Full wwPDB X-ray Structure Validation Report ⓘ

Aug 8, 2023 – 05:34 PM EDT

PDB ID	:	1Q86
Title	:	Crystal structure of CCA-Phe-cap-biotin bound simultaneously at half occupancy to both the A-site and P-site of the the 50S ribosomal Subunit.
Authors	:	Hansen, J.L.; Schmeing, T.M.; Moore, P.B.; Steitz, T.A.
Deposited on	:	2003-08-20
Resolution	:	3.00 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:

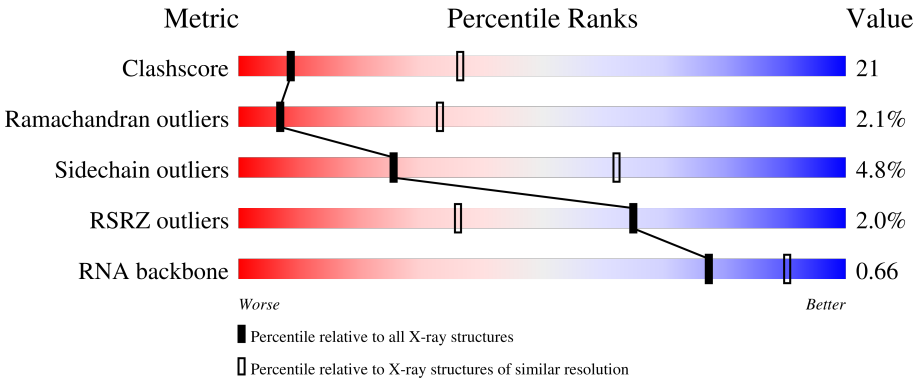
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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.



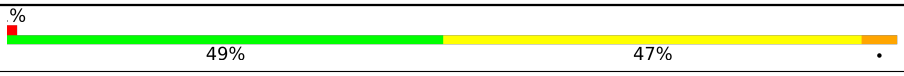
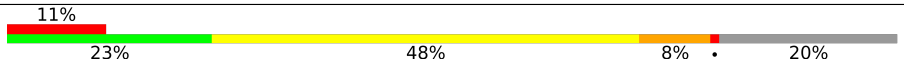
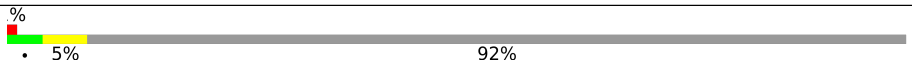
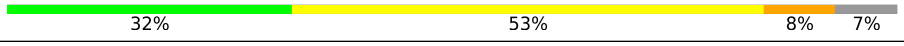
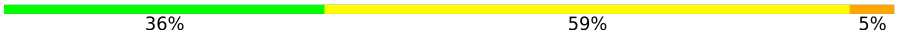
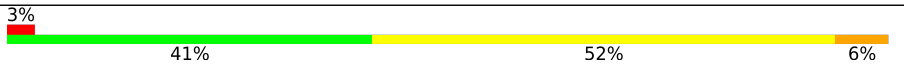
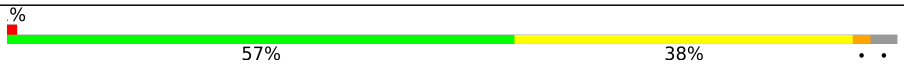
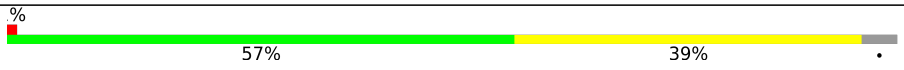
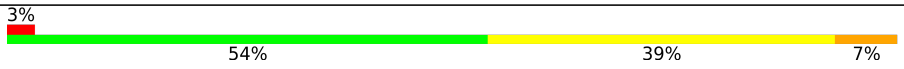
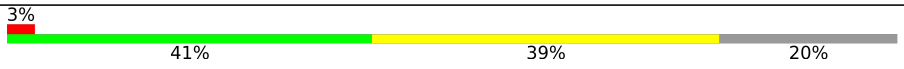
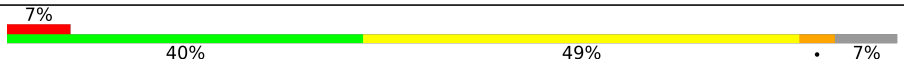
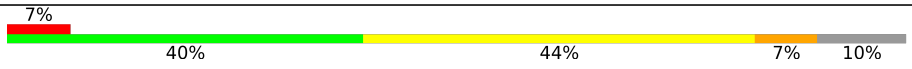
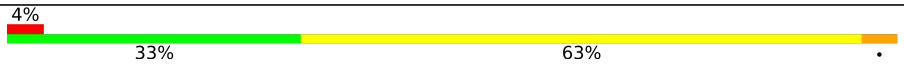
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (3.00-3.00)
RNA backbone	3102	1173 (3.30-2.70)

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 <=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	2922	% 53% 35% 5% 6%
2	B	122	5% 48% 39% 11%
3	5	3	33% 33% 33% 33%
3	6	3	100% 100%
4	C	239	3% 57% 36% 6%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
5	D	337	
6	E	246	
7	F	176	
8	G	177	
9	H	119	
10	I	348	
11	J	167	
12	K	145	
13	L	132	
14	M	164	
15	N	194	
16	O	186	
17	P	115	
18	Q	148	
19	R	95	
20	S	154	
21	T	84	
22	U	119	
23	V	66	
24	W	70	
25	X	154	
26	Y	91	
27	Z	240	
28	1	73	
29	2	56	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
30	3	48	
31	4	92	

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
32	MG	1	8105	-	-	-	X
32	MG	6	8118	-	-	-	X
32	MG	A	8024	-	-	-	X
34	NA	A	8328	-	-	-	X
34	NA	A	8350	-	-	-	X
34	NA	A	8352	-	-	-	X
34	NA	A	8354	-	-	-	X
34	NA	A	8359	-	-	-	X
34	NA	A	8372	-	-	-	X
34	NA	A	8375	-	-	-	X
34	NA	A	8377	-	-	-	X
34	NA	A	8384	-	-	-	X
34	NA	S	8386	-	-	-	X
34	NA	T	8312	-	-	-	X
36	PHA	5	77	-	-	-	X
36	PHA	6	77	-	-	-	X

2 Entry composition

There are 38 unique types of molecules in this entry. The entry contains 98659 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 23S ribosomal rna.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
1	A	2754	59017	26346	10878	19048	2745	0	0	0

- Molecule 2 is a RNA chain called 5S ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
2	B	122	2600	1160	472	847	121	0	0	0

- Molecule 3 is a RNA chain called CCA-phenylalanine-cariotic-acid-biotin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
3	5	3	59	28	11	18	2	0	0	0
			Total	C	N	O	P			
3	6	3	59	28	11	18	2	0	0	0

- Molecule 4 is a protein called 50S ribosomal protein L2P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	C	237	1754	1072	352	325	5	0	0	0

- Molecule 5 is a protein called 50S ribosomal protein L3P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
5	D	337	2624	1616	493	510	5	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	?	-	PRO	deletion	UNP P20279
D	310	ARG	PHE	conflict	UNP P20279

- Molecule 6 is a protein called 50S ribosomal protein L4E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	E	246	Total	C	N	O	S	0	0	0
			1858	1131	344	382	1			

- Molecule 7 is a protein called 50S ribosomal protein L5P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	F	140	Total	C	N	O	S	0	0	0
			1094	685	195	210	4			

- Molecule 8 is a protein called 50S ribosomal protein L6P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	G	172	Total	C	N	O	S	0	0	0
			1357	840	224	289	4			

- Molecule 9 is a protein called 50S ribosomal protein L7Ae.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	H	119	Total	C	N	O	S	0	0	0
			885	552	141	191	1			

- Molecule 10 is a protein called Acidic ribosomal protein P0 homolog.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	I	29	Total	C	N	O	S	0	0	0
			240	149	39	51	1			

- Molecule 11 is a protein called L10 Ribosomal Protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	J	156	Total	C	N	O	S	0	0	0
			1215	766	233	212	4			

- Molecule 12 is a protein called 50S ribosomal protein L13P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	K	142	Total	C	N	O	S	0	0	0
			1119	696	199	221	3			

- Molecule 13 is a protein called 50S ribosomal protein L14P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	L	132	Total	C	N	O	S	0	0	0
			993	609	189	191	4			

- Molecule 14 is a protein called 50S ribosomal protein L15P.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
14	M	145	Total	C	N	O	0	0	0
			1114	668	222	224			

- Molecule 15 is a protein called L15 Ribosomal Protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	N	194	Total	C	N	O	S	0	0	0
			1605	988	346	266	5			

- Molecule 16 is a protein called 50S ribosomal protein L18P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	O	186	Total	C	N	O	S	0	0	0
			1444	895	262	285	2			

- Molecule 17 is a protein called 50S ribosomal protein L18e.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
17	P	115	Total	C	N	O	0	0	0
			864	529	161	174			

- Molecule 18 is a protein called 50S ribosomal protein L19E.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
18	Q	143	Total	C	N	O	0	0	0
			1133	680	230	223			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Q	71	LYS	TYR	conflict	UNP P14119

- Molecule 19 is a protein called 50S ribosomal protein L21e.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
19	R	95	Total	C	N	O	0	0	0
			734	450	141	143			

- Molecule 20 is a protein called 50S ribosomal protein L22P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
20	S	150	Total	C	N	O	S	0	0	0
			1149	713	209	223	4			

- Molecule 21 is a protein called 50S ribosomal protein L23P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
21	T	81	Total	C	N	O	S	0	0	0
			641	389	111	138	3			

- Molecule 22 is a protein called 50S ribosomal protein L24P.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
22	U	119	Total	C	N	O	0	0	0
			949	568	180	201			

- Molecule 23 is a protein called 50S ribosomal protein L24E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	V	53	Total	C	N	O	S	0	0	0
			410	244	75	86	5			

- Molecule 24 is a protein called 50S ribosomal protein L29P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
24	W	65	Total	C	N	O	S	0	0	0
			499	304	94	100	1			

- Molecule 25 is a protein called 50S ribosomal protein L30P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
25	X	154	Total	C	N	O	S	0	0	0
			1195	737	209	243	6			

- Molecule 26 is a protein called 50S ribosomal protein L31e.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	Y	82	Total	C	N	O	S	0	0	0
			654	402	129	122	1			

- Molecule 27 is a protein called 50S ribosomal protein L32E.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
27	Z	142	Total	C	N	O	0	0	0
			1130	686	228	216			

- Molecule 28 is a protein called L37Ae 50S ribosomal protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
28	1	73	Total	C	N	O	S	0	0	0
			563	359	111	86	7			

- Molecule 29 is a protein called 50S ribosomal protein L37e.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
29	2	56	Total	C	N	O	S	0	0	0
			430	258	86	82	4			

- Molecule 30 is a protein called 50S ribosomal protein L39e.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
30	3	46	Total	C	N	O	S	0	0	0
			393	238	86	68	1			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
3	?	-	ARG	deletion	UNP P22452

- Molecule 31 is a protein called 50S ribosomal protein L44E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
31	4	92	Total	C	N	O	S	0	0	0
			755	458	153	137	7			

- Molecule 32 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
32	A	108	Total	Mg	0	0
			108	108		
32	B	1	Total	Mg	0	0
			1	1		
32	6	1	Total	Mg	0	0
			1	1		
32	C	1	Total	Mg	0	0
			1	1		
32	D	2	Total	Mg	0	0
			2	2		
32	L	1	Total	Mg	0	0
			1	1		
32	U	1	Total	Mg	0	0
			1	1		
32	Z	1	Total	Mg	0	0
			1	1		
32	1	1	Total	Mg	0	0
			1	1		
32	4	1	Total	Mg	0	0
			1	1		

- Molecule 33 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
33	A	2	Total	K	0	0
			2	2		

- Molecule 34 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
34	A	70	Total	Na	0	0
			70	70		
34	B	2	Total	Na	0	0
			2	2		
34	C	1	Total	Na	0	0
			1	1		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
34	E	1	Total Na 1 1	0	0
34	J	2	Total Na 2 2	0	0
34	K	1	Total Na 1 1	0	0
34	M	1	Total Na 1 1	0	0
34	N	2	Total Na 2 2	0	0
34	R	1	Total Na 1 1	0	0
34	S	3	Total Na 3 3	0	0
34	T	1	Total Na 1 1	0	0
34	U	1	Total Na 1 1	0	0

- Molecule 35 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

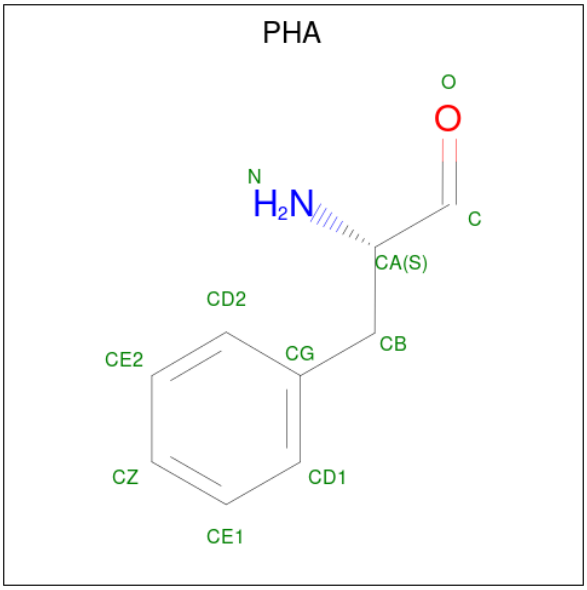
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
35	A	9	Total Cl 9 9	0	0
35	C	1	Total Cl 1 1	0	0
35	D	1	Total Cl 1 1	0	0
35	K	3	Total Cl 3 3	0	0
35	L	1	Total Cl 1 1	0	0
35	M	1	Total Cl 1 1	0	0
35	N	1	Total Cl 1 1	0	0
35	O	1	Total Cl 1 1	0	0
35	P	1	Total Cl 1 1	0	0
35	S	1	Total Cl 1 1	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
35	Z	1	Total Cl 1 1	0	0
35	4	1	Total Cl 1 1	0	0

- Molecule 36 is PHENYLALANINAL (three-letter code: PHA) (formula: $C_9H_{11}NO$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
36	5	1	Total C N O 11 9 1 1	0	0
36	6	1	Total C O 10 9 1	0	0

- Molecule 37 is CADMIUM ION (three-letter code: CD) (formula: Cd).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
37	P	1	Total Cd 1 1	0	0
37	V	1	Total Cd 1 1	0	0
37	1	1	Total Cd 1 1	0	0
37	2	1	Total Cd 1 1	0	0
37	4	1	Total Cd 1 1	0	0

- Molecule 38 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
38	A	5892	Total O 5892 5892	0	0
38	B	139	Total O 139 139	0	0
38	C	116	Total O 116 116	0	0
38	D	149	Total O 149 149	0	0
38	E	173	Total O 173 173	0	0
38	F	52	Total O 52 52	0	0
38	G	43	Total O 43 43	0	0
38	H	27	Total O 27 27	0	0
38	I	21	Total O 21 21	0	0
38	J	77	Total O 77 77	0	0
38	K	54	Total O 54 54	0	0
38	L	62	Total O 62 62	0	0
38	M	82	Total O 82 82	0	0
38	N	139	Total O 139 139	0	0
38	O	70	Total O 70 70	0	0
38	P	43	Total O 43 43	0	0
38	Q	67	Total O 67 67	0	0
38	R	54	Total O 54 54	0	0
38	S	84	Total O 84 84	0	0
38	T	37	Total O 37 37	0	0
38	U	44	Total O 44 44	0	0

Continued on next page...

Continued from previous page...

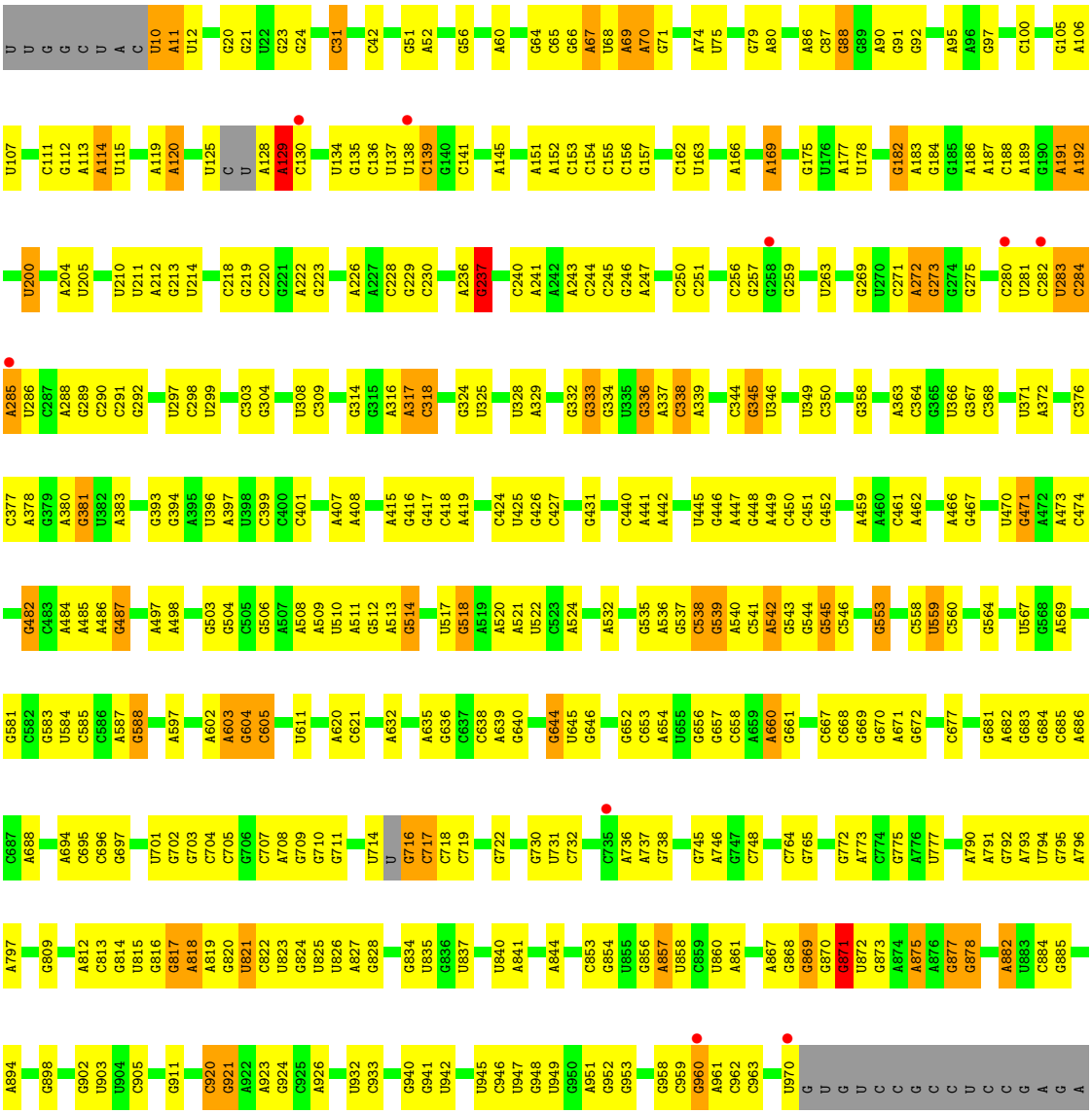
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
38	V	24	Total O 24 24	0	0
38	W	14	Total O 14 14	0	0
38	X	71	Total O 71 71	0	0
38	Y	31	Total O 31 31	0	0
38	Z	93	Total O 93 93	0	0
38	1	37	Total O 37 37	0	0
38	2	63	Total O 63 63	0	0
38	3	41	Total O 41 41	0	0
38	4	70	Total O 70 70	0	0

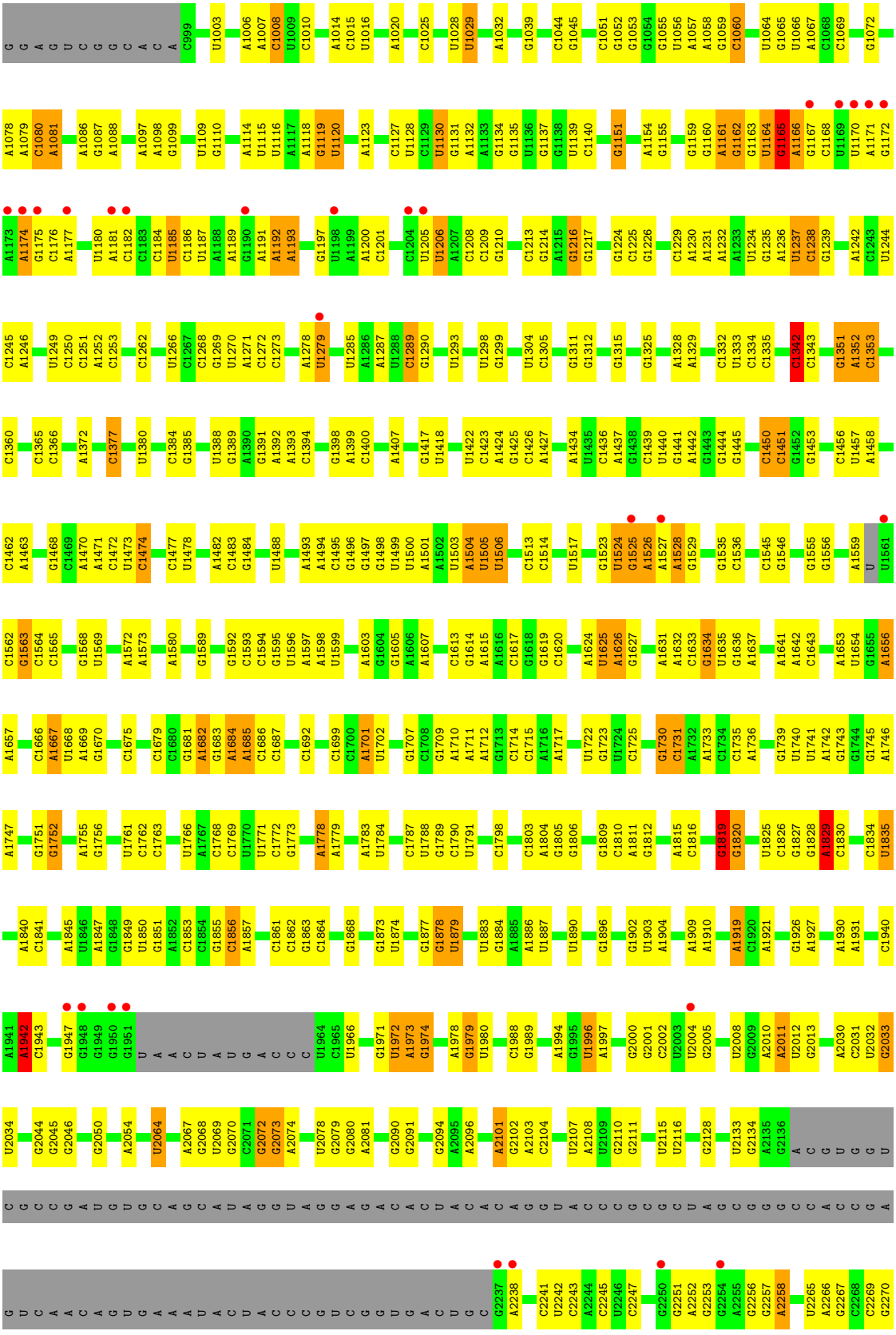
3 Residue-property plots (i)

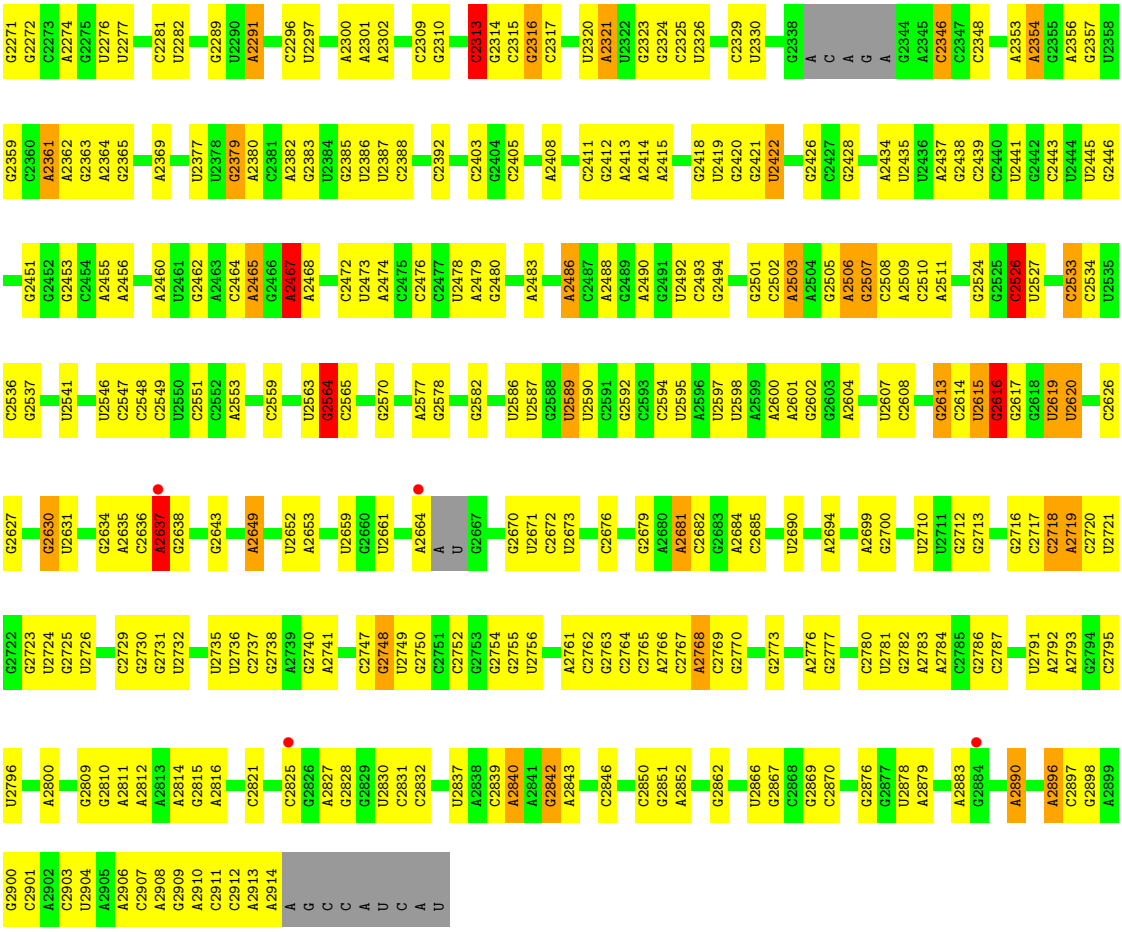
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: 23S ribosomal rna

Chain A:

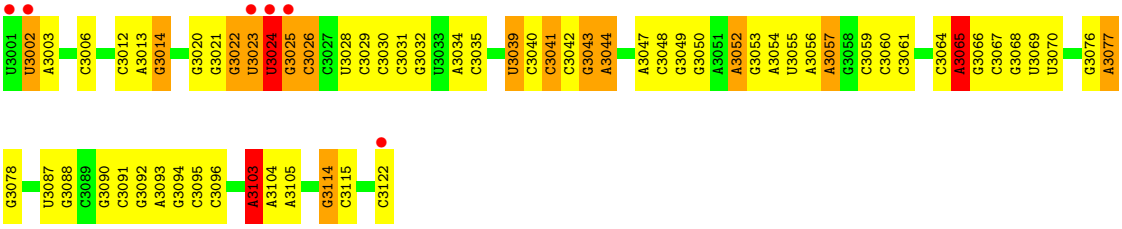






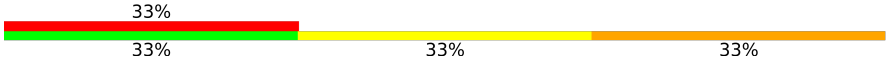
• Molecule 2: 5S ribosomal RNA

Chain B:



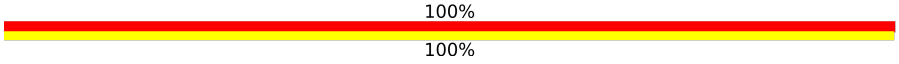
• Molecule 3: CCA-phenylalanine-cariotic-acid-biotin

Chain 5:

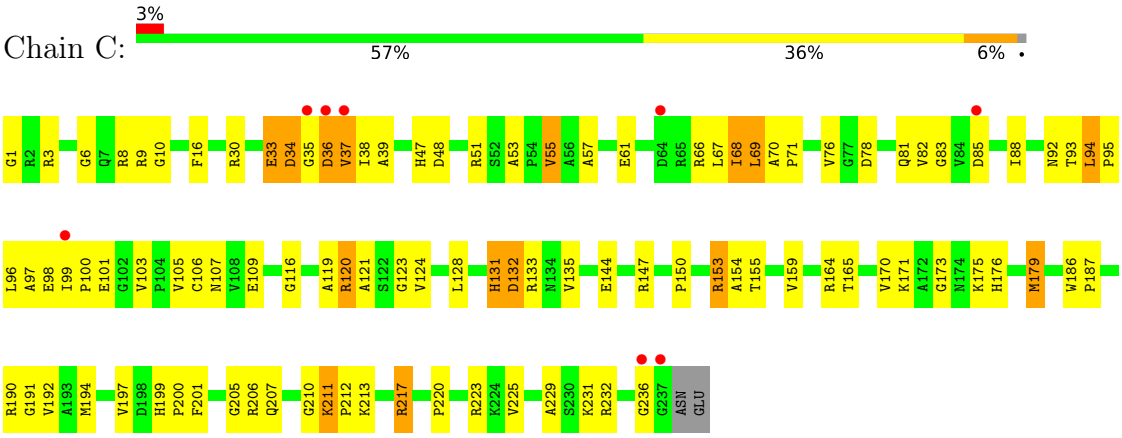


• Molecule 3: CCA-phenylalanine-cariotic-acid-biotin

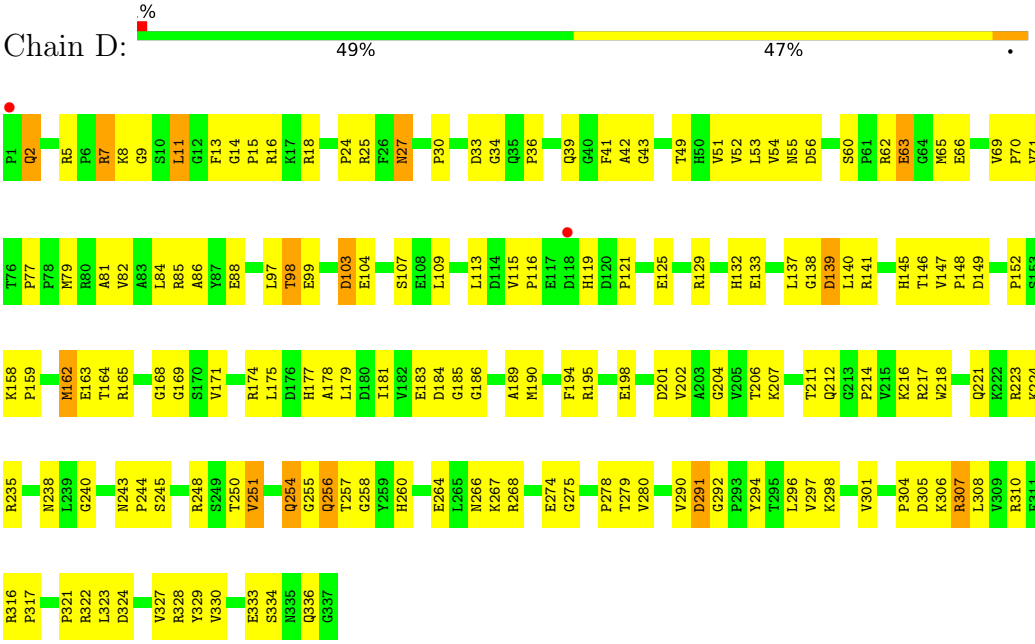
Chain 6:



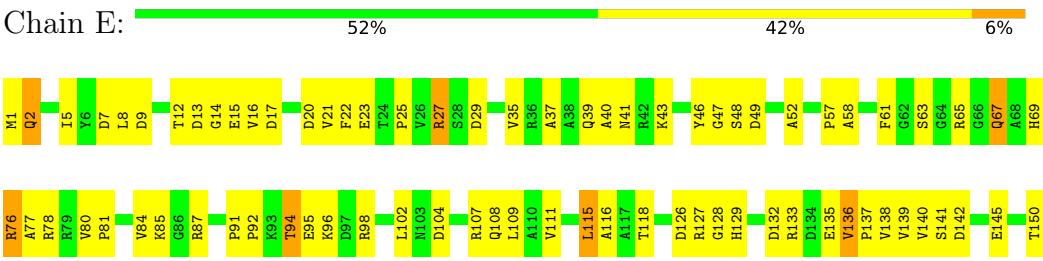
• Molecule 4: 50S ribosomal protein L2P

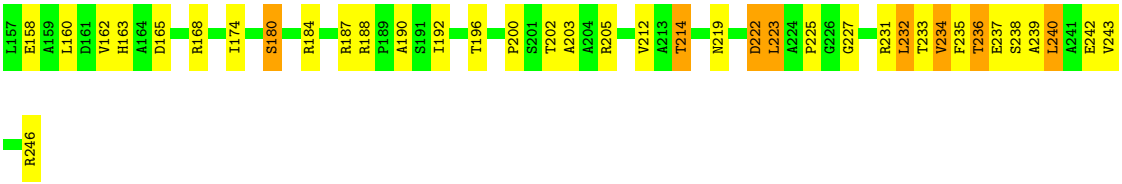


• Molecule 5: 50S ribosomal protein L3P

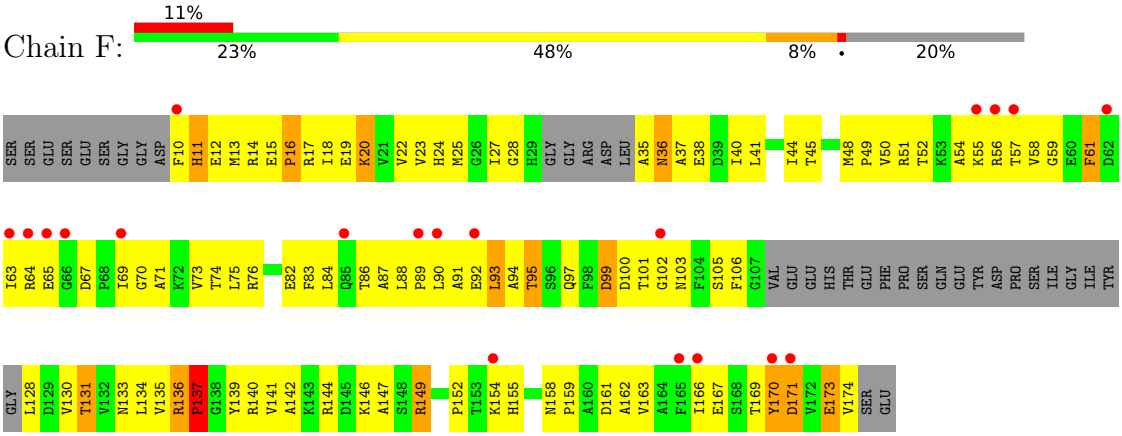


• Molecule 6: 50S ribosomal protein L4E

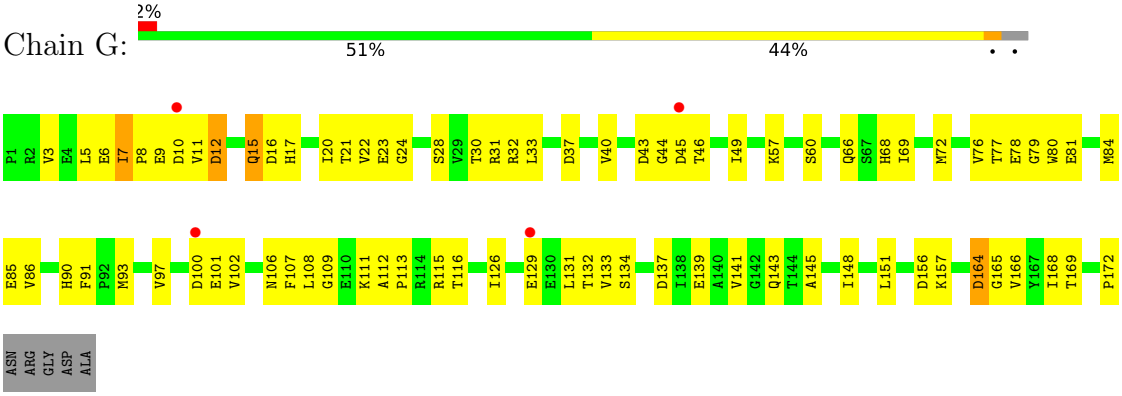




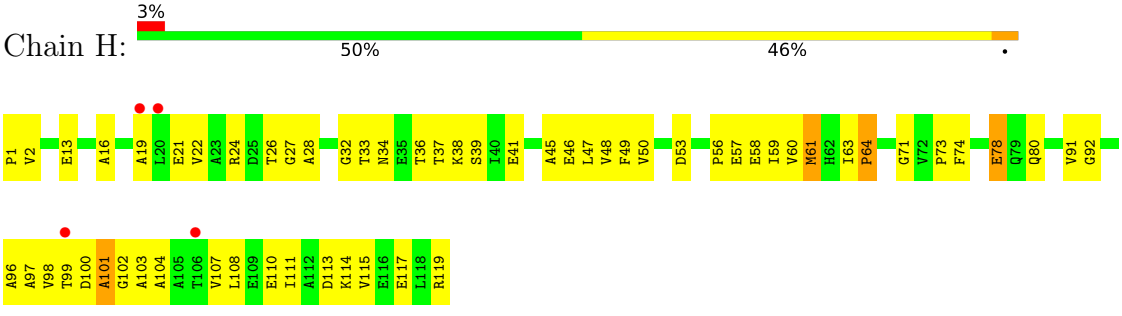
• Molecule 7: 50S ribosomal protein L5P



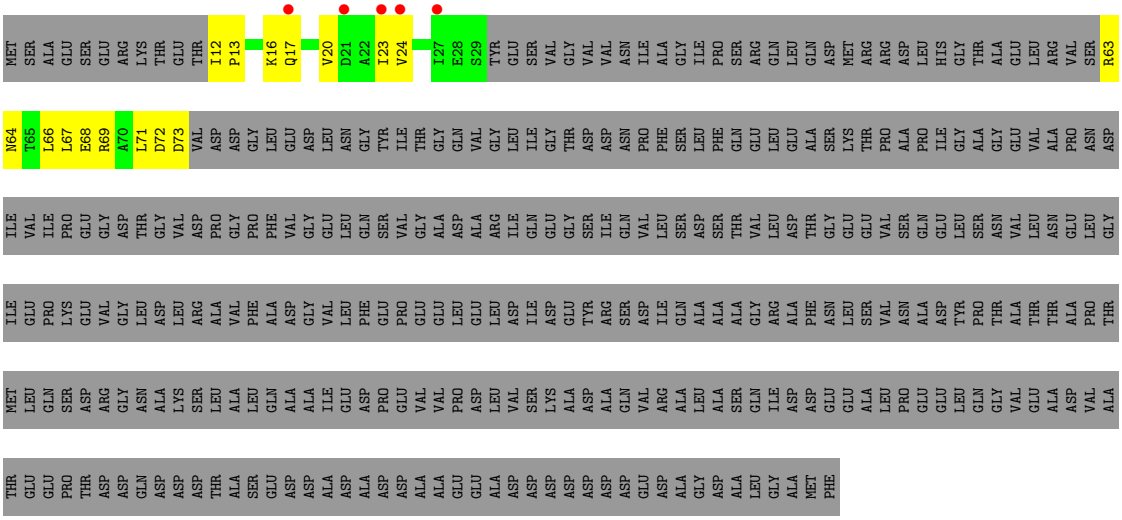
• Molecule 8: 50S ribosomal protein L6P



• Molecule 9: 50S ribosomal protein L7Ae

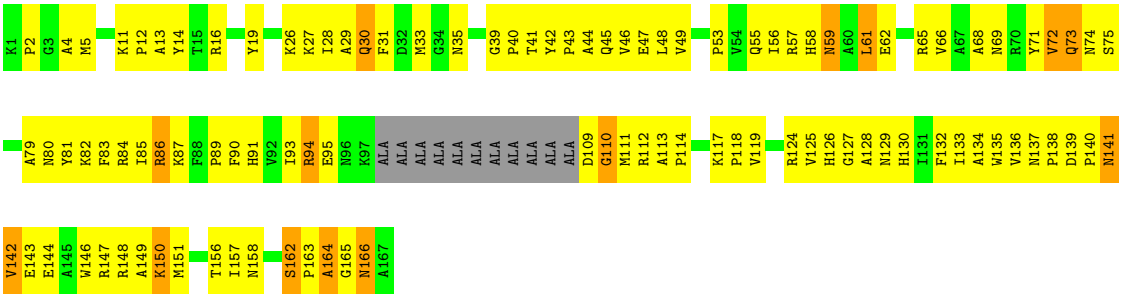


• Molecule 10: Acidic ribosomal protein P0 homolog



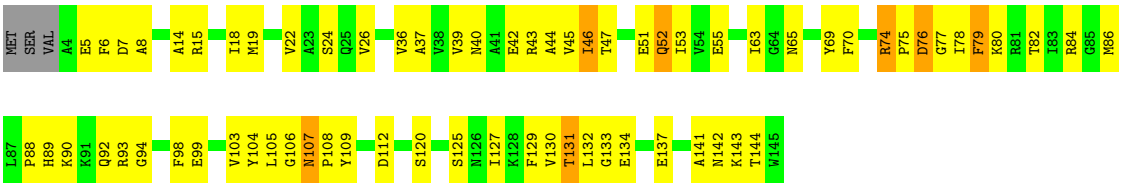
• Molecule 11: L10 Ribosomal Protein

Chain J:



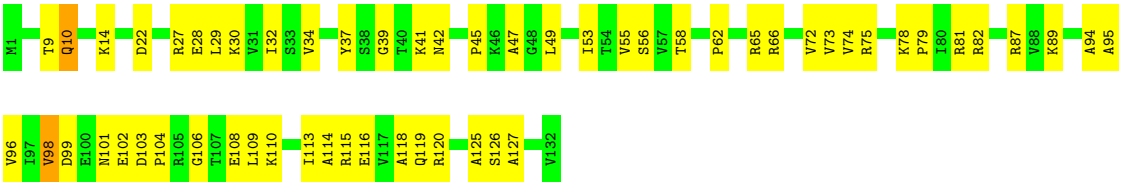
• Molecule 12: 50S ribosomal protein L13P

Chain K:



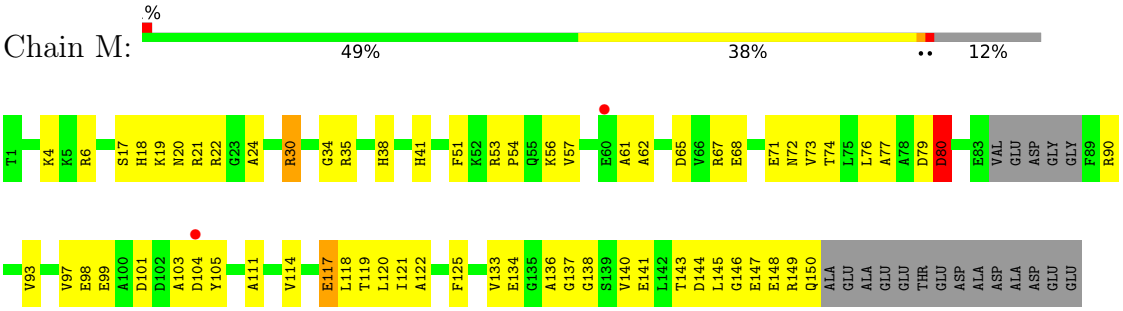
• Molecule 13: 50S ribosomal protein L14P

Chain L:



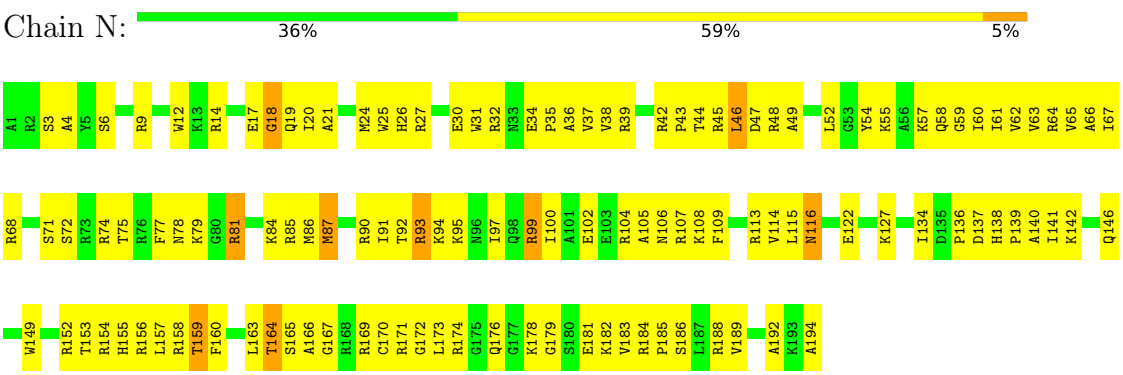
• Molecule 14: 50S ribosomal protein L15P

Chain M:



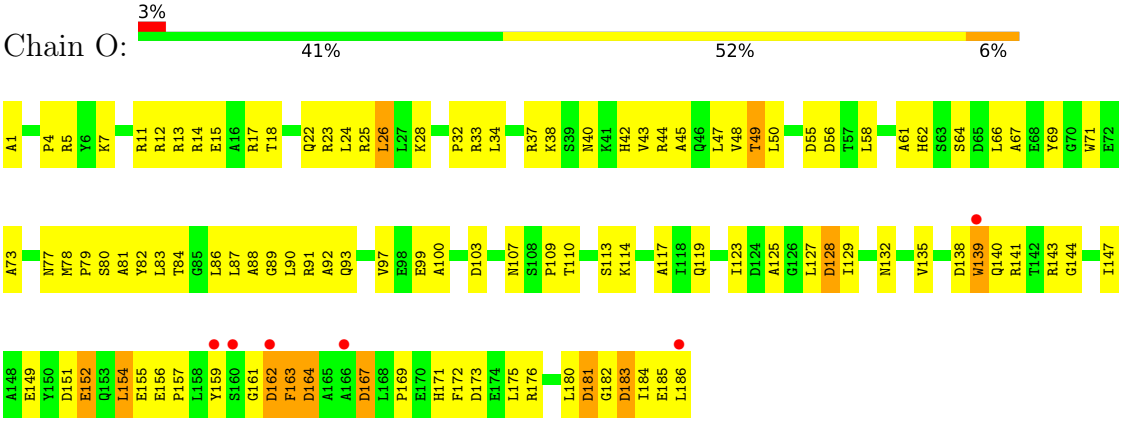
• Molecule 15: L15 Ribosomal Protein

Chain N:



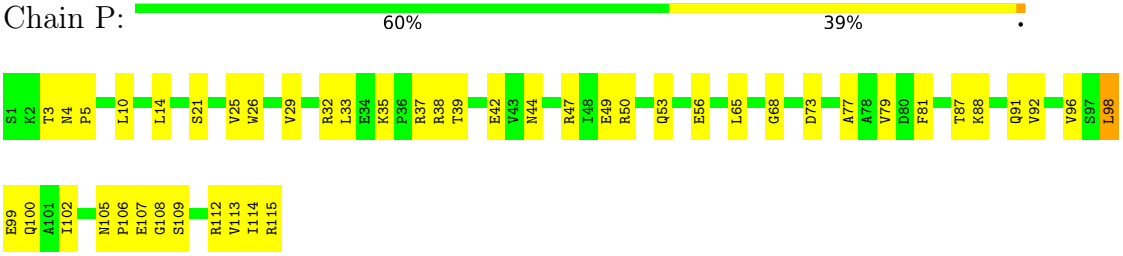
• Molecule 16: 50S ribosomal protein L18P

Chain O:



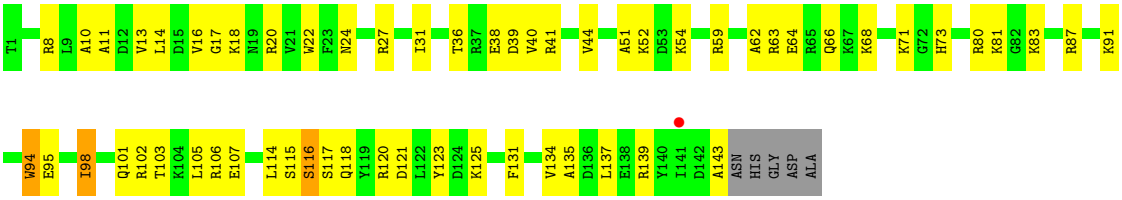
• Molecule 17: 50S ribosomal protein L18e

Chain P:



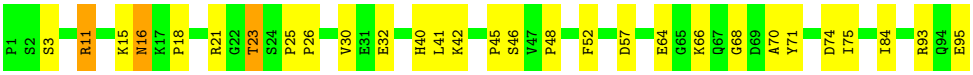
• Molecule 18: 50S ribosomal protein L19E

Chain Q:



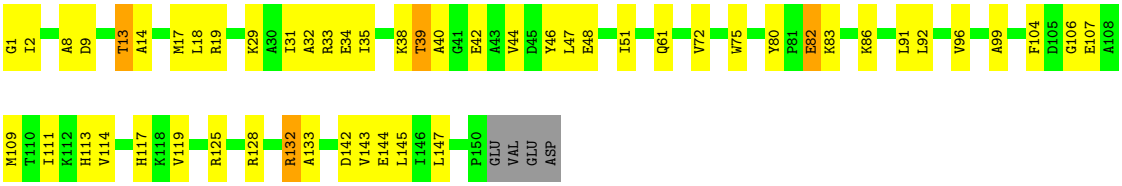
• Molecule 19: 50S ribosomal protein L21e

Chain R:



• Molecule 20: 50S ribosomal protein L22P

Chain S:

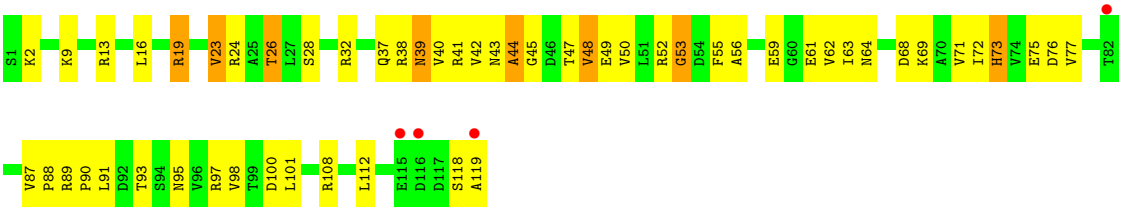


• Molecule 21: 50S ribosomal protein L23P

Chain T:

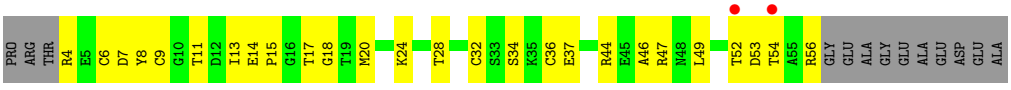
• Molecule 22: 50S ribosomal protein L24P

Chain U:



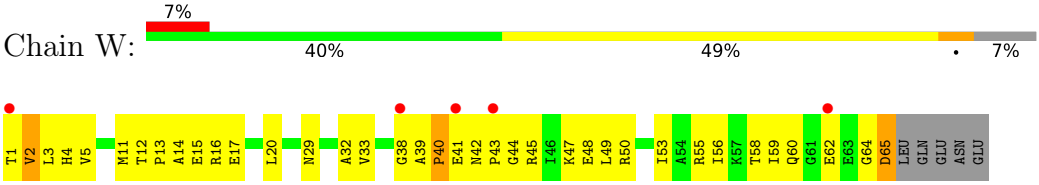
• Molecule 23: 50S ribosomal protein L24E

Chain V:



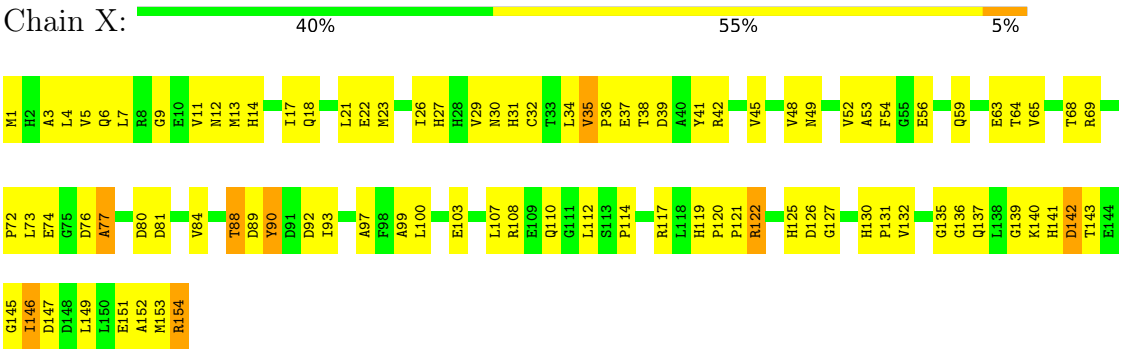
• Molecule 24: 50S ribosomal protein L29P

Chain W:



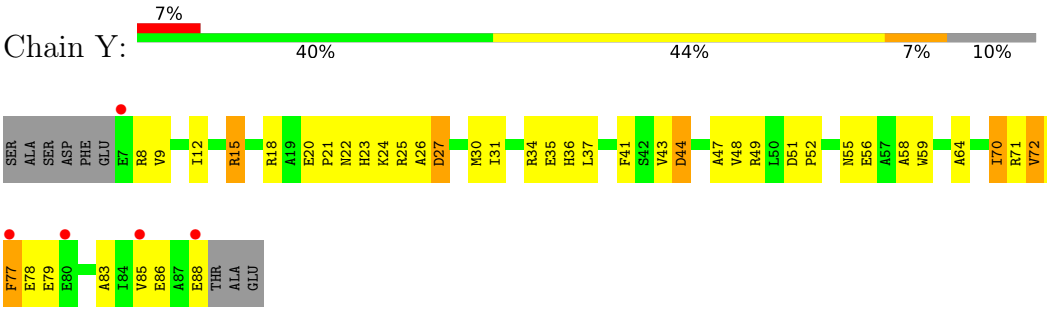
• Molecule 25: 50S ribosomal protein L30P

Chain X:



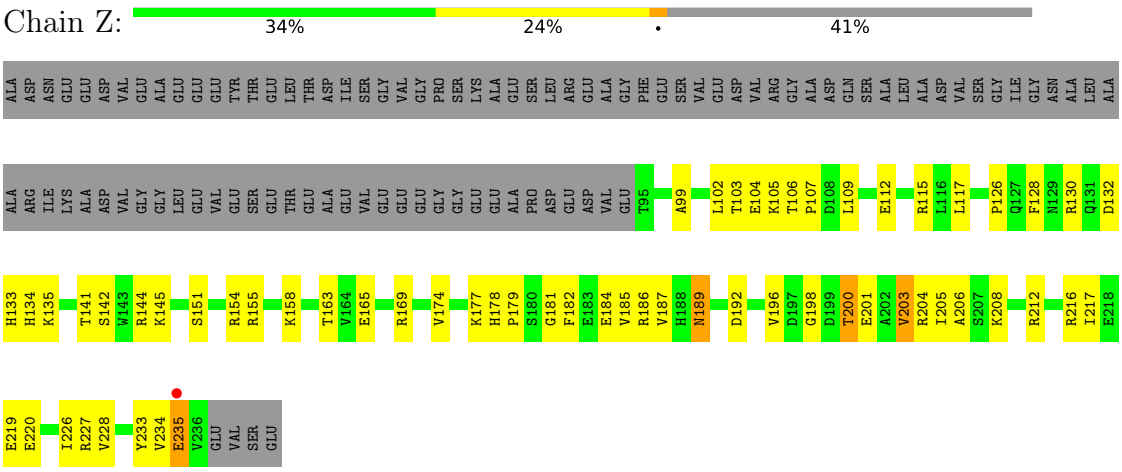
• Molecule 26: 50S ribosomal protein L31e

Chain Y:



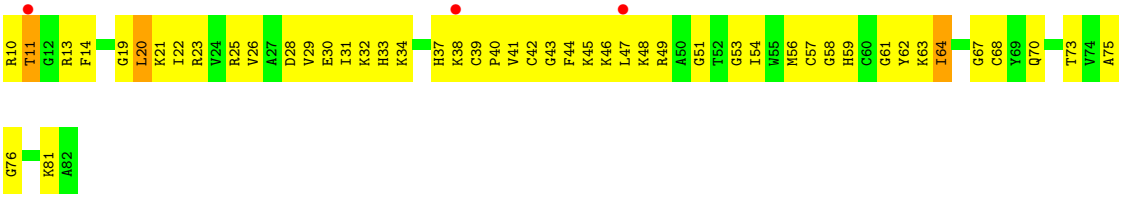
• Molecule 27: 50S ribosomal protein L32E

Chain Z:



• Molecule 28: L37Ae 50S ribosomal protein

Chain 1:

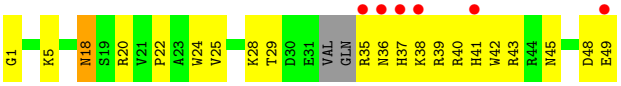


• Molecule 29: 50S ribosomal protein L37e

Chain 2:

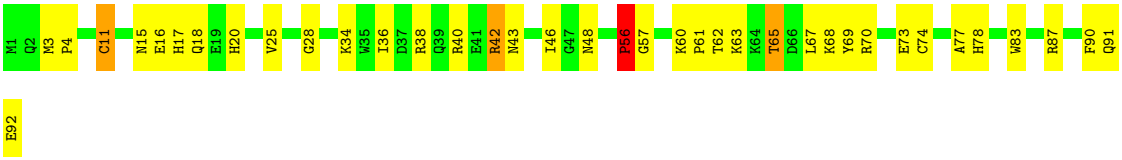
• Molecule 30: 50S ribosomal protein L39e

Chain 3:



• Molecule 31: 50S ribosomal protein L44E

Chain 4:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	213.16Å 301.29Å 575.40Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 3.00 49.62 – 2.80	Depositor EDS
% Data completeness (in resolution range)	95.6 (20.00-3.00) 92.8 (49.62-2.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.01 (at 2.81Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.234 , 0.264 0.234 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å^2)	47.1	Xtriage
Anisotropy	0.292	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 70.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.89	EDS
Total number of atoms	98659	wwPDB-VP
Average B, all atoms (Å^2)	53.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.50% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: K, MG, PHA, CD, CL, NA

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	0.41	1/66076 (0.0%)	0.70	24/103052 (0.0%)
2	B	0.37	0/2905	0.75	4/4528 (0.1%)
3	5	0.67	0/65	0.86	0/99
3	6	1.66	2/65 (3.1%)	1.27	0/99
4	C	0.32	0/1787	0.65	0/2409
5	D	0.34	0/2689	0.64	0/3652
6	E	0.38	0/1883	0.65	0/2551
7	F	0.32	0/1111	0.59	0/1498
8	G	0.33	0/1382	0.59	0/1880
9	H	0.31	0/896	0.58	0/1219
10	I	0.29	0/241	0.50	0/324
11	J	0.40	0/1246	0.77	4/1686 (0.2%)
12	K	0.38	0/1135	0.63	0/1530
13	L	0.35	0/1003	0.68	0/1351
14	M	0.32	0/1126	0.65	0/1504
15	N	0.38	0/1633	0.68	0/2180
16	O	0.29	0/1473	0.64	0/1999
17	P	0.34	0/873	0.61	0/1181
18	Q	0.34	0/1143	0.54	0/1521
19	R	0.37	0/748	0.69	1/1005 (0.1%)
20	S	0.36	0/1172	0.67	0/1578
21	T	0.33	0/648	0.58	0/875
22	U	0.31	0/957	0.62	0/1289
23	V	0.33	0/417	0.59	0/562
24	W	0.29	0/502	0.56	0/675
25	X	0.35	0/1218	0.64	0/1655
26	Y	0.35	0/664	0.60	0/895
27	Z	0.36	0/1146	0.65	0/1536
28	1	0.37	0/575	0.69	0/763
29	2	0.37	0/437	0.63	0/578
30	3	0.30	0/398	0.52	0/527
31	4	0.41	0/771	0.62	0/1024

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
All	All	0.39	3/98385 (0.0%)	0.68	33/147225 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	2	50
2	B	1	3
3	6	0	1
25	X	0	1
All	All	3	55

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	6	75	C	O5'-C5'	5.83	1.53	1.44
1	A	2620	U	N1-C6	5.47	1.42	1.38
3	6	74	C	C2'-O2'	5.05	1.48	1.41

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	1563	G	C2'-C3'-O3'	9.42	130.23	109.50
2	B	3024	U	C2'-C3'-O3'	9.17	129.68	109.50
1	A	2637	A	C4'-C3'-O3'	-7.22	94.24	109.40
2	B	3103	A	C5'-C4'-O4'	7.11	117.63	109.10
11	J	74	ASN	N-CA-C	-6.83	92.57	111.00
1	A	1942	A	C5'-C4'-C3'	6.56	126.50	116.00
2	B	3039	U	N1-C1'-C2'	6.47	122.42	114.00
1	A	1504	A	C1'-O4'-C4'	-6.41	104.77	109.90
1	A	871	G	C5'-C4'-O4'	-5.97	101.93	109.10
1	A	2616	G	C2'-C3'-O3'	5.94	123.21	113.70
1	A	2467	A	C1'-O4'-C4'	-5.92	105.17	109.90
1	A	2636	C	OP2-P-O3'	5.76	117.88	105.20
1	A	1979	G	C2'-C3'-O3'	5.74	122.89	113.70
1	A	1165	G	O5'-P-OP2	5.64	117.46	110.70
1	A	2313	C	C5'-C4'-O4'	5.61	115.83	109.10
11	J	110	GLY	N-CA-C	-5.50	99.36	113.10
1	A	2637	A	C1'-O4'-C4'	-5.49	105.51	109.90
1	A	1819	G	C5'-C4'-C3'	5.35	124.56	116.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	2316	G	C5'-C4'-C3'	-5.33	107.48	116.00
1	A	2291	A	N9-C1'-C2'	5.30	120.89	114.00
11	J	156	THR	N-CA-C	-5.29	96.72	111.00
1	A	2616	G	N9-C1'-C2'	5.27	120.86	114.00
1	A	2637	A	OP1-P-O3'	-5.25	93.66	105.20
1	A	1165	G	N9-C1'-C2'	5.20	120.76	114.00
19	R	68	GLY	N-CA-C	-5.15	100.23	113.10
1	A	1829	A	N9-C1'-C2'	-5.11	106.38	112.00
1	A	1504	A	N9-C1'-C2'	5.10	120.63	114.00
1	A	1120	U	C5'-C4'-C3'	-5.10	107.84	116.00
1	A	237	G	N9-C1'-C2'	-5.07	106.42	112.00
1	A	129	A	C2'-C3'-O3'	5.03	121.75	113.70
2	B	3103	A	C1'-O4'-C4'	-5.02	105.88	109.90
11	J	141	ASN	N-CA-C	-5.00	97.49	111.00
1	A	535	G	N9-C1'-C2'	5.00	120.50	114.00

All (3) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	1563	G	C3'
1	A	2616	G	C3'
2	B	3024	U	C3'

All (55) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	6	76	A	Sidechain
1	A	1039	G	Sidechain
1	A	1078	A	Sidechain
1	A	1226	G	Sidechain
1	A	1293	U	Sidechain
1	A	1342	C	Sidechain
1	A	1351	G	Sidechain
1	A	1417	G	Sidechain
1	A	1458	A	Sidechain
1	A	1599	U	Sidechain
1	A	1809	G	Sidechain
1	A	182	G	Sidechain
1	A	1829	A	Sidechain
1	A	1835	U	Sidechain
1	A	1861	C	Sidechain
1	A	1863	G	Sidechain

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
1	A	1877	G	Sidechain
1	A	1878	G	Sidechain
1	A	1972	U	Sidechain
1	A	2313	C	Sidechain
1	A	2465	A	Sidechain
1	A	2486	A	Sidechain
1	A	2492	U	Sidechain
1	A	2493	C	Sidechain
1	A	2503	A	Sidechain
1	A	2506	A	Sidechain
1	A	2526	C	Sidechain
1	A	2551	C	Sidechain
1	A	2564	G	Sidechain
1	A	2607	U	Sidechain
1	A	2615	U	Sidechain
1	A	2619	U	Sidechain
1	A	2630	G	Sidechain
1	A	2631	U	Sidechain
1	A	2637	A	Sidechain
1	A	2643	G	Sidechain
1	A	2673	U	Sidechain
1	A	2793	A	Sidechain
1	A	2840	A	Sidechain
1	A	2842	G	Sidechain
1	A	333	G	Sidechain
1	A	471	G	Sidechain
1	A	482	G	Sidechain
1	A	518	G	Sidechain
1	A	722	G	Sidechain
1	A	792	G	Sidechain
1	A	815	U	Sidechain
1	A	817	G	Sidechain
1	A	818	A	Sidechain
1	A	867	A	Sidechain
1	A	882	A	Sidechain
2	B	3065	A	Sidechain
2	B	3087	U	Sidechain
2	B	3090	G	Sidechain
25	X	90	TYR	Sidechain

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	59017	0	29805	1077	0
2	B	2600	0	1326	84	0
3	5	59	0	34	4	0
3	6	59	0	34	0	0
4	C	1754	0	1763	112	0
5	D	2624	0	2533	183	0
6	E	1858	0	1816	135	0
7	F	1094	0	1085	146	0
8	G	1357	0	1266	77	0
9	H	885	0	854	71	0
10	I	240	0	231	23	0
11	J	1215	0	1215	170	0
12	K	1119	0	1098	77	0
13	L	993	0	1027	72	0
14	M	1114	0	1072	66	0
15	N	1605	0	1676	182	0
16	O	1444	0	1401	129	0
17	P	864	0	873	53	0
18	Q	1133	0	1127	62	0
19	R	734	0	729	26	0
20	S	1149	0	1122	67	0
21	T	641	0	605	31	0
22	U	949	0	923	62	0
23	V	410	0	364	35	0
24	W	499	0	511	33	0
25	X	1195	0	1137	118	0
26	Y	654	0	653	51	0
27	Z	1130	0	1133	71	0
28	1	563	0	597	66	0
29	2	430	0	426	28	0
30	3	393	0	406	32	0
31	4	755	0	728	40	0
32	1	1	0	0	0	0
32	4	1	0	0	0	0
32	6	1	0	0	0	0
32	A	108	0	0	0	0
32	B	1	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
32	C	1	0	0	0	0
32	D	2	0	0	0	0
32	L	1	0	0	0	0
32	U	1	0	0	0	0
32	Z	1	0	0	0	0
33	A	2	0	0	0	0
34	A	70	0	0	0	0
34	B	2	0	0	0	0
34	C	1	0	0	0	0
34	E	1	0	0	0	0
34	J	2	0	0	0	0
34	K	1	0	0	0	0
34	M	1	0	0	0	0
34	N	2	0	0	0	0
34	R	1	0	0	0	0
34	S	3	0	0	0	0
34	T	1	0	0	0	0
34	U	1	0	0	0	0
35	4	1	0	0	0	0
35	A	9	0	0	0	0
35	C	1	0	0	0	0
35	D	1	0	0	0	0
35	K	3	0	0	1	0
35	L	1	0	0	1	0
35	M	1	0	0	0	0
35	N	1	0	0	1	0
35	O	1	0	0	0	0
35	P	1	0	0	0	0
35	S	1	0	0	0	0
35	Z	1	0	0	0	0
36	5	11	0	10	5	0
36	6	10	0	7	4	0
37	1	1	0	0	0	0
37	2	1	0	0	0	0
37	4	1	0	0	0	0
37	P	1	0	0	0	0
37	V	1	0	0	0	0
38	1	37	0	0	14	0
38	2	63	0	0	4	0
38	3	41	0	0	3	0
38	4	70	0	0	10	0
38	A	5892	0	0	227	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
38	B	139	0	0	14	0
38	C	116	0	0	12	0
38	D	149	0	0	30	0
38	E	173	0	0	37	0
38	F	52	0	0	22	0
38	G	43	0	0	12	0
38	H	27	0	0	11	0
38	I	21	0	0	6	0
38	J	77	0	0	23	0
38	K	54	0	0	5	0
38	L	62	0	0	11	0
38	M	82	0	0	18	0
38	N	139	0	0	23	0
38	O	70	0	0	17	0
38	P	43	0	0	13	0
38	Q	67	0	0	5	0
38	R	54	0	0	5	0
38	S	84	0	0	7	0
38	T	37	0	0	6	0
38	U	44	0	0	7	0
38	V	24	0	0	5	0
38	W	14	0	0	3	0
38	X	71	0	0	14	0
38	Y	31	0	0	5	0
38	Z	93	0	0	14	0
All	All	98659	0	59587	3106	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 21.

All (3106) 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)
6:E:236:THR:HG22	6:E:239:ALA:H	1.05	1.18
11:J:45:GLN:HB3	11:J:163:PRO:HD2	1.31	1.12
11:J:86:ARG:NH1	11:J:133:ILE:HG13	1.64	1.11
1:A:1119:G:H2'	12:K:52:GLN:HE22	1.10	1.10
1:A:156:C:H5"	15:N:171:ARG:HD3	1.29	1.09
24:W:12:THR:HG22	24:W:15:GLU:HG3	1.39	1.05
2:B:3023:U:H3'	2:B:3024:U:H5"	1.36	1.04
1:A:1242:A:H5'	12:K:82:THR:HG23	1.38	1.03

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:J:86:ARG:HH11	11:J:133:ILE:HG13	0.91	1.02
22:U:71:VAL:HG11	22:U:90:PRO:HB3	1.40	1.02
1:A:960:G:H4'	38:A:6921:HOH:O	1.58	1.02
5:D:201:ASP:HB2	5:D:312:ARG:HD2	1.43	1.00
11:J:29:ALA:HB3	11:J:65:ARG:HH12	1.23	1.00
1:A:856:G:H2'	38:A:4918:HOH:O	1.60	1.00
1:A:1119:G:H2'	12:K:52:GLN:NE2	1.77	1.00
1:A:2717:C:H2'	1:A:2718:C:H5"	1.45	0.98
13:L:10:GLN:NE2	13:L:10:GLN:H	1.61	0.98
6:E:127:ARG:NH2	6:E:225:PRO:HG2	1.79	0.98
3:5:74:C:H2'	3:5:75:C:H5'	1.44	0.98
7:F:134:LEU:HD11	7:F:166:ILE:HD11	1.44	0.97
2:B:3006:C:H5"	16:O:37:ARG:NH1	1.77	0.97
11:J:162:SER:HB2	11:J:163:PRO:HD3	1.44	0.97
2:B:3076:G:H3'	2:B:3077:A:H5"	1.46	0.97
15:N:52:LEU:HD11	38:N:8623:HOH:O	1.64	0.96
1:A:1160:G:H5'	1:A:1161:A:H5'	1.45	0.96
5:D:140:LEU:HA	38:D:8583:HOH:O	1.64	0.96
1:A:1134:G:H4'	11:J:151:MET:HE1	1.45	0.96
16:O:47:LEU:HD11	16:O:127:LEU:HD21	1.46	0.95
11:J:86:ARG:HH11	11:J:133:ILE:CG1	1.77	0.95
12:K:76:ASP:HA	38:K:5907:HOH:O	1.63	0.95
8:G:20:ILE:HD11	8:G:40:VAL:HG11	1.48	0.95
7:F:105:SER:HB2	7:F:131:THR:HG23	1.48	0.94
25:X:88:THR:HB	38:X:6679:HOH:O	1.66	0.94
22:U:9:LYS:HE3	22:U:13:ARG:NH1	1.82	0.94
7:F:154:LYS:H	7:F:154:LYS:HD2	1.32	0.94
7:F:25:MET:HE2	7:F:41:LEU:HG	1.50	0.93
2:B:3056:A:H2'	2:B:3057:A:H5"	1.50	0.93
5:D:238:ASN:HD22	5:D:240:GLY:H	0.97	0.93
20:S:99:ALA:HB1	20:S:109:MET:HE1	1.50	0.93
13:L:10:GLN:H	13:L:10:GLN:HE21	1.04	0.92
13:L:29:LEU:HB3	13:L:55:VAL:HG11	1.50	0.92
38:A:4711:HOH:O	13:L:39:GLY:HA2	1.68	0.92
11:J:165:GLY:HA3	38:J:8398:HOH:O	1.70	0.92
2:B:3103:A:H4'	38:B:8445:HOH:O	1.69	0.92
15:N:164:THR:HG22	15:N:167:GLY:H	1.33	0.92
26:Y:37:LEU:HD13	26:Y:85:VAL:HG21	1.52	0.91
28:1:10:ARG:HA	38:1:8415:HOH:O	1.68	0.91
1:A:1751:G:H2'	1:A:1752:G:H5"	1.51	0.91
1:A:1667:A:H5'	1:A:1667:A:H8	1.35	0.91

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:D:86:ALA:HA	38:D:8583:HOH:O	1.69	0.91
1:A:541:C:H2'	1:A:542:A:H5"	1.51	0.90
13:L:81:ARG:HB2	13:L:87:ARG:HH11	1.31	0.90
16:O:7:LYS:HE3	19:R:21:ARG:O	1.71	0.90
28:1:58:GLY:HA3	38:1:8438:HOH:O	1.70	0.90
1:A:871:G:H5'	1:A:871:G:H8	1.37	0.90
38:B:8474:HOH:O	16:O:23:ARG:HD3	1.72	0.90
2:B:3023:U:H3'	2:B:3024:U:C5'	2.01	0.89
1:A:871:G:H5'	1:A:871:G:C8	2.07	0.89
14:M:79:ASP:HB3	38:M:8560:HOH:O	1.71	0.89
4:C:211:LYS:HB3	4:C:212:PRO:HD2	1.55	0.88
11:J:75:SER:O	11:J:79:ALA:HB2	1.73	0.88
18:Q:115:SER:H	18:Q:118:GLN:NE2	1.71	0.88
15:N:106:ASN:HD22	15:N:114:VAL:HG23	1.36	0.88
7:F:27:ILE:HG22	7:F:28:GLY:H	1.38	0.88
14:M:67:ARG:O	14:M:71:GLU:HG3	1.74	0.88
1:A:1164:U:H4'	1:A:1165:G:OP1	1.73	0.88
11:J:59:ASN:H	11:J:59:ASN:HD22	1.14	0.88
28:1:38:LYS:HE2	28:1:45:LYS:HE2	1.56	0.88
1:A:1116:U:HO2'	1:A:1118:A:H2	0.89	0.87
1:A:545:G:H5'	1:A:545:G:H8	1.39	0.87
1:A:1474:C:H6	1:A:1474:C:H5'	1.39	0.87
6:E:236:THR:HG22	6:E:239:ALA:N	1.88	0.87
1:A:1701:A:H5'	38:A:5779:HOH:O	1.74	0.87
5:D:321:PRO:HA	38:D:8659:HOH:O	1.75	0.87
8:G:97:VAL:HG12	38:G:4191:HOH:O	1.73	0.87
1:A:1679:C:H5'	38:A:8839:HOH:O	1.74	0.87
12:K:52:GLN:HG3	12:K:53:ILE:N	1.88	0.87
15:N:35:PRO:HG2	15:N:38:VAL:HG23	1.55	0.87
4:C:223:ARG:HG3	38:C:8597:HOH:O	1.73	0.86
15:N:102:GLU:OE1	15:N:164:THR:HG21	1.73	0.86
11:J:41:THR:HA	38:J:8395:HOH:O	1.73	0.86
13:L:81:ARG:HB2	13:L:87:ARG:NH1	1.89	0.86
15:N:87:MET:HB3	31:4:46:ILE:HD13	1.57	0.86
15:N:106:ASN:ND2	35:N:8518:CL:CL	2.45	0.86
18:Q:115:SER:N	18:Q:118:GLN:HE21	1.71	0.86
1:A:1116:U:H3	1:A:1246:A:H62	1.22	0.86
13:L:10:GLN:HE21	13:L:10:GLN:N	1.73	0.86
30:3:41:HIS:H	30:3:45:ASN:HD22	1.23	0.86
1:A:381:G:H5"	38:A:3825:HOH:O	1.73	0.86
1:A:711:G:H1'	38:A:6586:HOH:O	1.74	0.86

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:L:74:VAL:HG11	13:L:113:ILE:HG12	1.57	0.86
1:A:2586:U:H3	1:A:2592:G:H22	1.24	0.86
1:A:1184:C:H1'	38:A:6959:HOH:O	1.75	0.85
13:L:14:LYS:HB2	13:L:45:PRO:HG2	1.56	0.85
1:A:2004:U:H4'	38:A:4800:HOH:O	1.76	0.85
11:J:26:LYS:HD2	11:J:28:ILE:HD12	1.59	0.85
1:A:542:A:H5'	1:A:542:A:H8	1.40	0.84
25:X:72:PRO:HG2	25:X:77:ALA:HB3	1.57	0.84
1:A:21:G:H5'	20:S:2:ILE:HA	1.59	0.84
38:A:3295:HOH:O	15:N:189:VAL:HG21	1.77	0.84
6:E:132:ASP:HB3	38:E:8365:HOH:O	1.77	0.84
12:K:52:GLN:HG3	12:K:53:ILE:H	1.43	0.84
25:X:4:LEU:HD22	25:X:52:VAL:HG21	1.60	0.84
11:J:139:ASP:N	11:J:140:PRO:HD3	1.93	0.84
7:F:20:LYS:HA	7:F:75:LEU:O	1.78	0.83
12:K:74:ARG:HB3	12:K:74:ARG:HH11	1.43	0.83
4:C:192:VAL:HB	38:C:8590:HOH:O	1.76	0.83
20:S:106:GLY:HA2	20:S:109:MET:HE3	1.59	0.83
1:A:2717:C:C2'	1:A:2718:C:H5"	2.09	0.83
1:A:2812:A:H2	1:A:2814:A:H62	1.24	0.83
16:O:49:THR:HG22	16:O:56:ASP:HB2	1.59	0.83
23:V:9:CYS:HA	23:V:52:THR:HG23	1.58	0.83
26:Y:78:GLU:HG2	26:Y:79:GLU:H	1.41	0.83
11:J:137:ASN:O	11:J:139:ASP:N	2.11	0.83
7:F:146:LYS:NZ	16:O:107:ASN:HD21	1.77	0.83
1:A:1835:U:H5	1:A:1840:A:N7	1.76	0.83
1:A:282:C:H1'	1:A:368:C:N4	1.94	0.82
1:A:1166:A:H1'	1:A:1192:A:C2	2.14	0.82
1:A:2506:A:HO2'	1:A:2507:G:H8	0.86	0.82
1:A:541:C:C2'	1:A:542:A:H5"	2.09	0.82
11:J:4:ALA:HB3	38:J:8366:HOH:O	1.78	0.82
9:H:96:ALA:HA	38:H:3111:HOH:O	1.77	0.82
14:M:133:VAL:HA	38:M:8575:HOH:O	1.79	0.82
16:O:144:GLY:O	16:O:147:ILE:HG22	1.79	0.82
20:S:8:ALA:HB1	20:S:13:THR:HG21	1.61	0.82
38:A:5791:HOH:O	7:F:99:ASP:HA	1.79	0.82
2:B:3024:U:O2'	2:B:3025:G:H4'	1.79	0.82
11:J:5:MET:HG3	38:J:8366:HOH:O	1.80	0.82
15:N:87:MET:HB2	15:N:91:ILE:HD11	1.61	0.82
11:J:27:LYS:H	11:J:58:HIS:HD2	1.26	0.81
27:Z:187:VAL:HG23	27:Z:192:ASP:HB2	1.60	0.81

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:182:G:H4'	15:N:157:LEU:HD13	1.61	0.81
5:D:62:ARG:HA	5:D:65:MET:CE	2.10	0.81
11:J:55:GLN:HE21	11:J:124:ARG:HE	1.24	0.81
15:N:35:PRO:CG	15:N:38:VAL:HG23	2.09	0.81
5:D:162:MET:HE3	5:D:308:LEU:HD21	1.59	0.81
1:A:962:C:H1'	16:O:5:ARG:NH1	1.96	0.81
4:C:109:GLU:HG2	4:C:116:GLY:H	1.46	0.81
1:A:2506:A:O2'	1:A:2507:G:H8	1.63	0.81
31:4:60:LYS:HG3	31:4:61:PRO:HD2	1.63	0.81
1:A:236:A:H4'	1:A:237:G:H5'	1.62	0.81
1:A:2533:C:H6	1:A:2533:C:H5'	1.45	0.81
1:A:870:G:H2'	1:A:871:G:H5"	1.61	0.80
38:A:6363:HOH:O	15:N:178:LYS:HB2	1.79	0.80
9:H:63:ILE:HB	9:H:64:PRO:HD3	1.64	0.80
9:H:91:VAL:HG12	9:H:92:GLY:N	1.96	0.80
22:U:52:ARG:HB2	22:U:95:ASN:HB3	1.63	0.80
9:H:91:VAL:HG12	9:H:92:GLY:H	1.43	0.80
11:J:162:SER:HB2	11:J:163:PRO:CD	2.10	0.80
38:A:5284:HOH:O	15:N:170:CYS:SG	2.40	0.80
6:E:242:GLU:HG3	38:E:8385:HOH:O	1.81	0.80
28:1:61:GLY:HA3	38:1:8425:HOH:O	1.82	0.80
1:A:1603:A:H5'	1:A:1605:G:O4'	1.81	0.80
11:J:47:GLU:HB3	11:J:133:ILE:HD13	1.64	0.80
11:J:49:VAL:O	11:J:157:ILE:HG23	1.81	0.80
6:E:115:LEU:HD13	6:E:223:LEU:HD21	1.62	0.80
11:J:14:TYR:H	11:J:91:HIS:CE1	2.00	0.80
20:S:99:ALA:HB1	20:S:109:MET:CE	2.11	0.80
4:C:69:LEU:HD21	4:C:120:ARG:HB3	1.61	0.80
31:4:25:VAL:HG22	31:4:68:LYS:HG3	1.62	0.80
1:A:657:G:OP1	6:E:27:ARG:NH2	2.15	0.79
5:D:62:ARG:HA	5:D:65:MET:HE2	1.62	0.79
38:A:4357:HOH:O	15:N:14:ARG:HG2	1.79	0.79
5:D:238:ASN:ND2	5:D:240:GLY:H	1.78	0.79
1:A:111:C:O2'	29:2:20:ARG:HG2	1.82	0.79
4:C:192:VAL:HG12	4:C:207:GLN:HB3	1.65	0.79
11:J:139:ASP:HA	38:J:8372:HOH:O	1.83	0.79
15:N:52:LEU:HD13	15:N:116:ASN:HB3	1.64	0.79
27:Z:220:GLU:HG2	38:Z:8545:HOH:O	1.80	0.79
16:O:83:LEU:HD13	16:O:175:LEU:HD23	1.65	0.79
1:A:1118:A:C8	1:A:1118:A:H3'	2.18	0.79
38:A:3234:HOH:O	15:N:157:LEU:HD11	1.83	0.78

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:F:64:ARG:HG2	7:F:67:ASP:HB3	1.64	0.78
1:A:282:C:H1'	1:A:368:C:H42	1.49	0.78
2:B:3023:U:H6	2:B:3023:U:H5"	1.46	0.78
1:A:1625:U:H4'	38:A:4165:HOH:O	1.84	0.78
6:E:5:ILE:HD11	6:E:16:VAL:HG23	1.65	0.78
2:B:3025:G:H3'	2:B:3026:C:H5'	1.64	0.78
6:E:115:LEU:HD21	6:E:243:VAL:HG13	1.64	0.78
8:G:81:GLU:HG2	8:G:134:SER:HB3	1.64	0.78
10:I:12:ILE:HA	38:I:4499:HOH:O	1.83	0.78
27:Z:186:ARG:HG2	27:Z:186:ARG:HH11	1.48	0.78
2:B:3006:C:H5"	16:O:37:ARG:HH12	1.48	0.78
6:E:1:MET:HG2	6:E:2:GLN:H	1.48	0.78
1:A:1118:A:H3'	1:A:1118:A:H8	1.47	0.77
1:A:1160:G:C5'	1:A:1161:A:H5'	2.13	0.77
2:B:3025:G:H3'	2:B:3026:C:C5'	2.14	0.77
6:E:236:THR:HG21	38:E:8376:HOH:O	1.83	0.77
1:A:182:G:H5'	38:A:4644:HOH:O	1.83	0.77
1:A:871:G:H8	1:A:871:G:C5'	1.98	0.77
5:D:179:LEU:O	5:D:183:GLU:HG2	1.84	0.77
3:5:74:C:H2'	3:5:75:C:C5'	2.13	0.77
16:O:113:SER:HB2	38:O:8560:HOH:O	1.84	0.77
1:A:2526:C:O2'	1:A:2527:U:H5'	1.85	0.77
5:D:238:ASN:HD22	5:D:240:GLY:N	1.80	0.77
13:L:74:VAL:CG1	13:L:113:ILE:HG12	2.13	0.76
28:1:40:PRO:HD3	28:1:47:LEU:HD11	1.65	0.76
1:A:1450:C:H4'	1:A:1451:C:OP2	1.86	0.76
11:J:2:PRO:HB2	38:J:8366:HOH:O	1.85	0.76
12:K:19:MET:HE3	12:K:132:LEU:HD11	1.66	0.76
1:A:1834:C:H2'	1:A:1840:A:N6	1.99	0.76
38:A:3191:HOH:O	15:N:79:LYS:HD3	1.84	0.76
3:5:74:C:C2'	3:5:75:C:H5'	2.14	0.76
14:M:143:THR:HG21	38:M:8541:HOH:O	1.86	0.76
16:O:87:LEU:HD12	16:O:186:LEU:HD21	1.67	0.76
1:A:2716:G:H5"	5:D:206:THR:HG21	1.67	0.76
7:F:25:MET:HE1	7:F:37:ALA:HB1	1.67	0.76
1:A:1684:A:H1'	30:3:43:ARG:HH22	1.48	0.76
1:A:2783:A:H3'	38:A:4722:HOH:O	1.86	0.76
15:N:172:GLY:O	15:N:183:VAL:HG11	1.84	0.76
15:N:139:PRO:O	15:N:140:ALA:HB3	1.85	0.76
1:A:877:G:H5'	1:A:878:G:OP1	1.85	0.76
1:A:2908:A:H2'	1:A:2909:G:O4'	1.87	0.76

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:D:162:MET:CE	5:D:308:LEU:HD21	2.16	0.75
5:D:168:GLY:N	5:D:174:ARG:HD3	2.01	0.75
14:M:148:GLU:HA	38:M:8574:HOH:O	1.85	0.75
18:Q:115:SER:OG	18:Q:118:GLN:HG3	1.86	0.75
4:C:35:GLY:O	4:C:36:ASP:HB3	1.85	0.75
12:K:93:ARG:HB3	12:K:93:ARG:HH11	1.48	0.75
7:F:55:LYS:HA	38:F:6752:HOH:O	1.86	0.75
8:G:166:VAL:HG12	38:G:3134:HOH:O	1.86	0.75
16:O:48:VAL:CG1	16:O:55:ASP:HB3	2.15	0.75
26:Y:72:VAL:HG22	26:Y:85:VAL:HG12	1.68	0.75
1:A:1878:G:H1'	38:A:5614:HOH:O	1.84	0.75
1:A:2676:C:H4'	12:K:70:PHE:CE1	2.21	0.75
38:A:5021:HOH:O	15:N:58:GLN:HG3	1.87	0.75
20:S:18:LEU:HD12	20:S:143:VAL:HG11	1.66	0.75
23:V:14:GLU:O	23:V:17:THR:HB	1.87	0.75
24:W:1:THR:HG23	24:W:2:VAL:H	1.49	0.75
5:D:190:MET:HE2	5:D:194:PHE:CD1	2.21	0.75
14:M:133:VAL:HB	38:M:8559:HOH:O	1.86	0.75
15:N:164:THR:HG23	15:N:165:SER:N	2.01	0.75
1:A:383:A:H4'	38:A:4821:HOH:O	1.86	0.75
25:X:21:LEU:HD21	25:X:48:VAL:CG1	2.17	0.75
15:N:64:ARG:HD2	38:N:8590:HOH:O	1.87	0.74
24:W:39:ALA:N	24:W:40:PRO:HD2	2.02	0.74
25:X:6:GLN:HB2	25:X:26:ILE:HD12	1.69	0.74
1:A:214:U:H5'	38:A:5633:HOH:O	1.87	0.74
1:A:450:C:OP1	6:E:184:ARG:NH2	2.19	0.74
4:C:199:HIS:HD2	4:C:201:PHE:HB2	1.53	0.74
13:L:22:ASP:HB2	38:L:5264:HOH:O	1.87	0.74
15:N:94:LYS:HE3	38:N:8587:HOH:O	1.87	0.74
5:D:41:PHE:HA	5:D:79:MET:HE2	1.69	0.74
1:A:289:G:H22	1:A:363:A:H2	1.35	0.74
5:D:168:GLY:H	5:D:174:ARG:HD3	1.51	0.74
5:D:217:ARG:HG3	5:D:257:THR:HG22	1.69	0.74
25:X:21:LEU:HD21	25:X:48:VAL:HG11	1.67	0.74
1:A:1666:C:O2'	1:A:1667:A:H5"	1.88	0.74
15:N:164:THR:HG22	15:N:167:GLY:N	2.02	0.74
1:A:1372:A:H3'	38:A:6680:HOH:O	1.88	0.74
5:D:212:GLN:HB2	5:D:257:THR:HG21	1.70	0.74
13:L:62:PRO:HG3	13:L:65:ARG:HH21	1.51	0.74
1:A:21:G:C5'	20:S:2:ILE:HA	2.17	0.74
1:A:338:C:H4'	6:E:174:ILE:CD1	2.18	0.74

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:396:U:H1'	38:A:7119:HOH:O	1.86	0.74
11:J:140:PRO:HB3	38:J:8381:HOH:O	1.88	0.74
29:2:1:THR:HB	38:2:8461:HOH:O	1.87	0.74
6:E:162:VAL:HG13	6:E:232:LEU:HD21	1.70	0.73
1:A:1328:A:OP1	27:Z:169:ARG:HD2	1.87	0.73
1:A:1187:U:HO2'	1:A:1189:A:H2	1.35	0.73
1:A:1474:C:H5'	1:A:1474:C:C6	2.21	0.73
1:A:2414:A:H2'	1:A:2415:A:C8	2.23	0.73
6:E:233:THR:HG22	6:E:234:VAL:H	1.53	0.73
17:P:32:ARG:O	17:P:32:ARG:HD3	1.88	0.73
27:Z:185:VAL:HG12	38:Z:8567:HOH:O	1.88	0.73
12:K:107:ASN:ND2	12:K:109:TYR:H	1.85	0.73
11:J:162:SER:CB	11:J:163:PRO:HD3	2.17	0.73
28:1:37:HIS:HB2	28:1:47:LEU:HB2	1.70	0.73
20:S:14:ALA:HB3	20:S:147:LEU:HB2	1.69	0.73
6:E:236:THR:HA	38:E:8454:HOH:O	1.88	0.73
8:G:20:ILE:CD1	8:G:40:VAL:HG11	2.19	0.73
11:J:47:GLU:HB3	11:J:133:ILE:CD1	2.19	0.73
25:X:22:GLU:HG2	25:X:27:HIS:CD2	2.23	0.73
1:A:506:G:H22	1:A:509:A:C5'	2.00	0.73
4:C:37:VAL:HG22	38:C:8592:HOH:O	1.88	0.73
7:F:88:LEU:HB2	7:F:89:PRO:HD3	1.71	0.73
25:X:4:LEU:HD22	25:X:52:VAL:CG2	2.18	0.73
1:A:1116:U:O2'	1:A:1118:A:H2	1.69	0.73
1:A:1191:A:H3'	1:A:1192:A:H5"	1.69	0.73
1:A:1164:U:H3	1:A:1192:A:H2	1.37	0.72
17:P:47:ARG:HH11	17:P:47:ARG:HG3	1.53	0.72
27:Z:216:ARG:HD3	38:Z:8566:HOH:O	1.89	0.72
7:F:135:VAL:HG21	7:F:139:TYR:CD1	2.24	0.72
26:Y:15:ARG:HB3	26:Y:15:ARG:HH11	1.53	0.72
1:A:272:A:H3'	38:A:7022:HOH:O	1.90	0.72
1:A:2851:G:O2'	1:A:2852:A:H5'	1.89	0.72
2:B:3048:C:H4'	16:O:141:ARG:HH21	1.54	0.72
6:E:2:GLN:HB3	38:E:8335:HOH:O	1.89	0.72
25:X:122:ARG:HG2	25:X:122:ARG:HH11	1.54	0.72
1:A:541:C:H2'	1:A:542:A:C5'	2.18	0.72
23:V:46:ALA:HB1	23:V:52:THR:HG21	1.72	0.72
1:A:56:G:H5"	24:W:50:ARG:HH12	1.55	0.72
12:K:19:MET:CE	12:K:132:LEU:HD11	2.20	0.72
16:O:159:TYR:HB3	16:O:162:ASP:HB2	1.72	0.72
19:R:11:ARG:HD3	38:R:5620:HOH:O	1.90	0.72

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:E:236:THR:CG2	6:E:239:ALA:H	1.94	0.72
7:F:57:THR:HG23	7:F:63:ILE:HG22	1.72	0.72
22:U:63:ILE:HD11	22:U:75:GLU:HB2	1.70	0.72
1:A:2420:G:O2'	1:A:2421:G:H5'	1.90	0.72
1:A:1667:A:H5'	1:A:1667:A:C8	2.23	0.72
4:C:153:ARG:HB2	4:C:153:ARG:HH11	1.55	0.72
12:K:131:THR:HG22	12:K:134:GLU:H	1.53	0.72
14:M:77:ALA:HB3	38:M:8531:HOH:O	1.90	0.72
1:A:962:C:H1'	16:O:5:ARG:HH12	1.55	0.71
1:A:1641:A:H2'	1:A:1642:A:H5'	1.72	0.71
28:1:46:LYS:HD3	28:1:59:HIS:HB2	1.70	0.71
1:A:284:C:H4'	1:A:285:A:O5'	1.88	0.71
7:F:64:ARG:CG	7:F:67:ASP:HB3	2.21	0.71
16:O:4:PRO:HD2	38:O:8558:HOH:O	1.90	0.71
25:X:4:LEU:HD23	25:X:54:PHE:HB3	1.69	0.71
1:A:2502:C:C2'	1:A:2503:A:H5'	2.20	0.71
1:A:2578:G:H5'	1:A:2578:G:H8	1.54	0.71
9:H:58:GLU:HA	9:H:61:MET:HE2	1.71	0.71
6:E:237:GLU:HB2	38:E:8435:HOH:O	1.89	0.71
1:A:1160:G:H5'	1:A:1161:A:C5'	2.20	0.71
1:A:2502:C:H4'	11:J:151:MET:HG2	1.72	0.71
2:B:3056:A:C2'	2:B:3057:A:H5"	2.20	0.71
9:H:99:THR:HA	38:H:3461:HOH:O	1.91	0.71
24:W:42:ASN:HB3	38:W:7247:HOH:O	1.90	0.71
25:X:13:MET:HE3	25:X:17:ILE:HG22	1.72	0.71
1:A:1701:A:H4'	1:A:1702:U:H5"	1.71	0.71
38:A:3063:HOH:O	15:N:152:ARG:HG3	1.89	0.71
5:D:195:ARG:HG2	5:D:323:LEU:HD22	1.71	0.71
12:K:99:GLU:HA	38:K:7377:HOH:O	1.88	0.71
4:C:191:GLY:HA2	4:C:194:MET:CE	2.21	0.71
25:X:88:THR:HG22	25:X:89:ASP:H	1.54	0.71
1:A:2359:G:H3'	38:A:5184:HOH:O	1.89	0.71
30:3:39:ARG:HG2	38:3:3143:HOH:O	1.89	0.71
1:A:281:U:H3'	38:A:6697:HOH:O	1.90	0.71
1:A:544:G:H2'	1:A:545:G:H5"	1.73	0.70
1:A:603:A:H5"	1:A:604:G:OP1	1.91	0.70
38:A:6516:HOH:O	4:C:211:LYS:HG2	1.90	0.70
11:J:150:LYS:HB2	11:J:157:ILE:HD12	1.73	0.70
11:J:142:VAL:HG13	38:J:8381:HOH:O	1.90	0.70
1:A:1182:C:H1'	1:A:1192:A:H8	1.57	0.70
7:F:136:ARG:HD2	7:F:155:HIS:O	1.90	0.70

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:J:59:ASN:HD22	11:J:59:ASN:N	1.87	0.70
1:A:31:C:H2'	38:A:7178:HOH:O	1.91	0.70
1:A:2827:A:H2'	1:A:2828:G:O4'	1.90	0.70
1:A:2890:A:H1'	23:V:56:ARG:NH2	2.06	0.70
9:H:53:ASP:OD1	9:H:80:GLN:HB2	1.90	0.70
11:J:45:GLN:HE21	11:J:135:TRP:HE1	1.39	0.70
20:S:9:ASP:O	20:S:13:THR:HB	1.91	0.70
7:F:41:LEU:HA	7:F:44:ILE:HG22	1.74	0.70
8:G:107:PHE:CE2	8:G:108:LEU:HD13	2.27	0.70
31:4:70:ARG:HD3	38:4:8538:HOH:O	1.90	0.70
4:C:170:VAL:HG22	28:1:22:ILE:HG23	1.72	0.70
11:J:46:VAL:HG12	11:J:146:TRP:HZ3	1.57	0.70
1:A:1185:U:H2'	1:A:1186:C:C6	2.27	0.70
1:A:1835:U:C5	1:A:1840:A:N7	2.60	0.70
22:U:61:GLU:HG3	38:U:3851:HOH:O	1.91	0.70
10:I:23:ILE:HD13	10:I:67:LEU:HD23	1.74	0.69
1:A:188:C:H5"	15:N:163:LEU:HD21	1.74	0.69
1:A:2031:C:O3'	38:A:4015:HOH:O	2.10	0.69
1:A:2862:G:H4'	5:D:336:GLN:O	1.91	0.69
4:C:131:HIS:O	4:C:132:ASP:HB2	1.91	0.69
38:A:7070:HOH:O	28:1:31:ILE:HG13	1.92	0.69
4:C:191:GLY:HA2	4:C:194:MET:HE3	1.72	0.69
7:F:27:ILE:HG22	7:F:28:GLY:N	2.07	0.69
26:Y:71:ARG:HB3	26:Y:88:GLU:OE1	1.92	0.69
4:C:94:LEU:HG	4:C:99:ILE:HD11	1.73	0.69
15:N:139:PRO:O	15:N:140:ALA:CB	2.40	0.69
11:J:55:GLN:NE2	11:J:124:ARG:HE	1.90	0.69
15:N:87:MET:HB3	31:4:46:ILE:HG21	1.73	0.69
1:A:1165:G:H4'	1:A:1174:A:O2'	1.93	0.69
1:A:1206:U:H6	1:A:1206:U:H5'	1.56	0.69
1:A:1505:U:H6	1:A:1505:U:H5'	1.56	0.69
4:C:105:VAL:HG11	4:C:154:ALA:HB1	1.74	0.69
22:U:9:LYS:HE3	22:U:13:ARG:HH11	1.58	0.69
1:A:338:C:H5"	38:E:8426:HOH:O	1.93	0.69
1:A:553:G:P	27:Z:204:ARG:HH22	2.16	0.69
2:B:3049:G:H5"	38:B:8465:HOH:O	1.92	0.69
4:C:100:PRO:HG2	4:C:103:VAL:HG21	1.73	0.69
6:E:47:GLY:HA2	6:E:92:PRO:HB2	1.74	0.69
6:E:236:THR:H	6:E:239:ALA:HB3	1.58	0.69
20:S:18:LEU:HB2	20:S:143:VAL:HG12	1.75	0.69
22:U:41:ARG:HG2	22:U:41:ARG:HH11	1.56	0.69

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:U:101:LEU:HD13	22:U:112:LEU:HD11	1.75	0.69
27:Z:99:ALA:HB2	27:Z:233:TYR:CZ	2.28	0.69
1:A:1751:G:C2'	1:A:1752:G:H5"	2.22	0.69
15:N:57:LYS:HE2	15:N:140:ALA:O	1.93	0.69
16:O:71:TRP:CE3	16:O:175:LEU:HD22	2.28	0.69
1:A:545:G:H5'	1:A:545:G:C8	2.26	0.69
1:A:871:G:C8	1:A:871:G:C5'	2.75	0.69
1:A:1118:A:H62	1:A:1244:U:H3	1.39	0.69
5:D:145:HIS:HD2	5:D:146:THR:O	1.76	0.69
2:B:3014:G:H5'	2:B:3014:G:H8	1.56	0.68
4:C:109:GLU:HG2	4:C:116:GLY:N	2.08	0.68
25:X:88:THR:HG23	25:X:110:GLN:HE21	1.57	0.68
1:A:56:G:H5"	24:W:50:ARG:NH1	2.09	0.68
24:W:12:THR:HG22	24:W:15:GLU:CG	2.22	0.68
1:A:2587:U:H2'	1:A:2589:U:H5"	1.74	0.68
1:A:2897:C:H2'	1:A:2898:G:H8	1.58	0.68
12:K:45:VAL:HG23	12:K:130:VAL:O	1.92	0.68
30:3:41:HIS:N	30:3:45:ASN:HD22	1.91	0.68
12:K:103:VAL:HG12	38:K:5907:HOH:O	1.92	0.68
1:A:2426:G:H1'	38:A:5585:HOH:O	1.93	0.68
1:A:2054:A:N3	20:S:128:ARG:NH2	2.41	0.68
20:S:18:LEU:HB2	20:S:143:VAL:CG1	2.24	0.68
5:D:304:PRO:HD2	5:D:307:ARG:HD2	1.76	0.68
1:A:2502:C:H2'	1:A:2503:A:H5'	1.76	0.68
16:O:48:VAL:HG11	16:O:55:ASP:HB3	1.76	0.68
16:O:183:ASP:OD2	16:O:186:LEU:HD12	1.93	0.68
26:Y:76:ARG:HH11	26:Y:76:ARG:HG3	1.58	0.68
1:A:281:U:H2'	1:A:282:C:O4'	1.94	0.67
11:J:35:ASN:ND2	11:J:80:ASN:HA	2.10	0.67
1:A:681:G:H5'	1:A:681:G:N3	2.10	0.67
1:A:2310:G:OP2	11:J:114:PRO:HD2	1.95	0.67
1:A:2638:G:H1'	38:A:7249:HOH:O	1.93	0.67
11:J:141:ASN:HA	38:J:8368:HOH:O	1.95	0.67
25:X:21:LEU:HD22	25:X:26:ILE:HD11	1.75	0.67
1:A:183:A:H5'	15:N:157:LEU:HD12	1.77	0.67
5:D:314:ALA:HB3	5:D:317:PRO:HG3	1.76	0.67
7:F:105:SER:CB	7:F:131:THR:HG23	2.22	0.67
10:I:64:ASN:O	10:I:68:GLU:HG3	1.94	0.67
27:Z:107:PRO:HB3	27:Z:182:PHE:CD2	2.29	0.67
27:Z:235:GLU:H	27:Z:235:GLU:CD	1.97	0.67
1:A:2878:U:H2'	1:A:2879:A:O4'	1.95	0.67

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:C:88:ILE:HD13	4:C:100:PRO:HD3	1.76	0.67
6:E:140:VAL:HB	38:E:8454:HOH:O	1.93	0.67
14:M:136:ALA:HB3	38:M:8575:HOH:O	1.94	0.67
1:A:1080:C:H4'	1:A:1081:A:OP1	1.94	0.67
1:A:1120:U:H6	1:A:1120:U:H5"	1.59	0.67
1:A:2533:C:H5'	1:A:2533:C:C6	2.28	0.67
26:Y:30:MET:HE1	26:Y:55:ASN:HA	1.76	0.67
1:A:2748:G:H5'	38:A:7033:HOH:O	1.95	0.67
5:D:18:ARG:HG3	5:D:256:GLN:HG3	1.76	0.67
5:D:175:LEU:HD23	5:D:175:LEU:C	2.14	0.67
18:Q:143:ALA:HA	38:Q:168:HOH:O	1.95	0.67
1:A:694:A:H2'	1:A:695:C:H5'	1.75	0.67
5:D:264:GLU:HG2	5:D:267:LYS:HE2	1.76	0.67
25:X:65:VAL:HA	25:X:68:THR:HG22	1.76	0.67
25:X:137:GLN:HE21	25:X:141:HIS:HE1	1.41	0.67
31:4:70:ARG:HG2	31:4:77:ALA:HB2	1.76	0.67
10:I:12:ILE:N	10:I:13:PRO:HD3	2.09	0.67
1:A:282:C:O2'	1:A:283:U:H5'	1.94	0.67
1:A:2301:A:H5"	1:A:2302:A:H5'	1.76	0.67
1:A:1119:G:N2	1:A:1246:A:C2	2.62	0.67
4:C:33:GLU:O	4:C:34:ASP:HB2	1.94	0.67
16:O:169:PRO:O	16:O:172:PHE:HB3	1.95	0.67
1:A:1596:U:H2'	1:A:1598:A:OP2	1.94	0.66
1:A:1771:U:H4'	28:1:20:LEU:HD21	1.75	0.66
8:G:11:VAL:HG12	8:G:12:ASP:N	2.11	0.66
18:Q:59:ARG:NH2	18:Q:66:GLN:HE22	1.92	0.66
21:T:23:LYS:HE2	38:T:8330:HOH:O	1.95	0.66
1:A:2676:C:H4'	12:K:70:PHE:HE1	1.60	0.66
6:E:76:ARG:HD3	38:E:8369:HOH:O	1.95	0.66
11:J:59:ASN:H	11:J:59:ASN:ND2	1.91	0.66
38:L:408:HOH:O	23:V:37:GLU:HB3	1.94	0.66
21:T:51:GLN:HE21	21:T:53:ASN:HD21	1.41	0.66
25:X:21:LEU:HD13	25:X:26:ILE:HD11	1.76	0.66
1:A:2256:G:H2'	1:A:2257:G:H5'	1.78	0.66
7:F:65:GLU:HG3	38:F:6752:HOH:O	1.94	0.66
15:N:37:VAL:HG21	15:N:108:LYS:HG3	1.76	0.66
15:N:65:VAL:HG21	15:N:105:ALA:HB2	1.77	0.66
15:N:138:HIS:ND1	15:N:139:PRO:O	2.23	0.66
27:Z:141:THR:HG23	38:Z:8586:HOH:O	1.95	0.66
1:A:558:C:H2'	1:A:559:U:H5'	1.75	0.66
14:M:54:PRO:HG2	14:M:57:VAL:HG21	1.78	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:N:169:ARG:HD2	38:N:8596:HOH:O	1.94	0.66
17:P:87:THR:O	17:P:91:GLN:HG3	1.96	0.66
1:A:470:U:O2'	29:2:16:HIS:HD2	1.77	0.66
1:A:1741:U:H5'	1:A:1742:A:OP1	1.96	0.66
1:A:2840:A:OP1	5:D:211:THR:HG23	1.94	0.66
4:C:105:VAL:CG1	4:C:154:ALA:HB1	2.25	0.66
6:E:162:VAL:HG12	6:E:192:ILE:HD11	1.78	0.66
11:J:56:ILE:HG22	11:J:61:LEU:HD22	1.77	0.66
16:O:164:ASP:CG	16:O:167:ASP:HA	2.16	0.66
1:A:1120:U:H5"	1:A:1120:U:C6	2.31	0.66
5:D:71:VAL:HG11	5:D:296:LEU:HB3	1.75	0.66
9:H:46:GLU:O	9:H:73:PRO:HD2	1.95	0.66
27:Z:151:SER:HB3	27:Z:154:ARG:HB3	1.77	0.66
29:2:25:LYS:HG2	29:2:25:LYS:O	1.94	0.66
1:A:1666:C:H2'	1:A:1667:A:H5'	1.76	0.66
38:A:4461:HOH:O	11:J:57:ARG:HG3	1.93	0.66
7:F:19:GLU:O	7:F:20:LYS:HG2	1.96	0.66
11:J:31:PHE:CD2	11:J:85:ILE:HG23	2.31	0.66
24:W:4:HIS:HB3	38:W:6622:HOH:O	1.95	0.66
6:E:214:THR:HG21	38:E:8408:HOH:O	1.94	0.66
7:F:140:ARG:O	7:F:144:ARG:HG2	1.96	0.66
12:K:39:VAL:HG12	12:K:40:ASN:ND2	2.11	0.66
14:M:68:GLU:HA	38:M:8545:HOH:O	1.95	0.66
14:M:143:THR:HG22	14:M:144:ASP:N	2.11	0.66
18:Q:64:GLU:HG2	38:Q:169:HOH:O	1.95	0.66
28:1:28:ASP:O	28:1:31:ILE:HG22	1.95	0.66
1:A:1130:U:H5'	38:A:7161:HOH:O	1.96	0.65
9:H:50:VAL:HG21	9:H:63:ILE:HG21	1.77	0.65
11:J:44:ALA:HA	11:J:163:PRO:O	1.96	0.65
25:X:90:TYR:CE2	25:X:99:ALA:HB2	2.31	0.65
1:A:1377:C:H6	1:A:1377:C:H5'	1.61	0.65
4:C:95:PRO:HG2	4:C:98:GLU:HG2	1.78	0.65
6:E:142:ASP:OD1	6:E:237:GLU:HB3	1.95	0.65
18:Q:115:SER:O	18:Q:117:SER:N	2.30	0.65
20:S:132:ARG:HG2	20:S:133:ALA:N	2.12	0.65
22:U:32:ARG:NH1	22:U:38:ARG:HH12	1.93	0.65
1:A:656:G:OP2	17:P:37:ARG:HD2	1.96	0.65
1:A:2508:C:H2'	38:A:6243:HOH:O	1.95	0.65
7:F:64:ARG:CD	7:F:67:ASP:HB3	2.25	0.65
11:J:84:ARG:NH2	11:J:135:TRP:HH2	1.95	0.65
15:N:52:LEU:HD21	38:N:8623:HOH:O	1.95	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:S:33:ARG:NH1	38:S:8544:HOH:O	2.29	0.65
25:X:88:THR:HG23	25:X:110:GLN:HB3	1.78	0.65
28:1:49:ARG:HD2	38:1:8427:HOH:O	1.97	0.65
1:A:1589:G:N2	1:A:1605:G:H1'	2.11	0.65
1:A:1593:C:H5'	18:Q:116:SER:O	1.96	0.65
1:A:1919:A:H4'	38:A:4344:HOH:O	1.96	0.65
16:O:143:ARG:HA	16:O:172:PHE:CD2	2.32	0.65
1:A:42:C:H1'	38:A:4174:HOH:O	1.95	0.65
6:E:5:ILE:HD11	6:E:16:VAL:CG2	2.26	0.65
7:F:146:LYS:HZ1	16:O:107:ASN:HD21	1.45	0.65
11:J:46:VAL:O	11:J:146:TRP:HH2	1.80	0.65
25:X:81:ASP:OD1	25:X:92:ASP:HB2	1.96	0.65
27:Z:187:VAL:HG23	27:Z:192:ASP:CB	2.25	0.65
27:Z:189:ASN:HD22	27:Z:189:ASN:C	2.00	0.65
28:1:25:ARG:O	28:1:29:VAL:HG23	1.97	0.65
1:A:2780:C:H1'	8:G:143:GLN:HE21	1.60	0.65
21:T:57:THR:HG22	21:T:59:ASP:H	1.61	0.65
1:A:1118:A:H8	1:A:1119:G:H5"	1.61	0.65
1:A:1209:C:H4'	38:A:4773:HOH:O	1.95	0.65
5:D:297:VAL:HB	38:D:8607:HOH:O	1.97	0.65
15:N:174:ARG:HG3	38:N:8521:HOH:O	1.96	0.65
18:Q:103:THR:HA	18:Q:106:ARG:NH1	2.12	0.65
26:Y:43:VAL:HG12	26:Y:44:ASP:N	2.11	0.65
6:E:104:ASP:HA	6:E:107:ARG:HH12	1.61	0.65
7:F:135:VAL:HG22	7:F:136:ARG:H	1.61	0.65
15:N:30:GLU:O	15:N:34:GLU:HG3	1.97	0.65
1:A:1028:U:H1'	38:A:3156:HOH:O	1.96	0.64
38:A:3171:HOH:O	15:N:79:LYS:HD2	1.96	0.64
5:D:55:ASN:HB3	5:D:63:GLU:HA	1.79	0.64
8:G:132:THR:HB	38:G:2227:HOH:O	1.96	0.64
11:J:130:HIS:CD2	11:J:133:ILE:HD11	2.32	0.64
15:N:34:GLU:HB3	15:N:35:PRO:HD2	1.79	0.64
1:A:2768:A:H2'	1:A:2769:C:O4'	1.96	0.64
6:E:139:VAL:HG13	38:E:8451:HOH:O	1.97	0.64
7:F:69:ILE:HG22	7:F:69:ILE:O	1.96	0.64
11:J:33:MET:HB2	11:J:83:PHE:HB3	1.80	0.64
16:O:154:LEU:O	16:O:155:GLU:HB3	1.98	0.64
25:X:68:THR:HG23	25:X:69:ARG:HG2	1.77	0.64
5:D:140:LEU:HD23	38:D:8583:HOH:O	1.98	0.64
12:K:133:GLY:O	12:K:137:GLU:HG3	1.97	0.64
17:P:42:GLU:HB2	38:P:2176:HOH:O	1.96	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2748:G:H2'	38:A:7033:HOH:O	1.97	0.64
4:C:81:GLN:HB2	4:C:92:ASN:ND2	2.11	0.64
6:E:78:ARG:HG3	6:E:78:ARG:HH11	1.61	0.64
17:P:44:ASN:OD1	17:P:65:LEU:HB2	1.96	0.64
27:Z:212:ARG:HD2	38:Z:8598:HOH:O	1.97	0.64
7:F:54:ALA:CB	7:F:69:ILE:HD12	2.28	0.64
7:F:67:ASP:O	7:F:69:ILE:HG13	1.98	0.64
16:O:164:ASP:OD2	16:O:167:ASP:HA	1.98	0.64
20:S:39:THR:HG23	20:S:107:GLU:O	1.98	0.64
31:4:73:GLU:HB3	38:4:8558:HOH:O	1.96	0.64
1:A:2472:C:O2'	1:A:2634:G:H4'	1.97	0.64
1:A:1266:U:H4'	27:Z:115:ARG:HH21	1.62	0.64
7:F:99:ASP:HB3	7:F:103:ASN:H	1.62	0.64
1:A:272:A:H5'	1:A:273:G:OP2	1.98	0.64
1:A:559:U:H2'	1:A:560:C:O4'	1.98	0.64
1:A:2346:C:O2'	7:F:52:THR:HG21	1.97	0.64
2:B:3023:U:C3'	2:B:3024:U:H5"	2.21	0.64
5:D:36:PRO:HA	5:D:168:GLY:CA	2.28	0.64
7:F:23:VAL:HG23	7:F:23:VAL:O	1.97	0.64
7:F:38:GLU:OE2	7:F:51:ARG:CZ	2.45	0.64
12:K:74:ARG:HH11	12:K:74:ARG:CB	2.11	0.64
16:O:71:TRP:HE3	16:O:175:LEU:HD22	1.63	0.64
17:P:96:VAL:HA	38:P:4258:HOH:O	1.98	0.64
23:V:14:GLU:OE1	23:V:15:PRO:HD2	1.98	0.64
1:A:506:G:H22	1:A:509:A:H5"	1.63	0.63
18:Q:103:THR:HB	38:Q:180:HOH:O	1.98	0.63
1:A:1285:U:H4'	25:X:74:GLU:OE1	1.98	0.63
8:G:7:ILE:HD11	8:G:11:VAL:C	2.18	0.63
13:L:49:LEU:HD21	13:L:74:VAL:O	1.99	0.63
17:P:32:ARG:HG2	38:P:2336:HOH:O	1.97	0.63
1:A:506:G:H22	1:A:509:A:H5'	1.62	0.63
1:A:2435:U:H1'	38:A:4921:HOH:O	1.97	0.63
2:B:3092:G:H2'	2:B:3093:A:C8	2.33	0.63
28:1:53:GLY:HA2	28:1:67:GLY:O	1.98	0.63
7:F:36:ASN:HA	38:F:7500:HOH:O	1.98	0.63
11:J:26:LYS:HD2	11:J:28:ILE:HB	1.78	0.63
15:N:38:VAL:C	15:N:63:VAL:HG13	2.19	0.63
16:O:86:LEU:HD12	16:O:125:ALA:HB2	1.79	0.63
25:X:21:LEU:HD22	25:X:26:ILE:CD1	2.29	0.63
38:A:3734:HOH:O	30:3:38:LYS:HE3	1.99	0.63
9:H:91:VAL:CG1	9:H:92:GLY:H	2.11	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2064:U:H4'	1:A:2653:A:OP1	1.98	0.63
5:D:305:ASP:O	5:D:306:LYS:HB2	1.98	0.63
8:G:15:GLN:HG3	8:G:20:ILE:HG12	1.81	0.63
38:A:8913:HOH:O	15:N:94:LYS:HE2	1.98	0.63
8:G:31:ARG:HH12	8:G:68:HIS:CD2	2.17	0.63
14:M:145:LEU:O	14:M:148:GLU:HG3	1.98	0.63
1:A:157:G:H4'	15:N:95:LYS:HE3	1.80	0.63
1:A:2320:U:H4'	1:A:2321:A:O4'	1.98	0.63
2:B:3023:U:H5"	2:B:3023:U:C6	2.31	0.63
11:J:48:LEU:HG	11:J:157:ILE:HG21	1.79	0.63
15:N:149:TRP:O	15:N:152:ARG:HG2	1.99	0.63
21:T:37:VAL:O	21:T:41:VAL:HG23	1.98	0.63
27:Z:189:ASN:ND2	27:Z:192:ASP:H	1.97	0.63
5:D:275:GLY:O	5:D:291:ASP:HA	1.99	0.63
6:E:20:ASP:O	6:E:23:GLU:HB2	1.99	0.63
11:J:27:LYS:N	11:J:58:HIS:HD2	1.95	0.63
11:J:127:GLY:O	11:J:128:ALA:HB3	1.98	0.63
15:N:157:LEU:HB3	15:N:160:PHE:HD1	1.64	0.63
25:X:122:ARG:HH22	25:X:154:ARG:C	2.02	0.63
1:A:280:C:H2'	1:A:281:U:O4'	1.99	0.62
1:A:560:C:H42	1:A:597:A:H61	1.45	0.62
21:T:57:THR:HG22	21:T:59:ASP:N	2.13	0.62
1:A:585:C:H5"	38:A:4365:HOH:O	1.97	0.62
1:A:1333:U:H2'	1:A:1334:C:C6	2.35	0.62
1:A:1559:A:H1'	38:A:5357:HOH:O	1.99	0.62
38:A:4043:HOH:O	11:J:151:MET:HE2	1.98	0.62
10:I:63:ARG:N	38:I:2569:HOH:O	2.30	0.62
20:S:17:MET:HE1	20:S:19:ARG:NH2	2.13	0.62
20:S:40:ALA:O	20:S:44:VAL:HG23	1.99	0.62
38:B:8465:HOH:O	16:O:147:ILE:HD12	1.98	0.62
18:Q:10:ALA:HA	18:Q:13:VAL:HG12	1.81	0.62
2:B:3029:C:H2'	2:B:3030:C:H5'	1.81	0.62
1:A:2265:U:H2'	1:A:2266:A:C8	2.35	0.62
38:A:5703:HOH:O	5:D:2:GLN:HA	1.99	0.62
5:D:66:GLU:OE1	5:D:328:ARG:HD2	1.99	0.62
7:F:51:ARG:HD3	38:F:7636:HOH:O	1.99	0.62
22:U:47:THR:HB	22:U:100:ASP:HB3	1.81	0.62
26:Y:25:ARG:HD2	38:Y:3861:HOH:O	1.99	0.62
4:C:8:ARG:HG2	38:C:8550:HOH:O	2.00	0.62
4:C:53:ALA:HB3	38:C:8602:HOH:O	1.98	0.62
7:F:86:THR:C	7:F:89:PRO:HD2	2.19	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:F:97:GLN:HG2	7:F:97:GLN:O	1.98	0.62
8:G:77:THR:OG1	8:G:78:GLU:N	2.33	0.62
11:J:28:ILE:HA	11:J:62:GLU:OE1	2.00	0.62
11:J:47:GLU:CB	11:J:133:ILE:HD13	2.29	0.62
28:1:29:VAL:O	28:1:33:HIS:HB2	1.99	0.62
1:A:714:U:H3'	38:A:6432:HOH:O	2.00	0.62
4:C:210:GLY:HA3	38:C:8583:HOH:O	1.98	0.62
6:E:12:THR:HB	38:E:8445:HOH:O	1.99	0.62
7:F:37:ALA:O	7:F:40:ILE:HG12	1.99	0.62
8:G:137:ASP:O	8:G:141:VAL:HG23	2.00	0.62
9:H:2:VAL:HG22	9:H:57:GLU:OE1	2.00	0.62
11:J:45:GLN:HG3	11:J:135:TRP:NE1	2.15	0.62
11:J:166:ASN:N	11:J:166:ASN:HD22	1.96	0.62
27:Z:200:THR:HG22	27:Z:201:GLU:CG	2.29	0.62
1:A:2346:C:O5'	1:A:2346:C:H6	1.83	0.62
5:D:54:VAL:HB	38:D:8614:HOH:O	1.98	0.62
16:O:163:PHE:HE1	16:O:171:HIS:HD1	1.47	0.62
18:Q:71:LYS:HG3	18:Q:71:LYS:O	1.99	0.62
1:A:2364:A:H5"	19:R:15:LYS:HD3	1.82	0.62
2:B:3035:C:H5"	38:B:8453:HOH:O	1.99	0.62
11:J:26:LYS:HG2	11:J:28:ILE:H	1.63	0.62
15:N:134:ILE:HG23	15:N:141:ILE:HD13	1.81	0.62
1:A:797:A:C4'	28:1:10:ARG:N	2.63	0.62
2:B:3006:C:C5'	16:O:37:ARG:NH1	2.60	0.62
2:B:3028:U:H2'	2:B:3029:C:C6	2.35	0.62
4:C:190:ARG:NH2	4:C:207:GLN:OE1	2.33	0.62
5:D:221:GLN:HE22	13:L:42:ASN:HD22	1.48	0.62
7:F:35:ALA:N	38:F:5576:HOH:O	2.33	0.62
20:S:39:THR:HG22	20:S:42:GLU:H	1.63	0.62
22:U:50:VAL:HG12	22:U:56:ALA:HA	1.81	0.62
1:A:1187:U:O2'	1:A:1189:A:H2	1.83	0.61
14:M:30:ARG:NH2	38:M:8520:HOH:O	2.32	0.61
17:P:14:LEU:HD23	17:P:102:ILE:HD11	1.80	0.61
25:X:38:THR:HG22	25:X:39:ASP:H	1.65	0.61
28:1:26:VAL:O	28:1:30:GLU:HG3	1.99	0.61
7:F:146:LYS:NZ	16:O:107:ASN:ND2	2.47	0.61
8:G:5:LEU:HD21	8:G:66:GLN:HG3	1.81	0.61
8:G:15:GLN:NE2	8:G:40:VAL:O	2.33	0.61
10:I:64:ASN:HD22	10:I:64:ASN:N	1.97	0.61
11:J:29:ALA:HB3	11:J:65:ARG:NH1	2.07	0.61
23:V:9:CYS:CA	23:V:52:THR:HG23	2.27	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:X:4:LEU:O	25:X:32:CYS:HA	2.00	0.61
26:Y:78:GLU:HG2	26:Y:79:GLU:N	2.15	0.61
1:A:1654:U:H2'	4:C:47:HIS:HD2	1.65	0.61
5:D:30:PRO:HB2	5:D:39:GLN:NE2	2.14	0.61
38:E:8358:HOH:O	17:P:3:THR:HG21	2.01	0.61
13:L:115:ARG:HG3	13:L:116:GLU:N	2.13	0.61
15:N:104:ARG:O	15:N:108:LYS:HE2	2.00	0.61
16:O:33:ARG:NH1	16:O:103:ASP:OD2	2.32	0.61
20:S:82:GLU:O	20:S:86:LYS:HG3	2.00	0.61
1:A:2256:G:C2'	1:A:2257:G:H5'	2.30	0.61
1:A:559:U:H5'	1:A:559:U:H6	1.65	0.61
1:A:1299:G:O6	14:M:6:ARG:HD3	2.00	0.61
1:A:2241:C:O2'	1:A:2242:U:H5'	2.01	0.61
14:M:148:GLU:HB2	38:M:8589:HOH:O	1.99	0.61
31:4:62:THR:HB	38:4:8548:HOH:O	1.99	0.61
36:5:77:PHA:N	36:6:77:PHA:C	2.64	0.61
15:N:60:ILE:C	15:N:61:ILE:HD12	2.21	0.61
25:X:90:TYR:N	25:X:90:TYR:CD1	2.67	0.61
31:4:3:MET:O	31:4:90:PHE:HA	1.99	0.61
6:E:214:THR:HB	38:E:8323:HOH:O	2.01	0.61
17:P:14:LEU:CD2	17:P:102:ILE:HD11	2.30	0.61
29:2:21:ARG:HD2	29:2:39:PHE:HB2	1.81	0.61
8:G:100:ASP:HB2	38:G:2789:HOH:O	2.01	0.61
1:A:820:G:O2'	1:A:856:G:H4'	2.01	0.61
1:A:1058:A:H2'	1:A:1060:C:H5"	1.81	0.61
5:D:98:THR:HG22	5:D:99:GLU:H	1.65	0.61
24:W:64:GLY:O	24:W:65:ASP:HB2	2.01	0.61
25:X:88:THR:HG23	25:X:110:GLN:NE2	2.16	0.61
1:A:80:A:H3'	22:U:43:ASN:OD1	2.01	0.60
1:A:1441:G:O2'	1:A:1442:A:H5'	2.00	0.60
4:C:94:LEU:N	4:C:94:LEU:HD23	2.16	0.60
10:I:16:LYS:O	10:I:20:VAL:HG23	2.01	0.60
11:J:83:PHE:HZ	11:J:146:TRP:HE1	1.45	0.60
1:A:338:C:H4'	6:E:174:ILE:HD11	1.83	0.60
1:A:1878:G:C1'	38:A:5614:HOH:O	2.47	0.60
5:D:82:VAL:O	5:D:82:VAL:HG12	2.00	0.60
6:E:233:THR:HG22	6:E:234:VAL:N	2.15	0.60
13:L:81:ARG:HD3	13:L:87:ARG:NH1	2.16	0.60
15:N:81:ARG:O	15:N:86:MET:HE2	2.01	0.60
1:A:1187:U:H2'	38:A:6385:HOH:O	2.02	0.60
1:A:285:A:H2'	1:A:286:U:O4'	2.01	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:E:129:HIS:CE1	6:E:231:ARG:HA	2.37	0.60
7:F:54:ALA:HB2	7:F:69:ILE:HD12	1.84	0.60
6:E:27:ARG:HG3	6:E:29:ASP:OD1	2.01	0.60
15:N:74:ARG:HH11	15:N:74:ARG:HG3	1.65	0.60
20:S:18:LEU:HD12	20:S:143:VAL:CG1	2.32	0.60
1:A:88:G:H5'	1:A:88:G:H8	1.66	0.60
1:A:1118:A:C8	1:A:1119:G:H5"	2.37	0.60
1:A:2756:U:H3	1:A:2896:A:H2	1.47	0.60
11:J:55:GLN:HE22	11:J:91:HIS:CD2	2.20	0.60
17:P:79:VAL:HA	38:P:6810:HOH:O	2.02	0.60
1:A:2548:C:OP2	5:D:5:ARG:NH2	2.33	0.60
2:B:3040:C:N4	7:F:51:ARG:HB2	2.16	0.60
5:D:7:ARG:HG2	5:D:7:ARG:HH11	1.67	0.60
5:D:177:HIS:O	5:D:181:ILE:HG13	2.02	0.60
20:S:104:PHE:HB2	20:S:109:MET:HE1	1.82	0.60
25:X:151:GLU:O	25:X:154:ARG:HB3	2.02	0.60
1:A:1118:A:C8	1:A:1118:A:C3'	2.82	0.60
1:A:2769:C:H2'	1:A:2770:G:O4'	2.02	0.60
5:D:279:THR:OG1	5:D:290:VAL:HB	2.02	0.60
15:N:186:SER:O	15:N:189:VAL:HG12	2.02	0.60
24:W:56:ILE:O	24:W:60:GLN:HG3	2.02	0.60
27:Z:133:HIS:HD2	38:Z:8579:HOH:O	1.85	0.60
1:A:870:G:C2'	1:A:871:G:H5"	2.29	0.60
1:A:1130:U:H2'	1:A:1131:G:O4'	2.02	0.60
2:B:3013:A:O2'	2:B:3014:G:H5"	2.02	0.60
2:B:3024:U:H3'	2:B:3025:G:C5'	2.30	0.60
7:F:86:THR:O	7:F:90:LEU:HG	2.02	0.60
1:A:542:A:H5'	1:A:542:A:C8	2.30	0.59
1:A:1768:C:H2'	1:A:1769:C:O4'	2.02	0.59
5:D:56:ASP:OD1	5:D:322:ARG:HB3	2.00	0.59
9:H:91:VAL:CG1	9:H:92:GLY:N	2.65	0.59
16:O:110:THR:HB	16:O:113:SER:OG	2.02	0.59
1:A:449:A:N7	6:E:43:LYS:HG2	2.18	0.59
1:A:2256:G:H2'	1:A:2257:G:C5'	2.32	0.59
1:A:2719:A:C2	5:D:70:PRO:HG3	2.37	0.59
1:A:2912:C:OP2	38:A:5044:HOH:O	2.17	0.59
4:C:36:ASP:HA	4:C:83:GLY:HA3	1.84	0.59
5:D:103:ASP:HB2	38:D:8594:HOH:O	2.02	0.59
15:N:61:ILE:HG13	38:N:8632:HOH:O	2.02	0.59
1:A:138:U:H5"	1:A:139:C:OP2	2.03	0.59
1:A:2453:G:H3'	38:A:5413:HOH:O	2.00	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:C:94:LEU:HG	4:C:99:ILE:CD1	2.32	0.59
8:G:137:ASP:OD1	8:G:139:GLU:HB2	2.02	0.59
13:L:74:VAL:HG13	13:L:113:ILE:HG23	1.85	0.59
14:M:143:THR:HG22	14:M:145:LEU:H	1.66	0.59
16:O:90:LEU:HB2	16:O:186:LEU:HD22	1.84	0.59
25:X:13:MET:HE1	25:X:18:GLN:HA	1.84	0.59
8:G:20:ILE:HD11	8:G:40:VAL:CG1	2.28	0.59
12:K:26:VAL:HG13	12:K:36:VAL:HG11	1.83	0.59
1:A:1329:A:H2	38:A:4181:HOH:O	1.84	0.59
9:H:58:GLU:HG3	9:H:61:MET:HE1	1.83	0.59
25:X:80:ASP:O	25:X:84:VAL:HG23	2.01	0.59
1:A:1234:U:N3	5:D:244:PRO:HB3	2.18	0.59
30:3:22:PRO:HG2	30:3:25:VAL:HG23	1.85	0.59
1:A:1244:U:OP1	12:K:18:ILE:HD13	2.03	0.59
1:A:1589:G:H22	1:A:1605:G:H1'	1.68	0.59
38:A:5011:HOH:O	5:D:298:LYS:HD3	2.02	0.59
11:J:57:ARG:HG3	11:J:57:ARG:HH11	1.68	0.59
23:V:52:THR:CG2	23:V:54:THR:HB	2.33	0.59
1:A:902:G:N7	14:M:18:HIS:HD2	2.01	0.59
1:A:2081:A:H4'	12:K:69:TYR:CE1	2.37	0.59
1:A:2755:G:H1'	38:A:4180:HOH:O	2.02	0.59
1:A:2910:A:H5"	38:A:3639:HOH:O	2.01	0.59
2:B:3054:A:O2'	2:B:3055:U:H5'	2.02	0.59
6:E:118:THR:O	6:E:136:VAL:HG13	2.02	0.59
11:J:150:LYS:HE2	38:J:8383:HOH:O	2.03	0.59
31:4:40:ARG:HD2	38:4:8546:HOH:O	2.02	0.59
1:A:1535:G:H2'	1:A:1536:C:C6	2.37	0.59
1:A:1834:C:H2'	1:A:1840:A:H62	1.67	0.59
9:H:47:LEU:HB2	9:H:108:LEU:HD11	1.85	0.59
9:H:61:MET:HB3	15:N:19:GLN:OE1	2.03	0.59
10:I:67:LEU:O	10:I:71:LEU:HG	2.03	0.59
18:Q:38:GLU:HA	18:Q:41:ARG:NH1	2.18	0.59
1:A:677:C:H4'	6:E:246:ARG:NH2	2.18	0.59
1:A:2270:G:H4'	4:C:223:ARG:HH12	1.68	0.59
7:F:44:ILE:HG12	7:F:83:PHE:HE1	1.66	0.59
18:Q:11:ALA:HB2	18:Q:18:LYS:HA	1.85	0.59
21:T:33:SER:O	21:T:37:VAL:HG23	2.02	0.59
1:A:1333:U:H2'	1:A:1334:C:H6	1.68	0.58
1:A:1527:A:H1'	1:A:1528:A:C8	2.38	0.58
1:A:1733:A:H4'	5:D:212:GLN:HA	1.84	0.58
1:A:2604:A:H5'	38:A:5282:HOH:O	2.02	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2795:C:O2'	1:A:2796:U:H5'	2.03	0.58
7:F:163:VAL:HA	38:F:6326:HOH:O	2.01	0.58
13:L:74:VAL:HG12	13:L:75:ARG:HG3	1.84	0.58
15:N:164:THR:CG2	15:N:165:SER:N	2.66	0.58
16:O:143:ARG:NH1	16:O:173:ASP:OD2	2.33	0.58
23:V:13:ILE:HG12	23:V:32:CYS:HB3	1.83	0.58
25:X:38:THR:HG22	25:X:39:ASP:N	2.17	0.58
1:A:288:A:H61	1:A:364:C:H42	1.50	0.58
6:E:246:ARG:HB3	6:E:246:ARG:NH1	2.17	0.58
22:U:44:ALA:HA	22:U:62:VAL:HG12	1.84	0.58
26:Y:12:ILE:HD12	26:Y:36:HIS:ND1	2.18	0.58
26:Y:71:ARG:HD3	38:Y:2171:HOH:O	2.03	0.58
1:A:1634:G:H3'	38:A:3405:HOH:O	2.03	0.58
1:A:2830:U:H3'	38:A:4718:HOH:O	2.03	0.58
38:A:3201:HOH:O	8:G:143:GLN:HG2	2.02	0.58
13:L:62:PRO:HG3	13:L:65:ARG:NH2	2.18	0.58
18:Q:105:LEU:HD21	18:Q:137:LEU:HD21	1.85	0.58
1:A:1008:C:H5"	11:J:16:ARG:HH12	1.67	0.58
5:D:314:ALA:CB	5:D:317:PRO:HG3	2.34	0.58
6:E:133:ARG:HD2	38:E:8415:HOH:O	2.03	0.58
7:F:25:MET:CE	7:F:37:ALA:HB1	2.31	0.58
12:K:74:ARG:O	12:K:78:ILE:HG12	2.03	0.58
16:O:24:LEU:HD13	19:R:26:PRO:HB3	1.83	0.58
16:O:151:ASP:O	16:O:154:LEU:HB2	2.03	0.58
21:T:43:GLU:HB3	38:T:8345:HOH:O	2.03	0.58
25:X:130:HIS:O	25:X:136:GLY:HA3	2.03	0.58
1:A:1197:G:N2	38:A:5728:HOH:O	2.36	0.58
1:A:1701:A:H4'	1:A:1702:U:C5'	2.33	0.58
1:A:2501:G:H1'	38:A:4043:HOH:O	2.03	0.58
1:A:2672:C:H1'	38:D:8635:HOH:O	2.04	0.58
18:Q:13:VAL:HG21	18:Q:41:ARG:HG2	1.84	0.58
25:X:39:ASP:HB2	38:X:3580:HOH:O	2.02	0.58
1:A:544:G:C2'	1:A:545:G:H5"	2.32	0.58
5:D:202:VAL:HG11	5:D:301:VAL:HG13	1.86	0.58
8:G:31:ARG:NH1	8:G:68:HIS:CG	2.72	0.58
8:G:79:GLY:HA3	38:G:7046:HOH:O	2.04	0.58
9:H:110:GLU:HG2	38:H:6926:HOH:O	2.04	0.58
16:O:89:GLY:O	16:O:92:ALA:HB3	2.04	0.58
22:U:9:LYS:HB2	38:U:7242:HOH:O	2.04	0.58
2:B:3006:C:OP1	16:O:37:ARG:NH1	2.36	0.58
13:L:82:ARG:NH2	13:L:115:ARG:HG2	2.19	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:U:53:GLY:HA3	38:U:6384:HOH:O	2.04	0.58
23:V:52:THR:HG22	23:V:54:THR:H	1.69	0.58
27:Z:155:ARG:NH1	38:Z:8555:HOH:O	2.36	0.58
27:Z:186:ARG:HG2	27:Z:186:ARG:NH1	2.18	0.58
31:4:42:ARG:HH11	31:4:42:ARG:HG3	1.68	0.58
1:A:21:G:H4'	20:S:2:ILE:HG22	1.86	0.58
1:A:797:A:H4'	28:1:10:ARG:N	2.19	0.58
1:A:1206:U:H5'	1:A:1206:U:C6	2.38	0.58
38:A:3267:HOH:O	22:U:9:LYS:HD2	2.03	0.58
6:E:111:VAL:HB	38:E:8320:HOH:O	2.03	0.58
11:J:26:LYS:HD2	11:J:28:ILE:CD1	2.32	0.58
11:J:139:ASP:H	11:J:140:PRO:HD3	1.69	0.58
28:1:62:TYR:CE2	28:1:64:ILE:HG23	2.39	0.58
1:A:1819:G:H2'	1:A:1820:G:H4'	1.84	0.58
8:G:6:GLU:HA	8:G:46:THR:HG22	1.85	0.58
23:V:52:THR:HG22	23:V:54:THR:N	2.19	0.58
26:Y:15:ARG:HH11	26:Y:15:ARG:CB	2.16	0.58
1:A:1189:A:H1'	1:A:1209:C:C1'	2.34	0.58
38:A:6948:HOH:O	5:D:211:THR:HG21	2.04	0.58
4:C:88:ILE:HG22	4:C:88:ILE:O	2.02	0.58
6:E:200:PRO:HB3	6:E:212:VAL:HG23	1.86	0.58
7:F:95:THR:C	7:F:97:GLN:H	2.07	0.58
8:G:31:ARG:HH12	8:G:68:HIS:CG	2.21	0.58
25:X:125:HIS:HE1	38:X:3071:HOH:O	1.86	0.58
1:A:2524:G:H21	1:A:2526:C:N4	2.02	0.57
1:A:2679:G:H2'	1:A:2681:A:OP2	2.04	0.57
5:D:51:VAL:HG13	5:D:53:LEU:HD13	1.85	0.57
29:2:28:HIS:HD2	29:2:30:LYS:H	1.51	0.57
1:A:1624:A:H5'	1:A:1626:A:O4'	2.04	0.57
1:A:2365:G:H4'	19:R:45:PRO:O	2.04	0.57
2:B:3014:G:H5'	2:B:3014:G:C8	2.39	0.57
4:C:192:VAL:HG12	4:C:192:VAL:O	2.04	0.57
6:E:104:ASP:HA	6:E:107:ARG:NH1	2.19	0.57
11:J:139:ASP:N	11:J:140:PRO:CD	2.66	0.57
16:O:24:LEU:O	16:O:28:LYS:HG2	2.04	0.57
16:O:61:ALA:HB3	16:O:88:ALA:HB2	1.85	0.57
17:P:113:VAL:O	17:P:114:ILE:HD13	2.04	0.57
22:U:71:VAL:HG11	22:U:90:PRO:CB	2.27	0.57
30:3:20:ARG:HB3	38:3:5444:HOH:O	2.03	0.57
1:A:1942:A:O2'	1:A:1943:C:H5'	2.05	0.57
4:C:232:ARG:NH2	4:C:236:GLY:O	2.34	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:L:34:VAL:HB	38:L:7169:HOH:O	2.04	0.57
16:O:152:GLU:C	16:O:154:LEU:H	2.06	0.57
24:W:39:ALA:N	24:W:40:PRO:CD	2.67	0.57
1:A:536:A:H3'	38:A:4538:HOH:O	2.04	0.57
1:A:2502:C:C4'	11:J:151:MET:HG2	2.33	0.57
5:D:294:TYR:HE2	38:D:8652:HOH:O	1.87	0.57
9:H:110:GLU:O	9:H:114:LYS:HG3	2.03	0.57
11:J:117:LYS:HB2	38:J:8339:HOH:O	2.05	0.57
14:M:114:VAL:HG11	38:M:8575:HOH:O	2.04	0.57
15:N:38:VAL:O	15:N:63:VAL:HG13	2.04	0.57
18:Q:115:SER:C	18:Q:117:SER:H	2.08	0.57
1:A:1636:G:O2'	1:A:1637:A:H5'	2.03	0.57
4:C:55:VAL:HG22	4:C:68:ILE:O	2.04	0.57
5:D:141:ARG:HB3	5:D:164:THR:O	2.05	0.57
6:E:72:LYS:HG2	6:E:77:ALA:HA	1.86	0.57
7:F:135:VAL:HG22	7:F:136:ARG:N	2.19	0.57
11:J:26:LYS:CD	11:J:28:ILE:HB	2.35	0.57
11:J:27:LYS:H	11:J:58:HIS:CD2	2.15	0.57
12:K:93:ARG:HB3	12:K:93:ARG:NH1	2.18	0.57
14:M:54:PRO:HG2	14:M:57:VAL:CG2	2.34	0.57
27:Z:130:ARG:HB2	27:Z:142:SER:O	2.04	0.57
29:2:25:LYS:HD2	30:3:48:ASP:HA	1.86	0.57
1:A:328:U:O4'	6:E:202:THR:HG22	2.03	0.57
1:A:1205:U:H2'	1:A:1206:U:H5"	1.86	0.57
6:E:145:GLU:HG3	38:E:8376:HOH:O	2.05	0.57
8:G:12:ASP:HA	38:G:1750:HOH:O	2.03	0.57
10:I:12:ILE:HD12	38:I:692:HOH:O	2.03	0.57
17:P:47:ARG:HG3	17:P:47:ARG:NH1	2.20	0.57
18:Q:27:ARG:O	18:Q:31:ILE:HG13	2.05	0.57
29:2:10:LYS:HG3	38:2:8434:HOH:O	2.05	0.57
31:4:3:MET:HG3	31:4:4:PRO:HD2	1.86	0.57
1:A:952:G:OP1	19:R:42:LYS:HE2	2.03	0.57
2:B:3055:U:H4'	2:B:3056:A:C8	2.39	0.57
5:D:307:ARG:HH11	5:D:307:ARG:HB2	1.69	0.57
7:F:174:VAL:HG13	38:F:6555:HOH:O	2.04	0.57
16:O:34:LEU:HA	16:O:47:LEU:HD23	1.86	0.57
22:U:37:GLN:OE1	22:U:118:SER:HA	2.05	0.57
29:2:21:ARG:HD2	29:2:37:CYS:SG	2.43	0.57
1:A:20:G:H21	20:S:117:HIS:HD2	1.53	0.57
1:A:175:G:H2'	15:N:192:ALA:HB3	1.85	0.57
2:B:3041:C:O4'	7:F:50:VAL:HG23	2.04	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:D:329:TYR:CE2	23:V:15:PRO:HG2	2.39	0.57
12:K:104:TYR:HA	38:K:2238:HOH:O	2.04	0.57
15:N:63:VAL:HG21	15:N:109:PHE:CE1	2.40	0.57
4:C:192:VAL:CG1	4:C:207:GLN:HB3	2.33	0.57
5:D:274:GLU:HA	5:D:292:GLY:O	2.05	0.57
8:G:86:VAL:CG1	8:G:129:GLU:HA	2.34	0.57
10:I:12:ILE:HG22	10:I:17:GLN:NE2	2.20	0.57
16:O:12:ARG:HD3	16:O:18:THR:OG1	2.05	0.57
1:A:1097:A:H5"	25:X:125:HIS:NE2	2.20	0.57
1:A:2846:C:OP1	5:D:158:LYS:HD3	2.05	0.57
2:B:3078:G:N2	2:B:3103:A:OP2	2.36	0.57
15:N:55:LYS:HB2	15:N:60:ILE:CD1	2.35	0.57
16:O:47:LEU:HD11	16:O:127:LEU:CD2	2.30	0.57
16:O:80:SER:HB2	38:O:8537:HOH:O	2.03	0.57
1:A:1015:C:H2'	1:A:1016:U:H6	1.70	0.56
1:A:1450:C:O2'	1:A:1494:A:H5'	2.05	0.56
1:A:1778:A:H2'	1:A:1779:A:H5'	1.86	0.56
1:A:2421:G:H3'	1:A:2422:U:H5"	1.87	0.56
1:A:2690:U:O2'	8:G:111:LYS:HE3	2.05	0.56
1:A:2769:C:C2'	1:A:2770:G:H5'	2.35	0.56
2:B:3024:U:H3'	2:B:3025:G:H5'	1.87	0.56
24:W:39:ALA:C	24:W:41:GLU:H	2.08	0.56
28:1:11:THR:HG23	28:1:23:ARG:HD2	1.87	0.56
28:1:11:THR:OG1	28:1:23:ARG:HB2	2.04	0.56
1:A:169:A:H1'	31:4:48:ASN:ND2	2.20	0.56
1:A:485:A:N3	1:A:487:G:H5"	2.20	0.56
1:A:775:G:OP1	29:2:16:HIS:HE1	1.88	0.56
1:A:1151:G:OP1	10:I:63:ARG:NH1	2.38	0.56
1:A:2266:A:OP2	15:N:90:ARG:NH2	2.38	0.56
5:D:85:ARG:NH1	38:D:8635:HOH:O	2.38	0.56
20:S:119:VAL:O	20:S:119:VAL:HG12	2.04	0.56
26:Y:78:GLU:CG	26:Y:79:GLU:H	2.17	0.56
1:A:31:C:H4'	38:U:7242:HOH:O	2.03	0.56
1:A:346:U:H4'	38:A:6332:HOH:O	2.03	0.56
1:A:1209:C:H2'	1:A:1210:G:H8	1.69	0.56
1:A:2291:A:C8	1:A:2309:C:H5'	2.40	0.56
1:A:2694:A:H4'	8:G:91:PHE:CE1	2.40	0.56
4:C:211:LYS:HB3	4:C:212:PRO:CD	2.33	0.56
8:G:81:GLU:HG2	8:G:134:SER:CB	2.34	0.56
10:I:12:ILE:HB	38:I:4714:HOH:O	2.05	0.56
15:N:74:ARG:HD3	15:N:91:ILE:HD12	1.87	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:O:132:ASN:O	16:O:135:VAL:HG12	2.05	0.56
20:S:106:GLY:HA2	20:S:109:MET:CE	2.32	0.56
21:T:51:GLN:NE2	21:T:53:ASN:HD21	2.02	0.56
21:T:77:VAL:O	21:T:80:ARG:HG2	2.04	0.56
26:Y:18:ARG:NH1	38:Y:4132:HOH:O	2.35	0.56
1:A:136:C:H2'	1:A:137:U:O4'	2.04	0.56
1:A:256:C:H2'	1:A:257:G:O4'	2.05	0.56
1:A:1615:A:H4'	38:A:5377:HOH:O	2.05	0.56
1:A:2780:C:H2'	1:A:2781:U:C6	2.40	0.56
2:B:3088:G:OP1	25:X:130:HIS:NE2	2.38	0.56
4:C:121:ALA:O	4:C:124:VAL:HG22	2.06	0.56
4:C:199:HIS:CD2	4:C:201:PHE:HB2	2.37	0.56
5:D:175:LEU:HD23	5:D:175:LEU:O	2.05	0.56
7:F:10:PHE:CG	7:F:11:HIS:N	2.73	0.56
15:N:9:ARG:HG3	38:N:8548:HOH:O	2.03	0.56
15:N:74:ARG:HG3	15:N:74:ARG:NH1	2.21	0.56
20:S:34:GLU:HG2	20:S:46:TYR:OH	2.05	0.56
30:3:48:ASP:O	30:3:49:GLU:HB2	2.05	0.56
1:A:558:C:O2'	1:A:559:U:H5"	2.06	0.56
1:A:2274:A:H1'	15:N:86:MET:SD	2.46	0.56
1:A:2434:A:O3'	31:4:28:GLY:HA3	2.05	0.56
6:E:1:MET:HG2	6:E:2:GLN:N	2.20	0.56
11:J:53:PRO:HA	11:J:125:VAL:O	2.05	0.56
12:K:107:ASN:C	12:K:107:ASN:HD22	2.09	0.56
19:R:25:PRO:HB2	38:R:4350:HOH:O	2.05	0.56
21:T:29:ASP:OD1	21:T:31:ARG:NH1	2.39	0.56
25:X:122:ARG:NH2	25:X:154:ARG:HD2	2.20	0.56
1:A:154:C:H2'	1:A:155:C:H6	1.70	0.56
1:A:794:U:H3	1:A:819:A:H61	1.53	0.56
1:A:2281:C:C2'	1:A:2282:U:H5'	2.36	0.56
4:C:36:ASP:OD2	4:C:85:ASP:HB2	2.05	0.56
7:F:99:ASP:HB2	7:F:103:ASN:HB2	1.85	0.56
8:G:37:ASP:OD1	12:K:125:SER:HB3	2.06	0.56
16:O:43:VAL:HG11	16:O:81:ALA:HA	1.87	0.56
25:X:119:HIS:HD2	25:X:120:PRO:O	1.88	0.56
1:A:184:G:H5"	15:N:153:THR:HG22	1.87	0.56
1:A:2070:G:H5"	38:A:3292:HOH:O	2.06	0.56
2:B:3023:U:C3'	2:B:3024:U:C5'	2.81	0.56
11:J:166:ASN:N	11:J:166:ASN:ND2	2.54	0.56
28:1:30:GLU:HA	28:1:33:HIS:HB3	1.86	0.56
1:A:1205:U:C2'	1:A:1206:U:H5"	2.36	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2630:G:O6	4:C:206:ARG:NH2	2.39	0.56
38:A:9674:HOH:O	15:N:87:MET:HE3	2.06	0.56
5:D:62:ARG:HG2	5:D:65:MET:HE3	1.87	0.56
7:F:102:GLY:O	7:F:134:LEU:HD12	2.06	0.56
9:H:50:VAL:HG13	9:H:60:VAL:HG11	1.87	0.56
16:O:77:ASN:OD1	16:O:80:SER:HB2	2.06	0.56
27:Z:200:THR:HG22	27:Z:201:GLU:HG2	1.88	0.56
29:2:8:GLN:HE22	29:2:11:LYS:NZ	2.03	0.56
1:A:247:A:H2'	38:A:3434:HOH:O	2.05	0.56
1:A:281:U:O2'	1:A:282:C:H5'	2.06	0.56
1:A:1020:A:O3'	38:A:3536:HOH:O	2.18	0.56
4:C:51:ARG:NH1	4:C:120:ARG:O	2.38	0.56
7:F:41:LEU:HA	7:F:44:ILE:CG2	2.35	0.56
16:O:37:ARG:NE	38:O:8534:HOH:O	2.39	0.56
26:Y:73:ARG:O	26:Y:85:VAL:HG13	2.06	0.56
1:A:1972:U:H2'	1:A:1973:A:H5'	1.87	0.56
1:A:2768:A:O2'	1:A:2769:C:H5'	2.06	0.56
2:B:3025:G:C3'	2:B:3026:C:H5'	2.33	0.56
4:C:170:VAL:HG22	28:1:22:ILE:CG2	2.36	0.56
15:N:67:ILE:CD1	15:N:104:ARG:HD2	2.36	0.56
15:N:104:ARG:O	15:N:108:LYS:HG2	2.05	0.56
23:V:52:THR:HG22	23:V:54:THR:HB	1.88	0.56
1:A:200:U:H2'	38:A:9953:HOH:O	2.06	0.55
1:A:669:G:O2'	1:A:670:G:H5'	2.05	0.55
1:A:1377:C:H5'	1:A:1377:C:C6	2.41	0.55
9:H:46:GLU:OE1	9:H:100:ASP:HA	2.06	0.55
21:T:81:ILE:HG23	38:T:8337:HOH:O	2.06	0.55
25:X:122:ARG:NE	38:X:5817:HOH:O	2.39	0.55
27:Z:185:VAL:HA	38:Z:8561:HOH:O	2.05	0.55
1:A:960:G:H2'	1:A:960:G:N3	2.21	0.55
1:A:2064:U:H5'	1:A:2652:U:O3'	2.07	0.55
1:A:2503:A:OP1	11:J:147:ARG:NH2	2.35	0.55
9:H:57:GLU:O	9:H:61:MET:HG3	2.05	0.55
11:J:144:GLU:OE1	11:J:144:GLU:HA	2.06	0.55
26:Y:75:ALA:O	26:Y:83:ALA:HA	2.06	0.55
1:A:1213:C:O2'	1:A:1214:G:H5'	2.07	0.55
1:A:2505:G:O2'	1:A:2506:A:H5'	2.06	0.55
5:D:62:ARG:HA	5:D:65:MET:HE3	1.85	0.55
6:E:78:ARG:HG3	6:E:78:ARG:NH1	2.21	0.55
6:E:104:ASP:O	6:E:108:GLN:HG3	2.05	0.55
15:N:46:LEU:HG	38:N:8630:HOH:O	2.05	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:O:100:ALA:O	16:O:129:ILE:HG23	2.06	0.55
22:U:48:VAL:HG22	22:U:98:VAL:HA	1.87	0.55
24:W:39:ALA:O	24:W:41:GLU:N	2.39	0.55
26:Y:72:VAL:HG22	26:Y:85:VAL:CG1	2.34	0.55
27:Z:106:THR:HG23	27:Z:107:PRO:HD2	1.88	0.55
1:A:1116:U:O2'	1:A:1118:A:C2	2.52	0.55
1:A:1864:C:OP1	15:N:75:THR:HG23	2.07	0.55
38:A:9211:HOH:O	5:D:254:GLN:HG3	2.05	0.55
7:F:99:ASP:CB	7:F:103:ASN:H	2.19	0.55
25:X:149:LEU:HG	25:X:153:MET:CE	2.36	0.55
27:Z:200:THR:HG22	27:Z:201:GLU:HG3	1.89	0.55
38:A:3572:HOH:O	5:D:27:ASN:HB2	2.05	0.55
2:B:3023:U:H6	2:B:3023:U:C5'	2.18	0.55
6:E:107:ARG:NE	38:E:8461:HOH:O	2.17	0.55
15:N:52:LEU:HD13	15:N:116:ASN:CB	2.36	0.55
18:Q:131:PHE:CD1	18:Q:137:LEU:HD13	2.40	0.55
24:W:12:THR:HG23	24:W:14:ALA:H	1.70	0.55
31:4:65:THR:HG23	31:4:67:LEU:HG	1.88	0.55
1:A:263:U:O4'	9:H:59:ILE:HD13	2.06	0.55
1:A:1123:A:C6	1:A:1238:C:H5'	2.41	0.55
1:A:1132:A:N6	1:A:1229:C:H2'	2.22	0.55
1:A:2276:U:H2'	1:A:2277:U:C6	2.41	0.55
1:A:2468:A:H61	31:4:48:ASN:HD21	1.53	0.55
5:D:152:PRO:HD2	38:D:8632:HOH:O	2.06	0.55
5:D:204:GLY:HA3	38:D:8655:HOH:O	2.06	0.55
6:E:115:LEU:O	6:E:118:THR:HB	2.06	0.55
7:F:91:ALA:HB1	38:F:5198:HOH:O	2.06	0.55
16:O:47:LEU:HD13	16:O:97:VAL:HG11	1.87	0.55
26:Y:74:ALA:CB	26:Y:85:VAL:HG22	2.37	0.55
31:4:17:HIS:O	31:4:18:GLN:HG3	2.07	0.55
1:A:371:U:H2'	1:A:372:A:H8	1.71	0.55
1:A:431:G:P	15:N:48:ARG:HH12	2.30	0.55
1:A:588:G:O6	25:X:154:ARG:NH1	2.39	0.55
7:F:95:THR:O	7:F:97:GLN:N	2.33	0.55
14:M:72:ASN:HB2	38:M:8584:HOH:O	2.07	0.55
15:N:37:VAL:HG21	15:N:108:LYS:CG	2.36	0.55
22:U:38:ARG:NH1	38:U:6217:HOH:O	2.38	0.55
23:V:9:CYS:HA	23:V:52:THR:CG2	2.34	0.55
23:V:17:THR:HG22	23:V:18:GLY:N	2.22	0.55
26:Y:31:ILE:O	26:Y:35:GLU:HG3	2.06	0.55
30:3:40:ARG:HG3	30:3:45:ASN:CB	2.37	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:3:41:HIS:H	30:3:45:ASN:ND2	1.98	0.55
1:A:21:G:H5"	20:S:1:GLY:O	2.07	0.55
38:A:3966:HOH:O	15:N:146:GLN:HG2	2.06	0.55
8:G:126:ILE:HB	8:G:131:LEU:CD2	2.37	0.55
16:O:78:MET:HB2	16:O:79:PRO:HD3	1.89	0.55
22:U:28:SER:O	22:U:32:ARG:HG3	2.07	0.55
25:X:13:MET:CE	25:X:17:ILE:HG22	2.36	0.55
26:Y:15:ARG:HB3	26:Y:15:ARG:NH1	2.22	0.55
28:1:57:CYS:SG	28:1:59:HIS:HB3	2.47	0.55
1:A:1189:A:H1'	1:A:1209:C:O4'	2.07	0.55
4:C:101:GLU:OE2	4:C:131:HIS:HB2	2.07	0.55
6:E:246:ARG:NE	38:E:8429:HOH:O	2.39	0.55
7:F:146:LYS:HZ3	16:O:107:ASN:HD21	1.53	0.55
18:Q:80:ARG:HG2	18:Q:87:ARG:CZ	2.37	0.55
19:R:23:THR:HA	38:R:4792:HOH:O	2.07	0.55
19:R:64:GLU:HG3	19:R:74:ASP:OD2	2.06	0.55
26:Y:51:ASP:OD2	26:Y:52:PRO:HD2	2.07	0.55
31:4:74:CYS:N	38:4:8558:HOH:O	2.39	0.55
1:A:814:G:H8	38:A:6700:HOH:O	1.90	0.55
1:A:2769:C:O2'	1:A:2770:G:H5'	2.06	0.55
5:D:72:THR:O	38:D:8607:HOH:O	2.18	0.55
6:E:214:THR:HG23	38:E:8440:HOH:O	2.07	0.55
12:K:107:ASN:HD21	12:K:109:TYR:HB2	1.72	0.55
1:A:1014:A:H2'	1:A:1015:C:H5'	1.90	0.54
1:A:1164:U:C4'	1:A:1165:G:OP1	2.53	0.54
1:A:1189:A:H1'	1:A:1209:C:H1'	1.90	0.54
1:A:1787:C:H4'	1:A:2883:A:O4'	2.07	0.54
1:A:2281:C:H2'	1:A:2282:U:H5'	1.90	0.54
1:A:2577:A:H5'	38:A:7241:HOH:O	2.07	0.54
4:C:217:ARG:HG2	4:C:229:ALA:HB2	1.88	0.54
5:D:36:PRO:HA	5:D:168:GLY:HA3	1.89	0.54
6:E:35:VAL:HG21	6:E:227:GLY:HA2	1.90	0.54
21:T:6:LYS:HD3	38:T:8324:HOH:O	2.07	0.54
24:W:5:VAL:HG23	38:W:2271:HOH:O	2.07	0.54
26:Y:41:PHE:O	26:Y:43:VAL:HG23	2.07	0.54
27:Z:109:LEU:HA	38:Z:8568:HOH:O	2.07	0.54
1:A:945:U:H2'	1:A:946:C:C6	2.43	0.54
1:A:1003:U:O2'	11:J:90:PHE:HE1	1.90	0.54
5:D:51:VAL:CG2	5:D:327:VAL:HG13	2.38	0.54
12:K:19:MET:HE2	12:K:79:PHE:HA	1.87	0.54
14:M:104:ASP:O	14:M:105:TYR:HB3	2.06	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:N:39:ARG:HA	15:N:63:VAL:HG22	1.89	0.54
18:Q:115:SER:H	18:Q:118:GLN:HE21	0.85	0.54
27:Z:112:GLU:CD	27:Z:115:ARG:NH1	2.60	0.54
6:E:107:ARG:NH1	6:E:107:ARG:HB3	2.23	0.54
15:N:12:TRP:CE2	15:N:20:ILE:HD11	2.43	0.54
1:A:2241:C:H2'	1:A:2242:U:C6	2.42	0.54
11:J:68:ALA:HB2	11:J:149:ALA:HB2	1.88	0.54
16:O:86:LEU:O	16:O:90:LEU:HG	2.07	0.54
1:A:67:A:H5"	1:A:69:A:C8	2.43	0.54
1:A:289:G:N2	1:A:363:A:H2	2.02	0.54
1:A:657:G:H2'	1:A:658:C:H6	1.72	0.54
1:A:1242:A:H5'	12:K:82:THR:CG2	2.24	0.54
1:A:1687:C:O2	29:2:9:GLY:HA2	2.06	0.54
1:A:2411:C:H4'	38:A:4443:HOH:O	2.07	0.54
7:F:22:VAL:HG22	7:F:74:THR:HG22	1.90	0.54
14:M:138:GLY:HA3	38:M:8555:HOH:O	2.05	0.54
16:O:11:ARG:HG3	16:O:14:ARG:NH1	2.22	0.54
16:O:141:ARG:N	38:O:8570:HOH:O	2.39	0.54
16:O:171:HIS:CE1	38:O:8567:HOH:O	2.61	0.54
25:X:122:ARG:NH2	38:X:4276:HOH:O	2.40	0.54
31:4:69:TYR:HB2	31:4:78:HIS:CE1	2.42	0.54
1:A:682:A:H2'	1:A:683:G:O4'	2.07	0.54
1:A:1185:U:H5'	38:A:6959:HOH:O	2.07	0.54
1:A:2252:A:C5	1:A:2253:G:H1'	2.42	0.54
1:A:2634:G:O2'	1:A:2635:A:H5'	2.08	0.54
6:E:246:ARG:NH2	38:E:8429:HOH:O	2.40	0.54
15:N:87:MET:CB	31:4:46:ILE:HG21	2.37	0.54
17:P:73:ASP:HA	17:P:92:VAL:O	2.08	0.54
24:W:58:THR:O	24:W:62:GLU:HG3	2.08	0.54
27:Z:107:PRO:HB3	27:Z:182:PHE:CE2	2.42	0.54
1:A:926:A:O2'	14:M:41:HIS:HD2	1.90	0.54
2:B:3041:C:C6	7:F:50:VAL:HG21	2.43	0.54
5:D:119:HIS:O	5:D:121:PRO:HD3	2.08	0.54
7:F:44:ILE:HG23	7:F:45:THR:HG23	1.90	0.54
12:K:75:PRO:HG2	12:K:105:LEU:CD2	2.37	0.54
15:N:172:GLY:C	15:N:183:VAL:HG11	2.27	0.54
16:O:91:ARG:HG3	16:O:186:LEU:HD23	1.89	0.54
21:T:33:SER:OG	21:T:36:GLU:HG3	2.08	0.54
1:A:538:C:OP2	27:Z:134:HIS:HE1	1.90	0.54
4:C:153:ARG:HH11	4:C:153:ARG:CB	2.20	0.54
5:D:329:TYR:HE2	23:V:15:PRO:HG2	1.73	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:E:246:ARG:CZ	38:E:8429:HOH:O	2.55	0.54
25:X:122:ARG:HH21	25:X:154:ARG:HD2	1.72	0.54
31:4:56:PRO:HA	38:4:8547:HOH:O	2.08	0.54
1:A:100:C:H4'	22:U:16:LEU:HB2	1.90	0.54
1:A:447:A:OP1	22:U:2:LYS:HG2	2.08	0.54
1:A:667:C:H2'	1:A:668:C:H6	1.72	0.54
1:A:1086:A:N6	25:X:11:VAL:HG11	2.22	0.54
1:A:1495:C:H1'	1:A:1573:A:H1'	1.90	0.54
1:A:2563:U:H2'	1:A:2565:C:O5'	2.08	0.54
1:A:2638:G:H1'	38:A:4083:HOH:O	2.07	0.54
2:B:3044:A:O4'	7:F:76:ARG:NE	2.41	0.54
22:U:49:GLU:HB3	22:U:59:GLU:HG3	1.89	0.54
27:Z:112:GLU:OE1	27:Z:112:GLU:HA	2.08	0.54
1:A:1182:C:H1'	1:A:1192:A:C8	2.42	0.54
38:A:5780:HOH:O	27:Z:158:LYS:HD3	2.08	0.54
5:D:7:ARG:HD3	5:D:9:GLY:O	2.08	0.54
5:D:41:PHE:HB3	5:D:190:MET:HE1	1.89	0.54
9:H:104:ALA:HA	38:H:6617:HOH:O	2.08	0.54
15:N:84:LYS:HE2	38:N:8580:HOH:O	2.06	0.54
17:P:77:ALA:HB1	17:P:98:LEU:HD12	1.89	0.54
18:Q:105:LEU:CD2	18:Q:137:LEU:HD21	2.38	0.54
1:A:1176:C:H1'	38:A:3441:HOH:O	2.07	0.53
1:A:1181:A:H2'	1:A:1182:C:O4'	2.08	0.53
1:A:1497:G:H4'	1:A:1627:G:O2'	2.08	0.53
38:A:9179:HOH:O	17:P:112:ARG:HD2	2.08	0.53
6:E:1:MET:HG2	6:E:2:GLN:NE2	2.24	0.53
7:F:25:MET:CE	7:F:41:LEU:HG	2.32	0.53
15:N:37:VAL:HG13	15:N:63:VAL:HG11	1.90	0.53
16:O:47:LEU:HD12	16:O:92:ALA:HB1	1.89	0.53
16:O:139:TRP:HA	16:O:139:TRP:CE3	2.43	0.53
25:X:63:GLU:HG2	25:X:93:ILE:HG22	1.89	0.53
29:2:37:CYS:SG	29:2:39:PHE:HB2	2.48	0.53
1:A:240:C:H4'	15:N:146:GLN:NE2	2.22	0.53
1:A:660:A:H4'	1:A:661:G:O5'	2.09	0.53
1:A:1790:C:H2'	1:A:1791:U:H6	1.72	0.53
1:A:2787:C:H5	38:A:4131:HOH:O	1.90	0.53
4:C:175:LYS:HE2	38:C:8572:HOH:O	2.08	0.53
5:D:36:PRO:HA	5:D:168:GLY:HA2	1.90	0.53
6:E:95:GLU:HG3	38:E:8476:HOH:O	2.08	0.53
6:E:235:PHE:HE2	6:E:243:VAL:HG21	1.72	0.53
11:J:58:HIS:HA	11:J:61:LEU:HD23	1.90	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:J:157:ILE:HG22	11:J:158:ASN:N	2.23	0.53
25:X:6:GLN:HB2	25:X:26:ILE:CD1	2.37	0.53
25:X:84:VAL:HG12	38:X:6679:HOH:O	2.07	0.53
1:A:241:A:C2	1:A:378:A:H4'	2.42	0.53
1:A:1717:A:H5"	18:Q:54:LYS:HB2	1.91	0.53
1:A:1730:G:H5'	1:A:1731:C:C5	2.43	0.53
1:A:2419:U:H5"	1:A:2420:G:H5'	1.90	0.53
1:A:2506:A:O2'	1:A:2507:G:O5'	2.26	0.53
5:D:148:PRO:HD2	38:D:8584:HOH:O	2.08	0.53
7:F:41:LEU:CA	7:F:44:ILE:HG22	2.37	0.53
24:W:64:GLY:O	24:W:65:ASP:CB	2.57	0.53
1:A:558:C:H2'	1:A:559:U:C5'	2.39	0.53
1:A:1119:G:H22	1:A:1246:A:H2	1.53	0.53
1:A:1268:C:H2'	1:A:1269:G:H8	1.74	0.53
2:B:3030:C:OP1	7:F:137:PRO:O	2.27	0.53
2:B:3064:C:H2'	2:B:3065:A:H5'	1.91	0.53
7:F:170:TYR:O	7:F:171:ASP:HB3	2.08	0.53
13:L:82:ARG:HH21	13:L:115:ARG:HG2	1.73	0.53
16:O:155:GLU:O	16:O:156:GLU:HG3	2.08	0.53
20:S:17:MET:CE	20:S:19:ARG:NH2	2.72	0.53
24:W:49:LEU:O	24:W:53:ILE:HG13	2.08	0.53
1:A:1304:U:H2'	1:A:1305:C:C6	2.44	0.53
1:A:1667:A:H2'	1:A:1668:U:C6	2.43	0.53
5:D:217:ARG:HG3	5:D:257:THR:CG2	2.37	0.53
7:F:94:ALA:O	7:F:95:THR:O	2.27	0.53
11:J:14:TYR:N	11:J:91:HIS:CE1	2.75	0.53
15:N:45:ARG:CZ	15:N:48:ARG:HG3	2.38	0.53
21:T:51:GLN:HE21	21:T:53:ASN:ND2	2.07	0.53
22:U:48:VAL:CG2	22:U:98:VAL:HA	2.38	0.53
22:U:75:GLU:O	22:U:76:ASP:HB2	2.07	0.53
23:V:6:CYS:C	23:V:8:TYR:H	2.12	0.53
25:X:88:THR:HG22	25:X:89:ASP:N	2.23	0.53
29:2:28:HIS:CD2	29:2:31:LYS:HG3	2.43	0.53
1:A:1711:A:O2'	1:A:1712:A:H5'	2.08	0.53
11:J:150:LYS:HG2	38:J:8383:HOH:O	2.07	0.53
15:N:81:ARG:HG3	15:N:85:ARG:HB2	1.90	0.53
17:P:38:ARG:NH1	38:P:7674:HOH:O	2.41	0.53
28:1:42:CYS:SG	28:1:44:PHE:HB2	2.48	0.53
1:A:154:C:H2'	1:A:155:C:C6	2.44	0.53
1:A:524:A:H5'	20:S:29:LYS:HE2	1.91	0.53
1:A:1525:G:H5'	1:A:1526:A:OP2	2.08	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1787:C:OP1	18:Q:68:LYS:HE2	2.09	0.53
2:B:3076:G:C3'	2:B:3077:A:H5"	2.30	0.53
5:D:221:GLN:HE22	13:L:42:ASN:ND2	2.05	0.53
7:F:94:ALA:HB3	7:F:174:VAL:HA	1.91	0.53
22:U:73:HIS:CD2	22:U:88:PRO:HG3	2.43	0.53
25:X:38:THR:O	25:X:42:ARG:HB2	2.09	0.53
25:X:110:GLN:NE2	25:X:110:GLN:HA	2.24	0.53
1:A:818:A:O2'	28:1:13:ARG:HD3	2.07	0.53
1:A:1766:U:O2	1:A:1778:A:H5'	2.08	0.53
5:D:223:ARG:HG3	5:D:232:TRP:O	2.08	0.53
7:F:154:LYS:H	7:F:154:LYS:CD	2.09	0.53
9:H:50:VAL:CG2	9:H:63:ILE:HG21	2.37	0.53
10:I:64:ASN:N	10:I:64:ASN:ND2	2.55	0.53
10:I:71:LEU:C	10:I:73:ASP:H	2.12	0.53
11:J:86:ARG:NH1	11:J:130:HIS:CD2	2.77	0.53
12:K:45:VAL:HG22	12:K:46:ILE:N	2.23	0.53
12:K:130:VAL:HG12	12:K:131:THR:N	2.23	0.53
14:M:73:VAL:HG23	14:M:74:THR:N	2.24	0.53
15:N:37:VAL:CG1	15:N:63:VAL:HG11	2.37	0.53
1:A:120:A:H2'	1:A:120:A:N3	2.23	0.53
1:A:259:G:H21	15:N:58:GLN:NE2	2.06	0.53
1:A:684:G:H2'	1:A:685:C:C6	2.44	0.53
1:A:1159:G:H21	1:A:1189:A:H8	1.55	0.53
8:G:49:ILE:HD11	8:G:69:ILE:HD12	1.91	0.53
20:S:39:THR:CG2	20:S:42:GLU:HG3	2.38	0.53
22:U:49:GLU:OE2	22:U:97:ARG:HD2	2.09	0.53
28:1:38:LYS:HG2	28:1:45:LYS:HG2	1.90	0.53
29:2:28:HIS:CD2	29:2:30:LYS:HB2	2.44	0.53
1:A:69:A:C8	1:A:69:A:H5'	2.43	0.53
1:A:1342:C:C2'	1:A:1343:C:H5'	2.39	0.53
2:B:3055:U:H4'	2:B:3056:A:H8	1.73	0.53
5:D:315:VAL:HG23	5:D:316:ARG:HG2	1.91	0.53
17:P:56:GLU:HB2	38:P:6111:HOH:O	2.09	0.53
28:1:46:LYS:O	28:1:57:CYS:HA	2.09	0.53
1:A:970:U:H2'	38:A:5822:HOH:O	2.08	0.52
1:A:1528:A:H2'	1:A:1529:G:O4'	2.09	0.52
1:A:2415:A:C2	16:O:25:ARG:HB3	2.44	0.52
1:A:2439:C:H5'	38:A:4977:HOH:O	2.07	0.52
2:B:3002:U:OP2	2:B:3003:A:H5'	2.08	0.52
4:C:220:PRO:HD2	4:C:223:ARG:HD3	1.90	0.52
6:E:16:VAL:HG12	6:E:17:ASP:N	2.24	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:J:71:TYR:C	11:J:73:GLN:H	2.12	0.52
27:Z:117:LEU:HD12	27:Z:174:VAL:CG1	2.39	0.52
27:Z:154:ARG:NH1	27:Z:155:ARG:HG3	2.24	0.52
30:3:35:ARG:HB2	38:3:2691:HOH:O	2.07	0.52
1:A:2721:U:H4'	13:L:87:ARG:HG3	1.91	0.52
1:A:2781:U:H1'	8:G:139:GLU:OE2	2.08	0.52
2:B:3048:C:H4'	16:O:141:ARG:NH2	2.24	0.52
5:D:51:VAL:HG23	5:D:330:VAL:HG22	1.91	0.52
11:J:53:PRO:HG3	11:J:127:GLY:H	1.72	0.52
20:S:39:THR:HB	20:S:42:GLU:CD	2.30	0.52
28:1:11:THR:CG2	28:1:23:ARG:HB2	2.39	0.52
1:A:869:G:OP1	15:N:79:LYS:HE2	2.10	0.52
1:A:1334:C:H2'	1:A:1335:C:H6	1.73	0.52
1:A:1351:G:OP1	6:E:96:LYS:NZ	2.33	0.52
1:A:1789:G:O6	18:Q:73:HIS:HE1	1.93	0.52
1:A:2851:G:C2'	1:A:2852:A:H5'	2.39	0.52
38:B:8465:HOH:O	16:O:147:ILE:HB	2.09	0.52
5:D:27:ASN:HD22	5:D:27:ASN:H	1.57	0.52
11:J:136:VAL:HG22	11:J:137:ASN:O	2.08	0.52
24:W:11:MET:HB3	24:W:15:GLU:HB2	1.91	0.52
24:W:20:LEU:HD22	24:W:60:GLN:HE22	1.74	0.52
1:A:602:A:O2'	1:A:605:C:H4'	2.08	0.52
1:A:894:A:C2	6:E:87:ARG:NH2	2.77	0.52
1:A:1353:C:P	38:A:4177:HOH:O	2.68	0.52
6:E:7:ASP:O	6:E:9:ASP:N	2.43	0.52
7:F:58:VAL:HG12	7:F:59:GLY:N	2.24	0.52
7:F:149:ARG:NH1	38:F:3066:HOH:O	2.29	0.52
8:G:126:ILE:HB	8:G:131:LEU:HD23	1.91	0.52
9:H:36:THR:HG23	9:H:97:ALA:HB2	1.91	0.52
9:H:48:VAL:HG12	9:H:97:ALA:CB	2.39	0.52
13:L:49:LEU:HA	13:L:73:VAL:HG12	1.91	0.52
14:M:72:ASN:O	14:M:76:LEU:HG	2.09	0.52
15:N:173:LEU:HD23	15:N:183:VAL:HG12	1.90	0.52
15:N:185:PRO:HG2	15:N:189:VAL:HG11	1.90	0.52
1:A:380:A:OP2	15:N:9:ARG:HD2	2.10	0.52
1:A:920:C:H5"	1:A:921:G:O5'	2.10	0.52
1:A:1098:A:H2'	1:A:1099:G:O4'	2.10	0.52
1:A:2815:G:OP2	12:K:99:GLU:HG2	2.09	0.52
7:F:11:HIS:O	7:F:12:GLU:HB3	2.09	0.52
8:G:69:ILE:HA	8:G:72:MET:CE	2.40	0.52
15:N:134:ILE:O	15:N:136:PRO:HD3	2.09	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:Q:16:VAL:HG12	18:Q:17:GLY:N	2.24	0.52
20:S:39:THR:HB	20:S:42:GLU:HG3	1.91	0.52
20:S:119:VAL:HG21	20:S:142:ASP:CG	2.29	0.52
21:T:57:THR:CG2	21:T:58:MET:N	2.71	0.52
25:X:5:VAL:HG22	25:X:32:CYS:HB2	1.91	0.52
25:X:137:GLN:HE21	25:X:141:HIS:CE1	2.26	0.52
27:Z:117:LEU:HD12	27:Z:174:VAL:HG11	1.90	0.52
30:3:40:ARG:HA	30:3:45:ASN:ND2	2.24	0.52
31:4:11:CYS:HB2	31:4:20:HIS:CE1	2.43	0.52
1:A:1015:C:H2'	1:A:1016:U:C6	2.45	0.52
1:A:2269:C:C2'	1:A:2270:G:H5'	2.40	0.52
1:A:2324:G:H4'	1:A:2418:G:O2'	2.10	0.52
36:5:77:PHA:H	36:6:77:PHA:C	2.21	0.52
11:J:45:GLN:HB3	11:J:163:PRO:CD	2.22	0.52
11:J:95:GLU:HB3	11:J:119:VAL:HG11	1.91	0.52
26:Y:70:ILE:O	26:Y:70:ILE:HG23	2.09	0.52
1:A:459:A:H4'	38:A:8966:HOH:O	2.10	0.52
1:A:1139:U:H2'	1:A:1140:C:C6	2.45	0.52
1:A:1166:A:H61	1:A:1180:U:H3	1.57	0.52
1:A:1471:A:H2'	1:A:1472:C:C6	2.43	0.52
1:A:2073:G:OP2	1:A:2490:A:H5'	2.09	0.52
38:A:3366:HOH:O	11:J:90:PHE:HD2	1.92	0.52
2:B:3114:G:O6	16:O:11:ARG:HD3	2.10	0.52
9:H:58:GLU:HG3	9:H:61:MET:CE	2.40	0.52
18:Q:16:VAL:CG1	18:Q:20:ARG:HB2	2.40	0.52
20:S:111:ILE:HG23	20:S:145:LEU:HD11	1.91	0.52
23:V:47:ARG:HG3	38:V:4381:HOH:O	2.10	0.52
27:Z:112:GLU:OE1	27:Z:115:ARG:NH1	2.42	0.52
1:A:795:G:H1'	1:A:817:G:N2	2.24	0.52
1:A:2684:A:H2'	1:A:2685:C:C6	2.44	0.52
13:L:9:THR:O	13:L:10:GLN:C	2.47	0.52
15:N:72:SER:HB2	15:N:93:ARG:HG2	1.92	0.52
31:4:16:GLU:HG3	31:4:18:GLN:HE21	1.75	0.52
31:4:38:ARG:O	31:4:42:ARG:HB2	2.10	0.52
1:A:113:A:OP2	1:A:114:A:H2'	2.09	0.52
1:A:2578:G:H5'	1:A:2578:G:C8	2.42	0.52
1:A:2815:G:N7	12:K:80:LYS:NZ	2.58	0.52
2:B:3039:U:H1'	2:B:3044:A:H61	1.73	0.52
5:D:49:THR:HG21	5:D:280:VAL:HG23	1.91	0.52
7:F:35:ALA:O	7:F:37:ALA:N	2.43	0.52
14:M:22:ARG:HG2	38:M:8523:HOH:O	2.10	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:O:37:ARG:NH2	38:O:8534:HOH:O	2.43	0.52
16:O:154:LEU:O	16:O:155:GLU:CB	2.58	0.52
16:O:163:PHE:HA	38:O:8519:HOH:O	2.10	0.52
20:S:18:LEU:HG	20:S:91:LEU:HD13	1.91	0.52
22:U:40:VAL:HG23	22:U:119:ALA:C	2.30	0.52
22:U:41:ARG:HG2	22:U:41:ARG:NH1	2.24	0.52
22:U:69:LYS:O	22:U:71:VAL:HG23	2.10	0.52
25:X:13:MET:HE2	25:X:18:GLN:N	2.24	0.52
1:A:69:A:H5'	1:A:69:A:H8	1.75	0.52
1:A:2780:C:H2'	1:A:2781:U:H6	1.75	0.52
4:C:57:ALA:HA	4:C:67:LEU:HD23	1.92	0.52
5:D:81:ALA:O	5:D:186:GLY:HA3	2.10	0.52
7:F:50:VAL:O	7:F:71:ALA:HA	2.10	0.52
15:N:35:PRO:HD2	15:N:38:VAL:CG2	2.40	0.52
15:N:113:ARG:NH2	15:N:156:ARG:HG2	2.25	0.52
17:P:35:LYS:HD3	38:P:3360:HOH:O	2.09	0.52
27:Z:115:ARG:NE	38:Z:8553:HOH:O	2.42	0.52
1:A:157:G:H4'	15:N:95:LYS:CE	2.40	0.51
1:A:1025:C:H5'	25:X:23:MET:O	2.10	0.51
1:A:1477:C:H5'	1:A:1868:G:C5'	2.40	0.51
1:A:1669:A:H2'	1:A:1670:G:C8	2.45	0.51
1:A:2421:G:H3'	1:A:2422:U:C5'	2.40	0.51
1:A:2564:G:OP2	1:A:2565:C:H5"	2.10	0.51
38:A:7115:HOH:O	15:N:156:ARG:HD3	2.09	0.51
10:I:12:ILE:N	10:I:13:PRO:CD	2.72	0.51
11:J:69:ASN:O	11:J:72:VAL:HG12	2.10	0.51
14:M:65:ASP:CG	14:M:111:ALA:HB3	2.30	0.51
15:N:87:MET:CB	31:4:46:ILE:HD13	2.35	0.51
25:X:38:THR:HG22	38:X:3580:HOH:O	2.10	0.51
27:Z:187:VAL:CG2	27:Z:192:ASP:HB2	2.36	0.51
1:A:156:C:H5"	15:N:171:ARG:CD	2.20	0.51
9:H:56:PRO:CG	15:N:44:THR:HA	2.39	0.51
16:O:180:LEU:O	16:O:181:ASP:HB3	2.10	0.51
1:A:1060:C:H6	1:A:1060:C:H5'	1.74	0.51
1:A:2906:A:H5'	1:A:2907:C:O4'	2.10	0.51
1:A:135:G:OP1	15:N:39:ARG:NH1	2.41	0.51
1:A:394:G:H1	15:N:181:GLU:CD	2.14	0.51
1:A:1134:G:C4'	11:J:151:MET:HE1	2.31	0.51
1:A:1192:A:H3'	1:A:1193:A:H5'	1.92	0.51
1:A:2251:G:H2'	1:A:2252:A:C8	2.45	0.51
1:A:2300:A:H4'	1:A:2301:A:O5'	2.11	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:3020:G:O2'	2:B:3021:G:H5'	2.11	0.51
4:C:173:GLY:O	4:C:176:HIS:HB3	2.11	0.51
4:C:200:PRO:HG2	4:C:225:VAL:HG21	1.91	0.51
5:D:16:ARG:NH1	38:D:8618:HOH:O	2.43	0.51
6:E:84:VAL:O	6:E:85:LYS:HB2	2.10	0.51
7:F:158:ASN:HB2	7:F:161:ASP:OD2	2.11	0.51
11:J:139:ASP:OD2	38:J:8392:HOH:O	2.19	0.51
20:S:44:VAL:O	20:S:48:GLU:HG3	2.11	0.51
21:T:57:THR:HG22	21:T:58:MET:N	2.24	0.51
23:V:34:SER:HA	23:V:37:GLU:OE1	2.10	0.51
25:X:1:MET:HB2	25:X:103:GLU:HG2	1.93	0.51
25:X:41:TYR:O	25:X:45:VAL:HG13	2.10	0.51
28:1:19:GLY:O	28:1:23:ARG:HG2	2.09	0.51
1:A:1500:U:P	18:Q:41:ARG:HH22	2.33	0.51
1:A:2720:C:O2	13:L:87:ARG:NH2	2.43	0.51
38:A:9579:HOH:O	20:S:83:LYS:HB3	2.10	0.51
4:C:36:ASP:O	4:C:38:ILE:N	2.44	0.51
5:D:141:ARG:HD2	5:D:163:GLU:OE2	2.10	0.51
5:D:207:LYS:HG2	5:D:304:PRO:HB3	1.90	0.51
5:D:248:ARG:O	5:D:251:VAL:HG13	2.09	0.51
7:F:166:ILE:HD12	38:F:6326:HOH:O	2.11	0.51
11:J:163:PRO:HG2	38:J:8338:HOH:O	2.10	0.51
15:N:77:PHE:HD2	38:N:8527:HOH:O	1.92	0.51
22:U:9:LYS:CE	22:U:13:ARG:NH1	2.66	0.51
1:A:229:G:O2'	1:A:230:C:H5'	2.10	0.51
1:A:2115:U:H2'	1:A:2116:U:C6	2.45	0.51
1:A:2265:U:H2'	1:A:2266:A:H8	1.75	0.51
6:E:235:PHE:CE2	6:E:243:VAL:HG21	2.45	0.51
8:G:7:ILE:HD11	8:G:11:VAL:O	2.11	0.51
11:J:47:GLU:HG2	11:J:133:ILE:HD12	1.92	0.51
15:N:20:ILE:O	15:N:24:MET:HG2	2.11	0.51
17:P:10:LEU:HD13	17:P:99:GLU:HG3	1.93	0.51
18:Q:94:TRP:CZ2	18:Q:98:ILE:HG13	2.45	0.51
18:Q:98:ILE:HD12	18:Q:102:ARG:NE	2.26	0.51
20:S:113:HIS:HE1	20:S:144:GLU:CD	2.14	0.51
25:X:65:VAL:HA	25:X:68:THR:CG2	2.40	0.51
1:A:440:C:O2'	1:A:441:A:H5'	2.11	0.51
1:A:653:C:H2'	1:A:654:A:C8	2.45	0.51
1:A:821:U:H2'	1:A:822:C:H6	1.75	0.51
1:A:1973:A:H2'	1:A:1974:G:O5'	2.10	0.51
38:A:3033:HOH:O	21:T:13:LYS:HE2	2.11	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:J:31:PHE:HE2	11:J:87:LYS:O	1.92	0.51
13:L:22:ASP:O	13:L:110:LYS:HE3	2.11	0.51
14:M:143:THR:CG2	14:M:144:ASP:N	2.73	0.51
28:1:34:LYS:HE2	38:1:8424:HOH:O	2.09	0.51
28:1:42:CYS:SG	28:1:43:GLY:N	2.84	0.51
1:A:419:A:H1'	1:A:1921:A:C2	2.45	0.51
1:A:542:A:H2'	1:A:543:G:O4'	2.10	0.51
1:A:709:G:O2'	17:P:25:VAL:HG12	2.11	0.51
38:A:9068:HOH:O	25:X:119:HIS:HE1	1.94	0.51
6:E:21:VAL:C	6:E:23:GLU:H	2.14	0.51
8:G:80:TRP:O	8:G:134:SER:HA	2.10	0.51
11:J:13:ALA:HA	11:J:91:HIS:CE1	2.46	0.51
11:J:86:ARG:HD3	11:J:130:HIS:HD2	1.76	0.51
12:K:22:VAL:O	12:K:26:VAL:HG23	2.10	0.51
13:L:89:LYS:HA	38:L:7064:HOH:O	2.09	0.51
14:M:73:VAL:HG11	14:M:118:LEU:HD21	1.92	0.51
16:O:157:PRO:HA	38:O:8526:HOH:O	2.10	0.51
18:Q:134:VAL:O	18:Q:137:LEU:HB3	2.10	0.51
1:A:1299:G:N7	14:M:6:ARG:NH1	2.59	0.51
1:A:1701:A:H5"	1:A:1702:U:H3'	1.93	0.51
1:A:1825:U:O2'	1:A:1826:C:H5'	2.11	0.51
1:A:1829:A:H2'	1:A:1830:C:H5'	1.93	0.51
1:A:1909:A:H2'	1:A:1910:A:C8	2.46	0.51
1:A:2269:C:H2'	1:A:2270:G:H5'	1.91	0.51
38:A:6195:HOH:O	27:Z:165:GLU:HB3	2.10	0.51
6:E:142:ASP:OD2	6:E:238:SER:OG	2.27	0.51
8:G:24:GLY:HA3	8:G:76:VAL:HB	1.93	0.51
11:J:35:ASN:HD21	11:J:80:ASN:HA	1.75	0.51
15:N:87:MET:HB2	15:N:91:ILE:CD1	2.36	0.51
16:O:119:GLN:O	16:O:123:ILE:HG13	2.11	0.51
1:A:95:A:H5"	1:A:97:G:O4'	2.11	0.51
1:A:244:C:O5'	1:A:244:C:H6	1.94	0.51
1:A:657:G:H2'	1:A:658:C:C6	2.46	0.51
1:A:2363:G:O2'	19:R:11:ARG:HG3	2.10	0.51
1:A:2710:U:H1'	38:A:7111:HOH:O	2.11	0.51
1:A:2781:U:C2'	1:A:2782:G:H5'	2.41	0.51
1:A:2821:C:H4'	5:D:116:PRO:HB3	1.93	0.51
2:B:3039:U:H1'	2:B:3044:A:N6	2.26	0.51
5:D:41:PHE:CE1	5:D:79:MET:HG3	2.46	0.51
7:F:59:GLY:C	7:F:61:PHE:H	2.15	0.51
9:H:99:THR:O	9:H:99:THR:HG23	2.10	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:J:13:ALA:HA	11:J:91:HIS:HE1	1.75	0.51
11:J:81:TYR:CD1	11:J:81:TYR:C	2.84	0.51
25:X:107:LEU:O	25:X:112:LEU:HB2	2.11	0.51
25:X:108:ARG:HE	25:X:114:PRO:HG3	1.76	0.51
1:A:702:G:O2'	1:A:703:G:H5'	2.11	0.50
1:A:1116:U:H3	1:A:1246:A:N6	2.02	0.50
1:A:1342:C:O2'	1:A:1343:C:H5'	2.11	0.50
1:A:1819:G:H5'	38:A:4207:HOH:O	2.11	0.50
1:A:2837:U:H2'	38:A:6328:HOH:O	2.09	0.50
7:F:57:THR:HG23	7:F:63:ILE:CG2	2.40	0.50
11:J:26:LYS:HG2	11:J:28:ILE:N	2.26	0.50
25:X:21:LEU:CD2	25:X:48:VAL:HG11	2.39	0.50
25:X:154:ARG:C	38:X:4276:HOH:O	2.49	0.50
26:Y:26:ALA:HB1	26:Y:59:TRP:CE2	2.46	0.50
27:Z:189:ASN:HA	27:Z:217:ILE:HD11	1.93	0.50
1:A:524:A:C5'	20:S:29:LYS:HE2	2.41	0.50
1:A:816:G:C6	1:A:817:G:N1	2.79	0.50
1:A:1114:A:O2'	1:A:1115:U:H5'	2.11	0.50
1:A:1555:G:O2'	1:A:1556:G:H5'	2.11	0.50
38:A:8873:HOH:O	29:2:1:THR:HA	2.12	0.50
5:D:60:SER:C	5:D:62:ARG:H	2.15	0.50
8:G:68:HIS:O	8:G:72:MET:HG3	2.11	0.50
19:R:93:ARG:HH11	19:R:93:ARG:HG3	1.77	0.50
28:1:30:GLU:HA	28:1:33:HIS:CB	2.42	0.50
1:A:567:U:H5"	38:X:5817:HOH:O	2.12	0.50
1:A:2613:G:O2'	1:A:2614:C:H5'	2.12	0.50
7:F:91:ALA:HB2	7:F:106:PHE:CD2	2.47	0.50
9:H:111:ILE:O	9:H:115:VAL:HG23	2.11	0.50
12:K:80:LYS:HE2	12:K:98:PHE:CZ	2.47	0.50
15:N:72:SER:OG	15:N:93:ARG:CZ	2.59	0.50
18:Q:120:ARG:NH2	18:Q:123:TYR:CD2	2.80	0.50
1:A:951:A:C2'	1:A:952:G:H5'	2.41	0.50
1:A:1189:A:O2'	1:A:1208:C:H2'	2.11	0.50
1:A:2445:U:H2'	1:A:2446:G:C8	2.46	0.50
1:A:2478:U:O2'	1:A:2479:A:H5'	2.11	0.50
7:F:94:ALA:HB3	7:F:174:VAL:CA	2.41	0.50
11:J:75:SER:HB3	11:J:79:ALA:CB	2.41	0.50
14:M:53:ARG:NH2	14:M:57:VAL:HG12	2.26	0.50
18:Q:38:GLU:HA	18:Q:41:ARG:HH11	1.75	0.50
19:R:26:PRO:O	19:R:30:VAL:HG23	2.12	0.50
22:U:64:ASN:HA	38:U:5927:HOH:O	2.10	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:X:21:LEU:HD21	25:X:48:VAL:HG13	1.93	0.50
1:A:134:U:C2	1:A:145:A:C2	3.00	0.50
1:A:513:A:N3	38:A:3169:HOH:O	2.35	0.50
1:A:736:A:H2'	1:A:737:A:O4'	2.11	0.50
1:A:1847:A:OP1	4:C:175:LYS:HG3	2.11	0.50
1:A:2773:G:H5'	38:A:6690:HOH:O	2.11	0.50
38:A:4120:HOH:O	4:C:6:GLY:HA3	2.12	0.50
6:E:150:THR:HA	6:E:203:ALA:O	2.11	0.50
6:E:160:LEU:O	6:E:162:VAL:HG23	2.11	0.50
7:F:64:ARG:HB3	7:F:67:ASP:OD2	2.12	0.50
8:G:106:ASN:ND2	8:G:109:GLY:HA2	2.26	0.50
9:H:49:PHE:HE1	9:H:98:VAL:HG23	1.77	0.50
11:J:139:ASP:HB2	38:J:8347:HOH:O	2.12	0.50
13:L:32:ILE:HD11	13:L:56:SER:HB3	1.93	0.50
13:L:34:VAL:HG22	13:L:47:ALA:HB2	1.93	0.50
16:O:61:ALA:CB	16:O:88:ALA:HB2	2.42	0.50
21:T:80:ARG:NH1	38:T:8347:HOH:O	2.44	0.50
23:V:17:THR:CG2	23:V:18:GLY:N	2.73	0.50
1:A:344:C:H2'	1:A:345:G:O4'	2.11	0.50
1:A:1252:A:H2'	1:A:1253:C:O4'	2.12	0.50
1:A:1468:G:H5"	38:A:6508:HOH:O	2.12	0.50
1:A:2460:A:OP1	31:4:63:LYS:NZ	2.37	0.50
14:M:104:ASP:HB3	38:M:8565:HOH:O	2.11	0.50
15:N:67:ILE:HD11	15:N:104:ARG:HD2	1.92	0.50
20:S:119:VAL:HG11	38:S:8584:HOH:O	2.11	0.50
25:X:26:ILE:HB	38:X:5420:HOH:O	2.11	0.50
28:1:13:ARG:NH1	28:1:14:PHE:CE2	2.79	0.50
1:A:125:U:H2'	38:A:3277:HOH:O	2.11	0.50
1:A:793:A:H5"	18:Q:83:LYS:HG2	1.94	0.50
1:A:1594:C:OP2	18:Q:120:ARG:HD2	2.11	0.50
1:A:2896:A:OP1	26:Y:15:ARG:NH1	2.44	0.50
8:G:81:GLU:HA	8:G:133:VAL:O	2.12	0.50
12:K:52:GLN:CG	12:K:53:ILE:N	2.67	0.50
17:P:25:VAL:O	17:P:29:VAL:HG23	2.12	0.50
25:X:141:HIS:HB2	25:X:146:ILE:HG12	1.94	0.50
28:1:75:ALA:HB3	38:1:8436:HOH:O	2.10	0.50
1:A:283:U:H5"	1:A:284:C:P	2.51	0.50
1:A:497:A:H5"	38:A:3106:HOH:O	2.10	0.50
1:A:694:A:C2'	1:A:695:C:H5'	2.41	0.50
1:A:746:A:C6	17:P:65:LEU:HD13	2.47	0.50
1:A:1249:U:H2'	1:A:1250:C:C6	2.46	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1735:C:O2'	1:A:1736:A:H5'	2.12	0.50
1:A:1743:G:H1'	38:A:4383:HOH:O	2.10	0.50
1:A:2323:G:H5'	38:A:6510:HOH:O	2.11	0.50
2:B:3034:A:H2'	2:B:3035:C:O4'	2.11	0.50
4:C:1:GLY:HA2	4:C:197:VAL:HG23	1.94	0.50
4:C:179:MET:HG2	4:C:186:TRP:CG	2.47	0.50
5:D:248:ARG:O	5:D:251:VAL:CG1	2.60	0.50
6:E:236:THR:O	6:E:237:GLU:C	2.49	0.50
15:N:155:HIS:CE1	15:N:158:ARG:HE	2.29	0.50
16:O:44:ARG:HG3	16:O:45:ALA:N	2.27	0.50
23:V:47:ARG:CG	38:V:4381:HOH:O	2.60	0.50
26:Y:9:VAL:HG22	26:Y:88:GLU:OE2	2.11	0.50
26:Y:43:VAL:CG1	26:Y:44:ASP:N	2.73	0.50
1:A:581:G:H5'	38:A:7172:HOH:O	2.10	0.50
1:A:1483:C:O2'	1:A:1484:G:H5'	2.12	0.50
1:A:1930:A:H2'	1:A:1931:A:C8	2.47	0.50
1:A:2385:G:H2'	1:A:2386:U:C6	2.46	0.50
1:A:2781:U:H2'	1:A:2782:G:H5'	1.93	0.50
38:A:9458:HOH:O	26:Y:23:HIS:HD2	1.94	0.50
4:C:164:ARG:HB2	28:1:68:CYS:SG	2.52	0.50
6:E:196:THR:HG23	38:E:8405:HOH:O	2.12	0.50
8:G:21:THR:HG23	8:G:30:THR:OG1	2.12	0.50
9:H:19:ALA:O	9:H:22:VAL:HG22	2.12	0.50
9:H:21:GLU:O	9:H:24:ARG:HG3	2.11	0.50
11:J:163:PRO:O	11:J:164:ALA:HB2	2.12	0.50
14:M:90:ARG:NH1	14:M:119:THR:HG21	2.27	0.50
15:N:87:MET:HG2	31:4:46:ILE:HG21	1.94	0.50
24:W:44:GLY:O	24:W:48:GLU:HG2	2.12	0.50
1:A:553:G:H5'	38:A:3008:HOH:O	2.12	0.49
1:A:1003:U:O2	11:J:90:PHE:CZ	2.65	0.49
1:A:1086:A:C6	25:X:11:VAL:HG11	2.47	0.49
1:A:1613:C:H2'	1:A:1614:G:O4'	2.12	0.49
1:A:1853:C:OP1	4:C:231:LYS:HG3	2.11	0.49
1:A:2078:U:O2'	1:A:2079:G:H5'	2.11	0.49
1:A:2392:C:H4'	38:A:3775:HOH:O	2.11	0.49
4:C:66:ARG:HB2	4:C:66:ARG:HH11	1.76	0.49
5:D:25:ARG:HA	5:D:310:ARG:HH21	1.76	0.49
5:D:254:GLN:HG2	5:D:255:GLY:N	2.26	0.49
6:E:22:PHE:HA	6:E:116:ALA:HA	1.94	0.49
6:E:129:HIS:HE1	6:E:231:ARG:HA	1.77	0.49
6:E:246:ARG:HB3	6:E:246:ARG:HH11	1.75	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:G:116:THR:HG22	8:G:151:LEU:HD22	1.93	0.49
9:H:113:ASP:O	9:H:117:GLU:HG3	2.12	0.49
11:J:26:LYS:CG	11:J:28:ILE:H	2.25	0.49
12:K:75:PRO:HG2	12:K:105:LEU:HD21	1.93	0.49
15:N:164:THR:HB	38:N:8519:HOH:O	2.12	0.49
25:X:6:GLN:HG2	25:X:29:VAL:HA	1.94	0.49
25:X:88:THR:CG2	25:X:110:GLN:NE2	2.75	0.49
1:A:317:A:H5"	22:U:52:ARG:HD2	1.94	0.49
1:A:1010:C:H4'	16:O:4:PRO:HB2	1.92	0.49
1:A:2243:C:H5"	38:A:3261:HOH:O	2.12	0.49
2:B:3067:C:H2'	2:B:3068:G:H8	1.77	0.49
2:B:3091:C:H2'	2:B:3092:G:O4'	2.12	0.49
4:C:186:TRP:CG	4:C:187:PRO:HA	2.48	0.49
18:Q:13:VAL:HG11	18:Q:40:VAL:CG1	2.41	0.49
30:3:36:ASN:HB3	30:3:39:ARG:NE	2.28	0.49
38:A:9404:HOH:O	12:K:46:ILE:HA	2.13	0.49
11:J:162:SER:CB	11:J:163:PRO:CD	2.82	0.49
17:P:32:ARG:HB2	38:P:4656:HOH:O	2.11	0.49
20:S:111:ILE:HG23	20:S:145:LEU:CD1	2.42	0.49
27:Z:99:ALA:HB2	27:Z:233:TYR:CE2	2.47	0.49
1:A:2326:U:H4'	1:A:2412:G:H4'	1.94	0.49
4:C:132:ASP:OD1	4:C:133:ARG:N	2.44	0.49
6:E:25:PRO:HG2	38:E:8321:HOH:O	2.10	0.49
8:G:23:GLU:HG2	8:G:28:SER:HB3	1.94	0.49
9:H:28:ALA:CB	9:H:99:THR:HG23	2.41	0.49
16:O:182:GLY:O	16:O:183:ASP:O	2.31	0.49
1:A:128:A:O2'	1:A:129:A:H5'	2.12	0.49
1:A:212:A:O4'	1:A:214:U:C6	2.66	0.49
1:A:415:A:O2'	1:A:416:G:H5'	2.13	0.49
1:A:638:C:H2'	1:A:639:A:C8	2.48	0.49
1:A:814:G:H4'	38:A:9641:HOH:O	2.12	0.49
1:A:1236:A:O2'	1:A:1237:U:H5'	2.12	0.49
1:A:1756:G:H1'	38:A:5760:HOH:O	2.11	0.49
1:A:1940:C:H4'	38:A:6838:HOH:O	2.13	0.49
1:A:2072:G:C6	1:A:2533:C:H1'	2.48	0.49
1:A:2676:C:H4'	12:K:70:PHE:CD1	2.47	0.49
4:C:191:GLY:HA2	4:C:194:MET:HE2	1.94	0.49
6:E:136:VAL:HA	6:E:137:PRO:C	2.32	0.49
8:G:7:ILE:HG22	8:G:45:ASP:O	2.12	0.49
13:L:14:LYS:NZ	35:L:8512:CL:CL	2.80	0.49
14:M:149:ARG:O	14:M:150:GLN:HB2	2.12	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:R:32:GLU:HA	19:R:71:TYR:OH	2.12	0.49
1:A:187:A:H3'	1:A:188:C:H6	1.78	0.49
1:A:512:G:O3'	1:A:513:A:H8	1.95	0.49
1:A:797:A:O4'	28:1:10:ARG:N	2.46	0.49
1:A:1666:C:C2'	1:A:1667:A:C5'	2.91	0.49
1:A:2010:A:H5"	38:A:3678:HOH:O	2.12	0.49
1:A:2064:U:H5'	1:A:2652:U:H4'	1.94	0.49
2:B:3057:A:O2'	7:F:152:PRO:HD2	2.12	0.49
5:D:125:GLU:O	5:D:129:ARG:HG3	2.12	0.49
6:E:219:ASN:O	6:E:222:ASP:OD1	2.31	0.49
9:H:110:GLU:HA	9:H:113:ASP:OD2	2.12	0.49
14:M:125:PHE:CZ	14:M:140:VAL:HG13	2.46	0.49
14:M:146:GLY:C	14:M:148:GLU:H	2.16	0.49
16:O:64:SER:C	16:O:66:LEU:H	2.16	0.49
20:S:96:VAL:HG13	20:S:106:GLY:HA3	1.93	0.49
1:A:470:U:O2'	29:2:16:HIS:CD2	2.63	0.49
1:A:958:G:H2'	1:A:959:C:C6	2.47	0.49
1:A:1840:A:H4'	1:A:1841:C:O5'	2.13	0.49
38:A:9964:HOH:O	15:N:36:ALA:HB1	2.13	0.49
4:C:51:ARG:HB2	38:C:8602:HOH:O	2.11	0.49
6:E:237:GLU:N	38:E:8451:HOH:O	2.46	0.49
7:F:35:ALA:C	7:F:37:ALA:H	2.15	0.49
8:G:31:ARG:NH1	38:G:5919:HOH:O	2.44	0.49
11:J:109:ASP:HB2	38:J:8346:HOH:O	2.12	0.49
22:U:23:VAL:CA	22:U:93:THR:HG21	2.43	0.49
26:Y:43:VAL:CG1	26:Y:47:ALA:HB3	2.42	0.49
1:A:521:A:H2'	1:A:522:U:H5'	1.95	0.49
1:A:703:G:O2'	1:A:704:C:H5'	2.13	0.49
1:A:1029:U:O2'	1:A:1273:C:OP1	2.26	0.49
1:A:1135:G:H5'	38:A:5420:HOH:O	2.11	0.49
1:A:2694:A:H4'	8:G:91:PHE:HE1	1.78	0.49
1:A:2730:G:O2'	1:A:2731:G:H5'	2.13	0.49
38:A:5815:HOH:O	7:F:55:LYS:HB2	2.12	0.49
6:E:13:ASP:OD1	6:E:13:ASP:O	2.30	0.49
11:J:85:ILE:HB	11:J:132:PHE:CE2	2.48	0.49
17:P:39:THR:HB	38:P:3360:HOH:O	2.12	0.49
18:Q:135:ALA:HB1	18:Q:139:ARG:HH12	1.76	0.49
28:1:11:THR:CG2	28:1:23:ARG:HD2	2.43	0.49
29:2:25:LYS:HE2	38:2:8463:HOH:O	2.12	0.49
1:A:128:A:H3'	1:A:128:A:C8	2.47	0.49
1:A:251:C:H1'	15:N:58:GLN:HE22	1.78	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:645:U:OP2	14:M:4:LYS:HE2	2.13	0.49
1:A:818:A:H5"	38:A:6078:HOH:O	2.13	0.49
1:A:1163:G:N2	38:A:5539:HOH:O	2.46	0.49
1:A:1418:U:OP1	30:3:42:TRP:HB3	2.13	0.49
1:A:1470:A:OP1	15:N:93:ARG:HD2	2.13	0.49
1:A:1741:U:O2'	1:A:2723:G:H4'	2.13	0.49
1:A:1896:G:H1'	38:A:3765:HOH:O	2.12	0.49
1:A:2044:G:OP1	26:Y:23:HIS:HE1	1.96	0.49
2:B:3023:U:H2'	38:B:8479:HOH:O	2.10	0.49
24:W:38:GLY:C	24:W:40:PRO:HD2	2.32	0.49
27:Z:187:VAL:HB	38:Z:8567:HOH:O	2.12	0.49
29:2:28:HIS:CE1	29:2:31:LYS:HE2	2.47	0.49
1:A:349:U:O2'	1:A:350:C:H5'	2.13	0.49
1:A:1398:G:H2'	1:A:1399:A:C8	2.48	0.49
7:F:101:THR:HG22	38:F:7400:HOH:O	2.13	0.49
25:X:13:MET:HE3	25:X:17:ILE:CG2	2.41	0.49
27:Z:184:GLU:OE1	27:Z:204:ARG:NH1	2.46	0.49
1:A:23:G:H1'	1:A:520:A:N6	2.28	0.48
1:A:2661:U:H3	1:A:2812:A:H62	1.59	0.48
6:E:7:ASP:C	6:E:9:ASP:H	2.17	0.48
7:F:35:ALA:C	7:F:37:ALA:N	2.66	0.48
16:O:139:TRP:HA	16:O:139:TRP:HE3	1.78	0.48
22:U:55:PHE:CD2	22:U:77:VAL:HG13	2.48	0.48
23:V:11:THR:HG22	23:V:53:ASP:OD2	2.13	0.48
25:X:1:MET:N	25:X:103:GLU:OE2	2.43	0.48
25:X:14:HIS:HB2	25:X:17:ILE:HG13	1.94	0.48
25:X:65:VAL:CA	25:X:68:THR:HG22	2.42	0.48
28:1:13:ARG:NH1	28:1:14:PHE:CZ	2.81	0.48
1:A:1170:U:O2'	1:A:1172:G:N7	2.33	0.48
1:A:1477:C:O2'	1:A:1478:U:H5'	2.12	0.48
1:A:2619:U:H2'	1:A:2620:U:C6	2.48	0.48
2:B:3064:C:C2'	2:B:3065:A:H5'	2.43	0.48
9:H:13:GLU:OE2	9:H:78:GLU:HG2	2.13	0.48
11:J:75:SER:C	11:J:79:ALA:HB2	2.32	0.48
13:L:125:ALA:C	13:L:127:ALA:H	2.16	0.48
22:U:32:ARG:NH1	22:U:38:ARG:NH1	2.60	0.48
30:3:18:ASN:HD21	30:3:40:ARG:H	1.61	0.48
1:A:299:U:H5'	38:A:6828:HOH:O	2.13	0.48
1:A:440:C:H2'	1:A:441:A:C8	2.48	0.48
1:A:517:U:H2'	1:A:518:G:H5'	1.94	0.48
1:A:941:G:O2'	1:A:942:U:H5'	2.12	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1656:A:H2'	1:A:1657:A:O4'	2.13	0.48
1:A:1772:C:H5'	1:A:1773:G:C5	2.48	0.48
1:A:2314:G:C2'	1:A:2315:C:H5'	2.44	0.48
38:A:9528:HOH:O	29:2:46:ARG:HA	2.13	0.48
8:G:43:ASP:HA	38:G:5864:HOH:O	2.14	0.48
9:H:117:GLU:C	9:H:119:ARG:H	2.15	0.48
11:J:117:LYS:O	11:J:119:VAL:HG13	2.12	0.48
15:N:107:ARG:NH1	38:N:8582:HOH:O	2.46	0.48
16:O:58:LEU:HD12	16:O:58:LEU:N	2.28	0.48
25:X:21:LEU:HB3	25:X:26:ILE:HG12	1.96	0.48
28:1:56:MET:CE	28:1:63:LYS:HE3	2.44	0.48
1:A:1545:C:H2'	1:A:1546:G:O4'	2.13	0.48
1:A:1762:C:H2'	1:A:1763:C:H6	1.78	0.48
1:A:2488:A:H61	1:A:2534:C:H42	1.61	0.48
1:A:2724:U:H2'	1:A:2725:G:O4'	2.12	0.48
2:B:3025:G:N2	38:B:8506:HOH:O	2.46	0.48
4:C:105:VAL:HG12	4:C:106:CYS:N	2.28	0.48
5:D:146:THR:O	5:D:159:PRO:HB3	2.12	0.48
7:F:141:VAL:HG13	7:F:144:ARG:HH21	1.79	0.48
11:J:127:GLY:O	11:J:128:ALA:CB	2.62	0.48
28:1:56:MET:HA	28:1:62:TYR:O	2.13	0.48
31:4:65:THR:HB	31:4:83:TRP:H	1.79	0.48
1:A:86:A:C2	30:3:25:VAL:HG13	2.48	0.48
1:A:1783:A:O2'	1:A:1784:U:H5'	2.13	0.48
1:A:1827:G:H2'	1:A:1828:G:C8	2.47	0.48
1:A:2377:U:O5'	1:A:2377:U:H6	1.96	0.48
1:A:2670:G:O2'	1:A:2671:U:H5'	2.13	0.48
38:A:9404:HOH:O	12:K:18:ILE:HG23	2.13	0.48
2:B:3014:G:O2'	16:O:1:ALA:HB2	2.14	0.48
5:D:16:ARG:NE	38:D:8555:HOH:O	2.36	0.48
5:D:162:MET:O	5:D:162:MET:HG2	2.13	0.48
5:D:255:GLY:O	5:D:257:THR:HG23	2.13	0.48
7:F:23:VAL:HG21	7:F:45:THR:CG2	2.44	0.48
14:M:101:ASP:C	14:M:103:ALA:H	2.16	0.48
22:U:49:GLU:OE2	22:U:97:ARG:NH1	2.42	0.48
26:Y:9:VAL:HG13	26:Y:88:GLU:OE2	2.12	0.48
1:A:324:G:O2'	1:A:325:U:H5'	2.13	0.48
1:A:539:G:H2'	1:A:540:A:C8	2.48	0.48
1:A:1423:C:O2'	1:A:1424:A:H5'	2.14	0.48
1:A:1473:U:C1'	29:2:42:SER:HB2	2.43	0.48
1:A:1666:C:H2'	1:A:1667:A:C5'	2.43	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2387:U:H2'	1:A:2388:C:C6	2.48	0.48
1:A:2615:U:H2'	1:A:2616:G:O4'	2.14	0.48
4:C:199:HIS:CD2	4:C:201:PHE:H	2.32	0.48
8:G:11:VAL:CG1	8:G:12:ASP:N	2.75	0.48
8:G:31:ARG:CZ	38:G:5919:HOH:O	2.61	0.48
9:H:22:VAL:HG21	9:H:104:ALA:HB2	1.96	0.48
14:M:117:GLU:HB3	14:M:137:GLY:O	2.13	0.48
15:N:97:ILE:HA	15:N:100:ILE:HD12	1.95	0.48
17:P:21:SER:OG	17:P:106:PRO:HB2	2.12	0.48
21:T:81:ILE:HG12	38:T:8337:HOH:O	2.13	0.48
22:U:43:ASN:HD22	22:U:108:ARG:CZ	2.27	0.48
26:Y:76:ARG:HG3	26:Y:76:ARG:NH1	2.25	0.48
31:4:91:GLN:O	31:4:92:GLU:HB2	2.13	0.48
1:A:1172:G:H1'	38:A:4463:HOH:O	2.13	0.48
1:A:1352:A:N1	6:E:48:SER:HB3	2.29	0.48
1:A:2547:C:OP2	5:D:5:ARG:NH1	2.46	0.48
4:C:76:VAL:HG23	28:1:63:LYS:HB3	1.94	0.48
7:F:59:GLY:O	7:F:61:PHE:N	2.38	0.48
11:J:157:ILE:CG2	11:J:158:ASN:N	2.77	0.48
13:L:87:ARG:NE	38:L:4854:HOH:O	2.47	0.48
16:O:159:TYR:HE2	16:O:163:PHE:HE2	1.61	0.48
1:A:1127:C:H2'	1:A:1128:U:H5'	1.96	0.48
1:A:1615:A:H5'	38:A:3690:HOH:O	2.12	0.48
4:C:105:VAL:HG11	4:C:154:ALA:CB	2.43	0.48
5:D:24:PRO:CG	5:D:204:GLY:HA2	2.44	0.48
5:D:260:HIS:HA	38:D:8628:HOH:O	2.13	0.48
7:F:19:GLU:HG3	38:F:6165:HOH:O	2.13	0.48
9:H:107:VAL:HG23	38:H:6617:HOH:O	2.14	0.48
10:I:69:ARG:NH1	38:I:3513:HOH:O	2.46	0.48
11:J:65:ARG:NH2	11:J:66:VAL:HG22	2.28	0.48
17:P:47:ARG:HA	17:P:50:ARG:NH1	2.29	0.48
18:Q:121:ASP:OD1	18:Q:125:LYS:HE3	2.13	0.48
23:V:49:LEU:CD1	38:V:3805:HOH:O	2.61	0.48
26:Y:21:PRO:HG2	26:Y:24:LYS:HD3	1.95	0.48
1:A:474:C:O3'	6:E:73:LEU:HD21	2.13	0.48
1:A:1617:C:C4	1:A:1643:C:H4'	2.49	0.48
1:A:2852:A:H5"	38:A:4724:HOH:O	2.14	0.48
2:B:3047:A:C2	2:B:3048:C:C2	3.02	0.48
4:C:107:ASN:OD1	4:C:120:ARG:HD2	2.14	0.48
5:D:279:THR:CG2	5:D:280:VAL:N	2.76	0.48
15:N:12:TRP:HB2	38:N:8607:HOH:O	2.14	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:N:27:ARG:NH2	15:N:44:THR:HG23	2.29	0.48
25:X:146:ILE:HG22	25:X:147:ASP:N	2.29	0.48
1:A:191:A:H2'	1:A:237:G:O6	2.14	0.48
1:A:820:G:H5'	1:A:821:U:H5'	1.95	0.48
1:A:820:G:C6	4:C:171:LYS:HB2	2.48	0.48
1:A:945:U:H2'	1:A:946:C:H6	1.78	0.48
1:A:1079:A:H4'	1:A:2078:U:H5'	1.96	0.48
1:A:1174:A:C5	1:A:1201:C:H4'	2.48	0.48
1:A:2896:A:H5"	38:A:5592:HOH:O	2.14	0.48
6:E:39:GLN:O	6:E:43:LYS:HD3	2.14	0.48
17:P:26:TRP:N	38:P:3062:HOH:O	2.46	0.48
25:X:52:VAL:HG22	25:X:53:ALA:H	1.79	0.48
25:X:122:ARG:HG2	25:X:152:ALA:O	2.13	0.48
28:1:41:VAL:HG12	28:1:42:CYS:N	2.28	0.48
1:A:399:C:H5'	15:N:179:GLY:O	2.15	0.47
1:A:812:A:H2'	1:A:813:C:C6	2.49	0.47
1:A:2904:U:H4'	26:Y:8:ARG:NH1	2.29	0.47
5:D:154:VAL:HG12	5:D:156:LYS:HG2	1.96	0.47
9:H:26:THR:HG21	9:H:103:ALA:HB2	1.95	0.47
10:I:12:ILE:HG13	38:I:6833:HOH:O	2.14	0.47
11:J:46:VAL:O	11:J:146:TRP:CH2	2.64	0.47
13:L:55:VAL:HG12	13:L:56:SER:N	2.29	0.47
15:N:47:ASP:CG	15:N:48:ARG:H	2.16	0.47
15:N:66:ALA:O	15:N:67:ILE:HD13	2.14	0.47
26:Y:30:MET:CE	26:Y:58:ALA:HB3	2.43	0.47
1:A:24:G:N2	1:A:518:G:H1'	2.29	0.47
1:A:656:G:H5'	17:P:3:THR:HB	1.95	0.47
1:A:877:G:H3'	38:A:9621:HOH:O	2.13	0.47
1:A:2441:U:HO2'	14:M:51:PHE:HE1	1.61	0.47
6:E:133:ARG:NH2	38:E:8431:HOH:O	2.46	0.47
6:E:138:VAL:O	6:E:234:VAL:HA	2.14	0.47
8:G:69:ILE:HA	8:G:72:MET:HE3	1.96	0.47
12:K:93:ARG:HH11	12:K:93:ARG:CB	2.21	0.47
13:L:29:LEU:HB3	13:L:55:VAL:CG1	2.33	0.47
17:P:105:ASN:HD21	17:P:109:SER:H	1.62	0.47
22:U:71:VAL:CG1	22:U:90:PRO:HB3	2.29	0.47
1:A:245:C:H2'	1:A:246:G:H5'	1.97	0.47
1:A:765:G:O3'	6:E:69:HIS:HB3	2.14	0.47
1:A:812:A:H2'	1:A:813:C:O4'	2.14	0.47
1:A:1503:U:H2'	1:A:1504:A:O4'	2.15	0.47
1:A:1504:A:H5'	38:A:3918:HOH:O	2.13	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1568:G:O2'	1:A:1569:U:H5'	2.13	0.47
1:A:1849:G:H1'	1:A:2011:A:N1	2.29	0.47
11:J:111:MET:O	11:J:114:PRO:HD3	2.14	0.47
1:A:661:G:C5	1:A:686:A:C2	3.02	0.47
1:A:903:U:O4	14:M:18:HIS:HB2	2.14	0.47
1:A:932:U:H2'	1:A:933:C:C6	2.49	0.47
1:A:1154:A:H2'	1:A:1155:G:C8	2.50	0.47
1:A:1947:G:N2	1:A:1966:U:C2	2.82	0.47
1:A:1994:A:P	13:L:66:ARG:HH22	2.38	0.47
5:D:16:ARG:NH2	38:D:8555:HOH:O	2.44	0.47
8:G:84:MET:HE1	8:G:148:ILE:HD12	1.97	0.47
9:H:39:SER:HB3	9:H:45:ALA:HB2	1.95	0.47
11:J:26:LYS:HD3	11:J:89:PRO:HG3	1.96	0.47
11:J:65:ARG:CZ	38:J:8385:HOH:O	2.61	0.47
12:K:39:VAL:HG13	12:K:106:GLY:O	2.14	0.47
15:N:87:MET:H	15:N:87:MET:HG3	1.30	0.47
15:N:154:ARG:HG3	38:N:8620:HOH:O	2.14	0.47
16:O:32:PRO:HD2	16:O:99:GLU:O	2.15	0.47
16:O:138:ASP:O	16:O:140:GLN:N	2.40	0.47
20:S:47:LEU:O	20:S:51:ILE:HG13	2.14	0.47
22:U:23:VAL:C	22:U:93:THR:HG21	2.34	0.47
23:V:20:MET:CG	23:V:28:THR:HG23	2.45	0.47
28:1:51:GLY:HA3	38:1:8416:HOH:O	2.13	0.47
1:A:1287:A:O4'	25:X:117:ARG:HD3	2.15	0.47
1:A:1439:C:H5"	30:3:41:HIS:CE1	2.50	0.47
1:A:2256:G:O2'	1:A:2257:G:H5'	2.13	0.47
1:A:2748:G:H1'	38:A:7391:HOH:O	2.14	0.47
5:D:149:ASP:HB2	38:D:8584:HOH:O	2.13	0.47
6:E:16:VAL:HG12	6:E:17:ASP:H	1.80	0.47
6:E:61:PHE:HB3	38:E:8448:HOH:O	2.14	0.47
7:F:128:LEU:HB2	38:F:6007:HOH:O	2.14	0.47
8:G:145:ALA:HB1	8:G:168:ILE:CD1	2.44	0.47
15:N:48:ARG:NH2	38:N:8564:HOH:O	2.48	0.47
16:O:67:ALA:HA	16:O:71:TRP:H	1.79	0.47
20:S:35:ILE:O	20:S:38:LYS:HB2	2.14	0.47
25:X:131:PRO:O	25:X:136:GLY:N	2.47	0.47
26:Y:25:ARG:NH1	38:Y:3861:HOH:O	2.47	0.47
1:A:1139:U:H2'	1:A:1140:C:H6	1.80	0.47
1:A:2405:C:H5'	38:A:6086:HOH:O	2.13	0.47
1:A:2464:C:H5"	1:A:2465:A:OP1	2.14	0.47
1:A:2718:C:H6	1:A:2718:C:H5'	1.80	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:D:43:GLY:O	5:D:308:LEU:HD12	2.14	0.47
5:D:132:HIS:HB2	5:D:137:LEU:HD22	1.96	0.47
5:D:140:LEU:HD13	5:D:175:LEU:HA	1.97	0.47
6:E:95:GLU:H	6:E:95:GLU:CD	2.18	0.47
7:F:84:LEU:C	7:F:86:THR:H	2.17	0.47
7:F:142:ALA:HA	7:F:149:ARG:O	2.15	0.47
13:L:109:LEU:HD13	13:L:113:ILE:HD11	1.95	0.47
14:M:53:ARG:HH22	14:M:57:VAL:HG12	1.79	0.47
14:M:134:GLU:HA	14:M:138:GLY:O	2.14	0.47
15:N:32:ARG:NH2	38:N:8604:HOH:O	2.47	0.47
15:N:42:ARG:HA	15:N:43:PRO:HD3	1.79	0.47
16:O:43:VAL:O	16:O:43:VAL:HG12	2.13	0.47
18:Q:22:TRP:CH2	18:Q:24:ASN:HA	2.50	0.47
25:X:29:VAL:O	25:X:30:ASN:HB2	2.14	0.47
1:A:377:C:H5	38:A:9815:HOH:O	1.98	0.47
1:A:695:C:H2'	1:A:696:C:C6	2.50	0.47
1:A:1505:U:H5'	1:A:1505:U:C6	2.44	0.47
1:A:1909:A:N1	1:A:2128:G:H1'	2.29	0.47
1:A:2270:G:H4'	4:C:223:ARG:NH1	2.29	0.47
38:A:5956:HOH:O	5:D:27:ASN:HB3	2.14	0.47
2:B:3049:G:O2'	2:B:3050:G:H5'	2.14	0.47
2:B:3059:C:H2'	2:B:3060:C:C6	2.50	0.47
4:C:135:VAL:HG11	4:C:147:ARG:NH2	2.30	0.47
7:F:41:LEU:O	7:F:44:ILE:HG22	2.15	0.47
8:G:10:ASP:HA	38:G:3707:HOH:O	2.14	0.47
9:H:21:GLU:O	9:H:24:ARG:CG	2.63	0.47
11:J:83:PHE:HE1	11:J:146:TRP:CZ2	2.32	0.47
13:L:28:GLU:HG2	13:L:58:THR:HB	1.96	0.47
15:N:55:LYS:O	15:N:60:ILE:HD12	2.15	0.47
15:N:166:ALA:HA	15:N:169:ARG:NH1	2.30	0.47
19:R:66:LYS:HB2	19:R:70:ALA:O	2.14	0.47
20:S:29:LYS:HD3	38:S:8531:HOH:O	2.14	0.47
22:U:19:ARG:NH1	22:U:68:ASP:O	2.48	0.47
25:X:7:LEU:HD12	25:X:53:ALA:HB2	1.97	0.47
25:X:76:ASP:O	25:X:77:ALA:C	2.53	0.47
25:X:122:ARG:HH11	25:X:122:ARG:CG	2.23	0.47
26:Y:85:VAL:HG12	26:Y:86:GLU:N	2.28	0.47
30:3:40:ARG:HG3	30:3:45:ASN:HB2	1.97	0.47
31:4:15:ASN:ND2	38:4:8545:HOH:O	2.47	0.47
1:A:949:U:O2'	19:R:40:HIS:HE1	1.98	0.47
1:A:1172:G:H5"	38:A:6752:HOH:O	2.13	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1393:A:H2'	1:A:1394:C:C6	2.50	0.47
1:A:2506:A:H1'	38:A:3257:HOH:O	2.13	0.47
4:C:194:MET:CE	4:C:199:HIS:HB2	2.45	0.47
5:D:41:PHE:CD1	5:D:79:MET:HE2	2.50	0.47
5:D:279:THR:HG22	5:D:280:VAL:N	2.29	0.47
15:N:78:ASN:C	15:N:79:LYS:HG2	2.36	0.47
16:O:37:ARG:CZ	38:O:8534:HOH:O	2.62	0.47
20:S:92:LEU:HD23	20:S:145:LEU:HD21	1.97	0.47
28:1:31:ILE:HG23	28:1:32:LYS:N	2.30	0.47
30:3:22:PRO:HG2	30:3:25:VAL:CG2	2.43	0.47
1:A:522:U:O2'	1:A:1366:C:H5'	2.14	0.47
1:A:825:U:H5"	1:A:826:U:OP1	2.15	0.47
1:A:1180:U:H2'	1:A:1181:A:O4'	2.15	0.47
1:A:1269:G:H2'	1:A:1270:U:C6	2.49	0.47
1:A:1641:A:C2'	1:A:1642:A:H5'	2.43	0.47
1:A:2251:G:H4'	38:A:6900:HOH:O	2.14	0.47
38:A:5744:HOH:O	23:V:56:ARG:HD3	2.14	0.47
38:A:7169:HOH:O	15:N:154:ARG:HB2	2.14	0.47
38:A:9077:HOH:O	5:D:267:LYS:HD3	2.14	0.47
7:F:19:GLU:O	7:F:133:ASN:HB3	2.14	0.47
7:F:65:GLU:HA	38:F:6752:HOH:O	2.14	0.47
7:F:167:GLU:OE2	7:F:173:GLU:HG2	2.14	0.47
9:H:28:ALA:HB3	9:H:99:THR:O	2.15	0.47
10:I:12:ILE:HG22	10:I:12:ILE:O	2.14	0.47
13:L:75:ARG:CZ	38:L:4172:HOH:O	2.62	0.47
15:N:38:VAL:O	15:N:38:VAL:HG12	2.14	0.47
16:O:97:VAL:HG12	16:O:127:LEU:HD11	1.97	0.47
16:O:184:ILE:HG22	16:O:185:GLU:HG3	1.97	0.47
17:P:49:GLU:HG2	38:P:5191:HOH:O	2.15	0.47
19:R:30:VAL:O	19:R:30:VAL:HG12	2.15	0.47
26:Y:76:ARG:O	26:Y:77:PHE:HB3	2.15	0.47
1:A:772:G:H2'	1:A:773:A:O4'	2.14	0.47
1:A:1268:C:H2'	1:A:1269:G:C8	2.50	0.47
1:A:1380:U:H5'	38:A:8733:HOH:O	2.14	0.47
1:A:1434:A:H2'	1:A:1436:C:C5	2.49	0.47
1:A:1805:G:H2'	1:A:1806:G:H8	1.79	0.47
4:C:9:ARG:HG2	4:C:16:PHE:CD2	2.49	0.47
7:F:23:VAL:HG22	7:F:73:VAL:HB	1.97	0.47
8:G:23:GLU:HG2	8:G:28:SER:CB	2.44	0.47
11:J:45:GLN:CB	11:J:163:PRO:HD2	2.23	0.47
13:L:113:ILE:HG22	13:L:114:ALA:O	2.14	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:M:90:ARG:NH2	14:M:121:ILE:HD11	2.30	0.47
16:O:161:GLY:O	16:O:162:ASP:C	2.53	0.47
1:A:251:C:H4'	15:N:140:ALA:HB2	1.98	0.46
1:A:1191:A:C3'	1:A:1192:A:H5"	2.40	0.46
1:A:1427:A:H61	1:A:1440:U:H1'	1.81	0.46
1:A:2101:A:H5"	6:E:63:SER:HB3	1.96	0.46
1:A:2694:A:H5"	8:G:90:HIS:CE1	2.50	0.46
38:A:4570:HOH:O	5:D:216:LYS:HA	2.14	0.46
5:D:175:LEU:C	5:D:175:LEU:CD2	2.82	0.46
6:E:154:VAL:O	6:E:158:GLU:HG3	2.14	0.46
8:G:172:PRO:HB3	38:G:6931:HOH:O	2.14	0.46
9:H:47:LEU:HD22	9:H:108:LEU:CD1	2.45	0.46
12:K:74:ARG:NH1	12:K:76:ASP:HB2	2.29	0.46
13:L:101:ASN:HB2	13:L:103:ASP:OD2	2.16	0.46
15:N:59:GLY:HA3	15:N:141:ILE:HD12	1.96	0.46
19:R:93:ARG:HG3	19:R:93:ARG:NH1	2.29	0.46
22:U:71:VAL:HG12	22:U:72:ILE:N	2.29	0.46
1:A:182:G:O3'	15:N:157:LEU:CD1	2.62	0.46
1:A:338:C:H4'	6:E:174:ILE:HD12	1.96	0.46
1:A:474:C:O3'	6:E:73:LEU:CD2	2.63	0.46
1:A:558:C:H5'	38:A:4750:HOH:O	2.14	0.46
1:A:652:G:H8	38:A:9520:HOH:O	1.97	0.46
1:A:1181:A:O2'	1:A:1182:C:H5'	2.16	0.46
1:A:2403:C:H3'	38:A:4701:HOH:O	2.13	0.46
5:D:198:GLU:HB3	38:D:8597:HOH:O	2.14	0.46
7:F:23:VAL:O	7:F:23:VAL:CG2	2.63	0.46
12:K:131:THR:HG22	12:K:133:GLY:N	2.30	0.46
13:L:98:VAL:HG13	13:L:102:GLU:HA	1.98	0.46
15:N:47:ASP:CG	15:N:48:ARG:N	2.69	0.46
16:O:93:GLN:HG2	38:O:8557:HOH:O	2.15	0.46
18:Q:8:ARG:HG3	38:Q:193:HOH:O	2.13	0.46
27:Z:196:VAL:CG1	27:Z:226:ILE:HD13	2.45	0.46
28:1:32:LYS:NZ	28:1:70:GLN:NE2	2.63	0.46
29:2:25:LYS:HG3	30:3:49:GLU:H	1.79	0.46
1:A:106:A:H2'	1:A:107:U:O4'	2.16	0.46
1:A:250:C:O2'	1:A:251:C:H5'	2.15	0.46
1:A:333:G:O2'	1:A:334:G:H5'	2.16	0.46
1:A:1154:A:H2'	1:A:1155:G:H8	1.81	0.46
1:A:1523:G:H2'	1:A:1524:U:C6	2.50	0.46
1:A:2507:G:H5'	38:A:3257:HOH:O	2.15	0.46
1:A:2866:U:H4'	1:A:2867:G:H5'	1.97	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:3042:C:H2'	38:B:8500:HOH:O	2.15	0.46
5:D:24:PRO:HG2	5:D:204:GLY:HA2	1.96	0.46
5:D:189:ALA:HB1	38:D:8568:HOH:O	2.14	0.46
7:F:52:THR:HB	7:F:70:GLY:O	2.15	0.46
9:H:37:THR:O	9:H:41:GLU:HG3	2.15	0.46
11:J:75:SER:HB3	11:J:79:ALA:HB1	1.96	0.46
1:A:289:G:O2'	1:A:290:C:H5'	2.15	0.46
1:A:558:C:C2'	1:A:559:U:C5'	2.93	0.46
1:A:1236:A:H2'	1:A:1237:U:O4'	2.15	0.46
1:A:1299:G:N2	38:A:4181:HOH:O	2.48	0.46
1:A:1589:G:H4'	38:A:6347:HOH:O	2.14	0.46
2:B:3069:U:OP1	16:O:4:PRO:HG3	2.15	0.46
4:C:39:ALA:HB3	4:C:61:GLU:OE2	2.15	0.46
6:E:180:SER:HB2	38:E:8449:HOH:O	2.15	0.46
7:F:11:HIS:C	7:F:13:MET:H	2.18	0.46
7:F:49:PRO:HA	7:F:73:VAL:HG22	1.98	0.46
11:J:59:ASN:N	11:J:59:ASN:ND2	2.54	0.46
12:K:19:MET:HE1	12:K:132:LEU:HD21	1.98	0.46
15:N:59:GLY:HA3	15:N:141:ILE:CD1	2.45	0.46
27:Z:234:VAL:HG12	27:Z:235:GLU:N	2.31	0.46
1:A:329:A:OP1	6:E:205:ARG:NE	2.45	0.46
1:A:1053:G:OP1	11:J:12:PRO:HG3	2.15	0.46
1:A:1699:C:H4'	38:A:5932:HOH:O	2.14	0.46
1:A:1746:A:O4'	1:A:1747:A:C2	2.68	0.46
1:A:1819:G:H2'	1:A:1820:G:C5'	2.46	0.46
38:A:9665:HOH:O	8:G:57:LYS:HE2	2.16	0.46
2:B:3012:C:H5'	2:B:3070:U:O4'	2.15	0.46
9:H:56:PRO:HG2	15:N:43:PRO:O	2.16	0.46
11:J:134:ALA:HB3	11:J:142:VAL:HG21	1.96	0.46
14:M:80:ASP:HB2	14:M:90:ARG:O	2.14	0.46
20:S:8:ALA:CB	20:S:13:THR:HG21	2.41	0.46
1:A:407:A:H5'	38:A:5517:HOH:O	2.15	0.46
1:A:1874:U:OP1	4:C:51:ARG:HD2	2.16	0.46
5:D:195:ARG:HD2	5:D:324:ASP:OD1	2.15	0.46
7:F:54:ALA:HB3	7:F:69:ILE:HD12	1.95	0.46
8:G:31:ARG:HH12	8:G:68:HIS:CE1	2.32	0.46
11:J:39:GLY:O	11:J:41:THR:N	2.49	0.46
16:O:114:LYS:O	16:O:117:ALA:HB3	2.16	0.46
18:Q:103:THR:O	18:Q:107:GLU:HG3	2.15	0.46
20:S:39:THR:HB	20:S:42:GLU:CG	2.45	0.46
25:X:4:LEU:CD2	25:X:54:PHE:HB3	2.43	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:Z:126:PRO:HG2	27:Z:128:PHE:CE1	2.50	0.46
1:A:65:C:O2'	1:A:66:G:H5'	2.15	0.46
1:A:484:A:N1	1:A:506:G:H4'	2.31	0.46
1:A:711:G:N2	1:A:718:C:C2	2.83	0.46
1:A:1819:G:H2'	1:A:1820:G:C4'	2.46	0.46
1:A:2549:C:H4'	38:A:7012:HOH:O	2.14	0.46
38:A:3355:HOH:O	11:J:11:LYS:HE2	2.16	0.46
2:B:3020:G:H3'	38:B:8432:HOH:O	2.15	0.46
9:H:48:VAL:HG23	9:H:74:PHE:CB	2.46	0.46
9:H:78:GLU:HG3	38:H:5966:HOH:O	2.16	0.46
11:J:83:PHE:CZ	11:J:146:TRP:NE1	2.81	0.46
12:K:107:ASN:HD22	12:K:109:TYR:H	1.63	0.46
13:L:53:ILE:HG13	13:L:55:VAL:CG2	2.45	0.46
15:N:35:PRO:CD	15:N:38:VAL:HG23	2.46	0.46
1:A:671:A:O2'	1:A:672:G:H2'	2.16	0.46
1:A:796:A:HO2'	28:1:10:ARG:N	2.13	0.46
1:A:816:G:H5'	1:A:1598:A:H4'	1.97	0.46
1:A:2890:A:H1'	23:V:56:ARG:HH21	1.77	0.46
6:E:234:VAL:O	6:E:234:VAL:HG22	2.16	0.46
7:F:23:VAL:HG23	7:F:41:LEU:HD22	1.98	0.46
7:F:92:GLU:O	7:F:93:LEU:O	2.33	0.46
9:H:46:GLU:N	38:H:3461:HOH:O	2.49	0.46
9:H:101:ALA:HB2	9:H:108:LEU:CD2	2.46	0.46
11:J:47:GLU:HG2	11:J:133:ILE:CD1	2.46	0.46
11:J:143:GLU:N	38:J:8381:HOH:O	2.47	0.46
12:K:107:ASN:HD22	12:K:108:PRO:N	2.14	0.46
13:L:14:LYS:CB	13:L:45:PRO:HG2	2.37	0.46
16:O:69:TYR:HE2	16:O:183:ASP:OD2	1.99	0.46
16:O:151:ASP:HB3	38:O:8528:HOH:O	2.15	0.46
18:Q:36:THR:O	18:Q:39:ASP:HB2	2.15	0.46
1:A:585:C:H6	38:A:5588:HOH:O	1.97	0.46
1:A:621:C:H5'	27:Z:132:ASP:OD2	2.16	0.46
1:A:681:G:H1'	1:A:683:G:O6	2.16	0.46
1:A:705:C:O2	1:A:705:C:H2'	2.16	0.46
1:A:2559:C:H4'	38:A:6749:HOH:O	2.14	0.46
2:B:3029:C:C2'	2:B:3030:C:H5'	2.46	0.46
6:E:27:ARG:HD2	17:P:5:PRO:HD2	1.97	0.46
8:G:93:MET:HE1	8:G:165:GLY:N	2.30	0.46
11:J:118:PRO:HD2	38:J:8339:HOH:O	2.14	0.46
13:L:109:LEU:CD1	13:L:113:ILE:HD11	2.46	0.46
14:M:73:VAL:HG23	14:M:74:THR:H	1.81	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:N:99:ARG:HD2	15:N:167:GLY:HA2	1.97	0.46
15:N:114:VAL:HG21	15:N:159:THR:HG21	1.97	0.46
25:X:149:LEU:HG	25:X:153:MET:HE2	1.97	0.46
27:Z:106:THR:HG22	27:Z:107:PRO:O	2.16	0.46
31:4:11:CYS:HB2	31:4:20:HIS:NE2	2.30	0.46
1:A:240:C:O2	1:A:240:C:H2'	2.15	0.46
1:A:514:G:N2	38:A:3588:HOH:O	2.48	0.46
1:A:719:C:O2'	17:P:112:ARG:NH2	2.48	0.46
1:A:790:A:H2'	1:A:791:A:O4'	2.16	0.46
1:A:1056:U:H2'	1:A:1057:A:O4'	2.16	0.46
1:A:1654:U:H2'	4:C:47:HIS:CD2	2.48	0.46
1:A:2316:G:H4'	38:A:5585:HOH:O	2.15	0.46
1:A:2325:C:H2'	1:A:2326:U:C6	2.51	0.46
1:A:2445:U:H2'	1:A:2446:G:H8	1.80	0.46
6:E:102:LEU:HD12	38:E:8315:HOH:O	2.16	0.46
16:O:154:LEU:HG	16:O:155:GLU:H	1.80	0.46
17:P:107:GLU:O	17:P:108:GLY:C	2.54	0.46
18:Q:103:THR:O	18:Q:106:ARG:HB3	2.16	0.46
20:S:132:ARG:CZ	38:S:8583:HOH:O	2.64	0.46
25:X:126:ASP:HB3	25:X:135:GLY:O	2.16	0.46
25:X:149:LEU:HG	25:X:153:MET:HE1	1.98	0.46
27:Z:144:ARG:CZ	38:Z:8608:HOH:O	2.64	0.46
1:A:297:U:H1'	38:A:3447:HOH:O	2.15	0.45
1:A:371:U:H2'	1:A:372:A:C8	2.50	0.45
1:A:1162:G:H2'	38:A:6073:HOH:O	2.15	0.45
1:A:2090:G:H2'	1:A:2091:G:C8	2.51	0.45
1:A:2413:A:N7	16:O:109:PRO:HB3	2.31	0.45
5:D:104:GLU:HG3	38:D:8594:HOH:O	2.15	0.45
6:E:57:PRO:HD2	6:E:73:LEU:HD22	1.98	0.45
7:F:95:THR:C	7:F:97:GLN:N	2.69	0.45
11:J:46:VAL:CG1	11:J:146:TRP:HZ3	2.28	0.45
15:N:35:PRO:HD2	15:N:38:VAL:HG21	1.98	0.45
25:X:122:ARG:CZ	38:X:5817:HOH:O	2.62	0.45
1:A:707:C:C2	1:A:708:A:C8	3.04	0.45
1:A:737:A:H2'	1:A:738:G:O4'	2.16	0.45
1:A:1167:G:O2'	1:A:1168:C:H5'	2.15	0.45
1:A:1594:C:O2'	1:A:1607:A:H4'	2.16	0.45
1:A:1804:A:H2'	1:A:1805:G:C8	2.50	0.45
1:A:1883:U:O2'	1:A:1884:G:H5'	2.16	0.45
1:A:1890:U:H4'	1:A:2010:A:C6	2.52	0.45
1:A:2473:U:O3'	1:A:2474:A:H3'	2.16	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:3039:U:H3'	2:B:3040:C:H5"	1.98	0.45
2:B:3114:G:H2'	2:B:3115:C:C6	2.52	0.45
5:D:141:ARG:HG2	5:D:165:ARG:HA	1.99	0.45
12:K:36:VAL:HG12	12:K:37:ALA:N	2.31	0.45
14:M:90:ARG:HG3	14:M:119:THR:CG2	2.46	0.45
15:N:65:VAL:CG2	15:N:105:ALA:HB2	2.46	0.45
17:P:14:LEU:HG	17:P:102:ILE:HD11	1.98	0.45
17:P:77:ALA:HA	17:P:96:VAL:O	2.16	0.45
18:Q:131:PHE:CE1	18:Q:137:LEU:HD13	2.51	0.45
1:A:88:G:N3	30:3:24:TRP:HB2	2.31	0.45
1:A:92:G:H4'	24:W:44:GLY:HA3	1.98	0.45
1:A:1064:U:H2'	1:A:1065:G:C8	2.52	0.45
1:A:1269:G:H2'	1:A:1270:U:H6	1.81	0.45
1:A:1855:G:H8	4:C:144:GLU:OE2	2.00	0.45
1:A:2361:A:H5'	1:A:2361:A:H8	1.82	0.45
5:D:195:ARG:NH1	5:D:324:ASP:OD1	2.43	0.45
15:N:181:GLU:OE1	15:N:181:GLU:N	2.41	0.45
16:O:184:ILE:HG22	16:O:185:GLU:N	2.31	0.45
21:T:25:GLN:HG2	21:T:65:VAL:HG22	1.97	0.45
25:X:54:PHE:CZ	25:X:140:LYS:HB2	2.50	0.45
1:A:820:G:C5	4:C:171:LYS:HB2	2.52	0.45
1:A:947:U:H2'	1:A:948:G:C8	2.51	0.45
1:A:2382:A:O2'	1:A:2383:G:H5'	2.15	0.45
1:A:2507:G:H2'	1:A:2510:C:H42	1.82	0.45
1:A:2731:G:H2'	1:A:2732:U:O4'	2.17	0.45
1:A:2735:U:H2'	1:A:2736:U:C6	2.51	0.45
1:A:2783:A:H2'	1:A:2784:A:C8	2.52	0.45
8:G:84:MET:HB2	8:G:131:LEU:HB2	1.98	0.45
11:J:46:VAL:HG12	11:J:146:TRP:CZ3	2.43	0.45
12:K:107:ASN:ND2	12:K:107:ASN:C	2.69	0.45
16:O:47:LEU:HD12	16:O:92:ALA:CB	2.47	0.45
22:U:16:LEU:HA	22:U:19:ARG:HG3	1.98	0.45
1:A:485:A:O2'	1:A:487:G:H5'	2.16	0.45
1:A:1278:A:H4'	1:A:1279:U:C4	2.52	0.45
1:A:1685:A:H4'	1:A:1686:C:OP2	2.16	0.45
1:A:2831:C:H2'	1:A:2832:C:H5'	1.98	0.45
1:A:2839:C:H2'	1:A:2840:A:H5"	1.98	0.45
5:D:138:GLY:O	5:D:139:ASP:O	2.34	0.45
7:F:64:ARG:O	7:F:67:ASP:OD2	2.34	0.45
13:L:30:LYS:O	13:L:55:VAL:HG13	2.17	0.45
15:N:122:GLU:OE2	15:N:127:LYS:HE2	2.16	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:O:73:ALA:N	38:O:8567:HOH:O	2.49	0.45
20:S:39:THR:HB	20:S:42:GLU:OE1	2.17	0.45
21:T:6:LYS:O	21:T:7:HIS:HB3	2.16	0.45
25:X:108:ARG:HE	25:X:114:PRO:CG	2.28	0.45
31:4:42:ARG:HH11	31:4:42:ARG:CG	2.29	0.45
1:A:1250:C:O2'	1:A:1251:C:H5'	2.16	0.45
1:A:2911:C:H2'	1:A:2912:C:C6	2.52	0.45
4:C:95:PRO:HA	4:C:153:ARG:HA	1.98	0.45
9:H:107:VAL:O	9:H:111:ILE:HG13	2.16	0.45
12:K:6:PHE:O	12:K:8:ALA:N	2.49	0.45
20:S:17:MET:HE3	20:S:19:ARG:CZ	2.46	0.45
1:A:283:U:H5	1:A:284:C:N4	2.14	0.45
1:A:290:C:O2'	1:A:291:C:H5'	2.16	0.45
1:A:645:U:H2'	1:A:646:G:C8	2.52	0.45
1:A:1634:G:H2'	1:A:1635:U:C6	2.51	0.45
1:A:2467:A:H2'	38:A:4948:HOH:O	2.16	0.45
5:D:316:ARG:N	5:D:317:PRO:HD3	2.32	0.45
7:F:27:ILE:CG2	7:F:28:GLY:H	2.20	0.45
8:G:107:PHE:CZ	8:G:108:LEU:HD13	2.51	0.45
11:J:72:VAL:O	11:J:72:VAL:HG13	2.16	0.45
11:J:136:VAL:HG23	38:J:8343:HOH:O	2.17	0.45
15:N:159:THR:HA	38:N:8519:HOH:O	2.16	0.45
18:Q:10:ALA:HA	18:Q:13:VAL:CG1	2.45	0.45
25:X:13:MET:CE	25:X:18:GLN:HA	2.47	0.45
1:A:64:G:H2'	1:A:65:C:O4'	2.17	0.45
1:A:241:A:N1	1:A:378:A:H4'	2.32	0.45
1:A:1450:C:C4'	1:A:1451:C:OP2	2.59	0.45
1:A:1973:A:C2'	1:A:1974:G:O5'	2.65	0.45
1:A:2900:G:H2'	1:A:2901:C:O4'	2.17	0.45
38:A:3805:HOH:O	27:Z:208:LYS:HD2	2.16	0.45
38:A:9859:HOH:O	19:R:16:ASN:HB2	2.16	0.45
4:C:96:LEU:HD22	4:C:128:LEU:HD13	1.99	0.45
5:D:147:VAL:O	5:D:147:VAL:HG12	2.17	0.45
5:D:275:GLY:C	38:D:8652:HOH:O	2.55	0.45
11:J:26:LYS:HD2	11:J:28:ILE:CG1	2.47	0.45
12:K:77:GLY:O	12:K:78:ILE:C	2.55	0.45
17:P:25:VAL:HG23	17:P:26:TRP:N	2.31	0.45
19:R:75:ILE:CD1	19:R:84:ILE:HD11	2.47	0.45
21:T:11:THR:H	21:T:14:ALA:HB3	1.80	0.45
27:Z:154:ARG:O	27:Z:154:ARG:HG2	2.16	0.45
28:1:73:THR:O	28:1:76:GLY:N	2.50	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:2:8:GLN:HE22	29:2:11:LYS:HZ2	1.64	0.45
29:2:26:SER:HB3	29:2:35:SER:OG	2.17	0.45
1:A:290:C:H2'	1:A:291:C:O4'	2.17	0.45
1:A:1444:G:O2'	1:A:1445:G:H5'	2.16	0.45
1:A:2326:U:H4'	1:A:2412:G:C4'	2.47	0.45
1:A:2455:A:H2'	1:A:2456:A:O4'	2.17	0.45
1:A:2594:C:O2'	1:A:2595:U:H5'	2.16	0.45
1:A:2754:G:H2'	1:A:2755:G:O4'	2.17	0.45
2:B:3041:C:H4'	7:F:48:MET:HB2	1.99	0.45
4:C:170:VAL:HG13	28:1:22:ILE:HG21	1.99	0.45
5:D:280:VAL:HG13	5:D:334:SER:HA	1.98	0.45
6:E:139:VAL:CG1	38:E:8451:HOH:O	2.62	0.45
8:G:32:ARG:O	8:G:33:LEU:HD23	2.17	0.45
19:R:25:PRO:HA	19:R:26:PRO:HD3	1.79	0.45
22:U:38:ARG:HH11	22:U:38:ARG:HG3	1.81	0.45
27:Z:145:LYS:NZ	38:Z:8565:HOH:O	2.46	0.45
28:1:33:HIS:HE1	28:1:49:ARG:NE	2.15	0.45
1:A:162:C:H2'	1:A:163:U:H5'	1.99	0.45
1:A:177:A:H2'	1:A:178:U:O4'	2.17	0.45
1:A:314:G:N2	1:A:316:A:H3'	2.31	0.45
1:A:318:C:H5'	1:A:339:A:C2	2.51	0.45
1:A:447:A:O2'	1:A:448:G:H5'	2.17	0.45
1:A:462:A:C2	30:3:37:HIS:HB3	2.52	0.45
1:A:716:G:C2'	1:A:717:C:O5'	2.65	0.45
1:A:920:C:H5'	1:A:921:G:C4	2.52	0.45
1:A:1681:G:H5"	1:A:1682:A:H5'	1.98	0.45
1:A:1805:G:O2'	1:A:1806:G:H5'	2.17	0.45
1:A:2909:G:O2'	1:A:2910:A:H5'	2.17	0.45
12:K:92:GLN:HB3	38:K:1405:HOH:O	2.16	0.45
15:N:164:THR:CG2	15:N:167:GLY:H	2.18	0.45
16:O:162:ASP:HB3	16:O:163:PHE:H	1.58	0.45
18:Q:13:VAL:HG11	18:Q:40:VAL:HG11	1.98	0.45
18:Q:16:VAL:HG12	18:Q:20:ARG:HB2	1.98	0.45
1:A:218:C:C5	1:A:220:C:C4	3.05	0.44
1:A:538:C:H5"	1:A:539:G:C8	2.52	0.44
1:A:553:G:O4'	1:A:1325:G:H5'	2.17	0.44
1:A:584:U:H3'	38:A:5588:HOH:O	2.16	0.44
1:A:1189:A:H3'	38:A:7170:HOH:O	2.16	0.44
1:A:1803:C:H2'	1:A:1804:A:C8	2.52	0.44
1:A:2716:G:O2'	1:A:2717:C:H5'	2.17	0.44
1:A:2831:C:H2'	1:A:2832:C:C5'	2.47	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:5:77:PHA:N	36:6:77:PHA:CA	2.80	0.44
5:D:304:PRO:HD2	5:D:307:ARG:NH1	2.32	0.44
11:J:47:GLU:CB	11:J:133:ILE:CD1	2.90	0.44
17:P:26:TRP:HB2	38:P:3062:HOH:O	2.16	0.44
24:W:1:THR:O	24:W:3:LEU:N	2.49	0.44
27:Z:103:THR:HG22	27:Z:104:GLU:OE2	2.17	0.44
1:A:745:G:O6	17:P:68:GLY:HA3	2.17	0.44
1:A:2329:C:O2'	1:A:2330:U:H5'	2.18	0.44
1:A:2761:A:C4	1:A:2763:G:C8	3.06	0.44
5:D:42:ALA:HB1	5:D:308:LEU:HD11	1.97	0.44
5:D:75:GLU:C	5:D:77:PRO:HD3	2.38	0.44
6:E:126:ASP:C	6:E:128:GLY:N	2.70	0.44
8:G:11:VAL:HG11	8:G:22:VAL:HG13	1.99	0.44
11:J:29:ALA:C	11:J:30:GLN:HG3	2.37	0.44
11:J:84:ARG:CZ	11:J:135:TRP:CH2	3.00	0.44
15:N:182:LYS:HB2	15:N:194:ALA:HB2	2.00	0.44
16:O:67:ALA:HA	16:O:71:TRP:HB3	1.99	0.44
1:A:553:G:P	27:Z:204:ARG:NH2	2.89	0.44
1:A:710:G:N2	1:A:719:C:C2	2.85	0.44
1:A:1119:G:N2	1:A:1246:A:H2	2.14	0.44
1:A:1943:C:O4'	4:C:212:PRO:HA	2.16	0.44
38:A:8976:HOH:O	20:S:83:LYS:HD3	2.18	0.44
5:D:268:ARG:NE	38:D:8609:HOH:O	2.50	0.44
5:D:304:PRO:CG	5:D:307:ARG:NH1	2.80	0.44
7:F:25:MET:SD	7:F:40:ILE:HD11	2.57	0.44
8:G:85:GLU:HG3	8:G:169:THR:OG1	2.17	0.44
8:G:108:LEU:HD11	8:G:164:ASP:HB2	1.99	0.44
9:H:58:GLU:OE1	15:N:27:ARG:NH2	2.38	0.44
9:H:100:ASP:HB3	38:H:5691:HOH:O	2.17	0.44
11:J:112:ARG:O	11:J:113:ALA:C	2.55	0.44
12:K:52:GLN:O	12:K:53:ILE:C	2.56	0.44
18:Q:101:GLN:HG3	38:Q:163:HOH:O	2.18	0.44
20:S:125:ARG:HG2	38:S:8542:HOH:O	2.16	0.44
1:A:396:U:O2'	1:A:418:C:H4'	2.17	0.44
1:A:441:A:H1'	1:A:442:A:N7	2.33	0.44
1:A:517:U:C2'	1:A:518:G:H5'	2.47	0.44
1:A:2502:C:H2'	1:A:2503:A:C5'	2.45	0.44
1:A:2590:U:O2	3:5:74:C:C2	2.71	0.44
4:C:36:ASP:HB2	4:C:85:ASP:H	1.82	0.44
6:E:77:ALA:O	6:E:78:ARG:HG3	2.17	0.44
7:F:55:LYS:O	7:F:56:ARG:HB2	2.18	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:H:26:THR:HG21	9:H:103:ALA:CB	2.47	0.44
12:K:46:ILE:HD11	12:K:53:ILE:HG23	1.98	0.44
13:L:34:VAL:CG2	13:L:47:ALA:HB2	2.48	0.44
13:L:72:VAL:O	13:L:95:ALA:HA	2.17	0.44
13:L:98:VAL:HG13	13:L:99:ASP:N	2.31	0.44
14:M:57:VAL:HG12	14:M:57:VAL:O	2.17	0.44
21:T:8:PRO:HD2	24:W:32:ALA:HA	1.98	0.44
23:V:49:LEU:HD11	38:V:3805:HOH:O	2.18	0.44
26:Y:30:MET:CE	26:Y:55:ASN:HA	2.45	0.44
1:A:911:G:H5'	1:A:932:U:OP1	2.17	0.44
1:A:1209:C:H2'	1:A:1210:G:C8	2.52	0.44
1:A:1365:C:H4'	38:A:4109:HOH:O	2.17	0.44
1:A:1439:C:H5"	30:3:41:HIS:HE1	1.82	0.44
1:A:1762:C:H2'	1:A:1763:C:C6	2.53	0.44
1:A:2266:A:H2'	1:A:2267:G:C8	2.53	0.44
1:A:2776:A:H2'	1:A:2777:G:O4'	2.17	0.44
1:A:2815:G:H4'	1:A:2816:A:OP2	2.18	0.44
1:A:2909:G:H2'	1:A:2910:A:H8	1.83	0.44
4:C:105:VAL:HG13	4:C:155:THR:O	2.18	0.44
6:E:76:ARG:HD2	38:E:8438:HOH:O	2.17	0.44
9:H:99:THR:O	9:H:100:ASP:HB2	2.17	0.44
16:O:42:HIS:CG	16:O:62:HIS:HE1	2.35	0.44
16:O:154:LEU:HG	16:O:155:GLU:N	2.32	0.44
27:Z:102:LEU:O	27:Z:227:ARG:HG3	2.17	0.44
1:A:68:U:O2'	1:A:69:A:H5"	2.18	0.44
1:A:1496:G:H5'	1:A:1572:A:H1'	2.00	0.44
1:A:1641:A:H2'	1:A:1642:A:C5'	2.43	0.44
1:A:2107:U:O2'	1:A:2108:A:H5'	2.18	0.44
1:A:2729:C:O2'	1:A:2730:G:H5'	2.18	0.44
2:B:3056:A:H1'	7:F:14:ARG:HG2	1.99	0.44
5:D:49:THR:CG2	5:D:280:VAL:CG2	2.96	0.44
7:F:18:ILE:HD13	7:F:84:LEU:CD1	2.48	0.44
7:F:35:ALA:HB2	38:F:5858:HOH:O	2.18	0.44
7:F:170:TYR:N	7:F:170:TYR:CD1	2.86	0.44
8:G:9:GLU:HA	38:G:5240:HOH:O	2.17	0.44
9:H:60:VAL:HG13	9:H:63:ILE:HG13	2.00	0.44
11:J:84:ARG:CZ	11:J:135:TRP:HH2	2.30	0.44
24:W:55:ARG:O	24:W:59:ILE:HG12	2.18	0.44
1:A:119:A:H2'	1:A:120:A:H5"	1.98	0.44
1:A:155:C:OP2	15:N:188:ARG:HD3	2.18	0.44
1:A:611:U:H6	1:A:611:U:O5'	2.01	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:639:A:H2'	1:A:640:G:C8	2.52	0.44
1:A:677:C:P	38:E:8461:HOH:O	2.76	0.44
1:A:1007:A:H2'	11:J:19:TYR:CZ	2.53	0.44
1:A:1453:G:N2	1:A:1675:C:C2	2.85	0.44
1:A:2000:G:O2'	1:A:2001:G:H5'	2.18	0.44
6:E:162:VAL:HG12	6:E:162:VAL:O	2.18	0.44
7:F:23:VAL:HG12	7:F:130:VAL:HG22	1.99	0.44
11:J:35:ASN:ND2	11:J:79:ALA:O	2.51	0.44
15:N:25:TRP:HE3	15:N:26:HIS:HD2	1.64	0.44
15:N:37:VAL:CG2	15:N:108:LYS:HG3	2.46	0.44
16:O:22:GLN:HG2	16:O:26:LEU:HD22	2.00	0.44
20:S:61:GLN:CD	38:S:8540:HOH:O	2.55	0.44
27:Z:205:ILE:O	27:Z:206:ALA:C	2.55	0.44
1:A:189:A:OP1	15:N:171:ARG:NH2	2.51	0.44
1:A:240:C:C5'	15:N:146:GLN:NE2	2.81	0.44
1:A:514:G:H8	1:A:514:G:O5'	2.00	0.44
1:A:960:G:N3	1:A:960:G:C2'	2.80	0.44
1:A:1236:A:C2'	1:A:1237:U:H5'	2.48	0.44
1:A:1603:A:H5"	1:A:1605:G:H5'	1.99	0.44
1:A:1635:U:O2'	1:A:1636:G:H5'	2.17	0.44
1:A:2348:C:C5'	7:F:22:VAL:HG21	2.48	0.44
38:A:8593:HOH:O	5:D:214:PRO:HD2	2.17	0.44
4:C:128:LEU:HG	38:C:8569:HOH:O	2.18	0.44
4:C:192:VAL:O	4:C:192:VAL:CG1	2.65	0.44
5:D:84:LEU:HD23	5:D:178:ALA:HB1	1.99	0.44
6:E:154:VAL:HG13	6:E:163:HIS:CE1	2.52	0.44
7:F:57:THR:HG23	7:F:63:ILE:CB	2.48	0.44
9:H:32:GLY:N	38:H:3111:HOH:O	2.50	0.44
15:N:18:GLY:O	15:N:21:ALA:HB3	2.17	0.44
15:N:84:LYS:O	15:N:87:MET:HG2	2.17	0.44
15:N:115:LEU:HD13	15:N:116:ASN:HB2	2.00	0.44
16:O:7:LYS:HE2	38:O:8514:HOH:O	2.17	0.44
21:T:6:LYS:HB2	21:T:27:ALA:O	2.17	0.44
23:V:36:CYS:O	23:V:37:GLU:C	2.57	0.44
25:X:35:VAL:HA	25:X:36:PRO:HD3	1.76	0.44
28:1:54:ILE:HD12	38:1:8416:HOH:O	2.18	0.44
29:2:10:LYS:N	38:2:8434:HOH:O	2.31	0.44
1:A:1811:A:C2	1:A:2752:C:H1'	2.52	0.44
1:A:2385:G:H2'	1:A:2386:U:H6	1.83	0.44
1:A:2626:C:H2'	1:A:2627:G:C8	2.53	0.44
2:B:3031:C:H2'	2:B:3032:G:O4'	2.18	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:D:248:ARG:NH2	38:D:8527:HOH:O	2.51	0.44
5:D:278:PRO:HD3	5:D:294:TYR:CZ	2.53	0.44
6:E:49:ASP:HB3	6:E:52:ALA:HB2	2.00	0.44
7:F:139:TYR:N	38:F:3723:HOH:O	2.47	0.44
11:J:85:ILE:HG23	11:J:85:ILE:O	2.18	0.44
25:X:3:ALA:O	25:X:54:PHE:HA	2.18	0.44
26:Y:20:GLU:CD	26:Y:21:PRO:HD2	2.38	0.44
28:1:48:LYS:NZ	38:1:8435:HOH:O	2.51	0.44
31:4:69:TYR:CB	31:4:78:HIS:CE1	3.01	0.44
1:A:90:A:H2'	1:A:91:G:O4'	2.17	0.43
1:A:841:A:OP2	20:S:128:ARG:HD2	2.18	0.43
1:A:2050:G:H5"	20:S:80:TYR:O	2.18	0.43
1:A:2506:A:C1'	38:A:5548:HOH:O	2.66	0.43
1:A:2684:A:H2'	1:A:2685:C:H6	1.80	0.43
1:A:2812:A:N7	38:A:7009:HOH:O	2.36	0.43
10:I:63:ARG:HB2	10:I:66:LEU:HG	1.99	0.43
11:J:165:GLY:C	11:J:166:ASN:HD22	2.21	0.43
13:L:28:GLU:OE2	13:L:58:THR:HG21	2.17	0.43
14:M:61:ALA:HA	38:M:8565:HOH:O	2.17	0.43
16:O:67:ALA:C	16:O:69:TYR:N	2.71	0.43
30:3:18:ASN:ND2	30:3:40:ARG:H	2.15	0.43
1:A:74:A:H2'	1:A:75:U:C6	2.52	0.43
1:A:1422:U:H2'	1:A:1423:C:C6	2.52	0.43
1:A:1595:G:O2'	1:A:1596:U:H5'	2.18	0.43
2:B:3093:A:H8	2:B:3093:A:O5'	2.02	0.43
5:D:74:ILE:HG13	38:D:8607:HOH:O	2.18	0.43
5:D:132:HIS:CE1	5:D:171:VAL:HG21	2.53	0.43
6:E:127:ARG:NH1	6:E:127:ARG:HG2	2.34	0.43
6:E:168:ARG:NH2	6:E:190:ALA:O	2.51	0.43
7:F:173:GLU:O	7:F:174:VAL:C	2.55	0.43
11:J:151:MET:HA	11:J:151:MET:HE3	2.00	0.43
13:L:75:ARG:HE	13:L:94:ALA:HB3	1.83	0.43
13:L:78:LYS:HA	13:L:79:PRO:HD3	1.87	0.43
14:M:93:VAL:HG12	14:M:97:VAL:HG23	2.01	0.43
15:N:18:GLY:HA3	38:N:8588:HOH:O	2.17	0.43
16:O:67:ALA:C	16:O:69:TYR:H	2.21	0.43
20:S:31:ILE:O	20:S:32:ALA:C	2.54	0.43
24:W:16:ARG:NH1	24:W:65:ASP:O	2.50	0.43
1:A:407:A:H8	38:A:3961:HOH:O	2.01	0.43
1:A:844:A:C6	1:A:882:A:C5	3.06	0.43
1:A:1168:C:H5	38:A:6989:HOH:O	2.01	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1653:A:N6	38:A:3770:HOH:O	2.51	0.43
1:A:2045:G:H2'	1:A:2046:G:O4'	2.19	0.43
1:A:2067:A:H2'	1:A:2068:G:O4'	2.18	0.43
1:A:2740:G:H2'	1:A:2741:A:O4'	2.18	0.43
38:A:3614:HOH:O	5:D:158:LYS:HB2	2.18	0.43
38:A:5852:HOH:O	4:C:205:GLY:HA3	2.18	0.43
7:F:10:PHE:CD1	7:F:11:HIS:N	2.86	0.43
7:F:25:MET:HE1	7:F:37:ALA:O	2.19	0.43
7:F:27:ILE:CG2	7:F:28:GLY:N	2.79	0.43
7:F:38:GLU:HB3	7:F:49:PRO:HG2	2.00	0.43
9:H:100:ASP:O	9:H:101:ALA:O	2.37	0.43
11:J:57:ARG:HG3	11:J:57:ARG:NH1	2.33	0.43
13:L:118:ALA:HA	13:L:125:ALA:HB2	1.98	0.43
13:L:118:ALA:O	13:L:120:ARG:N	2.51	0.43
14:M:121:ILE:HG12	14:M:141:GLU:HB2	1.99	0.43
14:M:122:ALA:HB3	14:M:125:PHE:CZ	2.54	0.43
21:T:49:VAL:HG13	21:T:66:VAL:HG13	2.00	0.43
25:X:11:VAL:O	25:X:12:ASN:HB2	2.18	0.43
25:X:38:THR:HG21	38:X:5390:HOH:O	2.18	0.43
28:1:32:LYS:HE2	28:1:32:LYS:HB3	1.83	0.43
1:A:175:G:C2'	15:N:192:ALA:HB3	2.47	0.43
1:A:2428:G:N7	31:4:60:LYS:NZ	2.64	0.43
1:A:2769:C:H2'	1:A:2770:G:C5'	2.48	0.43
38:A:3171:HOH:O	15:N:79:LYS:CD	2.59	0.43
36:5:77:PHA:H2	36:6:77:PHA:CA	2.31	0.43
4:C:105:VAL:CG1	4:C:106:CYS:N	2.81	0.43
5:D:240:GLY:HA3	38:D:8530:HOH:O	2.19	0.43
5:D:258:GLY:H	5:D:260:HIS:CE1	2.36	0.43
6:E:21:VAL:C	6:E:23:GLU:N	2.71	0.43
6:E:200:PRO:HB3	6:E:212:VAL:CG2	2.48	0.43
11:J:31:PHE:HD2	11:J:85:ILE:O	2.01	0.43
11:J:45:GLN:NE2	11:J:135:TRP:HE1	2.11	0.43
15:N:61:ILE:HD12	15:N:61:ILE:N	2.33	0.43
17:P:14:LEU:CG	17:P:102:ILE:HD11	2.48	0.43
18:Q:115:SER:C	18:Q:117:SER:N	2.70	0.43
20:S:39:THR:HG22	20:S:42:GLU:HG3	2.00	0.43
22:U:73:HIS:CD2	22:U:88:PRO:CG	3.01	0.43
1:A:138:U:OP2	1:A:139:C:H5	2.01	0.43
1:A:790:A:H1'	1:A:1710:A:H2'	2.00	0.43
1:A:875:A:C2	4:C:194:MET:SD	3.12	0.43
1:A:1289:C:O2'	1:A:1290:G:H5'	2.18	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1973:A:H5'	1:A:1973:A:H8	1.84	0.43
1:A:2353:A:H4'	1:A:2354:A:O5'	2.17	0.43
4:C:48:ASP:HB3	38:C:8602:HOH:O	2.18	0.43
5:D:129:ARG:O	5:D:133:GLU:HG3	2.18	0.43
6:E:65:ARG:HG3	6:E:67:GLN:HB2	2.01	0.43
6:E:107:ARG:NH2	38:E:8461:HOH:O	2.48	0.43
9:H:48:VAL:HG12	9:H:97:ALA:HB2	2.00	0.43
11:J:29:ALA:N	11:J:62:GLU:OE1	2.40	0.43
11:J:129:ASN:HD22	11:J:129:ASN:N	2.17	0.43
19:R:3:SER:HB3	38:R:5998:HOH:O	2.17	0.43
1:A:79:G:H22	1:A:97:G:H1'	1.84	0.43
1:A:192:A:C4'	15:N:176:GLN:HE22	2.32	0.43
1:A:407:A:H2'	1:A:408:A:C8	2.54	0.43
1:A:644:G:H1'	38:A:5897:HOH:O	2.17	0.43
1:A:716:G:H2'	1:A:717:C:O5'	2.19	0.43
1:A:738:G:H3'	38:A:6538:HOH:O	2.19	0.43
1:A:1044:C:H5"	38:A:8544:HOH:O	2.18	0.43
1:A:1235:G:C1'	12:K:63:ILE:HG23	2.48	0.43
1:A:1500:U:OP2	18:Q:41:ARG:NH2	2.51	0.43
1:A:1506:U:H6	1:A:1506:U:H5'	1.83	0.43
1:A:1513:C:O2'	1:A:1514:C:H5'	2.18	0.43
1:A:2104:C:O2	1:A:2486:A:C2	2.72	0.43
1:A:2766:A:O2'	1:A:2767:C:H5'	2.18	0.43
2:B:3024:U:C3'	2:B:3025:G:H5'	2.48	0.43
2:B:3060:C:O2'	2:B:3061:C:H5'	2.19	0.43
6:E:40:ALA:O	6:E:43:LYS:HB2	2.19	0.43
7:F:23:VAL:HG21	7:F:45:THR:HG21	2.00	0.43
7:F:99:ASP:CB	7:F:103:ASN:HB2	2.48	0.43
11:J:93:ILE:O	11:J:119:VAL:HG22	2.17	0.43
22:U:40:VAL:HG22	22:U:41:ARG:N	2.33	0.43
25:X:64:THR:O	25:X:68:THR:HG22	2.18	0.43
26:Y:34:ARG:NH1	26:Y:48:VAL:O	2.49	0.43
28:1:30:GLU:O	28:1:33:HIS:HB3	2.18	0.43
28:1:58:GLY:CA	38:1:8438:HOH:O	2.47	0.43
1:A:450:C:H4'	6:E:46:TYR:CE1	2.53	0.43
1:A:860:U:H2'	1:A:861:A:C8	2.53	0.43
1:A:941:G:C5	1:A:942:U:C4	3.07	0.43
1:A:1051:C:H2'	1:A:1052:G:O4'	2.18	0.43
1:A:1597:A:O4'	18:Q:95:GLU:HG2	2.19	0.43
1:A:1654:U:C6	4:C:47:HIS:CD2	3.07	0.43
1:A:2032:U:P	38:A:4015:HOH:O	2.76	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2451:G:O2'	31:4:38:ARG:NH2	2.52	0.43
38:A:3263:HOH:O	15:N:108:LYS:HD2	2.18	0.43
6:E:76:ARG:HG2	6:E:78:ARG:NH1	2.34	0.43
6:E:133:ARG:NE	6:E:135:GLU:O	2.52	0.43
8:G:145:ALA:HB1	8:G:168:ILE:HD11	1.99	0.43
12:K:6:PHE:HB3	12:K:109:TYR:OH	2.18	0.43
21:T:23:LYS:HD3	21:T:65:VAL:HG12	2.01	0.43
24:W:1:THR:C	24:W:3:LEU:N	2.71	0.43
27:Z:177:LYS:HD3	27:Z:181:GLY:O	2.19	0.43
28:1:32:LYS:HZ2	28:1:70:GLN:NE2	2.17	0.43
29:2:25:LYS:HD2	30:3:48:ASP:CA	2.49	0.43
1:A:152:A:O2'	1:A:153:C:H5'	2.19	0.43
1:A:290:C:H1'	38:A:5597:HOH:O	2.18	0.43
1:A:1878:G:C4'	38:A:5614:HOH:O	2.66	0.43
2:B:3029:C:H5"	7:F:140:ARG:HB3	2.00	0.43
5:D:88:GLU:O	5:D:88:GLU:HG3	2.18	0.43
6:E:139:VAL:CG2	6:E:240:LEU:HD12	2.49	0.43
12:K:131:THR:HB	12:K:134:GLU:OE1	2.18	0.43
21:T:17:ASP:HB3	21:T:23:LYS:HB2	2.00	0.43
22:U:24:ARG:HG2	22:U:24:ARG:HH11	1.83	0.43
22:U:40:VAL:HA	22:U:119:ALA:O	2.19	0.43
1:A:764:C:H2'	1:A:765:G:O4'	2.18	0.43
1:A:1862:C:H1'	38:A:6710:HOH:O	2.19	0.43
1:A:2362:A:H2'	1:A:2363:G:C8	2.53	0.43
1:A:2781:U:H2'	1:A:2782:G:C5'	2.49	0.43
7:F:93:LEU:HB3	7:F:97:GLN:OE1	2.19	0.43
7:F:159:PRO:O	7:F:162:ALA:HB3	2.18	0.43
11:J:31:PHE:HA	11:J:85:ILE:CG2	2.49	0.43
12:K:90:LYS:HB2	35:K:8502:CL:CL	2.56	0.43
38:L:6493:HOH:O	23:V:24:LYS:HG3	2.18	0.43
15:N:61:ILE:CG2	15:N:62:VAL:N	2.82	0.43
17:P:29:VAL:O	17:P:33:LEU:HG	2.19	0.43
28:1:40:PRO:HG2	28:1:64:ILE:HD13	2.00	0.43
1:A:731:U:H2'	1:A:732:C:C6	2.54	0.43
1:A:827:A:H2'	1:A:828:G:O4'	2.18	0.43
1:A:1388:U:H2'	1:A:1389:G:O4'	2.19	0.43
1:A:2598:U:O2	1:A:2600:A:H8	2.01	0.43
1:A:2812:A:C2	1:A:2814:A:N6	2.80	0.43
2:B:3002:U:OP2	2:B:3002:U:H4'	2.18	0.43
38:B:8517:HOH:O	16:O:107:ASN:HB3	2.18	0.43
7:F:84:LEU:HA	7:F:87:ALA:HB3	2.01	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:F:95:THR:HG21	7:F:174:VAL:HG22	2.00	0.43
8:G:11:VAL:HG12	8:G:12:ASP:H	1.84	0.43
11:J:72:VAL:HG11	11:J:81:TYR:CZ	2.54	0.43
12:K:84:ARG:HB2	12:K:98:PHE:CE1	2.54	0.43
13:L:14:LYS:HD2	13:L:45:PRO:HG3	2.00	0.43
15:N:31:TRP:HA	15:N:34:GLU:HG3	2.01	0.43
15:N:78:ASN:O	15:N:79:LYS:HG2	2.19	0.43
18:Q:14:LEU:HD13	18:Q:51:ALA:HB2	2.00	0.43
21:T:73:ASP:O	21:T:77:VAL:HG23	2.18	0.43
22:U:23:VAL:HA	22:U:93:THR:HG21	2.01	0.43
23:V:52:THR:HG21	23:V:54:THR:HB	2.00	0.43
28:1:22:ILE:O	28:1:26:VAL:HG23	2.18	0.43
28:1:39:CYS:HA	28:1:47:LEU:HD11	2.01	0.43
1:A:1165:G:H1'	1:A:1174:A:H1'	2.01	0.42
1:A:1384:C:H5'	26:Y:30:MET:HG2	2.00	0.42
1:A:1559:A:C1'	38:A:5357:HOH:O	2.62	0.42
1:A:1745:G:H5'	38:A:3836:HOH:O	2.19	0.42
1:A:1761:U:H5'	18:Q:81:LYS:O	2.19	0.42
1:A:2379:G:N7	1:A:2408:A:N1	2.67	0.42
38:A:9304:HOH:O	13:L:39:GLY:HA3	2.19	0.42
4:C:95:PRO:HG2	4:C:98:GLU:CG	2.47	0.42
4:C:192:VAL:HG13	38:C:8554:HOH:O	2.19	0.42
5:D:63:GLU:O	5:D:63:GLU:HG3	2.19	0.42
5:D:217:ARG:CG	5:D:257:THR:HG22	2.45	0.42
5:D:224:LYS:HD3	5:D:224:LYS:HA	1.79	0.42
6:E:46:TYR:CE2	6:E:98:ARG:NH1	2.87	0.42
6:E:236:THR:O	6:E:239:ALA:N	2.52	0.42
11:J:58:HIS:ND1	11:J:59:ASN:ND2	2.67	0.42
11:J:65:ARG:HD3	38:J:8385:HOH:O	2.18	0.42
12:K:77:GLY:O	12:K:80:LYS:N	2.51	0.42
13:L:74:VAL:HG21	13:L:96:VAL:HG23	2.01	0.42
13:L:106:GLY:HA3	38:L:5264:HOH:O	2.18	0.42
14:M:120:LEU:HD12	14:M:133:VAL:HG21	2.00	0.42
15:N:95:LYS:HG2	15:N:99:ARG:HB3	2.01	0.42
16:O:15:GLU:OE1	16:O:17:ARG:HD2	2.19	0.42
17:P:39:THR:O	17:P:115:ARG:NH2	2.52	0.42
22:U:38:ARG:NH1	22:U:38:ARG:HG3	2.33	0.42
23:V:4:ARG:N	38:V:5334:HOH:O	2.51	0.42
25:X:31:HIS:HB3	38:X:5420:HOH:O	2.19	0.42
25:X:122:ARG:NH1	25:X:152:ALA:O	2.51	0.42
27:Z:105:LYS:HE2	27:Z:198:GLY:O	2.19	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:222:A:H2'	1:A:223:G:O4'	2.18	0.42
1:A:228:C:H2'	1:A:229:G:H5'	1.99	0.42
1:A:795:G:N3	1:A:817:G:C2	2.87	0.42
1:A:853:C:H2'	1:A:854:G:O4'	2.19	0.42
1:A:1055:G:OP2	11:J:94:ARG:NH1	2.52	0.42
1:A:1165:G:O2'	1:A:1174:A:H4'	2.19	0.42
1:A:1682:A:O2'	1:A:1683:G:H5"	2.19	0.42
1:A:1878:G:O2'	1:A:1879:U:P	2.77	0.42
1:A:1988:C:O2'	1:A:1989:G:H5'	2.19	0.42
1:A:2004:U:O2	1:A:2004:U:H2'	2.19	0.42
1:A:2437:A:H2'	1:A:2438:G:C8	2.54	0.42
1:A:2597:U:H2'	1:A:2598:U:H5'	2.02	0.42
1:A:2756:U:N3	1:A:2896:A:H2	2.16	0.42
5:D:217:ARG:HD3	5:D:218:TRP:NE1	2.34	0.42
6:E:80:VAL:HA	6:E:81:PRO:HD3	1.85	0.42
13:L:37:TYR:HD2	38:L:7169:HOH:O	2.01	0.42
13:L:37:TYR:HE2	13:L:45:PRO:HA	1.84	0.42
14:M:6:ARG:NH2	38:M:8550:HOH:O	2.51	0.42
15:N:17:GLU:O	15:N:21:ALA:HB2	2.19	0.42
20:S:29:LYS:NZ	38:S:8540:HOH:O	2.51	0.42
22:U:55:PHE:CG	22:U:77:VAL:HG13	2.53	0.42
25:X:139:GLY:O	25:X:141:HIS:CD2	2.72	0.42
27:Z:126:PRO:HG2	27:Z:128:PHE:CZ	2.54	0.42
1:A:210:U:O2'	1:A:211:U:H5'	2.19	0.42
1:A:213:G:O2'	1:A:214:U:OP2	2.37	0.42
1:A:288:A:H2'	1:A:289:G:C8	2.54	0.42
1:A:1820:G:C6	1:A:2030:A:C2	3.07	0.42
1:A:2821:C:H4'	5:D:116:PRO:CB	2.49	0.42
5:D:7:ARG:CD	5:D:9:GLY:O	2.68	0.42
6:E:109:LEU:HD12	6:E:109:LEU:O	2.19	0.42
7:F:167:GLU:C	7:F:169:THR:H	2.23	0.42
10:I:71:LEU:C	10:I:73:ASP:N	2.72	0.42
12:K:14:ALA:HB1	12:K:44:ALA:HB2	2.00	0.42
13:L:103:ASP:O	13:L:104:PRO:C	2.56	0.42
15:N:49:ALA:C	15:N:54:TYR:HB3	2.39	0.42
16:O:37:ARG:HA	16:O:37:ARG:HD3	1.82	0.42
26:Y:25:ARG:O	26:Y:26:ALA:C	2.57	0.42
29:2:36:SER:O	29:2:46:ARG:HD3	2.19	0.42
30:3:36:ASN:HB3	30:3:39:ARG:HE	1.84	0.42
1:A:482:G:H4'	1:A:508:A:N1	2.34	0.42
1:A:1400:C:H4'	26:Y:56:GLU:HG2	2.01	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1855:G:H4'	1:A:1856:C:O5'	2.19	0.42
1:A:2737:C:H2'	38:A:5635:HOH:O	2.19	0.42
1:A:2897:C:H2'	1:A:2898:G:C8	2.46	0.42
5:D:243:ASN:HA	5:D:244:PRO:C	2.39	0.42
8:G:156:ASP:OD2	8:G:157:LYS:NZ	2.41	0.42
10:I:20:VAL:O	10:I:24:VAL:HG23	2.19	0.42
11:J:56:ILE:HG22	11:J:61:LEU:CD2	2.48	0.42
15:N:157:LEU:HD23	38:N:8637:HOH:O	2.18	0.42
15:N:169:ARG:NH2	38:N:8553:HOH:O	2.50	0.42
16:O:149:GLU:O	16:O:152:GLU:HB2	2.20	0.42
17:P:53:GLN:HG2	17:P:56:GLU:OE1	2.20	0.42
18:Q:20:ARG:NH1	18:Q:54:LYS:HD3	2.34	0.42
26:Y:22:ASN:C	26:Y:24:LYS:H	2.23	0.42
26:Y:27:ASP:OD2	26:Y:27:ASP:N	2.50	0.42
1:A:297:U:H2'	1:A:298:C:H6	1.85	0.42
1:A:366:U:H2'	1:A:367:G:O4'	2.19	0.42
1:A:545:G:H2'	1:A:546:C:O4'	2.20	0.42
1:A:1315:G:C4	27:Z:212:ARG:HB2	2.54	0.42
1:A:1887:U:OP1	28:1:21:LYS:HE3	2.20	0.42
1:A:2245:C:O5'	1:A:2245:C:H6	2.02	0.42
1:A:2379:G:H4'	1:A:2380:A:H5"	2.01	0.42
38:B:8474:HOH:O	16:O:23:ARG:NH1	2.52	0.42
7:F:86:THR:HG23	38:F:7477:HOH:O	2.19	0.42
9:H:28:ALA:HB3	9:H:99:THR:HG23	2.00	0.42
11:J:42:TYR:HA	11:J:43:PRO:HD3	1.87	0.42
11:J:49:VAL:HG22	11:J:130:HIS:HB3	2.02	0.42
11:J:58:HIS:CE1	11:J:59:ASN:ND2	2.88	0.42
12:K:45:VAL:HG21	12:K:129:PHE:CD1	2.54	0.42
16:O:13:ARG:NH1	16:O:13:ARG:O	2.51	0.42
20:S:72:VAL:HG11	20:S:75:TRP:HB3	2.02	0.42
22:U:89:ARG:C	22:U:89:ARG:HD2	2.39	0.42
24:W:13:PRO:O	24:W:17:GLU:HG3	2.20	0.42
25:X:4:LEU:HD23	25:X:4:LEU:HA	1.79	0.42
25:X:142:ASP:HB3	25:X:145:GLY:H	1.84	0.42
31:4:34:LYS:N	31:4:34:LYS:HD2	2.34	0.42
1:A:69:A:H2'	1:A:70:A:OP2	2.19	0.42
1:A:635:A:H2'	1:A:636:G:H5"	2.01	0.42
1:A:1052:G:N3	1:A:1052:G:H2'	2.34	0.42
1:A:1669:A:H2	38:A:3214:HOH:O	2.02	0.42
1:A:2842:G:H2'	1:A:2843:A:H5'	2.00	0.42
5:D:13:PHE:CD1	5:D:13:PHE:N	2.87	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:F:49:PRO:HG3	38:F:5828:HOH:O	2.18	0.42
7:F:154:LYS:HD3	38:F:1796:HOH:O	2.19	0.42
11:J:31:PHE:HD2	11:J:85:ILE:HG23	1.84	0.42
12:K:88:PRO:O	12:K:94:GLY:HA3	2.19	0.42
16:O:80:SER:CB	38:O:8537:HOH:O	2.65	0.42
16:O:176:ARG:O	16:O:180:LEU:HG	2.20	0.42
17:P:26:TRP:HA	17:P:26:TRP:CE3	2.55	0.42
25:X:7:LEU:CD1	25:X:53:ALA:HB2	2.50	0.42
25:X:125:HIS:CD2	25:X:127:GLY:H	2.37	0.42
1:A:451:C:O2'	1:A:452:G:H5'	2.19	0.42
1:A:1790:C:H2'	1:A:1791:U:C6	2.54	0.42
1:A:1902:G:H2'	1:A:1903:U:O4'	2.20	0.42
1:A:1942:A:H3'	38:A:6838:HOH:O	2.19	0.42
1:A:2570:G:H5"	38:A:4406:HOH:O	2.19	0.42
9:H:1:PRO:HB2	38:H:5897:HOH:O	2.20	0.42
9:H:108:LEU:O	9:H:111:ILE:N	2.50	0.42
11:J:26:LYS:HD3	11:J:89:PRO:CG	2.50	0.42
13:L:27:ARG:HD2	38:L:4747:HOH:O	2.19	0.42
14:M:24:ALA:HB2	14:M:30:ARG:HD2	2.01	0.42
15:N:49:ALA:HB1	15:N:54:TYR:CB	2.50	0.42
15:N:99:ARG:CD	15:N:167:GLY:HA2	2.50	0.42
24:W:45:ARG:C	24:W:47:LYS:N	2.73	0.42
28:1:45:LYS:HG3	38:1:8410:HOH:O	2.18	0.42
31:4:36:ILE:HD12	31:4:36:ILE:HA	1.95	0.42
1:A:51:G:O2'	1:A:52:A:H5'	2.20	0.42
1:A:503:G:H2'	1:A:504:G:H8	1.85	0.42
1:A:521:A:C2'	1:A:522:U:H5'	2.50	0.42
1:A:823:U:H2'	1:A:824:G:O4'	2.19	0.42
1:A:926:A:O2'	14:M:41:HIS:CD2	2.70	0.42
1:A:952:G:N3	1:A:2302:A:H2'	2.35	0.42
1:A:1329:A:C2	38:A:4181:HOH:O	2.56	0.42
1:A:1669:A:H2'	1:A:1670:G:H8	1.85	0.42
1:A:1730:G:C5'	1:A:1731:C:C6	3.02	0.42
1:A:1810:C:OP1	23:V:44:ARG:NE	2.38	0.42
1:A:1972:U:H2'	1:A:1973:A:C5'	2.50	0.42
1:A:2769:C:H2'	1:A:2770:G:H5'	2.02	0.42
38:A:4412:HOH:O	15:N:14:ARG:HB3	2.19	0.42
4:C:123:GLY:HA2	4:C:159:VAL:O	2.20	0.42
5:D:30:PRO:HG2	5:D:313:PRO:HD2	2.01	0.42
5:D:69:VAL:HA	5:D:70:PRO:HD3	1.91	0.42
9:H:26:THR:HB	9:H:102:GLY:HA3	2.02	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:I:63:ARG:O	10:I:67:LEU:HG	2.19	0.42
12:K:70:PHE:CD2	12:K:70:PHE:O	2.72	0.42
14:M:34:GLY:HA3	14:M:38:HIS:CE1	2.55	0.42
27:Z:235:GLU:CD	27:Z:235:GLU:N	2.70	0.42
31:4:87:ARG:NH1	38:4:8524:HOH:O	2.53	0.42
1:A:128:A:H3'	1:A:128:A:H8	1.85	0.42
1:A:283:U:H5"	1:A:284:C:OP2	2.20	0.42
1:A:583:G:H2'	1:A:584:U:H6	1.84	0.42
1:A:921:G:H4'	1:A:924:G:C6	2.55	0.42
1:A:1565:C:O4'	1:A:2738:G:H1'	2.20	0.42
1:A:2297:U:H1'	38:A:4665:HOH:O	2.20	0.42
1:A:2712:G:H5'	38:A:4711:HOH:O	2.20	0.42
4:C:35:GLY:O	4:C:36:ASP:CB	2.60	0.42
4:C:165:THR:O	4:C:165:THR:HG22	2.19	0.42
12:K:42:GLU:O	12:K:131:THR:HG23	2.20	0.42
12:K:142:ASN:O	12:K:144:THR:N	2.53	0.42
13:L:22:ASP:HA	13:L:108:GLU:O	2.20	0.42
14:M:144:ASP:HA	14:M:147:GLU:HG3	2.01	0.42
19:R:32:GLU:O	19:R:93:ARG:NH2	2.53	0.42
19:R:41:LEU:HB3	19:R:52:PHE:CZ	2.55	0.42
20:S:119:VAL:O	20:S:119:VAL:CG1	2.67	0.42
21:T:57:THR:C	21:T:59:ASP:H	2.22	0.42
25:X:21:LEU:HB3	25:X:26:ILE:CG1	2.50	0.42
25:X:73:LEU:HD12	25:X:73:LEU:HA	1.73	0.42
25:X:132:VAL:HG21	25:X:141:HIS:CD2	2.55	0.42
27:Z:189:ASN:C	27:Z:189:ASN:ND2	2.71	0.42
1:A:303:C:H2'	1:A:304:G:O4'	2.20	0.42
1:A:424:C:H2'	1:A:425:U:C6	2.55	0.42
1:A:873:G:H2'	1:A:875:A:N7	2.35	0.42
1:A:1755:A:H2'	1:A:1756:G:O4'	2.20	0.42
1:A:2269:C:H2'	1:A:2270:G:C5'	2.50	0.42
1:A:2699:A:H2'	1:A:2700:G:O4'	2.20	0.42
1:A:2846:C:H4'	5:D:156:LYS:HB3	2.01	0.42
38:A:9721:HOH:O	27:Z:135:LYS:HE3	2.20	0.42
2:B:3056:A:C3'	2:B:3057:A:H5"	2.49	0.42
2:B:3093:A:C5	2:B:3094:G:H1'	2.54	0.42
5:D:36:PRO:HG3	5:D:168:GLY:HA3	2.02	0.42
5:D:49:THR:HG21	5:D:280:VAL:CG2	2.50	0.42
6:E:37:ALA:O	6:E:41:ASN:ND2	2.53	0.42
7:F:15:GLU:HA	7:F:16:PRO:HD3	1.88	0.42
7:F:144:ARG:NH2	38:F:3839:HOH:O	2.48	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:H:50:VAL:CG1	9:H:60:VAL:HG11	2.49	0.42
16:O:71:TRP:CE2	16:O:73:ALA:HB3	2.55	0.42
17:P:81:PHE:CD1	17:P:81:PHE:N	2.87	0.42
22:U:9:LYS:HD2	38:U:7242:HOH:O	2.20	0.42
22:U:43:ASN:C	22:U:45:GLY:H	2.23	0.42
27:Z:178:HIS:CG	27:Z:179:PRO:HD2	2.55	0.42
30:3:40:ARG:HG2	30:3:40:ARG:HH11	1.85	0.42
1:A:486:A:H1'	38:A:6265:HOH:O	2.19	0.41
1:A:1066:U:H2'	1:A:1067:A:C8	2.55	0.41
1:A:1230:A:H4'	1:A:1231:A:O5'	2.20	0.41
1:A:1666:C:C2'	1:A:1667:A:H5"	2.49	0.41
1:A:1787:C:O2'	1:A:1788:U:H5'	2.20	0.41
1:A:1926:G:H2'	1:A:1927:A:C8	2.55	0.41
1:A:2032:U:O2'	1:A:2033:G:H5"	2.19	0.41
1:A:2094:G:H4'	5:D:245:SER:HB3	2.03	0.41
1:A:2589:U:H2'	1:A:2590:U:C6	2.55	0.41
38:A:5766:HOH:O	18:Q:63:ARG:NH2	2.53	0.41
5:D:16:ARG:HB3	5:D:217:ARG:NH2	2.35	0.41
5:D:60:SER:C	5:D:62:ARG:N	2.72	0.41
9:H:49:PHE:CD1	9:H:49:PHE:N	2.88	0.41
12:K:40:ASN:OD1	12:K:106:GLY:HA2	2.19	0.41
14:M:143:THR:HG22	14:M:144:ASP:H	1.85	0.41
15:N:184:ARG:CG	15:N:185:PRO:HA	2.50	0.41
19:R:46:SER:O	19:R:48:PRO:HD3	2.20	0.41
27:Z:186:ARG:NH1	27:Z:186:ARG:CG	2.80	0.41
31:4:18:GLN:OE1	31:4:73:GLU:HB3	2.19	0.41
1:A:1224:G:H2'	1:A:1225:C:C6	2.54	0.41
1:A:1311:G:C2	1:A:1312:G:C8	3.08	0.41
1:A:1391:G:H2'	1:A:1392:A:H5'	2.02	0.41
1:A:1456:C:H2'	1:A:1457:U:C6	2.55	0.41
1:A:1462:C:H2'	1:A:1463:A:C8	2.55	0.41
1:A:1484:G:H2'	38:A:8620:HOH:O	2.19	0.41
1:A:1811:A:H2'	1:A:1812:G:H5'	2.02	0.41
1:A:1850:U:H2'	1:A:1851:G:H8	1.85	0.41
1:A:1996:U:O2'	1:A:1997:A:H5'	2.19	0.41
1:A:2005:G:H3'	1:A:2005:G:OP2	2.20	0.41
1:A:2111:G:H1'	38:A:8566:HOH:O	2.19	0.41
1:A:2897:C:O2'	1:A:2898:G:H5'	2.21	0.41
2:B:3003:A:N6	2:B:3022:G:H1'	2.35	0.41
2:B:3042:C:H5'	2:B:3043:G:OP2	2.19	0.41
5:D:154:VAL:CG1	5:D:156:LYS:HG2	2.50	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:E:188:ARG:NH2	38:E:8322:HOH:O	2.50	0.41
7:F:40:ILE:HG23	38:F:5583:HOH:O	2.20	0.41
7:F:169:THR:C	7:F:170:TYR:HD1	2.23	0.41
8:G:7:ILE:HA	8:G:8:PRO:HD3	1.93	0.41
8:G:101:GLU:OE2	8:G:115:ARG:NH1	2.52	0.41
11:J:26:LYS:HD2	11:J:28:ILE:CB	2.45	0.41
11:J:126:HIS:O	11:J:127:GLY:C	2.59	0.41
11:J:136:VAL:HG22	11:J:137:ASN:N	2.35	0.41
15:N:184:ARG:HG3	15:N:185:PRO:HA	2.02	0.41
19:R:16:ASN:HD22	19:R:16:ASN:HA	1.62	0.41
19:R:18:PRO:O	19:R:21:ARG:HB2	2.20	0.41
25:X:59:GLN:NE2	25:X:97:ALA:HB3	2.35	0.41
1:A:11:A:H5'	1:A:12:U:OP2	2.20	0.41
1:A:711:G:C2	1:A:718:C:C2	3.08	0.41
1:A:816:G:C5	1:A:817:G:C6	3.08	0.41
1:A:902:G:N7	14:M:18:HIS:CD2	2.85	0.41
1:A:1332:C:O2'	1:A:1333:U:H5'	2.20	0.41
1:A:2079:G:H2'	1:A:2080:G:O4'	2.20	0.41
1:A:2781:U:O2'	1:A:2782:G:H5'	2.20	0.41
2:B:3059:C:H5'	38:B:8476:HOH:O	2.19	0.41
36:5:77:PHA:HD2	36:5:77:PHA:HA	1.82	0.41
4:C:100:PRO:HG2	4:C:103:VAL:CG2	2.45	0.41
4:C:211:LYS:HD3	38:C:8607:HOH:O	2.19	0.41
4:C:211:LYS:CB	4:C:212:PRO:CD	2.98	0.41
5:D:304:PRO:CD	5:D:307:ARG:NH1	2.84	0.41
7:F:59:GLY:C	7:F:61:PHE:N	2.74	0.41
8:G:112:ALA:HA	8:G:113:PRO:HD3	1.84	0.41
9:H:34:ASN:HA	15:N:4:ALA:HB2	2.02	0.41
13:L:87:ARG:CZ	38:L:4854:HOH:O	2.68	0.41
17:P:26:TRP:HA	17:P:26:TRP:HE3	1.85	0.41
22:U:87:VAL:HB	22:U:88:PRO:HD2	2.02	0.41
25:X:34:LEU:CD1	25:X:100:LEU:HD13	2.51	0.41
25:X:137:GLN:HG3	25:X:137:GLN:O	2.20	0.41
1:A:236:A:H4'	1:A:237:G:OP1	2.19	0.41
1:A:1003:U:O2	11:J:90:PHE:HZ	2.02	0.41
1:A:1271:A:H2'	1:A:1272:C:O4'	2.21	0.41
1:A:1470:A:O4'	15:N:93:ARG:HD3	2.21	0.41
1:A:1739:G:O2'	1:A:1740:U:H5'	2.20	0.41
1:A:2252:A:C6	1:A:2253:G:H1'	2.54	0.41
1:A:2659:U:H5"	38:A:3635:HOH:O	2.20	0.41
38:A:3267:HOH:O	22:U:9:LYS:CD	2.66	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:A:7197:HOH:O	6:E:94:THR:HG21	2.21	0.41
2:B:3028:U:H5"	16:O:40:ASN:ND2	2.35	0.41
2:B:3095:C:O2'	2:B:3096:C:H5'	2.21	0.41
4:C:97:ALA:HB2	4:C:150:PRO:HB2	2.02	0.41
5:D:82:VAL:O	5:D:82:VAL:CG1	2.68	0.41
9:H:38:LYS:NZ	15:N:3:SER:HA	2.35	0.41
14:M:17:SER:C	14:M:19:LYS:H	2.24	0.41
15:N:61:ILE:HA	38:N:8632:HOH:O	2.20	0.41
16:O:34:LEU:HD13	16:O:47:LEU:HD21	2.03	0.41
16:O:82:TYR:CD2	16:O:82:TYR:C	2.94	0.41
22:U:26:THR:HA	22:U:39:ASN:HB3	2.01	0.41
26:Y:25:ARG:HD3	26:Y:64:ALA:O	2.20	0.41
1:A:111:C:H2'	1:A:112:G:O4'	2.20	0.41
1:A:569:A:H5"	1:A:587:A:N1	2.34	0.41
1:A:1384:C:H2'	1:A:1385:G:O4'	2.20	0.41
1:A:1619:G:H2'	1:A:1620:C:O4'	2.20	0.41
1:A:2032:U:H5'	38:A:4015:HOH:O	2.19	0.41
4:C:30:ARG:HE	4:C:30:ARG:HB3	1.62	0.41
7:F:17:ARG:NH2	38:F:3723:HOH:O	2.54	0.41
10:I:71:LEU:O	10:I:73:ASP:N	2.53	0.41
11:J:65:ARG:HH21	11:J:66:VAL:HG22	1.85	0.41
16:O:38:LYS:HE3	16:O:38:LYS:HB2	1.76	0.41
18:Q:41:ARG:O	18:Q:44:VAL:HB	2.19	0.41
18:Q:59:ARG:HH22	18:Q:66:GLN:HE22	1.65	0.41
20:S:113:HIS:O	20:S:145:LEU:HD12	2.21	0.41
24:W:29:ASN:O	24:W:33:VAL:HG23	2.20	0.41
25:X:56:GLU:O	25:X:143:THR:HG23	2.20	0.41
26:Y:30:MET:HE1	26:Y:58:ALA:HB3	2.02	0.41
27:Z:117:LEU:HA	27:Z:174:VAL:HG11	2.02	0.41
1:A:275:G:C2	1:A:376:C:N3	2.89	0.41
1:A:1162:G:H2'	1:A:1162:G:N3	2.35	0.41
1:A:1245:C:O5'	1:A:1245:C:H6	2.04	0.41
1:A:1398:G:O2'	1:A:1399:A:H5'	2.21	0.41
1:A:1482:A:O2'	1:A:1483:C:H5'	2.21	0.41
1:A:1562:C:O2	1:A:1562:C:H2'	2.20	0.41
1:A:1593:C:OP1	18:Q:117:SER:HB3	2.21	0.41
1:A:1714:C:O2'	1:A:1715:C:H5'	2.21	0.41
1:A:1857:A:N6	1:A:2247:C:H1'	2.36	0.41
1:A:2506:A:O2'	1:A:2507:G:P	2.78	0.41
1:A:2582:G:O3'	13:L:41:LYS:HA	2.20	0.41
4:C:82:VAL:HG13	4:C:93:THR:HB	2.02	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:D:7:ARG:NH1	5:D:11:LEU:HD22	2.35	0.41
5:D:62:ARG:HG2	5:D:62:ARG:HH11	1.86	0.41
6:E:140:VAL:HG12	6:E:141:SER:N	2.34	0.41
6:E:165:ASP:O	6:E:168:ARG:HB3	2.20	0.41
11:J:113:ALA:N	11:J:114:PRO:HD3	2.36	0.41
13:L:65:ARG:O	13:L:66:ARG:HB2	2.21	0.41
13:L:99:ASP:C	13:L:99:ASP:OD1	2.58	0.41
15:N:63:VAL:HG21	15:N:109:PHE:CZ	2.55	0.41
17:P:96:VAL:CG1	17:P:100:GLN:HB2	2.51	0.41
18:Q:114:LEU:HD22	18:Q:118:GLN:HB2	2.02	0.41
1:A:137:U:OP1	1:A:259:G:O2'	2.38	0.41
1:A:243:A:H61	1:A:269:G:H1'	1.86	0.41
1:A:506:G:N2	1:A:508:A:H3'	2.35	0.41
1:A:564:G:N2	38:A:3904:HOH:O	2.43	0.41
1:A:669:G:H2'	1:A:670:G:H8	1.86	0.41
1:A:837:U:H4'	38:A:9903:HOH:O	2.20	0.41
1:A:857:A:H4'	4:C:176:HIS:CD2	2.56	0.41
1:A:951:A:O2'	1:A:952:G:H5'	2.21	0.41
1:A:1707:G:N2	1:A:1709:G:H3'	2.36	0.41
1:A:2505:G:H8	38:A:5130:HOH:O	2.03	0.41
1:A:2546:U:H4'	38:D:8587:HOH:O	2.20	0.41
2:B:3104:A:O2'	2:B:3105:A:H5'	2.21	0.41
9:H:27:GLY:HA3	38:H:5413:HOH:O	2.19	0.41
9:H:49:PHE:HE1	9:H:98:VAL:CG2	2.33	0.41
11:J:148:ARG:NE	38:J:8345:HOH:O	2.45	0.41
12:K:39:VAL:CG1	12:K:107:ASN:HB2	2.51	0.41
14:M:97:VAL:HG12	14:M:98:GLU:O	2.21	0.41
22:U:44:ALA:HA	22:U:62:VAL:CG1	2.50	0.41
22:U:71:VAL:HG13	22:U:91:LEU:O	2.20	0.41
25:X:1:MET:N	25:X:37:GLU:HG3	2.35	0.41
27:Z:144:ARG:NE	38:Z:8608:HOH:O	2.53	0.41
27:Z:189:ASN:ND2	27:Z:192:ASP:N	2.65	0.41
30:3:25:VAL:O	30:3:29:THR:HG23	2.21	0.41
1:A:88:G:C8	30:3:28:LYS:HB2	2.55	0.41
1:A:424:C:H2'	1:A:425:U:H6	1.85	0.41
1:A:946:C:H2'	1:A:947:U:C6	2.55	0.41
1:A:1058:A:H2'	1:A:1060:C:C5'	2.49	0.41
1:A:1151:G:H2'	38:A:4506:HOH:O	2.21	0.41
1:A:1436:C:O2'	1:A:1437:A:H5'	2.21	0.41
1:A:1477:C:H5'	1:A:1868:G:H5"	2.03	0.41
1:A:1517:U:C2	1:A:1670:G:N2	2.89	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1675:C:H3'	38:A:7301:HOH:O	2.19	0.41
1:A:1743:G:O4'	13:L:78:LYS:HD3	2.20	0.41
1:A:1878:G:O2'	1:A:1879:U:C6	2.70	0.41
1:A:2001:G:O2'	1:A:2002:C:H5'	2.21	0.41
1:A:2289:G:H21	1:A:2291:A:H2	1.63	0.41
1:A:2296:C:H5	38:R:5998:HOH:O	2.03	0.41
1:A:2346:C:O3'	7:F:52:THR:HG23	2.20	0.41
1:A:2478:U:H2'	1:A:2479:A:C8	2.56	0.41
1:A:2869:G:H2'	1:A:2870:C:C6	2.55	0.41
5:D:109:LEU:HG	5:D:113:LEU:HD12	2.02	0.41
6:E:14:GLY:O	6:E:15:GLU:HB3	2.21	0.41
8:G:16:ASP:O	8:G:17:HIS:HB2	2.20	0.41
12:K:130:VAL:CG1	12:K:131:THR:N	2.84	0.41
16:O:154:LEU:HD11	16:O:157:PRO:HA	2.02	0.41
16:O:181:ASP:HA	38:O:8571:HOH:O	2.20	0.41
18:Q:16:VAL:CG1	18:Q:17:GLY:N	2.83	0.41
22:U:71:VAL:CG1	22:U:72:ILE:N	2.83	0.41
24:W:42:ASN:O	24:W:44:GLY:N	2.54	0.41
26:Y:9:VAL:HG13	26:Y:88:GLU:OE1	2.20	0.41
1:A:69:A:C2'	1:A:70:A:OP2	2.69	0.41
1:A:128:A:C8	1:A:128:A:C3'	3.02	0.41
1:A:426:G:H2'	1:A:427:C:O4'	2.21	0.41
1:A:685:C:O2	1:A:748:C:H4'	2.20	0.41
1:A:1200:A:H4'	38:A:6832:HOH:O	2.20	0.41
1:A:1262:C:O2'	25:X:120:PRO:HD3	2.21	0.41
1:A:1477:C:C5'	1:A:1868:G:H5"	2.50	0.41
1:A:1631:A:H2'	1:A:1632:A:C8	2.55	0.41
1:A:1815:A:H2'	1:A:1816:C:O4'	2.21	0.41
1:A:1845:A:O3'	4:C:187:PRO:HB2	2.21	0.41
1:A:1942:A:HO2'	1:A:1943:C:H5'	1.85	0.41
1:A:2069:U:H5'	38:A:4259:HOH:O	2.20	0.41
1:A:2072:G:H3'	1:A:2073:G:C5'	2.51	0.41
1:A:2133:U:H4'	1:A:2134:G:H5'	2.02	0.41
1:A:2809:G:H2'	1:A:2810:G:O4'	2.21	0.41
1:A:2837:U:H1'	5:D:307:ARG:HH12	1.85	0.41
5:D:313:PRO:O	5:D:314:ALA:C	2.59	0.41
6:E:223:LEU:HD12	6:E:223:LEU:HA	1.82	0.41
9:H:16:ALA:HA	9:H:111:ILE:HD13	2.03	0.41
11:J:47:GLU:OE2	11:J:162:SER:OG	2.38	0.41
11:J:49:VAL:C	11:J:157:ILE:HG23	2.39	0.41
12:K:51:GLU:O	12:K:55:GLU:HG3	2.21	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:L:98:VAL:CG1	13:L:102:GLU:HA	2.51	0.41
15:N:114:VAL:HG21	15:N:159:THR:CG2	2.50	0.41
16:O:175:LEU:HA	16:O:175:LEU:HD12	1.86	0.41
17:P:4:ASN:HA	17:P:5:PRO:HD3	1.90	0.41
20:S:114:VAL:HA	20:S:144:GLU:O	2.20	0.41
21:T:32:ALA:HA	21:T:36:GLU:OE1	2.21	0.41
22:U:41:ARG:NH1	22:U:42:VAL:O	2.54	0.41
23:V:14:GLU:HA	23:V:15:PRO:HD2	1.87	0.41
24:W:12:THR:CG2	24:W:15:GLU:HG3	2.28	0.41
25:X:142:ASP:HB2	38:X:2729:HOH:O	2.20	0.41
27:Z:189:ASN:HD22	27:Z:192:ASP:H	1.67	0.41
27:Z:203:VAL:HG12	27:Z:228:VAL:HG22	2.03	0.41
28:1:38:LYS:HG3	38:1:8428:HOH:O	2.21	0.41
1:A:105:G:O2'	1:A:106:A:H5'	2.21	0.41
1:A:154:C:P	15:N:188:ARG:HH12	2.44	0.41
1:A:245:C:C2'	1:A:246:G:H5'	2.51	0.41
1:A:250:C:H2'	1:A:251:C:C6	2.56	0.41
1:A:704:C:H2'	1:A:705:C:H6	1.86	0.41
1:A:1069:C:H4'	1:A:1081:A:O2'	2.20	0.41
1:A:1425:G:O2'	1:A:1426:C:H5'	2.21	0.41
1:A:1771:U:O2'	1:A:1773:G:N7	2.47	0.41
1:A:1783:A:C2'	1:A:1784:U:H5'	2.51	0.41
1:A:1829:A:C2'	1:A:1830:C:H5'	2.50	0.41
1:A:2443:C:O3'	14:M:56:LYS:HE3	2.20	0.41
1:A:2494:G:H4'	11:J:5:MET:SD	2.60	0.41
38:A:6000:HOH:O	30:3:1:GLY:HA3	2.20	0.41
2:B:3052:A:H2'	2:B:3053:G:O4'	2.21	0.41
4:C:36:ASP:CB	4:C:85:ASP:H	2.34	0.41
5:D:14:GLY:HA2	5:D:15:PRO:C	2.40	0.41
7:F:57:THR:HA	7:F:63:ILE:HA	2.02	0.41
7:F:173:GLU:HG3	7:F:174:VAL:N	2.36	0.41
16:O:38:LYS:HD2	16:O:114:LYS:HE3	2.03	0.41
20:S:82:GLU:HG3	20:S:83:LYS:N	2.35	0.41
23:V:6:CYS:C	23:V:8:TYR:N	2.74	0.41
25:X:72:PRO:HB2	25:X:74:GLU:O	2.21	0.41
28:1:30:GLU:HB3	28:1:34:LYS:HE3	2.03	0.41
29:2:15:THR:O	29:2:29:THR:HG22	2.20	0.41
1:A:204:A:C2'	1:A:205:U:H5'	2.51	0.40
1:A:696:C:H4'	38:A:6771:HOH:O	2.20	0.40
1:A:963:C:O5'	1:A:963:C:H6	2.04	0.40
1:A:1114:A:H2'	1:A:1115:U:C6	2.56	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1450:C:O2'	1:A:1493:A:H2'	2.20	0.40
1:A:1675:C:H5"	30:3:5:LYS:HD2	2.03	0.40
1:A:1735:C:H2'	1:A:1736:A:C8	2.55	0.40
1:A:1873:G:H3'	38:A:4700:HOH:O	2.21	0.40
1:A:2134:G:C6	1:A:2258:A:C8	3.10	0.40
1:A:2912:C:H2'	1:A:2913:A:O4'	2.21	0.40
5:D:235:ARG:HA	38:D:8604:HOH:O	2.20	0.40
7:F:140:ARG:HG3	7:F:140:ARG:HH11	1.85	0.40
8:G:3:VAL:HG22	8:G:49:ILE:HB	2.03	0.40
12:K:19:MET:HE1	12:K:132:LEU:HD11	2.02	0.40
16:O:50:LEU:HD12	16:O:50:LEU:HA	1.94	0.40
16:O:73:ALA:HB2	16:O:163:PHE:CZ	2.56	0.40
17:P:47:ARG:HA	17:P:50:ARG:HH12	1.85	0.40
23:V:14:GLU:OE1	23:V:15:PRO:CD	2.65	0.40
28:1:11:THR:HG23	28:1:11:THR:O	2.21	0.40
28:1:46:LYS:NZ	38:1:8440:HOH:O	2.53	0.40
1:A:10:U:O4	1:A:532:A:OP2	2.38	0.40
1:A:291:C:H2'	1:A:292:G:O4'	2.21	0.40
1:A:445:U:H2'	1:A:446:G:H8	1.85	0.40
1:A:466:A:H2'	1:A:467:G:O4'	2.21	0.40
1:A:470:U:H2'	1:A:471:G:O4'	2.21	0.40
1:A:1127:C:C5	1:A:1128:U:C4	3.09	0.40
1:A:1942:A:O3'	4:C:213:LYS:HE2	2.21	0.40
1:A:2004:U:H2'	1:A:2005:G:OP1	2.21	0.40
1:A:2764:C:H2'	1:A:2765:C:H6	1.85	0.40
4:C:66:ARG:HH11	4:C:66:ARG:CB	2.34	0.40
4:C:186:TRP:CD1	4:C:187:PRO:HA	2.56	0.40
5:D:7:ARG:HG2	5:D:7:ARG:NH1	2.35	0.40
5:D:7:ARG:NH2	5:D:250:THR:O	2.54	0.40
5:D:52:VAL:N	5:D:329:TYR:O	2.46	0.40
6:E:118:THR:CG2	6:E:137:PRO:HB3	2.51	0.40
6:E:141:SER:HA	38:E:8383:HOH:O	2.21	0.40
7:F:64:ARG:NE	7:F:67:ASP:HB3	2.36	0.40
12:K:15:ARG:NH1	12:K:43:ARG:NH1	2.69	0.40
13:L:74:VAL:HG13	13:L:113:ILE:HG12	2.01	0.40
15:N:183:VAL:HG12	15:N:184:ARG:N	2.36	0.40
16:O:43:VAL:O	16:O:84:THR:HG21	2.20	0.40
17:P:105:ASN:CG	17:P:105:ASN:O	2.59	0.40
20:S:17:MET:CE	20:S:19:ARG:CZ	3.00	0.40
21:T:69:SER:C	21:T:71:ASP:N	2.75	0.40
1:A:226:A:H1'	1:A:393:G:C5	2.56	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:332:G:O2'	1:A:333:G:H5'	2.22	0.40
1:A:363:A:O5'	1:A:363:A:H8	2.04	0.40
1:A:401:C:O2'	15:N:92:THR:HB	2.21	0.40
1:A:559:U:H5'	1:A:559:U:C6	2.50	0.40
1:A:644:G:N3	1:A:644:G:H5'	2.36	0.40
1:A:697:G:H4'	1:A:730:G:O3'	2.21	0.40
1:A:1741:U:H3'	38:A:9274:HOH:O	2.20	0.40
1:A:2526:C:C2'	1:A:2527:U:H5'	2.50	0.40
1:A:2712:G:O2'	1:A:2713:G:H5'	2.22	0.40
1:A:2784:A:H1'	8:G:60:SER:OG	2.22	0.40
38:A:4899:HOH:O	4:C:164:ARG:NE	2.53	0.40
4:C:70:ALA:HA	4:C:71:PRO:HD3	1.78	0.40
5:D:266:ASN:OD1	5:D:317:PRO:HA	2.20	0.40
5:D:280:VAL:HG13	5:D:333:GLU:O	2.20	0.40
7:F:128:LEU:HD23	7:F:128:LEU:C	2.42	0.40
8:G:132:THR:O	8:G:132:THR:HG23	2.20	0.40
12:K:24:SER:HA	12:K:86:MET:SD	2.61	0.40
14:M:20:ASN:O	14:M:22:ARG:N	2.52	0.40
14:M:62:ALA:HB2	14:M:103:ALA:CB	2.51	0.40
15:N:152:ARG:HB3	38:N:8649:HOH:O	2.21	0.40
20:S:72:VAL:CG1	20:S:75:TRP:HB3	2.51	0.40
26:Y:71:ARG:CD	38:Y:2171:HOH:O	2.66	0.40
31:4:43:ASN:ND2	38:4:8506:HOH:O	2.50	0.40
1:A:204:A:H2'	1:A:205:U:H5'	2.02	0.40
1:A:316:A:N3	1:A:336:G:O2'	2.48	0.40
1:A:1298:U:H2'	1:A:1299:G:C8	2.56	0.40
1:A:1498:G:O2'	1:A:1499:U:H5'	2.21	0.40
1:A:1886:A:H4'	38:1:8405:HOH:O	2.20	0.40
1:A:2241:C:H2'	1:A:2242:U:H6	1.85	0.40
1:A:2361:A:H2'	1:A:2362:A:C8	2.56	0.40
1:A:2443:C:H3'	38:A:9982:HOH:O	2.21	0.40
1:A:2649:A:H5'	1:A:2649:A:H8	1.86	0.40
38:A:9052:HOH:O	18:Q:81:LYS:HG2	2.21	0.40
2:B:3023:U:H3'	38:B:8479:HOH:O	2.21	0.40
6:E:156:LEU:O	6:E:156:LEU:HD12	2.21	0.40
6:E:236:THR:C	38:E:8451:HOH:O	2.59	0.40
9:H:33:THR:HG21	9:H:59:ILE:O	2.22	0.40
12:K:39:VAL:HG11	12:K:107:ASN:HB2	2.02	0.40
13:L:30:LYS:C	13:L:55:VAL:HG13	2.42	0.40
14:M:148:GLU:HG3	38:M:8553:HOH:O	2.22	0.40
15:N:137:ASP:O	15:N:142:LYS:HE3	2.20	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:P:88:LYS:HB3	38:P:7061:HOH:O	2.20	0.40
18:Q:59:ARG:O	18:Q:62:ALA:HB3	2.21	0.40
25:X:121:PRO:CA	25:X:153:MET:HG2	2.51	0.40
27:Z:216:ARG:O	27:Z:219:GLU:HG2	2.21	0.40
1:A:473:A:O2'	1:A:474:C:H5'	2.22	0.40
1:A:656:G:H3'	17:P:37:ARG:HH12	1.86	0.40
1:A:940:G:O2'	1:A:1032:A:N1	2.51	0.40
1:A:1114:A:H2'	1:A:1115:U:H6	1.85	0.40
1:A:1216:G:O2'	1:A:1217:G:H5'	2.22	0.40
1:A:1501:A:H4'	38:A:5090:HOH:O	2.21	0.40
1:A:1656:A:H5'	38:A:3906:HOH:O	2.22	0.40
1:A:2356:A:H2'	1:A:2357:G:O4'	2.21	0.40
1:A:2382:A:H5'	38:4:8533:HOH:O	2.22	0.40
38:A:6557:HOH:O	20:S:33:ARG:HD3	2.20	0.40
38:A:8843:HOH:O	25:X:9:GLY:HA3	2.20	0.40
5:D:5:ARG:HD2	5:D:8:LYS:NZ	2.36	0.40
5:D:11:LEU:HA	38:D:8618:HOH:O	2.22	0.40
5:D:30:PRO:HB2	5:D:39:GLN:HE21	1.83	0.40
5:D:115:VAL:HA	5:D:116:PRO:HD3	1.88	0.40
5:D:183:GLU:HA	5:D:183:GLU:OE1	2.21	0.40
11:J:158:ASN:ND2	38:J:8388:HOH:O	2.54	0.40
16:O:128:ASP:HA	38:O:8562:HOH:O	2.21	0.40
28:1:31:ILE:CG2	28:1:32:LYS:N	2.84	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
4	C	235/239 (98%)	202 (86%)	27 (12%)	6 (3%)	5 27
5	D	335/337 (99%)	291 (87%)	36 (11%)	8 (2%)	6 29

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
6	E	244/246 (99%)	210 (86%)	31 (13%)	3 (1%)	13 48
7	F	134/176 (76%)	95 (71%)	28 (21%)	11 (8%)	1 4
8	G	170/177 (96%)	159 (94%)	10 (6%)	1 (1%)	25 64
9	H	117/119 (98%)	100 (86%)	13 (11%)	4 (3%)	3 20
10	I	25/348 (7%)	23 (92%)	1 (4%)	1 (4%)	3 17
11	J	152/167 (91%)	129 (85%)	18 (12%)	5 (3%)	4 21
12	K	140/145 (97%)	126 (90%)	8 (6%)	6 (4%)	2 15
13	L	130/132 (98%)	115 (88%)	13 (10%)	2 (2%)	10 42
14	M	141/164 (86%)	117 (83%)	22 (16%)	2 (1%)	11 43
15	N	192/194 (99%)	164 (85%)	25 (13%)	3 (2%)	9 40
16	O	184/186 (99%)	160 (87%)	17 (9%)	7 (4%)	3 18
17	P	113/115 (98%)	105 (93%)	8 (7%)	0	100 100
18	Q	141/148 (95%)	132 (94%)	8 (6%)	1 (1%)	22 60
19	R	93/95 (98%)	88 (95%)	4 (4%)	1 (1%)	14 50
20	S	148/154 (96%)	134 (90%)	14 (10%)	0	100 100
21	T	79/84 (94%)	71 (90%)	8 (10%)	0	100 100
22	U	117/119 (98%)	103 (88%)	12 (10%)	2 (2%)	9 39
23	V	51/66 (77%)	44 (86%)	6 (12%)	1 (2%)	7 34
24	W	63/70 (90%)	55 (87%)	5 (8%)	3 (5%)	2 13
25	X	152/154 (99%)	142 (93%)	8 (5%)	2 (1%)	12 45
26	Y	80/91 (88%)	70 (88%)	8 (10%)	2 (2%)	5 28
27	Z	140/240 (58%)	135 (96%)	5 (4%)	0	100 100
28	1	71/73 (97%)	59 (83%)	10 (14%)	2 (3%)	5 25
29	2	54/56 (96%)	51 (94%)	3 (6%)	0	100 100
30	3	42/48 (88%)	42 (100%)	0	0	100 100
31	4	90/92 (98%)	84 (93%)	4 (4%)	2 (2%)	6 31
All	All	3633/4235 (86%)	3206 (88%)	352 (10%)	75 (2%)	7 33

All (75) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	D	139	ASP
5	D	184	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
6	E	8	LEU
7	F	93	LEU
7	F	95	THR
7	F	173	GLU
9	H	101	ALA
11	J	138	PRO
11	J	162	SER
16	O	154	LEU
16	O	162	ASP
16	O	183	ASP
18	Q	116	SER
31	4	56	PRO
4	C	34	ASP
4	C	37	VAL
4	C	132	ASP
5	D	34	GLY
5	D	107	SER
5	D	169	GLY
7	F	11	HIS
7	F	20	LYS
7	F	137	PRO
7	F	171	ASP
11	J	164	ALA
12	K	5	GLU
14	M	80	ASP
15	N	18	GLY
16	O	164	ASP
24	W	43	PRO
25	X	77	ALA
28	1	20	LEU
31	4	57	GLY
6	E	58	ALA
7	F	16	PRO
7	F	36	ASN
7	F	147	ALA
10	I	72	ASP
12	K	7	ASP
12	K	143	LYS
13	L	119	GLN
13	L	126	SER
14	M	21	ARG
16	O	181	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
19	R	23	THR
6	E	232	LEU
7	F	82	GLU
8	G	44	GLY
9	H	64	PRO
12	K	65	ASN
15	N	6	SER
15	N	71	SER
22	U	53	GLY
23	V	7	ASP
25	X	49	ASN
26	Y	70	ILE
28	1	81	LYS
4	C	10	GLY
4	C	119	ALA
5	D	291	ASP
9	H	61	MET
11	J	40	PRO
12	K	89	HIS
12	K	141	ALA
16	O	139	TRP
22	U	44	ALA
24	W	40	PRO
9	H	71	GLY
16	O	167	ASP
26	Y	77	PHE
11	J	110	GLY
4	C	211	LYS
5	D	2	GLN
5	D	185	GLY
24	W	2	VAL

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all 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.

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	C	179/181 (99%)	166 (93%)	13 (7%)	14	44
5	D	282/282 (100%)	267 (95%)	15 (5%)	22	58
6	E	193/193 (100%)	177 (92%)	16 (8%)	11	39
7	F	117/147 (80%)	108 (92%)	9 (8%)	13	42
8	G	152/155 (98%)	147 (97%)	5 (3%)	38	73
9	H	92/92 (100%)	91 (99%)	1 (1%)	73	90
10	I	27/283 (10%)	27 (100%)	0	100	100
11	J	122/122 (100%)	111 (91%)	11 (9%)	9	35
12	K	118/121 (98%)	107 (91%)	11 (9%)	9	33
13	L	106/106 (100%)	104 (98%)	2 (2%)	57	84
14	M	112/126 (89%)	107 (96%)	5 (4%)	27	64
15	N	166/166 (100%)	157 (95%)	9 (5%)	22	57
16	O	149/149 (100%)	144 (97%)	5 (3%)	37	72
17	P	93/93 (100%)	92 (99%)	1 (1%)	73	90
18	Q	113/116 (97%)	109 (96%)	4 (4%)	36	71
19	R	79/79 (100%)	75 (95%)	4 (5%)	24	60
20	S	117/121 (97%)	113 (97%)	4 (3%)	37	72
21	T	71/73 (97%)	70 (99%)	1 (1%)	67	88
22	U	105/105 (100%)	99 (94%)	6 (6%)	20	56
23	V	44/52 (85%)	44 (100%)	0	100	100
24	W	51/56 (91%)	50 (98%)	1 (2%)	55	83
25	X	130/130 (100%)	124 (95%)	6 (5%)	27	64
26	Y	66/73 (90%)	61 (92%)	5 (8%)	13	43
27	Z	120/195 (62%)	115 (96%)	5 (4%)	30	66
28	1	56/56 (100%)	54 (96%)	2 (4%)	35	70
29	2	46/46 (100%)	46 (100%)	0	100	100
30	3	42/44 (96%)	41 (98%)	1 (2%)	49	79
31	4	79/79 (100%)	75 (95%)	4 (5%)	24	60
All	All	3027/3441 (88%)	2881 (95%)	146 (5%)	25	62

All (146) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	C	3	ARG
4	C	33	GLU
4	C	36	ASP
4	C	55	VAL
4	C	68	ILE
4	C	69	LEU
4	C	78	ASP
4	C	94	LEU
4	C	120	ARG
4	C	131	HIS
4	C	153	ARG
4	C	179	MET
4	C	217	ARG
5	D	7	ARG
5	D	11	LEU
5	D	27	ASN
5	D	33	ASP
5	D	63	GLU
5	D	97	LEU
5	D	98	THR
5	D	103	ASP
5	D	162	MET
5	D	234	ARG
5	D	251	VAL
5	D	254	GLN
5	D	256	GLN
5	D	307	ARG
5	D	312	ARG
6	E	2	GLN
6	E	27	ARG
6	E	67	GLN
6	E	76	ARG
6	E	91	PRO
6	E	94	THR
6	E	115	LEU
6	E	136	VAL
6	E	180	SER
6	E	187	ARG
6	E	214	THR
6	E	222	ASP
6	E	223	LEU
6	E	234	VAL
6	E	236	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
6	E	240	LEU
7	F	24	HIS
7	F	61	PHE
7	F	99	ASP
7	F	100	ASP
7	F	131	THR
7	F	136	ARG
7	F	137	PRO
7	F	149	ARG
7	F	170	TYR
8	G	7	ILE
8	G	12	ASP
8	G	15	GLN
8	G	102	VAL
8	G	164	ASP
9	H	78	GLU
11	J	30	GLN
11	J	59	ASN
11	J	61	LEU
11	J	72	VAL
11	J	73	GLN
11	J	82	LYS
11	J	86	ARG
11	J	94	ARG
11	J	142	VAL
11	J	150	LYS
11	J	166	ASN
12	K	46	ILE
12	K	47	THR
12	K	52	GLN
12	K	74	ARG
12	K	76	ASP
12	K	79	PHE
12	K	107	ASN
12	K	112	ASP
12	K	120	SER
12	K	127	ILE
12	K	131	THR
13	L	10	GLN
13	L	98	VAL
14	M	30	ARG
14	M	35	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
14	M	80	ASP
14	M	99	GLU
14	M	117	GLU
15	N	46	LEU
15	N	68	ARG
15	N	81	ARG
15	N	87	MET
15	N	93	ARG
15	N	99	ARG
15	N	116	ASN
15	N	159	THR
15	N	164	THR
16	O	26	LEU
16	O	49	THR
16	O	128	ASP
16	O	152	GLU
16	O	163	PHE
17	P	98	LEU
18	Q	52	LYS
18	Q	91	LYS
18	Q	94	TRP
18	Q	98	ILE
19	R	11	ARG
19	R	16	ASN
19	R	57	ASP
19	R	95	GLU
20	S	13	THR
20	S	39	THR
20	S	82	GLU
20	S	132	ARG
21	T	10	VAL
22	U	19	ARG
22	U	23	VAL
22	U	26	THR
22	U	39	ASN
22	U	48	VAL
22	U	73	HIS
24	W	65	ASP
25	X	35	VAL
25	X	88	THR
25	X	122	ARG
25	X	142	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
25	X	146	ILE
25	X	154	ARG
26	Y	15	ARG
26	Y	27	ASP
26	Y	44	ASP
26	Y	49	ARG
26	Y	72	VAL
27	Z	163	THR
27	Z	189	ASN
27	Z	200	THR
27	Z	203	VAL
27	Z	235	GLU
28	1	11	THR
28	1	64	ILE
30	3	18	ASN
31	4	11	CYS
31	4	42	ARG
31	4	56	PRO
31	4	65	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (97) such sidechains are listed below:

Mol	Chain	Res	Type
4	C	29	HIS
4	C	47	HIS
4	C	92	ASN
4	C	125	ASN
4	C	127	GLN
4	C	176	HIS
4	C	199	HIS
5	D	27	ASN
5	D	145	HIS
5	D	221	GLN
5	D	238	ASN
5	D	260	HIS
5	D	320	GLN
5	D	332	ASN
6	E	2	GLN
6	E	39	GLN
6	E	129	HIS
6	E	163	HIS
7	F	47	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
7	F	85	GLN
7	F	103	ASN
7	F	133	ASN
8	G	106	ASN
8	G	119	HIS
8	G	143	GLN
9	H	80	GLN
10	I	17	GLN
10	I	64	ASN
11	J	35	ASN
11	J	36	ASN
11	J	45	GLN
11	J	55	GLN
11	J	58	HIS
11	J	59	ASN
11	J	69	ASN
11	J	74	ASN
11	J	91	HIS
11	J	129	ASN
11	J	130	HIS
11	J	166	ASN
12	K	52	GLN
12	K	107	ASN
12	K	126	ASN
13	L	10	GLN
14	M	18	HIS
14	M	41	HIS
14	M	42	ASN
15	N	26	HIS
15	N	58	GLN
15	N	176	GLN
16	O	40	ASN
16	O	107	ASN
17	P	53	GLN
18	Q	50	GLN
18	Q	66	GLN
18	Q	73	HIS
18	Q	118	GLN
19	R	16	ASN
19	R	40	HIS
20	S	61	GLN
20	S	94	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
20	S	98	ASN
20	S	113	HIS
20	S	117	HIS
20	S	122	GLN
21	T	53	ASN
22	U	39	ASN
22	U	73	HIS
23	V	39	ASN
24	W	60	GLN
25	X	2	HIS
25	X	12	ASN
25	X	27	HIS
25	X	28	HIS
25	X	59	GLN
25	X	87	HIS
25	X	110	GLN
25	X	119	HIS
25	X	125	HIS
25	X	141	HIS
26	Y	23	HIS
27	Z	133	HIS
27	Z	134	HIS
27	Z	149	GLN
27	Z	189	ASN
28	1	33	HIS
28	1	70	GLN
29	2	8	GLN
29	2	16	HIS
29	2	28	HIS
30	3	16	ASN
30	3	18	ASN
30	3	41	HIS
30	3	45	ASN
31	4	15	ASN
31	4	30	GLN
31	4	48	ASN

5.3.3 RNA

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	2747/2922 (94%)	244 (8%)	32 (1%)

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	B	121/122 (99%)	16 (13%)	3 (2%)
3	5	2/3 (66%)	1 (50%)	0
3	6	2/3 (66%)	0	0
All	All	2872/3050 (94%)	261 (9%)	35 (1%)

All (261) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	11	A
1	A	31	C
1	A	60	A
1	A	67	A
1	A	69	A
1	A	70	A
1	A	71	G
1	A	87	C
1	A	88	G
1	A	114	A
1	A	115	U
1	A	120	A
1	A	130	C
1	A	139	C
1	A	141	C
1	A	151	A
1	A	166	A
1	A	169	A
1	A	186	A
1	A	191	A
1	A	192	A
1	A	200	U
1	A	219	G
1	A	237	G
1	A	271	C
1	A	272	A
1	A	273	G
1	A	283	U
1	A	284	C
1	A	285	A
1	A	308	U
1	A	309	C
1	A	317	A
1	A	318	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	336	G
1	A	337	A
1	A	345	G
1	A	358	G
1	A	381	G
1	A	397	A
1	A	417	G
1	A	461	C
1	A	487	G
1	A	498	A
1	A	510	U
1	A	511	A
1	A	514	G
1	A	537	G
1	A	538	C
1	A	539	G
1	A	542	A
1	A	545	G
1	A	553	G
1	A	559	U
1	A	588	G
1	A	604	G
1	A	605	C
1	A	620	A
1	A	632	A
1	A	644	G
1	A	660	A
1	A	688	A
1	A	701	U
1	A	717	C
1	A	777	U
1	A	809	G
1	A	821	U
1	A	835	U
1	A	840	U
1	A	857	A
1	A	858	U
1	A	868	G
1	A	869	G
1	A	871	G
1	A	872	U
1	A	875	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	877	G
1	A	878	G
1	A	884	C
1	A	885	G
1	A	898	G
1	A	905	C
1	A	920	C
1	A	921	G
1	A	923	A
1	A	953	G
1	A	960	G
1	A	961	A
1	A	1006	A
1	A	1008	C
1	A	1029	U
1	A	1045	G
1	A	1059	G
1	A	1060	C
1	A	1072	G
1	A	1081	A
1	A	1087	G
1	A	1088	A
1	A	1109	U
1	A	1110	G
1	A	1119	G
1	A	1130	U
1	A	1137	G
1	A	1151	G
1	A	1161	A
1	A	1162	G
1	A	1164	U
1	A	1165	G
1	A	1166	A
1	A	1171	A
1	A	1174	A
1	A	1175	G
1	A	1177	A
1	A	1185	U
1	A	1192	A
1	A	1193	A
1	A	1206	U
1	A	1216	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	1237	U
1	A	1238	C
1	A	1239	G
1	A	1279	U
1	A	1289	C
1	A	1342	C
1	A	1353	C
1	A	1360	C
1	A	1377	C
1	A	1407	A
1	A	1451	C
1	A	1474	C
1	A	1488	U
1	A	1505	U
1	A	1506	U
1	A	1524	U
1	A	1525	G
1	A	1526	A
1	A	1528	A
1	A	1564	C
1	A	1580	A
1	A	1592	G
1	A	1625	U
1	A	1626	A
1	A	1633	C
1	A	1634	G
1	A	1656	A
1	A	1667	A
1	A	1682	A
1	A	1684	A
1	A	1685	A
1	A	1692	C
1	A	1701	A
1	A	1722	U
1	A	1723	G
1	A	1725	C
1	A	1730	G
1	A	1731	C
1	A	1752	G
1	A	1778	A
1	A	1798	C
1	A	1819	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	1820	G
1	A	1829	A
1	A	1856	C
1	A	1879	U
1	A	1904	A
1	A	1919	A
1	A	1942	A
1	A	1971	G
1	A	1973	A
1	A	1974	G
1	A	1978	A
1	A	1980	U
1	A	1996	U
1	A	2008	U
1	A	2011	A
1	A	2012	U
1	A	2013	G
1	A	2033	G
1	A	2034	U
1	A	2064	U
1	A	2072	G
1	A	2073	G
1	A	2074	A
1	A	2096	A
1	A	2101	A
1	A	2102	G
1	A	2103	A
1	A	2110	G
1	A	2238	A
1	A	2258	A
1	A	2271	G
1	A	2272	G
1	A	2317	C
1	A	2321	A
1	A	2346	C
1	A	2354	A
1	A	2361	A
1	A	2369	A
1	A	2379	G
1	A	2422	U
1	A	2462	G
1	A	2467	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	2476	C
1	A	2480	G
1	A	2483	A
1	A	2507	G
1	A	2509	A
1	A	2511	A
1	A	2533	C
1	A	2537	G
1	A	2541	U
1	A	2553	A
1	A	2564	G
1	A	2589	U
1	A	2601	A
1	A	2602	G
1	A	2608	C
1	A	2613	G
1	A	2616	G
1	A	2617	G
1	A	2637	A
1	A	2649	A
1	A	2664	A
1	A	2681	A
1	A	2682	C
1	A	2719	A
1	A	2726	U
1	A	2747	C
1	A	2748	G
1	A	2749	U
1	A	2750	G
1	A	2762	C
1	A	2768	A
1	A	2786	G
1	A	2792	A
1	A	2800	A
1	A	2811	A
1	A	2825	C
1	A	2850	C
1	A	2876	G
1	A	2890	A
1	A	2896	A
1	A	2903	C
1	A	2914	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	3002	U
2	B	3014	G
2	B	3022	G
2	B	3023	U
2	B	3024	U
2	B	3025	G
2	B	3026	C
2	B	3041	C
2	B	3043	G
2	B	3044	A
2	B	3052	A
2	B	3057	A
2	B	3066	G
2	B	3077	A
2	B	3114	G
2	B	3122	C
3	5	75	C

All (35) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	10	U
1	A	129	A
1	A	284	C
1	A	338	C
1	A	603	A
1	A	604	G
1	A	716	G
1	A	834	G
1	A	857	A
1	A	871	G
1	A	877	G
1	A	898	G
1	A	1080	C
1	A	1232	A
1	A	1237	U
1	A	1352	A
1	A	1377	C
1	A	1450	C
1	A	1563	G
1	A	1667	A
1	A	1730	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	1856	C
1	A	1979	G
1	A	2011	A
1	A	2313	C
1	A	2467	A
1	A	2526	C
1	A	2536	C
1	A	2616	G
1	A	2649	A
1	A	2718	C
1	A	2791	U
2	B	3024	U
2	B	3065	A
2	B	3103	A

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 monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 235 ligands modelled in this entry, 233 are monoatomic - leaving 2 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	$\#\|Z\| > 2$
36	PHA	5	77	3	10,11,11	0.86	0	10,13,13	0.79	0
36	PHA	6	77	3	10,10,11	0.63	0	11,11,13	0.48	0

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
36	PHA	5	77	3	-	3/5/6/6	0/1/1/1
36	PHA	6	77	3	-	1/3/4/6	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
36	5	77	PHA	CA-CB-CG-CD1
36	5	77	PHA	CA-CB-CG-CD2
36	5	77	PHA	C-CA-CB-CG
36	6	77	PHA	C-CA-CB-CG

There are no ring outliers.

2 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
36	5	77	PHA	5	0
36	6	77	PHA	4	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

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, 95^{th} 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	2754/2922 (94%)	0.14	41 (1%) 73 46	19, 47, 95, 154	0
2	B	122/122 (100%)	0.11	6 (4%) 29 11	30, 62, 92, 154	0
3	5	3/3 (100%)	1.61	1 (33%) 0 0	29, 29, 31, 35	3 (100%)
3	6	3/3 (100%)	2.43	3 (100%) 0 0	15, 15, 17, 31	3 (100%)
4	C	237/239 (99%)	0.19	8 (3%) 45 19	27, 52, 91, 115	0
5	D	337/337 (100%)	0.02	2 (0%) 89 72	26, 55, 84, 96	0
6	E	246/246 (100%)	-0.25	0 100 100	19, 47, 71, 80	0
7	F	140/176 (79%)	0.87	20 (14%) 2 1	53, 101, 124, 131	0
8	G	172/177 (97%)	0.24	4 (2%) 60 31	41, 68, 91, 99	0
9	H	119/119 (100%)	0.44	4 (3%) 45 19	53, 77, 104, 111	0
10	I	29/348 (8%)	1.19	5 (17%) 1 0	66, 86, 97, 103	0
11	J	156/167 (93%)	-0.12	0 100 100	30, 52, 77, 81	0
12	K	142/145 (97%)	-0.21	0 100 100	34, 47, 71, 90	0
13	L	132/132 (100%)	-0.04	0 100 100	31, 53, 78, 86	0
14	M	145/164 (88%)	0.04	2 (1%) 75 49	21, 67, 108, 116	0
15	N	194/194 (100%)	-0.05	0 100 100	30, 47, 68, 80	0
16	O	186/186 (100%)	0.13	6 (3%) 47 20	35, 65, 112, 125	0
17	P	115/115 (100%)	-0.15	0 100 100	36, 54, 74, 83	0
18	Q	143/148 (96%)	0.33	1 (0%) 87 69	36, 57, 71, 80	0
19	R	95/95 (100%)	-0.28	0 100 100	32, 42, 57, 73	0
20	S	150/154 (97%)	-0.05	0 100 100	29, 43, 64, 75	0
21	T	81/84 (96%)	0.21	1 (1%) 79 54	41, 62, 81, 85	0
22	U	119/119 (100%)	0.28	4 (3%) 45 19	38, 60, 86, 105	0
23	V	53/66 (80%)	0.35	2 (3%) 40 16	42, 53, 71, 80	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
24	W	65/70 (92%)	0.72	5 (7%) 13 4	56, 79, 120, 125	0
25	X	154/154 (100%)	-0.42	0 100 100	29, 45, 62, 74	0
26	Y	82/91 (90%)	0.46	6 (7%) 15 4	42, 56, 79, 100	0
27	Z	142/240 (59%)	-0.17	1 (0%) 87 69	25, 45, 67, 86	0
28	1	73/73 (100%)	0.26	3 (4%) 37 14	43, 61, 76, 81	0
29	2	56/56 (100%)	-0.29	0 100 100	24, 33, 39, 41	0
30	3	46/48 (95%)	0.84	6 (13%) 3 1	34, 65, 118, 126	0
31	4	92/92 (100%)	0.00	0 100 100	39, 55, 69, 78	0
All	All	6583/7285 (90%)	0.11	131 (1%) 65 36	15, 52, 97, 154	6 (0%)

All (131) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
24	W	1	THR	11.8
2	B	3001	U	7.4
1	A	1172	G	5.1
1	A	2237	G	5.1
7	F	66	GLY	4.9
2	B	3025	G	4.3
24	W	43	PRO	4.2
1	A	1173	A	4.1
7	F	62	ASP	3.8
7	F	57	THR	3.8
7	F	63	ILE	3.8
26	Y	88	GLU	3.8
1	A	1177	A	3.8
9	H	106	THR	3.5
7	F	10	PHE	3.4
10	I	21	ASP	3.4
21	T	81	ILE	3.4
5	D	1	PRO	3.4
7	F	89	PRO	3.3
4	C	236	GLY	3.3
2	B	3023	U	3.3
16	O	162	ASP	3.3
30	3	41	HIS	3.3
7	F	90	LEU	3.3
1	A	1169	U	3.2
28	1	11	THR	3.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
4	C	36	ASP	3.2
16	O	186	LEU	3.1
1	A	735	C	3.1
1	A	1525	G	3.1
9	H	19	ALA	3.0
1	A	1171	A	3.0
30	3	36	ASN	2.9
1	A	1951	G	2.9
7	F	171	ASP	2.9
22	U	119	ALA	2.9
7	F	85	GLN	2.9
3	6	76	A	2.8
30	3	35	ARG	2.8
4	C	85	ASP	2.8
10	I	23	ILE	2.8
8	G	100	ASP	2.8
7	F	170	TYR	2.8
1	A	285	A	2.7
1	A	2238	A	2.7
4	C	37	VAL	2.7
1	A	1174	A	2.7
4	C	35	GLY	2.7
1	A	2637	A	2.7
5	D	118	ASP	2.7
7	F	92	GLU	2.7
1	A	970	U	2.7
27	Z	235	GLU	2.6
7	F	55	LYS	2.6
1	A	1950	G	2.6
7	F	69	ILE	2.6
1	A	1170	U	2.6
1	A	960	G	2.6
1	A	1181	A	2.6
22	U	82	THR	2.6
1	A	2254	G	2.6
7	F	102	GLY	2.5
7	F	154	LYS	2.5
16	O	159	TYR	2.5
30	3	38	LYS	2.5
9	H	20	LEU	2.5
1	A	1198	U	2.5
24	W	38	GLY	2.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	1190	G	2.5
1	A	1948	G	2.5
26	Y	80	GLU	2.5
1	A	138	U	2.5
16	O	166	ALA	2.5
1	A	2250	G	2.4
1	A	130	C	2.4
8	G	129	GLU	2.4
14	M	60	GLU	2.4
1	A	1204	C	2.4
2	B	3024	U	2.4
2	B	3122	C	2.4
1	A	1175	G	2.4
1	A	1167	G	2.4
4	C	237	GLY	2.3
10	I	24	VAL	2.3
1	A	2664	A	2.3
3	5	74	C	2.3
22	U	115	GLU	2.3
1	A	2825	C	2.3
9	H	99	THR	2.3
8	G	10	ASP	2.3
23	V	52	THR	2.3
1	A	1182	C	2.3
3	6	75	C	2.3
1	A	282	C	2.3
1	A	2884	G	2.2
26	Y	74	ALA	2.2
1	A	1205	U	2.2
8	G	45	ASP	2.2
24	W	41	GLU	2.2
10	I	27	ILE	2.2
3	6	74	C	2.2
4	C	99	ILE	2.2
2	B	3002	U	2.2
1	A	2004	U	2.2
7	F	165	PHE	2.2
16	O	139	TRP	2.2
30	3	49	GLU	2.2
1	A	1947	G	2.1
28	1	47	LEU	2.1
26	Y	7	GLU	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
16	O	160	SER	2.1
1	A	1561	U	2.1
4	C	64	ASP	2.1
1	A	258	G	2.1
7	F	64	ARG	2.1
7	F	56	ARG	2.1
7	F	166	ILE	2.1
18	Q	141	ILE	2.1
1	A	1279	U	2.1
1	A	1527	A	2.1
14	M	104	ASP	2.1
30	3	37	HIS	2.1
23	V	54	THR	2.0
28	1	38	LYS	2.0
1	A	280	C	2.0
22	U	116	ASP	2.0
26	Y	77	PHE	2.0
7	F	65	GLU	2.0
10	I	17	GLN	2.0
24	W	62	GLU	2.0
26	Y	85	VAL	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 monosaccharides 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, 95^{th} 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
34	NA	A	8384	1/1	0.23	0.68	101,101,101,101	0
34	NA	S	8386	1/1	0.37	0.78	63,63,63,63	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
32	MG	A	8046	1/1	0.40	0.19	45,45,45,45	0
32	MG	A	8114	1/1	0.44	0.28	51,51,51,51	0
34	NA	A	8366	1/1	0.46	0.26	51,51,51,51	0
32	MG	A	8076	1/1	0.54	0.16	37,37,37,37	0
32	MG	A	8041	1/1	0.56	0.20	79,79,79,79	0
32	MG	C	8065	1/1	0.58	0.16	40,40,40,40	0
34	NA	A	8369	1/1	0.60	0.39	59,59,59,59	0
34	NA	A	8324	1/1	0.60	0.31	58,58,58,58	0
32	MG	A	8106	1/1	0.60	0.17	45,45,45,45	0
34	NA	A	8359	1/1	0.61	0.73	48,48,48,48	0
34	NA	A	8385	1/1	0.63	0.28	43,43,43,43	0
34	NA	A	8372	1/1	0.64	0.56	55,55,55,55	0
32	MG	A	8029	1/1	0.64	0.14	53,53,53,53	0
32	MG	A	8040	1/1	0.65	0.17	71,71,71,71	0
32	MG	A	8024	1/1	0.65	0.81	95,95,95,95	0
32	MG	6	8118	1/1	0.65	0.69	61,61,61,61	0
34	NA	A	8317	1/1	0.66	0.20	63,63,63,63	0
32	MG	1	8105	1/1	0.67	0.46	30,30,30,30	0
32	MG	U	8073	1/1	0.68	0.23	52,52,52,52	0
34	NA	B	8351	1/1	0.69	0.30	85,85,85,85	0
36	PHA	6	77	10/11	0.69	0.43	35,38,41,41	10
36	PHA	5	77	11/11	0.70	0.52	24,25,29,29	11
32	MG	A	8113	1/1	0.70	0.18	43,43,43,43	0
34	NA	A	8382	1/1	0.71	0.25	54,54,54,54	0
34	NA	T	8312	1/1	0.71	0.47	108,108,108,108	0
32	MG	4	8078	1/1	0.72	0.13	63,63,63,63	0
32	MG	A	8011	1/1	0.73	0.10	37,37,37,37	0
35	CL	P	8508	1/1	0.73	0.22	72,72,72,72	0
32	MG	A	8080	1/1	0.73	0.15	33,33,33,33	0
32	MG	A	8059	1/1	0.73	0.20	65,65,65,65	0
37	CD	P	8405	1/1	0.73	0.12	184,184,184,184	0
32	MG	A	8115	1/1	0.74	0.20	36,36,36,36	0
32	MG	A	8096	1/1	0.74	0.18	46,46,46,46	0
34	NA	A	8327	1/1	0.74	0.21	34,34,34,34	0
34	NA	A	8329	1/1	0.74	0.38	65,65,65,65	0
34	NA	A	8377	1/1	0.74	0.41	76,76,76,76	0
32	MG	A	8044	1/1	0.75	0.20	50,50,50,50	0
32	MG	A	8110	1/1	0.75	0.14	29,29,29,29	0
34	NA	A	8352	1/1	0.75	0.43	51,51,51,51	0
32	MG	A	8071	1/1	0.76	0.19	80,80,80,80	0
34	NA	A	8328	1/1	0.76	0.55	54,54,54,54	0
32	MG	A	8016	1/1	0.76	0.21	38,38,38,38	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
35	CL	A	8514	1/1	0.76	0.29	55,55,55,55	0
34	NA	A	8340	1/1	0.77	0.31	38,38,38,38	0
34	NA	A	8350	1/1	0.77	0.43	36,36,36,36	0
32	MG	A	8104	1/1	0.77	0.29	51,51,51,51	0
32	MG	A	8081	1/1	0.77	0.09	51,51,51,51	0
32	MG	A	8035	1/1	0.77	0.11	54,54,54,54	0
34	NA	A	8319	1/1	0.77	0.15	33,33,33,33	0
34	NA	J	8322	1/1	0.77	0.31	68,68,68,68	0
35	CL	K	8501	1/1	0.78	0.13	69,69,69,69	0
32	MG	A	8090	1/1	0.78	0.34	62,62,62,62	0
34	NA	A	8374	1/1	0.78	0.27	60,60,60,60	0
34	NA	A	8375	1/1	0.78	0.73	63,63,63,63	0
32	MG	A	8092	1/1	0.78	0.33	92,92,92,92	0
34	NA	A	8370	1/1	0.79	0.29	50,50,50,50	0
34	NA	A	8307	1/1	0.79	0.22	53,53,53,53	0
34	NA	A	8354	1/1	0.79	0.55	31,31,31,31	0
34	NA	A	8336	1/1	0.79	0.18	41,41,41,41	0
32	MG	A	8091	1/1	0.79	0.09	53,53,53,53	0
32	MG	A	8111	1/1	0.79	0.15	67,67,67,67	0
34	NA	A	8368	1/1	0.80	0.22	69,69,69,69	0
34	NA	A	8320	1/1	0.80	0.25	24,24,24,24	0
34	NA	A	8310	1/1	0.80	0.38	33,33,33,33	0
32	MG	A	8116	1/1	0.80	0.12	67,67,67,67	0
32	MG	A	8117	1/1	0.80	0.14	26,26,26,26	0
32	MG	A	8019	1/1	0.81	0.09	15,15,15,15	0
34	NA	A	8357	1/1	0.81	0.09	53,53,53,53	0
34	NA	A	8330	1/1	0.81	0.39	42,42,42,42	0
34	NA	A	8313	1/1	0.81	0.26	44,44,44,44	0
32	MG	A	8084	1/1	0.82	0.14	56,56,56,56	0
35	CL	A	8515	1/1	0.82	0.58	85,85,85,85	0
32	MG	A	8054	1/1	0.82	0.12	37,37,37,37	0
35	CL	L	8512	1/1	0.82	0.16	47,47,47,47	0
34	NA	A	8381	1/1	0.83	0.16	54,54,54,54	0
32	MG	Z	8109	1/1	0.83	0.12	28,28,28,28	0
32	MG	A	8015	1/1	0.83	0.09	38,38,38,38	0
34	NA	A	8358	1/1	0.83	0.47	113,113,113,113	0
32	MG	A	8009	1/1	0.84	0.08	15,15,15,15	0
32	MG	A	8068	1/1	0.84	0.15	58,58,58,58	0
32	MG	A	8058	1/1	0.84	0.15	33,33,33,33	0
34	NA	C	8345	1/1	0.84	0.17	48,48,48,48	0
32	MG	A	8075	1/1	0.84	0.15	64,64,64,64	0
34	NA	A	8316	1/1	0.85	0.23	30,30,30,30	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
32	MG	A	8063	1/1	0.85	0.10	54,54,54,54	0
34	NA	A	8373	1/1	0.85	0.39	45,45,45,45	0
34	NA	K	8346	1/1	0.85	0.30	33,33,33,33	0
34	NA	S	8338	1/1	0.85	0.22	48,48,48,48	0
32	MG	A	8006	1/1	0.85	0.09	34,34,34,34	0
32	MG	A	8021	1/1	0.85	0.11	22,22,22,22	0
35	CL	A	8511	1/1	0.85	0.19	65,65,65,65	0
34	NA	A	8342	1/1	0.86	0.21	34,34,34,34	0
32	MG	A	8094	1/1	0.86	0.15	67,67,67,67	0
34	NA	A	8305	1/1	0.86	0.22	27,27,27,27	0
34	NA	N	8365	1/1	0.86	0.49	46,46,46,46	0
32	MG	A	8045	1/1	0.86	0.19	52,52,52,52	0
32	MG	A	8086	1/1	0.86	0.17	49,49,49,49	0
32	MG	A	8088	1/1	0.86	0.21	23,23,23,23	0
34	NA	A	8326	1/1	0.86	1.05	54,54,54,54	0
37	CD	1	8403	1/1	0.86	0.09	60,60,60,60	0
34	NA	A	8333	1/1	0.87	0.11	24,24,24,24	0
32	MG	A	8062	1/1	0.87	0.09	61,61,61,61	0
35	CL	A	8516	1/1	0.87	0.19	51,51,51,51	0
32	MG	A	8039	1/1	0.87	0.10	52,52,52,52	0
32	MG	A	8032	1/1	0.87	0.10	24,24,24,24	0
32	MG	A	8037	1/1	0.87	0.12	46,46,46,46	0
32	MG	A	8061	1/1	0.87	0.11	25,25,25,25	0
34	NA	A	8318	1/1	0.87	0.60	37,37,37,37	0
35	CL	A	8505	1/1	0.87	0.16	60,60,60,60	0
32	MG	A	8112	1/1	0.87	0.26	43,43,43,43	0
34	NA	B	8383	1/1	0.88	0.29	72,72,72,72	0
32	MG	A	8066	1/1	0.88	0.10	72,72,72,72	0
34	NA	A	8306	1/1	0.88	0.89	42,42,42,42	0
32	MG	A	8087	1/1	0.88	0.10	56,56,56,56	0
32	MG	A	8030	1/1	0.88	0.10	23,23,23,23	0
32	MG	A	8028	1/1	0.89	0.06	30,30,30,30	0
34	NA	N	8347	1/1	0.89	0.16	36,36,36,36	0
34	NA	A	8353	1/1	0.89	0.13	26,26,26,26	0
35	CL	K	8502	1/1	0.89	0.14	62,62,62,62	0
32	MG	A	8099	1/1	0.89	0.14	32,32,32,32	0
35	CL	M	8510	1/1	0.89	0.19	57,57,57,57	0
34	NA	A	8355	1/1	0.89	0.65	72,72,72,72	0
35	CL	Z	8520	1/1	0.89	0.12	39,39,39,39	0
33	K	A	8201	1/1	0.89	0.31	76,76,76,76	0
32	MG	D	8055	1/1	0.89	0.10	34,34,34,34	0
32	MG	A	8013	1/1	0.89	0.15	45,45,45,45	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
37	CD	V	8401	1/1	0.89	0.07	69,69,69,69	0
32	MG	A	8020	1/1	0.89	0.14	27,27,27,27	0
35	CL	A	8503	1/1	0.90	0.24	47,47,47,47	0
34	NA	A	8356	1/1	0.90	0.69	44,44,44,44	0
35	CL	O	8507	1/1	0.90	0.34	63,63,63,63	0
34	NA	A	8360	1/1	0.90	0.49	45,45,45,45	0
34	NA	A	8371	1/1	0.90	0.53	62,62,62,62	0
35	CL	4	8504	1/1	0.90	0.26	56,56,56,56	0
34	NA	S	8337	1/1	0.90	0.16	45,45,45,45	0
34	NA	A	8379	1/1	0.90	0.13	34,34,34,34	0
32	MG	A	8082	1/1	0.90	0.28	51,51,51,51	0
32	MG	A	8010	1/1	0.90	0.09	26,26,26,26	0
35	CL	K	8521	1/1	0.90	0.19	51,51,51,51	0
32	MG	A	8102	1/1	0.91	0.09	53,53,53,53	0
32	MG	A	8033	1/1	0.91	0.06	22,22,22,22	0
32	MG	A	8001	1/1	0.91	0.09	23,23,23,23	0
32	MG	A	8085	1/1	0.91	0.17	61,61,61,61	0
32	MG	A	8007	1/1	0.91	0.09	19,19,19,19	0
34	NA	A	8301	1/1	0.91	0.14	26,26,26,26	0
34	NA	A	8334	1/1	0.91	0.11	46,46,46,46	0
34	NA	A	8302	1/1	0.91	0.32	39,39,39,39	0
32	MG	A	8067	1/1	0.91	0.29	55,55,55,55	0
32	MG	A	8048	1/1	0.91	0.09	57,57,57,57	0
32	MG	A	8089	1/1	0.91	0.22	60,60,60,60	0
32	MG	A	8070	1/1	0.91	0.27	36,36,36,36	0
32	MG	A	8049	1/1	0.91	0.24	67,67,67,67	0
34	NA	A	8314	1/1	0.91	0.17	21,21,21,21	0
32	MG	A	8008	1/1	0.91	0.07	20,20,20,20	0
32	MG	B	8095	1/1	0.91	0.10	69,69,69,69	0
32	MG	A	8004	1/1	0.91	0.09	28,28,28,28	0
32	MG	A	8022	1/1	0.91	0.06	17,17,17,17	0
32	MG	A	8043	1/1	0.91	0.16	38,38,38,38	0
34	NA	A	8321	1/1	0.91	0.37	49,49,49,49	0
34	NA	A	8323	1/1	0.91	0.30	34,34,34,34	0
32	MG	L	8069	1/1	0.91	0.08	56,56,56,56	0
34	NA	A	8335	1/1	0.92	0.21	58,58,58,58	0
34	NA	A	8376	1/1	0.92	0.21	42,42,42,42	0
34	NA	E	8304	1/1	0.92	0.18	39,39,39,39	0
32	MG	A	8097	1/1	0.92	0.12	27,27,27,27	0
35	CL	S	8506	1/1	0.92	0.22	41,41,41,41	0
32	MG	A	8064	1/1	0.92	0.20	29,29,29,29	0
34	NA	A	8315	1/1	0.92	0.29	29,29,29,29	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
32	MG	A	8100	1/1	0.92	0.23	53,53,53,53	0
35	CL	A	8522	1/1	0.92	0.33	78,78,78,78	0
32	MG	D	8056	1/1	0.92	0.14	44,44,44,44	0
34	NA	A	8311	1/1	0.92	0.17	52,52,52,52	0
34	NA	A	8361	1/1	0.92	0.25	48,48,48,48	0
34	NA	U	8343	1/1	0.93	0.18	23,23,23,23	0
34	NA	A	8332	1/1	0.93	0.31	35,35,35,35	0
32	MG	A	8018	1/1	0.93	0.09	44,44,44,44	0
34	NA	A	8378	1/1	0.93	0.56	46,46,46,46	0
32	MG	A	8014	1/1	0.93	0.12	21,21,21,21	0
34	NA	A	8325	1/1	0.93	0.25	49,49,49,49	0
34	NA	A	8308	1/1	0.93	0.12	49,49,49,49	0
32	MG	A	8077	1/1	0.93	0.11	33,33,33,33	0
35	CL	D	8519	1/1	0.93	0.27	47,47,47,47	0
32	MG	A	8042	1/1	0.93	0.12	35,35,35,35	0
34	NA	A	8303	1/1	0.93	0.21	55,55,55,55	0
32	MG	A	8053	1/1	0.93	0.11	39,39,39,39	0
34	NA	A	8331	1/1	0.94	0.12	34,34,34,34	0
32	MG	A	8036	1/1	0.94	0.10	27,27,27,27	0
34	NA	M	8380	1/1	0.94	0.27	61,61,61,61	0
32	MG	A	8098	1/1	0.94	0.20	28,28,28,28	0
32	MG	A	8072	1/1	0.94	0.13	44,44,44,44	0
32	MG	A	8083	1/1	0.94	0.05	43,43,43,43	0
32	MG	A	8101	1/1	0.94	0.22	54,54,54,54	0
32	MG	A	8060	1/1	0.94	0.10	49,49,49,49	0
34	NA	A	8363	1/1	0.94	0.20	46,46,46,46	0
34	NA	A	8364	1/1	0.94	0.20	39,39,39,39	0
32	MG	A	8103	1/1	0.94	0.13	73,73,73,73	0
34	NA	A	8344	1/1	0.94	0.10	17,17,17,17	0
32	MG	A	8023	1/1	0.94	0.09	34,34,34,34	0
35	CL	A	8513	1/1	0.94	0.13	50,50,50,50	0
32	MG	A	8057	1/1	0.94	0.10	34,34,34,34	0
32	MG	A	8108	1/1	0.94	0.12	72,72,72,72	0
32	MG	A	8050	1/1	0.94	0.09	65,65,65,65	0
37	CD	2	8402	1/1	0.94	0.07	64,64,64,64	0
32	MG	A	8025	1/1	0.95	0.09	63,63,63,63	0
34	NA	A	8362	1/1	0.95	0.29	70,70,70,70	0
32	MG	A	8005	1/1	0.95	0.10	32,32,32,32	0
32	MG	A	8047	1/1	0.95	0.17	58,58,58,58	0
32	MG	A	8002	1/1	0.95	0.07	33,33,33,33	0
34	NA	A	8349	1/1	0.95	0.20	40,40,40,40	0
32	MG	A	8031	1/1	0.96	0.11	19,19,19,19	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
34	NA	A	8341	1/1	0.96	0.10	28,28,28,28	0
35	CL	N	8518	1/1	0.96	0.12	41,41,41,41	0
32	MG	A	8107	1/1	0.96	0.05	39,39,39,39	0
32	MG	A	8074	1/1	0.96	0.05	15,15,15,15	0
32	MG	A	8026	1/1	0.96	0.10	20,20,20,20	0
32	MG	A	8003	1/1	0.96	0.10	29,29,29,29	0
35	CL	A	8517	1/1	0.96	0.09	61,61,61,61	0
32	MG	A	8051	1/1	0.96	0.21	87,87,87,87	0
35	CL	C	8509	1/1	0.96	0.16	55,55,55,55	0
32	MG	A	8093	1/1	0.96	0.13	48,48,48,48	0
32	MG	A	8079	1/1	0.96	0.07	27,27,27,27	0
32	MG	A	8052	1/1	0.96	0.11	39,39,39,39	0
34	NA	J	8309	1/1	0.96	0.12	31,31,31,31	0
34	NA	A	8367	1/1	0.97	0.32	48,48,48,48	0
32	MG	A	8038	1/1	0.97	0.09	29,29,29,29	0
32	MG	A	8034	1/1	0.97	0.06	24,24,24,24	0
32	MG	A	8017	1/1	0.97	0.04	24,24,24,24	0
34	NA	A	8339	1/1	0.97	0.21	14,14,14,14	0
37	CD	4	8404	1/1	0.97	0.08	63,63,63,63	0
32	MG	A	8012	1/1	0.98	0.11	33,33,33,33	0
32	MG	A	8027	1/1	0.98	0.07	35,35,35,35	0
33	K	A	8202	1/1	0.98	0.08	53,53,53,53	0
34	NA	R	8348	1/1	0.99	0.10	29,29,29,29	0

6.5 Other polymers (i)

There are no such residues in this entry.