



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 07:18 AM UTC

PDB ID : 4OX9 / pdb_00004ox9
Title : Crystal structure of the aminoglycoside resistance methyltransferase NpmA bound to the 30S ribosomal subunit
Authors : Dunkle, J.A.; Conn, G.L.; Dunham, C.M.
Deposited on : 2014-02-04
Resolution : 3.80 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

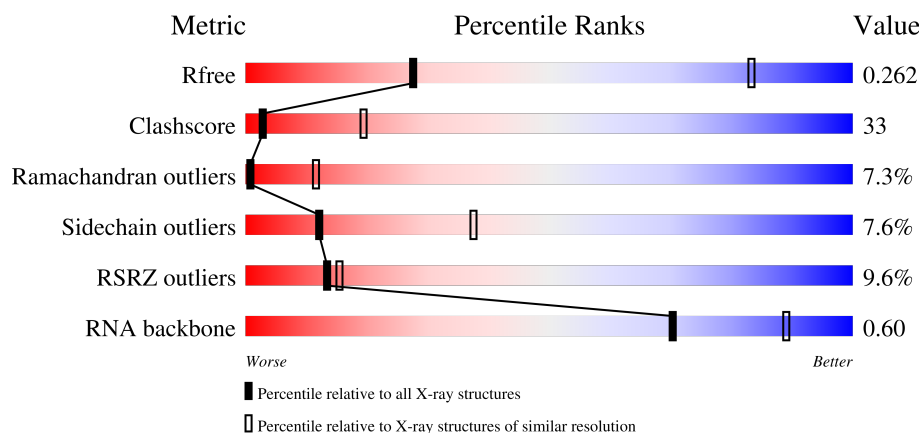
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.80 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1065 (3.96-3.64)
Clashscore	190562	1012 (3.94-3.66)
Ramachandran outliers	187476	1048 (3.96-3.64)
Sidechain outliers	187428	1043 (3.96-3.64)
RSRZ outliers	180081	1064 (3.96-3.64)
RNA backbone	3983	1007 (4.50-3.10)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. 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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	1513	6% 32% 52% 12% .
2	B	256	10% 24% 50% 15% . 9%
3	C	239	11% 25% 43% 16% . 14%
4	D	208	10% 38% 51% 10%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
5	E	161	
6	F	101	
7	G	155	
8	H	138	
9	I	128	
10	J	104	
11	K	129	
12	L	131	
13	M	126	
14	N	60	
15	O	88	
16	P	88	
17	Q	104	
18	R	88	
19	S	92	
20	T	106	
21	V	26	
22	Y	222	

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
23	MG	A	1604	-	-	-	X
23	MG	A	1611	-	-	-	X
23	MG	A	1620	-	-	-	X
23	MG	A	1621	-	-	-	X
23	MG	A	1624	-	-	-	X
23	MG	A	1626	-	-	-	X
23	MG	A	1629	-	-	-	X

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
23	MG	A	1637	-	-	-	X
23	MG	A	1647	-	-	-	X
23	MG	A	1650	-	-	-	X
23	MG	A	1652	-	-	-	X
23	MG	A	1677	-	-	-	X
23	MG	A	1699	-	-	-	X
23	MG	A	1703	-	-	-	X
23	MG	N	102	-	-	-	X

2 Entry composition

There are 25 unique types of molecules in this entry. The entry contains 53527 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1507	Total	C	N	O	P	0	0	0
			32394	14418	6002	10467	1507			

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	J	98	Total	C	N	O	S	0	0	0
			785	494	153	137	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	K	119	Total	C	N	O	S	0	0	0
			885	549	168	165	3			

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	Q	104	Total	C	N	O	S	0	0	0
			857	547	160	148	2			

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	S	80	Total	C	N	O	S	0	0	0
			647	414	119	112	2			

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

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

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

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

- Molecule 22 is a protein called 16S rRNA (adenine(1408)-N(1))-methyltransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	Y	219	Total	C	N	O	S	0	0	0
			1761	1138	294	328	1			

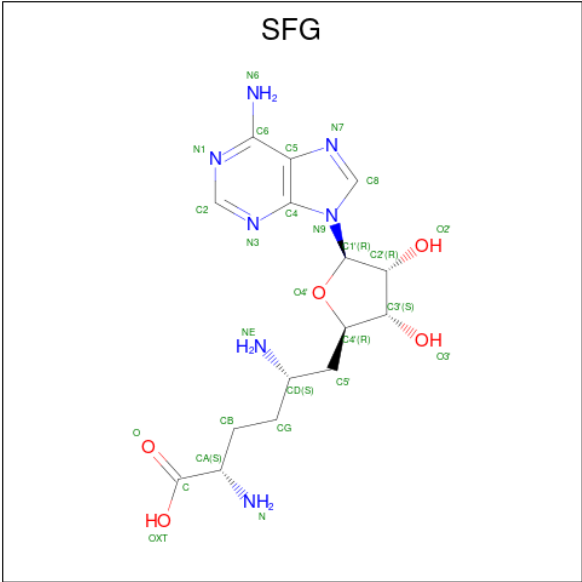
- Molecule 23 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
23	A	117	Total	Mg	0	0
			117	117		
23	B	1	Total	Mg	0	0
			1	1		
23	E	1	Total	Mg	0	0
			1	1		
23	N	1	Total	Mg	0	0
			1	1		

- Molecule 24 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
24	D	1	Total	Zn	0	0
			1	1		
24	N	1	Total	Zn	0	0
			1	1		

- Molecule 25 is SINEFUNGIN (CCD ID: SFG) (formula: C₁₅H₂₃N₇O₅).

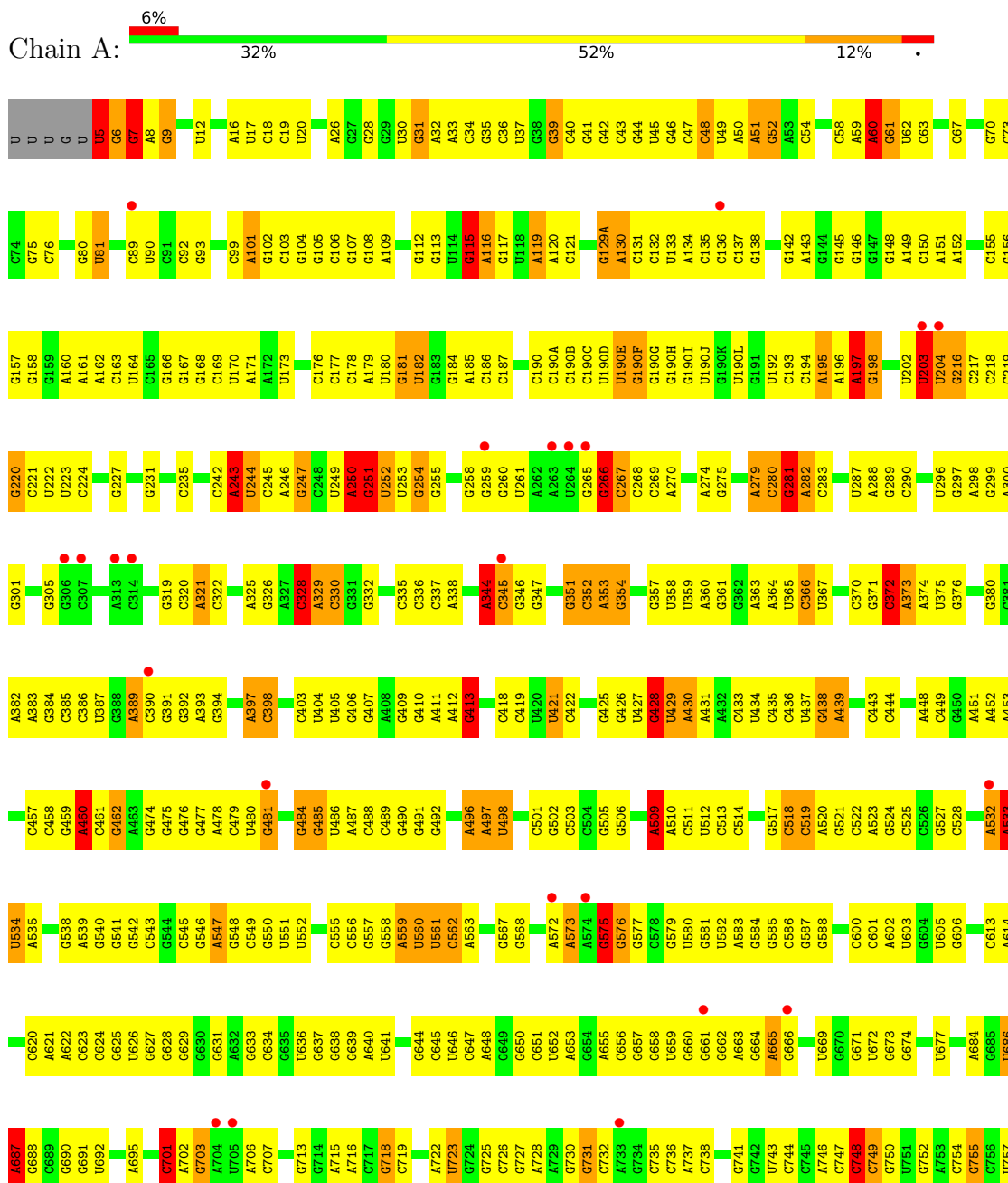


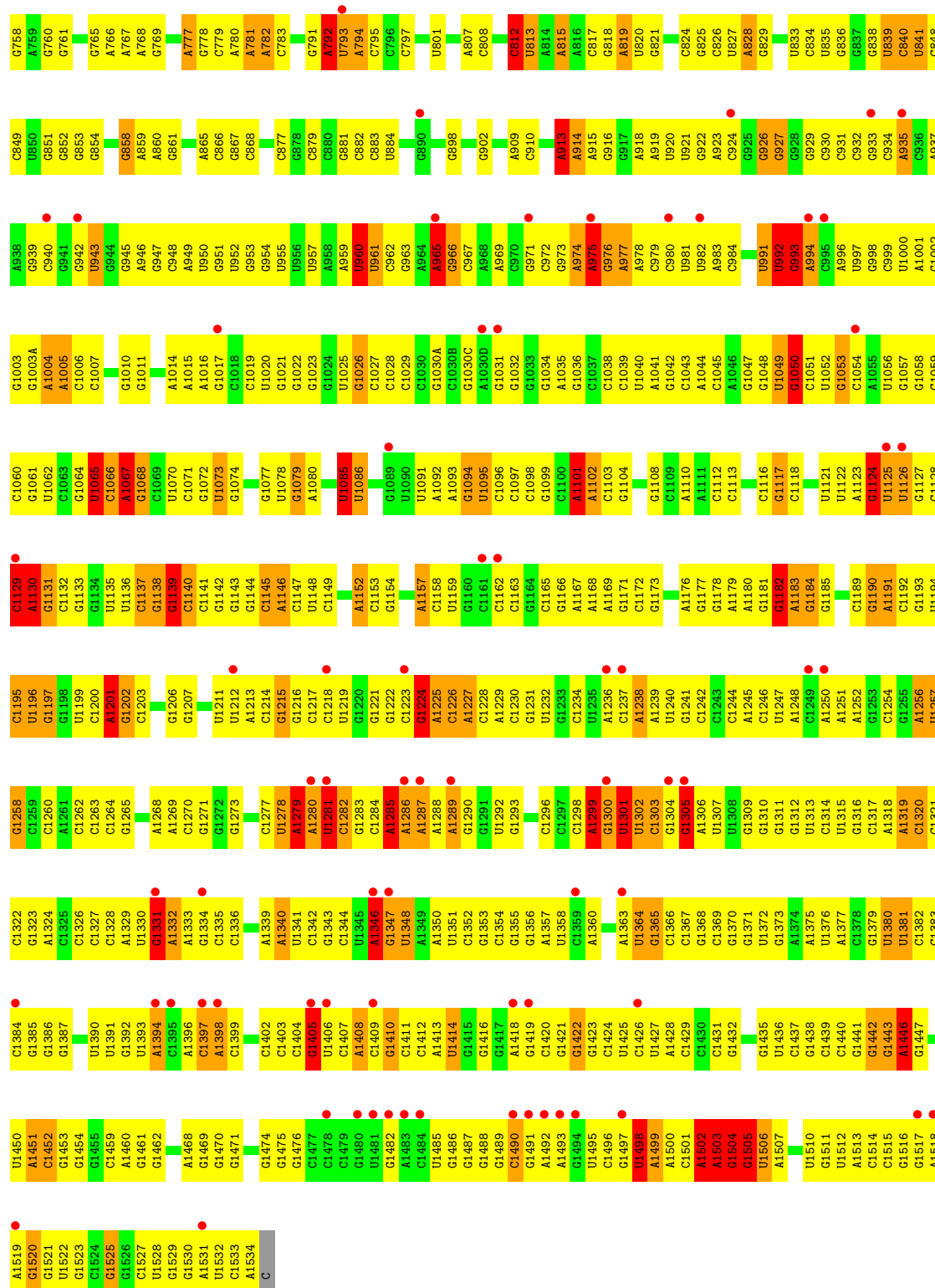
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
25	Y	1	Total	C	N	O	0	0
			27	15	7	5		

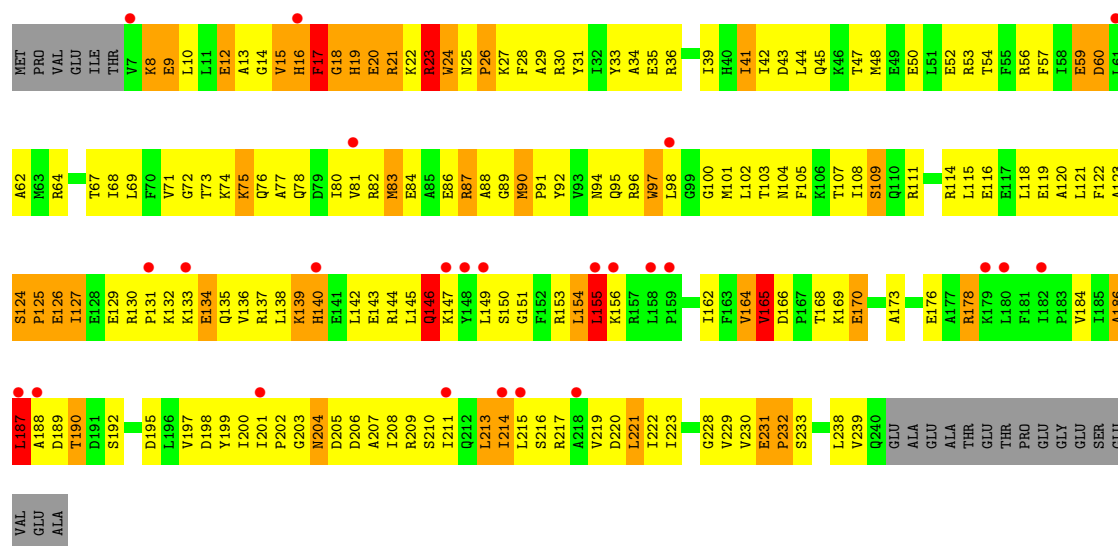
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

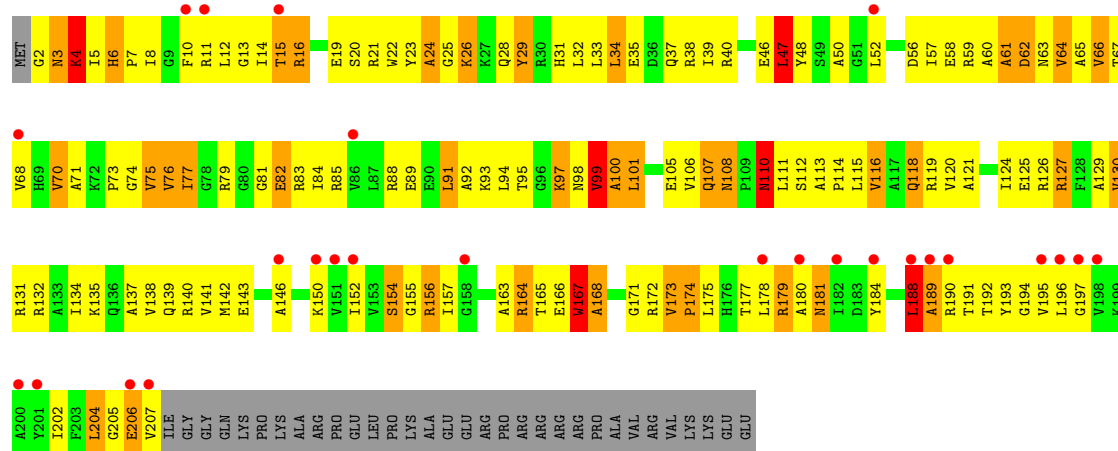
• Molecule 1: 16S rRNA



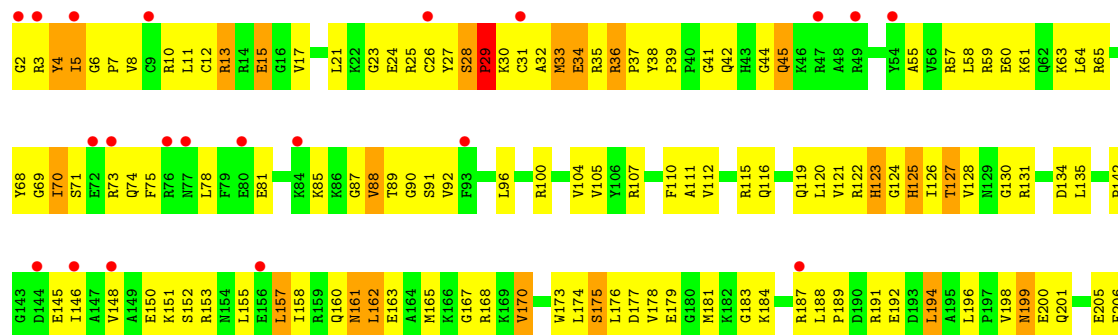




• Molecule 3: 30S ribosomal protein S3



• Molecule 4: 30S ribosomal protein S4



Y207
S208
R209

• Molecule 5: 30S ribosomal protein S5

Chain E:  3% 39% 40% 13% 7%

PRO GLU THR D5 F6 E7 M10 I11 I12 I13 I14 I15 I16 I17 I18 I19 M20 Q20 Q21 A21 G22 G23 G24 R25 R26 R27 A30 A31 L31 D36 D37 Q38 G39 R40 V41 G42 G43 G44 F45 G46 R47 V51 P52 L53 A54 V55 Q56 Q57 A58 G59 Y61 R64 R65 R66 R67 R68 V69

P70 L71 G74 I76 P77 E78 E79 I80 E81 E82 E83 I89 V90 L91 L92 K92 P93 I101 A102 G103 A104 V105 P106 A107 R108 V115 T116 D117 I118 L119 T120 K121 E122 L123 G124 S125 R126 N127 P128 I131 A132 M136 E137 Q141 L142 R143 T144 K145 A146 D147 V148 E149 R150

L151 R152 K153 G154 ALA ALA HIS ALA ALA ALA GLY

• Molecule 6: 30S ribosomal protein S6

Chain F:  8% 41% 50% 9%

H1 R2 R3 Y4 V5 V6 V7 W8 W9 L10 L15 D16 Q16 L19 A20 L21 E22 E23 E24 E25 I26 L30 Y33 G34 A35 R36 V37 E38 K39 V40 E41 E42 L43 G44 L45 R46 R47 L48 A49 Y50 P51 L52 A53 K54 D55 P56 Q57 G58 Y59 F60 Y63 G64 R65 E66 M67 P68

E69 D70 R71 W72 D74 L75 A76 R77 L78 L79 R80 R81 R82 R83 R84 R85 R86 R87 R88 R89 V90 V91 K92 S93 Q94 E95 P96 F97 M100 A101

• Molecule 7: 30S ribosomal protein S7

Chain G:  6% 41% 51% 8%

A2 R3 R4 R5 R6 A7 E8 V9 R10 R11 Q11 L12 Q13 Q14 D15 L16 V17 Y18 G19 R20 D21 V21 L22 V23 V24 A25 F26 I27 I30 M31 G34 L38 P112 E113 R114 R115 R116 A117 V118 R119 I120 A121 I49 I50 Q51 E52 K53 T54 G55 Q56 L59 Q64 A65 V66 E67 R68 V69 K70

P71 R72 V75 S77 R78 R79 R80 G81 G82 A83 R84 R85 Q86 R87 P93 R94 R95 A100 L101 R102 W103 L104 V105 Q106 A107 A108 R109 G110 R111 P112 E113 R114 R115 R116 A117 V118 R119 I120 A121 H122 M125 A134 V135 K138 E139 E142 R143 W144 A145 E146 V49 V69 N148

R149 A150 Y154 R155 A156

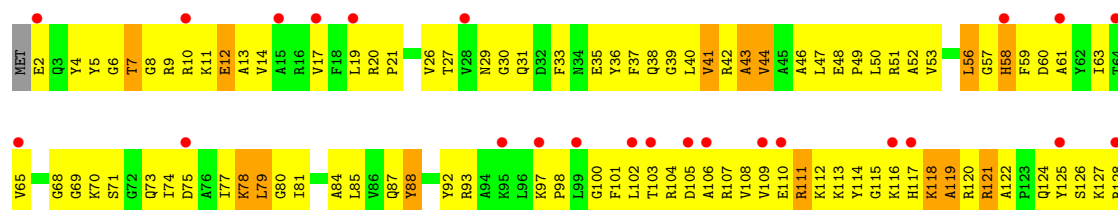
• Molecule 8: 30S ribosomal protein S8

Chain H:  4% 42% 45% 12%

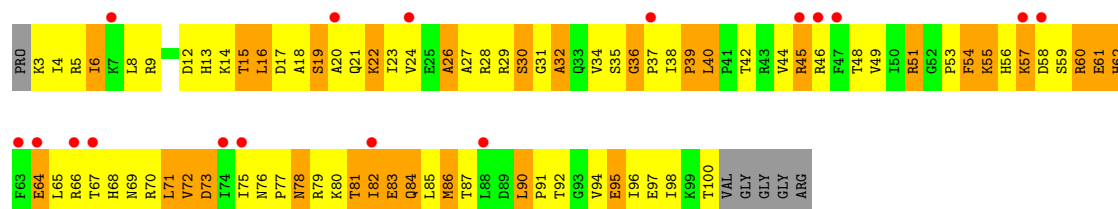
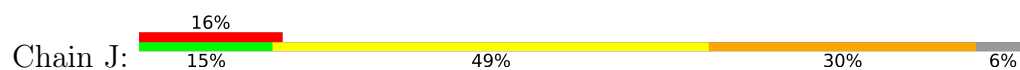
M1 L2 T3 I6 A7 D8 M9 L10 T11 T12 I13 I14 I15 A16 A17 R18 R19 V19 Y20 K21 E22 S23 S24 T24 V26 S29 R30 F31 K32 I35 L36 R37 L38 L39 I45 E49 R50 V51 D52 K56 L59 R60 V61 Y62 L63 K64 Y65 R68 D73 P74 R75 R76 P77



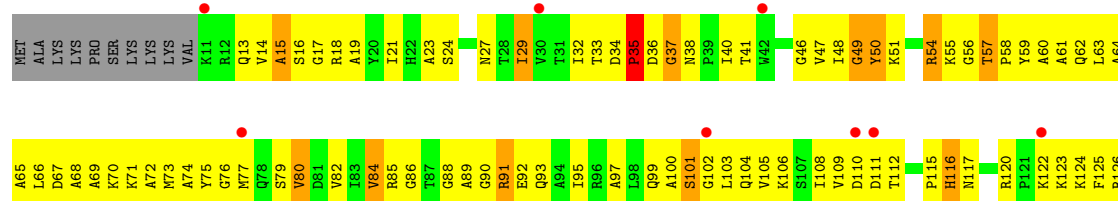
• Molecule 9: 30S ribosomal protein S9



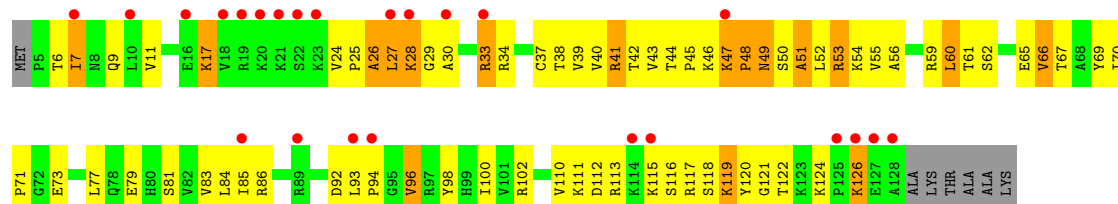
• Molecule 10: 30S ribosomal protein S10



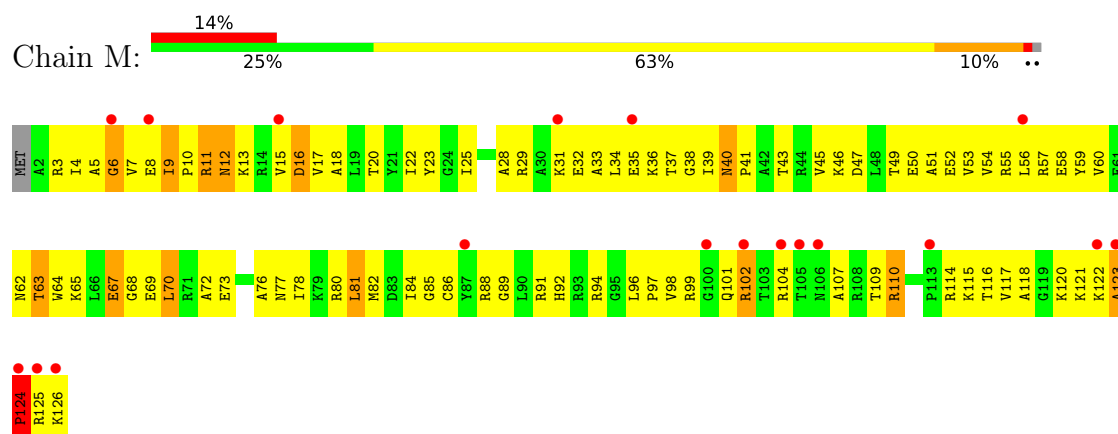
• Molecule 11: 30S ribosomal protein S11



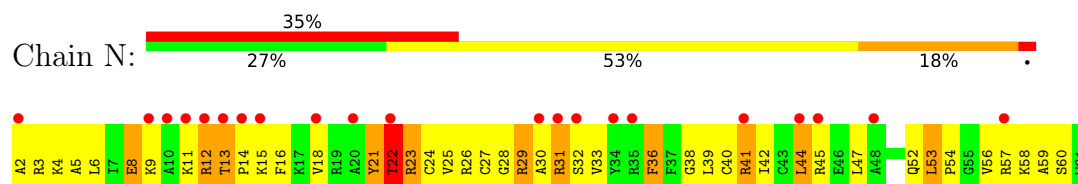
• Molecule 12: 30S ribosomal protein S12



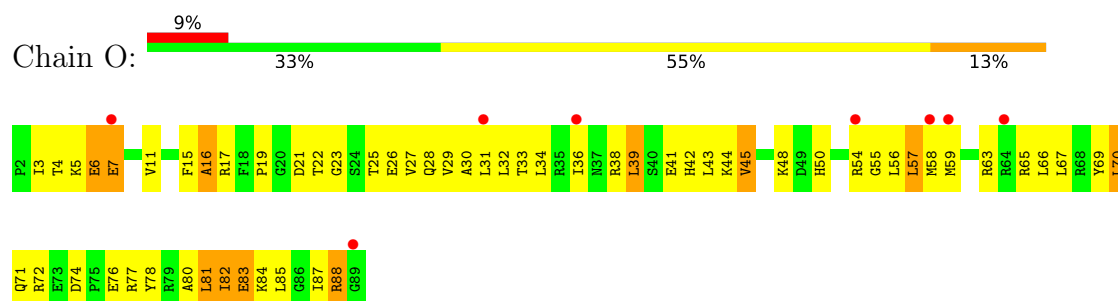
- Molecule 13: 30S ribosomal protein S13



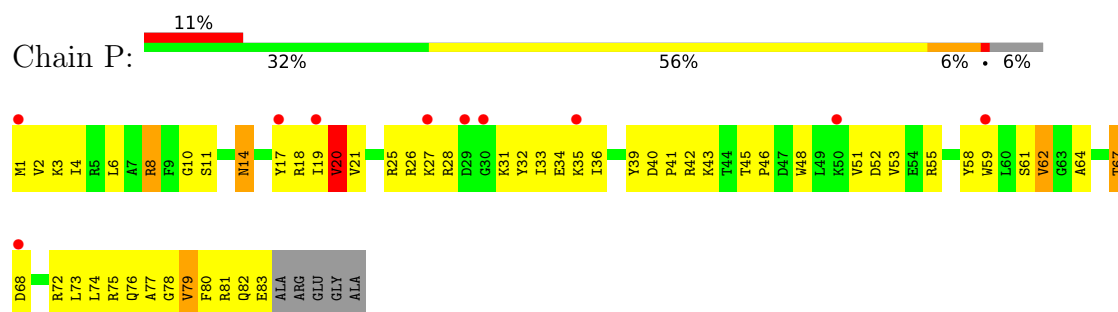
- Molecule 14: 30S ribosomal protein S14 type Z



- Molecule 15: 30S ribosomal protein S15

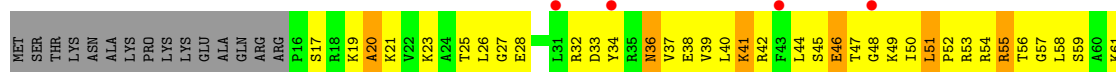
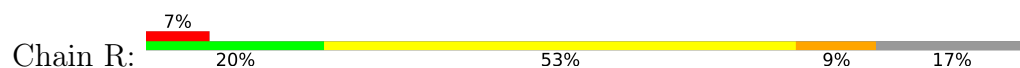


- Molecule 16: 30S ribosomal protein S16

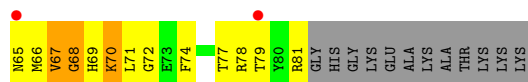
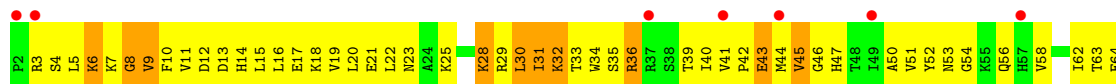
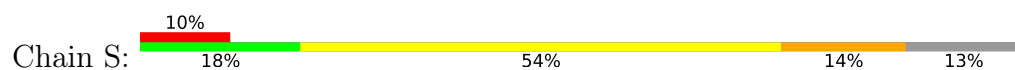




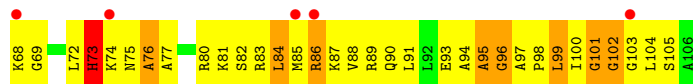
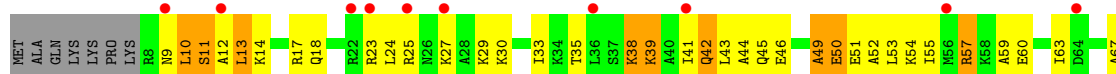
- Molecule 18: 30S ribosomal protein S18



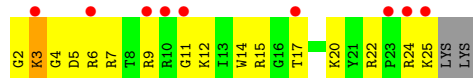
- Molecule 19: 30S ribosomal protein S19



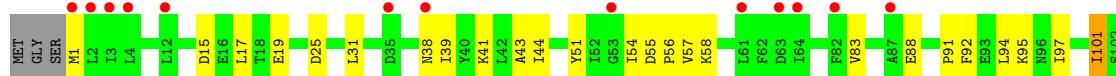
- Molecule 20: 30S ribosomal protein S20

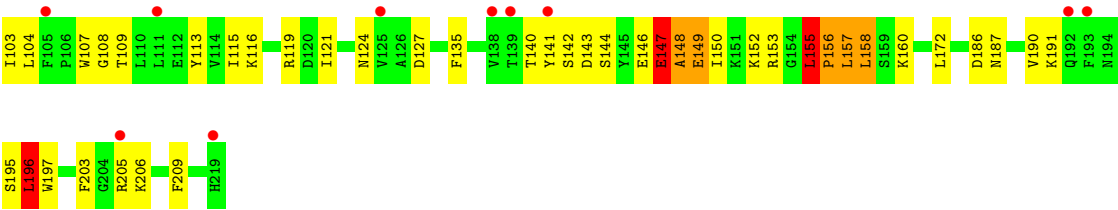


- Molecule 21: 30S ribosomal protein Thx



- Molecule 22: 16S rRNA (adenine(1408)-N(1))-methyltransferase





4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α , β , γ	403.52Å 403.52Å 176.61Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.72 – 3.80 49.72 – 3.80	Depositor EDS
% Data completeness (in resolution range)	99.7 (49.72-3.80) 94.0 (49.72-3.80)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.48 (at 3.77Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.233 , 0.257 0.238 , 0.262	Depositor DCC
R_{free} test set	7034 reflections (2.60%)	wwPDB-VP
Wilson B-factor (Å ²)	132.9	Xtriage
Anisotropy	0.320	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.26 , 60.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	53527	wwPDB-VP
Average B, all atoms (Å ²)	85.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.52% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: SFG, ZN, MG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.43	0/36262	0.72	79/56597 (0.1%)
2	B	0.56	4/1935 (0.2%)	1.10	17/2609 (0.7%)
3	C	0.54	3/1636 (0.2%)	1.04	11/2205 (0.5%)
4	D	0.53	4/1733 (0.2%)	0.96	7/2318 (0.3%)
5	E	0.92	2/1162 (0.2%)	1.23	14/1564 (0.9%)
6	F	0.53	1/856 (0.1%)	0.96	3/1154 (0.3%)
7	G	0.46	1/1276 (0.1%)	1.00	6/1709 (0.4%)
8	H	0.58	0/1136	1.13	9/1527 (0.6%)
9	I	0.41	0/1029	0.94	4/1379 (0.3%)
10	J	0.62	3/798 (0.4%)	1.13	8/1073 (0.7%)
11	K	0.51	0/900	1.07	4/1213 (0.3%)
12	L	0.52	0/986	1.08	4/1320 (0.3%)
13	M	0.50	1/1008 (0.1%)	0.99	2/1347 (0.1%)
14	N	0.44	0/501	1.21	7/664 (1.1%)
15	O	0.48	0/745	0.95	3/992 (0.3%)
16	P	0.52	0/716	1.17	8/963 (0.8%)
17	Q	0.59	1/870 (0.1%)	1.07	2/1159 (0.2%)
18	R	0.52	1/604 (0.2%)	0.97	4/801 (0.5%)
19	S	0.42	0/661	1.10	5/890 (0.6%)
20	T	0.58	1/765 (0.1%)	1.14	7/1007 (0.7%)
21	V	0.49	0/212	0.87	0/277
22	Y	0.62	0/1796	1.29	11/2418 (0.5%)
All	All	0.48	22/57587 (0.0%)	0.86	215/85186 (0.3%)

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
1	A	0	41

Continued on next page...

Continued from previous page...

Mol	Chain	#Chirality outliers	#Planarity outliers
22	Y	0	2
All	All	0	43

All (22) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	E	101	ILE	C-N	19.49	1.58	1.33
5	E	69	VAL	C-N	9.33	1.55	1.33
2	B	19	HIS	ND1-CE1	5.30	1.37	1.32
13	M	40	ASN	CG-OD1	5.26	1.33	1.23
17	Q	16	GLN	CD-OE1	5.26	1.33	1.23
6	F	94	GLN	CD-OE1	5.24	1.33	1.23
2	B	140	HIS	ND1-CE1	5.24	1.37	1.32
18	R	36	ASN	CG-OD1	5.21	1.33	1.23
10	J	78	ASN	CG-OD1	5.19	1.33	1.23
10	J	62	HIS	ND1-CE1	5.16	1.37	1.32
3	C	6	HIS	ND1-CE1	5.15	1.37	1.32
4	D	45	GLN	CD-OE1	5.15	1.33	1.23
10	J	84	GLN	CD-OE1	5.11	1.33	1.23
4	D	199	ASN	CG-OD1	5.09	1.33	1.23
7	G	106	GLN	CD-OE1	5.08	1.33	1.23
20	T	42	GLN	CD-OE1	5.06	1.33	1.23
4	D	199	ASN	CG-ND2	-5.04	1.22	1.33
3	C	118	GLN	CD-OE1	5.04	1.33	1.23
2	B	146	GLN	CD-OE1	5.03	1.33	1.23
3	C	110	ASN	CG-OD1	5.02	1.33	1.23
2	B	204	ASN	CG-OD1	5.01	1.33	1.23
4	D	161	ASN	CG-OD1	5.01	1.33	1.23

All (215) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	Y	155	LEU	CA-C-N	16.01	136.27	119.78
22	Y	155	LEU	C-N-CA	16.01	136.27	119.78
1	A	1498	U	C2'-C3'-O3'	14.53	131.29	109.50
1	A	243	A	C2'-C3'-O3'	13.88	130.32	109.50
1	A	559	A	C2'-C3'-O3'	13.42	129.63	109.50
3	C	167	TRP	N-CA-C	12.77	119.25	108.78
12	L	26	ALA	N-CA-C	-11.84	99.60	113.21
1	A	366	C	C2'-C3'-O3'	11.54	126.80	109.50
1	A	687	A	C2'-C3'-O3'	11.34	126.51	109.50
1	A	575	G	C2'-C3'-O3'	11.32	126.48	109.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	266	G	C2'-C3'-O3'	11.10	126.14	109.50
1	A	60	A	C2'-C3'-O3'	11.06	126.09	109.50
1	A	792	A	C2'-C3'-O3'	10.56	125.34	109.50
22	Y	157	LEU	N-CA-C	10.47	125.87	113.20
20	T	13	LEU	N-CA-C	-9.98	100.24	111.82
11	K	37	GLY	N-CA-C	9.90	125.37	113.79
5	E	23	GLY	N-CA-C	9.84	124.53	110.46
1	A	1067	A	C2'-C3'-O3'	9.84	124.25	109.50
14	N	31	ARG	N-CA-C	9.73	124.21	111.75
1	A	115	G	C2'-C3'-O3'	9.64	123.96	109.50
1	A	7	G	C2'-C3'-O3'	9.61	123.91	109.50
1	A	372	C	C2'-C3'-O3'	9.59	123.88	109.50
14	N	8	GLU	N-CA-C	-9.07	101.74	113.17
1	A	428	G	C2'-C3'-O3'	9.07	123.11	109.50
15	O	45	VAL	N-CA-C	-9.06	96.43	109.29
2	B	13	ALA	N-CA-C	-8.82	102.43	113.01
1	A	1299	A	N9-C1'-C2'	8.78	125.17	112.00
1	A	1380	U	C2'-C3'-O3'	8.62	122.43	109.50
1	A	484	G	C2'-C3'-O3'	8.45	122.17	109.50
1	A	960	U	C2'-C3'-O3'	8.25	121.87	109.50
7	G	154	TYR	N-CA-C	-8.19	101.45	112.26
22	Y	155	LEU	N-CA-C	8.19	127.91	109.81
16	P	27	LYS	N-CA-C	-8.05	99.88	110.43
11	K	116	HIS	N-CA-C	-8.05	101.30	112.25
2	B	59	GLU	N-CA-C	-8.02	102.49	111.07
1	A	1405	G	P-O3'-C3'	-7.98	108.22	120.20
5	E	21	ALA	N-CA-C	-7.90	100.39	110.19
1	A	1224	G	C2'-C3'-O3'	7.83	121.24	109.50
2	B	190	THR	N-CA-C	7.80	121.73	111.75
1	A	559	A	C4'-C3'-O3'	7.75	121.02	109.40
7	G	145	ALA	N-CA-C	-7.70	99.72	110.35
7	G	147	ALA	N-CA-C	-7.57	103.41	114.39
1	A	913	A	C2'-C3'-O3'	7.55	120.83	109.50
19	S	14	HIS	N-CA-C	-7.52	102.23	111.40
2	B	154	LEU	N-CA-C	7.45	119.05	111.07
5	E	64	ARG	N-CA-C	-7.44	97.56	109.76
2	B	187	LEU	N-CA-C	-7.41	96.47	108.41
22	Y	196	LEU	N-CA-C	-7.39	99.52	110.23
1	A	1301	U	C2'-C3'-O3'	7.33	120.50	109.50
14	N	21	TYR	N-CA-C	7.32	120.23	107.49
6	F	77	ARG	N-CA-C	-7.24	103.32	111.07
1	A	1364	U	C2'-C3'-O3'	7.21	120.32	109.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	250	A	C2'-C3'-O3'	7.20	120.30	109.50
1	A	748	C	C2'-C3'-O3'	7.19	120.29	109.50
1	A	1201	A	C2'-C3'-O3'	7.18	120.27	109.50
1	A	1505	G	C2'-C3'-O3'	7.18	124.47	113.70
5	E	20	GLN	N-CA-C	-7.17	98.45	109.14
1	A	1503	A	C2'-C3'-O3'	7.14	120.20	109.50
18	R	81	PHE	N-CA-C	-7.08	104.77	113.41
1	A	5	U	C2'-C3'-O3'	7.07	120.10	109.50
8	H	79	VAL	N-CA-C	-6.95	102.56	112.35
1	A	669	U	O3'-P-O5'	6.91	114.37	104.00
1	A	1335	C	C4'-C3'-O3'	-6.91	102.64	113.00
5	E	101	ILE	O-C-N	6.85	131.14	122.57
22	Y	149	GLU	N-CA-C	6.85	118.75	111.28
1	A	328	C	C2'-C3'-O3'	6.84	119.77	109.50
19	S	70	LYS	N-CA-C	6.84	119.78	108.49
1	A	1331	G	C2'-C3'-O3'	6.84	119.76	109.50
12	L	119	LYS	N-CA-C	-6.79	99.24	110.17
1	A	197	A	N9-C1'-C2'	6.78	124.17	114.00
4	D	33	MET	N-CA-C	-6.76	105.15	113.19
1	A	509	A	C2'-C3'-O3'	6.74	123.81	113.70
5	E	76	ILE	CA-C-N	6.70	126.65	119.28
5	E	76	ILE	C-N-CA	6.70	126.65	119.28
3	C	6	HIS	CB-CG-CD2	-6.70	122.50	131.20
11	K	91	ARG	N-CA-C	-6.66	105.29	113.41
20	T	44	ALA	N-CA-C	-6.65	104.04	111.28
1	A	460	A	N9-C1'-C2'	6.64	121.97	112.00
7	G	148	ASN	N-CA-C	-6.64	103.27	112.30
5	E	7	GLU	N-CA-C	-6.63	101.60	110.55
3	C	167	TRP	CB-CA-C	-6.62	107.54	117.07
1	A	1065	U	C2'-C3'-O3'	6.58	119.37	109.50
2	B	19	HIS	CB-CG-CD2	-6.57	122.66	131.20
1	A	965	A	C2'-C3'-O3'	6.55	119.33	109.50
1	A	243	A	C4'-C3'-O3'	6.54	119.21	109.40
2	B	105	PHE	N-CA-C	6.54	119.24	111.33
5	E	26	PHE	N-CA-C	6.53	120.18	110.52
1	A	1281	U	C2'-C3'-O3'	6.51	119.26	109.50
7	G	87	VAL	N-CA-C	6.50	114.22	108.63
2	B	140	HIS	CB-CG-CD2	-6.49	122.76	131.20
1	A	1085	U	C2'-C3'-O3'	6.48	119.21	109.50
22	Y	160	LYS	N-CA-C	-6.46	104.23	111.28
3	C	173	VAL	CA-C-N	6.46	127.92	119.84
3	C	173	VAL	C-N-CA	6.46	127.92	119.84

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	P	67	THR	N-CA-C	-6.46	101.97	110.43
10	J	62	HIS	CB-CG-CD2	-6.44	122.83	131.20
19	S	54	GLY	N-CA-C	-6.40	98.01	113.18
6	F	67	MET	N-CA-C	6.39	113.76	108.07
8	H	87	SER	N-CA-C	-6.32	100.93	110.28
12	L	61	THR	N-CA-C	-6.28	105.58	113.18
2	B	90	MET	N-CA-C	6.24	117.76	109.83
4	D	41	GLY	N-CA-C	6.21	120.51	112.68
12	L	66	VAL	N-CA-C	6.21	117.87	108.80
1	A	1124	G	N9-C1'-C2'	6.21	121.31	112.00
1	A	60	A	C4'-C3'-O3'	6.17	118.66	109.40
5	E	69	VAL	O-C-N	6.17	128.13	121.10
3	C	93	LYS	N-CA-C	-6.16	105.82	113.15
1	A	119	A	C2'-C3'-O3'	6.13	118.70	109.50
3	C	25	GLY	N-CA-C	6.09	119.69	110.18
17	Q	100	LYS	N-CA-C	-6.08	105.57	114.39
1	A	63	C	C5'-C4'-C3'	-6.08	106.89	116.00
20	T	76	ALA	N-CA-C	-6.04	104.69	111.28
1	A	1129	C	C2'-C3'-O3'	6.03	118.55	109.50
1	A	533	A	C2'-C3'-O3'	6.01	118.51	109.50
20	T	88	VAL	N-CA-C	6.00	116.17	110.53
1	A	115	G	N9-C1'-C2'	6.00	123.00	114.00
18	R	46	GLU	N-CA-C	-5.99	105.10	113.37
13	M	11	ARG	N-CA-C	5.96	118.24	109.24
10	J	51	ARG	N-CA-C	5.94	117.44	110.97
10	J	81	THR	N-CA-C	-5.92	104.74	111.07
19	S	36	ARG	N-CA-C	-5.92	106.04	113.20
4	D	12	CYS	N-CA-C	-5.90	104.03	111.11
1	A	413	G	C4'-C3'-O3'	-5.88	104.19	113.00
1	A	1504	G	C2'-C3'-O3'	5.87	118.30	109.50
13	M	107	ALA	N-CA-C	-5.83	105.04	113.21
22	Y	58	LYS	N-CA-C	5.83	118.59	111.82
8	H	75	ARG	CA-C-N	5.83	125.78	119.78
8	H	75	ARG	C-N-CA	5.83	125.78	119.78
1	A	701	C	C2'-C3'-O3'	5.81	118.22	109.50
16	P	77	ALA	N-CA-C	-5.79	106.83	112.97
6	F	60	PHE	N-CA-C	5.78	118.90	109.59
16	P	25	ARG	N-CA-C	5.77	120.16	113.18
15	O	44	LYS	N-CA-C	-5.76	105.13	111.82
1	A	281	G	C2'-C3'-O3'	5.76	118.13	109.50
10	J	62	HIS	N-CA-C	5.73	119.16	109.76
1	A	1182	G	C2'-C3'-O3'	5.72	118.08	109.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	19	HIS	CB-CG-ND1	5.71	131.27	122.70
1	A	1502	A	N9-C1'-C2'	5.71	122.56	114.00
8	H	56	LYS	CA-C-N	5.70	125.99	119.83
8	H	56	LYS	C-N-CA	5.70	125.99	119.83
5	E	101	ILE	CA-C-N	-5.69	112.55	121.87
5	E	101	ILE	C-N-CA	-5.69	112.55	121.87
4	D	11	LEU	N-CA-C	-5.68	104.70	111.69
19	S	34	TRP	N-CA-C	-5.66	106.14	113.16
1	A	993	G	C2'-C3'-O3'	5.65	117.98	109.50
4	D	13	ARG	N-CA-C	5.65	117.12	111.07
1	A	389	A	C5'-C4'-C3'	5.63	124.45	116.00
2	B	45	GLN	N-CA-C	-5.63	105.23	111.71
20	T	69	GLY	N-CA-C	-5.63	103.97	112.41
1	A	1285	A	C2'-C3'-O3'	5.62	117.94	109.50
1	A	413	G	N9-C1'-C2'	5.61	120.42	112.00
2	B	140	HIS	CB-CG-ND1	5.61	131.12	122.70
3	C	6	HIS	CB-CG-ND1	5.58	131.06	122.70
22	Y	147	GLU	N-CA-C	5.57	118.03	109.07
9	I	63	ILE	N-CA-C	5.56	116.29	108.17
1	A	266	G	C5'-C4'-C3'	-5.54	106.88	115.20
5	E	51	VAL	CB-CA-C	-5.52	108.45	113.70
2	B	23	ARG	N-CA-C	-5.52	99.04	110.80
1	A	812	C	C2'-C3'-O3'	5.51	117.77	109.50
2	B	186	ALA	N-CA-C	5.51	117.47	108.55
10	J	62	HIS	CB-CG-ND1	5.50	130.95	122.70
7	G	115	ARG	N-CA-C	5.49	117.69	108.96
3	C	99	VAL	N-CA-C	5.46	117.76	108.86
14	N	38	GLY	N-CA-C	-5.45	108.11	115.36
16	P	20	VAL	N-CA-C	5.42	117.90	108.95
20	T	38	LYS	N-CA-C	-5.42	105.06	110.97
1	A	1200	C	C2'-C3'-O3'	-5.42	105.58	113.70
4	D	28	SER	CA-C-N	5.41	126.60	119.84
4	D	28	SER	C-N-CA	5.41	126.60	119.84
14	N	53	LEU	CA-C-N	5.39	126.57	119.84
14	N	53	LEU	C-N-CA	5.39	126.57	119.84
1	A	1139	G	N9-C1'-C2'	5.38	120.07	112.00
5	E	11	ILE	N-CA-C	5.37	115.51	110.30
1	A	975	A	C2'-C3'-O3'	5.37	117.55	109.50
9	I	118	LYS	N-CA-C	5.34	116.71	110.41
22	Y	57	VAL	N-CA-C	5.33	114.42	106.85
15	O	5	LYS	N-CA-C	-5.33	105.47	111.28
1	A	687	A	C4'-C3'-O3'	5.31	117.36	109.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	167	TRP	CA-C-O	5.30	121.02	117.94
14	N	22	THR	N-CA-C	5.29	122.06	110.80
2	B	109	SER	N-CA-C	-5.28	105.20	111.69
3	C	4	LYS	N-CA-C	5.28	122.04	110.80
1	A	1299	A	C4'-C3'-O3'	-5.27	105.10	113.00
1	A	1050	G	C5'-C4'-C3'	5.27	123.90	116.00
1	A	661	G	C5'-C4'-C3'	-5.26	108.11	116.00
1	A	1346	A	C2'-C3'-O3'	5.26	117.39	109.50
1	A	344	A	C2'-C3'-O3'	5.25	117.38	109.50
10	J	18	ALA	N-CA-C	-5.25	104.46	111.24
18	R	51	LEU	CA-C-N	5.25	125.22	120.03
18	R	51	LEU	C-N-CA	5.25	125.22	120.03
20	T	75	ASN	N-CA-C	-5.23	106.85	113.18
11	K	88	GLY	N-CA-C	5.22	118.38	110.75
1	A	1279	A	N9-C1'-C2'	5.22	119.83	112.00
10	J	22	LYS	N-CA-C	-5.21	105.49	111.07
1	A	1305	G	N9-C1'-C2'	5.20	119.80	112.00
16	P	14	ASN	CA-C-N	5.20	125.12	119.76
16	P	14	ASN	C-N-CA	5.20	125.12	119.76
1	A	563	A	C4'-C3'-O3'	-5.19	105.21	113.00
1	A	1446	A	N9-C1'-C2'	5.19	119.79	112.00
2	B	134	GLU	N-CA-C	-5.17	106.65	113.12
1	A	197	A	C2'-C3'-O3'	5.17	117.25	109.50
1	A	1195	C	C4'-C3'-O3'	-5.15	105.27	113.00
1	A	992	U	C2'-C3'-O3'	5.15	117.22	109.50
1	A	1101	A	C2'-C3'-O3'	5.15	117.22	109.50
9	I	61	ALA	N-CA-C	5.15	117.75	108.48
1	A	1305	G	C4'-C3'-O3'	-5.14	105.29	113.00
8	H	103	VAL	N-CA-C	5.12	116.28	109.37
8	H	3	THR	N-CA-C	5.10	116.83	111.28
22	Y	156	PRO	CA-C-O	-5.09	115.66	121.56
8	H	135	CYS	N-CA-C	5.08	114.95	108.24
16	P	79	VAL	N-CA-C	-5.07	105.61	113.16
17	Q	49	GLU	N-CA-C	-5.06	106.69	112.86
10	J	55	LYS	N-CA-C	5.05	118.61	109.32
9	I	87	GLN	N-CA-C	-5.04	105.79	111.28
2	B	233	SER	N-CA-C	5.01	116.14	109.93

There are no chirality outliers.

All (43) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1048	G	Sidechain
1	A	1073	U	Sidechain
1	A	1079	G	Sidechain
1	A	1085	U	Sidechain
1	A	1092	A	Sidechain
1	A	1130	A	Sidechain
1	A	1139	G	Sidechain
1	A	12	U	Sidechain
1	A	1281	U	Sidechain
1	A	1289	A	Sidechain
1	A	1293	G	Sidechain
1	A	1299	A	Sidechain
1	A	1301	U	Sidechain
1	A	1305	G	Sidechain
1	A	1340	A	Sidechain
1	A	1360	A	Sidechain
1	A	1506	U	Sidechain
1	A	1525	G	Sidechain
1	A	197	A	Sidechain
1	A	203	U	Sidechain
1	A	220	G	Sidechain
1	A	231	G	Sidechain
1	A	249	U	Sidechain
1	A	250	A	Sidechain
1	A	251	G	Sidechain
1	A	254	G	Sidechain
1	A	266	G	Sidechain
1	A	274	A	Sidechain
1	A	290	C	Sidechain
1	A	297	G	Sidechain
1	A	305	G	Sidechain
1	A	380	G	Sidechain
1	A	413	G	Sidechain
1	A	481	G	Sidechain
1	A	573	A	Sidechain
1	A	575	G	Sidechain
1	A	603	U	Sidechain
1	A	727	G	Sidechain
1	A	879	C	Sidechain
1	A	898	G	Sidechain
1	A	982	U	Sidechain
22	Y	147	GLU	Peptide
22	Y	157	LEU	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	32394	0	16349	1175	0
2	B	1900	0	1951	223	0
3	C	1612	0	1677	224	0
4	D	1703	0	1764	143	0
5	E	1146	0	1207	108	0
6	F	843	0	857	70	0
7	G	1257	0	1296	95	0
8	H	1116	0	1177	70	0
9	I	1010	0	1037	119	0
10	J	785	0	823	128	0
11	K	885	0	904	88	0
12	L	970	0	1057	110	0
13	M	997	0	1072	122	0
14	N	492	0	529	76	0
15	O	734	0	771	64	0
16	P	700	0	720	59	0
17	Q	857	0	928	89	0
18	R	598	0	670	62	0
19	S	647	0	673	86	0
20	T	763	0	860	92	0
21	V	208	0	221	29	0
22	Y	1761	0	1792	51	0
23	A	117	0	0	0	0
23	B	1	0	0	0	0
23	E	1	0	0	0	0
23	N	1	0	0	0	0
24	D	1	0	0	0	0
24	N	1	0	0	0	0
25	Y	27	0	22	4	0
All	All	53527	0	38357	2996	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 33.

All (2996) 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)
9:I:57:GLY:O	9:I:58:HIS:HD2	1.22	1.18
20:T:54:LYS:HG3	20:T:100:ILE:CD1	1.73	1.18
12:L:41:ARG:HG2	12:L:42:THR:H	1.03	1.15
9:I:57:GLY:O	9:I:58:HIS:CD2	2.00	1.14
2:B:77:ALA:HB2	2:B:211:ILE:HD13	1.22	1.14
1:A:187:C:H1'	20:T:85:MET:HE2	1.17	1.12
1:A:1443:G:H5''	1:A:1446:A:H5'	1.28	1.10
9:I:8:GLY:HA2	9:I:79:LEU:HD12	1.32	1.09
4:D:36:ARG:H	4:D:37:PRO:HD3	1.19	1.07
11:K:110:ASP:HB2	18:R:88:LYS:HD2	1.35	1.07
1:A:243:A:H4'	1:A:244:U:H5'	1.36	1.05
4:D:150:GLU:HG3	4:D:153:ARG:HH21	1.19	1.04
10:J:51:ARG:HB2	10:J:59:SER:HB3	1.33	1.04
12:L:60:LEU:HD11	12:L:85:ILE:HD12	1.39	1.03
12:L:27:LEU:O	12:L:29:GLY:N	1.94	1.01
13:M:49:THR:HG22	13:M:51:ALA:H	1.26	1.00
1:A:664:G:H22	1:A:741:G:H1	1.08	0.99
2:B:178:ARG:HH11	2:B:178:ARG:HG3	1.21	0.99
3:C:52:LEU:HD23	3:C:52:LEU:H	1.26	0.99
8:H:113:SER:HB2	8:H:134:ILE:HD11	1.43	0.99
11:K:54:ARG:HB3	11:K:54:ARG:HH11	1.26	0.99
1:A:187:C:C1'	20:T:85:MET:HE2	1.93	0.98
19:S:28:LYS:HG2	19:S:29:ARG:H	1.26	0.98
1:A:539:A:OP2	12:L:115:LYS:HE2	1.63	0.97
20:T:50:GLU:O	20:T:100:ILE:HD12	1.62	0.97
3:C:6:HIS:HE1	3:C:8:ILE:HD12	1.25	0.97
20:T:54:LYS:HG3	20:T:100:ILE:HD13	0.99	0.97
1:A:1116:C:H2'	1:A:1117:G:H5''	1.46	0.97
1:A:1057:G:H5''	3:C:154:SER:HB2	1.47	0.96
3:C:91:LEU:HD21	3:C:99:VAL:HG13	1.48	0.96
20:T:50:GLU:HG3	20:T:99:LEU:CD1	1.96	0.96
20:T:53:LEU:CD1	20:T:101:GLY:N	2.30	0.95
12:L:27:LEU:C	12:L:29:GLY:H	1.74	0.95
20:T:54:LYS:CG	20:T:100:ILE:HD13	1.95	0.95
11:K:54:ARG:O	11:K:57:THR:HG22	1.66	0.95
1:A:1190:G:OP1	3:C:4:LYS:HA	1.67	0.94
3:C:14:ILE:HG22	3:C:15:THR:H	1.32	0.93
1:A:187:C:H1'	20:T:85:MET:CE	1.98	0.93
12:L:41:ARG:HG2	12:L:42:THR:N	1.83	0.93
17:Q:97:SER:HB2	17:Q:102:GLY:C	1.94	0.93
19:S:31:ILE:HG22	19:S:32:LYS:H	1.34	0.93
1:A:1256:A:H4'	1:A:1257:U:H5'	1.51	0.93

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:T:50:GLU:HG3	20:T:99:LEU:HD12	1.51	0.92
2:B:124:SER:HB2	2:B:125:PRO:HD2	1.49	0.92
16:P:58:TYR:O	16:P:61:SER:HB3	1.68	0.92
1:A:1137:C:H4'	1:A:1138:G:C2	2.05	0.92
3:C:131:ARG:HG2	3:C:135:LYS:HE3	1.50	0.92
1:A:35:G:O2'	12:L:118:SER:O	1.88	0.92
12:L:28:LYS:HD2	12:L:33:ARG:HH12	1.35	0.92
1:A:1086:U:H3	1:A:1099:G:H22	1.08	0.91
1:A:838:G:H2'	1:A:839:U:H5''	1.52	0.91
1:A:1305:G:HO2'	1:A:1306:A:H8	0.92	0.91
1:A:942:G:C2'	1:A:943:U:H5'	2.01	0.91
1:A:1101:A:H4'	1:A:1102:A:O5'	1.65	0.91
3:C:195:VAL:O	3:C:196:LEU:HD23	1.69	0.91
9:I:70:LYS:O	9:I:74:ILE:HG13	1.72	0.90
1:A:1502:A:H2	1:A:1505:G:H1	1.20	0.90
1:A:1394:A:C6	1:A:1501:C:H4'	2.06	0.90
3:C:58:GLU:HB3	10:J:92:THR:HG21	1.51	0.90
5:E:81:GLU:HG2	5:E:90:VAL:HG22	1.52	0.90
1:A:1497:G:O2'	1:A:1498:U:H5'	1.71	0.89
1:A:235:C:H5'	17:Q:70:ARG:HG2	1.51	0.89
10:J:8:LEU:HD21	10:J:96:ILE:HG12	1.54	0.89
2:B:91:PRO:HG2	2:B:155:LEU:HD23	1.54	0.89
2:B:59:GLU:HG2	2:B:221:LEU:HD11	1.51	0.88
1:A:186:C:O3'	20:T:82:SER:HB3	1.74	0.87
1:A:1125:U:H3	10:J:5:ARG:HH21	1.18	0.87
4:D:36:ARG:N	4:D:37:PRO:HD3	1.88	0.87
1:A:1435:G:H2'	1:A:1436:U:C6	2.10	0.86
4:D:150:GLU:HG3	4:D:153:ARG:NH2	1.90	0.86
13:M:10:PRO:HB2	13:M:18:ALA:HB1	1.57	0.86
3:C:70:VAL:HG21	3:C:76:VAL:HG21	1.58	0.86
2:B:116:GLU:HG2	2:B:153:ARG:HH12	1.39	0.86
12:L:25:PRO:C	12:L:27:LEU:H	1.79	0.86
6:F:30:LEU:HD23	6:F:75:LEU:HD21	1.57	0.86
5:E:115:VAL:HG11	5:E:118:ILE:HG13	1.57	0.86
19:S:41:VAL:HG22	19:S:44:MET:HE3	1.56	0.86
5:E:51:VAL:HB	5:E:52:PRO:HD3	1.55	0.85
6:F:10:LEU:HD12	6:F:59:TYR:HB3	1.55	0.85
1:A:1305:G:O2'	1:A:1306:A:H8	1.58	0.85
1:A:1394:A:C5	1:A:1501:C:H4'	2.11	0.85
1:A:1489:G:H2'	1:A:1490:C:H5''	1.59	0.85
10:J:22:LYS:HE2	10:J:90:LEU:HD12	1.57	0.85

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:190:ARG:HB3	3:C:190:ARG:NH1	1.92	0.85
2:B:102:LEU:HD21	2:B:162:ILE:HD11	1.57	0.85
6:F:95:GLU:CD	6:F:95:GLU:H	1.85	0.84
10:J:49:VAL:HG13	14:N:41:ARG:HB2	1.57	0.84
1:A:250:A:H4'	1:A:251:G:O5'	1.76	0.84
1:A:1131:G:H1	1:A:1143:G:H21	1.22	0.84
1:A:1064:G:H4'	1:A:1065:U:H5'	1.58	0.84
1:A:1497:G:C2'	1:A:1498:U:H5'	2.08	0.84
13:M:3:ARG:HG2	13:M:9:ILE:HG23	1.56	0.84
3:C:64:VAL:HB	3:C:99:VAL:HB	1.59	0.84
13:M:50:GLU:O	13:M:54:VAL:HG23	1.77	0.84
17:Q:27:PHE:CZ	17:Q:36:ILE:HD11	2.12	0.84
4:D:104:VAL:HG11	4:D:146:ILE:HD12	1.58	0.84
9:I:8:GLY:HA2	9:I:79:LEU:CD1	2.07	0.84
5:E:105:VAL:HB	5:E:106:PRO:HD3	1.60	0.83
6:F:36:ARG:HH12	6:F:38:GLU:HG2	1.43	0.83
1:A:1421:G:C2'	1:A:1422:G:H5'	2.08	0.83
3:C:190:ARG:HB3	3:C:190:ARG:HH11	1.44	0.83
3:C:172:ARG:HH12	3:C:174:PRO:HG3	1.43	0.83
4:D:61:LYS:HD2	4:D:207:TYR:OH	1.78	0.83
20:T:53:LEU:HD13	20:T:101:GLY:N	1.92	0.83
1:A:135:C:O2	16:P:1:MET:HB2	1.78	0.82
1:A:1281:U:H5'	1:A:1282:C:H5	1.44	0.82
1:A:1356:G:H2'	1:A:1357:A:C8	2.15	0.82
3:C:91:LEU:HD23	3:C:92:ALA:N	1.95	0.82
7:G:75:VAL:CG1	7:G:86:GLN:HB3	2.10	0.82
3:C:191:THR:HG22	3:C:193:TYR:H	1.44	0.82
4:D:25:ARG:C	4:D:27:TYR:H	1.85	0.82
3:C:8:ILE:HG23	3:C:16:ARG:HG2	1.60	0.82
15:O:78:TYR:CZ	15:O:82:ILE:HD11	2.15	0.81
4:D:150:GLU:H	4:D:150:GLU:CD	1.86	0.81
13:M:78:ILE:HA	13:M:81:LEU:HD21	1.62	0.81
19:S:29:ARG:O	19:S:30:LEU:HB2	1.80	0.81
4:D:150:GLU:HA	4:D:153:ARG:HE	1.44	0.81
6:F:30:LEU:HB3	6:F:35:ALA:HB3	1.62	0.81
10:J:19:SER:HB2	10:J:91:PRO:HG3	1.60	0.81
12:L:41:ARG:CG	12:L:42:THR:H	1.88	0.81
13:M:22:ILE:HD12	13:M:25:ILE:HD12	1.61	0.81
3:C:107:GLN:H	3:C:107:GLN:CD	1.87	0.81
2:B:101:MET:HA	2:B:108:ILE:HD12	1.63	0.81
1:A:1060:C:C5	3:C:2:GLY:HA3	2.14	0.81

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:70:ILE:HD13	12:L:77:LEU:HD12	1.63	0.81
2:B:27:LYS:HD3	2:B:195:ASP:OD2	1.81	0.80
17:Q:95:TYR:C	17:Q:97:SER:H	1.89	0.80
1:A:1410:G:H2'	1:A:1411:C:H5'	1.62	0.80
18:R:55:ARG:NH1	18:R:55:ARG:HB3	1.94	0.80
1:A:1285:A:H4'	1:A:1286:A:O5'	1.82	0.80
1:A:673:G:H2'	1:A:674:G:C8	2.17	0.80
7:G:75:VAL:HG11	7:G:86:GLN:HB3	1.64	0.80
10:J:8:LEU:CD2	10:J:96:ILE:HG12	2.11	0.79
20:T:53:LEU:HD13	20:T:101:GLY:CA	2.12	0.79
5:E:118:ILE:HG22	5:E:119:LEU:N	1.95	0.79
12:L:126:LYS:H	12:L:126:LYS:HD2	1.47	0.79
1:A:80:G:H3'	1:A:81:U:H5''	1.62	0.79
11:K:54:ARG:HB3	11:K:54:ARG:NH1	1.97	0.79
14:N:14:PRO:C	14:N:16:PHE:H	1.86	0.79
2:B:8:LYS:O	2:B:9:GLU:HB2	1.81	0.79
12:L:67:THR:HG22	12:L:96:VAL:HG13	1.63	0.79
12:L:120:TYR:O	12:L:122:THR:HG23	1.83	0.79
1:A:942:G:N1	1:A:1341:U:O2	2.13	0.79
1:A:1412:C:H42	1:A:1488:G:H1	1.31	0.78
2:B:132:LYS:HA	2:B:135:GLN:HB3	1.63	0.78
1:A:1116:C:C2'	1:A:1117:G:H5''	2.12	0.78
3:C:15:THR:O	3:C:16:ARG:HB2	1.82	0.78
2:B:84:GLU:OE1	2:B:216:SER:HA	1.83	0.78
5:E:43:LEU:HB2	5:E:136:MET:HE2	1.65	0.78
1:A:838:G:C2'	1:A:839:U:H5''	2.14	0.78
22:Y:108:GLY:HA2	22:Y:153:ARG:HH21	1.48	0.78
19:S:31:ILE:HG22	19:S:32:LYS:N	1.99	0.78
1:A:942:G:H2'	1:A:943:U:H5'	1.66	0.78
16:P:21:VAL:HG21	16:P:59:TRP:CD1	2.19	0.78
1:A:1226:C:H4'	1:A:1227:A:OP1	1.84	0.78
15:O:17:ARG:HG3	15:O:17:ARG:HH11	1.49	0.77
2:B:197:VAL:HB	2:B:200:ILE:HG12	1.66	0.77
5:E:64:ARG:O	5:E:65:ASN:HB3	1.84	0.77
7:G:66:VAL:HG12	7:G:70:LYS:HE3	1.65	0.77
1:A:761:G:H1'	17:Q:104:LYS:O	1.84	0.77
1:A:130:A:OP2	1:A:190(E):U:H2'	1.84	0.77
1:A:1250:A:H4'	9:I:68:GLY:H	1.47	0.77
1:A:1366:C:H2'	1:A:1367:C:H6	1.48	0.77
3:C:150:LYS:HE2	3:C:152:ILE:HD11	1.67	0.77
7:G:95:ARG:HG3	7:G:95:ARG:HH11	1.50	0.77

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:118:LYS:O	9:I:119:ALA:HB3	1.85	0.77
12:L:27:LEU:HG	12:L:28:LYS:H	1.49	0.77
15:O:16:ALA:HB1	15:O:21:ASP:HB3	1.64	0.77
1:A:243:A:C4'	1:A:244:U:H5'	2.13	0.77
3:C:110:ASN:O	3:C:111:LEU:HD23	1.85	0.77
1:A:1152:A:H5''	10:J:13:HIS:CD2	2.19	0.77
6:F:86:ARG:O	6:F:87:ARG:HG2	1.85	0.77
13:M:4:ILE:HG22	13:M:5:ALA:N	2.00	0.77
1:A:839:U:H5'	1:A:840:C:H5	1.50	0.76
8:H:90:GLY:O	8:H:91:ARG:HB2	1.82	0.76
1:A:1236:A:H4'	1:A:1304:G:H4'	1.67	0.76
2:B:57:PHE:O	2:B:60:ASP:HB3	1.85	0.76
3:C:6:HIS:CE1	3:C:8:ILE:HD12	2.17	0.76
12:L:126:LYS:H	12:L:126:LYS:CD	1.96	0.76
20:T:14:LYS:O	20:T:18:GLN:HG3	1.86	0.76
1:A:1256:A:N6	1:A:1278:U:H1'	2.00	0.76
21:V:5:ASP:O	21:V:11:GLY:HA3	1.85	0.76
17:Q:97:SER:OG	17:Q:103:GLY:HA2	1.85	0.76
2:B:139:LYS:O	2:B:143:GLU:HG2	1.86	0.76
16:P:74:LEU:O	16:P:79:VAL:HG23	1.85	0.76
3:C:19:GLU:HB3	3:C:40:ARG:HH21	1.50	0.76
1:A:328:C:O2	1:A:328:C:H2'	1.85	0.76
1:A:657:G:H4'	15:O:28:GLN:HG2	1.68	0.76
1:A:1025:U:H2'	1:A:1026:G:C8	2.21	0.76
2:B:36:ARG:HD2	2:B:41:ILE:HD12	1.68	0.76
10:J:82:ILE:O	10:J:86:MET:HB2	1.86	0.75
22:Y:109:THR:OG1	25:Y:301:SFG:N6	2.19	0.75
3:C:50:ALA:HB1	3:C:70:VAL:HG11	1.68	0.75
22:Y:156:PRO:HB2	22:Y:158:LEU:HD23	1.69	0.75
1:A:80:G:H3'	1:A:81:U:C5'	2.16	0.75
1:A:187:C:C1'	20:T:85:MET:CE	2.62	0.75
1:A:839:U:H5'	1:A:840:C:C5	2.22	0.75
10:J:96:ILE:HG22	10:J:97:GLU:H	1.52	0.75
19:S:16:LEU:O	19:S:19:VAL:HG12	1.87	0.75
3:C:116:VAL:HG21	3:C:202:ILE:HD11	1.67	0.75
12:L:48:PRO:HG2	12:L:49:ASN:H	1.52	0.75
13:M:3:ARG:HA	13:M:8:GLU:O	1.86	0.75
1:A:840:C:H5''	1:A:841:U:OP1	1.85	0.75
2:B:130:ARG:HH22	3:C:179:ARG:HH12	1.35	0.75
1:A:351:G:H4'	1:A:352:C:OP1	1.85	0.75
12:L:28:LYS:CD	12:L:33:ARG:HH12	1.99	0.74

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1234:C:H5'	1:A:1365:G:OP1	1.86	0.74
4:D:162:LEU:HD13	4:D:181:MET:HG2	1.68	0.74
1:A:579:G:H5'	1:A:728:A:H1'	1.69	0.74
1:A:1391:U:H2'	1:A:1392:G:C8	2.22	0.74
13:M:88:ARG:HD2	19:S:3:ARG:HH21	1.50	0.74
17:Q:95:TYR:O	17:Q:97:SER:N	2.19	0.74
12:L:28:LYS:HD2	12:L:33:ARG:NH1	2.02	0.74
19:S:40:ILE:HD13	19:S:62:ILE:HD13	1.68	0.74
19:S:17:GLU:O	19:S:21:GLU:HG3	1.87	0.74
20:T:53:LEU:CD1	20:T:101:GLY:H	1.97	0.74
1:A:1421:G:H2'	1:A:1422:G:H5'	1.70	0.74
2:B:16:HIS:NE2	2:B:214:ILE:HG12	2.02	0.74
2:B:72:GLY:HA3	2:B:81:VAL:HG21	1.69	0.74
2:B:77:ALA:HB2	2:B:211:ILE:CD1	2.11	0.74
2:B:178:ARG:HG3	2:B:178:ARG:NH1	1.92	0.74
15:O:33:THR:HG23	15:O:63:ARG:NH1	2.03	0.74
18:R:55:ARG:HB3	18:R:55:ARG:HH11	1.50	0.74
1:A:942:G:H2'	1:A:943:U:H6	1.51	0.74
1:A:1064:G:H4'	1:A:1065:U:C5'	2.18	0.74
1:A:1117:G:H4'	9:I:104:ARG:NH1	2.03	0.74
4:D:64:LEU:HD12	4:D:75:PHE:HZ	1.52	0.74
1:A:748:C:H1'	1:A:749:C:H5	1.53	0.74
1:A:792:A:H4'	1:A:793:U:H5''	1.68	0.74
6:F:69:GLU:HA	6:F:72:VAL:HG23	1.70	0.74
1:A:1125:U:H3	10:J:5:ARG:NH2	1.85	0.73
3:C:52:LEU:HD23	3:C:52:LEU:N	2.02	0.73
7:G:23:VAL:HG12	7:G:27:ILE:HD11	1.70	0.73
1:A:992:U:H4'	1:A:993:G:O5'	1.86	0.73
1:A:1279:A:H5''	1:A:1280:A:OP1	1.88	0.73
2:B:23:ARG:NH1	2:B:24:TRP:N	2.35	0.73
22:Y:147:GLU:HB2	22:Y:150:ILE:HG12	1.71	0.73
3:C:52:LEU:H	3:C:52:LEU:CD2	2.00	0.73
2:B:95:GLN:O	2:B:96:ARG:HD2	1.88	0.73
21:V:6:ARG:HD3	21:V:15:ARG:HH12	1.52	0.73
2:B:91:PRO:HG3	2:B:154:LEU:HB2	1.69	0.73
3:C:13:GLY:HA3	14:N:57:ARG:HH21	1.54	0.73
12:L:59:ARG:HD3	12:L:65:GLU:HG3	1.68	0.73
6:F:26:ILE:HG21	6:F:63:TYR:HE2	1.54	0.73
9:I:44:VAL:HG13	9:I:51:ARG:HH22	1.53	0.73
2:B:23:ARG:HH11	2:B:24:TRP:N	1.86	0.72
2:B:116:GLU:HG2	2:B:153:ARG:NH1	2.04	0.72

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:1:MET:HG2	8:H:2:LEU:N	2.05	0.72
1:A:1407:C:O2'	1:A:1408:A:OP1	2.06	0.72
10:J:39:PRO:O	10:J:40:LEU:HB2	1.89	0.72
20:T:10:LEU:O	20:T:12:ALA:N	2.22	0.72
4:D:3:ARG:HH22	4:D:74:GLN:CD	1.97	0.72
1:A:353:A:H5'	1:A:353:A:H8	1.53	0.72
1:A:434:U:H2'	1:A:435:C:C6	2.24	0.72
1:A:877:C:O2	8:H:3:THR:HG21	1.89	0.72
1:A:197:A:H4'	1:A:198:G:O5'	1.90	0.72
8:H:1:MET:HG2	8:H:2:LEU:H	1.54	0.72
18:R:26:LEU:HD12	18:R:27:GLY:H	1.53	0.72
1:A:161:A:H2'	1:A:162:A:C8	2.23	0.72
1:A:1152:A:H5''	10:J:13:HIS:HD2	1.53	0.72
1:A:1250:A:H4'	9:I:68:GLY:N	2.05	0.72
11:K:84:VAL:HG11	11:K:95:ILE:HD11	1.71	0.72
1:A:1148:U:H2'	1:A:1149:C:O4'	1.90	0.72
10:J:35:SER:HB2	10:J:72:VAL:O	1.90	0.72
17:Q:59:ILE:HG23	17:Q:71:PHE:HB3	1.70	0.72
18:R:45:SER:C	18:R:47:THR:H	1.97	0.72
1:A:974:A:OP1	14:N:31:ARG:HG2	1.89	0.71
1:A:1065:U:H4'	1:A:1066:C:O5'	1.89	0.71
9:I:4:TYR:CE2	9:I:88:TYR:HA	2.24	0.71
1:A:501:C:H2'	1:A:502:G:H8	1.53	0.71
3:C:195:VAL:C	3:C:196:LEU:HD23	2.15	0.71
18:R:33:ASP:OD2	18:R:36:ASN:HB2	1.90	0.71
1:A:1343:G:H2'	1:A:1344:C:C6	2.26	0.71
9:I:111:ARG:HD3	9:I:112:LYS:N	2.06	0.71
1:A:344:A:H4'	1:A:345:C:OP2	1.91	0.71
1:A:954:G:H5''	13:M:120:LYS:HD3	1.73	0.71
10:J:45:ARG:HH22	14:N:36:PHE:HD2	1.36	0.71
1:A:1281:U:H5'	1:A:1282:C:C5	2.25	0.71
19:S:15:LEU:HD12	19:S:16:LEU:N	2.06	0.71
1:A:977:A:H2'	1:A:978:A:H5''	1.73	0.71
22:Y:115:ILE:HD12	22:Y:156:PRO:HD2	1.73	0.71
1:A:706:A:O4'	11:K:29:ILE:HD11	1.91	0.70
2:B:19:HIS:CE1	2:B:206:ASP:HB3	2.26	0.70
8:H:108:GLY:HA3	8:H:138:TRP:HB3	1.70	0.70
9:I:65:VAL:HG21	9:I:73:GLN:HB3	1.72	0.70
13:M:40:ASN:HB3	13:M:43:THR:HG23	1.72	0.70
14:N:22:THR:HB	14:N:33:VAL:HG21	1.73	0.70
19:S:70:LYS:O	19:S:72:GLY:N	2.24	0.70

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:107:G:C2'	1:A:108:G:H5'	2.21	0.70
1:A:706:A:C1'	11:K:29:ILE:HD11	2.21	0.70
1:A:818:G:C3'	1:A:819:A:H5''	2.21	0.70
3:C:7:PRO:HG2	3:C:184:TYR:HB2	1.73	0.70
3:C:180:ALA:O	3:C:181:ASN:HB3	1.92	0.70
4:D:36:ARG:H	4:D:37:PRO:CD	2.02	0.70
10:J:78:ASN:O	10:J:80:LYS:N	2.24	0.70
13:M:6:GLY:O	13:M:7:VAL:HG22	1.91	0.70
5:E:102:ALA:HB1	5:E:120:THR:HG21	1.73	0.70
6:F:10:LEU:HD11	6:F:59:TYR:HD2	1.54	0.70
1:A:496:A:H4'	1:A:497:A:OP1	1.92	0.70
2:B:124:SER:HB2	2:B:125:PRO:CD	2.22	0.70
4:D:30:LYS:C	4:D:32:ALA:H	1.98	0.70
15:O:17:ARG:NH1	15:O:77:ARG:NH1	2.40	0.70
1:A:1278:U:H5''	1:A:1279:A:C5'	2.21	0.70
1:A:1351:U:H2'	1:A:1352:C:H6	1.55	0.70
4:D:70:ILE:HD11	4:D:100:ARG:CZ	2.21	0.70
10:J:65:LEU:HD23	10:J:65:LEU:O	1.90	0.70
13:M:49:THR:HG22	13:M:51:ALA:N	2.02	0.70
4:D:28:SER:O	4:D:30:LYS:N	2.25	0.70
5:E:74:GLY:HA3	5:E:116:THR:HG22	1.73	0.70
9:I:97:LYS:HG2	9:I:102:LEU:HD12	1.72	0.70
9:I:97:LYS:CG	9:I:102:LEU:HD12	2.22	0.70
10:J:61:GLU:OE1	14:N:45:ARG:NH1	2.25	0.70
18:R:39:VAL:O	18:R:42:ARG:HB2	1.90	0.70
1:A:1399:C:C2	1:A:1502:A:N6	2.60	0.70
17:Q:45:HIS:HB2	17:Q:65:ILE:HD13	1.71	0.70
1:A:438:G:H4'	1:A:439:A:OP1	1.90	0.70
1:A:1394:A:C6	1:A:1501:C:C4'	2.74	0.70
10:J:30:SER:O	10:J:78:ASN:HB2	1.92	0.70
1:A:1168:A:H2'	1:A:1169:A:C8	2.27	0.69
4:D:150:GLU:CG	4:D:153:ARG:HH21	2.02	0.69
1:A:254:G:OP1	17:Q:67:LYS:O	2.10	0.69
12:L:55:VAL:HG12	12:L:56:ALA:H	1.57	0.69
15:O:39:LEU:HD13	15:O:56:LEU:HB2	1.74	0.69
20:T:50:GLU:HG3	20:T:99:LEU:HD13	1.72	0.69
1:A:954:G:C5'	13:M:120:LYS:HD3	2.23	0.69
10:J:46:ARG:HH11	10:J:64:GLU:CB	2.05	0.69
13:M:81:LEU:O	13:M:86:CYS:HB3	1.92	0.69
1:A:352:C:H4'	1:A:354:G:OP1	1.91	0.69
1:A:1281:U:H4'	1:A:1282:C:OP2	1.92	0.69

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:30:SER:HB2	10:J:80:LYS:HB3	1.74	0.69
19:S:62:ILE:HD12	19:S:66:MET:HG3	1.75	0.69
12:L:28:LYS:HD2	12:L:33:ARG:HH22	1.57	0.69
1:A:1137:C:H4'	1:A:1138:G:N2	2.06	0.69
13:M:11:ARG:HG2	13:M:12:ASN:N	2.07	0.69
1:A:17:U:H2'	1:A:18:C:C6	2.28	0.69
1:A:392:G:H2'	1:A:393:A:H8	1.55	0.69
1:A:1418:A:H61	1:A:1482:G:H1'	1.56	0.69
11:K:108:ILE:HB	18:R:87:ARG:O	1.92	0.69
13:M:81:LEU:HD23	13:M:81:LEU:H	1.56	0.69
16:P:34:GLU:OE2	16:P:55:ARG:HD3	1.93	0.69
17:Q:24:GLU:OE2	17:Q:37:LYS:HD3	1.91	0.69
2:B:187:LEU:HD12	2:B:205:ASP:HA	1.74	0.69
6:F:36:ARG:NH1	6:F:38:GLU:HG2	2.08	0.69
12:L:47:LYS:CB	12:L:48:PRO:CD	2.71	0.69
17:Q:66:SER:O	17:Q:70:ARG:NH1	2.26	0.69
21:V:6:ARG:CD	21:V:15:ARG:HH12	2.06	0.69
4:D:64:LEU:HD12	4:D:75:PHE:CZ	2.28	0.69
10:J:42:THR:HG23	10:J:67:THR:O	1.92	0.69
4:D:64:LEU:HD23	4:D:198:VAL:HG21	1.75	0.68
9:I:93:ARG:HD3	9:I:97:LYS:HE3	1.75	0.68
1:A:477:G:H2'	1:A:478:A:H8	1.56	0.68
1:A:1443:G:C5'	1:A:1446:A:H5'	2.15	0.68
19:S:41:VAL:HG23	19:S:43:GLU:HG2	1.75	0.68
1:A:1141:C:H2'	1:A:1142:G:H8	1.57	0.68
19:S:5:LEU:O	19:S:6:LYS:HB2	1.92	0.68
1:A:701:C:H5'	1:A:703:G:O4'	1.93	0.68
13:M:81:LEU:HD12	13:M:88:ARG:HD3	1.74	0.68
1:A:731:G:OP1	1:A:766:A:H1'	1.94	0.68
4:D:151:LYS:N	4:D:151:LYS:HD2	2.08	0.68
12:L:126:LYS:HD2	12:L:126:LYS:N	2.07	0.68
1:A:948:C:OP1	13:M:109:THR:HG22	1.94	0.68
3:C:38:ARG:HH11	3:C:38:ARG:HG3	1.58	0.68
5:E:51:VAL:O	5:E:55:VAL:HG23	1.94	0.68
6:F:75:LEU:O	6:F:79:LEU:HG	1.94	0.68
19:S:43:GLU:H	19:S:43:GLU:CD	2.00	0.68
1:A:382:A:H2'	1:A:383:A:C8	2.28	0.68
1:A:1016:A:H2'	1:A:1017:G:O4'	1.93	0.68
2:B:22:LYS:HD2	2:B:35:GLU:OE1	1.93	0.68
1:A:99:C:H2'	1:A:101:A:C8	2.28	0.68
1:A:1064:G:C4'	1:A:1065:U:H5'	2.23	0.68

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1411:C:H2'	1:A:1412:C:C6	2.29	0.68
1:A:376:G:OP2	16:P:67:THR:HG21	1.94	0.68
5:E:151:LEU:HD11	8:H:77:GLU:OE2	1.94	0.68
12:L:27:LEU:C	12:L:29:GLY:N	2.37	0.68
18:R:45:SER:OG	18:R:49:LYS:HB2	1.94	0.68
1:A:173:U:H5'	1:A:197:A:O4'	1.94	0.67
1:A:942:G:O2'	1:A:943:U:H5'	1.94	0.67
15:O:55:GLY:O	15:O:59:MET:HG3	1.95	0.67
1:A:652:U:O4	1:A:752:G:O2'	2.09	0.67
1:A:939:G:H2'	1:A:940:C:C6	2.28	0.67
2:B:18:GLY:HA2	2:B:42:ILE:H	1.59	0.67
9:I:26:VAL:HB	9:I:33:PHE:HB2	1.76	0.67
12:L:47:LYS:HB2	12:L:48:PRO:CD	2.23	0.67
1:A:105:G:H2'	1:A:106:C:C6	2.29	0.67
1:A:1366:C:H2'	1:A:1367:C:C6	2.30	0.67
4:D:151:LYS:HD2	4:D:151:LYS:H	1.60	0.67
1:A:31:G:N1	1:A:48:C:H5''	2.09	0.67
1:A:760:G:N1	17:Q:104:LYS:O	2.28	0.67
3:C:82:GLU:O	3:C:85:ARG:HB3	1.94	0.67
16:P:20:VAL:HG11	16:P:32:TYR:HB3	1.74	0.67
17:Q:96:GLU:O	17:Q:96:GLU:HG2	1.94	0.67
3:C:179:ARG:HD3	3:C:206:GLU:HG2	1.76	0.67
8:H:91:ARG:HG3	12:L:7:ILE:HG13	1.77	0.67
18:R:26:LEU:HD21	18:R:39:VAL:CG2	2.25	0.67
1:A:328:C:H4'	1:A:329:A:O5'	1.94	0.67
1:A:1057:G:O2'	1:A:1058:G:H5'	1.95	0.67
1:A:1112:C:O2	3:C:179:ARG:HB3	1.95	0.67
1:A:1368:G:O2'	1:A:1369:C:H5'	1.95	0.67
1:A:1502:A:H2	1:A:1505:G:N1	1.90	0.67
3:C:26:LYS:H	3:C:26:LYS:HD3	1.58	0.67
3:C:190:ARG:HH11	3:C:190:ARG:CB	2.08	0.67
4:D:187:ARG:HH21	4:D:188:LEU:HD12	1.60	0.67
1:A:371:G:O2'	1:A:372:C:H5'	1.95	0.67
1:A:521:G:OP1	12:L:73:GLU:O	2.13	0.67
3:C:130:VAL:HG21	3:C:157:ILE:HG23	1.75	0.67
1:A:915:A:H2'	1:A:916:G:H5'	1.76	0.67
1:A:942:G:H2'	1:A:943:U:C6	2.30	0.67
13:M:33:ALA:HA	13:M:59:TYR:HE2	1.60	0.67
1:A:748:C:H1'	1:A:749:C:C5	2.30	0.66
1:A:967:C:H4'	9:I:128:ARG:HG3	1.75	0.66
1:A:1410:G:C2'	1:A:1411:C:H5'	2.25	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:12:LEU:HD13	5:E:31:LEU:HB2	1.77	0.66
10:J:94:VAL:HG12	10:J:95:GLU:N	2.10	0.66
11:K:14:VAL:O	11:K:15:ALA:HB3	1.95	0.66
18:R:47:THR:HG23	18:R:83:GLU:H	1.60	0.66
1:A:129(A):G:N3	1:A:190(E):U:H5'	2.10	0.66
1:A:686:U:HO2'	1:A:687:A:H8	1.40	0.66
10:J:49:VAL:O	10:J:60:ARG:HA	1.95	0.66
13:M:65:LYS:HG3	13:M:69:GLU:OE2	1.96	0.66
15:O:33:THR:HG23	15:O:63:ARG:HH12	1.59	0.66
17:Q:76:LEU:C	17:Q:76:LEU:HD23	2.20	0.66
1:A:80:G:C3'	1:A:81:U:H5''	2.25	0.66
4:D:32:ALA:C	4:D:34:GLU:H	2.04	0.66
11:K:66:LEU:HB3	11:K:70:LYS:HE3	1.78	0.66
1:A:650:G:O2'	1:A:651:C:H5'	1.94	0.66
20:T:85:MET:HE3	20:T:103:GLY:O	1.96	0.66
1:A:662:G:H2'	1:A:663:A:C8	2.30	0.66
3:C:155:GLY:O	3:C:156:ARG:HB2	1.96	0.66
10:J:60:ARG:O	10:J:61:GLU:HB3	1.95	0.66
20:T:87:LYS:O	20:T:91:LEU:HD12	1.96	0.66
2:B:71:VAL:O	2:B:165:VAL:HG23	1.96	0.66
1:A:427:U:OP1	4:D:13:ARG:NH2	2.29	0.66
1:A:1403:C:H1'	1:A:1500:A:N1	2.11	0.66
1:A:1405:G:O2'	1:A:1519:A:O4'	2.13	0.66
3:C:107:GLN:H	3:C:107:GLN:NE2	1.94	0.66
5:E:150:ARG:HG3	5:E:150:ARG:HH11	1.60	0.66
8:H:6:ILE:HD11	8:H:31:PHE:CD2	2.30	0.66
13:M:81:LEU:H	13:M:81:LEU:CD2	2.08	0.66
17:Q:97:SER:OG	17:Q:103:GLY:CA	2.44	0.66
1:A:353:A:H5'	1:A:353:A:C8	2.31	0.66
17:Q:67:LYS:HA	17:Q:70:ARG:HH12	1.60	0.66
1:A:266:G:O3'	17:Q:67:LYS:HB2	1.95	0.65
1:A:1216:G:H5''	14:N:5:ALA:CB	2.26	0.65
11:K:14:VAL:HG21	11:K:40:ILE:HD11	1.77	0.65
13:M:34:LEU:HD13	13:M:41:PRO:HA	1.77	0.65
19:S:33:THR:HG22	19:S:35:SER:H	1.60	0.65
22:Y:187:ASN:HD21	22:Y:206:LYS:HA	1.60	0.65
1:A:195:A:H4'	20:T:68:LYS:HE2	1.77	0.65
2:B:15:VAL:CG2	2:B:209:ARG:HG3	2.26	0.65
10:J:38:ILE:CG1	10:J:71:LEU:HB3	2.26	0.65
20:T:54:LYS:CG	20:T:100:ILE:CD1	2.65	0.65
1:A:443:C:H2'	1:A:444:C:H6	1.61	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:524:G:H2'	1:A:525:C:C6	2.31	0.65
1:A:1278:U:H5''	1:A:1279:A:H5'	1.77	0.65
1:A:1475:G:H2'	1:A:1476:G:H8	1.62	0.65
5:E:80:ILE:HD11	5:E:91:LEU:HD12	1.76	0.65
7:G:85:TYR:HD1	7:G:154:TYR:HE1	1.42	0.65
9:I:10:ARG:HG2	9:I:75:ASP:HB2	1.77	0.65
12:L:86:ARG:HH11	12:L:86:ARG:HG3	1.61	0.65
19:S:28:LYS:HG2	19:S:29:ARG:N	2.06	0.65
1:A:1224:G:H2'	19:S:78:ARG:HH22	1.62	0.65
3:C:83:ARG:C	3:C:85:ARG:H	2.04	0.65
12:L:33:ARG:HD3	12:L:62:SER:HB3	1.77	0.65
14:N:14:PRO:HB2	14:N:16:PHE:O	1.95	0.65
19:S:17:GLU:HA	19:S:20:LEU:HD11	1.78	0.65
2:B:18:GLY:HA3	2:B:41:ILE:HA	1.79	0.65
3:C:172:ARG:HB3	3:C:172:ARG:HH11	1.61	0.65
5:E:40:ARG:HG2	5:E:68:GLU:OE2	1.96	0.65
11:K:18:ARG:HB2	11:K:33:THR:HG23	1.78	0.65
1:A:1402:C:H2'	1:A:1403:C:O4'	1.97	0.65
10:J:96:ILE:HG22	10:J:97:GLU:N	2.10	0.65
21:V:6:ARG:HD3	21:V:15:ARG:NH1	2.12	0.65
1:A:1425:U:H2'	1:A:1426:C:C6	2.31	0.65
1:A:1522:U:O2'	1:A:1523:G:H5'	1.96	0.65
13:M:36:LYS:HD2	13:M:59:TYR:CZ	2.32	0.65
1:A:287:U:O2'	1:A:288:A:H5'	1.97	0.65
1:A:403:C:O2'	1:A:404:U:H5'	1.97	0.65
3:C:172:ARG:HB3	3:C:172:ARG:NH1	2.11	0.65
5:E:15:ARG:HD2	5:E:15:ARG:O	1.96	0.65
6:F:67:MET:HE2	6:F:72:VAL:HG22	1.76	0.65
15:O:29:VAL:HG12	15:O:85:LEU:CD1	2.27	0.65
1:A:562:C:O2'	12:L:17:LYS:HE3	1.95	0.65
13:M:33:ALA:HA	13:M:59:TYR:CE2	2.32	0.65
13:M:81:LEU:O	13:M:89:GLY:HA3	1.97	0.65
14:N:22:THR:CB	14:N:33:VAL:HG21	2.27	0.65
1:A:677:U:H3	1:A:713:G:H22	1.45	0.64
5:E:65:ASN:CG	5:E:65:ASN:O	2.41	0.64
1:A:168:G:O2'	1:A:169:C:H5'	1.97	0.64
1:A:392:G:H2'	1:A:393:A:C8	2.32	0.64
1:A:922:G:C2	1:A:1396:A:C6	2.86	0.64
4:D:187:ARG:NH2	4:D:188:LEU:HD12	2.10	0.64
7:G:50:ILE:O	7:G:54:THR:HB	1.96	0.64
19:S:64:GLU:O	19:S:67:VAL:HG23	1.97	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:203:U:H5''	1:A:204:U:OP1	1.97	0.64
1:A:397:A:H5'	1:A:398:C:OP1	1.98	0.64
1:A:738:C:OP2	6:F:92:LYS:HE3	1.97	0.64
9:I:49:PRO:O	9:I:52:ALA:HB3	1.97	0.64
9:I:118:LYS:O	9:I:119:ALA:CB	2.45	0.64
11:K:18:ARG:HB2	11:K:33:THR:CG2	2.28	0.64
1:A:281:G:O2'	1:A:282:A:OP2	2.12	0.64
1:A:393:A:O2'	1:A:394:G:H5'	1.98	0.64
6:F:21:LEU:O	6:F:24:GLU:HB3	1.97	0.64
20:T:53:LEU:CD1	20:T:101:GLY:CA	2.75	0.64
1:A:765:G:H1	1:A:812:C:H2'	1.62	0.64
1:A:818:G:H3'	1:A:819:A:C5'	2.27	0.64
1:A:918:A:H2'	1:A:919:A:C8	2.32	0.64
1:A:1489:G:C2'	1:A:1490:C:H5''	2.26	0.64
10:J:90:LEU:H	10:J:91:PRO:HD2	1.60	0.64
16:P:18:ARG:HD3	16:P:35:LYS:HE3	1.79	0.64
16:P:45:THR:HB	16:P:46:PRO:HD2	1.80	0.64
1:A:1040:U:H2'	1:A:1041:A:C8	2.33	0.64
3:C:188:LEU:O	3:C:189:ALA:HB2	1.96	0.64
5:E:115:VAL:CG1	5:E:118:ILE:HG13	2.25	0.64
11:K:74:ALA:C	11:K:76:GLY:H	2.05	0.64
12:L:110:VAL:O	12:L:122:THR:HG21	1.97	0.64
19:S:44:MET:O	19:S:47:HIS:HB2	1.97	0.64
3:C:177:THR:CG2	3:C:180:ALA:HB2	2.28	0.64
7:G:26:PHE:CE2	7:G:30:ILE:HD11	2.33	0.64
19:S:40:ILE:HB	19:S:67:VAL:O	1.98	0.64
1:A:1142:G:H2'	1:A:1143:G:O4'	1.97	0.64
1:A:1492:A:H2'	1:A:1493:A:O4'	1.97	0.64
3:C:64:VAL:HB	3:C:99:VAL:CB	2.27	0.64
5:E:120:THR:CG2	5:E:121:LYS:N	2.60	0.64
17:Q:101:ARG:HA	17:Q:101:ARG:HE	1.62	0.64
1:A:922:G:H2'	1:A:923:A:C8	2.33	0.64
1:A:1497:G:H2'	1:A:1498:U:H5'	1.78	0.64
2:B:215:LEU:O	2:B:219:VAL:HG23	1.97	0.64
1:A:1346:A:H2'	7:G:10:ARG:HH22	1.63	0.64
2:B:97:TRP:HH2	2:B:176:GLU:CD	2.06	0.64
3:C:112:SER:HB2	3:C:115:LEU:HD12	1.79	0.64
11:K:40:ILE:HG22	11:K:41:THR:HG23	1.80	0.64
11:K:48:ILE:HG22	11:K:49:GLY:H	1.61	0.64
12:L:55:VAL:HG12	12:L:56:ALA:N	2.13	0.64
21:V:6:ARG:CD	21:V:15:ARG:NH1	2.61	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1422:G:O2'	1:A:1423:G:H5'	1.97	0.63
1:A:1442:G:N3	1:A:1442:G:H2'	2.12	0.63
9:I:48:GLU:N	9:I:49:PRO:HD2	2.13	0.63
1:A:255:G:H1'	17:Q:16:GLN:OE1	1.97	0.63
2:B:74:LYS:NZ	2:B:206:ASP:HA	2.13	0.63
3:C:120:VAL:O	3:C:124:ILE:HG13	1.99	0.63
4:D:70:ILE:HD11	4:D:100:ARG:NE	2.13	0.63
7:G:42:ILE:HG22	7:G:120:ILE:HD12	1.80	0.63
14:N:27:CYS:SG	14:N:29:ARG:HB2	2.37	0.63
1:A:1141:C:H2'	1:A:1142:G:C8	2.32	0.63
1:A:1153:C:H2'	1:A:1154:G:H8	1.62	0.63
2:B:74:LYS:HZ1	2:B:206:ASP:HA	1.62	0.63
2:B:84:GLU:HB3	2:B:219:VAL:HG21	1.79	0.63
3:C:64:VAL:CB	3:C:99:VAL:HB	2.27	0.63
4:D:131:ARG:H	4:D:131:ARG:HD2	1.62	0.63
4:D:152:SER:HB3	4:D:155:LEU:HD12	1.80	0.63
5:E:79:GLU:HG3	5:E:93:PRO:HD2	1.79	0.63
7:G:114:ARG:HG2	7:G:114:ARG:HH11	1.63	0.63
20:T:53:LEU:HD13	20:T:102:GLY:N	2.12	0.63
1:A:1316:G:H4'	14:N:18:VAL:CG1	2.29	0.63
12:L:25:PRO:C	12:L:27:LEU:N	2.52	0.63
1:A:1020:U:H2'	1:A:1021:G:H8	1.63	0.63
1:A:1131:G:H1	1:A:1143:G:N2	1.95	0.63
2:B:82:ARG:O	2:B:86:GLU:HG3	1.98	0.63
3:C:155:GLY:O	3:C:196:LEU:HD22	1.98	0.63
1:A:1026:G:H2'	1:A:1027:C:H5'	1.80	0.63
2:B:95:GLN:OE1	2:B:95:GLN:HA	1.96	0.63
3:C:29:TYR:OH	14:N:54:PRO:HG2	1.97	0.63
3:C:91:LEU:CD2	3:C:99:VAL:HG13	2.27	0.63
9:I:111:ARG:HD3	9:I:112:LYS:C	2.24	0.63
19:S:39:THR:HA	19:S:70:LYS:HG2	1.81	0.63
1:A:243:A:H4'	1:A:244:U:C5'	2.22	0.63
1:A:1053:G:C3'	1:A:1054:C:H5'	2.29	0.63
1:A:1422:G:H2'	1:A:1423:G:O4'	1.98	0.63
2:B:68:ILE:HB	2:B:90:MET:HE3	1.80	0.63
2:B:130:ARG:NH2	3:C:207:VAL:HG22	2.14	0.63
5:E:150:ARG:HG3	5:E:150:ARG:NH1	2.14	0.63
1:A:1189:C:OP1	10:J:51:ARG:NH2	2.29	0.63
1:A:1238:A:H5'	1:A:1336:C:H41	1.64	0.63
2:B:20:GLU:HG2	2:B:189:ASP:OD2	1.99	0.63
2:B:132:LYS:HG2	2:B:135:GLN:OE1	1.99	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:102:ALA:CB	5:E:120:THR:HG21	2.29	0.63
5:E:116:THR:HG23	5:E:117:ASP:OD2	1.98	0.63
12:L:43:VAL:HG12	12:L:44:THR:N	2.14	0.63
1:A:1132:C:H2'	1:A:1133:G:H8	1.64	0.63
1:A:1229:A:OP2	13:M:114:ARG:HD3	1.99	0.63
1:A:1343:G:H1'	9:I:121:ARG:HH12	1.64	0.63
1:A:1405:G:O2'	1:A:1518:A:O2'	2.13	0.63
2:B:184:VAL:N	2:B:198:ASP:OD2	2.32	0.63
3:C:50:ALA:O	3:C:70:VAL:HG12	1.99	0.63
1:A:448:A:H2'	1:A:449:C:H6	1.64	0.62
1:A:556:C:O2'	1:A:557:G:H5'	1.99	0.62
1:A:1347:G:O2'	1:A:1348:U:P	2.57	0.62
1:A:1347:G:C4	9:I:107:ARG:NH1	2.67	0.62
2:B:73:THR:HB	2:B:170:GLU:OE2	1.99	0.62
6:F:9:VAL:HB	6:F:87:ARG:HB2	1.80	0.62
15:O:17:ARG:CZ	15:O:77:ARG:HH11	2.11	0.62
1:A:405:U:H3'	1:A:406:G:H5'	1.81	0.62
1:A:924:C:H5'	1:A:1399:C:OP2	1.98	0.62
1:A:1307:U:H5'	13:M:109:THR:HG21	1.81	0.62
3:C:177:THR:HG23	3:C:180:ALA:HB2	1.81	0.62
16:P:8:ARG:HB2	16:P:28:ARG:NH1	2.14	0.62
1:A:475:G:H2'	1:A:476:G:H8	1.63	0.62
1:A:1132:C:H2'	1:A:1133:G:C8	2.35	0.62
3:C:3:ASN:C	3:C:4:LYS:HG2	2.23	0.62
3:C:60:ALA:O	3:C:61:ALA:HB2	2.00	0.62
7:G:71:PRO:HD3	7:G:103:TRP:CZ3	2.33	0.62
1:A:1225:A:H2'	1:A:1225:A:N3	2.14	0.62
13:M:84:ILE:O	13:M:86:CYS:N	2.33	0.62
1:A:113:G:H1'	1:A:354:G:H5'	1.80	0.62
1:A:216:G:H2'	1:A:217:C:C6	2.35	0.62
1:A:501:C:H2'	1:A:502:G:C8	2.34	0.62
1:A:1260:C:O5'	1:A:1284:C:H4'	1.99	0.62
2:B:69:LEU:HD12	2:B:155:LEU:HD11	1.82	0.62
13:M:82:MET:HE2	13:M:92:HIS:HB3	1.80	0.62
13:M:84:ILE:C	13:M:86:CYS:H	2.08	0.62
14:N:14:PRO:C	14:N:16:PHE:N	2.56	0.62
17:Q:69:LYS:C	17:Q:70:ARG:HD2	2.24	0.62
1:A:760:G:C6	17:Q:105:ALA:HB2	2.35	0.62
1:A:976:G:OP1	14:N:32:SER:HA	1.98	0.62
2:B:186:ALA:HB3	2:B:197:VAL:HG11	1.81	0.62
7:G:23:VAL:O	7:G:27:ILE:HG13	2.00	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:T:53:LEU:HD12	20:T:101:GLY:N	2.13	0.62
22:Y:147:GLU:HG3	22:Y:150:ILE:HB	1.82	0.62
1:A:1370:G:O2'	1:A:1371:G:H5'	2.00	0.62
2:B:23:ARG:NH1	2:B:23:ARG:C	2.58	0.62
2:B:130:ARG:NH2	3:C:179:ARG:HH12	1.97	0.62
5:E:120:THR:HG23	5:E:121:LYS:N	2.15	0.62
1:A:542:G:OP1	4:D:10:ARG:NH2	2.33	0.62
4:D:30:LYS:C	4:D:32:ALA:N	2.58	0.62
7:G:155:ARG:O	7:G:156:TRP:HB3	1.99	0.62
12:L:33:ARG:CD	12:L:62:SER:HB3	2.29	0.62
1:A:1347:G:HO2'	1:A:1348:U:P	2.23	0.62
1:A:1425:U:H2'	1:A:1426:C:H6	1.65	0.62
2:B:115:LEU:HG	2:B:153:ARG:NH2	2.14	0.62
3:C:129:ALA:HB3	3:C:132:ARG:HD2	1.82	0.62
9:I:19:LEU:O	9:I:20:ARG:HG3	1.99	0.62
10:J:62:HIS:HB3	14:N:59:ALA:HB3	1.81	0.62
1:A:434:U:H2'	1:A:435:C:H6	1.64	0.62
1:A:1148:U:H4'	9:I:14:VAL:HG11	1.81	0.62
1:A:1182:G:H4'	1:A:1183:A:O5'	1.99	0.62
1:A:1407:C:HO2'	1:A:1408:A:P	2.23	0.62
1:A:1440:C:H2'	1:A:1441:G:H5'	1.82	0.62
4:D:148:VAL:CG1	4:D:158:ILE:HD13	2.30	0.62
5:E:71:LEU:HD21	5:E:115:VAL:HG22	1.80	0.62
1:A:476:G:O2'	1:A:477:G:H5'	2.00	0.61
1:A:706:A:H1'	11:K:29:ILE:HD11	1.81	0.61
1:A:1176:A:H2'	1:A:1177:G:C8	2.35	0.61
1:A:1178:G:P	9:I:97:LYS:HZ2	2.23	0.61
7:G:139:GLU:O	7:G:143:ARG:HG3	2.00	0.61
14:N:53:LEU:HB3	14:N:56:VAL:HG21	1.82	0.61
19:S:52:TYR:HA	19:S:56:GLN:O	1.99	0.61
1:A:37:U:OP1	12:L:124:LYS:N	2.26	0.61
1:A:959:A:H3'	1:A:960:U:H5''	1.82	0.61
2:B:80:ILE:HD11	2:B:208:ILE:HG23	1.81	0.61
17:Q:21:VAL:HG21	17:Q:59:ILE:HD11	1.82	0.61
19:S:31:ILE:CG2	19:S:32:LYS:H	2.10	0.61
1:A:193:C:H2'	1:A:194:C:C6	2.36	0.61
1:A:575:G:C5	1:A:881:G:C2	2.89	0.61
1:A:664:G:N2	1:A:741:G:H1	1.89	0.61
1:A:954:G:H21	1:A:1227:A:H62	1.49	0.61
4:D:25:ARG:O	4:D:27:TYR:N	2.34	0.61
5:E:80:ILE:CD1	5:E:91:LEU:HB2	2.30	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:78:ARG:HB2	7:G:156:TRP:CZ3	2.36	0.61
20:T:96:GLY:O	20:T:97:ALA:HB3	2.00	0.61
3:C:191:THR:HG22	3:C:192:THR:N	2.15	0.61
9:I:4:TYR:CZ	9:I:88:TYR:HD1	2.17	0.61
10:J:30:SER:OG	10:J:81:THR:HA	1.99	0.61
1:A:551:U:H2'	1:A:552:U:H6	1.64	0.61
1:A:1147:C:H4'	9:I:5:TYR:HE1	1.65	0.61
4:D:191:ARG:O	4:D:191:ARG:HD2	2.00	0.61
5:E:115:VAL:HG11	5:E:118:ILE:CG1	2.28	0.61
11:K:84:VAL:CG1	11:K:95:ILE:HD11	2.31	0.61
20:T:82:SER:C	20:T:84:LEU:H	2.08	0.61
1:A:386:C:O2'	1:A:387:U:H5'	2.00	0.61
1:A:1420:C:H2'	1:A:1421:G:H8	1.66	0.61
2:B:12:GLU:C	2:B:14:GLY:H	2.07	0.61
3:C:13:GLY:HA3	14:N:57:ARG:NH2	2.14	0.61
9:I:44:VAL:HG12	9:I:51:ARG:HH12	1.66	0.61
1:A:195:A:H4'	20:T:68:LYS:CE	2.30	0.61
2:B:34:ALA:O	2:B:41:ILE:N	2.31	0.61
4:D:23:GLY:HA3	4:D:112:VAL:CG1	2.30	0.61
7:G:38:LEU:HD12	7:G:38:LEU:O	2.01	0.61
16:P:4:ILE:HG13	16:P:64:ALA:HB1	1.83	0.61
1:A:107:G:H2'	1:A:108:G:H5'	1.83	0.61
1:A:1003:G:H2'	1:A:1003(A):G:C8	2.36	0.61
1:A:1053:G:C4'	1:A:1054:C:H5'	2.31	0.61
1:A:1091:U:O2	1:A:1093:A:C8	2.54	0.61
1:A:1226:C:N4	13:M:104:ARG:HD2	2.16	0.61
2:B:88:ALA:C	2:B:90:MET:H	2.09	0.61
17:Q:101:ARG:HA	17:Q:101:ARG:NE	2.16	0.61
1:A:1316:G:H4'	14:N:18:VAL:HG11	1.83	0.61
1:A:1475:G:H2'	1:A:1476:G:C8	2.36	0.61
2:B:115:LEU:O	2:B:119:GLU:HG3	2.00	0.61
3:C:191:THR:CG2	3:C:192:THR:N	2.64	0.61
5:E:80:ILE:HD11	5:E:91:LEU:HB2	1.83	0.61
13:M:54:VAL:O	13:M:58:GLU:HG2	2.01	0.61
1:A:1329:A:P	13:M:28:ALA:HB3	2.41	0.61
2:B:98:LEU:O	2:B:101:MET:HG3	2.01	0.61
10:J:46:ARG:HH11	10:J:64:GLU:HB3	1.64	0.61
11:K:48:ILE:HG22	11:K:49:GLY:N	2.16	0.61
1:A:104:G:N7	20:T:14:LYS:NZ	2.46	0.60
1:A:1495:U:H2'	1:A:1496:C:C6	2.36	0.60
4:D:148:VAL:HG11	4:D:158:ILE:HG21	1.81	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:40:VAL:O	12:L:40:VAL:HG12	1.99	0.60
18:R:52:PRO:O	18:R:56:THR:HG23	2.00	0.60
2:B:33:TYR:O	2:B:34:ALA:HB2	2.02	0.60
2:B:143:GLU:O	2:B:147:LYS:HG3	2.00	0.60
4:D:162:LEU:CD1	4:D:181:MET:HE2	2.31	0.60
17:Q:76:LEU:HD23	17:Q:77:VAL:N	2.15	0.60
4:D:25:ARG:C	4:D:27:TYR:N	2.55	0.60
8:H:64:LYS:HG2	8:H:79:VAL:HG21	1.84	0.60
16:P:67:THR:HG22	16:P:68:ASP:N	2.15	0.60
19:S:13:ASP:HA	19:S:16:LEU:HB3	1.83	0.60
1:A:390:C:H2'	1:A:391:G:H8	1.66	0.60
1:A:425:G:O2'	1:A:426:G:H5'	2.02	0.60
1:A:812:C:O2'	1:A:813:U:OP2	2.17	0.60
3:C:20:SER:HB3	3:C:22:TRP:HE1	1.67	0.60
5:E:43:LEU:HD11	5:E:132:ALA:HB1	1.84	0.60
7:G:72:ARG:HG2	7:G:142:GLU:OE1	2.02	0.60
10:J:71:LEU:O	10:J:72:VAL:HB	2.00	0.60
15:O:29:VAL:HG12	15:O:85:LEU:HD11	1.82	0.60
1:A:390:C:O3'	16:P:28:ARG:NH2	2.34	0.60
1:A:686:U:O2'	1:A:687:A:H8	1.84	0.60
1:A:953:G:H1'	13:M:125:ARG:CB	2.31	0.60
1:A:1381:U:O2'	1:A:1382:C:H5'	2.02	0.60
5:E:24:ARG:HG2	5:E:24:ARG:HH11	1.66	0.60
11:K:19:ALA:HB2	11:K:80:VAL:HG11	1.82	0.60
16:P:52:ASP:OD2	16:P:55:ARG:HG3	2.00	0.60
22:Y:141:TYR:HB2	22:Y:142:SER:C	2.26	0.60
1:A:112:G:H21	1:A:354:G:H5'	1.65	0.60
1:A:112:G:N2	1:A:354:G:H5'	2.16	0.60
1:A:1147:C:H4'	9:I:5:TYR:CE1	2.36	0.60
14:N:24:CYS:HB3	14:N:28:GLY:H	1.66	0.60
20:T:53:LEU:HD12	20:T:101:GLY:H	1.66	0.60
1:A:1305:G:H5'	21:V:4:GLY:HA3	1.84	0.60
2:B:114:ARG:NH1	2:B:118:LEU:HD21	2.15	0.60
3:C:33:LEU:HD11	14:N:53:LEU:CD2	2.32	0.60
3:C:47:LEU:HD23	3:C:68:VAL:HG11	1.83	0.60
7:G:78:ARG:HB2	7:G:156:TRP:HZ3	1.65	0.60
11:K:69:ALA:O	11:K:73:MET:HG2	2.02	0.60
17:Q:104:LYS:O	17:Q:105:ALA:HB2	2.02	0.60
1:A:449:C:O2	16:P:42:ARG:HD2	2.01	0.60
2:B:122:PHE:HE2	2:B:139:LYS:HG2	1.65	0.60
2:B:140:HIS:O	2:B:143:GLU:HB2	2.01	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:26:LYS:HD3	3:C:26:LYS:N	2.17	0.60
6:F:10:LEU:CD1	6:F:59:TYR:HB3	2.29	0.60
16:P:81:ARG:HG3	16:P:83:GLU:HG2	1.84	0.60
1:A:996:A:H2'	1:A:997:U:C6	2.37	0.60
1:A:1376:U:H2'	1:A:1377:A:C8	2.36	0.60
1:A:1470:G:O2'	1:A:1471:G:H5'	2.02	0.60
3:C:46:GLU:O	3:C:48:TYR:N	2.33	0.60
7:G:42:ILE:HG23	7:G:117:ALA:HA	1.84	0.60
13:M:10:PRO:O	13:M:45:VAL:HG11	2.01	0.60
1:A:435:C:H2'	1:A:436:C:H6	1.67	0.59
1:A:1306:A:N6	1:A:1331:G:H1'	2.17	0.59
3:C:47:LEU:H	3:C:47:LEU:CD1	2.15	0.59
4:D:162:LEU:HD13	4:D:181:MET:HE2	1.82	0.59
12:L:46:LYS:HG2	12:L:47:LYS:N	2.16	0.59
14:N:11:LYS:O	14:N:13:THR:N	2.34	0.59
1:A:502:G:H4'	1:A:550:G:H4'	1.83	0.59
1:A:505:G:H2'	1:A:506:G:C8	2.37	0.59
1:A:1231:G:H5''	9:I:126:SER:CB	2.33	0.59
3:C:79:ARG:HE	3:C:82:GLU:HG2	1.67	0.59
9:I:93:ARG:NH1	9:I:97:LYS:NZ	2.51	0.59
11:K:84:VAL:HG21	18:R:88:LYS:HD3	1.83	0.59
15:O:11:VAL:HG21	15:O:34:LEU:HD12	1.83	0.59
1:A:457:C:H2'	1:A:458:C:H6	1.67	0.59
1:A:839:U:O2	1:A:839:U:H2'	2.01	0.59
1:A:923:A:O4'	1:A:1398:A:C2	2.56	0.59
1:A:1130:A:H3'	1:A:1130:A:OP2	2.02	0.59
1:A:1405:G:C2'	1:A:1518:A:HO2'	2.14	0.59
5:E:118:ILE:CG2	5:E:119:LEU:N	2.65	0.59
9:I:5:TYR:CD2	9:I:6:GLY:N	2.71	0.59
11:K:110:ASP:HB2	18:R:88:LYS:CD	2.20	0.59
1:A:1352:C:H2'	1:A:1353:G:C8	2.37	0.59
2:B:97:TRP:HZ2	2:B:102:LEU:HD13	1.66	0.59
4:D:33:MET:O	4:D:37:PRO:HG3	2.02	0.59
7:G:95:ARG:HG3	7:G:95:ARG:NH1	2.17	0.59
1:A:972:C:OP1	10:J:57:LYS:NZ	2.28	0.59
2:B:101:MET:CA	2:B:108:ILE:HD12	2.33	0.59
4:D:151:LYS:H	4:D:151:LYS:CD	2.16	0.59
1:A:103:C:P	20:T:17:ARG:HH11	2.26	0.59
1:A:109:A:H2'	1:A:326:G:N2	2.17	0.59
1:A:1086:U:H3	1:A:1099:G:N2	1.91	0.59
8:H:83:ILE:HG23	8:H:83:ILE:O	2.03	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:94:ARG:HH22	19:S:81:ARG:NH1	2.00	0.59
13:M:125:ARG:HD2	13:M:125:ARG:C	2.27	0.59
1:A:1247:U:O2'	1:A:1248:A:H5'	2.02	0.59
1:A:1347:G:O2'	1:A:1348:U:OP2	2.16	0.59
1:A:1420:C:O2'	1:A:1421:G:H5'	2.02	0.59
22:Y:147:GLU:HA	22:Y:149:GLU:N	2.18	0.59
3:C:14:ILE:O	3:C:16:ARG:N	2.35	0.59
7:G:51:GLN:OE1	7:G:51:GLN:HA	2.02	0.59
10:J:3:LYS:N	10:J:77:PRO:HD3	2.18	0.59
10:J:46:ARG:NH1	10:J:64:GLU:HG2	2.18	0.59
12:L:55:VAL:CG1	12:L:67:THR:HG23	2.33	0.59
1:A:390:C:H2'	1:A:391:G:C8	2.38	0.59
1:A:457:C:H2'	1:A:458:C:C6	2.38	0.59
1:A:513:C:O2'	1:A:514:C:H5'	2.03	0.59
1:A:560:U:H4'	1:A:561:U:H5''	1.83	0.59
1:A:736:C:H2'	1:A:737:A:C8	2.38	0.59
1:A:1412:C:H2'	1:A:1413:A:O4'	2.03	0.59
2:B:12:GLU:C	2:B:14:GLY:N	2.59	0.59
2:B:120:ALA:O	2:B:124:SER:HB3	2.02	0.59
22:Y:147:GLU:HA	22:Y:149:GLU:H	1.67	0.59
7:G:122:HIS:HA	7:G:125:MET:HE3	1.85	0.59
10:J:60:ARG:HD2	10:J:60:ARG:N	2.17	0.59
10:J:82:ILE:O	10:J:82:ILE:HG22	2.03	0.59
13:M:81:LEU:HD23	13:M:81:LEU:N	2.17	0.59
16:P:51:VAL:O	16:P:51:VAL:HG12	2.02	0.59
18:R:86:VAL:O	18:R:87:ARG:HB2	2.02	0.59
1:A:39:G:O2'	1:A:40:C:H5'	2.03	0.58
1:A:1521:G:H2'	1:A:1522:U:C6	2.38	0.58
2:B:130:ARG:HD2	2:B:131:PRO:HD2	1.85	0.58
1:A:812:C:HO2'	1:A:813:U:P	2.26	0.58
1:A:991:U:O2'	1:A:992:U:H5'	2.02	0.58
1:A:1182:G:O2'	1:A:1183:A:OP2	2.20	0.58
1:A:1251:A:H4'	9:I:12:GLU:OE2	2.02	0.58
2:B:144:ARG:HG3	2:B:145:LEU:N	2.18	0.58
3:C:10:PHE:CZ	3:C:178:LEU:HD13	2.38	0.58
4:D:23:GLY:HA3	4:D:112:VAL:HG12	1.84	0.58
12:L:24:VAL:O	12:L:24:VAL:HG12	2.03	0.58
12:L:28:LYS:HD2	12:L:33:ARG:NH2	2.17	0.58
1:A:760:G:C2	17:Q:103:GLY:O	2.57	0.58
1:A:1410:G:H2'	1:A:1411:C:C5'	2.34	0.58
1:A:1441:G:H4'	1:A:1442:G:N7	2.19	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:10:LEU:C	2:B:12:GLU:H	2.12	0.58
3:C:64:VAL:HB	3:C:99:VAL:CG2	2.33	0.58
10:J:45:ARG:O	10:J:64:GLU:HA	2.03	0.58
14:N:8:GLU:O	14:N:11:LYS:HB2	2.02	0.58
1:A:518:C:H5''	1:A:519:C:C6	2.37	0.58
1:A:1003(A):G:C2	1:A:1004:A:H1'	2.39	0.58
1:A:1072:G:H2'	1:A:1073:U:C6	2.38	0.58
2:B:115:LEU:HG	2:B:153:ARG:HH21	1.68	0.58
2:B:133:LYS:O	2:B:137:ARG:HG3	2.03	0.58
1:A:60:A:H4'	1:A:61:G:O5'	2.03	0.58
1:A:1152:A:H5'	10:J:70:ARG:HH22	1.68	0.58
1:A:1316:G:N2	1:A:1318:A:H3'	2.18	0.58
1:A:1487:G:O2'	1:A:1488:G:H5'	2.03	0.58
8:H:17:THR:HG22	8:H:63:LEU:HG	1.86	0.58
9:I:5:TYR:O	9:I:84:ALA:HA	2.03	0.58
9:I:11:LYS:O	9:I:11:LYS:HG2	2.03	0.58
9:I:79:LEU:HD23	9:I:101:PHE:O	2.02	0.58
15:O:17:ARG:NH1	15:O:77:ARG:HH11	2.01	0.58
1:A:812:C:O2'	1:A:813:U:P	2.62	0.58
1:A:1117:G:H5'	1:A:1117:G:H8	1.66	0.58
2:B:10:LEU:HD23	2:B:48:MET:HG3	1.86	0.58
2:B:134:GLU:C	2:B:136:VAL:H	2.12	0.58
10:J:24:VAL:HG12	10:J:28:ARG:HE	1.68	0.58
13:M:94:ARG:NH2	19:S:81:ARG:HD3	2.19	0.58
14:N:44:LEU:C	14:N:44:LEU:HD12	2.29	0.58
15:O:87:ILE:O	15:O:88:ARG:HB2	2.04	0.58
1:A:1498:U:H4'	1:A:1519:A:H2	1.69	0.58
2:B:156:LYS:O	2:B:156:LYS:HD3	2.03	0.58
10:J:15:THR:HG23	10:J:94:VAL:HG22	1.85	0.58
10:J:51:ARG:HB2	10:J:59:SER:CB	2.23	0.58
14:N:9:LYS:HD3	14:N:9:LYS:C	2.28	0.58
20:T:50:GLU:CG	20:T:99:LEU:HD12	2.30	0.58
20:T:53:LEU:O	20:T:57:ARG:HD2	2.04	0.58
1:A:376:G:P	16:P:67:THR:HG21	2.44	0.58
1:A:765:G:H22	1:A:812:C:HO2'	1.51	0.58
1:A:1054:C:OP1	1:A:1197:G:OP1	2.21	0.58
2:B:76:GLN:HG3	2:B:206:ASP:OD1	2.04	0.58
3:C:33:LEU:HD23	3:C:33:LEU:C	2.29	0.58
5:E:122:GLU:O	5:E:123:LEU:HD23	2.03	0.58
9:I:46:ALA:HB1	9:I:77:ILE:HG22	1.86	0.58
12:L:85:ILE:HG23	12:L:98:TYR:HB3	1.86	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:120:LYS:HE2	13:M:123:ALA:HB2	1.86	0.58
1:A:411:A:N9	1:A:413:G:H1'	2.19	0.58
1:A:723:U:O2	1:A:723:U:H2'	2.04	0.58
1:A:818:G:C2'	1:A:819:A:H5''	2.34	0.58
1:A:976:G:OP2	1:A:1358:U:H1'	2.03	0.58
2:B:16:HIS:NE2	2:B:214:ILE:CG1	2.66	0.58
3:C:191:THR:HG21	3:C:193:TYR:CZ	2.39	0.58
4:D:32:ALA:C	4:D:34:GLU:N	2.60	0.58
10:J:86:MET:HA	10:J:86:MET:HE3	1.85	0.58
12:L:92:ASP:O	12:L:94:PRO:HD3	2.04	0.58
14:N:12:ARG:O	14:N:14:PRO:N	2.36	0.58
1:A:375:U:H4'	16:P:17:TYR:CE2	2.39	0.58
1:A:1228:C:OP1	13:M:115:LYS:HG3	2.03	0.58
3:C:10:PHE:CE2	3:C:178:LEU:HD13	2.38	0.58
7:G:15:ASP:OD1	7:G:17:VAL:N	2.37	0.58
9:I:93:ARG:NH1	9:I:97:LYS:HZ1	2.01	0.58
13:M:13:LYS:O	13:M:45:VAL:HG23	2.04	0.58
13:M:84:ILE:CG2	19:S:65:ASN:HD22	2.17	0.58
20:T:53:LEU:HD13	20:T:102:GLY:H	1.68	0.58
10:J:81:THR:C	10:J:83:GLU:H	2.10	0.57
11:K:109:VAL:HG13	18:R:85:LEU:O	2.04	0.57
12:L:26:ALA:O	12:L:27:LEU:O	2.22	0.57
1:A:1014:A:H2'	1:A:1015:A:C8	2.39	0.57
6:F:97:PHE:HB2	18:R:32:ARG:CZ	2.34	0.57
9:I:7:THR:HG21	9:I:9:ARG:NH1	2.19	0.57
9:I:17:VAL:HG21	9:I:80:GLY:HA3	1.86	0.57
11:K:40:ILE:HG23	11:K:75:TYR:CD2	2.38	0.57
14:N:24:CYS:HB3	14:N:28:GLY:N	2.19	0.57
16:P:17:TYR:HE1	16:P:41:PRO:HG2	1.69	0.57
1:A:1095:U:H2'	1:A:1096:C:C6	2.39	0.57
1:A:1504:G:H3'	1:A:1504:G:OP2	2.04	0.57
14:N:29:ARG:HG2	14:N:29:ARG:HH11	1.69	0.57
1:A:346:G:C2'	1:A:347:G:H5'	2.35	0.57
13:M:31:LYS:O	13:M:35:GLU:HB2	2.05	0.57
19:S:40:ILE:HG21	19:S:62:ILE:CD1	2.33	0.57
1:A:1298:C:C4	7:G:114:ARG:HD3	2.40	0.57
8:H:29:SER:OG	8:H:32:LYS:HB2	2.04	0.57
14:N:3:ARG:NH1	14:N:6:LEU:HD11	2.20	0.57
20:T:10:LEU:HD12	20:T:12:ALA:HB3	1.85	0.57
1:A:757:U:H2'	1:A:758:G:O4'	2.03	0.57
1:A:835:U:OP1	18:R:64:ARG:NH2	2.34	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:860:A:H2'	1:A:861:G:O4'	2.03	0.57
1:A:1015:A:H2'	1:A:1016:A:C8	2.40	0.57
1:A:1044:A:C2'	1:A:1045:C:H5'	2.34	0.57
1:A:1305:G:N2	1:A:1331:G:O2'	2.38	0.57
3:C:121:ALA:O	3:C:125:GLU:HG3	2.04	0.57
4:D:7:PRO:HG2	4:D:10:ARG:HD2	1.87	0.57
8:H:19:VAL:HG23	8:H:21:LYS:HD3	1.86	0.57
13:M:49:THR:HB	13:M:52:GLU:HG3	1.86	0.57
1:A:1347:G:N2	1:A:1373:G:H2'	2.19	0.57
2:B:223:ILE:HG21	2:B:230:VAL:CG2	2.35	0.57
19:S:25:LYS:H	19:S:25:LYS:HD2	1.68	0.57
1:A:1004:A:H5''	1:A:1025:U:C5	2.40	0.57
1:A:1230:C:H1'	13:M:126:LYS:HA	1.86	0.57
1:A:1241:G:H2'	1:A:1242:C:C6	2.39	0.57
2:B:15:VAL:HG11	2:B:209:ARG:C	2.30	0.57
4:D:35:ARG:O	4:D:36:ARG:HB2	2.04	0.57
6:F:80:ARG:NH1	6:F:88:VAL:HB	2.19	0.57
8:H:103:VAL:HG21	8:H:110:ALA:HB2	1.87	0.57
9:I:9:ARG:HA	9:I:13:ALA:O	2.05	0.57
13:M:13:LYS:HD3	13:M:17:VAL:HG11	1.86	0.57
1:A:192:U:O2'	1:A:193:C:H5'	2.05	0.57
2:B:209:ARG:HE	2:B:239:VAL:HG11	1.68	0.57
12:L:47:LYS:CB	12:L:48:PRO:HD3	2.35	0.57
14:N:3:ARG:O	14:N:4:LYS:C	2.48	0.57
18:R:47:THR:HG22	18:R:48:GLY:N	2.18	0.57
19:S:5:LEU:O	19:S:6:LYS:CB	2.52	0.57
19:S:7:LYS:HG3	19:S:7:LYS:O	2.03	0.57
1:A:1152:A:H5'	10:J:70:ARG:NH2	2.19	0.57
1:A:1372:U:OP1	9:I:71:SER:HB3	2.04	0.57
1:A:1491:G:H2'	1:A:1492:A:C8	2.40	0.57
1:A:1499:A:H1'	1:A:1520:G:H5'	1.87	0.57
3:C:83:ARG:C	3:C:85:ARG:N	2.63	0.57
3:C:84:ILE:O	3:C:88:ARG:HB2	2.05	0.57
3:C:91:LEU:HD11	3:C:99:VAL:HG13	1.87	0.57
3:C:188:LEU:HD13	3:C:195:VAL:HG13	1.86	0.57
5:E:80:ILE:HD12	5:E:80:ILE:O	2.05	0.57
8:H:123:GLU:O	8:H:127:LEU:HD23	2.05	0.57
12:L:6:THR:OG1	12:L:9:GLN:HG3	2.05	0.57
15:O:41:GLU:OE2	15:O:41:GLU:HA	2.05	0.57
20:T:67:ALA:HA	20:T:73:HIS:H	1.70	0.57
1:A:946:A:H2'	1:A:947:G:C8	2.40	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1317:C:H2'	1:A:1318:A:O4'	2.04	0.56
3:C:29:TYR:CZ	14:N:54:PRO:HG2	2.40	0.56
17:Q:59:ILE:HG22	17:Q:71:PHE:CD1	2.39	0.56
1:A:129(A):G:O2'	1:A:190(E):U:H2'	2.05	0.56
1:A:780:A:O2'	1:A:781:A:H5''	2.05	0.56
1:A:1278:U:H5''	1:A:1279:A:O4'	2.04	0.56
17:Q:5:VAL:HG22	17:Q:60:ILE:HG12	1.87	0.56
18:R:25:THR:O	18:R:26:LEU:HB2	2.04	0.56
1:A:760:G:O6	17:Q:105:ALA:HB2	2.05	0.56
1:A:818:G:H3'	1:A:819:A:H5''	1.87	0.56
1:A:1040:U:H2'	1:A:1041:A:H8	1.70	0.56
1:A:1256:A:H61	1:A:1278:U:H1'	1.70	0.56
2:B:126:GLU:HG2	2:B:129:GLU:OE1	2.05	0.56
3:C:32:LEU:HD23	3:C:32:LEU:O	2.05	0.56
5:E:101:ILE:O	5:E:120:THR:HB	2.05	0.56
8:H:60:ARG:HH11	8:H:60:ARG:HG3	1.70	0.56
13:M:17:VAL:O	13:M:20:THR:HB	2.05	0.56
15:O:3:ILE:HG22	15:O:7:GLU:HB3	1.86	0.56
19:S:28:LYS:CG	19:S:29:ARG:H	2.09	0.56
22:Y:156:PRO:HB2	22:Y:158:LEU:HB3	1.87	0.56
1:A:448:A:H2'	1:A:449:C:C6	2.40	0.56
1:A:915:A:C2'	1:A:916:G:H5'	2.35	0.56
1:A:1195:C:H3'	1:A:1196:U:C5'	2.35	0.56
1:A:1223:C:OP1	1:A:1224:G:H3'	2.05	0.56
1:A:1346:A:H4'	1:A:1347:G:O5'	2.06	0.56
2:B:47:THR:HA	2:B:202:PRO:HG2	1.87	0.56
2:B:98:LEU:HG	2:B:101:MET:HE3	1.88	0.56
3:C:33:LEU:HD23	3:C:33:LEU:O	2.04	0.56
5:E:12:LEU:HD22	5:E:12:LEU:C	2.29	0.56
6:F:2:ARG:CD	6:F:69:GLU:HG2	2.35	0.56
10:J:4:ILE:HA	10:J:100:THR:HA	1.88	0.56
13:M:8:GLU:OE1	13:M:22:ILE:HG12	2.06	0.56
13:M:15:VAL:HG23	13:M:43:THR:O	2.04	0.56
17:Q:59:ILE:CG2	17:Q:71:PHE:HB3	2.36	0.56
19:S:63:THR:HG22	19:S:64:GLU:H	1.71	0.56
7:G:146:GLU:HA	7:G:149:ARG:HB2	1.87	0.56
9:I:39:GLY:O	9:I:40:LEU:HD23	2.06	0.56
11:K:126:ARG:O	11:K:127:LYS:C	2.48	0.56
13:M:12:ASN:O	13:M:12:ASN:ND2	2.39	0.56
14:N:36:PHE:O	14:N:36:PHE:CD1	2.58	0.56
17:Q:67:LYS:O	17:Q:68:ARG:HB3	2.05	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:R:46:GLU:H	18:R:46:GLU:CD	2.14	0.56
1:A:1053:G:H4'	1:A:1054:C:H5'	1.88	0.56
1:A:1257:U:H4'	1:A:1258:G:O5'	2.06	0.56
1:A:1443:G:H5''	1:A:1446:A:C5'	2.19	0.56
4:D:6:GLY:O	4:D:8:VAL:HG23	2.06	0.56
4:D:57:ARG:HB3	4:D:206:PHE:HB2	1.88	0.56
10:J:12:ASP:HB3	10:J:15:THR:HB	1.88	0.56
10:J:22:LYS:CE	10:J:90:LEU:HD12	2.33	0.56
19:S:10:PHE:CD2	19:S:11:VAL:N	2.73	0.56
22:Y:55:ASP:OD1	22:Y:56:PRO:HD2	2.06	0.56
1:A:438:G:C4'	1:A:439:A:OP1	2.53	0.56
1:A:477:G:H2'	1:A:478:A:C8	2.40	0.56
1:A:1028:C:H2'	1:A:1029:C:C6	2.40	0.56
1:A:1339:A:H2'	1:A:1340:A:O4'	2.06	0.56
3:C:7:PRO:CG	3:C:184:TYR:HB2	2.35	0.56
3:C:108:ASN:C	3:C:110:ASN:H	2.12	0.56
8:H:105:ARG:HG3	8:H:105:ARG:HH11	1.71	0.56
1:A:1326:C:OP1	21:V:12:LYS:NZ	2.37	0.56
4:D:24:GLU:HG2	4:D:25:ARG:N	2.21	0.56
4:D:176:LEU:HA	4:D:183:GLY:HA2	1.87	0.56
5:E:79:GLU:CD	8:H:105:ARG:HD3	2.30	0.56
18:R:53:ARG:HD3	18:R:63:GLN:CB	2.36	0.56
19:S:10:PHE:CD2	19:S:10:PHE:C	2.83	0.56
19:S:40:ILE:HG21	19:S:62:ILE:HD11	1.88	0.56
1:A:665:A:H2'	1:A:725:G:N2	2.21	0.56
4:D:148:VAL:HG11	4:D:158:ILE:HD13	1.88	0.56
13:M:117:VAL:HG12	13:M:118:ALA:H	1.70	0.56
17:Q:103:GLY:O	17:Q:104:LYS:O	2.24	0.56
1:A:411:A:C4	1:A:413:G:H1'	2.41	0.56
1:A:933:G:OP2	7:G:3:ARG:HB2	2.06	0.56
1:A:1044:A:H2'	1:A:1045:C:C5'	2.36	0.56
1:A:1202:G:O2'	1:A:1203:C:H5'	2.06	0.56
2:B:74:LYS:HZ1	2:B:206:ASP:CA	2.18	0.56
10:J:81:THR:O	10:J:85:LEU:HG	2.06	0.56
1:A:166:G:O2'	1:A:167:G:H5'	2.06	0.55
1:A:652:U:H2'	1:A:752:G:N1	2.21	0.55
1:A:1216:G:H5''	14:N:5:ALA:HB1	1.88	0.55
1:A:1257:U:O2'	1:A:1258:G:OP2	2.21	0.55
4:D:24:GLU:H	4:D:112:VAL:CG1	2.19	0.55
5:E:118:ILE:HG22	5:E:119:LEU:H	1.67	0.55
16:P:26:ARG:HD2	16:P:31:LYS:O	2.06	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1042:G:O2'	1:A:1043:C:H5'	2.06	0.55
1:A:1405:G:C2	1:A:1497:G:C2	2.94	0.55
2:B:21:ARG:HG3	2:B:23:ARG:HD2	1.88	0.55
13:M:65:LYS:HE3	13:M:69:GLU:OE2	2.07	0.55
1:A:103:C:P	20:T:17:ARG:NH1	2.79	0.55
1:A:505:G:H2'	1:A:506:G:H8	1.69	0.55
1:A:1193:G:O2'	1:A:1194:U:H5'	2.07	0.55
2:B:15:VAL:HG22	2:B:209:ARG:HG3	1.88	0.55
20:T:86:ARG:O	20:T:90:GLN:HG3	2.06	0.55
2:B:23:ARG:HD3	2:B:23:ARG:N	2.22	0.55
10:J:24:VAL:HG21	10:J:37:PRO:HD3	1.88	0.55
16:P:81:ARG:CG	16:P:83:GLU:HG2	2.36	0.55
1:A:1236:A:H2'	1:A:1237:C:C6	2.41	0.55
1:A:1251:A:H2'	1:A:1252:A:C8	2.41	0.55
2:B:17:PHE:CD1	2:B:17:PHE:C	2.85	0.55
2:B:67:THR:HG22	2:B:68:ILE:N	2.21	0.55
3:C:33:LEU:HD11	14:N:53:LEU:HD22	1.87	0.55
6:F:69:GLU:HA	6:F:72:VAL:CG2	2.37	0.55
18:R:86:VAL:O	18:R:87:ARG:CB	2.55	0.55
1:A:18:C:H4'	1:A:1078:U:O2	2.07	0.55
1:A:490:G:H2'	1:A:491:G:H8	1.72	0.55
4:D:107:ARG:HH21	4:D:194:LEU:HD12	1.70	0.55
8:H:126:LYS:C	8:H:128:GLY:H	2.14	0.55
20:T:35:THR:O	20:T:39:LYS:HB2	2.06	0.55
20:T:94:ALA:O	20:T:95:ALA:HB3	2.06	0.55
1:A:227:G:O2'	16:P:62:VAL:HG11	2.05	0.55
1:A:620:C:H2'	1:A:621:A:O4'	2.07	0.55
1:A:1066:C:O2'	1:A:1067:A:H5'	2.07	0.55
1:A:1268:A:H2'	1:A:1269:A:C8	2.41	0.55
1:A:1460:A:H2'	1:A:1461:G:O4'	2.07	0.55
2:B:17:PHE:C	2:B:17:PHE:HD1	2.14	0.55
4:D:177:ASP:OD1	4:D:179:GLU:HB2	2.07	0.55
7:G:116:ALA:HA	7:G:119:ARG:NH2	2.21	0.55
9:I:7:THR:HG22	9:I:8:GLY:N	2.22	0.55
10:J:49:VAL:HG11	14:N:41:ARG:O	2.07	0.55
13:M:37:THR:HG22	13:M:37:THR:O	2.07	0.55
1:A:551:U:H2'	1:A:552:U:C6	2.41	0.55
1:A:954:G:H2'	1:A:955:U:C6	2.42	0.55
1:A:1442:G:H21	1:A:1446:A:H5''	1.72	0.55
3:C:38:ARG:HB3	3:C:94:LEU:HD21	1.89	0.55
6:F:46:ARG:HB2	6:F:60:PHE:HE1	1.71	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:76:ALA:O	6:F:80:ARG:HG3	2.06	0.55
12:L:43:VAL:HG12	12:L:44:THR:H	1.72	0.55
12:L:50:SER:O	12:L:51:ALA:HB2	2.05	0.55
22:Y:43:ALA:HA	22:Y:51:TYR:CE2	2.42	0.55
1:A:818:G:C3'	1:A:819:A:C5'	2.83	0.55
1:A:1404:C:H1'	1:A:1499:A:C2	2.42	0.55
3:C:52:LEU:HD21	3:C:118:GLN:OE1	2.07	0.55
1:A:532:A:H2'	1:A:533:A:H5''	1.89	0.55
1:A:939:G:H2'	1:A:940:C:H6	1.71	0.55
1:A:1006:C:H2'	1:A:1007:C:H6	1.72	0.55
1:A:1333:A:H2'	1:A:1334:G:O4'	2.07	0.55
1:A:1404:C:C1'	1:A:1499:A:N1	2.70	0.55
2:B:75:LYS:O	2:B:75:LYS:HD3	2.07	0.55
5:E:21:ALA:O	5:E:23:GLY:N	2.40	0.55
12:L:47:LYS:HB2	12:L:48:PRO:HD2	1.88	0.55
20:T:67:ALA:HB2	20:T:77:ALA:HB2	1.88	0.55
1:A:26:A:N6	1:A:558:G:H1'	2.21	0.54
1:A:190(F):G:H4'	1:A:190(G):G:OP2	2.07	0.54
1:A:193:C:H2'	1:A:194:C:H6	1.72	0.54
1:A:1319:A:H5'	1:A:1320:C:OP1	2.06	0.54
3:C:138:VAL:HG21	3:C:168:ALA:HB1	1.89	0.54
15:O:87:ILE:O	15:O:88:ARG:CB	2.54	0.54
17:Q:68:ARG:N	17:Q:70:ARG:NH1	2.55	0.54
1:A:54:C:H2'	1:A:352:C:H41	1.71	0.54
2:B:17:PHE:CD1	2:B:18:GLY:N	2.75	0.54
2:B:33:TYR:HB3	2:B:41:ILE:O	2.08	0.54
3:C:37:GLN:NE2	14:N:52:GLN:OE1	2.40	0.54
3:C:58:GLU:H	3:C:65:ALA:HB3	1.72	0.54
3:C:112:SER:CB	3:C:115:LEU:HD12	2.36	0.54
6:F:25:ILE:HD12	6:F:82:ARG:HD2	1.88	0.54
9:I:47:LEU:C	9:I:49:PRO:HD2	2.32	0.54
15:O:32:LEU:O	15:O:36:ILE:HG13	2.06	0.54
1:A:967:C:C4'	9:I:128:ARG:HG3	2.38	0.54
1:A:1128:C:H2'	1:A:1129:C:H5''	1.89	0.54
7:G:69:VAL:HG12	7:G:100:ALA:HA	1.89	0.54
8:H:36:LEU:HD12	8:H:59:LEU:HD13	1.88	0.54
8:H:56:LYS:HD2	8:H:56:LYS:N	2.23	0.54
17:Q:79:SER:O	17:Q:80:GLY:O	2.25	0.54
1:A:130:A:C8	17:Q:63:ARG:HG3	2.42	0.54
1:A:977:A:C2'	1:A:978:A:H5''	2.38	0.54
2:B:33:TYR:HB2	2:B:43:ASP:HB2	1.89	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:15:ARG:O	5:E:27:ARG:O	2.25	0.54
7:G:116:ALA:HA	7:G:119:ARG:CZ	2.37	0.54
10:J:51:ARG:H	10:J:59:SER:HB2	1.72	0.54
13:M:5:ALA:O	13:M:6:GLY:C	2.51	0.54
20:T:72:LEU:HD21	20:T:80:ARG:CZ	2.38	0.54
1:A:743:U:H2'	1:A:744:C:C6	2.43	0.54
1:A:1351:U:H2'	1:A:1352:C:C6	2.40	0.54
6:F:4:TYR:OH	6:F:69:GLU:HB3	2.07	0.54
7:G:18:TYR:CE2	7:G:59:LEU:HB2	2.42	0.54
7:G:113:GLU:HG2	7:G:119:ARG:HG2	1.90	0.54
10:J:3:LYS:N	10:J:75:ILE:HA	2.22	0.54
13:M:60:VAL:O	13:M:63:THR:HG22	2.07	0.54
13:M:94:ARG:HH22	19:S:81:ARG:HH11	1.54	0.54
1:A:195:A:H4'	20:T:68:LYS:NZ	2.22	0.54
1:A:1030(A):G:N2	1:A:1030(C):G:H3'	2.23	0.54
1:A:1320:C:N3	19:S:36:ARG:HG3	2.22	0.54
2:B:17:PHE:HD1	2:B:18:GLY:N	2.05	0.54
5:E:137:GLU:O	5:E:141:GLN:HG3	2.08	0.54
13:M:29:ARG:HB3	13:M:64:TRP:CH2	2.42	0.54
16:P:21:VAL:O	16:P:33:ILE:HB	2.07	0.54
17:Q:67:LYS:CA	17:Q:70:ARG:HH12	2.21	0.54
1:A:190:C:H2'	1:A:190(A):C:C6	2.43	0.54
1:A:960:U:H5'	1:A:960:U:O2	2.08	0.54
1:A:1459:C:OP1	20:T:27:LYS:HE2	2.08	0.54
2:B:187:LEU:HD23	2:B:214:ILE:HG21	1.90	0.54
3:C:77:ILE:HG22	3:C:81:GLY:HA2	1.90	0.54
3:C:150:LYS:CE	3:C:152:ILE:HD11	2.38	0.54
3:C:174:PRO:HB2	3:C:177:THR:HG22	1.89	0.54
6:F:26:ILE:HG21	6:F:63:TYR:CE2	2.40	0.54
9:I:85:LEU:O	9:I:92:TYR:HD1	1.91	0.54
15:O:27:VAL:O	15:O:31:LEU:HD13	2.07	0.54
17:Q:18:THR:HG23	17:Q:69:LYS:HE3	1.88	0.54
22:Y:41:LYS:O	22:Y:44:ILE:HG22	2.08	0.54
1:A:429:U:H2'	4:D:25:ARG:HH12	1.73	0.54
4:D:160:GLN:O	4:D:163:GLU:HB3	2.08	0.54
4:D:199:ASN:OD1	4:D:201:GLN:HB2	2.08	0.54
5:E:76:ILE:O	5:E:93:PRO:HB3	2.07	0.54
7:G:138:LYS:HE2	7:G:142:GLU:OE1	2.08	0.54
16:P:42:ARG:O	16:P:43:LYS:C	2.51	0.54
20:T:53:LEU:HB2	20:T:100:ILE:HB	1.89	0.54
1:A:281:G:O2'	1:A:282:A:P	2.65	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:429:U:H2'	4:D:25:ARG:NH1	2.22	0.54
1:A:750:G:H1'	15:O:22:THR:OG1	2.08	0.54
4:D:126:ILE:HG22	4:D:127:THR:N	2.23	0.54
5:E:104:ALA:O	5:E:105:VAL:C	2.49	0.54
1:A:475:G:H2'	1:A:476:G:C8	2.43	0.54
1:A:1222:G:P	19:S:77:THR:HG21	2.48	0.54
1:A:1318:A:H4'	19:S:10:PHE:CE1	2.42	0.54
1:A:1516:G:H2'	1:A:1518:A:OP2	2.08	0.54
3:C:116:VAL:O	3:C:120:VAL:HG23	2.07	0.54
8:H:119:LEU:HD12	8:H:124:ALA:HA	1.89	0.54
9:I:81:ILE:O	9:I:85:LEU:HB2	2.08	0.54
19:S:51:VAL:HG12	19:S:52:TYR:N	2.23	0.54
1:A:299:G:H2'	1:A:300:A:C8	2.43	0.53
1:A:933:G:C2	1:A:1385:G:C2	2.96	0.53
1:A:1218:C:H2'	1:A:1219:U:C6	2.42	0.53
1:A:1488:G:H2'	1:A:1489:G:C8	2.44	0.53
2:B:18:GLY:CA	2:B:42:ILE:H	2.20	0.53
6:F:100:ASN:OD1	18:R:23:LYS:HG2	2.08	0.53
7:G:44:TYR:HE1	9:I:41:VAL:HG11	1.72	0.53
15:O:70:LEU:HD11	15:O:77:ARG:HB2	1.89	0.53
16:P:11:SER:OG	16:P:14:ASN:HB3	2.08	0.53
1:A:35:G:H2'	1:A:36:C:C6	2.43	0.53
1:A:181:G:H4'	1:A:182:U:H5'	1.89	0.53
1:A:639:G:O2'	1:A:640:A:H5'	2.08	0.53
1:A:957:U:H4'	19:S:79:THR:HB	1.89	0.53
1:A:1347:G:C2'	1:A:1348:U:OP2	2.56	0.53
11:K:14:VAL:O	11:K:15:ALA:CB	2.57	0.53
13:M:53:VAL:O	13:M:57:ARG:HB2	2.08	0.53
1:A:983:A:H5'	1:A:984:C:OP2	2.07	0.53
3:C:91:LEU:HD21	3:C:99:VAL:CG1	2.30	0.53
3:C:113:ALA:HB3	3:C:114:PRO:HD3	1.90	0.53
5:E:79:GLU:OE1	8:H:105:ARG:HD3	2.08	0.53
7:G:42:ILE:CG2	7:G:120:ILE:HD12	2.38	0.53
16:P:43:LYS:HB3	16:P:48:TRP:CD1	2.43	0.53
20:T:93:GLU:HA	20:T:93:GLU:OE2	2.09	0.53
22:Y:1:MET:HE1	22:Y:17:LEU:HD22	1.90	0.53
1:A:101:A:O2'	1:A:102:G:H5'	2.07	0.53
1:A:1003:G:C2	1:A:1003(A):G:C6	2.96	0.53
1:A:1121:U:H2'	1:A:1122:U:H6	1.73	0.53
1:A:1157:A:H4'	1:A:1158:C:O5'	2.08	0.53
9:I:17:VAL:HG11	9:I:81:ILE:HA	1.90	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:8:GLU:OE1	13:M:22:ILE:HA	2.08	0.53
14:N:44:LEU:HD12	14:N:44:LEU:O	2.08	0.53
18:R:36:ASN:CG	18:R:39:VAL:HG12	2.34	0.53
20:T:76:ALA:O	20:T:80:ARG:HG2	2.09	0.53
1:A:382:A:H2'	1:A:383:A:H8	1.70	0.53
1:A:407:G:O2'	4:D:116:GLN:HG3	2.08	0.53
2:B:23:ARG:HH11	2:B:23:ARG:C	2.16	0.53
10:J:27:ALA:C	10:J:29:ARG:H	2.15	0.53
10:J:38:ILE:HG13	10:J:71:LEU:HB3	1.90	0.53
12:L:46:LYS:CG	12:L:47:LYS:N	2.71	0.53
16:P:19:ILE:HG22	16:P:36:ILE:HG13	1.90	0.53
22:Y:109:THR:HG1	25:Y:301:SFG:HN61	1.53	0.53
1:A:300:A:H2'	1:A:301:G:O4'	2.08	0.53
1:A:386:C:C2'	1:A:387:U:H5'	2.39	0.53
1:A:1003:G:N2	1:A:1039:C:C2	2.77	0.53
2:B:97:TRP:CH2	2:B:176:GLU:CD	2.85	0.53
3:C:32:LEU:HD21	3:C:59:ARG:HD2	1.91	0.53
5:E:78:HIS:HD2	8:H:107:LEU:HD12	1.74	0.53
7:G:6:ARG:O	7:G:7:ALA:C	2.52	0.53
8:H:80:ILE:O	8:H:80:ILE:HG22	2.08	0.53
9:I:97:LYS:O	9:I:100:GLY:N	2.36	0.53
19:S:42:PRO:O	19:S:45:VAL:HG23	2.09	0.53
20:T:38:LYS:O	20:T:39:LYS:C	2.51	0.53
22:Y:141:TYR:N	22:Y:141:TYR:CD1	2.77	0.53
1:A:33:A:H2'	1:A:34:C:H6	1.73	0.53
1:A:818:G:O2'	1:A:819:A:H5''	2.08	0.53
1:A:959:A:C2	1:A:1222:G:O4'	2.61	0.53
1:A:979:C:H2'	1:A:980:C:H5'	1.91	0.53
1:A:1286:A:H5''	21:V:25:LYS:HZ2	1.73	0.53
3:C:14:ILE:HG22	3:C:15:THR:N	2.12	0.53
5:E:18:ARG:HG2	5:E:19:MET:N	2.23	0.53
8:H:8:ASP:O	8:H:12:ARG:HG3	2.08	0.53
12:L:55:VAL:HG11	12:L:67:THR:HG23	1.91	0.53
17:Q:27:PHE:CE1	17:Q:36:ILE:HD11	2.42	0.53
1:A:33:A:H2'	1:A:34:C:C6	2.44	0.53
1:A:148:G:H2'	1:A:149:A:H8	1.74	0.53
1:A:1426:C:H2'	1:A:1427:U:C6	2.44	0.53
3:C:130:VAL:O	3:C:134:ILE:HG13	2.07	0.53
9:I:48:GLU:OE1	9:I:51:ARG:HD2	2.09	0.53
13:M:102:ARG:NH1	13:M:102:ARG:HB2	2.24	0.53
18:R:61:LYS:O	18:R:65:ILE:HG13	2.08	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:V:9:ARG:NH1	21:V:22:ARG:HA	2.23	0.53
1:A:179:A:H2'	1:A:180:U:C6	2.43	0.53
1:A:623:C:O2'	1:A:624:C:H5'	2.09	0.53
1:A:1117:G:H4'	9:I:104:ARG:HH11	1.72	0.53
1:A:1408:A:C6	22:Y:107:TRP:CE3	2.96	0.53
2:B:166:ASP:OD2	2:B:169:LYS:HB2	2.09	0.53
7:G:71:PRO:HD3	7:G:103:TRP:HZ3	1.74	0.53
10:J:44:VAL:HG22	10:J:66:ARG:HB3	1.91	0.53
12:L:47:LYS:HB3	12:L:48:PRO:HD3	1.91	0.53
12:L:53:ARG:HG2	12:L:69:TYR:HE1	1.73	0.53
13:M:11:ARG:CG	13:M:12:ASN:N	2.72	0.53
1:A:252:U:H2'	1:A:253:U:C6	2.44	0.53
1:A:370:C:O2'	1:A:371:G:H5'	2.09	0.53
1:A:373:A:O2'	1:A:374:A:H5'	2.09	0.53
1:A:656:C:O2'	15:O:28:GLN:OE1	2.23	0.53
1:A:666:G:H5'	1:A:726:C:H1'	1.90	0.53
1:A:937:A:C2	1:A:1379:G:C6	2.97	0.53
1:A:1184:G:H2'	1:A:1185:G:H8	1.74	0.53
2:B:23:ARG:O	2:B:24:TRP:O	2.27	0.53
4:D:6:GLY:O	4:D:7:PRO:C	2.50	0.53
6:F:75:LEU:C	6:F:75:LEU:HD13	2.34	0.53
9:I:31:GLN:HB3	9:I:35:GLU:HB3	1.91	0.53
1:A:101:A:H2'	1:A:102:G:H8	1.74	0.52
1:A:1068:G:OP2	1:A:1068:G:H8	1.91	0.52
2:B:124:SER:O	2:B:127:ILE:HG13	2.08	0.52
3:C:92:ALA:C	3:C:94:LEU:H	2.17	0.52
14:N:33:VAL:HA	14:N:40:CYS:HA	1.91	0.52
22:Y:39:ILE:HD12	22:Y:51:TYR:HB3	1.91	0.52
1:A:246:A:N6	1:A:281:G:H1'	2.24	0.52
1:A:1305:G:O2'	1:A:1306:A:C8	2.44	0.52
1:A:1513:A:H2'	1:A:1514:C:C6	2.44	0.52
2:B:213:LEU:C	2:B:213:LEU:CD2	2.82	0.52
5:E:12:LEU:CD1	5:E:31:LEU:HB2	2.39	0.52
22:Y:38:ASN:OD1	22:Y:195:SER:HB3	2.08	0.52
1:A:760:G:N1	17:Q:105:ALA:HB2	2.24	0.52
1:A:1006:C:H2'	1:A:1007:C:C6	2.44	0.52
3:C:23:TYR:CD2	3:C:24:ALA:N	2.78	0.52
3:C:70:VAL:O	3:C:106:VAL:HG23	2.09	0.52
6:F:43:LEU:H	6:F:43:LEU:CD2	2.22	0.52
6:F:94:GLN:OE1	18:R:32:ARG:HD3	2.09	0.52
7:G:69:VAL:HG21	7:G:104:LEU:HD21	1.90	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:13:GLN:HA	11:K:75:TYR:O	2.08	0.52
1:A:115:G:O2'	1:A:116:A:OP2	2.22	0.52
1:A:621:A:H2'	1:A:622:A:C8	2.44	0.52
1:A:657:G:C4'	15:O:28:GLN:HG2	2.36	0.52
1:A:953:G:H2'	1:A:954:G:O4'	2.09	0.52
1:A:1038:C:H2'	1:A:1039:C:C6	2.43	0.52
1:A:1038:C:H2'	1:A:1039:C:H6	1.74	0.52
1:A:1305:G:OP1	21:V:2:GLY:N	2.42	0.52
1:A:1397:C:H4'	1:A:1398:A:OP2	2.08	0.52
1:A:1423:G:O2'	1:A:1424:C:H5'	2.09	0.52
4:D:104:VAL:HG11	4:D:146:ILE:CD1	2.37	0.52
13:M:102:ARG:HB2	13:M:102:ARG:HH11	1.75	0.52
18:R:73:ALA:HB3	18:R:79:LEU:HD12	1.91	0.52
21:V:17:THR:O	21:V:22:ARG:HD3	2.10	0.52
1:A:684:A:H1'	11:K:38:ASN:HB3	1.91	0.52
1:A:1128:C:H1'	1:A:1146:A:H61	1.75	0.52
5:E:31:LEU:HD22	5:E:43:LEU:CD2	2.39	0.52
6:F:10:LEU:HD11	6:F:59:TYR:CD2	2.41	0.52
12:L:55:VAL:HG11	12:L:67:THR:CG2	2.39	0.52
13:M:117:VAL:HG12	13:M:118:ALA:N	2.24	0.52
15:O:36:ILE:HA	15:O:59:MET:HE3	1.91	0.52
19:S:13:ASP:O	19:S:17:GLU:HG2	2.10	0.52
1:A:560:U:O2'	1:A:561:U:OP2	2.27	0.52
4:D:65:ARG:HB2	4:D:75:PHE:CE1	2.45	0.52
8:H:14:ARG:O	8:H:18:ARG:HD3	2.10	0.52
11:K:77:MET:HE3	11:K:80:VAL:HG22	1.90	0.52
13:M:86:CYS:SG	13:M:88:ARG:HB3	2.49	0.52
14:N:12:ARG:O	14:N:13:THR:C	2.52	0.52
19:S:50:ALA:HA	19:S:58:VAL:O	2.10	0.52
21:V:24:ARG:O	21:V:25:LYS:HB2	2.10	0.52
1:A:142:G:O2'	1:A:196:A:N1	2.40	0.52
1:A:1405:G:O2'	1:A:1519:A:C4'	2.58	0.52
3:C:130:VAL:HG12	3:C:134:ILE:HD11	1.91	0.52
6:F:67:MET:CE	6:F:72:VAL:HA	2.40	0.52
8:H:25:ASP:OD1	8:H:60:ARG:HD3	2.09	0.52
1:A:115:G:H1'	1:A:116:A:N7	2.24	0.52
1:A:148:G:H2'	1:A:149:A:C8	2.45	0.52
1:A:582:U:H1'	17:Q:105:ALA:HA	1.92	0.52
1:A:605:U:O2'	1:A:606:G:H5'	2.10	0.52
1:A:791:G:H2'	1:A:792:A:H5'	1.91	0.52
1:A:1021:G:C2'	1:A:1022:G:H5'	2.40	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1167:A:H2'	1:A:1168:A:C8	2.45	0.52
1:A:1428:A:H2'	1:A:1429:C:C6	2.44	0.52
2:B:73:THR:HG23	2:B:95:GLN:O	2.09	0.52
2:B:130:ARG:HH22	3:C:179:ARG:NH1	2.05	0.52
3:C:22:TRP:CZ2	14:N:54:PRO:HG3	2.44	0.52
3:C:154:SER:O	3:C:165:THR:HA	2.09	0.52
11:K:17:GLY:O	11:K:80:VAL:HA	2.09	0.52
11:K:27:ASN:HA	11:K:56:GLY:HA2	1.92	0.52
1:A:190(E):U:O2'	17:Q:63:ARG:NH2	2.43	0.52
1:A:923:A:O2'	1:A:1398:A:H2'	2.10	0.52
1:A:935:A:O2'	1:A:1383:C:N3	2.39	0.52
1:A:1202:G:H2'	1:A:1203:C:O4'	2.10	0.52
1:A:1451:A:O2'	1:A:1452:C:OP1	2.26	0.52
2:B:215:LEU:O	2:B:216:SER:C	2.52	0.52
4:D:170:VAL:CG1	4:D:174:LEU:HB2	2.39	0.52
6:F:8:ILE:HD11	6:F:79:LEU:HD13	1.91	0.52
6:F:53:ALA:C	6:F:55:ASP:H	2.18	0.52
9:I:9:ARG:HG2	9:I:14:VAL:HG22	1.92	0.52
10:J:39:PRO:O	10:J:40:LEU:CB	2.57	0.52
16:P:20:VAL:CG1	16:P:32:TYR:HB3	2.40	0.52
18:R:19:LYS:O	18:R:20:ALA:HB2	2.10	0.52
21:V:24:ARG:O	21:V:25:LYS:CB	2.58	0.52
3:C:20:SER:HB3	3:C:22:TRP:NE1	2.24	0.52
11:K:62:GLN:HG3	11:K:97:ALA:HB2	1.92	0.52
22:Y:31:LEU:HB3	22:Y:103:ILE:HG12	1.91	0.52
1:A:1094:G:H5''	1:A:1095:U:H5	1.75	0.51
1:A:1424:C:O2'	1:A:1425:U:H5'	2.09	0.51
4:D:158:ILE:HG22	4:D:181:MET:HE2	1.93	0.51
13:M:73:GLU:O	13:M:76:ALA:HB3	2.09	0.51
1:A:163:C:O2'	1:A:164:U:H5'	2.10	0.51
1:A:357:G:O2'	1:A:358:U:H5'	2.09	0.51
1:A:443:C:H2'	1:A:444:C:C6	2.43	0.51
1:A:452:A:H4'	16:P:72:ARG:NH2	2.25	0.51
1:A:1416:G:N2	1:A:1485:U:H1'	2.24	0.51
1:A:1511:G:H2'	1:A:1512:U:O4'	2.09	0.51
3:C:107:GLN:CD	3:C:107:GLN:N	2.64	0.51
3:C:134:ILE:HG21	3:C:167:TRP:O	2.11	0.51
9:I:44:VAL:HG13	9:I:51:ARG:NH2	2.24	0.51
10:J:22:LYS:NZ	10:J:91:PRO:HD3	2.25	0.51
10:J:26:ALA:O	10:J:84:GLN:NE2	2.43	0.51
12:L:119:LYS:O	12:L:120:TYR:HB2	2.10	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:88:ARG:HG3	13:M:98:VAL:CG1	2.40	0.51
18:R:88:LYS:OXT	18:R:88:LYS:HG2	2.10	0.51
1:A:502:G:H1'	1:A:550:G:H5'	1.91	0.51
1:A:738:C:P	6:F:92:LYS:HE3	2.50	0.51
1:A:794:A:H2'	1:A:795:C:C6	2.45	0.51
1:A:1329:A:O2'	1:A:1330:U:H5'	2.11	0.51
2:B:126:GLU:O	2:B:129:GLU:HB2	2.11	0.51
5:E:40:ARG:HG2	5:E:40:ARG:HH11	1.76	0.51
8:H:24:THR:HG23	8:H:61:VAL:HB	1.92	0.51
8:H:91:ARG:HG2	12:L:7:ILE:HG21	1.92	0.51
14:N:21:TYR:HE2	14:N:23:ARG:NE	2.09	0.51
14:N:57:ARG:HG2	14:N:58:LYS:H	1.75	0.51
17:Q:97:SER:O	17:Q:98:LEU:C	2.54	0.51
1:A:828:A:H2'	1:A:829:G:O4'	2.10	0.51
3:C:94:LEU:HD22	3:C:95:THR:HG23	1.92	0.51
4:D:24:GLU:O	4:D:25:ARG:HB3	2.10	0.51
5:E:13:ILE:HG22	5:E:30:ALA:CB	2.40	0.51
7:G:102:ARG:O	7:G:106:GLN:HG3	2.11	0.51
9:I:115:GLY:HA2	10:J:58:ASP:OD1	2.10	0.51
10:J:20:ALA:O	10:J:24:VAL:HG23	2.11	0.51
10:J:23:ILE:N	10:J:23:ILE:HD12	2.26	0.51
12:L:42:THR:HG21	12:L:52:LEU:HB3	1.91	0.51
1:A:992:U:O2'	1:A:993:G:OP2	2.26	0.51
1:A:1059:C:O2'	1:A:1060:C:H5'	2.11	0.51
1:A:1191:A:H2'	1:A:1192:C:C6	2.45	0.51
1:A:1221:G:O3'	19:S:77:THR:HG21	2.10	0.51
1:A:1468:A:H2'	1:A:1469:G:O4'	2.09	0.51
3:C:84:ILE:O	3:C:84:ILE:HG12	2.10	0.51
3:C:137:ALA:HA	3:C:140:ARG:NH1	2.26	0.51
6:F:69:GLU:OE1	6:F:69:GLU:N	2.44	0.51
7:G:156:TRP:OXT	7:G:156:TRP:HD1	1.93	0.51
20:T:41:ILE:O	20:T:45:GLN:HB2	2.10	0.51
1:A:478:A:O2'	1:A:479:C:H5'	2.11	0.51
1:A:922:G:N2	1:A:1396:A:C4	2.79	0.51
1:A:1021:G:H2'	1:A:1022:G:O4'	2.11	0.51
1:A:1021:G:C2	1:A:1022:G:H1'	2.45	0.51
1:A:1241:G:H2'	1:A:1242:C:H6	1.76	0.51
1:A:1496:C:H2'	1:A:1497:G:O4'	2.11	0.51
1:A:1518:A:H2'	1:A:1519:A:C8	2.46	0.51
3:C:61:ALA:O	3:C:63:ASN:N	2.44	0.51
3:C:97:LYS:O	3:C:98:ASN:HB3	2.10	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:87:GLY:O	4:D:88:VAL:C	2.54	0.51
5:E:15:ARG:O	5:E:16:THR:O	2.28	0.51
5:E:89:ILE:HD13	5:E:90:VAL:H	1.75	0.51
5:E:127:ASN:O	5:E:128:PRO:C	2.53	0.51
9:I:125:TYR:CD2	9:I:125:TYR:N	2.79	0.51
9:I:127:LYS:N	9:I:127:LYS:HD2	2.24	0.51
12:L:27:LEU:HG	12:L:28:LYS:N	2.22	0.51
17:Q:15:MET:HE1	17:Q:43:LEU:HD22	1.92	0.51
17:Q:45:HIS:CB	17:Q:65:ILE:HD13	2.39	0.51
19:S:45:VAL:HG12	19:S:46:GLY:N	2.26	0.51
19:S:53:ASN:HB2	19:S:56:GLN:H	1.74	0.51
19:S:81:ARG:O	19:S:81:ARG:HG2	2.11	0.51
1:A:1003(A):G:N1	1:A:1004:A:H1'	2.25	0.51
1:A:1152:A:H2'	1:A:1153:C:C6	2.45	0.51
1:A:1346:A:C4	7:G:10:ARG:NH2	2.78	0.51
1:A:1486:G:H2'	1:A:1487:G:O4'	2.10	0.51
2:B:26:PRO:O	2:B:29:ALA:HB2	2.10	0.51
8:H:49:GLU:HG2	8:H:62:TYR:HE2	1.75	0.51
17:Q:45:HIS:HB2	17:Q:65:ILE:CD1	2.37	0.51
22:Y:115:ILE:HD12	22:Y:156:PRO:CD	2.41	0.51
22:Y:197:TRP:CD1	25:Y:301:SFG:HNE1	2.29	0.51
1:A:580:U:H2'	1:A:581:G:O4'	2.11	0.51
1:A:791:G:H2'	1:A:792:A:C5'	2.40	0.51
1:A:808:C:OP1	15:O:48:LYS:HE3	2.11	0.51
1:A:931:C:C2	1:A:1387:G:N1	2.79	0.51
1:A:1085:U:O3'	1:A:1086:U:C6	2.64	0.51
1:A:1126:U:OP2	1:A:1281:U:O2	2.29	0.51
1:A:1496:C:H6	1:A:1496:C:O5'	1.94	0.51
2:B:96:ARG:O	2:B:98:LEU:HD23	2.11	0.51
3:C:34:LEU:HD23	3:C:34:LEU:O	2.10	0.51
3:C:188:LEU:CD1	3:C:195:VAL:HG13	2.41	0.51
5:E:144:THR:C	5:E:146:ALA:N	2.67	0.51
6:F:9:VAL:HG22	6:F:60:PHE:CE2	2.46	0.51
10:J:69:ASN:O	10:J:70:ARG:HD3	2.11	0.51
1:A:7:G:H5'	1:A:298:A:O4'	2.11	0.51
1:A:1162:C:H2'	1:A:1163:C:C6	2.46	0.51
1:A:1396:A:H4'	1:A:1397:C:H5''	1.93	0.51
1:A:1495:U:H2'	1:A:1496:C:C5	2.45	0.51
2:B:53:ARG:NH1	2:B:53:ARG:HG2	2.26	0.51
4:D:81:GLU:O	4:D:85:LYS:HG3	2.11	0.51
5:E:61:TYR:O	5:E:64:ARG:O	2.29	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:115:VAL:HG12	5:E:116:THR:N	2.25	0.51
6:F:43:LEU:H	6:F:43:LEU:HD22	1.76	0.51
14:N:28:GLY:O	14:N:30:ALA:N	2.44	0.51
1:A:650:G:C2'	1:A:651:C:H5'	2.40	0.51
1:A:1097:C:H2'	1:A:1098:C:C6	2.45	0.51
1:A:1440:C:C2'	1:A:1441:G:H5'	2.41	0.51
2:B:97:TRP:CZ2	2:B:102:LEU:HD13	2.45	0.51
2:B:144:ARG:O	2:B:147:LYS:N	2.42	0.51
5:E:11:ILE:HB	5:E:31:LEU:HB3	1.93	0.51
9:I:27:THR:HG23	9:I:30:GLY:O	2.11	0.51
9:I:44:VAL:CG1	9:I:51:ARG:HH12	2.23	0.51
12:L:53:ARG:NH1	12:L:92:ASP:OD2	2.42	0.51
1:A:112:G:H21	1:A:354:G:C5'	2.24	0.50
1:A:160:A:H1'	1:A:344:A:C5	2.47	0.50
1:A:620:C:N1	4:D:135:LEU:HD13	2.26	0.50
1:A:1262:C:H42	1:A:1273:G:H1	1.59	0.50
1:A:1408:A:OP1	22:Y:205:ARG:NH1	2.44	0.50
2:B:124:SER:CB	2:B:125:PRO:HD2	2.32	0.50
3:C:47:LEU:CD1	3:C:47:LEU:N	2.74	0.50
9:I:17:VAL:CG2	9:I:80:GLY:HA3	2.41	0.50
21:V:2:GLY:C	21:V:4:GLY:N	2.69	0.50
1:A:149:A:O2'	1:A:150:C:H5'	2.12	0.50
1:A:853:G:O2'	1:A:854:G:H5'	2.11	0.50
1:A:942:G:C4	1:A:943:U:C5	2.99	0.50
1:A:1190:G:O2'	1:A:1191:A:P	2.69	0.50
3:C:112:SER:O	3:C:116:VAL:HG23	2.11	0.50
4:D:29:PRO:C	4:D:30:LYS:HG3	2.35	0.50
6:F:19:LEU:C	6:F:19:LEU:HD23	2.36	0.50
11:K:32:ILE:CG2	11:K:77:MET:HE2	2.42	0.50
14:N:29:ARG:O	14:N:33:VAL:HG13	2.11	0.50
1:A:1035:A:H2'	1:A:1036:G:H8	1.76	0.50
1:A:1283:G:O2'	1:A:1284:C:H5'	2.11	0.50
2:B:33:TYR:HB3	2:B:41:ILE:HG22	1.93	0.50
2:B:53:ARG:HG2	2:B:53:ARG:HH11	1.76	0.50
2:B:88:ALA:O	2:B:90:MET:N	2.44	0.50
2:B:121:LEU:O	2:B:127:ILE:HG12	2.11	0.50
3:C:58:GLU:O	3:C:59:ARG:HG2	2.11	0.50
4:D:7:PRO:HB2	4:D:10:ARG:HD2	1.92	0.50
14:N:22:THR:OG1	14:N:33:VAL:HG21	2.11	0.50
21:V:6:ARG:HD2	21:V:15:ARG:NH1	2.25	0.50
1:A:659:U:O2'	1:A:660:G:H5'	2.11	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:824:C:H2'	1:A:825:G:H8	1.76	0.50
1:A:960:U:H1'	1:A:1223:C:H5'	1.93	0.50
1:A:1278:U:C5'	1:A:1279:A:O4'	2.59	0.50
1:A:1305:G:C8	1:A:1305:G:OP2	2.64	0.50
1:A:1310:G:O2'	1:A:1311:G:H5'	2.12	0.50
1:A:1392:G:O2'	1:A:1502:A:H5''	2.11	0.50
5:E:21:ALA:C	5:E:23:GLY:H	2.19	0.50
7:G:69:VAL:HG12	7:G:69:VAL:O	2.12	0.50
10:J:71:LEU:O	10:J:72:VAL:CB	2.60	0.50
12:L:46:LYS:HG2	12:L:47:LYS:HG3	1.93	0.50
13:M:78:ILE:HA	13:M:81:LEU:CD2	2.38	0.50
17:Q:27:PHE:HB2	17:Q:28:PRO:HD2	1.94	0.50
1:A:222:U:H2'	1:A:223:U:C6	2.47	0.50
1:A:576:G:N7	1:A:881:G:H1'	2.27	0.50
1:A:792:A:H4'	1:A:793:U:C5'	2.40	0.50
1:A:839:U:O2	1:A:839:U:C2'	2.59	0.50
1:A:999:C:H2'	1:A:1000:U:C6	2.46	0.50
1:A:1136:U:H5''	1:A:1137:C:OP2	2.12	0.50
1:A:1393:U:O4'	1:A:1502:A:H5'	2.11	0.50
1:A:1498:U:H4'	1:A:1519:A:C2	2.45	0.50
4:D:151:LYS:N	4:D:151:LYS:CD	2.75	0.50
9:I:112:LYS:C	9:I:112:LYS:HD3	2.37	0.50
10:J:3:LYS:HA	10:J:75:ILE:HA	1.94	0.50
12:L:46:LYS:O	12:L:47:LYS:C	2.54	0.50
13:M:77:ASN:O	13:M:80:ARG:HB3	2.10	0.50
18:R:45:SER:C	18:R:47:THR:N	2.64	0.50
1:A:325:A:H2'	1:A:326:G:O4'	2.12	0.50
1:A:922:G:O2'	1:A:1398:A:N1	2.45	0.50
1:A:1096:C:H2'	1:A:1097:C:H6	1.77	0.50
1:A:1179:A:H2'	1:A:1180:A:O4'	2.11	0.50
1:A:1305:G:C5'	21:V:4:GLY:HA3	2.41	0.50
2:B:44:LEU:HA	2:B:47:THR:OG1	2.12	0.50
2:B:186:ALA:HB3	2:B:197:VAL:CG1	2.41	0.50
2:B:221:LEU:O	2:B:221:LEU:HD13	2.11	0.50
3:C:79:ARG:HG2	3:C:82:GLU:HG2	1.92	0.50
3:C:178:LEU:O	3:C:179:ARG:CB	2.60	0.50
5:E:121:LYS:HE3	5:E:123:LEU:HD21	1.93	0.50
6:F:38:GLU:O	6:F:39:LYS:HB3	2.12	0.50
9:I:120:ARG:O	9:I:121:ARG:C	2.54	0.50
10:J:27:ALA:HB1	10:J:81:THR:HG23	1.92	0.50
12:L:45:PRO:HD3	12:L:51:ALA:O	2.11	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:556:C:C2'	1:A:557:G:H5'	2.40	0.50
1:A:746:A:O2'	1:A:747:C:H5'	2.11	0.50
3:C:177:THR:HG23	3:C:177:THR:O	2.10	0.50
4:D:3:ARG:NH2	4:D:74:GLN:OE1	2.43	0.50
4:D:126:ILE:CG2	4:D:127:THR:N	2.75	0.50
7:G:102:ARG:HG2	7:G:106:GLN:NE2	2.27	0.50
9:I:19:LEU:C	9:I:20:ARG:HG3	2.37	0.50
11:K:74:ALA:C	11:K:76:GLY:N	2.69	0.50
17:Q:45:HIS:NE2	17:Q:47:PRO:HG3	2.27	0.50
17:Q:97:SER:HB2	17:Q:103:GLY:N	2.26	0.50
1:A:217:C:O2'	1:A:218:C:H5'	2.12	0.50
1:A:933:G:N2	1:A:1385:G:C4	2.80	0.50
1:A:1057:G:H5''	3:C:154:SER:CB	2.30	0.50
1:A:1306:A:H2'	1:A:1307:U:O4'	2.12	0.50
2:B:132:LYS:O	2:B:136:VAL:HG23	2.12	0.50
8:H:113:SER:HB2	8:H:134:ILE:CD1	2.29	0.50
9:I:46:ALA:HA	9:I:78:LYS:HB2	1.93	0.50
20:T:101:GLY:O	20:T:102:GLY:O	2.30	0.50
1:A:136:C:H2'	1:A:137:C:H6	1.77	0.50
1:A:664:G:OP1	18:R:64:ARG:HD2	2.12	0.50
1:A:1025:U:OP1	1:A:1025:U:H4'	2.11	0.50
1:A:1044:A:H2'	1:A:1045:C:H5'	1.92	0.50
1:A:1256:A:C4'	1:A:1257:U:H5'	2.35	0.50
4:D:8:VAL:HG11	4:D:21:LEU:HB3	1.94	0.50
4:D:8:VAL:HG13	4:D:21:LEU:HD13	1.93	0.50
7:G:18:TYR:HD2	7:G:59:LEU:HD22	1.76	0.50
7:G:38:LEU:O	7:G:42:ILE:HG13	2.12	0.50
9:I:10:ARG:HG2	9:I:75:ASP:CB	2.41	0.50
11:K:23:ALA:CB	11:K:91:ARG:HB2	2.42	0.50
11:K:51:LYS:O	11:K:55:LYS:HE3	2.11	0.50
11:K:65:ALA:HB3	11:K:97:ALA:HB3	1.93	0.50
11:K:82:VAL:HG23	11:K:105:VAL:HG13	1.93	0.50
17:Q:10:VAL:O	17:Q:53:LEU:HD12	2.12	0.50
20:T:50:GLU:C	20:T:100:ILE:HD12	2.36	0.50
1:A:89:C:H2'	1:A:90:U:O4'	2.12	0.49
1:A:255:G:O6	1:A:266:G:O6	2.29	0.49
1:A:430:A:C2'	1:A:431:A:H5'	2.42	0.49
1:A:575:G:C4	1:A:881:G:C2	3.00	0.49
1:A:959:A:H2'	1:A:960:U:O4'	2.12	0.49
1:A:1074:G:O3'	2:B:103:THR:HG22	2.12	0.49
1:A:1181:G:O2'	1:A:1184:G:H5'	2.11	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1499:A:O2'	1:A:1500:A:H5'	2.12	0.49
2:B:69:LEU:C	2:B:69:LEU:HD23	2.36	0.49
3:C:171:GLY:O	3:C:173:VAL:HG23	2.12	0.49
5:E:31:LEU:HD22	5:E:43:LEU:HD21	1.94	0.49
11:K:48:ILE:HD13	11:K:63:LEU:HB3	1.93	0.49
12:L:28:LYS:HD2	12:L:33:ARG:CZ	2.42	0.49
14:N:15:LYS:HB3	14:N:16:PHE:CD1	2.47	0.49
15:O:3:ILE:CG2	15:O:7:GLU:HB3	2.41	0.49
1:A:204:U:H4'	1:A:216:G:O5'	2.12	0.49
1:A:625:G:H2'	1:A:626:U:C6	2.47	0.49
1:A:1085:U:O3'	1:A:1086:U:H6	1.95	0.49
1:A:1165:C:O2'	1:A:1166:G:H5'	2.13	0.49
3:C:6:HIS:ND1	3:C:8:ILE:HB	2.27	0.49
3:C:47:LEU:N	3:C:47:LEU:HD12	2.27	0.49
7:G:108:ALA:O	7:G:119:ARG:HB3	2.12	0.49
9:I:36:TYR:HD2	9:I:37:PHE:CE2	2.30	0.49
11:K:124:LYS:HD2	11:K:125:PHE:CE1	2.47	0.49
17:Q:26:GLN:O	17:Q:27:PHE:HB3	2.12	0.49
18:R:87:ARG:HG2	18:R:87:ARG:HH11	1.76	0.49
1:A:245:C:O2	1:A:283:C:N3	2.46	0.49
1:A:647:C:H2'	1:A:648:A:H8	1.78	0.49
1:A:665:A:H2'	1:A:732:C:O2	2.12	0.49
1:A:1172:C:O2'	1:A:1173:G:H5'	2.11	0.49
1:A:1301:U:O2'	1:A:1302:U:OP1	2.30	0.49
2:B:30:ARG:HG3	2:B:31:TYR:CD2	2.48	0.49
3:C:14:ILE:CG2	3:C:15:THR:H	2.11	0.49
3:C:38:ARG:HG3	3:C:38:ARG:NH1	2.26	0.49
3:C:172:ARG:HH12	3:C:174:PRO:CG	2.22	0.49
8:H:38:ILE:N	8:H:38:ILE:HD12	2.27	0.49
10:J:60:ARG:O	10:J:61:GLU:CB	2.61	0.49
12:L:48:PRO:HG2	12:L:49:ASN:N	2.26	0.49
13:M:80:ARG:C	13:M:82:MET:H	2.20	0.49
13:M:84:ILE:C	13:M:86:CYS:N	2.70	0.49
15:O:36:ILE:HA	15:O:59:MET:CE	2.42	0.49
1:A:521:G:O2'	1:A:522:C:H5'	2.12	0.49
1:A:1323:G:H2'	1:A:1324:A:C8	2.47	0.49
2:B:124:SER:CB	2:B:125:PRO:CD	2.90	0.49
3:C:167:TRP:O	3:C:168:ALA:HB3	2.11	0.49
1:A:129(A):G:O2'	1:A:130:A:OP2	2.28	0.49
1:A:190:C:H2'	1:A:190(A):C:H6	1.75	0.49
1:A:218:C:H2'	1:A:219:C:C6	2.47	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:761:G:H5''	17:Q:102:GLY:HA3	1.95	0.49
1:A:1102:A:H2'	1:A:1103:C:C6	2.47	0.49
1:A:1365:G:O2'	1:A:1366:C:H5'	2.12	0.49
3:C:180:ALA:O	3:C:181:ASN:CB	2.61	0.49
6:F:43:LEU:HD22	6:F:43:LEU:N	2.27	0.49
7:G:85:TYR:CD1	7:G:154:TYR:HE1	2.28	0.49
9:I:36:TYR:HE2	9:I:73:GLN:NE2	2.10	0.49
12:L:45:PRO:HB2	12:L:49:ASN:O	2.13	0.49
15:O:4:THR:HB	15:O:6:GLU:HG2	1.94	0.49
15:O:17:ARG:HG3	15:O:17:ARG:NH1	2.23	0.49
15:O:34:LEU:O	15:O:34:LEU:HD23	2.12	0.49
15:O:39:LEU:HD12	15:O:59:MET:HE2	1.93	0.49
1:A:218:C:H2'	1:A:219:C:H6	1.76	0.49
1:A:489:C:H2'	1:A:490:G:H8	1.77	0.49
1:A:659:U:H2'	1:A:660:G:O4'	2.13	0.49
1:A:834:C:H2'	1:A:835:U:C6	2.48	0.49
1:A:1194:U:O2'	1:A:1195:C:H5'	2.12	0.49
1:A:1250:A:H2'	1:A:1251:A:C8	2.47	0.49
1:A:1366:C:C2	1:A:1367:C:C5	3.00	0.49
2:B:102:LEU:CD2	2:B:162:ILE:HD11	2.37	0.49
2:B:206:ASP:O	2:B:207:ALA:HB3	2.11	0.49
4:D:7:PRO:CG	4:D:10:ARG:HD2	2.43	0.49
13:M:94:ARG:CZ	19:S:81:ARG:HD3	2.43	0.49
1:A:149:A:H2'	1:A:150:C:C6	2.48	0.49
1:A:491:G:H2'	1:A:492:G:H8	1.77	0.49
1:A:1153:C:H2'	1:A:1154:G:C8	2.46	0.49
1:A:1503:A:O2'	1:A:1504:G:OP1	2.29	0.49
2:B:97:TRP:CH2	2:B:173:ALA:HA	2.47	0.49
4:D:38:TYR:CE1	4:D:45:GLN:HG3	2.48	0.49
4:D:78:LEU:HD22	4:D:96:LEU:HB3	1.94	0.49
5:E:36:ASP:O	5:E:37:ARG:HB2	2.13	0.49
6:F:100:ASN:O	18:R:28:GLU:HG3	2.13	0.49
7:G:85:TYR:HD1	7:G:154:TYR:CE1	2.27	0.49
17:Q:78:GLU:HG3	17:Q:78:GLU:O	2.12	0.49
18:R:34:TYR:HA	18:R:69:THR:HG23	1.93	0.49
1:A:1121:U:H2'	1:A:1122:U:C6	2.48	0.49
1:A:1162:C:H2'	1:A:1163:C:H6	1.78	0.49
1:A:1181:G:H4'	1:A:1184:G:H5'	1.94	0.49
1:A:1222:G:OP1	19:S:77:THR:HG21	2.13	0.49
1:A:1238:A:N7	1:A:1303:C:H1'	2.28	0.49
1:A:1279:A:O2'	1:A:1282:C:N4	2.46	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:168:THR:OG1	2:B:192:SER:HB3	2.12	0.49
4:D:119:GLN:CG	4:D:123:HIS:CE1	2.95	0.49
5:E:13:ILE:HG13	5:E:13:ILE:O	2.12	0.49
10:J:31:GLY:HA2	10:J:78:ASN:OD1	2.13	0.49
11:K:79:SER:OG	11:K:106:LYS:HG2	2.12	0.49
11:K:85:ARG:HH11	11:K:85:ARG:HG3	1.77	0.49
13:M:78:ILE:O	13:M:82:MET:HB2	2.12	0.49
20:T:54:LYS:HE3	20:T:100:ILE:HD11	1.94	0.49
1:A:346:G:H2'	1:A:347:G:H5'	1.94	0.49
1:A:393:A:C2	1:A:394:G:C8	3.00	0.49
1:A:586:C:O2'	1:A:587:G:H5'	2.13	0.49
1:A:760:G:C2	17:Q:104:LYS:O	2.66	0.49
1:A:760:G:O6	17:Q:105:ALA:CB	2.61	0.49
1:A:922:G:N2	1:A:1396:A:C5	2.80	0.49
1:A:1346:A:H1'	1:A:1348:U:C5	2.47	0.49
1:A:1404:C:C1'	1:A:1499:A:C2	2.96	0.49
2:B:213:LEU:C	2:B:213:LEU:HD23	2.37	0.49
3:C:116:VAL:O	3:C:119:ARG:HB3	2.13	0.49
3:C:139:GLN:O	3:C:143:GLU:N	2.37	0.49
3:C:191:THR:HG22	3:C:193:TYR:N	2.23	0.49
8:H:13:ILE:O	8:H:17:THR:HG23	2.13	0.49
8:H:65:TYR:HA	8:H:79:VAL:HG23	1.95	0.49
10:J:16:LEU:HD23	10:J:94:VAL:HG22	1.95	0.49
11:K:48:ILE:HD11	11:K:64:ALA:HA	1.95	0.49
16:P:51:VAL:O	16:P:51:VAL:CG1	2.60	0.49
25:Y:301:SFG:HB2	25:Y:301:SFG:H4'	1.95	0.49
1:A:178:C:O2'	1:A:179:A:H5'	2.13	0.49
1:A:220:G:O2'	1:A:221:C:H5'	2.12	0.49
1:A:265:G:O2'	1:A:266:G:H5'	2.13	0.49
1:A:1305:G:H22	1:A:1331:G:H2'	1.78	0.49
2:B:35:GLU:HA	2:B:39:ILE:O	2.13	0.49
8:H:60:ARG:HG3	8:H:60:ARG:NH1	2.28	0.49
8:H:103:VAL:CG2	8:H:110:ALA:HB2	2.43	0.49
15:O:30:ALA:HA	15:O:85:LEU:HD21	1.95	0.49
19:S:5:LEU:HD11	19:S:70:LYS:NZ	2.28	0.49
1:A:269:C:H2'	1:A:270:A:C8	2.48	0.48
1:A:722:A:H4'	1:A:723:U:C5	2.48	0.48
1:A:1505:G:C8	1:A:1505:G:H3'	2.48	0.48
4:D:196:LEU:C	4:D:198:VAL:H	2.21	0.48
9:I:50:LEU:C	9:I:52:ALA:N	2.69	0.48
10:J:38:ILE:HG13	10:J:71:LEU:CB	2.42	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:110:ASP:OD2	18:R:88:LYS:NZ	2.45	0.48
16:P:52:ASP:OD2	16:P:55:ARG:HB2	2.13	0.48
1:A:407:G:H5''	4:D:115:ARG:HB3	1.96	0.48
1:A:602:A:C2	1:A:637:G:C2	3.01	0.48
1:A:960:U:O2'	1:A:1223:C:H4'	2.13	0.48
1:A:974:A:OP2	14:N:41:ARG:NH1	2.45	0.48
1:A:1070:U:O2'	1:A:1071:C:H5'	2.13	0.48
1:A:1230:C:O2'	1:A:1231:G:H5'	2.13	0.48
1:A:1369:C:H2'	1:A:1370:G:C8	2.48	0.48
2:B:144:ARG:HG3	2:B:145:LEU:H	1.77	0.48
7:G:156:TRP:OXT	7:G:156:TRP:CD1	2.66	0.48
9:I:65:VAL:HG13	9:I:65:VAL:O	2.13	0.48
10:J:65:LEU:O	10:J:65:LEU:CD2	2.59	0.48
1:A:279:A:H5''	1:A:280:C:H3'	1.94	0.48
1:A:624:C:O2'	1:A:625:G:H5'	2.13	0.48
1:A:1490:C:N4	1:A:1491:G:O6	2.45	0.48
2:B:25:ASN:O	2:B:27:LYS:N	2.47	0.48
2:B:188:ALA:O	2:B:202:PRO:HA	2.13	0.48
3:C:79:ARG:C	3:C:81:GLY:H	2.21	0.48
3:C:173:VAL:N	3:C:174:PRO:CD	2.76	0.48
4:D:127:THR:CG2	4:D:128:VAL:N	2.75	0.48
7:G:138:LYS:HD3	7:G:138:LYS:C	2.38	0.48
10:J:32:ALA:HB2	10:J:76:ASN:HB2	1.94	0.48
16:P:1:MET:HE3	16:P:3:LYS:HG2	1.94	0.48
1:A:61:G:H2'	1:A:62:U:O4'	2.12	0.48
1:A:1102:A:H2'	1:A:1103:C:H6	1.77	0.48
1:A:1129:C:O2'	1:A:1130:A:OP2	2.24	0.48
1:A:1298:C:C5	7:G:114:ARG:HD3	2.48	0.48
1:A:1347:G:N7	9:I:10:ARG:NH2	2.61	0.48
1:A:1407:C:O2'	1:A:1408:A:P	2.69	0.48
1:A:1410:G:OP1	22:Y:148:ALA:HB2	2.13	0.48
2:B:17:PHE:HA	2:B:44:LEU:HD21	1.96	0.48
4:D:31:CYS:C	4:D:33:MET:H	2.21	0.48
4:D:36:ARG:N	4:D:37:PRO:CD	2.65	0.48
6:F:48:LEU:HD13	6:F:52:ILE:HG13	1.95	0.48
10:J:6:ILE:HG23	10:J:98:ILE:HG12	1.94	0.48
10:J:45:ARG:NH2	14:N:36:PHE:CD2	2.81	0.48
12:L:28:LYS:C	12:L:30:ALA:N	2.70	0.48
12:L:42:THR:CG2	12:L:52:LEU:HB3	2.44	0.48
12:L:83:VAL:HG21	12:L:100:ILE:HD13	1.95	0.48
17:Q:12:SER:HB3	17:Q:20:THR:HB	1.95	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:S:39:THR:HG22	19:S:40:ILE:N	2.28	0.48
1:A:184:G:H2'	1:A:185:A:H8	1.77	0.48
3:C:23:TYR:O	3:C:24:ALA:HB2	2.14	0.48
12:L:83:VAL:HG22	12:L:84:LEU:N	2.28	0.48
12:L:119:LYS:O	12:L:120:TYR:CB	2.61	0.48
15:O:25:THR:HG21	15:O:70:LEU:HD23	1.94	0.48
1:A:31:G:H1	1:A:48:C:H5''	1.77	0.48
1:A:1342:C:O2'	1:A:1343:G:H5'	2.13	0.48
1:A:1533:C:O2'	1:A:1534:A:H5'	2.14	0.48
2:B:230:VAL:HG13	2:B:231:GLU:OE2	2.13	0.48
3:C:138:VAL:O	3:C:142:MET:HB2	2.13	0.48
7:G:112:PRO:O	7:G:113:GLU:C	2.57	0.48
11:K:60:ALA:O	11:K:61:ALA:C	2.56	0.48
12:L:110:VAL:O	12:L:122:THR:CG2	2.62	0.48
20:T:43:LEU:HD13	20:T:51:GLU:HG3	1.96	0.48
1:A:337:C:H2'	1:A:338:A:C8	2.49	0.48
1:A:538:G:O2'	1:A:539:A:H5'	2.13	0.48
1:A:555:C:H2'	1:A:556:C:C6	2.48	0.48
1:A:954:G:H2'	1:A:955:U:H6	1.78	0.48
1:A:1195:C:H2'	1:A:1197:G:H5'	1.96	0.48
2:B:187:LEU:CD2	2:B:214:ILE:HG13	2.44	0.48
3:C:179:ARG:HD2	3:C:179:ARG:C	2.37	0.48
4:D:57:ARG:NH2	4:D:205:GLU:OE2	2.46	0.48
5:E:76:ILE:HD13	5:E:142:LEU:HD11	1.95	0.48
11:K:86:GLY:H	11:K:112:THR:HG23	1.79	0.48
17:Q:95:TYR:C	17:Q:97:SER:N	2.58	0.48
18:R:39:VAL:HG13	18:R:40:LEU:N	2.28	0.48
18:R:46:GLU:CD	18:R:46:GLU:N	2.72	0.48
1:A:926:G:H2'	1:A:1505:G:N3	2.28	0.48
1:A:1056:U:O2'	1:A:1057:G:H5'	2.14	0.48
1:A:1394:A:C6	1:A:1501:C:C5'	2.97	0.48
1:A:1422:G:C2'	1:A:1423:G:H5'	2.43	0.48
4:D:111:ALA:HB2	4:D:120:LEU:HD12	1.96	0.48
5:E:51:VAL:O	5:E:54:ALA:HB3	2.13	0.48
5:E:71:LEU:HD21	5:E:115:VAL:CG2	2.43	0.48
16:P:6:LEU:HB3	16:P:17:TYR:CD2	2.49	0.48
16:P:52:ASP:CG	16:P:52:ASP:O	2.57	0.48
17:Q:17:LYS:HA	17:Q:46:ASP:O	2.14	0.48
18:R:28:GLU:OE1	18:R:28:GLU:N	2.46	0.48
20:T:89:ARG:HE	20:T:104:LEU:HD22	1.78	0.48
1:A:421:U:H5'	1:A:422:C:C5	2.48	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:731:G:H5'	1:A:766:A:H4'	1.94	0.48
1:A:780:A:C2	1:A:801:U:C5	3.02	0.48
1:A:922:G:H5'	5:E:19:MET:O	2.14	0.48
1:A:1497:G:H2'	1:A:1498:U:C5'	2.42	0.48
2:B:12:GLU:HG2	2:B:213:LEU:HD11	1.95	0.48
2:B:111:ARG:HB3	2:B:149:LEU:HD11	1.95	0.48
6:F:46:ARG:HB2	6:F:60:PHE:CE1	2.48	0.48
11:K:58:PRO:HB2	11:K:93:GLN:HG3	1.95	0.48
12:L:53:ARG:HB3	12:L:93:LEU:HD11	1.94	0.48
15:O:41:GLU:O	15:O:42:HIS:C	2.57	0.48
17:Q:56:VAL:HG12	17:Q:77:VAL:HB	1.95	0.48
18:R:53:ARG:HD3	18:R:63:GLN:HB3	1.95	0.48
19:S:32:LYS:HG3	19:S:32:LYS:O	2.13	0.48
1:A:600:C:OP1	8:H:97:VAL:HG12	2.14	0.48
1:A:657:G:O2'	1:A:658:G:H5'	2.13	0.48
1:A:848:C:H2'	1:A:849:C:C6	2.49	0.48
1:A:1051:C:O2'	1:A:1052:U:H5'	2.13	0.48
1:A:1181:G:H4'	1:A:1184:G:C4'	2.43	0.48
4:D:3:ARG:O	4:D:5:ILE:HG13	2.13	0.48
5:E:148:VAL:O	5:E:152:ARG:HG3	2.14	0.48
7:G:64:GLN:O	7:G:67:GLU:HB3	2.14	0.48
10:J:39:PRO:HA	10:J:70:ARG:HH11	1.78	0.48
10:J:94:VAL:HG12	10:J:95:GLU:H	1.76	0.48
1:A:190(I):G:O2'	1:A:190(J):U:H5'	2.14	0.47
1:A:513:C:H2'	1:A:514:C:C6	2.49	0.47
1:A:625:G:H2'	1:A:626:U:H6	1.79	0.47
1:A:825:G:H2'	1:A:826:C:H6	1.78	0.47
1:A:1047:G:H5''	14:N:4:LYS:HD2	1.96	0.47
1:A:1127:G:N2	1:A:1147:C:N4	2.62	0.47
1:A:1347:G:H3'	9:I:108:VAL:O	2.14	0.47
4:D:200:GLU:OE1	4:D:200:GLU:N	2.46	0.47
9:I:111:ARG:HG3	9:I:111:ARG:NH1	2.28	0.47
1:A:497:A:O2'	1:A:498:U:OP1	2.32	0.47
1:A:528:C:H5'	1:A:535:A:C6	2.49	0.47
1:A:655:A:C2	1:A:754:C:C4	3.01	0.47
1:A:761:G:O4'	17:Q:103:GLY:O	2.31	0.47
9:I:117:HIS:HB2	9:I:121:ARG:HD2	1.95	0.47
18:R:47:THR:HA	18:R:83:GLU:HB2	1.97	0.47
20:T:59:ALA:O	20:T:63:ILE:HG13	2.14	0.47
1:A:185:A:N3	20:T:81:LYS:NZ	2.61	0.47
1:A:613:C:O2'	1:A:614:A:H5'	2.14	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1329:A:C2'	1:A:1330:U:H5'	2.43	0.47
2:B:108:ILE:O	2:B:108:ILE:HG22	2.13	0.47
2:B:115:LEU:O	2:B:115:LEU:HD12	2.13	0.47
4:D:105:VAL:HG13	4:D:110:PHE:HB2	1.95	0.47
12:L:53:ARG:HG2	12:L:93:LEU:HD11	1.95	0.47
17:Q:68:ARG:O	17:Q:69:LYS:HB2	2.13	0.47
19:S:10:PHE:HE2	19:S:12:ASP:OD1	1.97	0.47
22:Y:196:LEU:O	22:Y:197:TRP:HB2	2.14	0.47
1:A:155:C:H2'	1:A:156:G:H8	1.79	0.47
1:A:1057:G:C2'	1:A:1058:G:H5'	2.44	0.47
2:B:59:GLU:O	2:B:60:ASP:C	2.57	0.47
2:B:75:LYS:HE3	2:B:78:GLN:OE1	2.14	0.47
3:C:8:ILE:O	3:C:11:ARG:N	2.47	0.47
3:C:35:GLU:O	3:C:38:ARG:N	2.47	0.47
3:C:100:ALA:O	3:C:101:LEU:HB2	2.14	0.47
4:D:174:LEU:O	4:D:175:SER:HB3	2.13	0.47
7:G:54:THR:HG22	7:G:56:GLN:H	1.79	0.47
12:L:34:ARG:HG3	12:L:34:ARG:O	2.13	0.47
12:L:86:ARG:HG3	12:L:86:ARG:NH1	2.28	0.47
1:A:19:C:H2'	1:A:20:U:H6	1.80	0.47
1:A:41:G:H2'	1:A:42:G:C8	2.49	0.47
2:B:15:VAL:HG12	2:B:210:SER:HB2	1.97	0.47
2:B:125:PRO:C	2:B:127:ILE:H	2.22	0.47
7:G:21:VAL:HG23	7:G:22:LEU:N	2.29	0.47
7:G:77:SER:O	7:G:156:TRP:HZ3	1.98	0.47
10:J:27:ALA:HB2	10:J:85:LEU:HD21	1.96	0.47
10:J:30:SER:CB	10:J:80:LYS:HB3	2.45	0.47
13:M:39:ILE:CD1	13:M:56:LEU:HG	2.44	0.47
13:M:40:ASN:OD1	13:M:41:PRO:CD	2.62	0.47
20:T:53:LEU:HD13	20:T:101:GLY:C	2.39	0.47
1:A:51:A:H4'	1:A:52:G:C5'	2.45	0.47
1:A:518:C:HO2'	12:L:50:SER:HB3	1.79	0.47
1:A:560:U:O5'	1:A:560:U:H6	1.98	0.47
1:A:606:G:H2'	1:A:631:G:N2	2.30	0.47
1:A:768:A:H2'	1:A:769:G:O4'	2.14	0.47
1:A:927:G:H4'	1:A:1503:A:N7	2.29	0.47
1:A:1286:A:H5''	21:V:25:LYS:NZ	2.29	0.47
2:B:142:LEU:HD22	2:B:146:GLN:OE1	2.14	0.47
3:C:131:ARG:HA	3:C:134:ILE:HD12	1.96	0.47
3:C:167:TRP:HB3	3:C:168:ALA:H	1.32	0.47
6:F:4:TYR:CZ	6:F:72:VAL:HG21	2.49	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:67:MET:HE2	6:F:72:VAL:HA	1.96	0.47
7:G:23:VAL:HG12	7:G:27:ILE:CD1	2.41	0.47
7:G:65:ALA:O	7:G:66:VAL:C	2.58	0.47
9:I:111:ARG:HG3	9:I:111:ARG:HH11	1.80	0.47
12:L:26:ALA:C	12:L:27:LEU:O	2.58	0.47
17:Q:97:SER:CB	17:Q:102:GLY:C	2.78	0.47
1:A:51:A:H4'	1:A:52:G:O5'	2.15	0.47
1:A:435:C:O2'	1:A:436:C:H5'	2.15	0.47
1:A:998:G:O2'	1:A:999:C:H5'	2.15	0.47
1:A:1112:C:N3	3:C:178:LEU:N	2.62	0.47
1:A:1202:G:O4'	14:N:29:ARG:HD3	2.14	0.47
1:A:1231:G:H4'	9:I:126:SER:OG	2.14	0.47
1:A:1286:A:H2'	1:A:1287:A:H4'	1.96	0.47
1:A:1292:U:P	7:G:41:ARG:HH22	2.36	0.47
1:A:1420:C:H2'	1:A:1421:G:C8	2.48	0.47
3:C:79:ARG:HG2	3:C:82:GLU:CG	2.45	0.47
3:C:130:VAL:CG2	3:C:157:ILE:HG23	2.41	0.47
4:D:24:GLU:CG	4:D:25:ARG:N	2.77	0.47
7:G:46:ALA:O	7:G:50:ILE:HG13	2.15	0.47
10:J:94:VAL:CG1	10:J:95:GLU:N	2.77	0.47
11:K:33:THR:OG1	11:K:37:GLY:C	2.58	0.47
11:K:72:ALA:HB1	11:K:77:MET:HG3	1.97	0.47
19:S:15:LEU:HD12	19:S:16:LEU:H	1.77	0.47
20:T:29:LYS:O	20:T:33:ILE:HG13	2.14	0.47
21:V:3:LYS:HB3	21:V:14:TRP:CD1	2.50	0.47
22:Y:141:TYR:N	22:Y:141:TYR:HD1	2.12	0.47
1:A:913:A:O2'	1:A:914:A:P	2.73	0.47
1:A:942:G:N3	1:A:943:U:C6	2.83	0.47
1:A:1123:A:O3'	10:J:36:GLY:HA3	2.14	0.47
1:A:1194:U:H2'	1:A:1195:C:C6	2.50	0.47
1:A:1300:G:O2'	1:A:1301:U:H6	1.98	0.47
1:A:1367:C:H4'	10:J:48:THR:HG21	1.97	0.47
2:B:18:GLY:CA	2:B:41:ILE:HA	2.44	0.47
4:D:162:LEU:HD13	4:D:181:MET:CG	2.42	0.47
6:F:2:ARG:NE	6:F:69:GLU:HG2	2.29	0.47
14:N:53:LEU:HB3	14:N:56:VAL:CG2	2.45	0.47
16:P:51:VAL:O	16:P:52:ASP:C	2.58	0.47
19:S:15:LEU:O	19:S:19:VAL:N	2.48	0.47
22:Y:115:ILE:HB	22:Y:156:PRO:HG2	1.96	0.47
1:A:190(H):G:O2'	1:A:190(I):G:H5'	2.14	0.47
1:A:924:C:C4'	1:A:1399:C:OP2	2.63	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1074:G:O2'	1:A:1101:A:N1	2.45	0.47
1:A:1413:A:H2	1:A:1487:G:H22	1.63	0.47
1:A:1515:C:H2'	1:A:1516:G:C8	2.50	0.47
2:B:53:ARG:NH1	2:B:199:TYR:CD2	2.83	0.47
3:C:167:TRP:O	3:C:168:ALA:CB	2.63	0.47
4:D:163:GLU:C	4:D:165:MET:N	2.72	0.47
6:F:2:ARG:HD2	6:F:69:GLU:HG2	1.96	0.47
8:H:126:LYS:C	8:H:128:GLY:N	2.73	0.47
10:J:22:LYS:HE2	10:J:90:LEU:HB2	1.97	0.47
11:K:80:VAL:HG21	11:K:103:LEU:HD13	1.97	0.47
15:O:77:ARG:O	15:O:80:ALA:HB3	2.15	0.47
16:P:43:LYS:HG2	16:P:48:TRP:CE2	2.50	0.47
20:T:11:SER:C	20:T:13:LEU:H	2.22	0.47
22:Y:54:ILE:HG12	22:Y:83:VAL:HB	1.96	0.47
1:A:184:G:C4'	1:A:224:C:H4'	2.44	0.47
1:A:517:G:H5'	1:A:519:C:C2	2.50	0.47
1:A:951:G:O2'	1:A:952:U:H5'	2.15	0.47
1:A:1001:A:H2'	1:A:1002:G:H8	1.79	0.47
1:A:1245:A:H2'	1:A:1246:C:C6	2.50	0.47
2:B:50:GLU:HB3	2:B:200:ILE:O	2.15	0.47
5:E:74:GLY:CA	5:E:116:THR:HG22	2.43	0.47
12:L:54:LYS:N	12:L:54:LYS:HD2	2.30	0.47
1:A:321:A:O2'	1:A:322:C:H5'	2.15	0.46
1:A:542:G:H2'	1:A:543:C:H6	1.80	0.46
1:A:633:G:H2'	1:A:634:C:C6	2.49	0.46
1:A:1232:U:H5''	9:I:124:GLN:O	2.14	0.46
1:A:1240:U:P	7:G:116:ALA:HB2	2.56	0.46
1:A:1326:C:H5''	21:V:12:LYS:NZ	2.30	0.46
1:A:1510:U:H2'	1:A:1511:G:C8	2.50	0.46
2:B:62:ALA:C	2:B:64:ARG:H	2.23	0.46
5:E:18:ARG:HG2	5:E:19:MET:H	1.81	0.46
5:E:107:ARG:HG2	5:E:108:ALA:N	2.29	0.46
9:I:104:ARG:O	9:I:105:ASP:C	2.59	0.46
13:M:82:MET:CE	13:M:92:HIS:HB3	2.44	0.46
17:Q:66:SER:OG	17:Q:69:LYS:HB3	2.15	0.46
1:A:9:G:OP2	5:E:121:LYS:NZ	2.41	0.46
1:A:538:G:P	12:L:115:LYS:HG3	2.55	0.46
1:A:781:A:H2'	1:A:782:A:H5'	1.98	0.46
1:A:952:U:O2'	1:A:953:G:H5'	2.14	0.46
1:A:1051:C:H2'	1:A:1052:U:H6	1.80	0.46
1:A:1238:A:H5'	1:A:1336:C:N4	2.29	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1262:C:H2'	1:A:1263:C:H6	1.79	0.46
1:A:1277:C:C2'	1:A:1278:U:H5'	2.45	0.46
1:A:1320:C:H2'	1:A:1321:C:O4'	2.16	0.46
1:A:1490:C:C5'	1:A:1490:C:H6	2.28	0.46
2:B:15:VAL:CG1	2:B:209:ARG:HG3	2.46	0.46
3:C:173:VAL:O	3:C:173:VAL:HG12	2.14	0.46
4:D:111:ALA:HB1	4:D:116:GLN:HB3	1.96	0.46
9:I:48:GLU:N	9:I:49:PRO:CD	2.77	0.46
13:M:36:LYS:C	13:M:38:GLY:H	2.24	0.46
13:M:97:PRO:HB2	13:M:101:GLN:OE1	2.14	0.46
20:T:94:ALA:O	20:T:95:ALA:CB	2.63	0.46
1:A:582:U:C1'	17:Q:105:ALA:HA	2.44	0.46
1:A:976:G:C8	1:A:1358:U:C2	3.04	0.46
1:A:1404:C:O4'	1:A:1499:A:C2	2.69	0.46
1:A:1489:G:C3'	1:A:1490:C:H5''	2.45	0.46
3:C:64:VAL:CG2	3:C:99:VAL:HB	2.46	0.46
6:F:50:TYR:CE1	18:R:77:GLY:HA2	2.49	0.46
10:J:48:THR:OG1	10:J:62:HIS:CD2	2.68	0.46
10:J:96:ILE:CG2	10:J:97:GLU:H	2.25	0.46
12:L:48:PRO:CG	12:L:49:ASN:H	2.25	0.46
12:L:59:ARG:NH1	12:L:65:GLU:HG2	2.31	0.46
13:M:49:THR:CG2	13:M:51:ALA:H	2.13	0.46
13:M:62:ASN:O	13:M:63:THR:HB	2.16	0.46
15:O:66:LEU:O	15:O:69:TYR:HB3	2.15	0.46
1:A:41:G:H2'	1:A:42:G:H8	1.79	0.46
1:A:458:C:H2'	1:A:459:G:H8	1.80	0.46
1:A:1004:A:N6	1:A:1035:A:H62	2.13	0.46
1:A:1405:G:H1'	1:A:1519:A:O4'	2.16	0.46
2:B:10:LEU:C	2:B:12:GLU:N	2.72	0.46
2:B:42:ILE:HD12	2:B:203:GLY:HA2	1.98	0.46
4:D:39:PRO:HG2	4:D:44:GLY:HA2	1.97	0.46
5:E:20:GLN:C	5:E:21:ALA:O	2.51	0.46
7:G:15:ASP:O	7:G:19:GLY:HA2	2.16	0.46
7:G:135:VAL:O	7:G:139:GLU:HG3	2.15	0.46
12:L:60:LEU:HD21	12:L:66:VAL:HG22	1.97	0.46
15:O:83:GLU:C	15:O:83:GLU:OE1	2.58	0.46
17:Q:63:ARG:HG2	17:Q:64:PRO:HD2	1.97	0.46
1:A:5:U:O2'	1:A:6:G:P	2.73	0.46
1:A:92:C:O2'	1:A:93:G:H5'	2.15	0.46
1:A:518:C:H5''	1:A:519:C:H6	1.78	0.46
1:A:1301:U:O2'	1:A:1302:U:P	2.74	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1442:G:N2	1:A:1446:A:C8	2.80	0.46
2:B:83:MET:HG3	2:B:238:LEU:CD1	2.46	0.46
6:F:100:ASN:O	6:F:100:ASN:ND2	2.41	0.46
7:G:20:ASP:OD1	7:G:22:LEU:HB3	2.15	0.46
10:J:49:VAL:CG1	14:N:41:ARG:HB2	2.38	0.46
11:K:16:SER:O	11:K:35:PRO:HD3	2.16	0.46
11:K:48:ILE:O	11:K:49:GLY:C	2.59	0.46
11:K:50:TYR:HD1	11:K:60:ALA:HB2	1.80	0.46
11:K:59:TYR:O	11:K:62:GLN:HB3	2.15	0.46
12:L:37:CYS:O	12:L:79:GLU:O	2.34	0.46
18:R:59:SER:OG	18:R:62:GLU:HG3	2.15	0.46
19:S:22:LEU:CD1	19:S:31:ILE:HD11	2.46	0.46
20:T:67:ALA:O	20:T:73:HIS:ND1	2.47	0.46
1:A:129(A):G:O2'	1:A:190(E):U:H5''	2.16	0.46
1:A:624:C:H2'	1:A:625:G:H8	1.81	0.46
1:A:707:C:OP1	11:K:85:ARG:NH1	2.49	0.46
1:A:1367:C:H5'	10:J:60:ARG:NH1	2.31	0.46
2:B:97:TRP:CH2	2:B:176:GLU:OE2	2.69	0.46
2:B:134:GLU:C	2:B:136:VAL:N	2.71	0.46
2:B:228:GLY:O	2:B:229:VAL:C	2.58	0.46
3:C:154:SER:OG	3:C:155:GLY:N	2.48	0.46
7:G:154:TYR:O	7:G:156:TRP:N	2.49	0.46
8:H:92:ARG:HG2	8:H:94:TYR:OH	2.16	0.46
9:I:33:PHE:CE2	9:I:47:LEU:HD11	2.51	0.46
11:K:34:ASP:O	11:K:36:ASP:N	2.48	0.46
11:K:84:VAL:HG23	11:K:109:VAL:O	2.16	0.46
13:M:40:ASN:OD1	13:M:41:PRO:HD2	2.15	0.46
13:M:46:LYS:HG3	13:M:47:ASP:N	2.30	0.46
15:O:34:LEU:HD23	15:O:34:LEU:C	2.40	0.46
20:T:82:SER:C	20:T:84:LEU:N	2.74	0.46
1:A:279:A:C6	17:Q:98:LEU:HD13	2.51	0.46
1:A:390:C:H6	1:A:390:C:O5'	1.99	0.46
1:A:743:U:H2'	1:A:744:C:H6	1.79	0.46
1:A:828:A:H5''	1:A:859:A:C2	2.51	0.46
1:A:1171:G:H2'	1:A:1172:C:C6	2.51	0.46
1:A:1474:G:O2'	1:A:1475:G:H5'	2.16	0.46
2:B:78:GLN:O	2:B:94:ASN:OD1	2.33	0.46
4:D:173:TRP:CD2	4:D:189:PRO:HB3	2.51	0.46
5:E:78:HIS:CD2	8:H:107:LEU:HD12	2.51	0.46
6:F:44:GLY:HA2	6:F:59:TYR:CE1	2.50	0.46
10:J:24:VAL:CG1	10:J:28:ARG:HE	2.29	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:54:ARG:H	11:K:54:ARG:HG2	1.47	0.46
12:L:71:PRO:O	12:L:102:ARG:HD2	2.16	0.46
13:M:5:ALA:O	13:M:8:GLU:N	2.45	0.46
14:N:12:ARG:O	14:N:14:PRO:HD3	2.16	0.46
19:S:53:ASN:ND2	19:S:56:GLN:HB2	2.31	0.46
20:T:63:ILE:HG23	20:T:72:LEU:CD1	2.46	0.46
21:V:2:GLY:O	21:V:4:GLY:N	2.49	0.46
1:A:834:C:H2'	1:A:835:U:H6	1.79	0.46
1:A:1049:U:H4'	1:A:1050:G:OP2	2.16	0.46
1:A:1190:G:HO2'	1:A:1191:A:P	2.39	0.46
1:A:1221:G:O2'	1:A:1222:G:H5'	2.15	0.46
1:A:1238:A:OP1	1:A:1336:C:H5	1.98	0.46
1:A:1300:G:O2'	1:A:1301:U:P	2.73	0.46
3:C:21:ARG:NH2	3:C:56:ASP:OD2	2.48	0.46
3:C:23:TYR:CG	3:C:24:ALA:N	2.84	0.46
3:C:174:PRO:O	3:C:177:THR:HG22	2.15	0.46
5:E:121:LYS:HE3	5:E:123:LEU:CD2	2.46	0.46
8:H:23:SER:OG	8:H:60:ARG:HD2	2.15	0.46
9:I:97:LYS:HG3	9:I:102:LEU:HD12	1.96	0.46
10:J:62:HIS:CB	14:N:59:ALA:HB3	2.45	0.46
11:K:100:ALA:O	11:K:101:SER:C	2.57	0.46
13:M:59:TYR:O	13:M:63:THR:HB	2.15	0.46
1:A:70:G:H2'	1:A:73:C:C6	2.51	0.46
1:A:132:C:O2'	1:A:133:U:H5'	2.15	0.46
1:A:458:C:H2'	1:A:459:G:O4'	2.16	0.46
1:A:1044:A:O2'	1:A:1045:C:H5'	2.15	0.46
1:A:1230:C:O2'	13:M:126:LYS:HA	2.16	0.46
1:A:1237:C:H2'	1:A:1336:C:C5	2.51	0.46
1:A:1309:G:N7	13:M:99:ARG:NH2	2.61	0.46
1:A:1405:G:H1'	1:A:1519:A:C1'	2.45	0.46
3:C:129:ALA:HB3	3:C:132:ARG:CD	2.45	0.46
3:C:164:ARG:HB3	3:C:164:ARG:HH11	1.81	0.46
4:D:145:GLU:HG2	4:D:184:LYS:HE2	1.96	0.46
4:D:162:LEU:HD13	4:D:181:MET:CE	2.46	0.46
5:E:144:THR:O	5:E:145:LYS:C	2.59	0.46
7:G:107:ALA:O	7:G:110:GLN:HB2	2.16	0.46
8:H:116:LYS:NZ	8:H:127:LEU:HD12	2.31	0.46
9:I:48:GLU:OE1	9:I:48:GLU:HA	2.16	0.46
10:J:53:PRO:O	10:J:54:PHE:O	2.34	0.46
16:P:72:ARG:O	16:P:72:ARG:HG2	2.16	0.46
1:A:151:A:H2'	1:A:152:A:O4'	2.15	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:160:A:H1'	1:A:344:A:N7	2.32	0.46
1:A:421:U:H5'	1:A:422:C:H5	1.80	0.46
1:A:513:C:H2'	1:A:514:C:H6	1.80	0.46
1:A:1152:A:O2'	1:A:1153:C:H5'	2.16	0.46
1:A:1225:A:H5'	1:A:1226:C:OP2	2.16	0.46
1:A:1230:C:H2'	1:A:1231:G:H8	1.81	0.46
1:A:1390:U:H2'	1:A:1391:U:C6	2.51	0.46
1:A:1435:G:H2'	1:A:1436:U:H6	1.69	0.46
1:A:1461:G:O2'	1:A:1462:G:H5'	2.16	0.46
2:B:22:LYS:O	2:B:23:ARG:HG3	2.16	0.46
2:B:95:GLN:C	2:B:96:ARG:HD2	2.40	0.46
4:D:121:VAL:O	4:D:134:ASP:HA	2.16	0.46
4:D:152:SER:HA	4:D:155:LEU:HG	1.97	0.46
5:E:15:ARG:NE	5:E:26:PHE:CD2	2.84	0.46
8:H:6:ILE:HD12	8:H:35:ILE:HD12	1.97	0.46
19:S:18:LYS:HG2	19:S:18:LYS:O	2.15	0.46
1:A:690:G:H2'	1:A:691:G:O4'	2.15	0.45
1:A:909:A:H2'	1:A:910:C:O4'	2.16	0.45
1:A:975:A:H4'	1:A:976:G:H5'	1.97	0.45
1:A:1049:U:H1'	1:A:1201:A:N7	2.31	0.45
1:A:1515:C:H2'	1:A:1516:G:H8	1.81	0.45
1:A:1515:C:O2'	1:A:1516:G:H5'	2.16	0.45
1:A:1532:U:O5'	1:A:1532:U:H6	1.99	0.45
2:B:52:GLU:O	2:B:56:ARG:HB2	2.17	0.45
3:C:108:ASN:C	3:C:110:ASN:N	2.73	0.45
3:C:131:ARG:O	3:C:135:LYS:HG3	2.16	0.45
8:H:45:ILE:O	8:H:45:ILE:HG13	2.16	0.45
9:I:85:LEU:O	9:I:92:TYR:CD1	2.69	0.45
12:L:38:THR:HG22	12:L:39:VAL:HG23	1.97	0.45
12:L:46:LYS:CG	12:L:47:LYS:H	2.29	0.45
13:M:37:THR:HG23	13:M:55:ARG:CB	2.46	0.45
17:Q:80:GLY:O	17:Q:81:ARG:HB3	2.15	0.45
1:A:877:C:H5''	8:H:88:LYS:HD3	1.97	0.45
1:A:882:C:O2'	1:A:883:C:H5'	2.16	0.45
1:A:947:G:H2'	1:A:948:C:O4'	2.15	0.45
1:A:1039:C:O2'	1:A:1040:U:H5'	2.16	0.45
1:A:1131:G:H2'	1:A:1132:C:C6	2.51	0.45
1:A:1256:A:O2'	1:A:1257:U:P	2.74	0.45
2:B:129:GLU:O	2:B:130:ARG:HB2	2.15	0.45
2:B:178:ARG:NH1	2:B:178:ARG:CG	2.67	0.45
3:C:99:VAL:CG2	3:C:100:ALA:N	2.80	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:63:LYS:O	4:D:64:LEU:C	2.58	0.45
4:D:157:LEU:HD22	4:D:161:ASN:OD1	2.16	0.45
10:J:4:ILE:HG12	10:J:100:THR:CB	2.47	0.45
13:M:49:THR:O	13:M:53:VAL:HG23	2.16	0.45
19:S:20:LEU:O	19:S:23:ASN:HB2	2.15	0.45
1:A:19:C:OP1	5:E:125:SER:OG	2.19	0.45
1:A:190(B):C:H2'	1:A:190(C):C:O4'	2.17	0.45
1:A:242:C:H2'	1:A:243:A:H5'	1.99	0.45
1:A:755:G:H1'	8:H:1:MET:HE3	1.97	0.45
1:A:1019:C:O2'	1:A:1020:U:H5'	2.17	0.45
1:A:1202:G:C2'	1:A:1203:C:H5'	2.46	0.45
1:A:1216:G:H5''	14:N:5:ALA:HB2	1.99	0.45
1:A:1296:C:H4'	1:A:1302:U:C5	2.51	0.45
4:D:130:GLY:O	4:D:131:ARG:C	2.58	0.45
5:E:15:ARG:CD	5:E:26:PHE:CD2	2.99	0.45
6:F:101:ALA:HB2	18:R:28:GLU:HB3	1.97	0.45
8:H:114:THR:C	8:H:116:LYS:H	2.22	0.45
10:J:51:ARG:HG3	10:J:60:ARG:O	2.17	0.45
11:K:40:ILE:HG23	11:K:75:TYR:CE2	2.51	0.45
13:M:51:ALA:O	13:M:55:ARG:HG3	2.16	0.45
14:N:21:TYR:HE2	14:N:23:ARG:HE	1.63	0.45
14:N:39:LEU:CD1	14:N:47:LEU:HD12	2.47	0.45
19:S:63:THR:HG22	19:S:64:GLU:N	2.32	0.45
20:T:39:LYS:HD2	20:T:55:ILE:HD13	1.97	0.45
1:A:17:U:O2'	1:A:1079:G:H1'	2.16	0.45
1:A:28:G:O2'	1:A:296:U:OP1	2.33	0.45
1:A:58:C:O2'	1:A:59:A:H5'	2.16	0.45
1:A:575:G:C8	1:A:881:G:N2	2.85	0.45
1:A:686:U:O4	1:A:703:G:H1'	2.17	0.45
1:A:808:C:OP2	15:O:48:LYS:HE2	2.17	0.45
1:A:975:A:H4'	1:A:976:G:OP2	2.16	0.45
1:A:1158:C:N3	1:A:1181:G:N2	2.61	0.45
1:A:1250:A:H4'	9:I:68:GLY:CA	2.47	0.45
1:A:1318:A:H4'	19:S:10:PHE:CD1	2.51	0.45
1:A:1405:G:C2'	1:A:1518:A:O2'	2.65	0.45
3:C:126:ARG:C	3:C:127:ARG:HG3	2.42	0.45
5:E:102:ALA:HB2	5:E:120:THR:CB	2.46	0.45
5:E:115:VAL:HG11	5:E:118:ILE:CD1	2.46	0.45
7:G:77:SER:O	7:G:156:TRP:CZ3	2.69	0.45
10:J:8:LEU:HD12	10:J:20:ALA:HB2	1.97	0.45
10:J:54:PHE:O	10:J:55:LYS:HG2	2.17	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:115:PRO:C	11:K:117:ASN:H	2.25	0.45
12:L:117:ARG:HD2	12:L:122:THR:OG1	2.17	0.45
15:O:71:GLN:O	15:O:72:ARG:C	2.59	0.45
18:R:41:LYS:O	18:R:41:LYS:HG2	2.13	0.45
1:A:113:G:H1'	1:A:354:G:C5'	2.46	0.45
1:A:260:G:O2'	1:A:261:U:H5'	2.16	0.45
1:A:474:G:O2'	1:A:475:G:H5'	2.16	0.45
1:A:848:C:H2'	1:A:849:C:H6	1.80	0.45
1:A:920:U:H2'	1:A:921:U:C6	2.52	0.45
1:A:1196:U:H4'	1:A:1197:G:OP2	2.15	0.45
1:A:1206:G:C6	1:A:1207:G:C5	3.04	0.45
1:A:1501:C:OP2	1:A:1504:G:H2'	2.17	0.45
2:B:71:VAL:HB	2:B:164:VAL:HG23	1.99	0.45
2:B:137:ARG:O	2:B:140:HIS:HB2	2.16	0.45
2:B:223:ILE:HG21	2:B:230:VAL:HG23	1.99	0.45
3:C:157:ILE:HD11	3:C:166:GLU:HB2	1.97	0.45
3:C:188:LEU:O	3:C:189:ALA:CB	2.59	0.45
4:D:4:TYR:O	4:D:5:ILE:HB	2.17	0.45
4:D:142:PRO:HG2	4:D:187:ARG:NH1	2.32	0.45
14:N:26:ARG:NH1	14:N:47:LEU:HD21	2.32	0.45
18:R:74:ARG:HB3	18:R:81:PHE:CE1	2.51	0.45
19:S:67:VAL:O	19:S:69:HIS:N	2.49	0.45
1:A:411:A:C6	1:A:429:U:C4	3.04	0.45
1:A:533:A:O2'	1:A:534:U:P	2.75	0.45
1:A:820:U:H4'	1:A:821:G:OP2	2.15	0.45
1:A:826:C:H2'	1:A:827:U:H6	1.82	0.45
1:A:1044:A:H2'	1:A:1045:C:O4'	2.17	0.45
1:A:1254:C:OP1	10:J:45:ARG:HD3	2.16	0.45
2:B:88:ALA:C	2:B:90:MET:N	2.71	0.45
2:B:100:GLY:O	2:B:104:ASN:N	2.45	0.45
5:E:45:PHE:CD2	5:E:47:LYS:HE3	2.52	0.45
6:F:33:TYR:HB2	6:F:75:LEU:HD23	1.98	0.45
9:I:36:TYR:CD2	9:I:37:PHE:CE2	3.04	0.45
14:N:25:VAL:O	14:N:25:VAL:HG13	2.16	0.45
1:A:319:G:O2'	1:A:320:C:H5'	2.16	0.45
1:A:439:A:C4	1:A:497:A:C2	3.05	0.45
1:A:627:G:O2'	1:A:628:G:H5'	2.17	0.45
1:A:797:C:OP1	11:K:124:LYS:HG3	2.17	0.45
1:A:976:G:C8	1:A:1358:U:O2	2.70	0.45
1:A:1108:G:H4'	1:A:1191:A:O4'	2.17	0.45
1:A:1305:G:N2	1:A:1331:G:C2'	2.79	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1305:G:C5'	21:V:4:GLY:C	2.90	0.45
1:A:1331:G:O2'	1:A:1332:A:OP2	2.31	0.45
3:C:12:LEU:HD23	3:C:12:LEU:HA	1.76	0.45
4:D:3:ARG:NE	4:D:71:SER:HB3	2.31	0.45
12:L:85:ILE:HG23	12:L:98:TYR:CB	2.46	0.45
12:L:115:LYS:C	12:L:117:ARG:H	2.24	0.45
14:N:12:ARG:O	14:N:14:PRO:CD	2.65	0.45
22:Y:150:ILE:HD13	22:Y:155:LEU:HD23	1.99	0.45
1:A:75:G:O2'	1:A:76:C:H5'	2.17	0.45
1:A:403:C:H2'	1:A:404:U:H6	1.81	0.45
1:A:1060:C:C4	3:C:2:GLY:HA3	2.52	0.45
1:A:1404:C:H2'	1:A:1405:G:C8	2.52	0.45
1:A:1408:A:C5	22:Y:107:TRP:CE3	3.05	0.45
1:A:1413:A:H2'	1:A:1414:U:O4'	2.16	0.45
2:B:23:ARG:CZ	2:B:23:ARG:HB2	2.47	0.45
3:C:108:ASN:OD1	3:C:110:ASN:HB2	2.16	0.45
3:C:204:LEU:O	3:C:205:GLY:C	2.59	0.45
5:E:102:ALA:HB2	5:E:120:THR:HB	1.97	0.45
7:G:18:TYR:CD2	7:G:59:LEU:HB2	2.52	0.45
9:I:40:LEU:O	9:I:42:ARG:N	2.50	0.45
9:I:117:HIS:C	9:I:118:LYS:HG3	2.41	0.45
9:I:121:ARG:HG2	9:I:121:ARG:HH11	1.81	0.45
16:P:20:VAL:CG1	16:P:21:VAL:N	2.76	0.45
16:P:82:GLN:O	16:P:83:GLU:C	2.59	0.45
17:Q:104:LYS:HB3	17:Q:105:ALA:H	1.48	0.45
18:R:47:THR:HG22	18:R:48:GLY:H	1.79	0.45
18:R:58:LEU:HD22	18:R:62:GLU:HB3	1.99	0.45
18:R:70:ILE:O	18:R:74:ARG:HG3	2.17	0.45
20:T:42:GLN:O	20:T:45:GLN:HB3	2.16	0.45
1:A:197:A:H1'	1:A:198:G:O4'	2.17	0.45
1:A:509:A:H5''	4:D:55:ALA:HB2	1.99	0.45
1:A:600:C:O2'	1:A:601:C:H5'	2.17	0.45
1:A:1044:A:H2'	1:A:1045:C:C4'	2.46	0.45
1:A:1450:U:H2'	1:A:1452:C:C5	2.52	0.45
2:B:195:ASP:O	8:H:74:PRO:HG3	2.16	0.45
3:C:60:ALA:O	3:C:61:ALA:CB	2.63	0.45
3:C:113:ALA:N	3:C:114:PRO:CD	2.80	0.45
7:G:38:LEU:HD11	7:G:42:ILE:HD11	1.99	0.45
9:I:103:THR:HG22	9:I:104:ARG:N	2.31	0.45
13:M:9:ILE:HD12	13:M:9:ILE:N	2.32	0.45
14:N:29:ARG:HB3	14:N:40:CYS:HB3	1.99	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:O:48:LYS:O	15:O:50:HIS:N	2.50	0.45
17:Q:18:THR:HG23	17:Q:69:LYS:CE	2.47	0.45
19:S:72:GLY:C	19:S:74:PHE:H	2.25	0.45
1:A:258:G:H2'	1:A:259:G:H8	1.82	0.45
1:A:452:A:O2'	1:A:453:A:O4'	2.34	0.45
1:A:583:A:H2'	1:A:584:G:O4'	2.17	0.45
1:A:645:C:O2'	1:A:646:U:H5'	2.16	0.45
1:A:735:C:O2'	1:A:736:C:H5'	2.17	0.45
1:A:924:C:C5'	1:A:1399:C:OP2	2.63	0.45
1:A:1279:A:O2'	1:A:1281:U:OP2	2.33	0.45
1:A:1353:G:H2'	1:A:1354:C:H6	1.82	0.45
1:A:1391:U:H2'	1:A:1392:G:H8	1.74	0.45
4:D:78:LEU:HA	4:D:78:LEU:HD23	1.78	0.45
11:K:23:ALA:HB2	11:K:91:ARG:HB2	1.99	0.45
11:K:69:ALA:O	11:K:70:LYS:C	2.60	0.45
16:P:55:ARG:O	16:P:58:TYR:HB3	2.17	0.45
20:T:24:LEU:HD12	20:T:24:LEU:O	2.17	0.45
20:T:50:GLU:HG2	20:T:100:ILE:HG13	1.99	0.45
20:T:100:ILE:C	20:T:102:GLY:N	2.74	0.45
20:T:100:ILE:O	20:T:102:GLY:N	2.50	0.45
1:A:173:U:H5''	1:A:197:A:H5'	1.99	0.44
1:A:1074:G:O3'	2:B:103:THR:CG2	2.65	0.44
1:A:1300:G:O2'	1:A:1301:U:C6	2.70	0.44
1:A:1372:U:O2'	1:A:1373:G:H5'	2.17	0.44
1:A:1408:A:H8	22:Y:146:GLU:OE2	2.00	0.44
1:A:1408:A:C8	22:Y:146:GLU:OE2	2.70	0.44
1:A:1503:A:O2'	1:A:1504:G:P	2.75	0.44
3:C:11:ARG:NH1	3:C:177:THR:O	2.50	0.44
5:E:13:ILE:HG22	5:E:30:ALA:HB2	1.99	0.44
6:F:40:VAL:CG2	6:F:41:GLU:N	2.80	0.44
10:J:27:ALA:CB	10:J:81:THR:HG23	2.48	0.44
13:M:84:ILE:HG21	19:S:65:ASN:HD22	1.81	0.44
17:Q:81:ARG:HG3	17:Q:81:ARG:O	2.17	0.44
1:A:45:U:H2'	1:A:46:G:C8	2.53	0.44
1:A:384:G:H2'	1:A:385:C:C6	2.53	0.44
1:A:393:A:C2'	1:A:394:G:H5'	2.46	0.44
1:A:485:G:C2'	1:A:486:U:OP2	2.65	0.44
1:A:662:G:H2'	1:A:663:A:H8	1.79	0.44
1:A:691:G:O2'	1:A:797:C:H4'	2.17	0.44
1:A:865:A:H2'	1:A:866:C:C6	2.53	0.44
1:A:975:A:O5'	1:A:976:G:H5'	2.17	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1128:C:O2'	1:A:1130:A:C8	2.62	0.44
1:A:1347:G:C5	9:I:107:ARG:NH1	2.86	0.44
2:B:92:TYR:CE1	2:B:151:GLY:HA3	2.51	0.44
2:B:107:THR:C	2:B:109:SER:N	2.75	0.44
4:D:8:VAL:HG21	4:D:115:ARG:CZ	2.46	0.44
7:G:12:LEU:HD12	7:G:12:LEU:N	2.32	0.44
10:J:8:LEU:CD1	10:J:20:ALA:HB2	2.48	0.44
13:M:34:LEU:HD13	13:M:41:PRO:CA	2.45	0.44
13:M:84:ILE:HG13	13:M:86:CYS:HB2	2.00	0.44
13:M:110:ARG:HG2	13:M:110:ARG:HH11	1.82	0.44
14:N:23:ARG:HD3	14:N:30:ALA:HB2	1.99	0.44
16:P:20:VAL:CG1	16:P:32:TYR:CB	2.95	0.44
22:Y:101:ILE:O	22:Y:135:PHE:HA	2.17	0.44
1:A:807:A:H2'	1:A:808:C:C6	2.52	0.44
1:A:981:U:H5'	14:N:21:TYR:CE1	2.53	0.44
1:A:1005:A:H2'	1:A:1006:C:O4'	2.17	0.44
1:A:1263:C:H2'	1:A:1264:C:H6	1.83	0.44
1:A:1319:A:H5''	19:S:5:LEU:HD21	1.98	0.44
2:B:54:THR:O	2:B:57:PHE:HB3	2.18	0.44
7:G:143:ARG:O	7:G:145:ALA:O	2.34	0.44
10:J:3:LYS:CA	10:J:75:ILE:HA	2.48	0.44
10:J:46:ARG:NH1	10:J:64:GLU:CG	2.80	0.44
10:J:68:HIS:N	10:J:68:HIS:CD2	2.85	0.44
14:N:9:LYS:HG3	14:N:21:TYR:O	2.17	0.44
15:O:87:ILE:CG2	15:O:88:ARG:N	2.80	0.44
20:T:30:LYS:O	20:T:33:ILE:HB	2.18	0.44
1:A:50:A:N6	1:A:361:G:H4'	2.33	0.44
1:A:129(A):G:C2	1:A:190(E):U:H5'	2.52	0.44
1:A:950:U:H2'	1:A:951:G:C8	2.52	0.44
3:C:28:GLN:O	3:C:31:HIS:N	2.46	0.44
4:D:24:GLU:CG	4:D:25:ARG:H	2.30	0.44
8:H:114:THR:C	8:H:116:LYS:N	2.75	0.44
9:I:46:ALA:O	9:I:49:PRO:HD2	2.17	0.44
10:J:6:ILE:O	10:J:71:LEU:O	2.35	0.44
11:K:51:LYS:O	11:K:55:LYS:CE	2.65	0.44
12:L:111:LYS:O	12:L:112:ASP:HB2	2.18	0.44
13:M:39:ILE:HD12	13:M:56:LEU:HG	1.98	0.44
15:O:82:ILE:O	15:O:83:GLU:C	2.61	0.44
16:P:20:VAL:HG13	16:P:21:VAL:N	2.32	0.44
19:S:45:VAL:C	19:S:47:HIS:H	2.25	0.44
1:A:321:A:H2'	1:A:322:C:C6	2.52	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:389:A:H2'	1:A:390:C:C5'	2.48	0.44
1:A:532:A:H2'	1:A:533:A:C5'	2.48	0.44
1:A:644:G:O2'	1:A:645:C:H5'	2.17	0.44
1:A:761:G:H4'	17:Q:102:GLY:C	2.43	0.44
1:A:792:A:H1'	1:A:794:A:N7	2.31	0.44
1:A:1095:U:H2'	1:A:1096:C:H6	1.83	0.44
1:A:1152:A:H2'	1:A:1153:C:H6	1.82	0.44
1:A:1299:A:C8	1:A:1301:U:H1'	2.53	0.44
1:A:1404:C:C2	1:A:1499:A:N6	2.86	0.44
1:A:1421:G:O2'	1:A:1422:G:H5'	2.17	0.44
5:E:36:ASP:OD2	5:E:40:ARG:HD3	2.18	0.44
7:G:95:ARG:NH1	7:G:95:ARG:CG	2.79	0.44
8:H:91:ARG:CG	12:L:7:ILE:HG13	2.44	0.44
10:J:72:VAL:O	10:J:73:ASP:HB2	2.18	0.44
11:K:95:ILE:HD13	11:K:108:ILE:HG21	1.99	0.44
13:M:120:LYS:HE2	13:M:123:ALA:CB	2.47	0.44
17:Q:104:LYS:O	17:Q:105:ALA:CB	2.65	0.44
3:C:46:GLU:C	3:C:48:TYR:H	2.22	0.44
3:C:95:THR:C	3:C:97:LYS:N	2.74	0.44
9:I:10:ARG:O	9:I:11:LYS:C	2.60	0.44
10:J:81:THR:C	10:J:83:GLU:N	2.76	0.44
10:J:85:LEU:O	10:J:87:THR:N	2.50	0.44
16:P:43:LYS:HA	16:P:48:TRP:HB3	2.00	0.44
20:T:96:GLY:O	20:T:97:ALA:CB	2.66	0.44
22:Y:187:ASN:ND2	22:Y:206:LYS:HA	2.29	0.44
1:A:103:C:OP2	20:T:17:ARG:NH1	2.51	0.44
1:A:397:A:H3'	1:A:397:A:N3	2.32	0.44
1:A:460:A:N7	1:A:462:G:C6	2.86	0.44
1:A:755:G:OP2	15:O:65:ARG:HD2	2.17	0.44
1:A:921:U:O2'	5:E:19:MET:O	2.26	0.44
1:A:962:C:H2'	1:A:963:G:O4'	2.18	0.44
1:A:1097:C:H2'	1:A:1098:C:H6	1.82	0.44
1:A:1288:A:O4'	1:A:1353:G:H4'	2.18	0.44
1:A:1289:A:H2'	1:A:1290:G:H5'	2.00	0.44
2:B:219:VAL:O	2:B:220:ASP:C	2.61	0.44
7:G:145:ALA:C	7:G:147:ALA:H	2.25	0.44
9:I:50:LEU:C	9:I:52:ALA:H	2.26	0.44
13:M:80:ARG:C	13:M:82:MET:N	2.73	0.44
13:M:110:ARG:HH11	13:M:110:ARG:CG	2.31	0.44
20:T:42:GLN:HA	20:T:45:GLN:HB2	1.99	0.44
20:T:63:ILE:HD13	20:T:80:ARG:CB	2.48	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:540:G:H2'	1:A:541:G:O4'	2.18	0.44
1:A:677:U:O2	1:A:777:A:O2'	2.33	0.44
1:A:922:G:C2	1:A:1396:A:C5	3.05	0.44
1:A:953:G:H1'	13:M:125:ARG:HB3	1.99	0.44
1:A:1113:C:H1'	3:C:178:LEU:HD21	1.99	0.44
1:A:1440:C:H2'	1:A:1441:G:C5'	2.48	0.44
2:B:90:MET:HA	2:B:91:PRO:HD3	1.70	0.44
4:D:8:VAL:HG11	4:D:21:LEU:CB	2.47	0.44
7:G:78:ARG:HG2	7:G:80:VAL:HG23	1.99	0.44
7:G:108:ALA:O	7:G:119:ARG:HD2	2.18	0.44
8:H:7:ALA:HB2	8:H:85:ARG:HD2	1.99	0.44
8:H:73:ASP:OD2	8:H:75:ARG:HB2	2.18	0.44
8:H:103:VAL:HG21	8:H:109:ILE:O	2.18	0.44
9:I:93:ARG:CD	9:I:97:LYS:HE3	2.47	0.44
13:M:67:GLU:HB3	13:M:68:GLY:H	1.58	0.44
15:O:27:VAL:O	15:O:28:GLN:C	2.61	0.44
16:P:6:LEU:HB3	16:P:17:TYR:HD2	1.81	0.44
17:Q:68:ARG:H	17:Q:70:ARG:NH1	2.15	0.44
17:Q:76:LEU:C	17:Q:76:LEU:CD2	2.90	0.44
18:R:25:THR:O	18:R:25:THR:HG22	2.17	0.44
20:T:53:LEU:CD1	20:T:101:GLY:HA2	2.47	0.44
20:T:72:LEU:O	20:T:73:HIS:O	2.35	0.44
21:V:15:ARG:O	21:V:17:THR:HG23	2.18	0.44
22:Y:191:LYS:HE2	22:Y:203:PHE:CE1	2.53	0.44
1:A:116:A:H2'	1:A:117:G:O4'	2.18	0.44
1:A:1010:G:O2'	1:A:1011:G:H5'	2.18	0.44
1:A:1229:A:H2'	1:A:1230:C:H6	1.83	0.44
1:A:1314:C:OP2	19:S:6:LYS:CD	2.66	0.44
1:A:1533:C:O2	1:A:1533:C:H2'	2.17	0.44
9:I:121:ARG:C	9:I:121:ARG:HD3	2.42	0.44
16:P:39:TYR:CZ	16:P:41:PRO:HA	2.52	0.44
19:S:31:ILE:CG2	19:S:32:LYS:N	2.70	0.44
22:Y:155:LEU:HA	22:Y:156:PRO:HD3	1.53	0.44
1:A:253:U:H2'	1:A:254:G:C8	2.53	0.43
1:A:760:G:N2	17:Q:103:GLY:O	2.51	0.43
1:A:760:G:H1	17:Q:105:ALA:HB2	1.83	0.43
1:A:761:G:O2'	17:Q:104:LYS:HA	2.18	0.43
1:A:1314:C:H2'	1:A:1315:U:C6	2.52	0.43
2:B:92:TYR:CD1	2:B:151:GLY:HA3	2.53	0.43
6:F:22:GLU:OE2	6:F:84:ASN:HB2	2.18	0.43
9:I:69:GLY:O	9:I:73:GLN:HG3	2.18	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:O:29:VAL:HG11	15:O:67:LEU:HD21	2.00	0.43
19:S:10:PHE:C	19:S:10:PHE:HD2	2.26	0.43
22:Y:107:TRP:CD1	22:Y:108:GLY:H	2.35	0.43
1:A:718:G:C8	11:K:116:HIS:HB3	2.53	0.43
1:A:1031:G:H2'	1:A:1032:G:H8	1.83	0.43
1:A:1131:G:H2'	1:A:1132:C:H6	1.82	0.43
1:A:1231:G:OP1	9:I:127:LYS:NZ	2.50	0.43
1:A:1525:G:P	11:K:120:ARG:HH22	2.40	0.43
2:B:10:LEU:CD2	2:B:48:MET:HE2	2.48	0.43
4:D:10:ARG:HH11	4:D:10:ARG:HG3	1.83	0.43
4:D:24:GLU:HG2	4:D:25:ARG:H	1.81	0.43
4:D:55:ALA:O	4:D:59:ARG:HG2	2.19	0.43
9:I:78:LYS:HE2	9:I:78:LYS:HB3	1.87	0.43
10:J:75:ILE:HG22	10:J:76:ASN:N	2.33	0.43
11:K:85:ARG:HG3	11:K:85:ARG:NH1	2.33	0.43
11:K:100:ALA:O	11:K:102:GLY:N	2.51	0.43
12:L:115:LYS:O	12:L:117:ARG:N	2.37	0.43
13:M:123:ALA:O	13:M:124:PRO:C	2.60	0.43
15:O:54:ARG:O	15:O:58:MET:HG3	2.17	0.43
18:R:37:VAL:O	18:R:41:LYS:HB3	2.18	0.43
20:T:57:ARG:HE	20:T:100:ILE:CG2	2.31	0.43
1:A:409:G:OP1	4:D:24:GLU:O	2.36	0.43
1:A:1305:G:N2	1:A:1331:G:HO2'	2.16	0.43
2:B:83:MET:HG3	2:B:238:LEU:HD11	2.00	0.43
3:C:19:GLU:HB3	3:C:40:ARG:NH2	2.25	0.43
3:C:99:VAL:HG22	3:C:100:ALA:O	2.18	0.43
4:D:178:VAL:O	4:D:178:VAL:HG12	2.18	0.43
5:E:80:ILE:CD1	5:E:91:LEU:HD12	2.46	0.43
7:G:24:THR:HA	7:G:27:ILE:HD12	2.00	0.43
11:K:50:TYR:N	11:K:50:TYR:CD2	2.84	0.43
12:L:28:LYS:C	12:L:30:ALA:H	2.25	0.43
12:L:70:ILE:CD1	12:L:77:LEU:HD12	2.42	0.43
16:P:20:VAL:HG13	16:P:32:TYR:HB2	2.00	0.43
16:P:67:THR:CG2	16:P:68:ASP:N	2.81	0.43
18:R:26:LEU:HD21	18:R:39:VAL:HG23	2.00	0.43
22:Y:88:GLU:H	22:Y:88:GLU:CD	2.26	0.43
1:A:16:A:O2'	1:A:17:U:H5'	2.18	0.43
1:A:80:G:C2'	1:A:81:U:H5''	2.48	0.43
1:A:143:A:H2	1:A:220:G:H22	1.66	0.43
1:A:267:C:H2'	1:A:268:C:C6	2.53	0.43
1:A:363:A:O2'	1:A:364:A:H5'	2.19	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:430:A:H2'	1:A:431:A:H5'	1.99	0.43
1:A:640:A:C2'	1:A:641:U:H5'	2.48	0.43
1:A:838:G:C3'	1:A:839:U:H5''	2.48	0.43
1:A:1051:C:H2'	1:A:1052:U:C6	2.53	0.43
1:A:1053:G:O2'	1:A:1199:U:H5	2.01	0.43
1:A:1497:G:C2'	1:A:1498:U:C5'	2.87	0.43
3:C:82:GLU:CD	3:C:82:GLU:C	2.87	0.43
3:C:134:ILE:HG22	3:C:168:ALA:CB	2.48	0.43
3:C:188:LEU:HD22	3:C:188:LEU:HA	1.79	0.43
6:F:15:ASP:O	6:F:16:GLN:C	2.61	0.43
8:H:16:ALA:O	8:H:21:LYS:HG2	2.18	0.43
10:J:56:HIS:O	10:J:58:ASP:N	2.52	0.43
11:K:77:MET:CE	11:K:80:VAL:HG22	2.48	0.43
12:L:7:ILE:O	12:L:11:VAL:HG23	2.18	0.43
12:L:60:LEU:CD2	12:L:66:VAL:HG22	2.49	0.43
16:P:75:ARG:O	16:P:78:GLY:N	2.49	0.43
22:Y:15:ASP:O	22:Y:19:GLU:HG2	2.17	0.43
22:Y:115:ILE:HG13	22:Y:116:LYS:N	2.33	0.43
1:A:383:A:H2'	1:A:384:G:H5'	1.99	0.43
1:A:436:C:H2'	1:A:437:U:C6	2.53	0.43
1:A:502:G:C1'	1:A:550:G:H5'	2.49	0.43
1:A:961:U:C2'	1:A:962:C:H5'	2.48	0.43
1:A:1286:A:H4'	21:V:25:LYS:HE3	2.01	0.43
2:B:74:LYS:HD2	2:B:166:ASP:HB2	2.00	0.43
2:B:107:THR:C	2:B:109:SER:H	2.25	0.43
3:C:7:PRO:HG2	3:C:184:TYR:CB	2.45	0.43
7:G:75:VAL:HG13	7:G:86:GLN:HB3	1.95	0.43
8:H:86:ILE:HD12	8:H:133:LEU:HD22	2.00	0.43
19:S:12:ASP:HB2	19:S:35:SER:OG	2.19	0.43
1:A:254:G:O2'	1:A:255:G:H5'	2.18	0.43
1:A:718:G:H1'	11:K:116:HIS:HA	2.00	0.43
1:A:765:G:N2	1:A:812:C:O2'	2.51	0.43
1:A:851:G:H2'	1:A:852:G:H8	1.84	0.43
1:A:1152:A:OP1	10:J:13:HIS:HB2	2.18	0.43
1:A:1346:A:C4	7:G:10:ARG:CZ	3.02	0.43
2:B:17:PHE:H	2:B:44:LEU:HD21	1.83	0.43
2:B:41:ILE:O	2:B:41:ILE:HG22	2.19	0.43
3:C:116:VAL:HG11	3:C:141:VAL:HG21	2.01	0.43
3:C:188:LEU:HD13	3:C:189:ALA:H	1.84	0.43
9:I:106:ALA:O	9:I:108:VAL:HG23	2.19	0.43
10:J:46:ARG:HH11	10:J:64:GLU:CG	2.31	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:23:TYR:CE2	13:M:70:LEU:HD13	2.54	0.43
15:O:15:PHE:O	15:O:16:ALA:C	2.62	0.43
15:O:17:ARG:HH11	15:O:17:ARG:CG	2.25	0.43
16:P:80:PHE:O	16:P:81:ARG:C	2.60	0.43
17:Q:97:SER:O	17:Q:98:LEU:HD12	2.19	0.43
19:S:3:ARG:O	19:S:4:SER:HB3	2.18	0.43
1:A:433:C:O2'	1:A:434:U:H5'	2.19	0.43
1:A:935:A:H1'	1:A:1384:C:N3	2.33	0.43
2:B:14:GLY:C	2:B:15:VAL:HG23	2.44	0.43
2:B:28:PHE:CD2	2:B:190:THR:HA	2.54	0.43
2:B:119:GLU:OE1	2:B:153:ARG:NH2	2.51	0.43
3:C:191:THR:HB	3:C:194:GLY:O	2.18	0.43
4:D:15:GLU:C	4:D:17:VAL:N	2.76	0.43
4:D:198:VAL:HG12	4:D:199:ASN:N	2.33	0.43
5:E:105:VAL:HB	5:E:106:PRO:CD	2.40	0.43
5:E:118:ILE:CG2	5:E:119:LEU:H	2.28	0.43
7:G:148:ASN:C	7:G:150:ALA:H	2.26	0.43
11:K:46:GLY:O	11:K:47:VAL:C	2.62	0.43
15:O:78:TYR:CE2	15:O:82:ILE:HD11	2.53	0.43
19:S:8:GLY:O	19:S:9:VAL:C	2.62	0.43
1:A:359:U:O2'	1:A:360:A:H5'	2.18	0.43
1:A:448:A:C4	1:A:487:A:C2	3.07	0.43
1:A:730:G:C5	1:A:731:G:H1'	2.54	0.43
1:A:913:A:O2'	1:A:914:A:OP2	2.36	0.43
1:A:1135:U:H6	1:A:1135:U:O5'	2.01	0.43
2:B:146:GLN:O	2:B:150:SER:HB3	2.18	0.43
4:D:25:ARG:HH21	4:D:30:LYS:HD3	1.82	0.43
4:D:104:VAL:O	4:D:105:VAL:C	2.59	0.43
4:D:127:THR:HG23	4:D:128:VAL:N	2.34	0.43
5:E:6:PHE:CZ	5:E:66:MET:HE2	2.53	0.43
5:E:21:ALA:C	5:E:23:GLY:N	2.76	0.43
5:E:24:ARG:HG2	5:E:24:ARG:NH1	2.32	0.43
5:E:143:ARG:HD3	5:E:143:ARG:HA	1.71	0.43
6:F:77:ARG:O	6:F:81:ILE:HG13	2.18	0.43
16:P:40:ASP:HB3	16:P:48:TRP:HB2	2.00	0.43
19:S:40:ILE:HG23	19:S:44:MET:SD	2.59	0.43
20:T:63:ILE:HD13	20:T:80:ARG:HB3	2.01	0.43
1:A:137:C:O2'	1:A:138:G:H5'	2.18	0.43
1:A:157:G:O2'	1:A:158:G:H5'	2.18	0.43
1:A:487:A:H2'	1:A:488:C:O4'	2.19	0.43
1:A:628:G:H2'	1:A:629:G:H8	1.84	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:719:C:O2	18:R:50:ILE:HG13	2.19	0.43
1:A:1126:U:H2'	1:A:1127:G:O4'	2.18	0.43
1:A:1262:C:H2'	1:A:1263:C:C6	2.54	0.43
1:A:1394:A:N6	1:A:1501:C:C5'	2.82	0.43
1:A:1397:C:O2'	1:A:1398:A:P	2.77	0.43
1:A:1441:G:H4'	1:A:1442:G:C8	2.54	0.43
3:C:28:GLN:O	3:C:29:TYR:C	2.62	0.43
3:C:70:VAL:HG12	3:C:71:ALA:H	1.84	0.43
3:C:191:THR:HG21	3:C:193:TYR:CE1	2.53	0.43
3:C:193:TYR:HE1	3:C:196:LEU:HD11	1.83	0.43
4:D:120:LEU:HD23	4:D:125:HIS:CD2	2.54	0.43
8:H:68:ARG:HG2	8:H:68:ARG:HH11	1.84	0.43
9:I:97:LYS:HB2	9:I:98:PRO:HD3	2.01	0.43
13:M:33:ALA:HB2	13:M:64:TRP:CH2	2.54	0.43
14:N:14:PRO:O	14:N:16:PHE:N	2.44	0.43
16:P:4:ILE:HG23	16:P:36:ILE:HD11	2.01	0.43
16:P:39:TYR:CD2	16:P:73:LEU:HD11	2.54	0.43
17:Q:60:ILE:HD13	17:Q:61:GLU:N	2.34	0.43
19:S:25:LYS:HD2	19:S:25:LYS:N	2.34	0.43
20:T:84:LEU:O	20:T:84:LEU:HD22	2.18	0.43
1:A:247:G:OP2	17:Q:100:LYS:HG3	2.19	0.43
1:A:370:C:C2'	1:A:371:G:H5'	2.48	0.43
1:A:451:A:N6	1:A:480:U:H2'	2.33	0.43
1:A:522:C:O2'	1:A:523:A:H5'	2.19	0.43
1:A:647:C:H2'	1:A:648:A:C8	2.54	0.43
1:A:782:A:H2'	1:A:783:C:O4'	2.19	0.43
1:A:991:U:O2	1:A:993:G:H8	2.02	0.43
1:A:1064:G:H1'	1:A:1190:G:H21	1.84	0.43
1:A:1125:U:H5''	1:A:1126:U:H5	1.83	0.43
1:A:1270:C:H4'	1:A:1313:U:O2'	2.19	0.43
1:A:1331:G:O2'	1:A:1332:A:P	2.76	0.43
1:A:1504:G:OP1	1:A:1507:A:H4'	2.19	0.43
2:B:130:ARG:HH22	3:C:207:VAL:HG22	1.82	0.43
3:C:134:ILE:HD13	3:C:166:GLU:HB3	2.01	0.43
5:E:16:THR:HG23	5:E:27:ARG:O	2.18	0.43
5:E:80:ILE:HD12	5:E:80:ILE:H	1.84	0.43
12:L:33:ARG:HD2	12:L:62:SER:HB3	2.01	0.43
21:V:2:GLY:C	21:V:4:GLY:H	2.26	0.43
22:Y:124:ASN:O	22:Y:127:ASP:HB2	2.19	0.43
1:A:176:C:H2'	1:A:177:C:H6	1.83	0.42
1:A:518:C:O2'	12:L:50:SER:HB3	2.18	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:858:G:O2'	1:A:859:A:H5'	2.18	0.42
1:A:1230:C:H1'	13:M:125:ARG:O	2.19	0.42
1:A:1376:U:H2'	1:A:1377:A:H8	1.80	0.42
1:A:1404:C:O4'	1:A:1499:A:N1	2.52	0.42
1:A:1438:G:H2'	1:A:1439:C:C6	2.54	0.42
10:J:55:LYS:O	10:J:56:HIS:HB2	2.19	0.42
17:Q:45:HIS:CD2	17:Q:47:PRO:HG3	2.54	0.42
19:S:20:LEU:HD12	19:S:21:GLU:N	2.34	0.42
22:Y:140:THR:HG21	22:Y:209:PHE:CE1	2.54	0.42
1:A:160:A:H2'	1:A:161:A:O4'	2.18	0.42
1:A:418:C:H2'	1:A:419:C:H6	1.84	0.42
1:A:512:U:H1'	4:D:42:GLN:OE1	2.19	0.42
1:A:636:U:H2'	1:A:637:G:C8	2.54	0.42
1:A:1004:A:H5''	1:A:1025:U:C4	2.53	0.42
1:A:1305:G:H22	1:A:1331:G:C2'	2.33	0.42
1:A:1305:G:H5''	21:V:4:GLY:C	2.44	0.42
2:B:43:ASP:C	2:B:43:ASP:OD1	2.61	0.42
5:E:40:ARG:NH1	5:E:68:GLU:OE1	2.51	0.42
5:E:115:VAL:CG1	5:E:116:THR:N	2.82	0.42
6:F:30:LEU:HB3	6:F:35:ALA:CB	2.41	0.42
6:F:75:LEU:O	6:F:75:LEU:HD13	2.18	0.42
9:I:78:LYS:HD3	9:I:101:PHE:CD2	2.54	0.42
14:N:12:ARG:C	14:N:14:PRO:HD3	2.44	0.42
17:Q:59:ILE:CG2	17:Q:71:PHE:CD1	3.02	0.42
1:A:413:G:N2	1:A:428:G:H1'	2.34	0.42
1:A:640:A:O2'	1:A:641:U:H5'	2.20	0.42
1:A:960:U:O2	1:A:960:U:H2'	2.18	0.42
1:A:994:A:N7	1:A:1216:G:H4'	2.35	0.42
1:A:1157:A:O4'	1:A:1158:C:C2	2.72	0.42
2:B:8:LYS:O	2:B:9:GLU:CB	2.60	0.42
3:C:11:ARG:O	3:C:14:ILE:O	2.36	0.42
3:C:74:GLY:O	3:C:75:VAL:C	2.62	0.42
5:E:80:ILE:HD12	5:E:91:LEU:HB2	2.00	0.42
7:G:31:MET:SD	7:G:34:GLY:HA2	2.60	0.42
7:G:38:LEU:HD12	7:G:38:LEU:C	2.45	0.42
10:J:17:ASP:O	10:J:21:GLN:HB2	2.19	0.42
11:K:21:ILE:HD12	11:K:95:ILE:HG12	2.00	0.42
11:K:104:GLN:OE1	11:K:106:LYS:HE2	2.19	0.42
13:M:96:LEU:HB3	13:M:97:PRO:HD2	2.00	0.42
20:T:86:ARG:O	20:T:87:LYS:C	2.62	0.42
22:Y:146:GLU:O	22:Y:149:GLU:HG2	2.20	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:173:U:C5'	1:A:197:A:O4'	2.65	0.42
1:A:243:A:N6	1:A:281:G:O2'	2.51	0.42
1:A:545:C:O2'	1:A:549:C:OP1	2.37	0.42
1:A:1057:G:H4'	3:C:197:GLY:H	1.85	0.42
1:A:1104:G:OP1	2:B:111:ARG:HD2	2.18	0.42
1:A:1126:U:H2'	1:A:1127:G:H8	1.84	0.42
1:A:1353:G:H2'	1:A:1354:C:C6	2.54	0.42
3:C:14:ILE:O	3:C:15:THR:C	2.62	0.42
3:C:50:ALA:O	3:C:70:VAL:CG1	2.67	0.42
6:F:19:LEU:HD21	6:F:23:LYS:HD2	2.02	0.42
7:G:38:LEU:HD12	7:G:42:ILE:HG13	2.00	0.42
10:J:53:PRO:O	10:J:54:PHE:C	2.63	0.42
19:S:41:VAL:HB	19:S:43:GLU:OE2	2.20	0.42
20:T:10:LEU:C	20:T:12:ALA:H	2.26	0.42
22:Y:113:TYR:CD2	22:Y:121:ILE:HG21	2.55	0.42
1:A:409:G:H2'	1:A:410:G:O4'	2.18	0.42
1:A:833:U:H2'	1:A:834:C:C6	2.55	0.42
1:A:839:U:C5'	1:A:840:C:H5	2.27	0.42
1:A:932:C:C2	1:A:1386:G:C2	3.08	0.42
1:A:1060:C:O2'	1:A:1061:G:H5'	2.18	0.42
1:A:1091:U:O2	1:A:1093:A:H8	2.02	0.42
1:A:1181:G:O2'	1:A:1182:G:H5'	2.19	0.42
1:A:1217:C:O2'	1:A:1218:C:H5'	2.19	0.42
1:A:1244:C:O2'	1:A:1245:A:H5'	2.19	0.42
1:A:1288:A:H1'	1:A:1353:G:O4'	2.19	0.42
1:A:1347:G:HO2'	1:A:1373:G:H1	1.66	0.42
1:A:1487:G:C2'	1:A:1488:G:H5'	2.50	0.42
4:D:8:VAL:CG1	4:D:21:LEU:HD13	2.49	0.42
7:G:155:ARG:O	7:G:156:TRP:CB	2.64	0.42
10:J:32:ALA:HB2	10:J:75:ILE:O	2.19	0.42
11:K:57:THR:OG1	11:K:58:PRO:HD2	2.20	0.42
14:N:23:ARG:C	14:N:33:VAL:HG11	2.43	0.42
15:O:39:LEU:HD12	15:O:59:MET:CE	2.48	0.42
20:T:49:ALA:O	20:T:50:GLU:C	2.62	0.42
1:A:80:G:H2'	1:A:81:U:H5''	2.01	0.42
1:A:162:A:H2'	1:A:163:C:O4'	2.20	0.42
1:A:576:G:C6	1:A:881:G:O4'	2.73	0.42
1:A:1129:C:O2'	1:A:1130:A:P	2.78	0.42
1:A:1202:G:C2	14:N:42:ILE:HG21	2.55	0.42
1:A:1327:C:O2'	1:A:1328:C:H5'	2.19	0.42
1:A:1346:A:C8	7:G:10:ARG:NH2	2.87	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:187:LEU:HD21	2:B:214:ILE:HG13	2.00	0.42
3:C:64:VAL:HG12	3:C:65:ALA:H	1.84	0.42
4:D:25:ARG:HA	4:D:28:SER:OG	2.19	0.42
6:F:40:VAL:HG22	6:F:41:GLU:N	2.34	0.42
8:H:75:ARG:HA	8:H:76:PRO:HD3	1.70	0.42
10:J:12:ASP:OD1	10:J:14:LYS:N	2.50	0.42
10:J:22:LYS:HZ3	10:J:91:PRO:HD3	1.84	0.42
13:M:7:VAL:O	13:M:7:VAL:HG23	2.18	0.42
16:P:76:GLN:C	16:P:78:GLY:H	2.28	0.42
20:T:10:LEU:C	20:T:12:ALA:N	2.76	0.42
22:Y:92:PHE:CD1	22:Y:95:LYS:HD2	2.55	0.42
1:A:169:C:O2'	1:A:170:U:H5'	2.19	0.42
1:A:397:A:H5'	1:A:398:C:P	2.60	0.42
1:A:825:G:H2'	1:A:826:C:C6	2.53	0.42
2:B:14:GLY:C	2:B:15:VAL:CG2	2.92	0.42
2:B:17:PHE:CA	2:B:44:LEU:HD21	2.49	0.42
2:B:22:LYS:HD2	2:B:35:GLU:CD	2.45	0.42
4:D:70:ILE:HD11	4:D:100:ARG:CD	2.49	0.42
12:L:41:ARG:CB	12:L:41:ARG:NH1	2.82	0.42
15:O:38:ARG:O	15:O:41:GLU:HB3	2.20	0.42
18:R:44:LEU:HD23	18:R:44:LEU:HA	1.89	0.42
20:T:42:GLN:O	20:T:46:GLU:HG3	2.19	0.42
21:V:9:ARG:HH11	21:V:22:ARG:HA	1.85	0.42
1:A:418:C:H2'	1:A:419:C:C6	2.54	0.42
1:A:502:G:H2'	1:A:503:C:H6	1.84	0.42
1:A:974:A:P	14:N:41:ARG:HH12	2.42	0.42
1:A:1271:G:H5'	1:A:1314:C:OP1	2.20	0.42
1:A:1306:A:O2'	13:M:109:THR:HG21	2.19	0.42
2:B:73:THR:O	2:B:74:LYS:C	2.61	0.42
3:C:23:TYR:OH	10:J:9:ARG:HD3	2.20	0.42
4:D:89:THR:O	4:D:90:GLY:C	2.61	0.42
9:I:56:LEU:O	9:I:58:HIS:N	2.49	0.42
12:L:41:ARG:HB3	12:L:41:ARG:HH11	1.84	0.42
13:M:46:LYS:HB2	13:M:46:LYS:HE3	1.86	0.42
1:A:145:G:O2'	1:A:146:G:H5'	2.20	0.42
1:A:252:U:O2'	1:A:275:G:N2	2.53	0.42
1:A:584:G:H2'	1:A:585:G:C8	2.54	0.42
1:A:930:C:O2'	1:A:931:C:H5'	2.20	0.42
1:A:965:A:C2	13:M:124:PRO:HB2	2.55	0.42
1:A:974:A:OP1	1:A:974:A:H8	2.03	0.42
2:B:8:LYS:HB2	2:B:9:GLU:H	1.58	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:87:ARG:NH2	2:B:220:ASP:OD1	2.51	0.42
2:B:187:LEU:HA	2:B:201:ILE:HB	2.02	0.42
6:F:45:LEU:O	6:F:46:ARG:HG2	2.20	0.42
9:I:110:GLU:HG2	9:I:113:LYS:NZ	2.35	0.42
11:K:86:GLY:H	11:K:112:THR:CG2	2.32	0.42
13:M:16:ASP:O	13:M:17:VAL:C	2.63	0.42
18:R:17:SER:HB2	18:R:54:ARG:HH21	1.85	0.42
1:A:373:A:H2'	1:A:374:A:H8	1.85	0.42
1:A:413:G:H22	1:A:428:G:H1'	1.85	0.42
1:A:951:G:C6	1:A:1231:G:C6	3.08	0.42
1:A:961:U:O2'	1:A:962:C:H5'	2.20	0.42
1:A:1056:U:H5'	3:C:163:ALA:HB2	2.02	0.42
1:A:1060:C:OP1	14:N:45:ARG:NH2	2.53	0.42
1:A:1260:C:H4'	1:A:1284:C:H5'	2.01	0.42
1:A:1375:A:OP1	7:G:12:LEU:HD21	2.20	0.42
1:A:1405:G:O2'	1:A:1519:A:C5'	2.68	0.42
1:A:1426:C:H2'	1:A:1427:U:H6	1.84	0.42
1:A:1505:G:H3'	1:A:1505:G:H8	1.85	0.42
3:C:38:ARG:CB	3:C:94:LEU:HD21	2.50	0.42
3:C:77:ILE:CG2	3:C:81:GLY:HA2	2.50	0.42
3:C:139:GLN:O	3:C:140:ARG:C	2.62	0.42
4:D:8:VAL:CG1	4:D:21:LEU:CD1	2.98	0.42
5:E:24:ARG:O	5:E:25:ARG:HG2	2.20	0.42
6:F:42:GLU:C	6:F:44:GLY:N	2.78	0.42
17:Q:40:LYS:HD3	17:Q:42:TYR:OH	2.20	0.42
18:R:48:GLY:O	18:R:74:ARG:NH2	2.41	0.42
20:T:54:LYS:HA	20:T:57:ARG:HD3	2.02	0.42
1:A:192:U:O2	20:T:60:GLU:OE1	2.38	0.41
1:A:490:G:H2'	1:A:491:G:C8	2.54	0.41
1:A:767:A:H2'	1:A:768:A:O4'	2.20	0.41
1:A:825:G:O2'	1:A:826:C:H5'	2.20	0.41
1:A:977:A:H2'	1:A:978:A:C5'	2.46	0.41
1:A:1061:G:C2'	1:A:1062:U:H5'	2.50	0.41
1:A:1277:C:H1'	1:A:1282:C:O2	2.20	0.41
2:B:23:ARG:C	2:B:24:TRP:HD1	2.28	0.41
4:D:60:GLU:OE1	4:D:60:GLU:HA	2.20	0.41
6:F:48:LEU:HD13	6:F:52:ILE:CG1	2.50	0.41
7:G:15:ASP:OD2	7:G:23:VAL:HG11	2.20	0.41
7:G:93:PRO:HG2	7:G:94:ARG:H	1.85	0.41
9:I:42:ARG:O	9:I:43:ALA:C	2.63	0.41
9:I:120:ARG:O	9:I:122:ALA:N	2.53	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:80:LYS:HA	10:J:83:GLU:HB2	2.02	0.41
11:K:32:ILE:HG21	11:K:77:MET:HE2	2.01	0.41
11:K:111:ASP:CG	18:R:84:LYS:HE2	2.45	0.41
17:Q:95:TYR:N	17:Q:95:TYR:CD1	2.88	0.41
18:R:51:LEU:HA	18:R:52:PRO:HD3	1.80	0.41
20:T:43:LEU:HD12	20:T:55:ILE:HD12	2.02	0.41
1:A:867:G:O2'	1:A:868:C:H5'	2.20	0.41
1:A:1034:G:O2'	1:A:1035:A:H5'	2.20	0.41
1:A:1213:A:N1	1:A:1215:G:H1'	2.35	0.41
1:A:1264:C:H2'	1:A:1265:G:H8	1.85	0.41
1:A:1264:C:H2'	1:A:1265:G:C8	2.54	0.41
1:A:1346:A:C5	7:G:10:ARG:CZ	3.02	0.41
2:B:127:ILE:C	2:B:129:GLU:H	2.29	0.41
2:B:156:LYS:HD3	2:B:156:LYS:C	2.46	0.41
3:C:61:ALA:O	3:C:62:ASP:C	2.63	0.41
3:C:134:ILE:HG22	3:C:168:ALA:HB3	2.01	0.41
4:D:205:GLU:O	4:D:208:SER:HB2	2.20	0.41
8:H:6:ILE:O	8:H:10:LEU:HG	2.20	0.41
13:M:32:GLU:O	13:M:35:GLU:N	2.53	0.41
16:P:19:ILE:HG22	16:P:36:ILE:CG1	2.51	0.41
17:Q:63:ARG:O	17:Q:64:PRO:C	2.63	0.41
1:A:47:C:C6	1:A:365:U:H2'	2.56	0.41
1:A:184:G:O4'	1:A:224:C:H4'	2.19	0.41
1:A:550:G:O2'	1:A:551:U:H5'	2.20	0.41
1:A:628:G:O2'	1:A:629:G:H5'	2.20	0.41
1:A:778:G:O2'	1:A:779:C:H5'	2.19	0.41
1:A:965:A:O2'	1:A:966:G:C5'	2.67	0.41
1:A:1127:G:N2	1:A:1144:G:N2	2.69	0.41
1:A:1531:A:O5'	1:A:1531:A:H8	2.03	0.41
2:B:165:VAL:O	2:B:187:LEU:O	2.38	0.41
4:D:24:GLU:H	4:D:112:VAL:HG11	1.85	0.41
5:E:51:VAL:HB	5:E:52:PRO:CD	2.37	0.41
8:H:51:VAL:CG1	8:H:52:ASP:N	2.82	0.41
1:A:547:A:H4'	1:A:548:G:O5'	2.19	0.41
1:A:655:A:C2	1:A:754:C:N4	2.88	0.41
1:A:1371:G:H2'	1:A:1372:U:H6	1.86	0.41
2:B:142:LEU:O	2:B:143:GLU:C	2.63	0.41
7:G:69:VAL:O	7:G:69:VAL:CG1	2.68	0.41
9:I:59:PHE:HB3	9:I:60:ASP:H	1.56	0.41
9:I:110:GLU:HG2	9:I:113:LYS:HZ2	1.85	0.41
10:J:3:LYS:HG3	10:J:75:ILE:HG23	2.01	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:117:ARG:O	12:L:118:SER:C	2.64	0.41
13:M:115:LYS:HZ2	13:M:115:LYS:HB3	1.86	0.41
1:A:489:C:H2'	1:A:490:G:C8	2.54	0.41
1:A:546:G:OP1	4:D:73:ARG:HB2	2.21	0.41
1:A:866:C:H2'	1:A:867:G:O4'	2.20	0.41
1:A:1030(A):G:H21	1:A:1030(C):G:H3'	1.84	0.41
1:A:1094:G:OP2	1:A:1095:U:C5	2.74	0.41
1:A:1137:C:H4'	1:A:1138:G:N1	2.33	0.41
1:A:1322:C:OP1	19:S:78:ARG:NH2	2.54	0.41
1:A:1350:A:C6	1:A:1351:U:N3	2.89	0.41
1:A:1453:G:H2'	1:A:1454:G:O4'	2.21	0.41
2:B:22:LYS:C	2:B:23:ARG:HG3	2.45	0.41
3:C:89:GLU:C	3:C:91:LEU:N	2.76	0.41
3:C:112:SER:HB2	3:C:115:LEU:HB2	2.01	0.41
5:E:40:ARG:NH1	5:E:68:GLU:OE2	2.49	0.41
5:E:131:ILE:HD13	5:E:131:ILE:HA	1.93	0.41
8:H:108:GLY:CA	8:H:138:TRP:HB3	2.46	0.41
8:H:126:LYS:O	8:H:128:GLY:N	2.54	0.41
10:J:3:LYS:CG	10:J:75:ILE:HG23	2.51	0.41
15:O:70:LEU:HD12	15:O:78:TYR:HB2	2.01	0.41
15:O:87:ILE:HG22	15:O:88:ARG:N	2.34	0.41
17:Q:95:TYR:N	17:Q:95:TYR:HD1	2.18	0.41
21:V:7:ARG:O	21:V:7:ARG:HG3	2.19	0.41
22:Y:38:ASN:ND2	22:Y:104:LEU:HD12	2.35	0.41
22:Y:94:LEU:O	22:Y:97:ILE:HG22	2.21	0.41
1:A:67:C:O2'	1:A:171:A:H1'	2.20	0.41
1:A:520:A:O2'	12:L:73:GLU:OE2	2.35	0.41
1:A:1126:U:P	1:A:1126:U:H6	2.43	0.41
1:A:1145:C:O2'	1:A:1146:A:O5'	2.39	0.41
1:A:1145:C:HO2'	1:A:1146:A:H8	1.63	0.41
1:A:1239:A:C4	1:A:1298:C:N4	2.88	0.41
1:A:1262:C:N4	1:A:1273:G:H1	2.18	0.41
1:A:1311:G:H2'	1:A:1312:G:O4'	2.20	0.41
1:A:1431:C:H2'	1:A:1432:G:O4'	2.21	0.41
3:C:73:PRO:HD3	3:C:105:GLU:HG3	2.03	0.41
3:C:206:GLU:O	3:C:207:VAL:C	2.63	0.41
9:I:110:GLU:OE2	9:I:113:LYS:NZ	2.53	0.41
11:K:86:GLY:N	11:K:112:THR:HG23	2.35	0.41
11:K:127:LYS:HD3	11:K:127:LYS:HA	1.78	0.41
12:L:53:ARG:CB	12:L:93:LEU:HD11	2.50	0.41
12:L:83:VAL:HG22	12:L:84:LEU:H	1.85	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:78:ILE:CA	13:M:81:LEU:HD21	2.43	0.41
16:P:4:ILE:CG1	16:P:64:ALA:HB1	2.49	0.41
22:Y:186:ASP:O	22:Y:190:VAL:HG23	2.20	0.41
1:A:43:C:H2'	1:A:44:G:O4'	2.21	0.41
1:A:107:G:O2'	1:A:108:G:H5'	2.19	0.41
1:A:1228:C:H4'	13:M:116:THR:HA	2.02	0.41
1:A:1292:U:P	7:G:41:ARG:NH2	2.94	0.41
1:A:1390:U:H2'	1:A:1391:U:H6	1.86	0.41
2:B:90:MET:HE2	2:B:222:ILE:HD13	2.03	0.41
4:D:148:VAL:HG13	4:D:158:ILE:HD13	2.01	0.41
5:E:58:ALA:O	5:E:59:GLY:C	2.63	0.41
7:G:45:ASP:O	7:G:49:ILE:HG13	2.20	0.41
8:H:82:HIS:O	8:H:83:ILE:HB	2.21	0.41
9:I:108:VAL:HG12	9:I:109:VAL:N	2.36	0.41
10:J:75:ILE:O	10:J:76:ASN:HB2	2.21	0.41
12:L:60:LEU:HD21	12:L:66:VAL:CG2	2.50	0.41
16:P:1:MET:HE1	16:P:3:LYS:HE2	2.02	0.41
18:R:21:LYS:HG3	18:R:57:GLY:CA	2.51	0.41
19:S:5:LEU:HD23	19:S:5:LEU:HA	1.88	0.41
22:Y:91:PRO:HD2	22:Y:94:LEU:HD12	2.02	0.41
1:A:382:A:C2	1:A:383:A:C4	3.08	0.41
1:A:436:C:H2'	1:A:437:U:H6	1.86	0.41
1:A:439:A:N6	1:A:497:A:H1'	2.35	0.41
1:A:620:C:C2	4:D:135:LEU:HD13	2.56	0.41
1:A:625:G:O2'	1:A:626:U:H5'	2.20	0.41
1:A:665:A:H2'	1:A:725:G:H22	1.83	0.41
1:A:692:U:O2	1:A:695:A:C8	2.73	0.41
1:A:1077:G:N2	1:A:1080:A:OP2	2.50	0.41
1:A:1116:C:O2'	9:I:108:VAL:HG21	2.21	0.41
1:A:1352:C:OP1	21:V:3:LYS:NZ	2.51	0.41
1:A:1404:C:C2	1:A:1499:A:C6	3.08	0.41
2:B:116:GLU:CG	2:B:153:ARG:NH1	2.80	0.41
2:B:125:PRO:HG2	2:B:126:GLU:H	1.86	0.41
3:C:179:ARG:O	3:C:179:ARG:CG	2.69	0.41
4:D:23:GLY:HA3	4:D:112:VAL:HG13	2.02	0.41
5:E:66:MET:HE3	5:E:66:MET:HB3	1.98	0.41
6:F:48:LEU:HD13	6:F:52:ILE:HD12	2.03	0.41
8:H:39:LEU:HD13	8:H:39:LEU:HA	1.86	0.41
11:K:99:GLN:HG2	11:K:105:VAL:HG21	2.02	0.41
16:P:43:LYS:HA	16:P:48:TRP:CB	2.51	0.41
22:Y:196:LEU:HD13	22:Y:196:LEU:HA	1.92	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:134:A:H1'	1:A:325:A:C5	2.56	0.41
1:A:335:C:H2'	1:A:336:C:H6	1.85	0.41
1:A:519:C:H2'	1:A:520:A:C8	2.56	0.41
1:A:736:C:H2'	1:A:737:A:H8	1.83	0.41
1:A:913:A:H1'	1:A:914:A:O4'	2.21	0.41
1:A:953:G:H1'	13:M:125:ARG:HA	2.03	0.41
1:A:976:G:OP1	14:N:31:ARG:O	2.39	0.41
1:A:1096:C:H2'	1:A:1097:C:C6	2.56	0.41
1:A:1195:C:H3'	1:A:1196:U:H5''	2.02	0.41
1:A:1203:C:OP1	14:N:2:ALA:HB3	2.20	0.41
1:A:1231:G:H5''	9:I:126:SER:HB3	2.01	0.41
1:A:1286:A:H2'	1:A:1287:A:O5'	2.21	0.41
1:A:1402:C:H2'	1:A:1403:C:H6	1.85	0.41
1:A:1404:C:H1'	1:A:1499:A:N1	2.35	0.41
2:B:15:VAL:HG11	2:B:210:SER:N	2.36	0.41
2:B:130:ARG:NH2	3:C:207:VAL:CG2	2.82	0.41
3:C:70:VAL:O	3:C:106:VAL:N	2.51	0.41
3:C:174:PRO:HB2	3:C:177:THR:CG2	2.50	0.41
3:C:191:THR:HG21	3:C:193:TYR:CE2	2.56	0.41
4:D:91:SER:O	4:D:92:VAL:C	2.64	0.41
4:D:167:GLY:O	4:D:168:ARG:C	2.63	0.41
5:E:36:ASP:OD1	5:E:38:GLN:N	2.39	0.41
5:E:119:LEU:HD23	5:E:119:LEU:HA	1.84	0.41
6:F:33:TYR:HA	6:F:71:ARG:NH2	2.36	0.41
6:F:78:GLU:HA	6:F:81:ILE:CD1	2.51	0.41
6:F:91:VAL:HG13	18:R:72:ARG:NH2	2.36	0.41
7:G:23:VAL:HG13	7:G:43:PHE:CE2	2.56	0.41
9:I:114:TYR:C	9:I:116:LYS:H	2.29	0.41
10:J:15:THR:HG23	10:J:94:VAL:CG2	2.48	0.41
10:J:53:PRO:HA	14:N:41:ARG:HH21	1.85	0.41
11:K:65:ALA:O	11:K:68:ALA:HB3	2.20	0.41
12:L:46:LYS:NZ	12:L:47:LYS:HE3	2.36	0.41
13:M:4:ILE:HG22	13:M:5:ALA:H	1.83	0.41
15:O:34:LEU:C	15:O:34:LEU:CD2	2.94	0.41
15:O:43:LEU:C	15:O:45:VAL:O	2.64	0.41
17:Q:97:SER:O	17:Q:99:SER:N	2.53	0.41
19:S:16:LEU:O	19:S:20:LEU:HG	2.21	0.41
1:A:836:G:C6	1:A:851:G:C6	3.09	0.41
1:A:883:C:O2'	1:A:884:U:H5'	2.21	0.41
1:A:942:G:C4	1:A:943:U:C6	3.09	0.41
1:A:948:C:O2'	1:A:949:A:H5'	2.21	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1057:G:H2'	1:A:1058:G:O4'	2.20	0.41
1:A:1110:A:O5'	1:A:1110:A:H8	2.04	0.41
1:A:1257:U:H4'	1:A:1258:G:C5'	2.50	0.41
2:B:134:GLU:HG2	2:B:137:ARG:HH21	1.86	0.41
3:C:67:THR:O	3:C:67:THR:HG22	2.21	0.41
3:C:79:ARG:NE	3:C:82:GLU:HG2	2.34	0.41
4:D:124:GLY:C	4:D:126:ILE:H	2.29	0.41
5:E:31:LEU:HD23	5:E:31:LEU:HA	1.74	0.41
7:G:104:LEU:HD23	7:G:134:ALA:HB1	2.03	0.41
11:K:67:ASP:OD2	11:K:71:LYS:HE3	2.21	0.41
12:L:55:VAL:CG1	12:L:67:THR:CG2	2.96	0.41
15:O:57:LEU:HD12	15:O:57:LEU:HA	1.86	0.41
15:O:74:ASP:OD1	15:O:76:GLU:HB3	2.21	0.41
15:O:81:LEU:HD22	15:O:85:LEU:HD12	2.02	0.41
1:A:19:C:O2'	1:A:20:U:H5'	2.20	0.40
1:A:190(L):U:H3	20:T:105:SER:HB2	1.87	0.40
1:A:502:G:H2'	1:A:503:C:C6	2.56	0.40
1:A:637:G:O2'	1:A:638:G:H5'	2.21	0.40
1:A:750:G:N3	15:O:23:GLY:HA3	2.37	0.40
1:A:913:A:O2'	1:A:914:A:O4'	2.27	0.40
1:A:919:A:O2'	1:A:920:U:H5'	2.22	0.40
1:A:1124:G:C8	1:A:1145:C:C5	3.09	0.40
1:A:1263:C:H2'	1:A:1264:C:C6	2.56	0.40
2:B:53:ARG:NH1	2:B:199:TYR:HD2	2.19	0.40
2:B:145:LEU:HA	2:B:145:LEU:HD23	1.84	0.40
2:B:217:ARG:C	2:B:219:VAL:N	2.78	0.40
3:C:57:ILE:O	3:C:57:ILE:HG22	2.20	0.40
3:C:65:ALA:O	3:C:66:VAL:HB	2.21	0.40
4:D:68:TYR:O	4:D:69:GLY:C	2.63	0.40
6:F:30:LEU:CB	6:F:35:ALA:HB3	2.41	0.40
7:G:41:ARG:O	7:G:42:ILE:C	2.64	0.40
8:H:29:SER:O	8:H:30:ARG:C	2.64	0.40
10:J:23:ILE:N	10:J:23:ILE:CD1	2.85	0.40
11:K:95:ILE:O	11:K:95:ILE:HG22	2.20	0.40
11:K:122:LYS:O	11:K:123:LYS:C	2.63	0.40
15:O:26:GLU:HG3	15:O:81:LEU:HG	2.03	0.40
16:P:34:GLU:HG2	16:P:35:LYS:N	2.36	0.40
17:Q:6:LEU:O	17:Q:58:GLU:HA	2.21	0.40
20:T:49:ALA:O	20:T:52:ALA:HB3	2.21	0.40
20:T:53:LEU:C	20:T:57:ARG:HD2	2.46	0.40
1:A:660:G:C2	1:A:746:A:C2	3.09	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:929:G:OP1	1:A:1533:C:N4	2.55	0.40
1:A:952:U:H2'	1:A:953:G:H8	1.85	0.40
1:A:973:G:H8	1:A:973:G:O5'	2.04	0.40
1:A:1138:G:N1	1:A:1140:C:C2	2.89	0.40
1:A:1331:G:HO2'	1:A:1332:A:P	2.44	0.40
1:A:1372:U:H5''	9:I:71:SER:CB	2.51	0.40
1:A:1428:A:H2'	1:A:1429:C:O4'	2.21	0.40
2:B:14:GLY:O	2:B:15:VAL:HG22	2.22	0.40
2:B:60:ASP:O	2:B:64:ARG:HB2	2.20	0.40
3:C:47:LEU:H	3:C:47:LEU:HD13	1.83	0.40
3:C:77:ILE:O	3:C:83:ARG:HB3	2.21	0.40
4:D:194:LEU:HD22	4:D:194:LEU:N	2.37	0.40
4:D:196:LEU:C	4:D:198:VAL:N	2.79	0.40
5:E:118:ILE:HG21	5:E:118:ILE:HD13	1.74	0.40
6:F:74:ASP:O	6:F:75:LEU:C	2.64	0.40
8:H:19:VAL:CG2	8:H:21:LYS:HD3	2.52	0.40
8:H:89:PRO:HA	8:H:92:ARG:NH1	2.37	0.40
10:J:28:ARG:C	10:J:29:ARG:HG3	2.46	0.40
12:L:55:VAL:CG1	12:L:56:ALA:N	2.83	0.40
15:O:74:ASP:CG	15:O:77:ARG:HG3	2.46	0.40
18:R:44:LEU:HD22	18:R:48:GLY:O	2.21	0.40
1:A:359:U:H2'	1:A:360:A:C8	2.57	0.40
1:A:547:A:OP2	4:D:2:GLY:N	2.54	0.40
1:A:567:G:H2'	1:A:568:G:O4'	2.21	0.40
1:A:818:G:H3'	1:A:819:A:H5'	2.01	0.40
1:A:1003(A):G:H2'	1:A:1004:A:H4'	2.03	0.40
1:A:1028:C:H2'	1:A:1029:C:H6	1.84	0.40
1:A:1118:C:H1'	1:A:1179:A:C4	2.56	0.40
1:A:1355:G:O2'	1:A:1356:G:H5'	2.21	0.40
1:A:1392:G:H2'	1:A:1393:U:H6	1.86	0.40
2:B:216:SER:OG	2:B:217:ARG:N	2.54	0.40
4:D:8:VAL:C	4:D:10:ARG:N	2.79	0.40
4:D:58:LEU:HD23	4:D:206:PHE:CE1	2.57	0.40
8:H:111:ILE:O	8:H:134:ILE:HB	2.20	0.40
9:I:20:ARG:O	9:I:21:PRO:C	2.64	0.40
10:J:44:VAL:HG11	10:J:46:ARG:NH1	2.37	0.40
10:J:65:LEU:HD12	14:N:56:VAL:HG22	2.04	0.40
17:Q:92:ARG:O	17:Q:95:TYR:HB2	2.21	0.40
18:R:26:LEU:CD1	18:R:27:GLY:H	2.29	0.40
19:S:77:THR:HG22	19:S:78:ARG:N	2.36	0.40
1:A:16:A:C2'	1:A:17:U:H5'	2.51	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:458:C:H2'	1:A:459:G:C8	2.57	0.40
1:A:671:G:H2'	1:A:672:U:O4'	2.22	0.40
1:A:715:A:H2'	1:A:716:A:C8	2.57	0.40
1:A:769:G:H4'	1:A:1513:A:H4'	2.03	0.40
1:A:939:G:C6	1:A:940:C:N4	2.89	0.40
1:A:965:A:O2'	1:A:966:G:P	2.80	0.40
1:A:1298:C:H2'	7:G:114:ARG:HH12	1.86	0.40
1:A:1327:C:H5''	21:V:20:LYS:HB3	2.04	0.40
2:B:14:GLY:O	2:B:15:VAL:CG2	2.69	0.40
2:B:134:GLU:O	2:B:138:LEU:HG	2.21	0.40
3:C:33:LEU:C	3:C:33:LEU:CD2	2.94	0.40
3:C:126:ARG:O	3:C:127:ARG:HB2	2.22	0.40
5:E:143:ARG:NH1	8:H:77:GLU:CD	2.80	0.40
6:F:48:LEU:HD13	6:F:52:ILE:CD1	2.51	0.40
10:J:59:SER:O	10:J:60:ARG:HB2	2.21	0.40
12:L:43:VAL:CG1	12:L:44:THR:N	2.81	0.40
13:M:91:ARG:HD2	13:M:91:ARG:HA	1.85	0.40
13:M:96:LEU:O	13:M:110:ARG:NH1	2.54	0.40
14:N:39:LEU:HD11	14:N:47:LEU:HD12	2.02	0.40
15:O:70:LEU:O	15:O:71:GLN:C	2.64	0.40
19:S:67:VAL:HG12	19:S:68:GLY:N	2.35	0.40
1:A:155:C:H2'	1:A:156:G:C8	2.57	0.40
1:A:176:C:H2'	1:A:177:C:C6	2.56	0.40
1:A:330:C:H6	1:A:330:C:H5''	1.86	0.40
1:A:815:A:N3	1:A:1527:C:O2'	2.44	0.40
1:A:1116:C:H2'	1:A:1117:G:C5'	2.34	0.40
1:A:1312:G:N7	19:S:4:SER:HB3	2.36	0.40
1:A:1372:U:H5''	9:I:71:SER:HB2	2.04	0.40
1:A:1437:C:H2'	1:A:1438:G:H8	1.86	0.40
2:B:33:TYR:O	2:B:34:ALA:CB	2.67	0.40
2:B:130:ARG:HB3	2:B:134:GLU:OE1	2.20	0.40
2:B:154:LEU:O	2:B:155:LEU:C	2.65	0.40
2:B:208:ILE:O	2:B:209:ARG:C	2.64	0.40
3:C:70:VAL:C	3:C:106:VAL:HG23	2.46	0.40
3:C:110:ASN:OD1	3:C:140:ARG:HB3	2.21	0.40
5:E:118:ILE:HG22	5:E:119:LEU:O	2.21	0.40
10:J:94:VAL:CG1	10:J:95:GLU:H	2.35	0.40
13:M:37:THR:HG23	13:M:55:ARG:HB2	2.04	0.40
13:M:63:THR:HG23	13:M:64:TRP:CD2	2.56	0.40
13:M:69:GLU:O	13:M:72:ALA:HB3	2.21	0.40
14:N:3:ARG:NH1	14:N:6:LEU:CD1	2.84	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:T:23:ARG:HG2	20:T:23:ARG:NH1	2.36	0.40
20:T:68:LYS:HD2	20:T:68:LYS:HA	1.92	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 X-ray entries followed by that with respect to entries of similar resolution.

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	232/256 (91%)	174 (75%)	34 (15%)	24 (10%)	0	6
3	C	204/239 (85%)	135 (66%)	41 (20%)	28 (14%)	0	3
4	D	206/208 (99%)	166 (81%)	31 (15%)	9 (4%)	2	19
5	E	148/161 (92%)	130 (88%)	13 (9%)	5 (3%)	3	23
6	F	99/101 (98%)	79 (80%)	19 (19%)	1 (1%)	12	43
7	G	153/155 (99%)	127 (83%)	16 (10%)	10 (6%)	1	14
8	H	136/138 (99%)	125 (92%)	7 (5%)	4 (3%)	3	25
9	I	125/128 (98%)	88 (70%)	27 (22%)	10 (8%)	1	10
10	J	96/104 (92%)	59 (62%)	20 (21%)	17 (18%)	0	2
11	K	117/129 (91%)	88 (75%)	20 (17%)	9 (8%)	1	11
12	L	122/131 (93%)	97 (80%)	16 (13%)	9 (7%)	1	11
13	M	123/126 (98%)	88 (72%)	27 (22%)	8 (6%)	1	14
14	N	58/60 (97%)	40 (69%)	11 (19%)	7 (12%)	0	4
15	O	86/88 (98%)	70 (81%)	11 (13%)	5 (6%)	1	15
16	P	81/88 (92%)	65 (80%)	15 (18%)	1 (1%)	10	40
17	Q	102/104 (98%)	84 (82%)	10 (10%)	8 (8%)	1	11
18	R	71/88 (81%)	62 (87%)	7 (10%)	2 (3%)	4	26
19	S	78/92 (85%)	49 (63%)	18 (23%)	11 (14%)	0	3

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
20	T	97/106 (92%)	63 (65%)	21 (22%)	13 (13%)	0	3
21	V	22/26 (85%)	19 (86%)	2 (9%)	1 (4%)	2	18
22	Y	217/222 (98%)	206 (95%)	6 (3%)	5 (2%)	5	30
All	All	2573/2750 (94%)	2014 (78%)	372 (14%)	187 (7%)	1	11

All (187) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	9	GLU
2	B	15	VAL
2	B	16	HIS
2	B	17	PHE
2	B	21	ARG
2	B	24	TRP
3	C	4	LYS
3	C	15	THR
3	C	16	ARG
3	C	26	LYS
3	C	47	LEU
3	C	61	ALA
3	C	62	ASP
3	C	97	LYS
3	C	101	LEU
3	C	146	ALA
3	C	154	SER
3	C	179	ARG
3	C	189	ALA
4	D	29	PRO
4	D	36	ARG
5	E	16	THR
5	E	153	LYS
7	G	7	ALA
7	G	155	ARG
8	H	24	THR
8	H	83	ILE
8	H	91	ARG
9	I	58	HIS
9	I	88	TYR
10	J	32	ALA
10	J	39	PRO
10	J	54	PHE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
10	J	57	LYS
10	J	79	ARG
10	J	86	MET
11	K	57	THR
11	K	127	LYS
12	L	27	LEU
12	L	28	LYS
12	L	47	LYS
13	M	63	THR
13	M	67	GLU
13	M	121	LYS
13	M	122	LYS
13	M	124	PRO
14	N	22	THR
14	N	29	ARG
15	O	88	ARG
17	Q	69	LYS
17	Q	80	GLY
17	Q	81	ARG
17	Q	96	GLU
17	Q	98	LEU
17	Q	104	LYS
18	R	87	ARG
19	S	6	LYS
19	S	71	LEU
20	T	11	SER
20	T	73	HIS
22	Y	143	ASP
2	B	8	LYS
2	B	18	GLY
2	B	20	GLU
2	B	97	TRP
2	B	123	ALA
2	B	232	PRO
3	C	29	TYR
3	C	156	ARG
3	C	168	ALA
3	C	181	ASN
3	C	206	GLU
4	D	4	TYR
4	D	26	CYS
4	D	88	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
4	D	125	HIS
4	D	175	SER
5	E	22	GLY
5	E	104	ALA
6	F	37	VAL
7	G	52	GLU
9	I	41	VAL
10	J	30	SER
10	J	34	VAL
10	J	40	LEU
10	J	72	VAL
11	K	15	ALA
11	K	49	GLY
11	K	50	TYR
11	K	89	ALA
12	L	41	ARG
12	L	48	PRO
12	L	51	ALA
12	L	116	SER
12	L	121	GLY
13	M	6	GLY
13	M	85	GLY
16	P	10	GLY
18	R	20	ALA
19	S	9	VAL
19	S	45	VAL
19	S	67	VAL
19	S	68	GLY
20	T	9	ASN
20	T	49	ALA
20	T	50	GLU
20	T	95	ALA
20	T	99	LEU
20	T	102	GLY
2	B	26	PRO
2	B	60	ASP
2	B	83	MET
2	B	89	GLY
2	B	204	ASN
5	E	65	ASN
7	G	5	ARG
8	H	127	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
9	I	56	LEU
10	J	19	SER
10	J	60	ARG
10	J	61	GLU
10	J	90	LEU
11	K	35	PRO
11	K	101	SER
12	L	49	ASN
14	N	13	THR
14	N	23	ARG
17	Q	97	SER
19	S	28	LYS
19	S	30	LEU
19	S	32	LYS
20	T	74	LYS
20	T	83	ARG
22	Y	144	SER
22	Y	155	LEU
2	B	126	GLU
2	B	165	VAL
3	C	39	ILE
3	C	100	ALA
3	C	188	LEU
7	G	4	ARG
7	G	81	GLY
7	G	112	PRO
9	I	7	THR
9	I	12	GLU
9	I	119	ALA
13	M	123	ALA
14	N	12	ARG
14	N	60	SER
15	O	16	ALA
17	Q	33	GLY
21	V	3	LYS
22	Y	148	ALA
2	B	155	LEU
3	C	24	ALA
3	C	66	VAL
3	C	127	ARG
4	D	123	HIS
7	G	53	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
9	I	121	ARG
14	N	36	PHE
15	O	84	LYS
19	S	31	ILE
2	B	127	ILE
3	C	108	ASN
3	C	174	PRO
4	D	5	ILE
9	I	43	ALA
10	J	26	ALA
22	Y	152	LYS
2	B	124	SER
2	B	214	ILE
7	G	14	PRO
10	J	82	ILE
20	T	98	PRO
2	B	125	PRO
3	C	76	VAL
3	C	77	ILE
7	G	17	VAL
10	J	36	GLY
15	O	82	ILE
19	S	8	GLY
9	I	44	VAL
15	O	19	PRO
20	T	96	GLY
20	T	101	GLY
11	K	90	GLY

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	B	202/220 (92%)	184 (91%)	18 (9%)	9	32
3	C	160/188 (85%)	141 (88%)	19 (12%)	5	22
4	D	180/180 (100%)	169 (94%)	11 (6%)	17	43

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	E	115/122 (94%)	98 (85%)	17 (15%)	3	16
6	F	90/90 (100%)	85 (94%)	5 (6%)	19	45
7	G	126/126 (100%)	121 (96%)	5 (4%)	28	52
8	H	119/119 (100%)	107 (90%)	12 (10%)	7	27
9	I	98/99 (99%)	91 (93%)	7 (7%)	13	39
10	J	86/91 (94%)	77 (90%)	9 (10%)	6	26
11	K	90/99 (91%)	83 (92%)	7 (8%)	11	36
12	L	104/108 (96%)	95 (91%)	9 (9%)	9	33
13	M	100/101 (99%)	92 (92%)	8 (8%)	11	36
14	N	49/49 (100%)	47 (96%)	2 (4%)	27	51
15	O	79/79 (100%)	72 (91%)	7 (9%)	9	32
16	P	72/74 (97%)	67 (93%)	5 (7%)	14	40
17	Q	96/96 (100%)	90 (94%)	6 (6%)	16	42
18	R	64/77 (83%)	60 (94%)	4 (6%)	16	42
19	S	71/79 (90%)	70 (99%)	1 (1%)	59	70
20	T	76/82 (93%)	69 (91%)	7 (9%)	8	31
21	V	19/21 (90%)	19 (100%)	0	100	100
22	Y	193/195 (99%)	186 (96%)	7 (4%)	31	54
All	All	2189/2295 (95%)	2023 (92%)	166 (8%)	12	37

All (166) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	12	GLU
2	B	17	PHE
2	B	23	ARG
2	B	41	ILE
2	B	75	LYS
2	B	87	ARG
2	B	139	LYS
2	B	146	GLN
2	B	155	LEU
2	B	164	VAL
2	B	165	VAL
2	B	170	GLU
2	B	178	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	187	LEU
2	B	213	LEU
2	B	221	LEU
2	B	231	GLU
2	B	232	PRO
3	C	3	ASN
3	C	5	ILE
3	C	34	LEU
3	C	47	LEU
3	C	64	VAL
3	C	70	VAL
3	C	75	VAL
3	C	82	GLU
3	C	91	LEU
3	C	99	VAL
3	C	107	GLN
3	C	110	ASN
3	C	116	VAL
3	C	130	VAL
3	C	164	ARG
3	C	167	TRP
3	C	175	LEU
3	C	188	LEU
3	C	204	LEU
4	D	15	GLU
4	D	29	PRO
4	D	34	GLU
4	D	70	ILE
4	D	122	ARG
4	D	127	THR
4	D	157	LEU
4	D	162	LEU
4	D	170	VAL
4	D	192	GLU
4	D	194	LEU
5	E	10	MET
5	E	12	LEU
5	E	18	ARG
5	E	26	PHE
5	E	31	LEU
5	E	38	GLN
5	E	41	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
5	E	43	LEU
5	E	53	LEU
5	E	56	GLN
5	E	65	ASN
5	E	68	GLU
5	E	79	GLU
5	E	80	ILE
5	E	89	ILE
5	E	120	THR
5	E	150	ARG
6	F	10	LEU
6	F	37	VAL
6	F	43	LEU
6	F	69	GLU
6	F	100	ASN
7	G	8	GLU
7	G	11	GLN
7	G	38	LEU
7	G	113	GLU
7	G	146	GLU
8	H	2	LEU
8	H	21	LYS
8	H	26	VAL
8	H	39	LEU
8	H	52	ASP
8	H	63	LEU
8	H	85	ARG
8	H	92	ARG
8	H	105	ARG
8	H	112	LEU
8	H	119	LEU
8	H	127	LEU
9	I	2	GLU
9	I	29	ASN
9	I	38	GLN
9	I	53	VAL
9	I	78	LYS
9	I	79	LEU
9	I	111	ARG
10	J	6	ILE
10	J	15	THR
10	J	16	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
10	J	45	ARG
10	J	64	GLU
10	J	71	LEU
10	J	73	ASP
10	J	83	GLU
10	J	95	GLU
11	K	24	SER
11	K	29	ILE
11	K	35	PRO
11	K	54	ARG
11	K	80	VAL
11	K	84	VAL
11	K	92	GLU
12	L	7	ILE
12	L	17	LYS
12	L	33	ARG
12	L	53	ARG
12	L	60	LEU
12	L	81	SER
12	L	96	VAL
12	L	113	ARG
12	L	126	LYS
13	M	9	ILE
13	M	12	ASN
13	M	16	ASP
13	M	70	LEU
13	M	81	LEU
13	M	102	ARG
13	M	110	ARG
13	M	124	PRO
14	N	41	ARG
14	N	44	LEU
15	O	6	GLU
15	O	7	GLU
15	O	39	LEU
15	O	57	LEU
15	O	70	LEU
15	O	81	LEU
15	O	83	GLU
16	P	2	VAL
16	P	8	ARG
16	P	20	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
16	P	53	VAL
16	P	62	VAL
17	Q	34	LYS
17	Q	38	ARG
17	Q	60	ILE
17	Q	68	ARG
17	Q	74	LEU
17	Q	98	LEU
18	R	38	GLU
18	R	41	LYS
18	R	55	ARG
18	R	75	ILE
19	S	43	GLU
20	T	10	LEU
20	T	25	ARG
20	T	39	LYS
20	T	57	ARG
20	T	73	HIS
20	T	84	LEU
20	T	86	ARG
22	Y	25	ASP
22	Y	101	ILE
22	Y	119	ARG
22	Y	155	LEU
22	Y	158	LEU
22	Y	172	LEU
22	Y	196	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	94	ASN
2	B	240	GLN
3	C	104	GLN
3	C	107	GLN
5	E	38	GLN
9	I	58	HIS
10	J	56	HIS
10	J	69	ASN
12	L	8	ASN
13	M	77	ASN
20	T	18	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
22	Y	134	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	1507/1513 (99%)	230 (15%)	90 (5%)

All (230) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	6	G
1	A	8	A
1	A	9	G
1	A	31	G
1	A	32	A
1	A	39	G
1	A	48	C
1	A	49	U
1	A	51	A
1	A	52	G
1	A	61	G
1	A	81	U
1	A	101	A
1	A	116	A
1	A	120	A
1	A	121	C
1	A	129(A)	G
1	A	130	A
1	A	131	C
1	A	182	U
1	A	190(D)	U
1	A	190(E)	U
1	A	190(F)	G
1	A	195	A
1	A	197	A
1	A	198	G
1	A	202	U
1	A	203	U
1	A	204	U
1	A	216	G
1	A	244	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	247	G
1	A	251	G
1	A	252	U
1	A	266	G
1	A	267	C
1	A	280	C
1	A	282	A
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	344	A
1	A	345	C
1	A	352	C
1	A	353	A
1	A	354	G
1	A	367	U
1	A	373	A
1	A	397	A
1	A	398	C
1	A	412	A
1	A	413	G
1	A	421	U
1	A	428	G
1	A	429	U
1	A	430	A
1	A	439	A
1	A	460	A
1	A	461	C
1	A	462	G
1	A	481	G
1	A	484	G
1	A	485	G
1	A	497	A
1	A	498	U
1	A	509	A
1	A	510	A
1	A	511	C
1	A	518	C
1	A	519	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	527	G
1	A	532	A
1	A	533	A
1	A	534	U
1	A	547	A
1	A	559	A
1	A	560	U
1	A	561	U
1	A	562	C
1	A	572	A
1	A	573	A
1	A	575	G
1	A	576	G
1	A	577	G
1	A	588	G
1	A	653	A
1	A	665	A
1	A	686	U
1	A	687	A
1	A	688	G
1	A	702	A
1	A	703	G
1	A	718	G
1	A	723	U
1	A	731	G
1	A	749	C
1	A	755	G
1	A	777	A
1	A	781	A
1	A	782	A
1	A	793	U
1	A	794	A
1	A	813	U
1	A	815	A
1	A	817	C
1	A	819	A
1	A	828	A
1	A	839	U
1	A	840	C
1	A	841	U
1	A	858	G
1	A	902	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	913	A
1	A	914	A
1	A	926	G
1	A	927	G
1	A	934	C
1	A	935	A
1	A	943	U
1	A	945	G
1	A	960	U
1	A	961	U
1	A	966	G
1	A	969	A
1	A	971	G
1	A	974	A
1	A	975	A
1	A	976	G
1	A	977	A
1	A	991	U
1	A	992	U
1	A	993	G
1	A	994	A
1	A	1004	A
1	A	1005	A
1	A	1023	G
1	A	1026	G
1	A	1050	G
1	A	1053	G
1	A	1065	U
1	A	1066	C
1	A	1067	A
1	A	1068	G
1	A	1085	U
1	A	1086	U
1	A	1094	G
1	A	1095	U
1	A	1101	A
1	A	1102	A
1	A	1117	G
1	A	1124	G
1	A	1125	U
1	A	1126	U
1	A	1129	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	1130	A
1	A	1131	G
1	A	1137	C
1	A	1138	G
1	A	1139	G
1	A	1140	C
1	A	1145	C
1	A	1146	A
1	A	1152	A
1	A	1157	A
1	A	1159	U
1	A	1183	A
1	A	1184	G
1	A	1191	A
1	A	1196	U
1	A	1197	G
1	A	1201	A
1	A	1202	G
1	A	1211	U
1	A	1212	U
1	A	1215	G
1	A	1225	A
1	A	1226	C
1	A	1227	A
1	A	1238	A
1	A	1257	U
1	A	1258	G
1	A	1279	A
1	A	1280	A
1	A	1281	U
1	A	1282	C
1	A	1285	A
1	A	1286	A
1	A	1287	A
1	A	1299	A
1	A	1300	G
1	A	1301	U
1	A	1302	U
1	A	1303	C
1	A	1305	G
1	A	1320	C
1	A	1332	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	1347	G
1	A	1348	U
1	A	1363	A
1	A	1364	U
1	A	1365	G
1	A	1381	U
1	A	1394	A
1	A	1398	A
1	A	1405	G
1	A	1406	U
1	A	1408	A
1	A	1409	C
1	A	1410	G
1	A	1414	U
1	A	1419	G
1	A	1422	G
1	A	1442	G
1	A	1443	G
1	A	1446	A
1	A	1447	G
1	A	1452	C
1	A	1490	C
1	A	1499	A
1	A	1502	A
1	A	1504	G
1	A	1505	G
1	A	1506	U
1	A	1517	G
1	A	1520	G
1	A	1529	G
1	A	1530	G

All (90) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	5	U
1	A	7	G
1	A	30	U
1	A	48	C
1	A	51	A
1	A	60	A
1	A	115	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	119	A
1	A	129(A)	G
1	A	181	G
1	A	197	A
1	A	202	U
1	A	203	U
1	A	204	U
1	A	243	A
1	A	250	A
1	A	251	G
1	A	266	G
1	A	279	A
1	A	281	G
1	A	328	C
1	A	329	A
1	A	344	A
1	A	351	G
1	A	353	A
1	A	366	C
1	A	372	C
1	A	428	G
1	A	429	U
1	A	438	G
1	A	484	G
1	A	496	A
1	A	497	A
1	A	509	A
1	A	518	C
1	A	533	A
1	A	559	A
1	A	560	U
1	A	575	G
1	A	576	G
1	A	687	A
1	A	701	C
1	A	748	C
1	A	792	A
1	A	812	C
1	A	840	C
1	A	913	A
1	A	960	U
1	A	965	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	975	A
1	A	976	G
1	A	992	U
1	A	993	G
1	A	1049	U
1	A	1065	U
1	A	1067	A
1	A	1085	U
1	A	1101	A
1	A	1129	C
1	A	1145	C
1	A	1182	G
1	A	1183	A
1	A	1190	G
1	A	1196	U
1	A	1201	A
1	A	1214	C
1	A	1224	G
1	A	1226	C
1	A	1256	A
1	A	1257	U
1	A	1278	U
1	A	1281	U
1	A	1285	A
1	A	1300	G
1	A	1301	U
1	A	1302	U
1	A	1319	A
1	A	1331	G
1	A	1346	A
1	A	1347	G
1	A	1364	U
1	A	1380	U
1	A	1397	C
1	A	1409	C
1	A	1451	A
1	A	1498	U
1	A	1503	A
1	A	1504	G
1	A	1505	G
1	A	1528	U

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 123 ligands modelled in this entry, 122 are monoatomic - leaving 1 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
25	SFG	Y	301	-	28,29,29	0.82	0	34,42,42	1.99	7 (20%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	SFG	Y	301	-	-	4/17/33/33	0/3/3/3

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	Y	301	SFG	C5-C4-N3	-5.60	119.01	126.72
25	Y	301	SFG	N3-C4-N9	4.53	134.87	127.17
25	Y	301	SFG	N3-C2-N1	-4.06	122.44	128.58
25	Y	301	SFG	C5-N7-C8	3.81	109.43	103.45
25	Y	301	SFG	C2-N3-C4	3.63	120.70	111.83
25	Y	301	SFG	C4-C5-N7	-3.04	107.11	110.58
25	Y	301	SFG	N9-C8-N7	-2.78	110.00	113.94

There are no chirality outliers.

All (4) torsion outliers are listed below:

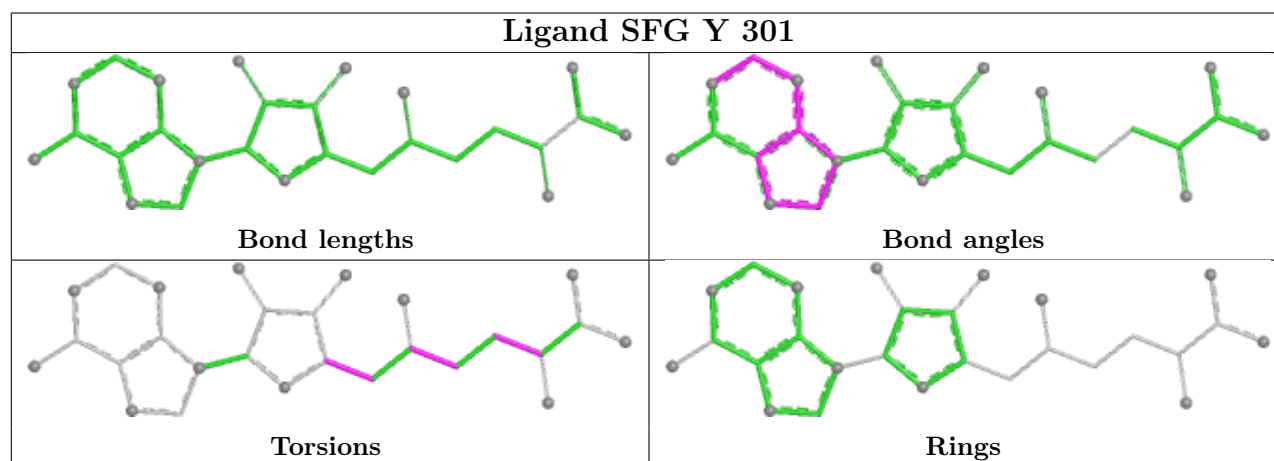
Mol	Chain	Res	Type	Atoms
25	Y	301	SFG	C5'-CD-CG-CB
25	Y	301	SFG	N-CA-CB-CG
25	Y	301	SFG	C-CA-CB-CG
25	Y	301	SFG	C3'-C4'-C5'-CD

There are no ring outliers.

1 monomer is involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
25	Y	301	SFG	4	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	1507/1513 (99%)	0.43	95 (6%) 26 21	18, 71, 170, 260	0
2	B	234/256 (91%)	0.72	25 (10%) 11 14	29, 94, 152, 190	0
3	C	206/239 (86%)	0.72	26 (12%) 8 11	44, 104, 145, 171	0
4	D	208/208 (100%)	0.74	21 (10%) 12 14	25, 79, 127, 182	0
5	E	150/161 (93%)	0.23	5 (3%) 49 34	18, 56, 106, 148	0
6	F	101/101 (100%)	0.53	8 (7%) 18 17	48, 103, 142, 156	0
7	G	155/155 (100%)	0.37	9 (5%) 29 23	40, 96, 148, 172	0
8	H	138/138 (100%)	0.40	5 (3%) 46 32	11, 41, 81, 116	0
9	I	127/128 (99%)	1.04	24 (18%) 3 5	40, 105, 144, 165	0
10	J	98/104 (94%)	1.15	17 (17%) 4 6	55, 123, 165, 188	0
11	K	119/129 (92%)	0.79	11 (9%) 14 16	36, 81, 129, 171	0
12	L	124/131 (94%)	1.09	24 (19%) 3 5	18, 74, 120, 165	0
13	M	125/126 (99%)	0.95	18 (14%) 6 9	56, 97, 137, 185	0
14	N	60/60 (100%)	1.64	21 (35%) 1 1	44, 102, 136, 160	0
15	O	88/88 (100%)	0.63	8 (9%) 15 16	17, 63, 122, 167	0
16	P	83/88 (94%)	0.73	10 (12%) 9 12	21, 56, 95, 122	0
17	Q	104/104 (100%)	0.66	8 (7%) 19 18	13, 56, 119, 198	0
18	R	73/88 (82%)	0.83	6 (8%) 17 17	35, 82, 143, 191	0
19	S	80/92 (86%)	0.83	9 (11%) 10 13	73, 124, 155, 197	0
20	T	99/106 (93%)	1.00	15 (15%) 5 8	38, 80, 118, 156	0
21	V	24/26 (92%)	2.27	9 (37%) 1 1	51, 88, 137, 141	0
22	Y	219/222 (98%)	0.75	23 (10%) 11 14	64, 119, 160, 196	0
All	All	4122/4263 (96%)	0.64	397 (9%) 13 15	11, 82, 153, 260	0

All (397) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
13	M	124	PRO	9.3
1	A	1492	A	8.3
14	N	22	THR	8.1
2	B	133	LYS	6.7
11	K	127	LYS	6.4
4	D	49	ARG	6.2
21	V	25	LYS	6.1
14	N	44	LEU	6.1
12	L	19	ARG	5.9
4	D	3	ARG	5.9
3	C	201	TYR	5.8
6	F	95	GLU	5.8
13	M	123	ALA	5.8
9	I	105	ASP	5.6
3	C	15	THR	5.5
10	J	57	LYS	5.5
22	Y	82	PHE	5.4
13	M	104	ARG	5.4
11	K	129	SER	5.4
19	S	3	ARG	5.3
19	S	37	ARG	5.3
17	Q	104	LYS	5.1
10	J	64	GLU	5.0
21	V	24	ARG	5.0
1	A	1237	C	5.0
9	I	65	VAL	4.9
1	A	1493	A	4.8
1	A	1031	G	4.8
4	D	31	CYS	4.8
10	J	46	ARG	4.7
2	B	16	HIS	4.7
9	I	110	GLU	4.7
12	L	89	ARG	4.7
13	M	122	LYS	4.7
9	I	128	ARG	4.7
21	V	6	ARG	4.7
20	T	103	GLY	4.5
3	C	182	ILE	4.5
22	Y	63	ASP	4.4
2	B	218	ALA	4.4
11	K	42	TRP	4.4
22	Y	35	ASP	4.4
15	O	7	GLU	4.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
3	C	10	PHE	4.3
11	K	128	ALA	4.3
2	B	7	VAL	4.3
14	N	13	THR	4.2
2	B	215	LEU	4.2
12	L	16	GLU	4.1
1	A	306	G	4.1
14	N	11	LYS	4.1
18	R	31	LEU	4.0
15	O	54	ARG	4.0
1	A	1491	G	4.0
4	D	9	CYS	4.0
14	N	20	ALA	4.0
1	A	264	U	3.9
10	J	58	ASP	3.9
14	N	10	ALA	3.9
22	Y	4	LEU	3.9
22	Y	111	LEU	3.8
9	I	15	ALA	3.8
6	F	89	MET	3.8
1	A	1125	U	3.8
1	A	1484	C	3.8
12	L	114	LYS	3.8
1	A	1030(D)	A	3.8
1	A	1418	A	3.8
22	Y	3	ILE	3.8
9	I	75	ASP	3.8
5	E	81	GLU	3.8
3	C	188	LEU	3.7
12	L	21	LYS	3.7
4	D	77	ASN	3.7
13	M	113	PRO	3.7
12	L	128	ALA	3.7
3	C	207	VAL	3.7
1	A	203	U	3.6
1	A	1517	G	3.6
21	V	9	ARG	3.6
18	R	72	ARG	3.6
21	V	23	PRO	3.6
9	I	106	ALA	3.6
9	I	103	THR	3.6
22	Y	38	ASN	3.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	1519	A	3.6
18	R	43	PHE	3.5
7	G	34	GLY	3.5
1	A	1126	U	3.5
20	T	64	ASP	3.5
21	V	10	ARG	3.5
3	C	190	ARG	3.5
4	D	144	ASP	3.5
1	A	1359	C	3.5
10	J	47	PHE	3.5
10	J	63	PHE	3.5
1	A	793	U	3.4
1	A	1494	G	3.4
4	D	187	ARG	3.4
19	S	2	PRO	3.4
1	A	532	A	3.4
14	N	2	ALA	3.4
1	A	1419	G	3.4
3	C	198	VAL	3.4
11	K	111	ASP	3.4
9	I	102	LEU	3.4
13	M	15	VAL	3.4
7	G	5	ARG	3.4
8	H	84	ARG	3.4
12	L	33	ARG	3.4
4	D	26	CYS	3.3
3	C	151	VAL	3.3
1	A	1331	G	3.3
12	L	20	LYS	3.3
22	Y	139	THR	3.3
1	A	1405	G	3.3
4	D	72	GLU	3.3
22	Y	193	PHE	3.3
2	B	214	ILE	3.3
12	L	47	LYS	3.3
1	A	994	A	3.3
20	T	74	LYS	3.3
12	L	125	PRO	3.2
2	B	179	LYS	3.2
2	B	211	ILE	3.2
17	Q	68	ARG	3.2
20	T	12	ALA	3.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	B	182	ILE	3.2
1	A	1281	U	3.2
18	R	48	GLY	3.2
9	I	10	ARG	3.2
1	A	1054	C	3.2
1	A	1395	C	3.2
14	N	18	VAL	3.2
4	D	73	ARG	3.1
15	O	89	GLY	3.1
12	L	28	LYS	3.1
21	V	11	GLY	3.1
1	A	1482	G	3.1
10	J	37	PRO	3.1
16	P	1	MET	3.1
20	T	56	MET	3.1
1	A	1397	C	3.1
12	L	115	LYS	3.1
14	N	12	ARG	3.1
6	F	65	VAL	3.1
13	M	102	ARG	3.1
16	P	19	ILE	3.0
20	T	86	ARG	3.0
1	A	1304	G	3.0
7	G	82	GLY	3.0
1	A	1394	A	3.0
3	C	158	GLY	3.0
6	F	57	GLN	3.0
12	L	23	LYS	3.0
10	J	20	ALA	3.0
7	G	85	TYR	3.0
14	N	45	ARG	3.0
12	L	7	ILE	3.0
1	A	1346	A	3.0
1	A	1531	A	3.0
3	C	178	LEU	3.0
19	S	79	THR	3.0
2	B	131	PRO	2.9
22	Y	192	GLN	2.9
1	A	733	A	2.9
8	H	18	ARG	2.9
12	L	18	VAL	2.9
2	B	156	LYS	2.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	B	180	LEU	2.9
16	P	29	ASP	2.9
18	R	34	TYR	2.9
4	D	80	GLU	2.9
13	M	126	LYS	2.9
9	I	58	HIS	2.9
11	K	110	ASP	2.9
20	T	22	ARG	2.9
1	A	1250	A	2.8
5	E	108	ALA	2.8
1	A	307	C	2.8
13	M	31	LYS	2.8
10	J	24	VAL	2.8
22	Y	1	MET	2.8
6	F	46	ARG	2.8
3	C	150	LYS	2.8
22	Y	12	LEU	2.8
10	J	75	ILE	2.8
1	A	136	C	2.8
1	A	265	G	2.8
1	A	1236	A	2.7
9	I	117	HIS	2.7
6	F	49	ALA	2.7
1	A	314	C	2.7
12	L	127	GLU	2.7
1	A	971	G	2.7
1	A	1481	U	2.7
14	N	14	PRO	2.7
13	M	8	GLU	2.7
19	S	65	ASN	2.7
2	B	140	HIS	2.6
16	P	68	ASP	2.6
2	B	61	LEU	2.6
22	Y	138	VAL	2.6
13	M	6	GLY	2.6
3	C	184	TYR	2.6
13	M	35	GLU	2.6
1	A	572	A	2.6
12	L	126	LYS	2.6
14	N	9	LYS	2.6
17	Q	13	ASP	2.6
1	A	661	G	2.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
13	M	125	ARG	2.6
14	N	57	ARG	2.6
9	I	95	LYS	2.6
13	M	100	GLY	2.6
1	A	263	A	2.6
1	A	1212	U	2.6
9	I	99	LEU	2.6
1	A	666	G	2.6
10	J	82	ILE	2.6
12	L	85	ILE	2.6
4	D	2	GLY	2.6
7	G	79	ARG	2.5
11	K	11	LYS	2.5
12	L	22	SER	2.5
16	P	50	LYS	2.5
7	G	4	ARG	2.5
9	I	109	VAL	2.5
1	A	259	G	2.5
1	A	942	G	2.5
1	A	1129	C	2.5
22	Y	105	PHE	2.5
17	Q	103	GLY	2.5
1	A	924	C	2.5
1	A	1161	C	2.5
10	J	45	ARG	2.5
20	T	85	MET	2.5
19	S	41	VAL	2.5
20	T	68	LYS	2.4
2	B	155	LEU	2.4
3	C	196	LEU	2.4
10	J	66	ARG	2.4
1	A	1017	G	2.4
1	A	1483	A	2.4
17	Q	32	TYR	2.4
8	H	136	GLU	2.4
20	T	27	LYS	2.4
19	S	57	HIS	2.4
2	B	188	ALA	2.4
3	C	180	ALA	2.4
14	N	35	ARG	2.4
1	A	1363	A	2.4
1	A	1398	A	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	B	148	TYR	2.4
3	C	206	GLU	2.4
4	D	93	PHE	2.4
22	Y	125	VAL	2.4
20	T	36	LEU	2.4
1	A	1249	C	2.4
5	E	83	GLU	2.4
1	A	1497	G	2.4
15	O	31	LEU	2.4
7	G	39	ALA	2.4
14	N	30	ALA	2.4
22	Y	87	ALA	2.4
16	P	27	LYS	2.4
1	A	1218	C	2.3
1	A	1223	C	2.3
1	A	1286	A	2.3
1	A	1384	C	2.3
1	A	1490	C	2.3
22	Y	61	LEU	2.3
1	A	1480	G	2.3
10	J	7	LYS	2.3
17	Q	14	LYS	2.3
12	L	30	ALA	2.3
3	C	197	GLY	2.3
10	J	88	LEU	2.3
17	Q	64	PRO	2.3
2	B	81	VAL	2.3
1	A	313	A	2.3
1	A	704	A	2.3
1	A	940	C	2.3
1	A	1305	G	2.3
1	A	1518	A	2.3
4	D	76	ARG	2.3
2	B	201	ILE	2.3
11	K	77	MET	2.3
9	I	61	ALA	2.3
1	A	390	C	2.3
14	N	15	LYS	2.3
16	P	30	GLY	2.3
13	M	106	ASN	2.2
2	B	149	LEU	2.2
4	D	146	ILE	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
11	K	122	LYS	2.2
18	R	68	LYS	2.2
9	I	17	VAL	2.2
1	A	1089	G	2.2
14	N	41	ARG	2.2
9	I	19	LEU	2.2
10	J	67	THR	2.2
10	J	74	ILE	2.2
1	A	1287	A	2.2
9	I	97	LYS	2.2
9	I	116	LYS	2.2
22	Y	141	TYR	2.2
3	C	52	LEU	2.2
14	N	48	ALA	2.2
16	P	59	TRP	2.2
1	A	933	G	2.2
1	A	1347	G	2.2
6	F	6	VAL	2.2
9	I	28	VAL	2.2
11	K	102	GLY	2.2
1	A	1280	A	2.2
13	M	105	THR	2.2
20	T	41	ILE	2.2
1	A	345	C	2.2
1	A	980	C	2.2
1	A	1426	C	2.2
22	Y	219	HIS	2.2
7	G	83	ALA	2.2
2	B	158	LEU	2.2
6	F	47	ARG	2.2
13	M	87	TYR	2.2
17	Q	78	GLU	2.2
1	A	204	U	2.2
1	A	982	U	2.2
3	C	146	ALA	2.2
3	C	189	ALA	2.2
3	C	200	ALA	2.2
1	A	1300	G	2.2
1	A	1334	G	2.2
15	O	64	ARG	2.2
3	C	195	VAL	2.2
4	D	54	TYR	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
19	S	49	ILE	2.2
5	E	149	GLU	2.2
4	D	84	LYS	2.2
15	O	58	MET	2.2
2	B	159	PRO	2.1
12	L	10	LEU	2.1
1	A	1478	C	2.1
3	C	152	ILE	2.1
14	N	34	TYR	2.1
21	V	3	LYS	2.1
4	D	156	GLU	2.1
22	Y	205	ARG	2.1
4	D	148	VAL	2.1
1	A	574	A	2.1
1	A	935	A	2.1
1	A	965	A	2.1
5	E	154	GLY	2.1
13	M	56	LEU	2.1
22	Y	2	LEU	2.1
1	A	481	G	2.1
1	A	890	G	2.1
8	H	1	MET	2.1
19	S	44	MET	2.1
21	V	17	THR	2.1
1	A	1162	C	2.1
8	H	102	ARG	2.1
14	N	31	ARG	2.1
1	A	1406	U	2.1
11	K	30	VAL	2.1
7	G	81	GLY	2.1
12	L	94	PRO	2.1
3	C	11	ARG	2.1
1	A	1289	A	2.1
15	O	36	ILE	2.1
20	T	9	ASN	2.1
1	A	1409	C	2.1
9	I	125	TYR	2.1
15	O	59	MET	2.1
20	T	23	ARG	2.1
1	A	705	U	2.1
2	B	147	LYS	2.1
2	B	187	LEU	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
4	D	5	ILE	2.0
9	I	2	GLU	2.0
22	Y	64	ILE	2.0
1	A	89	C	2.0
2	B	98	LEU	2.0
3	C	86	VAL	2.0
22	Y	53	GLY	2.0
16	P	17	TYR	2.0
4	D	47	ARG	2.0
12	L	93	LEU	2.0
14	N	32	SER	2.0
1	A	975	A	2.0
3	C	68	VAL	2.0
16	P	35	LYS	2.0
20	T	25	ARG	2.0
9	I	64	THR	2.0
1	A	995	C	2.0
12	L	27	LEU	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
23	MG	A	1677	1/1	-0.02	0.56	63,63,63,63	0
23	MG	A	1617	1/1	0.29	0.34	76,76,76,76	0
23	MG	A	1665	1/1	0.31	0.40	107,107,107,107	0
23	MG	A	1631	1/1	0.33	0.26	46,46,46,46	0
23	MG	A	1686	1/1	0.36	0.27	62,62,62,62	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
23	MG	A	1689	1/1	0.36	0.26	58,58,58,58	0
23	MG	A	1601	1/1	0.38	0.23	42,42,42,42	0
23	MG	A	1629	1/1	0.41	1.25	70,70,70,70	0
23	MG	A	1667	1/1	0.42	0.20	76,76,76,76	0
23	MG	A	1614	1/1	0.42	0.24	59,59,59,59	0
23	MG	B	301	1/1	0.43	0.15	59,59,59,59	0
23	MG	A	1656	1/1	0.44	0.28	33,33,33,33	0
23	MG	A	1644	1/1	0.46	0.26	54,54,54,54	0
23	MG	A	1624	1/1	0.46	0.67	70,70,70,70	0
23	MG	N	102	1/1	0.48	0.51	24,24,24,24	0
23	MG	A	1612	1/1	0.49	0.24	46,46,46,46	0
23	MG	A	1628	1/1	0.51	0.37	54,54,54,54	0
23	MG	A	1695	1/1	0.52	0.35	52,52,52,52	0
23	MG	A	1647	1/1	0.54	0.49	70,70,70,70	0
23	MG	A	1613	1/1	0.54	0.31	63,63,63,63	0
23	MG	A	1699	1/1	0.56	0.45	43,43,43,43	0
23	MG	A	1646	1/1	0.57	0.25	18,18,18,18	0
23	MG	A	1621	1/1	0.58	0.44	59,59,59,59	0
23	MG	A	1661	1/1	0.61	0.18	93,93,93,93	0
23	MG	A	1607	1/1	0.62	0.13	61,61,61,61	0
23	MG	A	1606	1/1	0.66	0.31	37,37,37,37	0
23	MG	A	1616	1/1	0.66	0.36	19,19,19,19	0
23	MG	A	1662	1/1	0.67	0.29	67,67,67,67	0
23	MG	A	1669	1/1	0.67	0.30	33,33,33,33	0
23	MG	A	1645	1/1	0.67	0.32	12,12,12,12	0
23	MG	A	1611	1/1	0.69	0.80	57,57,57,57	0
23	MG	A	1703	1/1	0.69	0.91	70,70,70,70	0
23	MG	A	1653	1/1	0.69	0.33	11,11,11,11	0
23	MG	A	1626	1/1	0.69	0.72	70,70,70,70	0
23	MG	A	1680	1/1	0.70	0.40	22,22,22,22	0
23	MG	A	1712	1/1	0.71	0.22	36,36,36,36	0
23	MG	A	1604	1/1	0.71	0.66	70,70,70,70	0
23	MG	A	1704	1/1	0.71	0.22	29,29,29,29	0
23	MG	A	1716	1/1	0.72	0.19	42,42,42,42	0
23	MG	A	1627	1/1	0.72	0.39	52,52,52,52	0
23	MG	A	1620	1/1	0.72	0.42	15,15,15,15	0
23	MG	A	1600	1/1	0.73	0.15	63,63,63,63	0
23	MG	A	1705	1/1	0.73	0.29	16,16,16,16	0
23	MG	A	1682	1/1	0.74	0.30	36,36,36,36	0
23	MG	A	1655	1/1	0.74	0.13	47,47,47,47	0
23	MG	A	1666	1/1	0.74	0.15	26,26,26,26	0
23	MG	A	1643	1/1	0.74	0.34	10,10,10,10	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
23	MG	A	1625	1/1	0.76	0.39	0,0,0,0	0
23	MG	A	1637	1/1	0.76	0.74	70,70,70,70	0
23	MG	A	1652	1/1	0.77	0.47	42,42,42,42	0
23	MG	A	1648	1/1	0.77	0.25	4,4,4,4	0
23	MG	A	1700	1/1	0.78	0.31	10,10,10,10	0
23	MG	A	1650	1/1	0.78	0.81	57,57,57,57	0
23	MG	A	1685	1/1	0.78	0.35	36,36,36,36	0
23	MG	A	1674	1/1	0.78	0.17	8,8,8,8	0
23	MG	A	1609	1/1	0.80	0.27	33,33,33,33	0
23	MG	A	1690	1/1	0.81	0.56	33,33,33,33	0
23	MG	A	1711	1/1	0.81	0.21	9,9,9,9	0
23	MG	A	1630	1/1	0.81	0.35	7,7,7,7	0
23	MG	A	1615	1/1	0.82	0.54	27,27,27,27	0
23	MG	A	1673	1/1	0.82	0.33	3,3,3,3	0
23	MG	A	1707	1/1	0.82	0.68	42,42,42,42	0
23	MG	A	1688	1/1	0.82	0.32	28,28,28,28	0
23	MG	A	1708	1/1	0.83	0.17	21,21,21,21	0
23	MG	A	1681	1/1	0.83	0.29	41,41,41,41	0
23	MG	A	1608	1/1	0.84	0.11	56,56,56,56	0
23	MG	A	1622	1/1	0.84	0.27	29,29,29,29	0
23	MG	A	1694	1/1	0.84	0.27	14,14,14,14	0
23	MG	A	1633	1/1	0.84	0.27	27,27,27,27	0
23	MG	A	1649	1/1	0.85	0.29	15,15,15,15	0
23	MG	A	1610	1/1	0.85	0.21	63,63,63,63	0
23	MG	A	1687	1/1	0.85	0.30	17,17,17,17	0
23	MG	A	1632	1/1	0.85	0.23	27,27,27,27	0
23	MG	A	1671	1/1	0.86	0.43	10,10,10,10	0
23	MG	A	1636	1/1	0.86	0.26	1,1,1,1	0
23	MG	A	1692	1/1	0.86	0.18	23,23,23,23	0
23	MG	A	1683	1/1	0.86	0.24	38,38,38,38	0
23	MG	A	1657	1/1	0.86	0.33	0,0,0,0	0
23	MG	A	1696	1/1	0.86	0.41	27,27,27,27	0
23	MG	A	1603	1/1	0.86	0.28	36,36,36,36	0
23	MG	A	1678	1/1	0.86	0.33	27,27,27,27	0
23	MG	A	1651	1/1	0.86	0.28	8,8,8,8	0
23	MG	A	1634	1/1	0.87	0.28	3,3,3,3	0
23	MG	A	1679	1/1	0.87	0.23	27,27,27,27	0
23	MG	A	1710	1/1	0.87	0.29	20,20,20,20	0
23	MG	A	1663	1/1	0.87	0.26	16,16,16,16	0
23	MG	A	1670	1/1	0.88	0.18	34,34,34,34	0
23	MG	A	1676	1/1	0.88	0.28	5,5,5,5	0
23	MG	A	1642	1/1	0.88	0.41	33,33,33,33	0

Continued on next page...

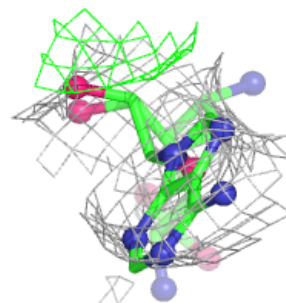
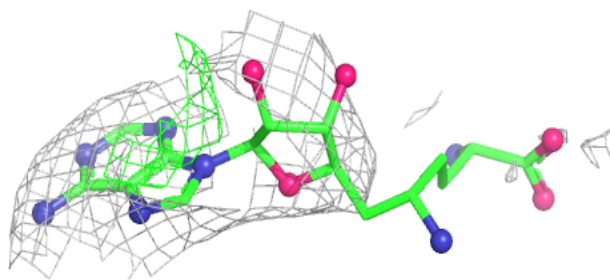
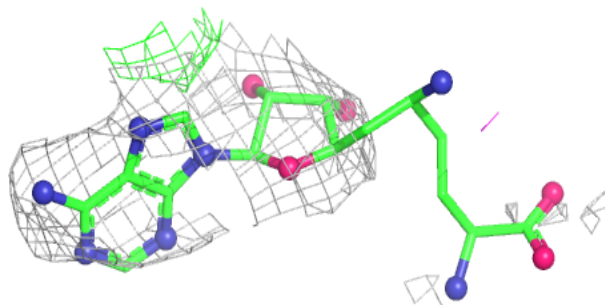
Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
23	MG	A	1640	1/1	0.88	0.24	33,33,33,33	0
23	MG	A	1641	1/1	0.89	0.26	0,0,0,0	0
23	MG	A	1697	1/1	0.89	0.39	38,38,38,38	0
23	MG	E	201	1/1	0.89	0.44	21,21,21,21	0
23	MG	A	1715	1/1	0.89	0.26	9,9,9,9	0
23	MG	A	1658	1/1	0.90	0.27	40,40,40,40	0
23	MG	A	1635	1/1	0.90	0.39	25,25,25,25	0
25	SFG	Y	301	27/27	0.90	0.17	110,110,110,110	0
23	MG	A	1668	1/1	0.91	0.38	15,15,15,15	0
23	MG	A	1701	1/1	0.91	0.22	6,6,6,6	0
23	MG	A	1713	1/1	0.91	0.21	39,39,39,39	0
23	MG	A	1639	1/1	0.92	0.21	15,15,15,15	0
23	MG	A	1691	1/1	0.92	0.15	2,2,2,2	0
23	MG	A	1702	1/1	0.92	0.24	32,32,32,32	0
23	MG	A	1654	1/1	0.93	0.34	16,16,16,16	0
23	MG	A	1693	1/1	0.93	0.59	18,18,18,18	0
23	MG	A	1638	1/1	0.93	0.14	47,47,47,47	0
23	MG	A	1714	1/1	0.93	0.40	19,19,19,19	0
23	MG	A	1664	1/1	0.93	0.23	7,7,7,7	0
23	MG	A	1602	1/1	0.94	0.58	22,22,22,22	0
23	MG	A	1698	1/1	0.94	0.28	23,23,23,23	0
23	MG	A	1709	1/1	0.95	0.29	34,34,34,34	0
23	MG	A	1684	1/1	0.95	0.37	17,17,17,17	0
23	MG	A	1619	1/1	0.95	0.13	40,40,40,40	0
23	MG	A	1675	1/1	0.96	0.24	43,43,43,43	0
23	MG	A	1660	1/1	0.96	0.18	4,4,4,4	0
23	MG	A	1618	1/1	0.96	0.92	69,69,69,69	0
23	MG	A	1672	1/1	0.97	0.08	15,15,15,15	0
23	MG	A	1706	1/1	0.97	0.16	30,30,30,30	0
23	MG	A	1623	1/1	0.97	0.37	30,30,30,30	0
23	MG	A	1605	1/1	0.97	0.31	8,8,8,8	0
23	MG	A	1659	1/1	0.98	0.10	12,12,12,12	0
24	ZN	N	101	1/1	0.99	0.04	108,108,108,108	0
24	ZN	D	301	1/1	0.99	0.25	34,34,34,34	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around SFG Y 301:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers [i](#)

There are no such residues in this entry.