:CE1	2.53	0.43
25:Z:158:VAL:HA	25:Z:174:LEU:HA	1.99	0.43
25:Z:179:LYS:HB3	26:X:5:G:H22	1.83	0.43
25:Z:91:ILE:O	26:X:24:U:N3	2.46	0.43
1:A:464:U:C2	1:A:466:A:H5''	2.53	0.43
1:A:1102:A:O2'	2:B:98:GLY:HA3	2.18	0.43
7:G:80:VAL:HG12	7:G:81:GLY:N	2.34	0.43
8:H:41:LYS:HD2	8:H:48:ASP:HA	2.00	0.43
12:L:47:SER:OG	22:V:35:TYR:CZ	2.71	0.43
17:Q:49:GLU:O	17:Q:50:ASN:HB2	2.18	0.43
23:W:647:GLU:O	23:W:651:ARG:HG3	2.18	0.43
26:X:71:C:H2'	26:X:72:A:H8	0.48	0.43
25:Z:123:LYS:HG3	26:X:11:A:O2'	2.18	0.43
1:A:7:A:C2'	5:E:106:ILE:CD1	2.52	0.43
2:B:138:THR:O	2:B:142:GLU:N	2.42	0.43
5:E:83:HIS:HB3	8:H:97:ALA:HB2	2.00	0.43
8:H:93:PRO:HG3	8:H:125:ILE:HD13	2.00	0.43
10:J:5:ARG:HG2	10:J:77:VAL:HA	1.99	0.43
23:W:451:PHE:CD1	23:W:451:PHE:N	2.86	0.43
23:W:575:ASP:OD1	23:W:576:LYS:N	2.51	0.43
25:Z:92:GLN:C	26:X:11:A:H2	2.22	0.43
2:B:126:PHE:CG	2:B:127:ASP:N	2.84	0.43
2:B:28:LYS:N	2:B:29:PRO:CD	2.81	0.43
2:B:19:GLN:HA	2:B:38:VAL:HA	2.01	0.43
9:I:36:GLU:HA	9:I:45:ARG:HE	1.83	0.43
9:I:91:ASP:O	9:I:92:GLU:CB	2.67	0.43
1:A:1493:A:C5	22:V:18:PRO:O	2.72	0.43
23:W:796:GLY:H	23:W:879:VAL:HG13	1.83	0.43
24:Y:58:ARG:HD2	24:Y:60:MET:CE	2.49	0.43
25:Z:149:LYS:HE3	25:Z:158:VAL:HG21	1.99	0.43
1:A:368:U:H3'	23:W:593:LYS:HZ2	1.79	0.43
1:A:7:A:H2'	5:E:124:LEU:CD2	2.47	0.43
1:A:80:A:N6	1:A:89:U:O4	2.45	0.43
4:D:95:GLU:OE2	4:D:104:ARG:CZ	2.67	0.43
7:G:72:THR:HG22	7:G:142:HIS:NE2	2.33	0.43
10:J:53:ILE:HG22	10:J:61:ALA:O	2.18	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:U:6:VAL:HG22	21:U:15:ALA:HB1	1.99	0.43
23:W:390:ARG:HD3	23:W:559:ALA:HB2	2.01	0.43
26:X:29:G:H1	26:X:41:C:H42	1.66	0.43
1:A:1493:A:H1'	22:V:20:ALA:O	1.61	0.43
1:A:701:U:H3'	24:Y:64:LYS:H	0.60	0.43
1:A:1103:C:C5'	2:B:98:GLY:H	2.14	0.43
5:E:95:PHE:CZ	5:E:97:GLN:HG3	2.54	0.43
7:G:111:ARG:O	7:G:119:ARG:NH2	2.48	0.43
9:I:50:GLN:N	9:I:51:PRO:HD2	2.34	0.43
13:M:89:LEU:HD23	13:M:92:ARG:HH21	1.84	0.43
22:V:17:LEU:HB2	22:V:21:THR:HB	2.00	0.43
1:A:1494:G:N9	22:V:18:PRO:CD	2.77	0.43
26:X:76:A:C2'	27:X:101:FME:O1	2.64	0.43
1:A:1111:A:O5'	2:B:132:LYS:CD	2.67	0.43
14:N:54:ASP:OD1	14:N:59:ARG:NE	2.47	0.43
22:V:23:ARG:O	22:V:24:VAL:C	2.57	0.43
23:W:390:ARG:NH1	23:W:463:ASP:OD2	2.52	0.43
23:W:566:SER:O	23:W:587:ARG:N	2.50	0.43
23:W:790:LEU:O	23:W:791:LYS:HD3	2.19	0.43
23:W:794:ILE:HA	23:W:880:PHE:HB3	2.00	0.43
26:X:22:G:O2'	26:X:23:C:P	2.77	0.43
26:X:51:C:H1'	26:X:64:G:H22	1.83	0.43
26:X:51:C:H42	26:X:62:C:N4	2.16	0.43
1:A:1496:C:H4'	25:Z:99:ARG:HE	1.84	0.43
1:A:920:U:O2'	1:A:1082:A:C5'	2.61	0.43
22:V:15:GLU:CD	22:V:16:ALA:H	2.21	0.43
23:W:644:VAL:HG21	23:W:650:ALA:HB2	2.01	0.43
23:W:794:ILE:HA	23:W:880:PHE:CB	2.48	0.43
25:Z:179:LYS:HG2	26:X:69:C:O2	2.19	0.43
1:A:1497:G:OP1	25:Z:99:ARG:CD	2.66	0.43
1:A:1141:C:HO2'	1:A:1142:G:P	2.41	0.43
1:A:1152:A:H5''	10:J:15:HIS:CD2	2.54	0.43
1:A:566:G:H5''	5:E:86:LYS:HZ1	1.84	0.43
5:E:90:THR:HG22	5:E:91:GLY:N	2.34	0.43
11:K:107:ILE:HG13	21:U:12:PHE:CE1	2.54	0.43
22:V:33:LEU:O	22:V:34:ALA:O	2.36	0.43
23:W:470:ALA:HB3	23:W:473:ASP:HB2	2.01	0.43
25:Z:144:VAL:O	25:Z:148:VAL:HG23	2.19	0.43
1:A:157:U:H2'	1:A:158:G:H5'	2.01	0.43
3:C:155:GLY:HA2	3:C:163:ALA:HB1	2.00	0.43
10:J:56:HIS:O	10:J:57:VAL:HG12	2.19	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:Y:65:PHE:O	24:Y:69:GLN:HG2	2.19	0.43
1:A:1102:A:O2'	2:B:98:GLY:CA	2.67	0.42
4:D:58:LYS:HD3	4:D:203:LEU:HD23	2.01	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
19:S:63:THR:HG22	19:S:65:GLU:H	1.84	0.42
22:V:22:PHE:HE1	22:V:36:ILE:HD11	1.84	0.42
22:V:7:ILE:O	22:V:56:GLU:HA	2.19	0.42
26:X:2:G:N3	26:X:2:G:H2'	2.33	0.42
1:A:141:G:H2'	1:A:142:G:H5''	2.01	0.42
1:A:1494:G:N7	22:V:18:PRO:CG	2.77	0.42
1:A:518:C:OP2	22:V:39:LYS:HE3	2.17	0.42
1:A:920:U:O3'	1:A:1082:A:C4'	2.65	0.42
2:B:47:VAL:N	2:B:48:PRO:HD2	2.34	0.42
16:P:75:ILE:HA	16:P:78:VAL:HG12	2.01	0.42
20:T:28:MET:HE2	20:T:32:ILE:HD11	2.01	0.42
23:W:445:THR:OG1	23:W:446:PRO:HD2	2.19	0.42
23:W:812:ILE:HG12	26:X:76:A:O4'	2.10	0.42
26:X:46:A:O2'	26:X:47:U:H5''	2.19	0.42
25:Z:94:LYS:NZ	26:X:24:U:C2'	2.81	0.42
2:B:124:GLY:O	2:B:125:THR:HG22	2.19	0.42
3:C:156:ARG:H	3:C:163:ALA:HA	1.83	0.42
5:E:161:VAL:CB	8:H:114:ARG:HH12	2.13	0.42
8:H:29:SER:HB3	8:H:57:PRO:HB2	2.00	0.42
10:J:22:THR:HG21	10:J:39:PRO:CB	2.49	0.42
23:W:396:ILE:HA	23:W:466:VAL:O	2.19	0.42
23:W:540:GLY:CA	23:W:542:ASP:N	2.81	0.42
23:W:804:PHE:C	23:W:812:ILE:HG22	2.40	0.42
1:A:1193:G:O2'	5:E:27:GLY:CA	2.67	0.42
9:I:24:GLY:N	9:I:61:LEU:HA	2.34	0.42
11:K:28:ASN:O	11:K:57:LYS:HD3	2.20	0.42
14:N:54:ASP:HA	14:N:59:ARG:HD3	2.02	0.42
23:W:727:GLY:C	23:W:748:VAL:HG21	2.38	0.42
23:W:838:TYR:CG	23:W:839:GLU:N	2.87	0.42
26:X:2:G:N3	26:X:2:G:C2'	2.82	0.42
26:X:41:C:C2'	26:X:42:G:H5''	2.49	0.42
24:Y:49:ALA:HB2	26:X:19:G:C5	2.28	0.42
4:D:11:LEU:O	4:D:15:GLU:HG2	2.20	0.42
5:E:157:ARG:CD	8:H:101:ILE:HG12	2.45	0.42
6:F:99:ALA:HB1	6:F:103:VAL:HB	2.01	0.42
10:J:29:ALA:HA	10:J:32:THR:HG22	2.00	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:W:495:VAL:HG11	23:W:520:LEU:HD11	2.01	0.42
26:X:23:C:O2'	26:X:24:U:P	2.78	0.42
25:Z:176:PRO:HD2	26:X:12:G:O4'	2.08	0.42
1:A:7:A:O2'	5:E:124:LEU:CA	2.67	0.42
1:A:1111:A:C5'	2:B:132:LYS:HE3	2.48	0.42
5:E:163:GLU:CG	8:H:98:GLY:O	2.61	0.42
12:L:74:LEU:HD21	12:L:104:CYS:SG	2.60	0.42
22:V:66:ARG:CB	22:V:66:ARG:CZ	2.98	0.42
23:W:578:ARG:HB3	23:W:629:LEU:HD11	2.01	0.42
1:A:1431:A:C6	1:A:1432:G:C6	3.08	0.42
1:A:475:C:H2'	1:A:476:U:O4'	2.19	0.42
1:A:68:G:C5	1:A:69:G:H1'	2.55	0.42
1:A:925:G:N9	1:A:927:G:C8	2.88	0.42
5:E:161:VAL:O	5:E:164:ILE:N	2.47	0.42
5:E:157:ARG:HG3	8:H:45:PHE:CZ	2.42	0.42
1:A:501:C:OP1	12:L:114:ARG:NH2	2.52	0.42
13:M:103:LYS:HG2	13:M:104:THR:HG23	2.01	0.42
23:W:477:PRO:HA	23:W:480:ILE:HG22	2.01	0.42
26:X:20:H2U:O2	26:X:20:H2U:H2'	2.19	0.42
1:A:1417:G:C6	1:A:1482:G:C6	3.08	0.42
25:Z:90:VAL:CG2	26:X:22:G:N1	2.69	0.42
26:X:38:A:H2'	26:X:39:C:O4'	2.19	0.42
26:X:53:G:H2'	26:X:54:5MU:O4'	2.20	0.42
1:A:1082:A:H2'	1:A:1083:U:O4'	2.20	0.42
10:J:93:ALA:HB3	10:J:96:VAL:HG23	2.01	0.42
20:T:29:ARG:O	20:T:33:LYS:HG3	2.20	0.42
1:A:1494:G:H1'	22:V:17:LEU:HA	1.26	0.42
22:V:43:HIS:O	22:V:45:ILE:HG13	2.20	0.42
23:W:748:VAL:CG2	23:W:749:ARG:N	2.81	0.42
23:W:778:VAL:CG2	23:W:779:LYS:N	2.82	0.42
9:I:24:GLY:H	9:I:61:LEU:HA	1.84	0.42
22:V:38:GLY:O	22:V:39:LYS:C	2.58	0.42
23:W:598:LEU:HD12	23:W:650:ALA:HB1	2.01	0.42
23:W:774:LEU:O	23:W:778:VAL:HG13	2.20	0.42
1:A:1064:G:H1'	1:A:1190:G:N2	2.35	0.41
1:A:865:A:P	1:A:1077:G:C5'	3.08	0.41
1:A:1397:C:O2'	1:A:1398:A:OP1	2.34	0.41
1:A:16:A:C2'	1:A:1080:A:C2'	2.70	0.41
1:A:1377:A:N3	7:G:2:PRO:HG3	2.35	0.41
1:A:933:G:O6	7:G:3:ARG:NH1	2.49	0.41
22:V:40:MET:CE	22:V:70:ARG:HB3	2.50	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:W:493:VAL:HG11	23:W:519:ILE:HD11	2.01	0.41
1:A:368:U:C5	23:W:608:ALA:HB2	2.55	0.41
23:W:796:GLY:O	23:W:879:VAL:CG1	2.65	0.41
23:W:838:TYR:CE2	23:W:839:GLU:O	2.74	0.41
1:A:1217:C:OP2	14:N:9:ARG:NH2	2.43	0.41
7:G:44:TYR:O	7:G:48:GLU:N	2.40	0.41
8:H:75:ILE:HG23	8:H:75:ILE:O	2.19	0.41
9:I:30:ILE:HA	9:I:65:ILE:HG13	2.02	0.41
9:I:57:MET:HG3	9:I:61:LEU:H	1.85	0.41
9:I:80:ARG:O	9:I:84:THR:HG23	2.20	0.41
23:W:404:LYS:NZ	23:W:445:THR:O	2.46	0.41
1:A:585:G:N3	1:A:879:C:H4'	2.34	0.41
1:A:662:U:H2'	1:A:663:A:C8	2.56	0.41
1:A:842:U:H3'	1:A:843:U:H4'	2.02	0.41
1:A:1074:G:C4'	2:B:103:ASN:CB	2.97	0.41
1:A:1096:C:C5'	2:B:139:ARG:HE	2.31	0.41
3:C:85:GLU:HB2	3:C:88:ARG:NH2	2.36	0.41
7:G:6:VAL:HG12	7:G:7:ILE:N	2.36	0.41
10:J:35:GLN:HB2	10:J:77:VAL:HB	2.01	0.41
13:M:6:GLY:HA2	13:M:66:GLU:HG3	2.01	0.41
22:V:70:ARG:O	22:V:71:LYS:HD2	2.19	0.41
23:W:388:GLU:HG3	23:W:561:ARG:HG2	2.02	0.41
25:Z:93:VAL:C	26:X:24:U:H2'	2.39	0.41
24:Y:28:ILE:HD12	24:Y:28:ILE:H	1.84	0.41
1:A:1405:G:O4'	1:A:1519:MA6:H4'	2.20	0.41
1:A:1402:4OC:HM42	1:A:1500:A:H61	1.85	0.41
13:M:107:ARG:NH2	13:M:113:ARG:HB3	2.35	0.41
15:O:87:LEU:O	15:O:88:ARG:CB	2.68	0.41
22:V:23:ARG:HH21	22:V:33:LEU:CD2	2.33	0.41
23:W:794:ILE:HA	23:W:880:PHE:HA	2.03	0.41
1:A:457:G:O6	1:A:475:C:N4	2.45	0.41
1:A:559:A:P	5:E:126:LYS:HZ2	2.42	0.41
13:M:12:HIS:HA	13:M:45:ILE:HG13	2.02	0.41
23:W:399:HIS:CD2	23:W:478:GLN:HB3	2.55	0.41
1:A:367:U:H4'	23:W:605:ARG:HH21	1.85	0.41
23:W:862:GLY:HA2	27:X:101:FME:HB2	2.02	0.41
1:A:510:A:H5''	1:A:511:C:P	2.61	0.41
5:E:94:VAL:HG22	5:E:111:MET:HE1	2.01	0.41
16:P:48:GLU:HG2	16:P:49:GLY:H	1.85	0.41
1:A:263:A:P	20:T:74:ARG:HH11	2.43	0.41
1:A:920:U:C4'	1:A:1081:A:HO2'	2.28	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:925:G:C2	1:A:927:G:N9	2.86	0.41
5:E:107:ALA:HB2	5:E:125:ALA:HB3	2.02	0.41
13:M:33:ILE:O	13:M:37:ALA:N	2.46	0.41
10:J:65:TYR:CB	14:N:96:LEU:HD11	2.50	0.41
22:V:26:LEU:N	22:V:30:PRO:O	2.53	0.41
23:W:540:GLY:CA	23:W:541:ILE:CB	2.85	0.41
23:W:545:LEU:HD12	23:W:545:LEU:HA	1.83	0.41
23:W:676:ASN:ND2	23:W:678:PHE:O	2.53	0.41
1:A:1224:U:H3'	1:A:1225:A:H5'	2.03	0.41
1:A:1449:C:C2	1:A:1455:G:C2	3.08	0.41
4:D:58:LYS:NZ	4:D:59:GLN:OE1	2.48	0.41
9:I:85:ARG:HA	9:I:88:MET:HE3	2.03	0.41
23:W:396:ILE:HG22	23:W:404:LYS:CG	2.50	0.41
12:L:102:LEU:C	23:W:662:ARG:HH21	2.21	0.41
24:Y:77:ARG:HH22	26:X:16:C:H5	0.66	0.41
1:A:108:G:N3	1:A:108:G:H5'	2.36	0.41
1:A:108:G:C5'	1:A:108:G:N3	2.84	0.41
1:A:18:C:O2'	1:A:1078:U:C1'	2.66	0.41
1:A:501:C:H2'	1:A:502:A:C8	2.55	0.41
1:A:841:C:C6	1:A:843:U:H5'	2.55	0.41
9:I:30:ILE:HB	9:I:65:ILE:HD11	2.03	0.41
1:A:1494:G:C1'	22:V:16:ALA:C	2.62	0.41
25:Z:179:LYS:CB	26:X:5:G:N2	2.83	0.41
1:A:1095:U:H2'	1:A:1096:C:C6	2.56	0.41
1:A:1152:A:H5'	10:J:72:ARG:HH22	1.85	0.41
1:A:925:G:N7	1:A:927:G:N7	2.64	0.41
17:Q:10:GLY:HA3	17:Q:25:ILE:HD13	2.03	0.41
19:S:40:ILE:HD11	19:S:71:LEU:HD23	2.03	0.41
23:W:706:ASP:O	23:W:710:LYS:HG3	2.21	0.41
26:X:22:G:O2'	26:X:23:C:C5'	2.69	0.41
25:Z:125:LYS:NZ	26:X:26:G:H5'	2.09	0.41
25:Z:90:VAL:N	26:X:22:G:N2	2.69	0.41
1:A:1053:G:H5''	1:A:1055:A:OP1	2.21	0.41
1:A:17:U:O2'	1:A:1080:A:O5'	2.14	0.41
1:A:188:C:H2'	1:A:189:A:O4'	2.21	0.41
1:A:196:A:OP1	20:T:64:LYS:NZ	2.47	0.41
1:A:597:G:C2	1:A:644:U:C2	3.09	0.41
4:D:95:GLU:OE2	4:D:104:ARG:NH1	2.53	0.41
5:E:149:SER:H	5:E:152:MET:HG3	1.86	0.41
12:L:49:LEU:O	12:L:51:LYS:NZ	2.48	0.41
17:Q:59:VAL:HG21	17:Q:75:LEU:HD13	2.03	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:S:31:LEU:N	19:S:31:LEU:HD12	2.36	0.41
22:V:11:GLY:HA3	22:V:26:LEU:HA	2.03	0.41
22:V:6:THR:HG21	22:V:56:GLU:HG2	2.03	0.41
1:A:358:U:H5'	23:W:607:ARG:CZ	2.49	0.41
23:W:589:GLY:H	23:W:622:PRO:HB3	1.85	0.41
23:W:728:ILE:C	23:W:729:THR:CG2	2.89	0.41
23:W:824:ARG:HE	23:W:845:LEU:HB3	1.86	0.41
1:A:1049:U:H2'	14:N:3:LYS:HE3	2.03	0.40
1:A:1149:C:OP2	9:I:11:ARG:NH2	2.54	0.40
1:A:1239:A:H62	1:A:1299:A:N6	2.19	0.40
1:A:234:C:H4'	17:Q:66:PRO:HG3	2.03	0.40
1:A:925:G:C2'	1:A:927:G:O4'	2.64	0.40
1:A:6:G:H1'	5:E:124:LEU:HD11	1.85	0.40
21:U:4:ILE:HG23	21:U:18:ARG:NH1	2.36	0.40
23:W:425:THR:O	23:W:446:PRO:HB3	2.21	0.40
23:W:728:ILE:CG2	23:W:729:THR:N	2.84	0.40
23:W:815:CYS:N	27:X:101:FME:SD	2.93	0.40
26:X:47:U:C4	26:X:50:U:H5''	2.56	0.40
1:A:18:C:O2'	1:A:1078:U:H3'	2.22	0.40
1:A:182:A:N1	1:A:223:A:O2'	2.53	0.40
7:G:131:LYS:HA	7:G:135:VAL:HG21	2.02	0.40
9:I:19:VAL:HA	9:I:65:ILE:HG22	2.02	0.40
22:V:25:LYS:HD2	22:V:26:LEU:N	2.37	0.40
1:A:1095:U:H2'	1:A:1096:C:O4'	2.21	0.40
1:A:4:U:C2'	1:A:5:U:OP2	2.69	0.40
1:A:925:G:N3	1:A:927:G:N9	2.68	0.40
1:A:983:A:H5''	1:A:984:C:OP2	2.22	0.40
5:E:82:GLN:CD	5:E:150:PRO:HD3	2.41	0.40
6:F:45:ARG:HH21	6:F:102:MET:HG3	1.87	0.40
19:S:29:LYS:CB	19:S:30:PRO:CD	2.99	0.40
11:K:89:PRO:HG3	21:U:32:VAL:HG11	2.02	0.40
11:K:109:ASN:ND2	21:U:5:LYS:HB3	2.36	0.40
22:V:20:ALA:CB	22:V:36:ILE:HD12	2.49	0.40
25:Z:123:LYS:HB3	26:X:11:A:C2	2.55	0.40
1:A:1111:A:C5	2:B:130:THR:HG21	2.57	0.40
1:A:173:U:H6	1:A:198:G:HO2'	1.69	0.40
1:A:702:A:P	24:Y:64:LYS:HE2	2.62	0.40
1:A:1096:C:H5''	2:B:139:ARG:CZ	2.52	0.40
5:E:161:VAL:HG12	5:E:162:GLU:N	2.35	0.40
9:I:54:LEU:N	9:I:54:LEU:HD12	2.36	0.40
1:A:1312:G:H5'	19:S:6:LYS:CE	2.51	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:W:716:VAL:CG2	23:W:786:LEU:CD2	2.98	0.40
1:A:1390:U:H4'	1:A:1391:U:H5'	1.61	0.40
1:A:1449:C:H2'	1:A:1450:U:H5'	2.03	0.40
5:E:57:PRO:HA	5:E:60:ILE:CG1	2.51	0.40
10:J:18:ILE:CG2	10:J:19:ASP:N	2.85	0.40
14:N:62:ASN:HB3	14:N:73:PHE:CD2	2.56	0.40
23:W:719:LYS:HG3	23:W:721:ILE:HD11	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
2	B	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

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
16	P	80/102 (78%)	72 (90%)	7 (9%)	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%)	14 (20%)	8 (12%)	0	9
23	W	497/890 (56%)	479 (96%)	17 (3%)	1 (0%)	52	86
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	3070/3845 (80%)	2861 (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
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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
23	W	788	PRO
19	S	29	LYS
22	V	45	ILE
22	V	49	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	B	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
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

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
22	V	62/63 (98%)	54 (87%)	8 (13%)	5	28
23	W	402/713 (56%)	399 (99%)	3 (1%)	88	94
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%)	2500 (97%)	82 (3%)	50	76

All (82) 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
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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
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
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	861	CYS
24	Y	21	GLN
24	Y	26	LEU
24	Y	42	ASN
24	Y	43	LEU
24	Y	73	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
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 (14) such sidechains are listed below:

Mol	Chain	Res	Type
7	G	52	GLN
12	L	75	GLN
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
24	Y	69	GLN
25	Z	92	GLN
25	Z	108	GLN
25	Z	180	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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
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
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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
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
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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
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
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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
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
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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
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
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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
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
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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
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
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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
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 ⓘ

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	1.13	2 (11%)	21,38,41	2.37	7 (33%)
1	4OC	A	1402	1	15,23,24	0.65	0	21,32,35	1.90	3 (14%)
1	5MC	A	1407	1	14,22,23	1.48	1 (7%)	17,32,35	1.04	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	2.11	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	0.89	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	2.27	5 (23%)
1	2MG	A	966	1	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	0.58	0	4,11,13	1.16	0
26	H2U	X	20	26	17,21,22	0.79	0	23,30,33	1.32	5 (21%)
26	5MU	X	54	26	13,22,23	0.77	0	16,32,35	2.61	2 (12%)
26	PSU	X	55	26	15,21,22	1.39	1 (6%)	16,30,33	2.36	5 (31%)
26	4SU	X	8	26	12,21,22	1.15	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	-	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
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'	-4.39	1.48	1.52
26	X	8	4SU	C2-N3	-2.22	1.33	1.38
1	A	1519	MA6	C5-C4	2.51	1.46	1.40
26	X	8	4SU	O4'-C1'	2.58	1.44	1.41
1	A	1516	2MG	C5-C4	2.76	1.46	1.40
1	A	1516	2MG	C6-C5	2.90	1.47	1.41
1	A	1207	2MG	C5-C4	2.92	1.47	1.40
1	A	1518	MA6	C5-C4	2.93	1.47	1.40
1	A	1207	2MG	C6-C5	3.11	1.47	1.41
1	A	516	PSU	C4-N3	3.20	1.38	1.33
1	A	966	2MG	C5-C4	3.20	1.47	1.40
1	A	966	2MG	C6-C5	3.38	1.48	1.41
1	A	527	G7M	C6-C5	3.76	1.48	1.41
1	A	967	5MC	C5-C4	4.28	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(°)	Ideal(°)
26	X	54	5MU	C5-C4-N3	-7.46	119.09	125.35
1	A	1519	MA6	N3-C2-N1	-7.33	123.11	128.87
1	A	1402	4OC	CM4-N4-C4	-6.26	117.59	122.87
1	A	1518	MA6	N3-C2-N1	-5.94	124.20	128.87
1	A	527	G7M	C1'-N9-C4	-4.87	121.37	126.81
1	A	527	G7M	C5-C6-N1	-4.81	117.24	123.52
1	A	966	2MG	C5-C6-N1	-4.65	117.44	123.52
1	A	1207	2MG	C5-C6-N1	-4.33	117.86	123.52
1	A	966	2MG	CM2-N2-C2	-4.06	118.47	123.03
1	A	1519	MA6	C1'-N9-C4	-3.83	122.54	126.81
1	A	1207	2MG	CM2-N2-C2	-3.81	118.75	123.03
26	X	55	PSU	C5-C6-N1	-3.70	119.22	124.38
1	A	1516	2MG	C5-C6-N1	-3.60	118.82	123.52
26	X	8	4SU	C5-C4-N3	-3.42	119.94	123.56
1	A	527	G7M	N3-C2-N1	-3.30	123.07	127.56
1	A	1207	2MG	C6-C5-C4	-3.29	117.10	120.86
26	X	55	PSU	C5-C1'-C2'	-3.23	109.95	115.44
1	A	1516	2MG	C6-C5-C4	-3.23	117.17	120.86
1	A	1516	2MG	CM2-N2-C2	-3.06	119.59	123.03
1	A	966	2MG	C6-C5-C4	-2.86	117.59	120.86
26	X	20	H2U	C4-N3-C2	-2.62	123.39	125.77
26	X	8	4SU	O4'-C4'-C3'	-2.60	99.89	105.16
1	A	1207	2MG	N3-C2-N1	-2.56	122.36	126.19
1	A	516	PSU	C5-C6-N1	-2.45	120.96	124.38
1	A	527	G7M	C6-C5-C4	-2.45	118.06	120.86
1	A	1516	2MG	C1'-N9-C4	-2.39	124.14	126.81
26	X	20	H2U	C5-C6-N1	-2.25	108.29	110.76
26	X	8	4SU	C2'-C1'-N1	-2.13	107.74	113.46
1	A	966	2MG	N3-C2-N1	-2.09	123.05	126.19
1	A	1516	2MG	C2'-C1'-N9	-2.01	108.10	113.47
26	X	20	H2U	C3'-C2'-C1'	2.20	105.86	101.44
26	X	20	H2U	C6-N1-C2	2.21	125.58	122.16
26	X	55	PSU	O4'-C1'-C2'	2.30	107.18	104.69
1	A	516	PSU	O4'-C1'-C2'	2.38	107.26	104.69
1	A	1207	2MG	N2-C2-N1	2.39	119.72	116.94
1	A	1407	5MC	N4-C4-N3	2.53	120.63	116.92
26	X	20	H2U	C1'-N1-C2	2.54	121.75	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	2.91	118.56	117.42
26	X	8	4SU	O3'-C3'-C4'	3.17	120.47	111.01
26	X	55	PSU	C3'-C2'-C1'	3.40	105.74	101.71
1	A	967	5MC	N4-C4-N3	3.48	122.01	116.92

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1518	MA6	C2-N1-C6	4.13	121.39	111.64
1	A	1516	2MG	C6-N1-C2	4.16	121.20	115.24
1	A	1519	MA6	C2-N1-C6	4.36	121.93	111.64
1	A	1402	4OC	C2-N3-C4	4.47	121.12	115.43
1	A	1516	2MG	C2-N3-C4	4.72	120.17	114.99
1	A	966	2MG	C2-N3-C4	4.84	120.30	114.99
1	A	516	PSU	C4-N3-C2	4.94	119.28	115.16
1	A	966	2MG	C6-N1-C2	4.95	122.32	115.24
1	A	1207	2MG	C2-N3-C4	5.00	120.47	114.99
1	A	527	G7M	C6-N1-C2	5.08	121.84	115.88
1	A	1207	2MG	C6-N1-C2	5.21	122.70	115.24
26	X	55	PSU	C4-N3-C2	6.46	120.55	115.16
26	X	54	5MU	C4-N3-C2	6.55	120.62	115.16

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

9 monomers are involved in 29 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	1	0
1	A	527	G7M	2	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

There are no carbohydrates in this entry.

5.6 Ligand geometry

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	0.39	0	8,8,11	1.48	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(°)	Ideal(°)
27	X	101	FME	CA-N-CN	-2.68	120.66	124.12
27	X	101	FME	O1-CN-N	-2.64	120.77	124.80

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 19 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
27	X	101	FME	19	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
23	W	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	W	791:LYS	C	792:GLN	N	5.71
1	A	926:G	O3'	927:G	P	2.61
1	A	1390:U	O3'	1391:U	P	2.53