



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 15, 2026 – 01:50 AM UTC

PDB ID : 1VQ4 / pdb_00001vq4
Title : The structure of the transition state analogue "DAA" bound to the large ribosomal subunit of Haloarcula marismortui
Authors : Schmeing, T.M.; Steitz, T.A.
Deposited on : 2004-12-16
Resolution : 2.70 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

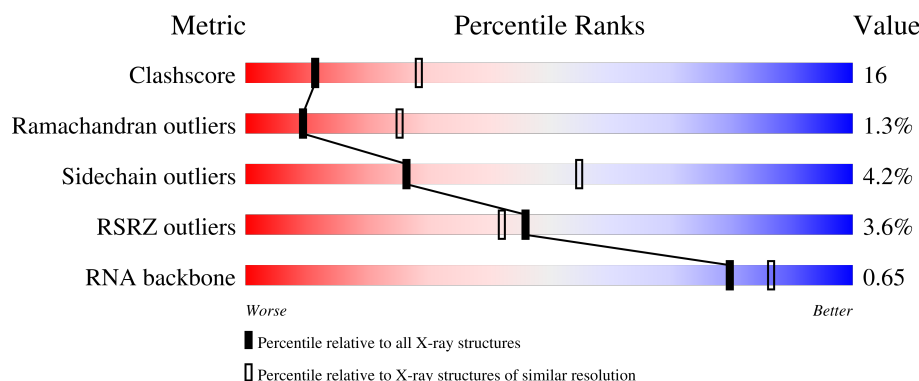
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)
RSRZ outliers	180081	3538 (2.70-2.70)
RNA backbone	3983	1044 (2.90-2.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	0	2922	59% 30% 5% 6%
2	9	122	4% 53% 34% 11%
3	4	8	38% 50% 12%
4	A	240	2% 52% 40% 6%
5	B	338	49% 44% 6%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
6	C	246	
7	D	177	
8	E	178	
9	F	120	
10	G	348	
11	H	171	
12	J	145	
13	K	132	
14	L	165	
15	M	194	
16	N	187	
17	O	116	
18	P	149	
19	Q	96	
20	R	155	
21	S	85	
22	T	120	
23	U	66	
24	V	71	
25	W	154	
26	X	92	
27	Y	241	
28	Z	83	
29	1	57	
30	2	50	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
31	3	92	2%61%36%
32	I	162	19%19%23%57%

2 Entry composition

There are 38 unique types of molecules in this entry. The entry contains 98999 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
1	0	2754	Total	C	N	O	P	0	0	0
			59021	26350	10878	19048	2745			

There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
0	628	1MA	A	modified residue	GB 3377779
0	2587	OMU	U	modified residue	GB 3377779
0	2588	OMG	G	modified residue	GB 3377779
0	2619	UR3	U	modified residue	GB 3377779
0	2621	PSU	U	modified residue	GB 3377779

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	9	122	Total	C	N	O	P	0	0	0
			2600	1160	472	847	121			

- Molecule 3 is a RNA chain called 5'-R(*CP*CP*(5AA)P*(2OP)P*(PO2)P*(DA)P*C*C)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	4	8	Total	C	N	O	P	0	0	0
			127	61	23	38	5			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	A	237	Total	C	N	O	S	0	0	0
			1753	1072	352	324	5			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	B	337	Total	C	N	O	S	0	0	0
			2625	1616	493	511	5			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	C	246	Total	C	N	O	S	0	0	0
			1859	1131	344	383	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	D	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	E	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	F	119	Total	C	N	O	S	0	0	0
			890	551	141	197	1			

- Molecule 10 is a protein called ACIDIC RIBOSOMAL PROTEIN P0 HOMOLOG.

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

- Molecule 11 is a protein called 50S RIBOSOMAL PROTEIN L10E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	H	160	Total	C	N	O	S	0	0	0
			1266	785	237	238	6			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	J	142	Total	C	N	O	S	0	0	0
			1120	696	199	222	3			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	K	132	Total	C	N	O	S	0	0	0
			992	609	187	192	4			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
K	44	LEU	HIS	conflict	UNP P22450

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	L	145	Total	C	N	O	S	0	0	0
			1118	670	222	226				

- Molecule 15 is a protein called 50S Ribosomal Protein L15E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	M	194	Total	C	N	O	S	0	0	0
			1560	943	332	284	1			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
M	13	GLU	LYS	conflict	GB 55231501
M	194	ALA	GLY	conflict	GB 55231501

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	N	186	Total	C	N	O	S	0	0	0
			1445	895	262	286	2			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
17	O	115	Total	C	N	O	0	0	0
			865	529	161	175			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
18	P	143	Total	C	N	O	0	0	0
			1136	683	229	224			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
19	Q	95	Total	C	N	O	0	0	0
			735	450	141	144			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
20	R	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	S	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	T	119	Total	C	N	O	0	0	0
			950	568	180	202			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	U	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	V	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	W	154	Total	C	N	O	S	0	0	0
			1196	737	209	244	6			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	X	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	Y	142	Total	C	N	O	S	0	0	0
			1130	686	228	216				

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
28	Z	73	Total	C	N	O	S	0	0	0
			578	346	116	111	5			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Z	10	ARG	SER	conflict	GB 55231162

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
29	1	56	Total	C	N	O	S	0	0	0
			431	258	86	83	4			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
30	2	46	Total	C	N	O	S	0	0	0
			396	239	89	67	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
31	3	92	Total	C	N	O	S	0	0	0
			755	458	153	137	7			

- Molecule 32 is a protein called 50S RIBOSOMAL PROTEIN L11P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
32	I	70	Total	C	N	O	S	0	0	0
			519	323	81	114	1			

- Molecule 33 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
33	0	108	Total	Mg	0	0
			108	108		
33	9	2	Total	Mg	0	0
			2	2		
33	A	2	Total	Mg	0	0
			2	2		
33	B	1	Total	Mg	0	0
			1	1		
33	K	1	Total	Mg	0	0
			1	1		
33	T	1	Total	Mg	0	0
			1	1		
33	Y	1	Total	Mg	0	0
			1	1		
33	3	1	Total	Mg	0	0
			1	1		

- Molecule 34 is POTASSIUM ION (CCD ID: K) (formula: K).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
34	0	3	Total	K	0	0
			3	3		

- Molecule 35 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
35	0	72	Total Na 72 72	0	0
35	9	2	Total Na 2 2	0	0
35	A	1	Total Na 1 1	0	0
35	C	1	Total Na 1 1	0	0
35	H	2	Total Na 2 2	0	0
35	J	1	Total Na 1 1	0	0
35	L	1	Total Na 1 1	0	0
35	M	1	Total Na 1 1	0	0
35	Q	1	Total Na 1 1	0	0
35	R	3	Total Na 3 3	0	0
35	S	1	Total Na 1 1	0	0

- Molecule 36 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
36	0	10	Total Cl 10 10	0	0
36	A	1	Total Cl 1 1	0	0
36	B	1	Total Cl 1 1	0	0
36	J	3	Total Cl 3 3	0	0
36	K	1	Total Cl 1 1	0	0
36	L	1	Total Cl 1 1	0	0
36	M	1	Total Cl 1 1	0	0
36	N	1	Total Cl 1 1	0	0
36	O	1	Total Cl 1 1	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
36	R	1	Total	Cl	0	0
			1	1		
36	3	1	Total	Cl	0	0
			1	1		

- Molecule 37 is CADMIUM ION (CCD ID: CD) (formula: Cd).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
37	O	1	Total	Cd	0	0
			1	1		
37	U	1	Total	Cd	0	0
			1	1		
37	Z	1	Total	Cd	0	0
			1	1		
37	1	1	Total	Cd	0	0
			1	1		
37	3	1	Total	Cd	0	0
			1	1		

- Molecule 38 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
38	0	5764	Total	O	0	0
			5764	5764		
38	9	133	Total	O	0	0
			133	133		
38	4	3	Total	O	0	0
			3	3		
38	A	116	Total	O	0	0
			116	116		
38	B	143	Total	O	0	0
			143	143		
38	C	173	Total	O	0	0
			173	173		
38	D	44	Total	O	0	0
			44	44		
38	E	43	Total	O	0	0
			43	43		
38	F	24	Total	O	0	0
			24	24		
38	G	17	Total	O	0	0
			17	17		

Continued on next page...

Continued from previous page...

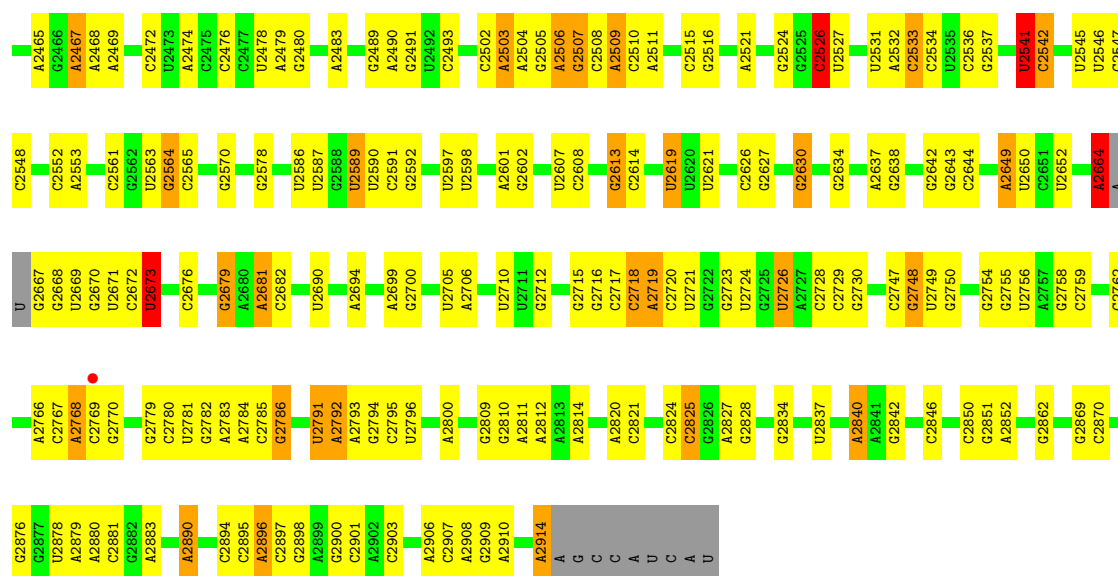
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
38	H	66	Total 66	O 66	0	0
38	J	52	Total 52	O 52	0	0
38	K	57	Total 57	O 57	0	0
38	L	81	Total 81	O 81	0	0
38	M	115	Total 115	O 115	0	0
38	N	61	Total 61	O 61	0	0
38	O	45	Total 45	O 45	0	0
38	P	63	Total 63	O 63	0	0
38	Q	52	Total 52	O 52	0	0
38	R	89	Total 89	O 89	0	0
38	S	31	Total 31	O 31	0	0
38	T	36	Total 36	O 36	0	0
38	U	26	Total 26	O 26	0	0
38	V	13	Total 13	O 13	0	0
38	W	70	Total 70	O 70	0	0
38	X	31	Total 31	O 31	0	0
38	Y	93	Total 93	O 93	0	0
38	Z	31	Total 31	O 31	0	0
38	1	61	Total 61	O 61	0	0
38	2	42	Total 42	O 42	0	0
38	3	71	Total 71	O 71	0	0

Continued on next page...

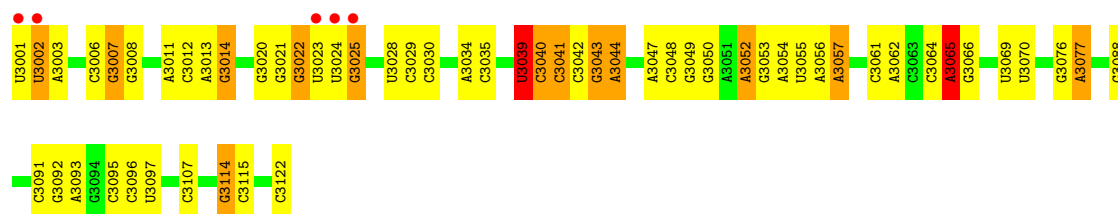
Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
38	I	9	Total	O	0	0
			9	9		

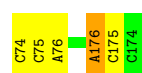
[illegible]



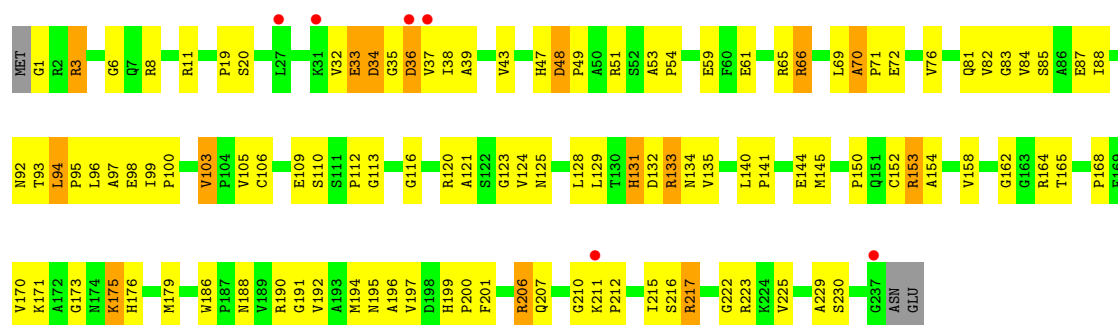
• Molecule 2: 5S ribosomal RNA



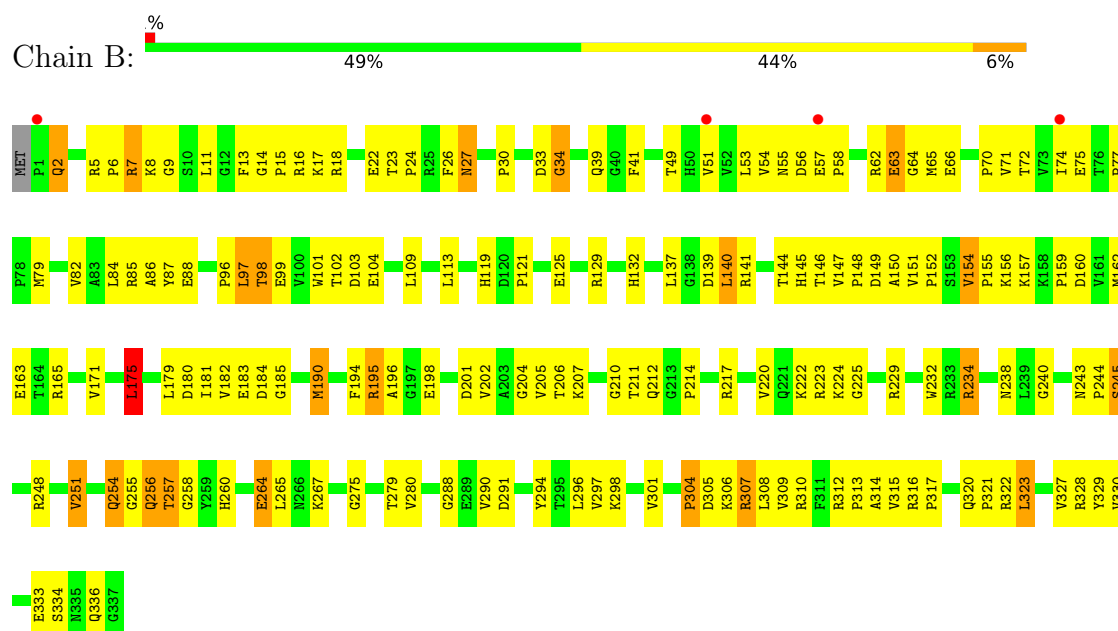
• Molecule 3: 5'-R(*CP*CP*(5AA)P*(2OP)P*(PO2)P*(DA)P*C*C)-3'



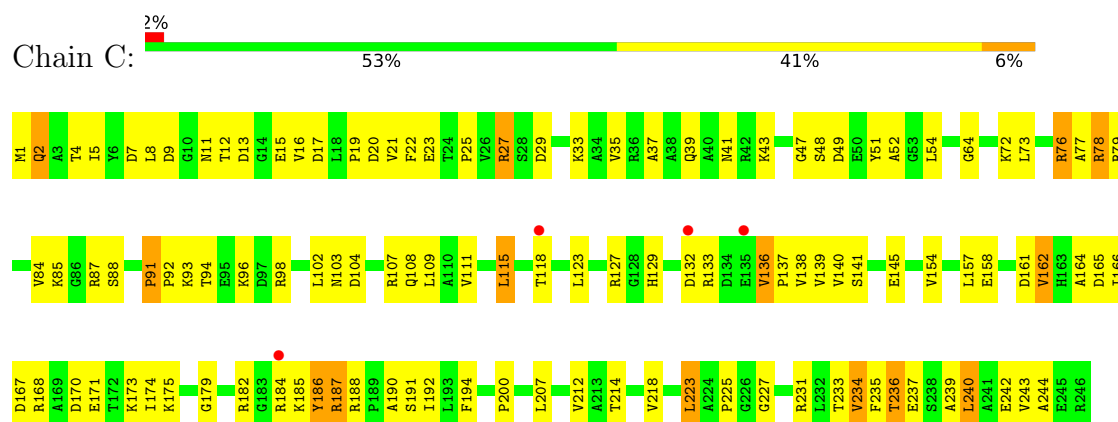
• Molecule 4: 50S ribosomal protein L2P



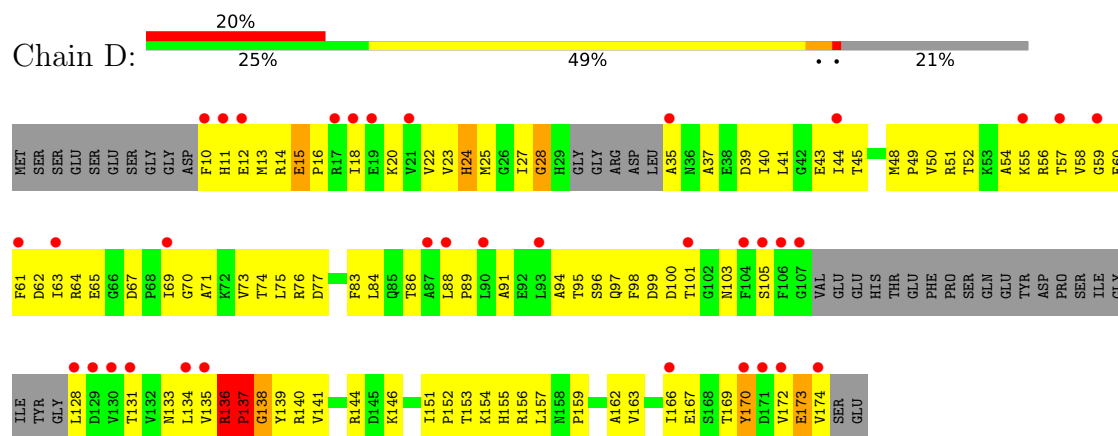
• Molecule 5: 50S ribosomal protein L3P



• Molecule 6: 50S ribosomal protein L4E

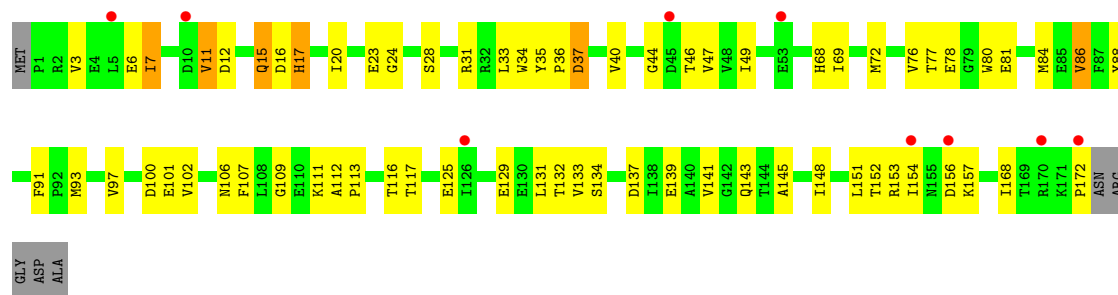


• Molecule 7: 50S ribosomal protein L5P

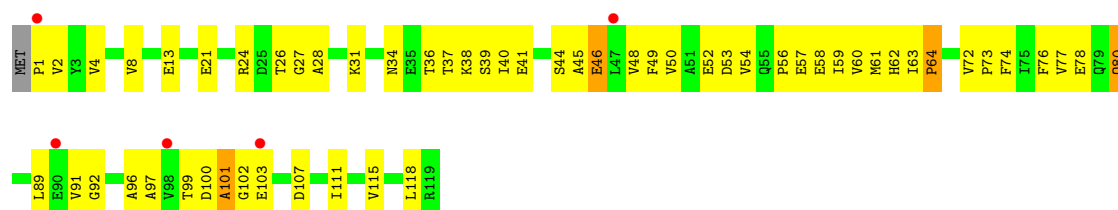


• Molecule 8: 50S ribosomal protein L6P

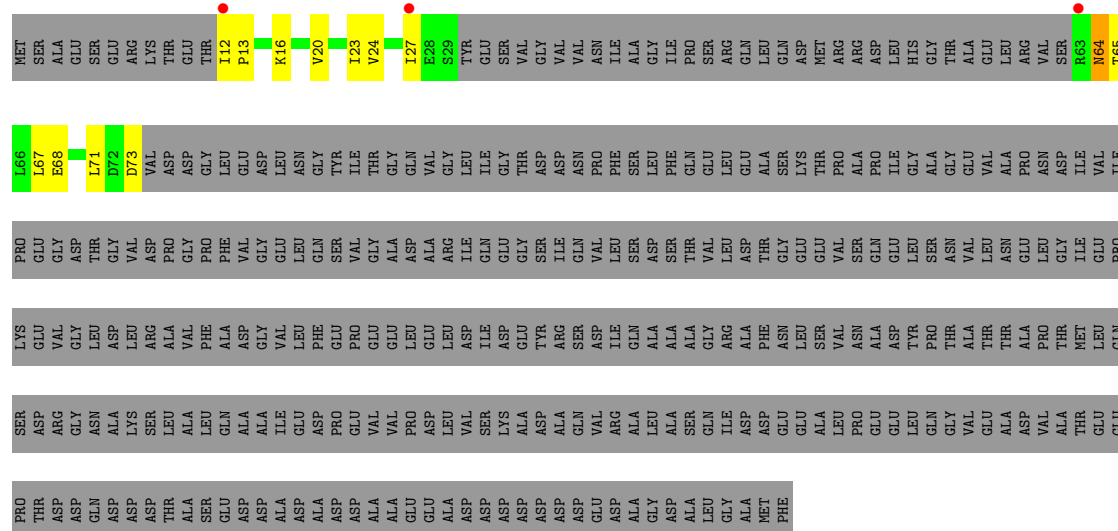




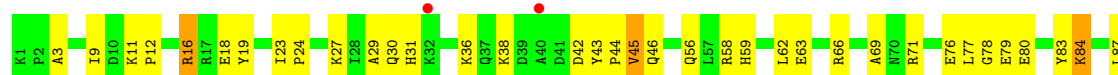
• Molecule 9: 50S ribosomal protein L7AE



• Molecule 10: ACIDIC RIBOSOMAL PROTEIN P0 HOMOLOG



• Molecule 11: 50S RIBOSOMAL PROTEIN L10E

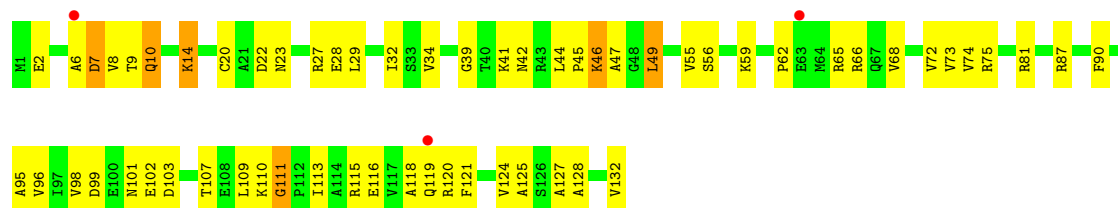




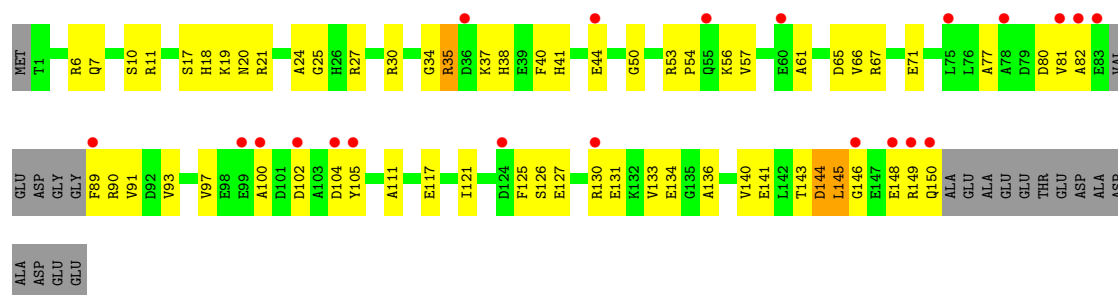
- Molecule 12: 50S ribosomal protein L13P



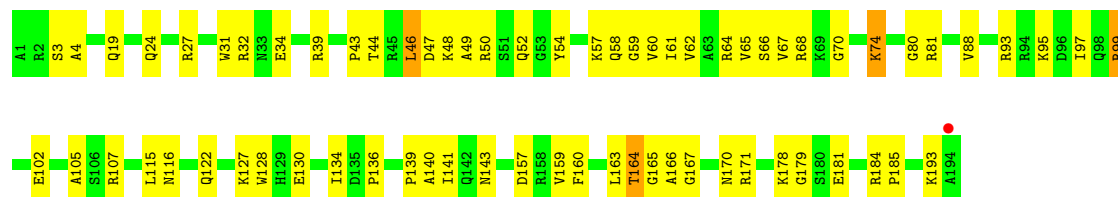
- Molecule 13: 50S ribosomal protein L14P



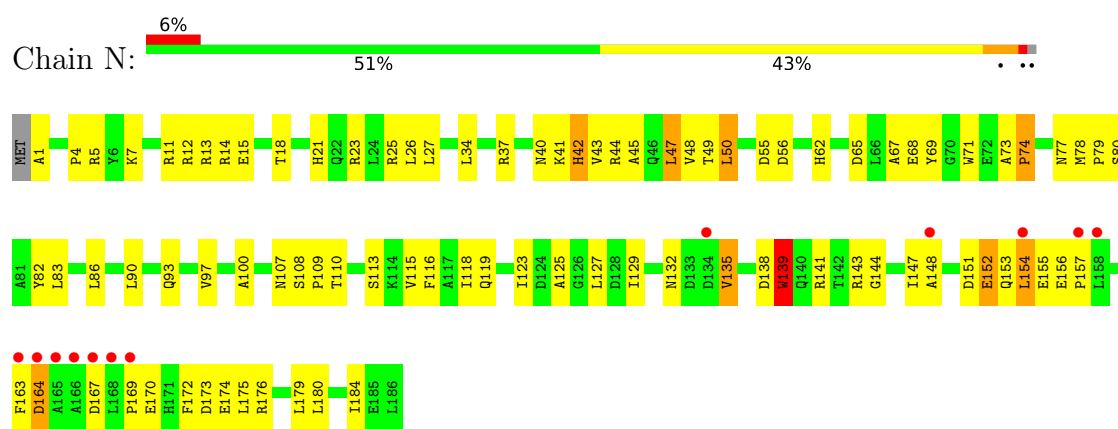
- Molecule 14: 50S ribosomal protein L15P



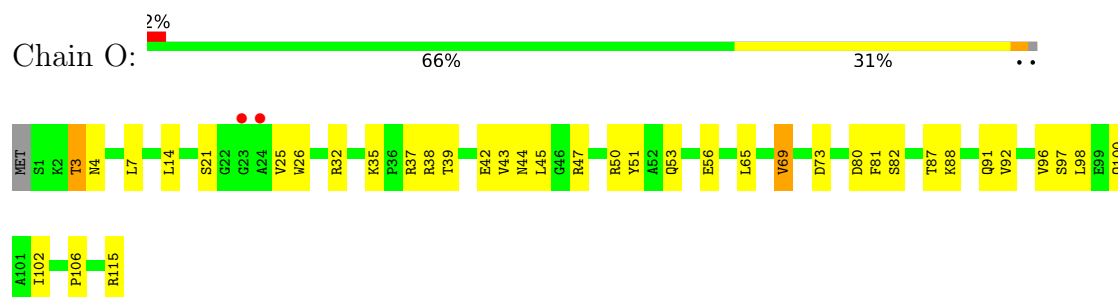
- Molecule 15: 50S Ribosomal Protein L15E



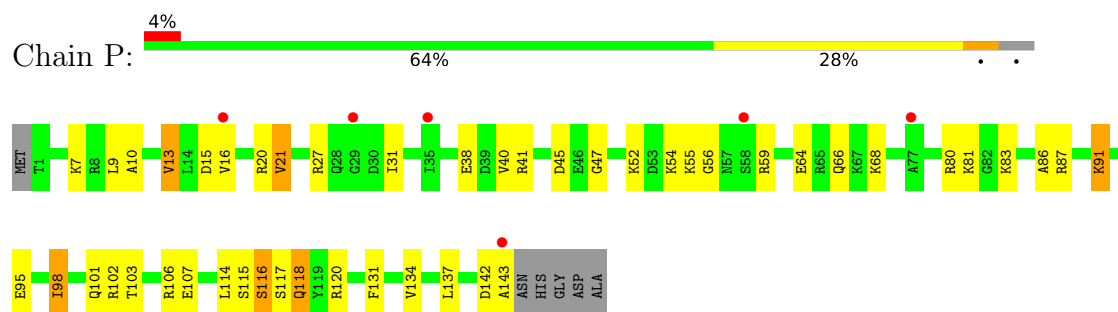
- Molecule 16: 50S ribosomal protein L18P



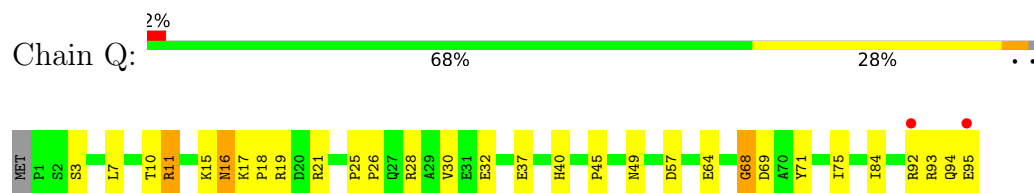
- Molecule 17: 50S ribosomal protein L18e



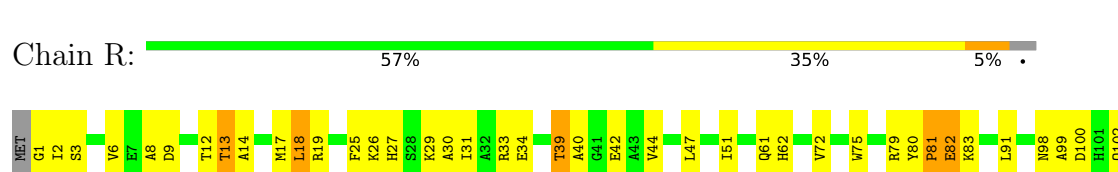
- Molecule 18: 50S ribosomal protein L19E

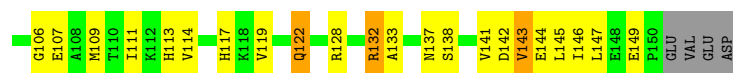


- Molecule 19: 50S ribosomal protein L21e

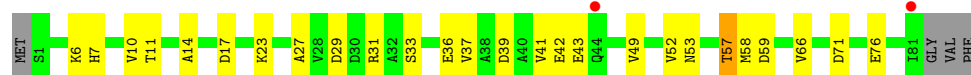


- Molecule 20: 50S ribosomal protein L22P

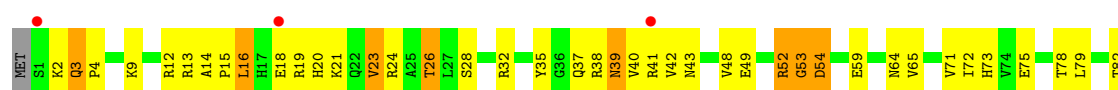




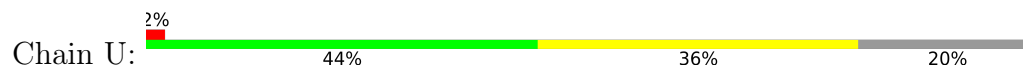
- Molecule 21: 50S ribosomal protein L23P



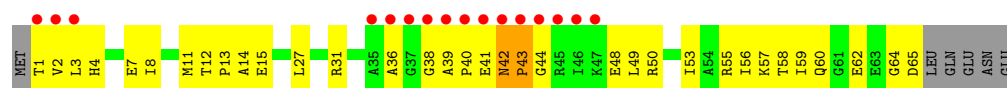
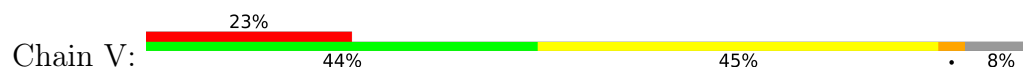
- Molecule 22: 50S ribosomal protein L24P



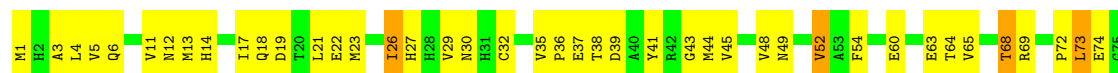
- Molecule 23: 50S ribosomal protein L24E



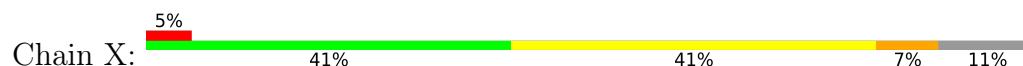
- Molecule 24: 50S ribosomal protein L29P

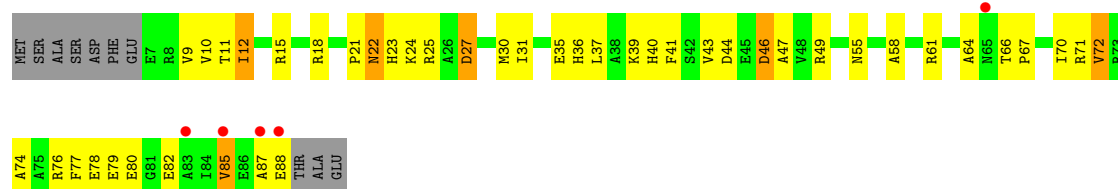


- Molecule 25: 50S ribosomal protein L30P

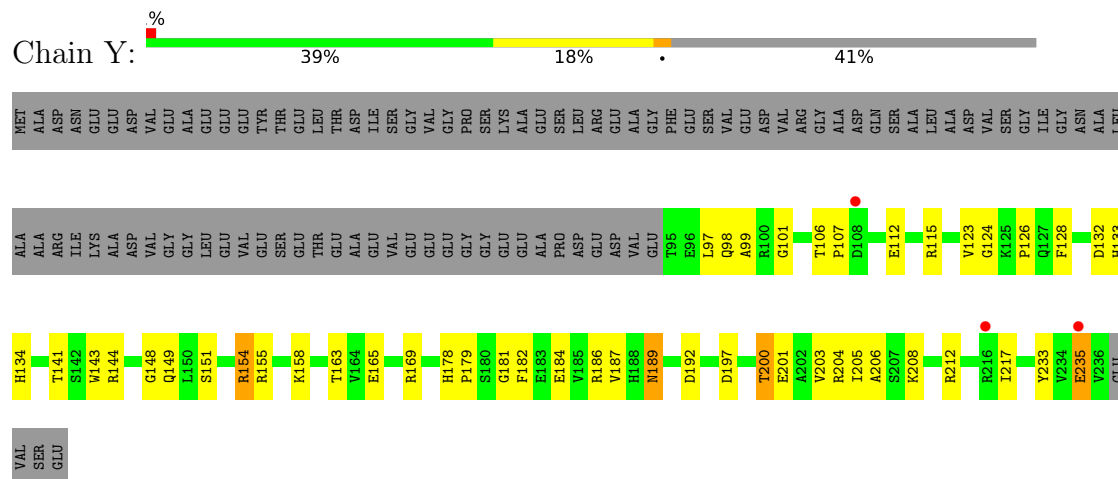


- Molecule 26: 50S ribosomal protein L31e

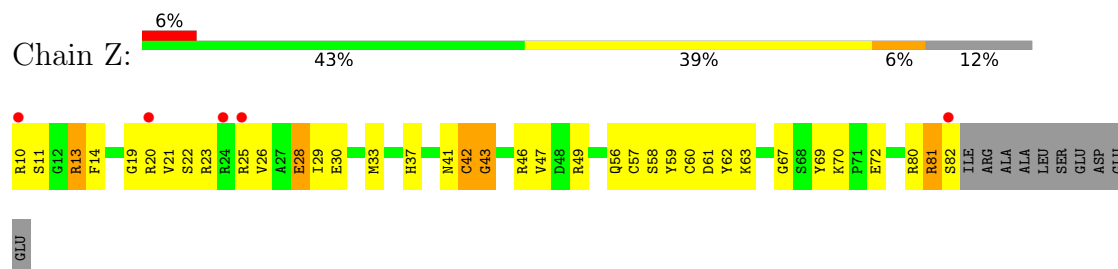




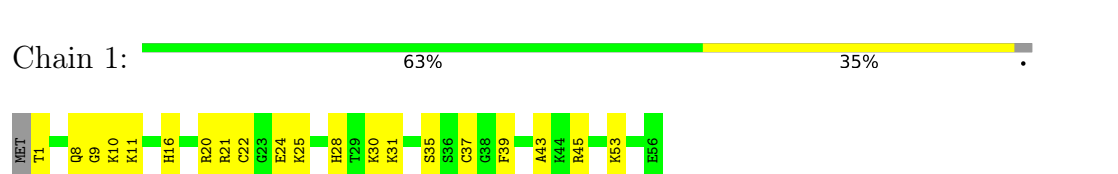
• Molecule 27: 50S ribosomal protein L32E



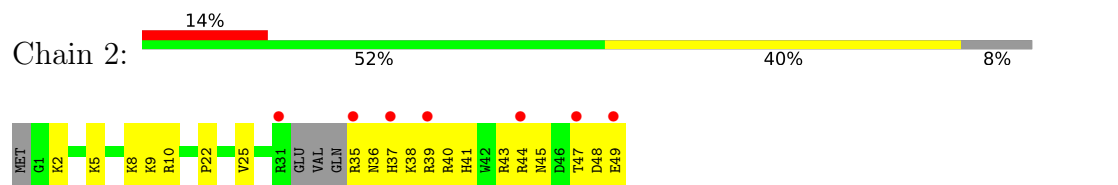
• Molecule 28: 50S ribosomal protein L37Ae



• Molecule 29: 50S ribosomal protein L37e

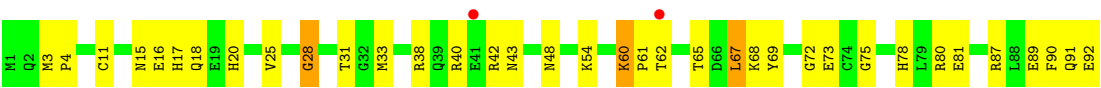


• Molecule 30: 50S ribosomal protein L39e

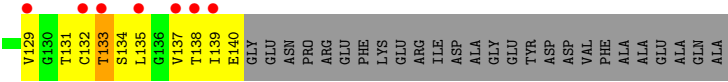
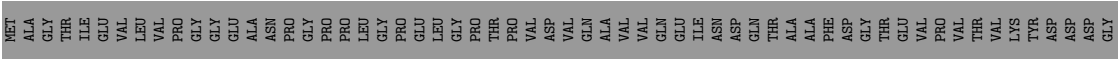


• Molecule 31: 50S ribosomal protein L44E





● Molecule 32: 50S RIBOSOMAL PROTEIN L11P



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	213.00Å 301.03Å 575.27Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.70 50.00 – 2.70	Depositor EDS
% Data completeness (in resolution range)	99.8 (50.00-2.70) 95.2 (50.00-2.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.80 (at 2.69Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.190 , 0.230 0.184 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	53.6	Xtriage
Anisotropy	0.306	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 56.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	98999	wwPDB-VP
Average B, all atoms (Å ²)	58.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.58% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: NA, CL, 5AA, UR3, 2OP, CD, MG, PO2, OMU, OMG, 1MA, K, PSU

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	0	0.38	0/65959	0.62	25/102870 (0.0%)
2	9	0.37	0/2905	0.62	4/4528 (0.1%)
3	4	0.35	0/102	0.79	0/149
4	A	0.41	0/1786	1.01	8/2408 (0.3%)
5	B	0.42	0/2690	1.01	13/3652 (0.4%)
6	C	0.46	0/1884	1.01	5/2551 (0.2%)
7	D	0.34	0/1111	0.86	7/1498 (0.5%)
8	E	0.39	0/1382	0.86	2/1880 (0.1%)
9	F	0.37	0/901	0.90	5/1224 (0.4%)
10	G	0.37	0/241	0.75	0/324
11	H	0.41	0/1287	0.97	7/1725 (0.4%)
12	J	0.44	0/1136	0.99	6/1530 (0.4%)
13	K	0.45	0/1001	1.03	4/1347 (0.3%)
14	L	0.38	0/1130	0.93	6/1509 (0.4%)
15	M	0.40	0/1584	0.92	3/2119 (0.1%)
16	N	0.37	0/1474	1.02	4/1999 (0.2%)
17	O	0.41	0/874	0.87	2/1181 (0.2%)
18	P	0.40	0/1147	0.84	1/1528 (0.1%)
19	Q	0.44	0/749	1.09	4/1005 (0.4%)
20	R	0.47	0/1172	0.96	5/1578 (0.3%)
21	S	0.37	0/648	0.88	2/875 (0.2%)
22	T	0.37	0/958	0.94	5/1289 (0.4%)
23	U	0.42	0/417	0.93	1/562 (0.2%)
24	V	0.35	0/502	0.91	2/675 (0.3%)
25	W	0.49	0/1219	1.01	4/1655 (0.2%)
26	X	0.45	0/664	0.94	2/895 (0.2%)
27	Y	0.44	0/1146	0.95	3/1536 (0.2%)
28	Z	0.41	0/589	0.93	0/787
29	1	0.41	0/438	0.92	1/578 (0.2%)
30	2	0.39	0/401	0.74	0/529
31	3	0.42	0/771	0.86	5/1024 (0.5%)
32	I	0.37	0/526	0.87	0/716

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
All	All	0.39	0/98794	0.72	136/147726 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	0	0	47
2	9	0	2
3	4	0	1
25	W	0	1
All	All	0	51

There are no bond length outliers.

All (136) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	0	1563	G	C2'-C3'-O3'	12.52	128.28	109.50
1	0	1979	G	C2'-C3'-O3'	9.97	124.45	109.50
16	N	135	VAL	N-CA-C	-9.06	104.31	113.10
1	0	1942	A	C5'-C4'-C3'	8.71	129.06	116.00
18	P	118	GLN	N-CA-C	-8.70	101.27	112.23
5	B	157	LYS	N-CA-C	-8.57	103.41	114.04
12	J	68	GLY	N-CA-C	8.32	122.61	111.72
11	H	160	SER	N-CA-C	-8.20	98.39	110.52
19	Q	17	LYS	N-CA-C	-8.18	99.44	109.83
4	A	222	GLY	N-CA-C	-8.09	104.86	114.48
25	W	68	THR	N-CA-C	7.29	119.22	111.28
5	B	154	VAL	CA-C-N	7.20	126.73	119.24
5	B	154	VAL	C-N-CA	7.20	126.73	119.24
8	E	11	VAL	N-CA-C	7.12	120.14	109.17
6	C	64	GLY	N-CA-C	7.09	122.91	114.48
16	N	13	ARG	N-CA-C	-7.08	104.77	113.41
5	B	265	LEU	N-CA-C	6.97	120.80	110.48
5	B	323	LEU	N-CA-C	6.97	119.30	110.24
2	9	3039	U	N1-C1'-C2'	6.79	122.18	112.00
1	0	2291	A	N9-C1'-C2'	6.78	122.16	112.00
2	9	3065	A	N9-C1'-C2'	6.76	122.14	112.00
29	1	43	ALA	N-CA-C	-6.69	104.07	111.36
15	M	193	LYS	N-CA-C	6.62	121.00	112.26
21	S	57	THR	N-CA-C	6.62	119.83	110.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	N	153	GLN	N-CA-C	-6.61	104.21	113.20
6	C	179	GLY	N-CA-C	-6.61	104.77	112.83
5	B	222	LYS	N-CA-C	-6.57	99.95	110.14
4	A	103	VAL	N-CA-C	6.47	115.11	107.73
21	S	27	ALA	N-CA-C	-6.43	98.24	108.73
12	J	22	VAL	N-CA-C	-6.38	104.53	110.53
1	0	920	C	C2'-C3'-O3'	-6.38	104.13	113.70
27	Y	143	TRP	N-CA-C	6.37	119.59	110.10
1	0	834	G	C2'-C3'-O3'	-6.34	104.20	113.70
4	A	48	ASP	CA-C-N	6.30	126.21	119.28
4	A	48	ASP	C-N-CA	6.30	126.21	119.28
12	J	112	ASP	N-CA-C	-6.29	99.01	109.46
20	R	141	VAL	N-CA-C	6.28	117.53	108.48
11	H	113	MET	N-CA-C	-6.25	105.30	113.17
4	A	70	ALA	N-CA-C	6.22	117.50	109.72
2	9	3039	U	C4'-C3'-O3'	-6.19	103.72	113.00
5	B	175	LEU	N-CA-C	-6.19	104.46	111.14
12	J	105	LEU	N-CA-C	-6.16	100.48	110.20
26	X	22	ASN	N-CA-C	6.09	118.70	111.33
1	0	2541	U	C2'-C3'-O3'	6.08	122.83	113.70
4	A	133	ARG	N-CA-C	-6.08	105.86	113.28
25	W	35	VAL	N-CA-C	6.04	114.48	107.89
6	C	78	ARG	N-CA-C	6.03	117.06	108.74
15	M	70	GLY	N-CA-C	6.00	120.57	112.17
22	T	54	ASP	N-CA-C	-5.96	105.97	113.18
1	0	1504	A	N9-C1'-C2'	5.96	120.94	112.00
19	Q	68	GLY	N-CA-C	-5.89	101.33	111.47
22	T	52	ARG	N-CA-C	5.88	123.32	110.80
5	B	151	VAL	CA-C-N	5.87	126.01	119.32
5	B	151	VAL	C-N-CA	5.87	126.01	119.32
1	0	206	G	C5'-C4'-C3'	-5.86	107.22	116.00
1	0	2526	C	N1-C1'-C2'	5.85	120.77	112.00
7	D	100	ASP	N-CA-C	-5.81	106.03	113.23
7	D	170	TYR	N-CA-C	5.80	119.86	111.56
13	K	124	VAL	N-CA-C	-5.76	106.09	111.45
1	0	871	G	C5'-C4'-O4'	-5.75	101.17	109.80
24	V	42	ASN	CA-C-N	5.73	127.00	119.84
24	V	42	ASN	C-N-CA	5.73	127.00	119.84
20	R	122	GLN	N-CA-C	-5.73	99.79	108.67
15	M	74	LYS	N-CA-C	5.72	118.80	109.59
31	3	43	ASN	N-CA-C	5.71	119.98	113.19
13	K	8	VAL	N-CA-C	5.71	116.70	108.48

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	D	151	ILE	N-CA-C	5.69	113.52	108.63
2	9	3065	A	C4'-C3'-O3'	-5.65	104.53	113.00
14	L	80	ASP	N-CA-C	5.65	118.26	110.35
4	A	135	VAL	N-CA-C	5.63	116.59	108.48
27	Y	181	GLY	N-CA-C	-5.63	106.76	114.64
14	L	145	LEU	N-CA-C	-5.61	105.26	111.71
12	J	47	THR	N-CA-C	5.58	117.27	110.41
20	R	137	ASN	N-CA-C	5.58	118.71	110.46
13	K	14	LYS	N-CA-C	-5.57	101.80	110.10
14	L	20	ASN	N-CA-C	5.57	119.68	111.04
1	0	2012	U	N1-C1'-C2'	5.56	120.34	112.00
23	U	50	GLU	N-CA-C	5.55	118.86	111.75
1	0	2301	A	N9-C1'-C2'	5.55	120.33	112.00
1	0	2673	U	N1-C1'-C2'	5.55	120.32	112.00
9	F	8	VAL	N-CA-C	5.48	112.97	107.55
7	D	15	GLU	CA-C-N	5.46	126.67	119.84
7	D	15	GLU	C-N-CA	5.46	126.67	119.84
11	H	166	SER	CA-C-N	-5.46	113.02	119.84
11	H	166	SER	C-N-CA	-5.46	113.02	119.84
1	0	921	G	N9-C1'-C2'	5.44	120.15	112.00
1	0	2313	C	C5'-C4'-C3'	5.43	124.15	116.00
5	B	220	VAL	N-CA-C	-5.41	104.15	110.05
17	O	69	VAL	N-CA-C	5.40	116.25	108.48
26	X	12	ILE	N-CA-C	5.39	113.21	107.76
5	B	22	GLU	N-CA-C	-5.38	105.97	112.54
25	W	142	ASP	N-CA-C	-5.38	103.28	110.55
22	T	3	GLN	CA-C-N	5.38	124.83	119.24
22	T	3	GLN	C-N-CA	5.38	124.83	119.24
16	N	42	HIS	N-CA-C	5.37	117.14	109.14
1	0	2726	U	N1-C1'-C2'	5.36	120.04	112.00
31	3	28	GLY	N-CA-C	-5.34	105.45	112.82
1	0	874	A	C4'-C3'-O3'	-5.33	105.00	113.00
11	H	159	PRO	N-CA-C	5.33	118.68	111.22
14	L	7	GLN	N-CA-C	5.30	117.97	111.82
25	W	123	GLY	N-CA-C	-5.27	108.36	115.21
6	C	175	LYS	N-CA-C	5.25	117.85	110.23
20	R	34	GLU	N-CA-C	5.24	117.08	111.36
1	0	129	A	C2'-C3'-O3'	5.23	121.54	113.70
7	D	136	ARG	CA-C-N	5.22	126.37	119.84
7	D	136	ARG	C-N-CA	5.22	126.37	119.84
11	H	116	ALA	N-CA-C	5.21	119.48	113.18
1	0	1819	G	C5'-C4'-C3'	5.20	123.80	116.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	0	2664	A	N9-C1'-C2'	5.17	119.76	112.00
4	A	110	SER	N-CA-C	-5.16	107.11	113.41
31	3	81	GLU	N-CA-C	-5.16	103.34	110.35
9	F	118	LEU	N-CA-C	-5.15	106.97	113.20
9	F	80	GLN	N-CA-C	-5.15	107.55	113.88
22	T	16	LEU	N-CA-C	5.11	117.24	111.11
1	0	1261	A	N9-C1'-C2'	5.11	119.66	112.00
11	H	45	VAL	N-CA-C	5.11	115.32	108.17
8	E	37	ASP	N-CA-C	5.10	119.09	112.86
1	0	922	A	C4'-C3'-O3'	-5.09	105.37	113.00
9	F	62	HIS	N-CA-C	5.08	117.71	111.82
12	J	44	ALA	N-CA-C	-5.08	103.82	110.53
19	Q	19	ARG	N-CA-C	5.08	117.71	111.82
19	Q	49	ASN	N-CA-C	5.08	117.96	110.59
14	L	44	GLU	N-CA-C	-5.08	103.07	110.08
1	0	1592	G	N9-C1'-C2'	5.07	119.60	112.00
27	Y	101	GLY	N-CA-C	5.07	121.49	112.22
31	3	67	LEU	N-CA-C	5.06	117.98	110.14
9	F	72	VAL	N-CA-C	5.04	113.89	108.95
17	O	82	SER	N-CA-C	-5.04	103.39	110.50
1	0	1479	A	C5'-C4'-C3'	-5.04	108.44	116.00
5	B	23	THR	CA-C-N	5.04	124.97	119.78
5	B	23	THR	C-N-CA	5.04	124.97	119.78
31	3	60	LYS	N-CA-C	-5.04	103.34	110.29
6	C	186	TYR	N-CA-C	5.02	118.20	110.42
14	L	144	ASP	N-CA-C	-5.02	105.81	111.28
20	R	18	LEU	N-CA-C	-5.01	101.98	109.95
13	K	46	LYS	N-CA-C	5.00	118.22	110.17

There are no chirality outliers.

All (51) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	0	1078	A	Sidechain
1	0	1340	G	Sidechain
1	0	1342	C	Sidechain
1	0	1351	G	Sidechain
1	0	1377	C	Sidechain
1	0	1417	G	Sidechain
1	0	1614	G	Sidechain
1	0	1681	G	Sidechain
1	0	1744	G	Sidechain

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
1	0	1829	A	Sidechain
1	0	1835	U	Sidechain
1	0	1845	A	Sidechain
1	0	1861	C	Sidechain
1	0	1863	G	Sidechain
1	0	1867	G	Sidechain
1	0	1877	G	Sidechain
1	0	1878	G	Sidechain
1	0	191	A	Sidechain
1	0	1970	G	Sidechain
1	0	221	G	Sidechain
1	0	2312	G	Sidechain
1	0	2316	G	Sidechain
1	0	2395	A	Sidechain
1	0	24	G	Sidechain
1	0	2412	G	Sidechain
1	0	2465	A	Sidechain
1	0	2493	C	Sidechain
1	0	2503	A	Sidechain
1	0	2506	A	Sidechain
1	0	2526	C	Sidechain
1	0	2552	C	Sidechain
1	0	2564	G	Sidechain
1	0	2607	U	Sidechain
1	0	2630	G	Sidechain
1	0	2673	U	Sidechain
1	0	2679	G	Sidechain
1	0	2840	A	Sidechain
1	0	2842	G	Sidechain
1	0	417	G	Sidechain
1	0	471	G	Sidechain
1	0	482	G	Sidechain
1	0	518	G	Sidechain
1	0	781	C	Sidechain
1	0	817	G	Sidechain
1	0	867	A	Sidechain
1	0	882	A	Sidechain
1	0	952	G	Sidechain
3	4	176	DA	Sidechain
2	9	3039	U	Sidechain
2	9	3065	A	Sidechain
25	W	90	TYR	Sidechain

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	0	59021	0	29812	854	0
2	9	2600	0	1326	65	0
3	4	127	0	75	4	0
4	A	1753	0	1766	126	0
5	B	2625	0	2533	164	0
6	C	1859	0	1816	128	0
7	D	1094	0	1085	95	0
8	E	1357	0	1266	70	0
9	F	890	0	843	54	0
10	G	240	0	231	14	0
11	H	1266	0	1268	70	0
12	J	1120	0	1098	57	0
13	K	992	0	1031	65	0
14	L	1118	0	1076	55	0
15	M	1560	0	1568	70	0
16	N	1445	0	1401	106	0
17	O	865	0	873	39	0
18	P	1136	0	1123	45	0
19	Q	735	0	729	24	0
20	R	1149	0	1122	64	0
21	S	641	0	605	22	0
22	T	950	0	923	62	0
23	U	410	0	364	26	0
24	V	499	0	511	35	0
25	W	1196	0	1137	99	0
26	X	654	0	653	49	0
27	Y	1130	0	1133	58	0
28	Z	578	0	539	30	0
29	1	431	0	426	31	0
30	2	396	0	413	28	0
31	3	755	0	728	33	0
32	I	519	0	500	55	0
33	0	108	0	0	0	0
33	3	1	0	0	0	0
33	9	2	0	0	0	0
33	A	2	0	0	0	0
33	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
33	K	1	0	0	0	0
33	T	1	0	0	0	0
33	Y	1	0	0	0	0
34	0	3	0	0	0	0
35	0	72	0	0	0	0
35	9	2	0	0	0	0
35	A	1	0	0	0	0
35	C	1	0	0	0	0
35	H	2	0	0	0	0
35	J	1	0	0	0	0
35	L	1	0	0	0	0
35	M	1	0	0	0	0
35	Q	1	0	0	0	0
35	R	3	0	0	0	0
35	S	1	0	0	0	0
36	0	10	0	0	1	0
36	3	1	0	0	0	0
36	A	1	0	0	0	0
36	B	1	0	0	0	0
36	J	3	0	0	1	0
36	K	1	0	0	0	0
36	L	1	0	0	0	0
36	M	1	0	0	1	0
36	N	1	0	0	1	0
36	O	1	0	0	0	0
36	R	1	0	0	0	0
37	1	1	0	0	0	0
37	3	1	0	0	0	0
37	O	1	0	0	0	0
37	U	1	0	0	0	0
37	Z	1	0	0	0	0
38	0	5764	0	0	97	0
38	1	61	0	0	3	0
38	2	42	0	0	3	0
38	3	71	0	0	6	0
38	4	3	0	0	0	0
38	9	133	0	0	4	0
38	A	116	0	0	19	0
38	B	143	0	0	23	0
38	C	173	0	0	21	0
38	D	44	0	0	8	0
38	E	43	0	0	5	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
38	F	24	0	0	4	0
38	G	17	0	0	0	0
38	H	66	0	0	9	0
38	I	9	0	0	2	0
38	J	52	0	0	3	0
38	K	57	0	0	7	0
38	L	81	0	0	11	0
38	M	115	0	0	4	0
38	N	61	0	0	10	0
38	O	45	0	0	6	0
38	P	63	0	0	3	0
38	Q	52	0	0	1	0
38	R	89	0	0	4	0
38	S	31	0	0	2	0
38	T	36	0	0	2	0
38	U	26	0	0	0	0
38	V	13	0	0	1	0
38	W	70	0	0	5	0
38	X	31	0	0	5	0
38	Y	93	0	0	7	0
38	Z	31	0	0	1	0
All	All	98999	0	59974	2429	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 16.

All (2429) 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)
2:9:3006:C:H5''	16:N:37:ARG:NH1	1.64	1.13
6:C:236:THR:HG22	6:C:239:ALA:H	1.11	1.13
11:H:46:GLN:HB3	11:H:167:PRO:HD2	1.32	1.11
20:R:99:ALA:HB1	20:R:109:MET:HE1	1.31	1.09
2:9:3006:C:H5''	16:N:37:ARG:HH12	1.08	1.07
1:0:1160:G:H5'	1:0:1161:A:H5'	1.34	1.04
6:C:127:ARG:NH2	6:C:225:PRO:HG2	1.71	1.04
1:0:156:C:H5''	15:M:171:ARG:HD3	1.38	1.03
1:0:1242:A:H5'	12:J:82:THR:HG23	1.40	1.03
26:X:37:LEU:HD13	26:X:85:VAL:HG21	1.39	1.02
11:H:56:GLN:HE21	11:H:126:ARG:HE	1.02	1.01
4:A:194:MET:HE3	4:A:199:HIS:HB2	1.43	1.01

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:Z:10:ARG:HA	38:Z:9216:HOH:O	1.57	1.01
5:B:238:ASN:HD22	5:B:240:GLY:H	1.06	1.00
13:K:10:GLN:HE21	13:K:10:GLN:H	1.05	1.00
4:A:211:LYS:HB3	4:A:212:PRO:HD2	1.43	0.99
1:O:2364:A:H5''	19:Q:15:LYS:HD3	1.45	0.98
1:O:871:G:H5'	1:O:871:G:H8	1.27	0.97
22:T:71:VAL:HG11	22:T:90:PRO:HB3	1.44	0.97
8:E:36:PRO:HD3	12:J:127:ILE:HD12	1.45	0.96
1:O:871:G:H5'	1:O:871:G:C8	1.99	0.96
7:D:134:LEU:HD11	7:D:166:ILE:HD11	1.46	0.96
1:O:56:G:H5''	24:V:50:ARG:HH12	1.31	0.95
1:O:1751:G:H2'	1:O:1752:G:H5''	1.46	0.95
24:V:12:THR:HG22	24:V:15:GLU:HG3	1.47	0.95
1:O:870:G:H2'	1:O:871:G:H5''	1.45	0.94
7:D:25:MET:HE2	7:D:41:LEU:HG	1.48	0.94
2:9:3056:A:H2'	2:9:3057:A:H5''	1.48	0.94
18:P:115:SER:H	18:P:118:GLN:HE21	0.96	0.94
1:O:2506:A:HO2'	1:O:2507:G:H8	1.03	0.93
25:W:149:LEU:HG	25:W:153:MET:HE2	1.50	0.92
9:F:91:VAL:HG12	9:F:92:GLY:H	1.32	0.92
7:D:154:LYS:H	7:D:154:LYS:HD2	1.31	0.92
25:W:5:VAL:HG11	25:W:153:MET:HE1	1.50	0.91
1:O:1187:U:HO2'	1:O:1189:A:H2	1.10	0.91
1:O:1474:C:H6	1:O:1474:C:H5'	1.36	0.91
20:R:39:THR:HG22	20:R:42:GLU:H	1.35	0.91
13:K:39:GLY:HA2	38:K:4183:HOH:O	1.71	0.91
1:O:1835:U:H5	1:O:1840:A:N7	1.69	0.90
2:9:3076:G:H3'	2:9:3077:A:H5''	1.52	0.90
26:X:76:ARG:HH11	26:X:76:ARG:HG3	1.33	0.90
21:S:57:THR:HG22	21:S:59:ASP:H	1.37	0.90
1:O:2717:C:H2'	1:O:2718:C:H5''	1.53	0.90
15:M:164:THR:HG22	15:M:167:GLY:H	1.36	0.89
13:K:10:GLN:H	13:K:10:GLN:NE2	1.70	0.89
1:O:2717:C:C2'	1:O:2718:C:H5''	2.03	0.88
1:O:1116:U:HO2'	1:O:1118:A:H2	0.89	0.88
8:E:81:GLU:HG2	8:E:134:SER:HB3	1.56	0.88
5:B:212:GLN:HB2	5:B:257:THR:HG21	1.55	0.88
22:T:9:LYS:HE3	22:T:13:ARG:NH1	1.89	0.88
1:O:2812:A:H2	1:O:2814:A:H62	1.22	0.88
11:H:46:GLN:HE21	11:H:137:TYR:HE2	1.15	0.88
13:K:74:VAL:HG11	13:K:113:ILE:HG12	1.53	0.87

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:V:1:THR:HG23	24:V:2:VAL:H	1.36	0.87
20:R:8:ALA:HB1	20:R:13:THR:HG21	1.56	0.87
6:C:1:MET:HG2	6:C:2:GLN:H	1.38	0.87
1:0:506:G:H22	1:0:509:A:H5'	1.40	0.87
1:0:56:G:H5''	24:V:50:ARG:NH1	1.90	0.87
20:R:106:GLY:HA2	20:R:109:MET:HE3	1.58	0.86
14:L:121:ILE:HG12	14:L:141:GLU:HB2	1.56	0.85
18:P:115:SER:N	18:P:118:GLN:HE21	1.74	0.85
1:0:282:C:H1'	1:0:368:C:N4	1.91	0.85
5:B:179:LEU:O	5:B:183:GLU:HG2	1.75	0.85
16:N:144:GLY:O	16:N:147:ILE:HG22	1.76	0.85
20:R:17:MET:HE1	20:R:19:ARG:NH2	1.92	0.84
1:0:2533:C:H5'	1:0:2533:C:H6	1.42	0.84
1:0:1162:G:H1'	32:I:117:LEU:HD11	1.59	0.84
25:W:88:THR:HG22	25:W:89:ASP:H	1.41	0.84
6:C:236:THR:HG22	6:C:239:ALA:N	1.90	0.84
1:0:1667:A:H8	1:0:1667:A:H5'	1.42	0.84
5:B:18:ARG:HG3	5:B:256:GLN:HG3	1.59	0.83
13:K:62:PRO:HG3	13:K:65:ARG:HH21	1.42	0.83
12:J:74:ARG:HB3	12:J:74:ARG:HH11	1.44	0.83
1:0:21:G:H5'	20:R:2:ILE:HA	1.61	0.83
1:0:1160:G:C5'	1:0:1161:A:H5'	2.08	0.83
32:I:99:ASP:OD1	32:I:138:THR:HB	1.77	0.83
1:0:545:G:H5'	1:0:545:G:H8	1.44	0.83
5:B:264:GLU:HG2	5:B:267:LYS:HE2	1.61	0.82
25:W:6:GLN:HB2	25:W:26:ILE:HD12	1.59	0.82
30:2:41:HIS:H	30:2:45:ASN:HD22	1.23	0.82
6:C:78:ARG:HH11	6:C:78:ARG:HG3	1.44	0.82
1:0:2506:A:O2'	1:0:2507:G:H8	1.61	0.82
1:0:2890:A:H1'	23:U:56:ARG:NH2	1.94	0.82
25:W:4:LEU:HD23	25:W:54:PHE:HB3	1.60	0.82
15:M:99:ARG:HD2	15:M:167:GLY:HA2	1.62	0.82
31:3:60:LYS:HG3	31:3:61:PRO:HD2	1.62	0.82
5:B:190:MET:HE2	5:B:194:PHE:CD1	2.15	0.81
18:P:115:SER:H	18:P:118:GLN:NE2	1.76	0.81
25:W:88:THR:HB	38:W:6679:HOH:O	1.80	0.81
11:H:56:GLN:NE2	11:H:126:ARG:HE	1.79	0.81
13:K:10:GLN:HE21	13:K:10:GLN:N	1.79	0.81
24:V:57:LYS:HA	24:V:60:GLN:HE21	1.46	0.81
1:0:1372:A:H3'	38:0:7376:HOH:O	1.81	0.80
11:H:29:ALA:HB3	11:H:66:ARG:HH12	1.44	0.80

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:E:69:ILE:HA	8:E:72:MET:HE3	1.63	0.80
15:M:102:GLU:OE1	15:M:164:THR:HG21	1.81	0.80
4:A:36:ASP:OD2	4:A:85:SER:HB2	1.79	0.80
2:9:3006:C:C5'	16:N:37:ARG:NH1	2.45	0.80
1:0:1593:C:H5'	18:P:116:SER:O	1.81	0.80
25:W:88:THR:HG23	25:W:110:GLN:HE21	1.46	0.79
1:0:559:U:H6	1:0:559:U:H5'	1.47	0.79
26:X:30:MET:HE1	26:X:58:ALA:HB3	1.63	0.79
1:0:870:G:C2'	1:0:871:G:H5''	2.11	0.79
1:0:2270:G:H4'	4:A:223:ARG:HH12	1.48	0.79
4:A:88:ILE:HD13	4:A:100:PRO:HD3	1.63	0.79
9:F:46:GLU:O	9:F:73:PRO:HD2	1.83	0.79
13:K:32:ILE:HD11	13:K:56:SER:HB3	1.64	0.79
1:0:1116:U:O2'	1:0:1118:A:H2	1.66	0.79
25:W:72:PRO:HG2	25:W:77:ALA:HB3	1.64	0.79
9:F:38:LYS:HZ1	15:M:3:SER:HA	1.48	0.78
29:1:8:GLN:HE22	29:1:11:LYS:NZ	1.81	0.78
1:0:506:G:H22	1:0:509:A:C5'	1.95	0.78
1:0:542:A:H5'	1:0:542:A:H8	1.48	0.78
16:N:176:ARG:HE	16:N:180:LEU:HD21	1.48	0.78
13:K:14:LYS:HB2	13:K:45:PRO:HG2	1.65	0.78
16:N:48:VAL:CG1	16:N:55:ASP:HB3	2.13	0.78
12:J:93:ARG:HB3	12:J:93:ARG:HH11	1.49	0.78
4:A:100:PRO:HG2	4:A:103:VAL:HG21	1.66	0.78
12:J:19:MET:HE3	12:J:132:LEU:HD11	1.66	0.78
7:D:99:ASP:HB3	7:D:103:ASN:H	1.47	0.78
16:N:164:ASP:CG	16:N:167:ASP:HA	2.09	0.78
1:0:21:G:C5'	20:R:2:ILE:HA	2.14	0.77
1:0:1116:U:H3	1:0:1246:A:H62	1.32	0.77
1:0:1180:U:H4'	32:I:91:GLU:HG2	1.64	0.77
1:0:1450:C:H4'	1:0:1451:C:OP2	1.82	0.77
8:E:6:GLU:HA	8:E:46:THR:HG22	1.67	0.77
5:B:238:ASN:HD22	5:B:240:GLY:N	1.83	0.77
1:0:541:C:H2'	1:0:542:A:H5''	1.65	0.77
13:K:74:VAL:HG13	13:K:113:ILE:HG23	1.66	0.77
22:T:48:VAL:HG11	22:T:96:VAL:HG13	1.66	0.77
13:K:29:LEU:HB3	13:K:55:VAL:HG11	1.66	0.76
1:0:541:C:C2'	1:0:542:A:H5''	2.16	0.76
28:Z:26:VAL:O	28:Z:30:GLU:HG3	1.85	0.76
32:I:132:CYS:HB3	32:I:137:VAL:HB	1.67	0.76
6:C:182:ARG:HB2	6:C:184:ARG:NH1	1.99	0.76

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:W:68:THR:HG23	25:W:69:ARG:HG2	1.68	0.76
28:Z:46:ARG:HD2	28:Z:59:TYR:HB2	1.66	0.76
1:0:2908:A:H2'	1:0:2909:G:O4'	1.86	0.76
2:9:3014:G:H5'	2:9:3014:G:H8	1.50	0.76
1:0:188:C:H5''	15:M:163:LEU:HD21	1.68	0.76
1:0:1603:A:H5'	1:0:1605:G:O4'	1.86	0.76
29:1:21:ARG:HD2	29:1:39:PHE:HB2	1.68	0.76
2:9:3039:U:H1'	2:9:3044:A:H61	1.50	0.76
23:U:20:MET:HE2	23:U:30:HIS:NE2	2.01	0.76
1:0:871:G:H8	1:0:871:G:C5'	1.99	0.76
1:0:1118:A:C8	1:0:1118:A:H3'	2.21	0.76
1:0:1120:U:H6	1:0:1120:U:H5'	1.51	0.75
1:0:2291:A:C8	1:0:2309:C:H5'	2.21	0.75
1:0:2716:G:H5''	5:B:206:THR:HG21	1.66	0.75
1:0:1474:C:H5'	1:0:1474:C:C6	2.21	0.75
16:N:113:SER:HB2	38:N:9357:HOH:O	1.86	0.75
9:F:63:ILE:HB	9:F:64:PRO:HD3	1.69	0.75
4:A:153:ARG:HB2	4:A:153:ARG:HH11	1.52	0.75
16:N:83:LEU:HD13	16:N:175:LEU:HD23	1.66	0.75
1:0:236:A:H4'	1:0:237:G:H5'	1.69	0.74
8:E:3:VAL:HG22	8:E:49:ILE:HB	1.69	0.74
25:W:6:GLN:HB2	25:W:26:ILE:CD1	2.16	0.74
32:I:75:THR:HA	32:I:112:LYS:HZ1	1.51	0.74
1:0:1118:A:H3'	1:0:1118:A:H8	1.51	0.74
8:E:31:ARG:HH12	8:E:68:HIS:CG	2.04	0.74
1:0:111:C:O2'	29:1:20:ARG:HG2	1.87	0.74
13:K:74:VAL:CG1	13:K:113:ILE:HG12	2.17	0.74
1:0:1181:A:H5'	32:I:94:GLU:OE2	1.88	0.74
1:0:1684:A:H1'	30:2:43:ARG:HH22	1.52	0.74
5:B:320:GLN:HE21	5:B:321:PRO:HD2	1.53	0.74
32:I:102:VAL:HG12	32:I:106:LYS:HE3	1.69	0.74
5:B:320:GLN:NE2	5:B:321:PRO:HD2	2.03	0.74
6:C:236:THR:H	6:C:239:ALA:HB3	1.53	0.73
1:0:1189:A:H1'	1:0:1209:C:O4'	1.89	0.73
2:9:3056:A:C2'	2:9:3057:A:H5''	2.18	0.73
25:W:21:LEU:HD22	25:W:26:ILE:CD1	2.18	0.73
1:0:1160:G:H5'	1:0:1161:A:C5'	2.15	0.73
31:3:17:HIS:O	31:3:18:GLN:HG3	1.88	0.73
25:W:88:THR:HG23	25:W:110:GLN:NE2	2.03	0.73
1:0:657:G:OP1	6:C:27:ARG:NH2	2.21	0.73
1:0:1328:A:OP1	27:Y:169:ARG:HD2	1.89	0.73

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:98:THR:HG22	5:B:99:GLU:H	1.53	0.73
5:B:238:ASN:ND2	5:B:240:GLY:H	1.86	0.73
1:0:2548:C:OP2	5:B:5:ARG:NH2	2.22	0.73
1:0:1234:U:N3	5:B:244:PRO:HB3	2.03	0.72
6:C:27:ARG:HG3	6:C:29:ASP:OD1	1.88	0.72
13:K:62:PRO:HG3	13:K:65:ARG:NH2	2.04	0.72
22:T:9:LYS:HE3	22:T:13:ARG:HH11	1.54	0.72
1:0:396:U:H1'	38:0:7793:HOH:O	1.90	0.72
1:0:289:G:H22	1:0:363:A:H2	1.38	0.72
20:R:17:MET:HE1	20:R:19:ARG:CZ	2.17	0.72
10:G:16:LYS:O	10:G:20:VAL:HG23	1.90	0.72
1:0:272:A:H5'	1:0:273:G:OP2	1.90	0.72
1:0:877:G:H5'	1:0:878:G:OP1	1.89	0.72
1:0:1206:U:H5'	1:0:1206:U:H6	1.55	0.72
16:N:132:ASN:O	16:N:135:VAL:HG12	1.89	0.72
25:W:137:GLN:HE21	25:W:141:HIS:HE1	1.36	0.72
31:3:25:VAL:HG22	31:3:68:LYS:HG3	1.72	0.72
1:0:2524:G:H21	1:0:2526:C:N4	1.88	0.72
4:A:36:ASP:HB2	4:A:83:GLY:HA3	1.72	0.72
11:H:99:LYS:HD3	11:H:119:LYS:HD3	1.71	0.72
21:S:57:THR:HG22	21:S:59:ASP:N	2.04	0.72
9:F:38:LYS:NZ	15:M:3:SER:HA	2.04	0.72
13:K:98:VAL:CG1	13:K:102:GLU:HA	2.20	0.72
5:B:125:GLU:O	5:B:129:ARG:HG3	1.90	0.71
15:M:164:THR:CG2	15:M:167:GLY:H	2.02	0.71
26:X:78:GLU:HG2	26:X:79:GLU:H	1.55	0.71
1:0:541:C:H2'	1:0:542:A:C5'	2.19	0.71
1:0:2426:G:H1'	38:0:6331:HOH:O	1.89	0.71
8:E:100:ASP:HB2	38:E:2789:HOH:O	1.89	0.71
9:F:2:VAL:HG22	9:F:57:GLU:OE1	1.91	0.71
26:X:37:LEU:CD1	26:X:85:VAL:HG21	2.18	0.71
1:0:1167:G:H4'	32:I:135:LEU:HD22	1.72	0.71
1:0:2769:C:H2'	1:0:2770:G:O4'	1.90	0.71
1:0:1165:G:H4'	1:0:1174:A:O2'	1.89	0.71
16:N:7:LYS:HE3	19:Q:21:ARG:O	1.90	0.71
1:0:1119:G:N2	1:0:1246:A:C2	2.58	0.71
4:A:43:VAL:HG21	4:A:59:GLU:HG3	1.71	0.71
8:E:84:MET:HE2	8:E:133:VAL:CG2	2.21	0.71
1:0:2524:G:H21	1:0:2526:C:H41	1.37	0.71
1:0:962:C:H1'	16:N:5:ARG:NH1	2.06	0.71
14:L:133:VAL:HA	38:L:9372:HOH:O	1.91	0.71

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:R:14:ALA:HB3	20:R:147:LEU:HB2	1.70	0.71
17:O:73:ASP:HA	17:O:92:VAL:O	1.91	0.71
20:R:39:THR:HG23	20:R:107:GLU:O	1.90	0.71
11:H:169:GLY:HA3	38:H:9187:HOH:O	1.91	0.70
1:O:1058:A:H2'	1:O:1060:C:H5''	1.71	0.70
1:O:2533:C:H5'	1:O:2533:C:C6	2.25	0.70
6:C:139:VAL:HG13	38:C:9249:HOH:O	1.89	0.70
7:D:136:ARG:HD2	7:D:155:HIS:O	1.91	0.70
29:1:8:GLN:HE22	29:1:11:LYS:HZ2	1.38	0.70
1:O:1751:G:C2'	1:O:1752:G:H5''	2.20	0.70
7:D:28:GLY:HA2	7:D:69:ILE:HG23	1.71	0.70
27:Y:187:VAL:HG23	27:Y:192:ASP:HB2	1.72	0.70
25:W:21:LEU:HD22	25:W:26:ILE:HD13	1.74	0.70
27:Y:187:VAL:HG23	27:Y:192:ASP:CB	2.22	0.70
11:H:9:ILE:HG23	11:H:126:ARG:CZ	2.21	0.70
26:X:72:VAL:HG22	26:X:85:VAL:HG12	1.72	0.70
24:V:56:ILE:O	24:V:60:GLN:HG3	1.90	0.70
15:M:164:THR:HG22	15:M:167:GLY:N	2.07	0.70
1:O:2587:OMU:H2'	1:O:2589:U:H5''	1.74	0.70
7:D:146:LYS:NZ	16:N:107:ASN:HD21	1.90	0.70
1:O:1119:G:H2'	12:J:52:GLN:NE2	2.06	0.70
30:2:39:ARG:HG2	38:2:3143:HOH:O	1.92	0.70
1:O:2586:U:H3	1:O:2592:G:H22	1.38	0.69
1:O:553:G:P	27:Y:204:ARG:HH22	2.16	0.69
4:A:94:LEU:HG	4:A:99:ILE:HD11	1.73	0.69
1:O:1118:A:H62	1:O:1244:U:H3	1.39	0.69
1:O:1201:C:H2'	1:O:1202:A:H5'	1.74	0.69
13:K:81:ARG:HB2	13:K:87:ARG:NH1	2.07	0.69
18:P:103:THR:HA	18:P:106:ARG:NH1	2.06	0.69
1:O:544:G:H2'	1:O:545:G:H5''	1.73	0.69
11:H:166:SER:HB2	11:H:167:PRO:CD	2.22	0.69
27:Y:189:ASN:HA	27:Y:217:ILE:HD11	1.74	0.69
12:J:19:MET:HE1	12:J:78:ILE:HG22	1.74	0.69
23:U:52:THR:CG2	23:U:54:THR:HB	2.23	0.69
9:F:53:ASP:OD1	9:F:80:GLN:HB2	1.93	0.69
13:K:14:LYS:CB	13:K:45:PRO:HG2	2.23	0.69
18:P:59:ARG:NH2	18:P:66:GLN:HE22	1.91	0.69
24:V:12:THR:HG22	24:V:15:GLU:CG	2.23	0.69
1:O:1205:U:H2'	1:O:1206:U:C5'	2.23	0.68
27:Y:144:ARG:CZ	38:Y:8197:HOH:O	2.40	0.68
1:O:1351:G:OP1	6:C:96:LYS:NZ	2.25	0.68

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:C:115:LEU:HD21	6:C:243:VAL:HG13	1.75	0.68
24:V:44:GLY:O	24:V:48:GLU:HG2	1.94	0.68
1:O:797:A:H4'	28:Z:10:ARG:N	2.08	0.68
12:J:76:ASP:HA	38:J:9361:HOH:O	1.92	0.68
17:O:32:ARG:HE	17:O:35:LYS:HD2	1.57	0.68
1:O:1205:U:H2'	1:O:1206:U:H5''	1.75	0.68
1:O:2768:A:H2'	1:O:2769:C:O4'	1.93	0.68
1:O:2768:A:H5''	38:O:4707:HOH:O	1.94	0.68
6:C:78:ARG:HG3	6:C:78:ARG:NH1	2.09	0.68
12:J:131:THR:HG22	12:J:134:GLU:H	1.57	0.68
16:N:154:LEU:HD11	16:N:157:PRO:HA	1.75	0.68
11:H:58:ARG:HH11	11:H:58:ARG:HG3	1.57	0.68
12:J:90:LYS:HB2	36:J:9302:CL:CL	2.31	0.68
24:V:39:ALA:N	24:V:40:PRO:HD2	2.09	0.68
26:X:76:ARG:HG3	26:X:76:ARG:NH1	2.06	0.68
32:I:93:GLN:HA	32:I:96:PHE:HE2	1.58	0.68
32:I:138:THR:HG22	32:I:139:ILE:H	1.58	0.68
2:9:3039:U:H1'	2:9:3044:A:N6	2.08	0.68
14:L:37:LYS:HG2	38:L:9334:HOH:O	1.92	0.68
17:O:32:ARG:O	17:O:32:ARG:HD3	1.94	0.68
2:9:3064:C:H2'	2:9:3065:A:H5'	1.76	0.68
5:B:201:ASP:HB2	5:B:312:ARG:HD2	1.76	0.68
7:D:37:ALA:O	7:D:40:ILE:HG12	1.94	0.68
25:W:13:MET:HE2	25:W:18:GLN:HA	1.75	0.68
1:O:656:G:OP2	17:O:37:ARG:HD2	1.94	0.68
30:2:41:HIS:HD2	30:2:44:ARG:H	1.41	0.68
1:O:2468:A:H61	31:3:48:ASN:HD21	1.41	0.67
5:B:202:VAL:HG11	5:B:301:VAL:HG13	1.77	0.67
9:F:58:GLU:HA	9:F:61:MET:HG3	1.75	0.67
22:T:38:ARG:HG3	22:T:38:ARG:HH11	1.57	0.67
30:2:36:ASN:O	30:2:39:ARG:HG3	1.93	0.67
5:B:41:PHE:CD1	5:B:79:MET:HE2	2.29	0.67
7:D:50:VAL:O	7:D:71:ALA:HA	1.95	0.67
25:W:4:LEU:HD22	25:W:52:VAL:HG21	1.76	0.67
4:A:65:ARG:C	4:A:66:ARG:HG3	2.19	0.67
1:O:157:G:H4'	15:M:95:LYS:HE2	1.77	0.67
1:O:2252:A:C5	1:O:2253:G:H1'	2.30	0.67
5:B:304:PRO:HD2	5:B:307:ARG:HD2	1.76	0.67
21:S:33:SER:O	21:S:37:VAL:HG23	1.93	0.67
22:T:52:ARG:HB2	22:T:95:ASN:HB3	1.76	0.67
24:V:64:GLY:O	24:V:65:ASP:HB2	1.94	0.67

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:W:81:ASP:OD1	25:W:92:ASP:HB2	1.95	0.67
1:O:1119:G:H2'	12:J:52:GLN:HE22	1.58	0.67
1:O:871:G:C8	1:O:871:G:C5'	2.76	0.67
1:O:1666:C:O2'	1:O:1667:A:H5''	1.95	0.67
1:O:1819:G:H5'	38:O:4985:HOH:O	1.93	0.67
4:A:192:VAL:HG12	4:A:207:GLN:HB3	1.75	0.67
1:O:2054:A:N3	20:R:128:ARG:NH2	2.42	0.67
1:O:1080:C:H4'	1:O:1081:A:OP1	1.94	0.67
1:O:1701:A:H5'	38:O:6518:HOH:O	1.93	0.67
9:F:46:GLU:OE1	9:F:100:ASP:HA	1.95	0.67
6:C:16:VAL:HG12	6:C:17:ASP:H	1.59	0.66
6:C:236:THR:CG2	6:C:239:ALA:H	1.99	0.66
6:C:7:ASP:OD2	6:C:9:ASP:HB2	1.95	0.66
10:G:20:VAL:O	10:G:24:VAL:HG23	1.96	0.66
1:O:1244:U:OP1	12:J:18:ILE:HD13	1.95	0.66
15:M:59:GLY:HA3	15:M:141:ILE:HD11	1.77	0.66
29:1:25:LYS:HD2	30:2:49:GLU:H	1.59	0.66
32:I:129:VAL:HG13	32:I:139:ILE:HD11	1.75	0.66
38:O:5785:HOH:O	15:M:58:GLN:HG3	1.95	0.66
5:B:5:ARG:HD2	5:B:8:LYS:NZ	2.10	0.66
5:B:62:ARG:HA	5:B:65:MET:HE3	1.77	0.66
13:K:81:ARG:HB2	13:K:87:ARG:HH11	1.59	0.66
22:T:101:LEU:HD13	22:T:112:LEU:HD11	1.77	0.66
25:W:88:THR:HG22	25:W:89:ASP:N	2.10	0.66
1:O:1641:A:H2'	1:O:1642:A:H5'	1.76	0.66
1:O:2649:A:H5'	1:O:2649:A:H8	1.60	0.66
1:O:1666:C:H2'	1:O:1667:A:H5'	1.77	0.66
4:A:191:GLY:HA2	4:A:194:MET:HE2	1.78	0.66
5:B:190:MET:HE2	5:B:194:PHE:HD1	1.60	0.66
25:W:4:LEU:CD2	25:W:54:PHE:HB3	2.26	0.66
25:W:88:THR:HG23	25:W:110:GLN:HB3	1.78	0.66
20:R:6:VAL:HG21	20:R:113:HIS:CD2	2.31	0.66
25:W:65:VAL:HA	25:W:68:THR:HG22	1.78	0.66
1:O:2851:G:O2'	1:O:2852:A:H5'	1.96	0.66
38:O:7598:HOH:O	22:T:9:LYS:HB2	1.93	0.66
9:F:52:GLU:HG3	9:F:77:VAL:O	1.96	0.66
15:M:60:VAL:C	15:M:61:ILE:HD12	2.20	0.66
32:I:110:GLU:HA	32:I:113:HIS:CD2	2.31	0.65
7:D:135:VAL:HG21	7:D:139:TYR:CD1	2.31	0.65
1:O:470:U:O2'	29:1:16:HIS:HD2	1.80	0.65
1:O:1130:U:H2'	1:O:1131:G:O4'	1.97	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:9:3029:C:O3'	7:D:138:GLY:HA2	1.97	0.65
7:D:54:ALA:HB2	7:D:69:ILE:HD12	1.78	0.65
7:D:88:LEU:HB2	7:D:89:PRO:HD3	1.78	0.65
32:I:125:ALA:O	32:I:129:VAL:HG23	1.96	0.65
1:0:1189:A:H1'	1:0:1209:C:C1'	2.27	0.65
27:Y:189:ASN:C	27:Y:189:ASN:HD22	2.03	0.65
1:0:558:C:O2'	1:0:559:U:H5''	1.96	0.65
1:0:870:G:OP2	4:A:3:ARG:HD3	1.97	0.65
2:9:3029:C:H2'	2:9:3030:C:H5'	1.78	0.65
27:Y:235:GLU:CD	27:Y:235:GLU:H	2.03	0.65
1:0:560:C:H42	1:0:597:A:H61	1.43	0.65
10:G:27:ILE:HD13	10:G:71:LEU:HD23	1.78	0.65
11:H:166:SER:CB	11:H:167:PRO:HD3	2.26	0.65
5:B:162:MET:CE	5:B:308:LEU:HD21	2.27	0.65
1:0:820:G:C6	4:A:171:LYS:HB2	2.32	0.65
16:N:152:GLU:C	16:N:154:LEU:H	2.03	0.65
1:0:1681:G:H5''	1:0:1682:A:H5'	1.78	0.65
14:L:67:ARG:O	14:L:71:GLU:HG3	1.96	0.65
22:T:71:VAL:HG11	22:T:90:PRO:CB	2.26	0.65
23:U:39:ASN:ND2	23:U:44:ARG:HH11	1.95	0.65
27:Y:186:ARG:HG2	27:Y:186:ARG:HH11	1.62	0.65
32:I:118:SER:HB2	32:I:123:ASN:HB2	1.78	0.65
12:J:52:GLN:HG3	12:J:53:ILE:N	2.11	0.64
12:J:74:ARG:NH1	12:J:76:ASP:HB2	2.12	0.64
1:0:777:U:O2'	29:1:11:LYS:HG2	1.97	0.64
27:Y:99:ALA:HB2	27:Y:233:TYR:CZ	2.32	0.64
1:0:1701:A:H4'	1:0:1702:U:H5''	1.78	0.64
8:E:84:MET:HE1	8:E:148:ILE:CD1	2.27	0.64
10:G:64:ASN:HD22	10:G:64:ASN:N	1.95	0.64
13:K:98:VAL:HG11	13:K:102:GLU:HA	1.78	0.64
19:Q:18:PRO:O	19:Q:21:ARG:HB2	1.97	0.64
22:T:48:VAL:HG11	22:T:96:VAL:CG1	2.27	0.64
1:0:2827:A:H2'	1:0:2828:G:O4'	1.98	0.64
16:N:119:GLN:O	16:N:123:ILE:HG13	1.97	0.64
20:R:18:LEU:HB2	20:R:143:VAL:HG12	1.79	0.64
1:0:545:G:H5'	1:0:545:G:C8	2.31	0.64
4:A:81:GLN:HB2	4:A:92:ASN:ND2	2.12	0.64
12:J:75:PRO:HG2	12:J:105:LEU:HD21	1.79	0.64
20:R:111:ILE:HG23	20:R:145:LEU:HD11	1.78	0.64
1:0:538:C:OP2	27:Y:134:HIS:HE1	1.81	0.64
20:R:18:LEU:HD12	20:R:143:VAL:HG11	1.80	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:C:5:ILE:HD11	6:C:16:VAL:HG23	1.78	0.64
21:S:52:VAL:C	21:S:53:ASN:HD22	2.06	0.64
25:W:21:LEU:HD21	25:W:48:VAL:HG11	1.78	0.64
1:0:380:A:H2'	38:0:7412:HOH:O	1.97	0.64
1:0:2690:U:O2'	8:E:111:LYS:HE3	1.98	0.64
2:9:3014:G:H5'	2:9:3014:G:C8	2.32	0.64
12:J:93:ARG:HB3	12:J:93:ARG:NH1	2.12	0.64
1:0:558:C:H2'	1:0:559:U:H5'	1.79	0.64
1:0:1667:A:H5'	1:0:1667:A:C8	2.31	0.64
1:0:2491:G:H1'	38:0:7076:HOH:O	1.98	0.64
5:B:62:ARG:HG2	5:B:65:MET:HE3	1.79	0.64
1:0:1060:C:H6	1:0:1060:C:H5'	1.63	0.63
1:0:1819:G:H2'	1:0:1820:G:H4'	1.79	0.63
7:D:57:THR:HG23	7:D:63:ILE:HA	1.79	0.63
7:D:105:SER:HB2	7:D:131:THR:HG23	1.80	0.63
8:E:69:ILE:HA	8:E:72:MET:CE	2.28	0.63
11:H:27:LYS:H	11:H:59:HIS:HD2	1.46	0.63
1:0:281:U:H2'	1:0:282:C:O4'	1.98	0.63
1:0:2896:A:H5''	38:0:6338:HOH:O	1.98	0.63
16:N:169:PRO:O	16:N:172:PHE:HB3	1.99	0.63
18:P:134:VAL:O	18:P:137:LEU:HB3	1.98	0.63
1:0:285:A:H2'	1:0:286:U:O4'	1.98	0.63
1:0:2570:G:H5''	38:0:5188:HOH:O	1.99	0.63
14:L:143:THR:HG22	14:L:144:ASP:N	2.14	0.63
1:0:447:A:OP1	22:T:2:LYS:HG2	1.98	0.63
7:D:99:ASP:HA	38:D:5675:HOH:O	1.97	0.63
8:E:145:ALA:HB1	8:E:168:ILE:HD11	1.81	0.63
18:P:91:LYS:O	18:P:95:GLU:HG3	1.99	0.63
38:0:7629:HOH:O	6:C:188:ARG:HD2	1.96	0.63
25:W:125:HIS:HD2	25:W:127:GLY:H	1.46	0.63
7:D:54:ALA:CB	7:D:69:ILE:HD12	2.28	0.63
1:0:2414:A:H2'	1:0:2415:A:C8	2.34	0.63
4:A:129:LEU:CD1	4:A:145:MET:HE1	2.29	0.63
7:D:57:THR:HG23	7:D:63:ILE:HG22	1.80	0.63
1:0:1377:C:H5'	1:0:1377:C:H6	1.64	0.63
1:0:1741:U:H5'	1:0:1742:A:OP1	1.98	0.63
38:0:4132:HOH:O	11:H:11:LYS:HE2	1.99	0.63
4:A:194:MET:HE3	4:A:199:HIS:CB	2.24	0.63
16:N:170:GLU:HA	16:N:173:ASP:OD2	1.98	0.63
32:I:75:THR:HA	32:I:112:LYS:NZ	2.14	0.63
1:0:1184:C:H1'	38:0:7636:HOH:O	1.99	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:S:11:THR:H	21:S:14:ALA:HB3	1.64	0.63
1:0:1130:U:H5'	38:0:7834:HOH:O	1.98	0.62
1:0:1299:G:O6	14:L:6:ARG:HD3	1.98	0.62
12:J:19:MET:HE2	12:J:79:PHE:HA	1.81	0.62
16:N:43:VAL:HG13	16:N:118:ILE:HD11	1.81	0.62
1:0:1159:G:H21	1:0:1189:A:H8	1.45	0.62
1:0:1834:C:H2'	1:0:1840:A:N6	2.14	0.62
16:N:47:LEU:HD11	16:N:127:LEU:HD21	1.81	0.62
1:0:564:G:H1'	38:0:6543:HOH:O	1.99	0.62
1:0:2756:U:H3	1:0:2896:A:H2	1.47	0.62
15:M:134:ILE:HG23	15:M:141:ILE:HD13	1.81	0.62
26:X:41:PHE:O	26:X:43:VAL:HG23	1.98	0.62
1:0:2320:U:H4'	1:0:2321:A:O4'	1.98	0.62
2:9:3114:G:O6	16:N:11:ARG:HD3	1.98	0.62
22:T:9:LYS:CE	22:T:13:ARG:NH1	2.61	0.62
1:0:1187:U:O2'	1:0:1189:A:H2	1.80	0.62
6:C:145:GLU:HG3	38:C:9175:HOH:O	1.99	0.62
7:D:41:LEU:HA	7:D:44:ILE:HG22	1.82	0.62
14:L:149:ARG:O	14:L:150:GLN:HB2	1.98	0.62
25:W:13:MET:HE2	25:W:18:GLN:CA	2.29	0.62
1:0:797:A:C4'	28:Z:10:ARG:N	2.62	0.62
4:A:200:PRO:HG2	4:A:225:VAL:HG21	1.82	0.62
1:0:2251:G:H2'	1:0:2252:A:C8	2.34	0.62
38:0:7228:HOH:O	4:A:211:LYS:HG2	2.00	0.62
7:D:58:VAL:CG1	7:D:60:GLU:HG2	2.28	0.62
1:0:1165:G:H4'	1:0:1174:A:HO2'	1.64	0.62
1:0:2004:U:H4'	38:0:5568:HOH:O	1.99	0.62
7:D:95:THR:OG1	7:D:174:VAL:HG22	1.99	0.62
16:N:154:LEU:O	16:N:155:GLU:HB3	2.00	0.62
22:T:32:ARG:NH1	22:T:38:ARG:HH12	1.97	0.62
2:9:3002:U:OP2	2:9:3003:A:H5'	1.99	0.62
20:R:9:ASP:O	20:R:13:THR:HB	1.99	0.62
22:T:48:VAL:CG1	22:T:96:VAL:HG13	2.30	0.62
5:B:254:GLN:HG2	5:B:255:GLY:N	2.15	0.62
13:K:118:ALA:HA	13:K:125:ALA:HB2	1.82	0.62
16:N:110:THR:HB	16:N:113:SER:OG	2.00	0.62
32:I:134:SER:O	32:I:135:LEU:HD23	2.00	0.62
1:0:544:G:C2'	1:0:545:G:H5''	2.30	0.61
6:C:127:ARG:HH21	6:C:225:PRO:HG2	1.61	0.61
16:N:23:ARG:HD3	38:N:9346:HOH:O	1.99	0.61
1:0:926:A:O2'	14:L:41:HIS:HD2	1.81	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:E:31:ARG:NH1	8:E:68:HIS:CG	2.68	0.61
9:F:21:GLU:O	9:F:24:ARG:HG3	2.00	0.61
14:L:143:THR:HG21	38:L:9336:HOH:O	1.99	0.61
15:M:24:GLN:NE2	15:M:27:ARG:HH11	1.98	0.61
1:O:1086:A:C6	25:W:11:VAL:HG11	2.35	0.61
1:O:2840:A:OP1	5:B:211:THR:HG23	2.00	0.61
26:X:25:ARG:HD2	38:X:3861:HOH:O	1.99	0.61
31:3:62:THR:HB	38:3:9349:HOH:O	2.00	0.61
1:O:399:C:H5'	15:M:179:GLY:O	2.01	0.61
5:B:5:ARG:NH1	5:B:8:LYS:HE2	2.16	0.61
8:E:11:VAL:HG12	8:E:12:ASP:N	2.16	0.61
1:O:1625:U:H4'	38:O:4940:HOH:O	2.00	0.61
1:O:2256:G:C2'	1:O:2257:G:H5'	2.31	0.61
38:O:7081:HOH:O	15:M:178:LYS:HB2	2.00	0.61
2:9:3055:U:H4'	2:9:3056:A:C8	2.36	0.61
16:N:48:VAL:HG11	16:N:55:ASP:HB3	1.82	0.61
22:T:48:VAL:HG13	22:T:97:ARG:O	2.00	0.61
1:O:902:G:N7	14:L:18:HIS:HD2	1.98	0.61
5:B:297:VAL:HB	38:B:9406:HOH:O	2.00	0.61
13:K:74:VAL:HG12	13:K:75:ARG:HG3	1.83	0.61
16:N:143:ARG:HA	16:N:172:PHE:CD2	2.36	0.61
22:T:71:VAL:CG1	22:T:90:PRO:HB3	2.24	0.61
25:W:125:HIS:CD2	25:W:127:GLY:H	2.19	0.61
32:I:131:THR:O	32:I:135:LEU:HG	2.01	0.61
8:E:137:ASP:O	8:E:141:VAL:HG23	2.01	0.61
1:O:1166:A:H1'	1:O:1192:A:C2	2.36	0.61
4:A:129:LEU:HD12	4:A:145:MET:HE1	1.83	0.61
7:D:146:LYS:HZ3	16:N:107:ASN:HD21	1.47	0.61
12:J:6:PHE:HB3	12:J:109:TYR:OH	2.01	0.61
1:O:848:C:H5'	38:O:7455:HOH:O	1.99	0.60
1:O:2346:C:H6	1:O:2346:C:O5'	1.84	0.60
38:O:7626:HOH:O	5:B:211:THR:HG21	2.01	0.60
4:A:66:ARG:HH11	4:A:66:ARG:HB2	1.66	0.60
5:B:140:LEU:HD23	38:B:9378:HOH:O	1.99	0.60
6:C:16:VAL:HG12	6:C:17:ASP:N	2.16	0.60
15:M:64:ARG:HD2	38:M:9378:HOH:O	2.00	0.60
1:O:1189:A:O2'	1:O:1208:C:H2'	2.00	0.60
6:C:104:ASP:HA	6:C:107:ARG:HH12	1.65	0.60
22:T:38:ARG:HG3	22:T:38:ARG:NH1	2.17	0.60
25:W:38:THR:HG22	25:W:39:ASP:H	1.67	0.60
1:O:1266:U:H4'	27:Y:115:ARG:HH21	1.65	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:F:50:VAL:HG21	9:F:63:ILE:HG21	1.83	0.60
11:H:166:SER:CB	11:H:167:PRO:CD	2.78	0.60
12:J:99:GLU:HA	38:J:9371:HOH:O	2.01	0.60
1:O:282:C:O2'	1:O:283:U:H5'	2.01	0.60
1:O:2256:G:H2'	1:O:2257:G:H5'	1.83	0.60
11:H:23:ILE:HA	11:H:120:ILE:HG21	1.82	0.60
1:O:449:A:N7	6:C:43:LYS:HG2	2.16	0.60
1:O:2502:C:C2'	1:O:2503:A:H5'	2.32	0.60
11:H:63:GLU:HA	38:H:9177:HOH:O	2.00	0.60
5:B:162:MET:HE1	5:B:308:LEU:HD21	1.83	0.60
16:N:11:ARG:HG3	16:N:14:ARG:NH1	2.16	0.60
1:O:793:A:H5''	18:P:83:LYS:HG2	1.83	0.60
1:O:2504:A:H4'	11:H:71:ARG:HH11	1.67	0.60
7:D:13:MET:HA	7:D:137:PRO:HG2	1.83	0.60
4:A:210:GLY:HA3	38:A:9380:HOH:O	2.02	0.60
6:C:33:LYS:HE2	38:C:9160:HOH:O	2.01	0.60
11:H:45:VAL:HA	11:H:167:PRO:O	2.01	0.60
25:W:4:LEU:HD22	25:W:52:VAL:CG2	2.32	0.60
25:W:5:VAL:HG22	25:W:32:CYS:HB2	1.83	0.60
4:A:105:VAL:HG11	4:A:154:ALA:HB1	1.83	0.60
28:Z:57:CYS:SG	28:Z:59:TYR:HB3	2.42	0.60
1:O:338:C:H4'	6:C:174:ILE:CD1	2.32	0.60
1:O:1119:G:H8	12:J:52:GLN:HE22	1.48	0.60
1:O:2837:U:H1'	5:B:307:ARG:HH12	1.67	0.60
6:C:233:THR:HG22	6:C:234:VAL:N	2.17	0.60
17:O:14:LEU:CD2	17:O:102:ILE:HD11	2.32	0.60
4:A:192:VAL:CG1	4:A:207:GLN:HB3	2.32	0.59
7:D:86:THR:C	7:D:89:PRO:HD2	2.27	0.59
14:L:136:ALA:HB3	38:L:9372:HOH:O	2.01	0.59
16:N:27:LEU:HD13	16:N:50:LEU:HD21	1.82	0.59
23:U:46:ALA:HB1	23:U:52:THR:HG21	1.84	0.59
4:A:211:LYS:HB3	4:A:212:PRO:CD	2.25	0.59
5:B:150:ALA:O	5:B:152:PRO:HD3	2.02	0.59
10:G:64:ASN:O	10:G:68:GLU:HG3	2.02	0.59
1:O:485:A:N3	1:O:487:G:H5''	2.17	0.59
2:9:3055:U:H4'	2:9:3056:A:H8	1.67	0.59
4:A:88:ILE:O	4:A:88:ILE:HG22	1.99	0.59
15:M:164:THR:HG23	15:M:165:GLY:N	2.17	0.59
29:1:10:LYS:HG3	38:1:9236:HOH:O	2.01	0.59
1:O:120:A:H5'	29:1:20:ARG:HH21	1.68	0.59
1:O:1441:G:O2'	1:O:1442:A:H5'	2.02	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1926:G:H2'	1:0:1927:A:C8	2.36	0.59
5:B:329:TYR:CE2	23:U:15:PRO:HG2	2.36	0.59
12:J:19:MET:HE1	12:J:132:LEU:HD21	1.83	0.59
14:L:61:ALA:HA	38:L:9363:HOH:O	2.03	0.59
1:0:1118:A:H2'	1:0:1120:U:H5''	1.84	0.59
1:0:2748:G:H5'	38:0:7705:HOH:O	2.02	0.59
7:D:22:VAL:HG22	7:D:74:THR:HG22	1.84	0.59
8:E:23:GLU:HG2	8:E:28:SER:HB3	1.84	0.59
13:K:34:VAL:HG22	13:K:47:ALA:HB2	1.84	0.59
26:X:43:VAL:HG12	26:X:44:ASP:N	2.17	0.59
1:0:121:U:OP2	30:2:10:ARG:NH2	2.32	0.59
1:0:1299:G:N7	14:L:6:ARG:NH1	2.50	0.59
2:9:3064:C:C2'	2:9:3065:A:H5'	2.33	0.59
25:W:38:THR:HG22	25:W:39:ASP:N	2.18	0.59
1:0:65:C:O2'	1:0:66:G:H5'	2.02	0.59
1:0:625:U:H5''	1:0:1044:C:N4	2.17	0.59
1:0:2668:G:H2'	1:0:2669:U:C6	2.38	0.59
4:A:94:LEU:HG	4:A:99:ILE:CD1	2.31	0.59
4:A:94:LEU:HD23	4:A:94:LEU:N	2.18	0.59
5:B:79:MET:HE3	5:B:144:THR:HG21	1.84	0.59
7:D:10:PHE:CG	7:D:11:HIS:N	2.71	0.59
2:9:3028:U:H5''	16:N:40:ASN:HD21	1.67	0.59
7:D:166:ILE:HB	38:D:6326:HOH:O	2.03	0.59
8:E:35:TYR:HA	12:J:127:ILE:HD12	1.84	0.59
9:F:91:VAL:HG12	9:F:92:GLY:N	2.09	0.59
12:J:19:MET:CE	12:J:132:LEU:HD21	2.33	0.59
12:J:74:ARG:HH11	12:J:74:ARG:CB	2.13	0.59
18:P:80:ARG:HG2	18:P:87:ARG:CZ	2.33	0.59
24:V:38:GLY:C	24:V:40:PRO:HD2	2.27	0.59
30:2:5:LYS:O	30:2:9:LYS:HG3	2.03	0.59
32:I:76:ALA:O	32:I:80:LYS:HG3	2.01	0.59
1:0:88:G:H8	1:0:88:G:H5'	1.68	0.59
1:0:1213:C:O2'	1:0:1214:G:H5'	2.03	0.59
1:0:1733:A:H4'	5:B:212:GLN:HA	1.84	0.59
1:0:1813:U:O2'	18:P:81:LYS:HE3	2.03	0.59
4:A:39:ALA:HB3	4:A:61:GLU:OE2	2.02	0.59
14:L:143:THR:HG22	14:L:145:LEU:H	1.66	0.59
16:N:139:TRP:HA	16:N:139:TRP:CE3	2.38	0.59
27:Y:212:ARG:HD2	38:Y:8187:HOH:O	2.02	0.59
4:A:105:VAL:CG1	4:A:154:ALA:HB1	2.33	0.59
5:B:16:ARG:NH1	38:B:9416:HOH:O	2.36	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:X:25:ARG:HD3	26:X:64:ALA:O	2.01	0.59
31:3:73:GLU:HB3	38:3:9360:HOH:O	2.02	0.59
38:0:7333:HOH:O	29:1:1:THR:HB	2.01	0.58
5:B:16:ARG:HB3	5:B:217:ARG:NH2	2.18	0.58
20:R:25:PHE:CE2	20:R:29:LYS:HE2	2.38	0.58
28:Z:42:CYS:SG	28:Z:43:GLY:N	2.76	0.58
1:0:381:G:H5'	38:0:4603:HOH:O	2.02	0.58
1:0:2502:C:H2'	1:0:2503:A:H5'	1.84	0.58
1:0:2649:A:H5'	1:0:2649:A:C8	2.38	0.58
1:0:2779:G:H21	8:E:143:GLN:NE2	2.01	0.58
2:9:3069:U:OP1	16:N:4:PRO:HG3	2.03	0.58
2:9:3092:G:H2'	2:9:3093:A:C8	2.38	0.58
4:A:8:ARG:HG2	38:A:9349:HOH:O	2.03	0.58
4:A:217:ARG:HH11	4:A:217:ARG:HG3	1.67	0.58
27:Y:106:THR:HG23	27:Y:107:PRO:HD2	1.84	0.58
1:0:2717:C:H2'	1:0:2718:C:C5'	2.31	0.58
11:H:167:PRO:O	11:H:168:ALA:HB2	2.02	0.58
12:J:75:PRO:HG2	12:J:105:LEU:CD2	2.32	0.58
20:R:40:ALA:O	20:R:44:VAL:HG23	2.03	0.58
1:0:1450:C:O2'	1:0:1494:A:H5'	2.03	0.58
1:0:1730:G:H5'	1:0:1731:C:C5	2.38	0.58
1:0:2546:U:H5	5:B:2:GLN:HE22	1.50	0.58
2:9:3048:C:H4'	16:N:141:ARG:HH21	1.67	0.58
5:B:307:ARG:HH11	5:B:307:ARG:HB2	1.68	0.58
5:B:312:ARG:HD3	5:B:315:VAL:HG13	1.84	0.58
20:R:132:ARG:HG2	20:R:133:ALA:N	2.17	0.58
27:Y:107:PRO:HB3	27:Y:182:PHE:CE2	2.38	0.58
1:0:2094:G:H4'	5:B:245:SER:HB3	1.84	0.58
1:0:2365:G:H4'	19:Q:45:PRO:O	2.03	0.58
1:0:2524:G:N2	1:0:2526:C:H41	2.01	0.58
6:C:154:VAL:O	6:C:158:GLU:HG3	2.03	0.58
28:Z:30:GLU:HA	28:Z:33:MET:HE3	1.84	0.58
1:0:31:C:H4'	38:0:7598:HOH:O	2.03	0.58
1:0:1741:U:O2'	1:0:2723:G:H4'	2.04	0.58
1:0:2241:C:H2'	1:0:2242:U:C6	2.39	0.58
1:0:2578:G:H5'	1:0:2578:G:H8	1.69	0.58
4:A:190:ARG:NH2	4:A:207:GLN:OE1	2.37	0.58
26:X:31:ILE:O	26:X:35:GLU:HG3	2.03	0.58
28:Z:11:SER:CB	28:Z:23:ARG:HB2	2.34	0.58
32:I:72:VAL:HG13	32:I:73:PRO:HD2	1.85	0.58
32:I:139:ILE:HG22	32:I:140:GLU:N	2.19	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1527:A:H1'	1:0:1528:A:C8	2.38	0.58
6:C:182:ARG:HB2	6:C:184:ARG:HH12	1.68	0.58
13:K:62:PRO:CG	13:K:65:ARG:HH21	2.16	0.58
1:0:447:A:O2'	1:0:448:G:H5'	2.04	0.58
11:H:120:ILE:N	11:H:120:ILE:HD12	2.19	0.58
20:R:145:LEU:HD12	20:R:146:ILE:N	2.19	0.58
25:W:4:LEU:O	25:W:32:CYS:HA	2.04	0.58
1:0:182:G:H5'	38:0:5426:HOH:O	2.03	0.58
1:0:962:C:H1'	16:N:5:ARG:HH12	1.68	0.58
1:0:1180:U:H1'	38:0:3528:HOH:O	2.03	0.58
1:0:1790:C:H2'	1:0:1791:U:H6	1.69	0.58
8:E:31:ARG:HH12	8:E:68:HIS:CD2	2.22	0.58
15:M:31:TRP:HA	15:M:34:GLU:HG3	1.84	0.58
17:O:37:ARG:HG3	38:O:3002:HOH:O	2.03	0.58
1:0:1835:U:C5	1:0:1840:A:N7	2.61	0.57
6:C:168:ARG:NH2	6:C:190:ALA:O	2.37	0.57
9:F:50:VAL:HG13	9:F:60:VAL:HG11	1.86	0.57
1:0:644:G:H5'	1:0:644:G:N3	2.18	0.57
23:U:17:THR:HG22	23:U:18:GLY:N	2.19	0.57
25:W:84:VAL:HG12	38:W:6679:HOH:O	2.03	0.57
25:W:108:ARG:HE	25:W:114:PRO:CG	2.17	0.57
32:I:92:PRO:C	32:I:94:GLU:H	2.10	0.57
32:I:138:THR:HG22	32:I:139:ILE:N	2.19	0.57
1:0:2256:G:H2'	1:0:2257:G:C5'	2.35	0.57
5:B:55:ASN:HB3	5:B:63:GLU:HA	1.86	0.57
11:H:76:GLU:C	11:H:77:LEU:HD23	2.29	0.57
18:P:9:LEU:O	18:P:13:VAL:HG12	2.03	0.57
20:R:47:LEU:O	20:R:51:ILE:HG13	2.04	0.57
4:A:109:GLU:HG2	4:A:116:GLY:N	2.18	0.57
4:A:121:ALA:O	4:A:124:VAL:HG22	2.04	0.57
7:D:39:ASP:O	7:D:43:GLU:HG3	2.03	0.57
22:T:48:VAL:HG12	22:T:49:GLU:N	2.18	0.57
25:W:122:ARG:HG2	25:W:122:ARG:HH11	1.70	0.57
25:W:149:LEU:CG	25:W:153:MET:HE2	2.29	0.57
1:0:1008:C:H5''	11:H:16:ARG:HH12	1.70	0.57
1:0:2878:U:H2'	1:0:2879:A:O4'	2.04	0.57
15:M:61:ILE:HD12	15:M:61:ILE:N	2.19	0.57
27:Y:151:SER:HB3	27:Y:154:ARG:HB3	1.87	0.57
27:Y:200:THR:HG22	27:Y:201:GLU:HG2	1.86	0.57
1:0:1182:C:H1'	1:0:1192:A:H8	1.68	0.57
13:K:55:VAL:HG12	13:K:56:SER:N	2.20	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:K:81:ARG:HD3	13:K:87:ARG:NH1	2.19	0.57
25:W:13:MET:HE3	25:W:17:ILE:HG22	1.84	0.57
25:W:88:THR:CG2	25:W:110:GLN:NE2	2.68	0.57
1:0:2508:C:H2'	38:0:6966:HOH:O	2.04	0.57
1:0:2679:G:H2'	1:0:2681:A:OP2	2.05	0.57
18:P:64:GLU:HG2	38:P:170:HOH:O	2.05	0.57
1:0:703:G:O2'	1:0:704:C:H5'	2.05	0.57
4:A:153:ARG:HH11	4:A:153:ARG:CB	2.18	0.57
5:B:275:GLY:O	5:B:291:ASP:HA	2.05	0.57
16:N:80:SER:HB2	38:N:9336:HOH:O	2.04	0.57
1:0:1163:G:H5'	32:I:115:ASP:O	2.05	0.57
7:D:25:MET:HE2	7:D:41:LEU:CG	2.30	0.57
8:E:80:TRP:O	8:E:134:SER:HA	2.05	0.57
17:O:87:THR:O	17:O:91:GLN:HG3	2.04	0.57
20:R:18:LEU:HB2	20:R:143:VAL:CG1	2.34	0.57
29:1:25:LYS:HD2	30:2:48:ASP:HA	1.87	0.57
30:2:36:ASN:HB3	30:2:39:ARG:HE	1.70	0.57
1:0:960:G:N3	1:0:960:G:H2'	2.20	0.57
1:0:1118:A:C8	1:0:1118:A:C3'	2.85	0.57
1:0:1926:G:H2'	1:0:1927:A:H8	1.70	0.57
5:B:5:ARG:HD2	5:B:8:LYS:HZ1	1.70	0.57
5:B:280:VAL:CG1	5:B:334:SER:HA	2.35	0.57
6:C:35:VAL:HG21	6:C:227:GLY:HA2	1.86	0.57
21:S:17:ASP:HB3	21:S:23:LYS:HB2	1.87	0.57
1:0:256:C:H2'	1:0:257:G:O4'	2.05	0.56
12:J:107:ASN:C	12:J:107:ASN:HD22	2.13	0.56
14:L:77:ALA:HB3	38:L:9329:HOH:O	2.05	0.56
20:R:145:LEU:HD12	20:R:146:ILE:H	1.70	0.56
1:0:1189:A:H3'	38:0:7842:HOH:O	2.04	0.56
1:0:1462:C:H2'	1:0:1463:A:C8	2.41	0.56
1:0:2265:U:H2'	1:0:2266:A:C8	2.40	0.56
1:0:2346:C:O2'	7:D:52:THR:HG21	2.04	0.56
2:9:3041:C:H4'	7:D:48:MET:HB2	1.87	0.56
4:A:82:VAL:HG13	4:A:93:THR:HB	1.87	0.56
9:F:96:ALA:HA	38:F:3111:HOH:O	2.04	0.56
1:0:280:C:H2'	1:0:281:U:O4'	2.05	0.56
1:0:1657:A:H2'	1:0:1658:A:C8	2.40	0.56
1:0:2256:G:O2'	1:0:2257:G:H5'	2.05	0.56
7:D:135:VAL:HG22	7:D:136:ARG:N	2.20	0.56
9:F:58:GLU:OE1	15:M:27:ARG:NH2	2.34	0.56
24:V:39:ALA:N	24:V:40:PRO:CD	2.69	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:2415:A:C2	16:N:25:ARG:HB3	2.41	0.56
1:0:2563:U:H2'	1:0:2565:C:O5'	2.05	0.56
2:9:3054:A:O2'	2:9:3055:U:H5'	2.06	0.56
5:B:305:ASP:O	5:B:306:LYS:HB2	2.06	0.56
13:K:34:VAL:CG2	13:K:47:ALA:HB2	2.35	0.56
21:S:33:SER:OG	21:S:36:GLU:HG3	2.06	0.56
23:U:9:CYS:HA	23:U:52:THR:HG23	1.87	0.56
1:0:1314:U:H2'	38:0:6124:HOH:O	2.03	0.56
38:0:4274:HOH:O	22:T:82:THR:HA	2.06	0.56
1:0:602:A:O2'	1:0:605:C:H4'	2.04	0.56
1:0:1535:G:H2'	1:0:1536:C:C6	2.41	0.56
1:0:1682:A:H5''	38:0:9763:HOH:O	2.06	0.56
22:T:35:TYR:CD2	22:T:112:LEU:HD22	2.40	0.56
1:0:119:A:H2'	1:0:120:A:H5''	1.88	0.56
22:T:24:ARG:HH21	22:T:39:ASN:ND2	2.04	0.56
23:U:14:GLU:O	23:U:17:THR:HB	2.05	0.56
30:2:22:PRO:HG2	30:2:25:VAL:HG23	1.88	0.56
32:I:75:THR:CA	32:I:112:LYS:HZ1	2.19	0.56
1:0:709:G:O2'	17:O:25:VAL:HG12	2.05	0.56
1:0:820:G:OP2	4:A:171:LYS:NZ	2.37	0.56
18:P:7:LYS:HD3	18:P:21:VAL:CG2	2.36	0.56
22:T:24:ARG:HH21	22:T:39:ASN:HD22	1.52	0.56
25:W:22:GLU:HG2	25:W:27:HIS:CD2	2.40	0.56
29:1:25:LYS:O	29:1:25:LYS:HG2	2.05	0.56
31:3:87:ARG:HD2	31:3:89:GLU:OE2	2.06	0.56
1:0:136:C:H2'	1:0:137:U:O4'	2.06	0.56
1:0:2271:G:H5'	38:0:5025:HOH:O	2.06	0.56
2:9:3049:G:O2'	2:9:3050:G:H5'	2.05	0.56
11:H:77:LEU:HD12	11:H:83:TYR:CD2	2.41	0.56
23:U:52:THR:HG21	23:U:54:THR:HB	1.87	0.56
1:0:1778:A:H2'	1:0:1779:A:H5'	1.88	0.55
7:D:51:ARG:HD3	38:D:7636:HOH:O	2.06	0.55
16:N:143:ARG:NH1	16:N:173:ASP:OD2	2.39	0.55
20:R:3:SER:HA	38:R:9348:HOH:O	2.06	0.55
23:U:52:THR:HG22	23:U:54:THR:N	2.21	0.55
24:V:1:THR:HG23	24:V:2:VAL:N	2.15	0.55
1:0:2769:C:C2'	1:0:2770:G:H5'	2.36	0.55
2:9:3013:A:O2'	2:9:3014:G:H5''	2.05	0.55
6:C:109:LEU:HD12	6:C:109:LEU:O	2.05	0.55
8:E:23:GLU:HG2	8:E:28:SER:CB	2.35	0.55
8:E:137:ASP:OD1	8:E:139:GLU:HB2	2.06	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:P:115:SER:O	18:P:117:SER:N	2.36	0.55
1:0:426:G:H2'	1:0:427:C:O4'	2.07	0.55
22:T:92:ASP:OD1	22:T:94:SER:HB3	2.06	0.55
1:0:290:C:H1'	38:0:6342:HOH:O	2.05	0.55
1:0:2718:C:H6	1:0:2718:C:H5'	1.71	0.55
2:9:3006:C:OP1	16:N:37:ARG:NH1	2.39	0.55
4:A:35:GLY:O	4:A:36:ASP:HB3	2.06	0.55
4:A:76:VAL:HG23	28:Z:63:LYS:HB3	1.87	0.55
5:B:198:GLU:HA	38:B:9454:HOH:O	2.06	0.55
8:E:20:ILE:HD11	8:E:40:VAL:HG11	1.88	0.55
1:0:660:A:H4'	1:0:661:G:O5'	2.07	0.55
1:0:1766:U:O2	1:0:1778:A:H5'	2.07	0.55
1:0:1909:A:H2'	1:0:1910:A:C8	2.40	0.55
1:0:2453:G:H4'	14:L:50:GLY:C	2.31	0.55
1:0:2755:G:H1'	38:0:4956:HOH:O	2.06	0.55
3:4:176:DA:O4'	3:4:175:C:H2'	2.06	0.55
13:K:115:ARG:HG3	13:K:116:GLU:N	2.20	0.55
25:W:73:LEU:O	25:W:74:GLU:HG3	2.06	0.55
1:0:968:G:O2'	1:0:969:G:H5'	2.07	0.55
1:0:1506:U:H6	1:0:1506:U:H5'	1.72	0.55
4:A:153:ARG:HB2	4:A:153:ARG:NH1	2.20	0.55
6:C:111:VAL:HB	38:C:9123:HOH:O	2.07	0.55
25:W:119:HIS:HD2	25:W:120:PRO:O	1.89	0.55
1:0:1687:C:O2	29:1:9:GLY:HA2	2.06	0.55
1:0:1972:U:H2'	1:0:1973:A:H5'	1.88	0.55
1:0:2505:G:O2'	1:0:2506:A:H5'	2.07	0.55
5:B:71:VAL:HG11	5:B:296:LEU:HD22	1.88	0.55
5:B:88:GLU:HB3	5:B:97:LEU:HG	1.89	0.55
20:R:39:THR:HB	20:R:42:GLU:HG3	1.89	0.55
1:0:681:G:N3	1:0:681:G:H5'	2.22	0.55
1:0:1242:A:C5'	12:J:82:THR:HG23	2.25	0.55
1:0:1505:U:H6	1:0:1505:U:H5'	1.70	0.55
1:0:2768:A:O2'	1:0:2769:C:H5'	2.07	0.55
21:S:37:VAL:O	21:S:41:VAL:HG23	2.06	0.55
28:Z:11:SER:HB3	28:Z:23:ARG:HB2	1.88	0.55
1:0:2613:G:O2'	1:0:2614:C:H5'	2.07	0.55
8:E:84:MET:HE1	8:E:148:ILE:HD12	1.88	0.55
9:F:107:ASP:O	9:F:111:ILE:HG13	2.07	0.55
11:H:9:ILE:O	11:H:9:ILE:HG22	2.07	0.55
17:O:21:SER:OG	17:O:106:PRO:HB2	2.07	0.55
18:P:143:ALA:HA	38:P:190:HOH:O	2.07	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:W:80:ASP:O	25:W:84:VAL:HG23	2.06	0.55
28:Z:13:ARG:NH1	28:Z:14:PHE:CZ	2.75	0.55
28:Z:25:ARG:O	28:Z:29:ILE:HG13	2.06	0.55
1:O:2630:G:O6	4:A:206:ARG:NH2	2.41	0.54
38:O:4897:HOH:O	4:A:6:GLY:HA3	2.07	0.54
6:C:107:ARG:NH1	6:C:107:ARG:HB3	2.22	0.54
11:H:166:SER:HB2	11:H:167:PRO:HD3	1.86	0.54
26:X:78:GLU:HG2	26:X:79:GLU:N	2.20	0.54
32:I:89:SER:HB3	32:I:97:VAL:CG2	2.37	0.54
1:O:2526:C:O2'	1:O:2527:U:H5'	2.07	0.54
1:O:2783:A:H3'	38:O:5494:HOH:O	2.07	0.54
7:D:84:LEU:C	7:D:86:THR:H	2.16	0.54
17:O:47:ARG:HH11	17:O:47:ARG:HG3	1.72	0.54
20:R:99:ALA:CB	20:R:109:MET:HE1	2.22	0.54
25:W:139:GLY:O	25:W:141:HIS:CD2	2.59	0.54
27:Y:187:VAL:CG2	27:Y:192:ASP:HB2	2.36	0.54
1:O:1234:U:C4	5:B:244:PRO:HB3	2.43	0.54
1:O:1289:C:H3'	38:O:6638:HOH:O	2.06	0.54
1:O:2509:A:H2'	1:O:2510:C:O4'	2.08	0.54
1:O:2676:C:H4'	12:J:70:PHE:CE1	2.42	0.54
25:W:21:LEU:HD13	25:W:26:ILE:HD11	1.88	0.54
26:X:22:ASN:O	26:X:25:ARG:HG3	2.07	0.54
1:O:21:G:H4'	20:R:2:ILE:HG22	1.87	0.54
1:O:92:G:H4'	24:V:44:GLY:HA3	1.89	0.54
1:O:282:C:H1'	1:O:368:C:H42	1.68	0.54
1:O:2862:G:H4'	5:B:336:GLN:O	2.07	0.54
2:9:3001:U:H5''	2:9:3003:A:OP1	2.08	0.54
2:9:3028:U:H5''	16:N:40:ASN:ND2	2.22	0.54
2:9:3091:C:H2'	2:9:3092:G:O4'	2.07	0.54
4:A:217:ARG:HH11	4:A:217:ARG:CG	2.20	0.54
5:B:51:VAL:HG13	5:B:53:LEU:HD13	1.89	0.54
5:B:119:HIS:O	5:B:121:PRO:HD3	2.08	0.54
6:C:77:ALA:O	6:C:78:ARG:HG3	2.07	0.54
7:D:25:MET:SD	7:D:40:ILE:HD11	2.48	0.54
8:E:84:MET:HB2	8:E:131:LEU:HB2	1.90	0.54
10:G:64:ASN:N	10:G:64:ASN:ND2	2.54	0.54
26:X:80:GLU:HB3	38:X:5564:HOH:O	2.07	0.54
27:Y:99:ALA:HB2	27:Y:233:TYR:CE2	2.42	0.54
32:I:139:ILE:HG22	32:I:140:GLU:H	1.71	0.54
1:O:2717:C:O2'	1:O:2718:C:H5''	2.06	0.54
5:B:75:GLU:C	5:B:77:PRO:HD3	2.33	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:J:103:VAL:HG12	38:J:9361:HOH:O	2.07	0.54
27:Y:184:GLU:OE1	27:Y:204:ARG:NH1	2.39	0.54
1:O:776:A:OP1	29:1:28:HIS:HE1	1.91	0.54
6:C:1:MET:HG2	6:C:2:GLN:N	2.15	0.54
1:O:583:G:H2'	1:O:584:U:C6	2.42	0.54
6:C:235:PHE:HE2	6:C:243:VAL:HG21	1.72	0.54
9:F:27:GLY:HA3	9:F:101:ALA:O	2.08	0.54
13:K:27:ARG:HD2	38:K:4747:HOH:O	2.07	0.54
16:N:151:ASP:OD1	16:N:154:LEU:HD13	2.08	0.54
20:R:99:ALA:HB1	20:R:109:MET:CE	2.22	0.54
25:W:13:MET:HE3	25:W:17:ILE:CG2	2.37	0.54
27:Y:112:GLU:HA	27:Y:112:GLU:OE1	2.07	0.54
27:Y:189:ASN:ND2	27:Y:192:ASP:H	2.05	0.54
32:I:72:VAL:CG1	32:I:73:PRO:HD2	2.37	0.54
1:O:1847:A:OP1	4:A:175:LYS:HG3	2.08	0.54
5:B:146:THR:O	5:B:159:PRO:HB3	2.08	0.54
6:C:140:VAL:HB	38:C:9252:HOH:O	2.07	0.54
16:N:67:ALA:C	16:N:69:TYR:H	2.14	0.54
16:N:139:TRP:HA	16:N:139:TRP:HE3	1.72	0.54
25:W:106:THR:OG1	25:W:109:GLU:HG3	2.07	0.54
1:O:1278:A:H4'	1:O:1279:U:C4	2.43	0.54
1:O:1342:C:O2'	1:O:1343:C:H5'	2.08	0.54
20:R:17:MET:CE	20:R:19:ARG:CZ	2.85	0.54
23:U:52:THR:HG22	23:U:54:THR:HB	1.90	0.54
25:W:122:ARG:HG3	25:W:152:ALA:O	2.07	0.54
27:Y:133:HIS:HD2	38:Y:8168:HOH:O	1.90	0.54
1:O:371:U:H2'	1:O:372:A:H8	1.73	0.54
1:O:1116:U:O2'	1:O:1118:A:C2	2.51	0.54
2:9:3003:A:N6	2:9:3022:G:H1'	2.23	0.54
5:B:162:MET:HG3	5:B:310:ARG:CZ	2.38	0.54
14:L:104:ASP:O	14:L:105:TYR:HB3	2.06	0.54
19:Q:28:ARG:HD2	19:Q:92:ARG:NH1	2.23	0.54
1:O:56:G:C5'	24:V:50:ARG:HH12	2.12	0.53
1:O:2300:A:H4'	1:O:2301:A:O5'	2.09	0.53
1:O:2720:C:O2	13:K:87:ARG:NH2	2.41	0.53
6:C:2:GLN:HB3	38:C:9186:HOH:O	2.07	0.53
8:E:84:MET:HE1	8:E:148:ILE:HD13	1.90	0.53
16:N:100:ALA:O	16:N:129:ILE:HG23	2.08	0.53
16:N:164:ASP:OD2	16:N:167:ASP:HA	2.08	0.53
22:T:16:LEU:HA	22:T:19:ARG:HG3	1.90	0.53
9:F:58:GLU:HA	9:F:61:MET:HE2	1.90	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:O:14:LEU:HD23	17:O:102:ILE:HD11	1.90	0.53
32:I:75:THR:CA	32:I:112:LYS:NZ	2.71	0.53
1:O:1942:A:O2'	1:O:1943:C:H5'	2.09	0.53
16:N:37:ARG:NE	38:N:9334:HOH:O	2.41	0.53
25:W:108:ARG:HE	25:W:114:PRO:HG3	1.73	0.53
27:Y:144:ARG:NH1	38:Y:8163:HOH:O	2.41	0.53
2:9:3042:C:H5'	2:9:3043:G:OP2	2.08	0.53
4:A:36:ASP:HB2	4:A:83:GLY:CA	2.39	0.53
6:C:127:ARG:HG2	6:C:127:ARG:NH1	2.24	0.53
12:J:45:VAL:HG22	12:J:130:VAL:O	2.09	0.53
1:O:407:A:H2'	1:O:408:A:C8	2.43	0.53
1:O:657:G:H2'	1:O:658:C:C6	2.43	0.53
1:O:1164:U:H3	1:O:1192:A:H2	1.56	0.53
1:O:2064:U:H5'	1:O:2652:U:H4'	1.90	0.53
38:O:9668:HOH:O	29:1:1:THR:HA	2.07	0.53
5:B:294:TYR:HE2	38:B:9446:HOH:O	1.90	0.53
38:C:9168:HOH:O	22:T:2:LYS:HE2	2.06	0.53
9:F:50:VAL:CG2	9:F:63:ILE:HG21	2.37	0.53
16:N:23:ARG:O	16:N:27:LEU:HG	2.08	0.53
1:O:1014:A:H2'	1:O:1015:C:H5'	1.91	0.53
1:O:2597:U:H2'	1:O:2598:U:H5'	1.90	0.53
25:W:41:TYR:HA	25:W:44:MET:HE3	1.90	0.53
25:W:63:GLU:HG2	25:W:93:ILE:HG22	1.89	0.53
1:O:1667:A:H2'	1:O:1668:U:C6	2.44	0.53
7:D:153:THR:HA	7:D:156:ARG:HG3	1.91	0.53
9:F:48:VAL:HG12	9:F:97:ALA:CB	2.39	0.53
25:W:21:LEU:HB3	25:W:26:ILE:HG12	1.91	0.53
27:Y:186:ARG:HG2	27:Y:186:ARG:NH1	2.23	0.53
32:I:102:VAL:CG1	32:I:106:LYS:HE3	2.37	0.53
1:O:90:A:H2'	1:O:91:G:O4'	2.09	0.53
1:O:539:G:H2'	1:O:540:A:C8	2.43	0.53
1:O:1377:C:H5'	1:O:1377:C:C6	2.44	0.53
1:O:2769:C:O2'	1:O:2770:G:H5'	2.09	0.53
5:B:212:GLN:HB2	5:B:257:THR:CG2	2.34	0.53
6:C:133:ARG:NE	6:C:138:VAL:HG22	2.23	0.53
9:F:58:GLU:CD	15:M:27:ARG:HH22	2.17	0.53
1:O:289:G:N2	1:O:363:A:H2	2.04	0.53
5:B:41:PHE:CZ	5:B:79:MET:HG3	2.44	0.53
9:F:101:ALA:HA	38:F:5413:HOH:O	2.09	0.53
2:9:3044:A:O4'	7:D:76:ARG:NE	2.42	0.53
38:9:4707:HOH:O	16:N:147:ILE:HB	2.08	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:27:ASN:HD22	5:B:27:ASN:H	1.57	0.53
6:C:236:THR:O	6:C:237:GLU:C	2.52	0.53
15:M:46:LEU:HG	38:M:9411:HOH:O	2.09	0.53
25:W:6:GLN:CB	25:W:26:ILE:HD12	2.35	0.53
25:W:21:LEU:HD21	25:W:48:VAL:CG1	2.39	0.53
1:0:1175:G:H1'	1:0:1193:A:H2'	1.91	0.52
1:0:2324:G:H4'	1:0:2418:G:O2'	2.09	0.52
5:B:17:LYS:O	5:B:260:HIS:HD2	1.92	0.52
6:C:184:ARG:CZ	38:C:9216:HOH:O	2.57	0.52
8:E:15:GLN:HG3	8:E:20:ILE:HG12	1.91	0.52
12:J:39:VAL:HG12	12:J:40:ASN:ND2	2.25	0.52
22:T:78:THR:OG1	22:T:86:GLU:HG2	2.08	0.52
25:W:122:ARG:CZ	38:W:5817:HOH:O	2.57	0.52
1:0:338:C:H4'	6:C:174:ILE:HD11	1.91	0.52
15:M:59:GLY:HA3	15:M:141:ILE:CD1	2.38	0.52
16:N:37:ARG:HD3	36:N:9307:CL:CL	2.47	0.52
20:R:114:VAL:HG13	20:R:114:VAL:O	2.09	0.52
23:U:11:THR:HG22	23:U:53:ASP:OD2	2.10	0.52
31:3:3:MET:HG3	31:3:4:PRO:HD2	1.90	0.52
1:0:814:G:H4'	38:0:3429:HOH:O	2.09	0.52
1:0:2909:G:H2'	1:0:2910:A:H8	1.74	0.52
6:C:139:VAL:HG21	6:C:240:LEU:HD12	1.92	0.52
11:H:24:PRO:HD3	11:H:120:ILE:HG22	1.90	0.52
11:H:31:HIS:HD2	11:H:87:LEU:O	1.93	0.52
16:N:176:ARG:O	16:N:180:LEU:HD13	2.09	0.52
17:O:4:ASN:HB3	17:O:7:LEU:HB3	1.92	0.52
18:P:83:LYS:O	18:P:86:ALA:HB3	2.09	0.52
18:P:114:LEU:HA	18:P:118:GLN:NE2	2.25	0.52
20:R:106:GLY:HA2	20:R:109:MET:CE	2.35	0.52
22:T:28:SER:O	22:T:32:ARG:HG3	2.08	0.52
25:W:139:GLY:O	25:W:141:HIS:HD2	1.92	0.52
1:0:120:A:H2'	1:0:120:A:N3	2.25	0.52
1:0:475:G:H5'	6:C:73:LEU:HD23	1.91	0.52
1:0:1342:C:C2'	1:0:1343:C:H5'	2.40	0.52
38:0:4516:HOH:O	30:2:38:LYS:HE3	2.10	0.52
9:F:26:THR:HG21	9:F:102:GLY:C	2.34	0.52
12:J:93:ARG:HH11	12:J:93:ARG:CB	2.20	0.52
25:W:13:MET:CE	25:W:17:ILE:HG22	2.39	0.52
28:Z:56:GLN:HA	28:Z:62:TYR:O	2.10	0.52
1:0:553:G:O4'	1:0:1325:G:H5'	2.09	0.52
1:0:1634:G:H3'	38:0:4181:HOH:O	2.09	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:2758:G:H2'	1:0:2759:C:C6	2.45	0.52
5:B:51:VAL:CG2	5:B:327:VAL:HG13	2.40	0.52
7:D:128:LEU:C	7:D:128:LEU:HD23	2.35	0.52
8:E:11:VAL:CG1	8:E:12:ASP:N	2.72	0.52
6:C:127:ARG:HG2	6:C:127:ARG:HH11	1.75	0.52
6:C:132:ASP:HB3	38:C:9162:HOH:O	2.09	0.52
15:M:59:GLY:C	15:M:141:ILE:HD11	2.35	0.52
26:X:9:VAL:HG13	26:X:88:GLU:OE2	2.10	0.52
1:0:503:G:H2'	1:0:504:G:H8	1.75	0.52
1:0:1119:G:H8	12:J:52:GLN:NE2	2.08	0.52
1:0:1423:C:O2'	1:0:1424:A:H5'	2.10	0.52
1:0:2364:A:OP1	19:Q:11:ARG:NH1	2.42	0.52
26:X:21:PRO:HD3	38:X:6179:HOH:O	2.09	0.52
1:0:542:A:H2'	1:0:543:G:O4'	2.10	0.52
1:0:816:G:H5'	1:0:1598:A:H4'	1.91	0.52
1:0:1654:U:H2'	4:A:47:HIS:HD2	1.75	0.52
38:0:7598:HOH:O	22:T:9:LYS:HD2	2.10	0.52
2:9:3003:A:OP2	2:9:3025:G:N2	2.42	0.52
5:B:14:GLY:HA2	5:B:15:PRO:C	2.35	0.52
5:B:54:VAL:HB	38:B:9412:HOH:O	2.09	0.52
22:T:71:VAL:HG13	22:T:91:LEU:O	2.10	0.52
24:V:39:ALA:C	24:V:41:GLU:H	2.18	0.52
25:W:11:VAL:O	25:W:12:ASN:HB2	2.10	0.52
1:0:69:A:H5'	1:0:69:A:C8	2.45	0.52
1:0:259:G:O2'	1:0:260:C:H5'	2.10	0.52
1:0:1874:U:OP1	4:A:51:ARG:HD2	2.10	0.52
4:A:66:ARG:HH11	4:A:66:ARG:CB	2.22	0.52
6:C:115:LEU:HD13	6:C:223:LEU:HD21	1.90	0.52
15:M:66:SER:HB3	15:M:128:TRP:CD1	2.45	0.52
16:N:179:LEU:HD23	16:N:184:ILE:CD1	2.40	0.52
26:X:25:ARG:HG2	38:X:5356:HOH:O	2.10	0.52
7:D:146:LYS:NZ	16:N:107:ASN:ND2	2.56	0.52
8:E:34:TRP:O	12:J:127:ILE:HD11	2.10	0.52
27:Y:126:PRO:HG2	27:Y:128:PHE:CE1	2.45	0.52
28:Z:37:HIS:HB2	28:Z:47:VAL:HB	1.92	0.52
1:0:960:G:H4'	38:0:7605:HOH:O	2.10	0.51
1:0:1855:G:H8	4:A:144:GLU:OE2	1.93	0.51
5:B:214:PRO:HD2	38:B:9321:HOH:O	2.09	0.51
8:E:20:ILE:CD1	8:E:40:VAL:HG11	2.40	0.51
11:H:154:TYR:CD1	11:H:154:TYR:C	2.87	0.51
12:J:15:ARG:NH1	12:J:43:ARG:NH1	2.57	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:N:78:MET:HB2	16:N:79:PRO:HD3	1.91	0.51
26:X:71:ARG:HB3	26:X:88:GLU:OE1	2.09	0.51
31:3:69:TYR:CZ	31:3:80:ARG:HD2	2.45	0.51
32:I:112:LYS:C	32:I:114:PRO:HD2	2.35	0.51
1:0:67:A:H5''	1:0:69:A:C8	2.46	0.51
1:0:1205:U:C2'	1:0:1206:U:H5''	2.40	0.51
4:A:88:ILE:HD13	4:A:100:PRO:CD	2.35	0.51
5:B:162:MET:HG3	5:B:310:ARG:HD3	1.92	0.51
5:B:258:GLY:H	5:B:260:HIS:CE1	2.27	0.51
11:H:3:ALA:HA	11:H:58:ARG:NH1	2.25	0.51
14:L:145:LEU:O	14:L:148:GLU:HG3	2.10	0.51
15:M:65:VAL:HG21	15:M:105:ALA:HB2	1.90	0.51
15:M:107:ARG:HD2	38:M:9370:HOH:O	2.09	0.51
16:N:11:ARG:O	16:N:15:GLU:HG3	2.10	0.51
25:W:137:GLN:HE21	25:W:141:HIS:CE1	2.22	0.51
26:X:30:MET:CE	26:X:58:ALA:HB3	2.39	0.51
1:0:512:G:O3'	1:0:513:A:H8	1.94	0.51
1:0:1850:U:H2'	1:0:1851:G:H8	1.74	0.51
1:0:2081:A:H4'	12:J:69:TYR:CE1	2.45	0.51
1:0:2894:C:O2'	1:0:2895:C:H5'	2.10	0.51
25:W:76:ASP:O	25:W:77:ALA:C	2.52	0.51
27:Y:107:PRO:HB3	27:Y:182:PHE:CD2	2.45	0.51
28:Z:46:ARG:HD3	28:Z:58:SER:OG	2.11	0.51
29:1:8:GLN:NE2	29:1:11:LYS:NZ	2.55	0.51
4:A:36:ASP:CB	4:A:83:GLY:HA3	2.41	0.51
4:A:199:HIS:CD2	4:A:201:PHE:H	2.28	0.51
5:B:62:ARG:HA	5:B:65:MET:CE	2.40	0.51
5:B:310:ARG:HD2	38:B:9444:HOH:O	2.08	0.51
20:R:111:ILE:HG23	20:R:145:LEU:CD1	2.40	0.51
22:T:35:TYR:CG	22:T:112:LEU:HD22	2.46	0.51
24:V:27:LEU:HA	24:V:49:LEU:HD13	1.92	0.51
1:0:159:G:OP1	15:M:74:LYS:HE3	2.10	0.51
5:B:141:ARG:HD2	5:B:163:GLU:OE2	2.11	0.51
11:H:148:GLU:OE1	11:H:148:GLU:HA	2.10	0.51
14:L:146:GLY:C	14:L:148:GLU:H	2.18	0.51
30:2:48:ASP:O	30:2:49:GLU:HB2	2.10	0.51
1:0:775:G:OP1	29:1:16:HIS:HE1	1.94	0.51
1:0:1180:U:H2'	1:0:1181:A:C8	2.46	0.51
1:0:2897:C:H2'	1:0:2898:G:H8	1.74	0.51
10:G:23:ILE:O	10:G:27:ILE:HG13	2.10	0.51
14:L:90:ARG:NH2	14:L:121:ILE:HD11	2.26	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:3:40:ARG:HD2	38:3:9357:HOH:O	2.10	0.51
1:0:638:C:H2'	1:0:639:A:C8	2.46	0.51
1:0:1500:U:P	18:P:41:ARG:HH22	2.33	0.51
4:A:179:MET:HG3	4:A:186:TRP:CG	2.46	0.51
11:H:166:SER:HB3	11:H:167:PRO:HD3	1.93	0.51
17:O:42:GLU:HB2	38:O:2176:HOH:O	2.09	0.51
20:R:132:ARG:CZ	38:R:9385:HOH:O	2.59	0.51
21:S:43:GLU:HB3	38:S:9141:HOH:O	2.10	0.51
26:X:10:VAL:HG11	26:X:36:HIS:HE1	1.75	0.51
27:Y:126:PRO:HG2	27:Y:128:PHE:CZ	2.46	0.51
32:I:101:SER:OG	32:I:104:GLN:HG3	2.11	0.51
1:0:419:A:H1'	1:0:1921:A:C2	2.45	0.51
1:0:474:C:O3'	6:C:73:LEU:CD2	2.59	0.51
1:0:1252:A:H2'	1:0:1253:C:O4'	2.11	0.51
1:0:2036:C:O4'	13:K:44:LEU:HG	2.11	0.51
15:M:59:GLY:CA	15:M:141:ILE:HD11	2.41	0.51
15:M:157:ASP:HB3	15:M:160:PHE:HD1	1.75	0.51
23:U:39:ASN:HD22	23:U:44:ARG:HH11	1.57	0.51
23:U:53:ASP:O	23:U:54:THR:C	2.54	0.51
1:0:263:U:C4	9:F:54:VAL:HG13	2.45	0.51
1:0:583:G:H2'	1:0:584:U:H6	1.76	0.51
1:0:694:A:H2'	1:0:695:C:H5'	1.93	0.51
1:0:702:G:O2'	1:0:703:G:H5'	2.11	0.51
1:0:790:A:H2'	1:0:791:A:O4'	2.10	0.51
1:0:1167:G:H2'	1:0:1168:C:O4'	2.11	0.51
1:0:1422:U:H2'	1:0:1423:C:C6	2.46	0.51
38:O:9863:HOH:O	25:W:119:HIS:HE1	1.93	0.51
6:C:233:THR:HG22	6:C:234:VAL:H	1.76	0.51
11:H:36:LYS:HA	11:H:84:LYS:NZ	2.26	0.51
14:L:17:SER:C	14:L:19:LYS:H	2.18	0.51
15:M:49:ALA:C	15:M:54:TYR:HB3	2.35	0.51
16:N:151:ASP:O	16:N:154:LEU:HB2	2.10	0.51
18:P:7:LYS:HD3	18:P:21:VAL:HG21	1.92	0.51
25:W:130:HIS:O	25:W:136:GLY:HA3	2.10	0.51
27:Y:97:LEU:C	27:Y:98:GLN:HG2	2.36	0.51
32:I:91:GLU:HB3	32:I:94:GLU:OE2	2.11	0.51
1:0:1528:A:H2'	1:0:1529:G:O4'	2.11	0.51
1:0:1555:G:H4'	1:0:1630:A:H2	1.75	0.51
1:0:2361:A:H5'	1:0:2361:A:H8	1.76	0.51
4:A:105:VAL:HG12	4:A:106:CYS:N	2.26	0.51
4:A:217:ARG:HG2	4:A:229:ALA:HB2	1.93	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:C:13:ASP:OD1	6:C:13:ASP:O	2.27	0.51
24:V:42:ASN:O	24:V:44:GLY:N	2.43	0.51
25:W:36:PRO:HD2	25:W:41:TYR:CE1	2.46	0.51
1:0:945:U:H2'	1:0:946:C:C6	2.46	0.50
1:0:1730:G:H5''	1:0:1731:C:H6	1.76	0.50
1:0:2533:C:H6	1:0:2533:C:C5'	2.20	0.50
4:A:211:LYS:HB2	38:A:9412:HOH:O	2.10	0.50
13:K:6:ALA:CB	13:K:116:GLU:HG2	2.41	0.50
18:P:55:LYS:HG2	18:P:56:GLY:N	2.25	0.50
1:0:243:A:H61	1:0:269:G:H1'	1.76	0.50
1:0:289:G:O2'	1:0:290:C:H5'	2.11	0.50
1:0:366:U:H2'	1:0:367:G:O4'	2.11	0.50
1:0:1189:A:H1'	1:0:1209:C:H1'	1.92	0.50
6:C:242:GLU:HG3	38:C:9183:HOH:O	2.11	0.50
9:F:56:PRO:HG2	15:M:43:PRO:O	2.11	0.50
13:K:109:LEU:HD13	13:K:113:ILE:HD11	1.94	0.50
16:N:170:GLU:O	16:N:174:GLU:HG3	2.10	0.50
17:O:53:GLN:HG2	17:O:56:GLU:OE1	2.12	0.50
32:I:106:LYS:O	32:I:110:GLU:HG3	2.12	0.50
1:0:451:C:O2'	1:0:452:G:H5'	2.11	0.50
1:0:1904:A:H2'	1:0:1905:U:O4'	2.12	0.50
38:O:3252:HOH:O	26:X:23:HIS:HD2	1.93	0.50
4:A:164:ARG:CZ	38:A:9383:HOH:O	2.59	0.50
5:B:7:ARG:HG2	5:B:7:ARG:HH11	1.76	0.50
5:B:41:PHE:HB3	5:B:190:MET:HE1	1.93	0.50
5:B:315:VAL:HG23	5:B:316:ARG:HG2	1.94	0.50
6:C:136:VAL:HG22	6:C:137:PRO:HA	1.92	0.50
14:L:35:ARG:C	14:L:35:ARG:HD3	2.36	0.50
23:U:13:ILE:HG12	23:U:32:CYS:HB3	1.93	0.50
1:0:241:A:C2	1:0:378:A:H4'	2.46	0.50
1:0:559:U:H2'	1:0:560:C:O4'	2.11	0.50
1:0:657:G:H2'	1:0:658:C:H6	1.75	0.50
1:0:1236:A:H2'	1:0:1237:U:O4'	2.11	0.50
1:0:1594:C:OP2	18:P:120:ARG:HD2	2.11	0.50
1:0:2419:U:H5''	1:0:2420:G:H5'	1.94	0.50
5:B:41:PHE:CD2	5:B:190:MET:HE3	2.47	0.50
5:B:304:PRO:CG	5:B:307:ARG:NH1	2.74	0.50
7:D:23:VAL:HG11	7:D:83:PHE:CZ	2.46	0.50
11:H:170:ASN:HD22	11:H:170:ASN:N	2.08	0.50
13:K:22:ASP:HB2	38:K:5264:HOH:O	2.10	0.50
14:L:54:PRO:HG2	14:L:57:VAL:CG2	2.41	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:L:148:GLU:HA	38:L:9371:HOH:O	2.10	0.50
1:O:263:U:O4'	9:F:59:ILE:HD13	2.11	0.50
1:O:2507:G:H2'	1:O:2510:C:H42	1.77	0.50
4:A:33:GLU:O	4:A:34:ASP:HB2	2.11	0.50
5:B:145:HIS:HD2	5:B:146:THR:O	1.94	0.50
7:D:35:ALA:C	7:D:37:ALA:H	2.18	0.50
16:N:67:ALA:C	16:N:69:TYR:N	2.69	0.50
20:R:18:LEU:HD12	20:R:143:VAL:CG1	2.42	0.50
1:O:113:A:OP2	1:O:114:A:H2'	2.11	0.50
2:9:3057:A:O2'	7:D:152:PRO:HD2	2.12	0.50
6:C:104:ASP:HA	6:C:107:ARG:NH1	2.27	0.50
6:C:237:GLU:HB2	38:C:9234:HOH:O	2.11	0.50
9:F:99:THR:HA	38:F:3461:HOH:O	2.11	0.50
17:O:38:ARG:HD3	38:O:7674:HOH:O	2.10	0.50
22:T:49:GLU:OE2	22:T:97:ARG:HD2	2.11	0.50
25:W:21:LEU:HD22	25:W:26:ILE:HD11	1.92	0.50
1:O:1289:C:O2'	1:O:1290:G:H5'	2.11	0.50
1:O:1304:U:H2'	1:O:1305:C:C6	2.47	0.50
1:O:1563:G:O2'	1:O:1564:C:OP2	2.25	0.50
1:O:1641:A:C2'	1:O:1642:A:H5'	2.42	0.50
8:E:24:GLY:HA3	8:E:76:VAL:HB	1.93	0.50
12:J:117:ASP:O	12:J:119:THR:HG23	2.12	0.50
14:L:54:PRO:HG2	14:L:57:VAL:HG21	1.93	0.50
26:X:18:ARG:NH1	38:X:4132:HOH:O	2.41	0.50
1:O:189:A:OP1	15:M:171:ARG:NH2	2.45	0.50
1:O:1205:U:H2'	1:O:1206:U:H5'	1.92	0.50
1:O:2353:A:H4'	1:O:2354:A:O5'	2.12	0.50
1:O:2851:G:C2'	1:O:2852:A:H5'	2.41	0.50
3:4:74:C:H2'	3:4:75:C:H5'	1.93	0.50
4:A:109:GLU:CD	4:A:113:GLY:H	2.20	0.50
6:C:72:LYS:HG2	6:C:77:ALA:HA	1.94	0.50
6:C:104:ASP:O	6:C:108:GLN:HG3	2.11	0.50
6:C:136:VAL:HA	6:C:137:PRO:C	2.37	0.50
15:M:122:GLN:OE1	15:M:127:LYS:HE2	2.11	0.50
16:N:73:ALA:HB1	16:N:74:PRO:HD2	1.93	0.50
16:N:77:ASN:OD1	16:N:79:PRO:HD2	2.12	0.50
1:O:1183:C:N4	1:O:1184:C:H41	2.09	0.50
1:O:2509:A:OP2	1:O:2510:C:H5	1.94	0.50
4:A:97:ALA:HB2	4:A:150:PRO:HB2	1.94	0.50
7:D:52:THR:N	7:D:70:GLY:O	2.45	0.50
13:K:72:VAL:HG11	13:K:121:PHE:CD1	2.46	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:M:99:ARG:HD2	15:M:167:GLY:CA	2.39	0.50
16:N:49:THR:HG22	16:N:56:ASP:HB2	1.94	0.50
29:1:25:LYS:HD2	30:2:49:GLU:N	2.26	0.50
1:0:475:G:OP1	6:C:73:LEU:HD22	2.12	0.49
5:B:147:VAL:HG12	5:B:150:ALA:H	1.76	0.49
6:C:129:HIS:HD2	6:C:165:ASP:OD2	1.95	0.49
9:F:31:LYS:HD3	9:F:89:LEU:HG	1.94	0.49
22:T:65:VAL:HG22	22:T:72:ILE:HG22	1.94	0.49
22:T:106:GLU:HG3	38:T:4913:HOH:O	2.12	0.49
24:V:64:GLY:O	24:V:65:ASP:CB	2.60	0.49
1:0:69:A:H5'	1:0:69:A:H8	1.77	0.49
1:0:396:U:O2'	1:0:418:C:H4'	2.12	0.49
1:0:944:G:H21	25:W:44:MET:CE	2.25	0.49
1:0:1180:U:H2'	1:0:1181:A:O4'	2.12	0.49
1:0:1593:C:OP1	18:P:117:SER:HB3	2.12	0.49
1:0:1730:G:C5'	1:0:1731:C:C6	2.95	0.49
12:J:19:MET:CE	12:J:132:LEU:HD11	2.38	0.49
12:J:75:PRO:HB3	12:J:132:LEU:HB3	1.95	0.49
16:N:49:THR:CG2	16:N:56:ASP:HB2	2.42	0.49
22:T:53:GLY:HA3	38:T:6384:HOH:O	2.11	0.49
23:U:6:CYS:C	23:U:8:TYR:H	2.20	0.49
1:0:316:A:H5'	22:T:54:ASP:OD2	2.12	0.49
1:0:1406:A:H4'	1:0:1407:A:H5''	1.93	0.49
6:C:139:VAL:CG2	6:C:240:LEU:HD12	2.43	0.49
13:K:20:CYS:HB2	13:K:29:LEU:HG	1.94	0.49
16:N:154:LEU:O	16:N:155:GLU:CB	2.60	0.49
18:P:38:GLU:HA	18:P:41:ARG:NH1	2.27	0.49
22:T:79:LEU:HG	22:T:89:ARG:HB2	1.94	0.49
31:3:18:GLN:OE1	31:3:73:GLU:HB3	2.13	0.49
1:0:500:G:H21	20:R:98:ASN:HD21	1.58	0.49
1:0:1701:A:H4'	1:0:1702:U:C5'	2.42	0.49
1:0:1735:C:OP2	5:B:234:ARG:HG3	2.12	0.49
1:0:2241:C:O2'	1:0:2242:U:H5'	2.12	0.49
1:0:2506:A:O2'	1:0:2507:G:O5'	2.30	0.49
38:0:5245:HOH:O	11:H:58:ARG:HG3	2.12	0.49
4:A:99:ILE:O	4:A:131:HIS:HE1	1.95	0.49
4:A:179:MET:HA	4:A:179:MET:HE3	1.94	0.49
15:M:80:GLY:O	15:M:81:ARG:HD3	2.12	0.49
16:N:47:LEU:CD1	16:N:97:VAL:HG11	2.42	0.49
17:O:25:VAL:HG23	17:O:26:TRP:N	2.26	0.49
19:Q:3:SER:HB3	38:Q:5998:HOH:O	2.13	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:T:48:VAL:CG1	22:T:49:GLU:N	2.74	0.49
26:X:30:MET:CE	26:X:55:ASN:HA	2.41	0.49
1:0:317:A:OP1	22:T:52:ARG:O	2.30	0.49
1:0:1537:C:H1'	38:0:6807:HOH:O	2.12	0.49
6:C:170:ASP:O	6:C:171:GLU:HG3	2.12	0.49
8:E:125:GLU:HB2	8:E:132:THR:CG2	2.43	0.49
15:M:57:LYS:HE2	15:M:140:ALA:O	2.12	0.49
18:P:55:LYS:CG	18:P:56:GLY:N	2.75	0.49
27:Y:123:VAL:HG12	27:Y:124:GLY:O	2.12	0.49
1:0:80:A:H3'	22:T:43:ASN:OD1	2.11	0.49
1:0:1166:A:H61	1:0:1180:U:H3	1.61	0.49
1:0:1804:A:H2'	1:0:1805:G:C8	2.48	0.49
1:0:2793:A:H2'	1:0:2794:G:H5'	1.94	0.49
2:9:3008:G:O6	16:N:11:ARG:NH1	2.46	0.49
4:A:132:ASP:OD1	4:A:133:ARG:N	2.45	0.49
5:B:243:ASN:HA	5:B:244:PRO:C	2.37	0.49
6:C:118:THR:HG22	6:C:137:PRO:HB3	1.94	0.49
7:D:159:PRO:O	7:D:163:VAL:HG23	2.13	0.49
8:E:106:ASN:ND2	8:E:109:GLY:HA2	2.27	0.49
12:J:107:ASN:ND2	12:J:109:TYR:H	2.11	0.49
13:K:101:ASN:HB2	13:K:103:ASP:OD2	2.13	0.49
16:N:86:LEU:HD12	16:N:125:ALA:HB2	1.94	0.49
25:W:60:GLU:O	25:W:63:GLU:HB2	2.13	0.49
27:Y:178:HIS:CG	27:Y:179:PRO:HD2	2.48	0.49
31:3:65:THR:HG23	31:3:67:LEU:HG	1.94	0.49
32:I:123:ASN:HA	32:I:126:LYS:HD2	1.94	0.49
1:0:542:A:H5'	1:0:542:A:C8	2.37	0.49
1:0:1086:A:N6	25:W:11:VAL:HG11	2.28	0.49
1:0:2834:G:OP1	26:X:39:LYS:HE2	2.12	0.49
2:9:3034:A:H2'	2:9:3035:C:O4'	2.12	0.49
5:B:248:ARG:O	5:B:251:VAL:HG13	2.13	0.49
15:M:134:ILE:O	15:M:136:PRO:HD3	2.13	0.49
17:O:96:VAL:CG1	17:O:100:GLN:HB2	2.43	0.49
25:W:126:ASP:HB3	25:W:135:GLY:O	2.12	0.49
1:0:371:U:H2'	1:0:372:A:C8	2.48	0.49
1:0:569:A:H5''	1:0:587:A:N1	2.27	0.49
1:0:894:A:C2	6:C:87:ARG:NH2	2.80	0.49
1:0:1311:G:O6	6:C:173:LYS:HE3	2.13	0.49
1:0:1787:C:H4'	1:0:2883:A:O4'	2.12	0.49
1:0:2587:OMU:O5'	1:0:2587:OMU:H6	2.13	0.49
1:0:2721:U:H4'	13:K:87:ARG:HG3	1.95	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:O:9527:HOH:O	4:A:11:ARG:HD3	2.13	0.49
6:C:25:PRO:HG2	38:C:9124:HOH:O	2.11	0.49
20:R:72:VAL:CG1	20:R:75:TRP:HB3	2.43	0.49
21:S:10:VAL:HG11	24:V:36:ALA:HA	1.94	0.49
23:U:17:THR:CG2	23:U:18:GLY:N	2.75	0.49
27:Y:200:THR:HG22	27:Y:201:GLU:CG	2.42	0.49
29:1:22:CYS:SG	29:1:24:GLU:HB2	2.53	0.49
32:I:132:CYS:C	32:I:134:SER:H	2.21	0.49
1:O:432:G:O2'	1:O:433:C:H5'	2.12	0.49
1:O:603:A:H5''	1:O:604:G:OP1	2.12	0.49
1:O:1393:A:H2'	1:O:1394:C:C6	2.48	0.49
1:O:2073:G:OP2	1:O:2490:A:H5'	2.13	0.49
1:O:2619:UR3:H6	1:O:2619:UR3:O5'	2.13	0.49
6:C:39:GLN:O	6:C:43:LYS:HD3	2.13	0.49
7:D:23:VAL:HG23	7:D:23:VAL:O	2.13	0.49
1:O:541:C:H2'	1:O:542:A:H5'	1.95	0.49
1:O:1878:G:H1'	38:O:6359:HOH:O	2.13	0.49
4:A:168:PRO:O	4:A:170:VAL:HG23	2.12	0.49
6:C:118:THR:O	6:C:136:VAL:HG13	2.13	0.49
8:E:7:ILE:HD11	8:E:11:VAL:C	2.37	0.49
14:L:81:VAL:HG12	14:L:82:ALA:N	2.28	0.49
15:M:47:ASP:CG	15:M:48:LYS:N	2.71	0.49
1:O:383:A:H4'	38:O:5588:HOH:O	2.13	0.48
1:O:482:G:H4'	1:O:508:A:N1	2.28	0.48
1:O:506:G:N2	1:O:509:A:H5'	2.20	0.48
38:O:6921:HOH:O	27:Y:165:GLU:HB3	2.11	0.48
5:B:132:HIS:CE1	5:B:171:VAL:HG21	2.48	0.48
5:B:180:ASP:O	5:B:181:ILE:C	2.55	0.48
6:C:47:GLY:HA2	6:C:92:PRO:HB2	1.94	0.48
8:E:101:GLU:HB2	8:E:116:THR:O	2.13	0.48
9:F:111:ILE:O	9:F:115:VAL:HG23	2.12	0.48
11:H:46:GLN:CB	11:H:167:PRO:HD2	2.22	0.48
11:H:80:GLU:HA	38:H:9182:HOH:O	2.13	0.48
13:K:125:ALA:C	13:K:127:ALA:H	2.21	0.48
20:R:39:THR:HG22	20:R:42:GLU:N	2.16	0.48
1:O:1206:U:H2'	1:O:1207:A:O4'	2.13	0.48
1:O:1636:G:O2'	1:O:1637:A:H5'	2.12	0.48
1:O:2269:C:H2'	1:O:2270:G:H5'	1.94	0.48
1:O:2890:A:C1'	23:U:56:ARG:NH2	2.72	0.48
4:A:211:LYS:CB	4:A:212:PRO:HD2	2.28	0.48
5:B:85:ARG:NH1	38:B:9431:HOH:O	2.45	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:H:83:TYR:CD1	11:H:83:TYR:C	2.91	0.48
11:H:120:ILE:N	11:H:120:ILE:CD1	2.76	0.48
30:2:41:HIS:CD2	30:2:44:ARG:H	2.27	0.48
1:0:214:U:H5'	38:0:6378:HOH:O	2.13	0.48
1:0:440:C:H2'	1:0:441:A:C8	2.48	0.48
1:0:777:U:HO2'	29:1:11:LYS:HG2	1.77	0.48
1:0:926:A:O2'	14:L:41:HIS:CD2	2.65	0.48
1:0:1507:C:H4'	38:0:3891:HOH:O	2.14	0.48
5:B:74:ILE:HD13	5:B:309:VAL:HG21	1.95	0.48
17:O:32:ARG:HH21	17:O:35:LYS:NZ	2.11	0.48
27:Y:184:GLU:OE2	27:Y:204:ARG:HD2	2.13	0.48
32:I:135:LEU:HB2	32:I:137:VAL:HG23	1.95	0.48
1:0:1053:G:OP1	11:H:12:PRO:HG3	2.12	0.48
1:0:2780:C:H1'	8:E:143:GLN:HE21	1.77	0.48
4:A:164:ARG:HA	28:Z:69:TYR:CE1	2.48	0.48
7:D:39:ASP:HB2	38:D:5583:HOH:O	2.14	0.48
8:E:31:ARG:NH1	38:E:5919:HOH:O	2.46	0.48
18:P:115:SER:OG	18:P:118:GLN:HG3	2.13	0.48
22:T:23:VAL:C	22:T:93:THR:HG21	2.38	0.48
22:T:26:THR:HA	22:T:39:ASN:HB3	1.94	0.48
25:W:14:HIS:HB2	25:W:17:ILE:HG13	1.95	0.48
1:0:920:C:H5''	1:0:921:G:O5'	2.13	0.48
1:0:1029:U:O2'	1:0:1273:C:OP1	2.29	0.48
1:0:2428:G:N7	31:3:60:LYS:HE2	2.29	0.48
4:A:53:ALA:HB3	38:A:9401:HOH:O	2.12	0.48
4:A:72:GLU:OE1	28:Z:72:GLU:HA	2.13	0.48
5:B:98:THR:HG22	5:B:99:GLU:N	2.26	0.48
5:B:132:HIS:HB2	5:B:137:LEU:HD22	1.95	0.48
6:C:185:LYS:HD3	6:C:186:TYR:CE1	2.49	0.48
8:E:116:THR:HG22	8:E:151:LEU:HD22	1.94	0.48
13:K:75:ARG:CZ	38:K:4172:HOH:O	2.61	0.48
22:T:41:ARG:HG2	22:T:41:ARG:HH11	1.79	0.48
24:V:55:ARG:O	24:V:59:ILE:HG12	2.14	0.48
25:W:13:MET:HE2	25:W:18:GLN:N	2.28	0.48
1:0:152:A:O2'	1:0:153:C:H5'	2.13	0.48
1:0:1132:A:N6	1:0:1229:C:H2'	2.29	0.48
1:0:1333:U:H2'	1:0:1334:C:C6	2.49	0.48
1:0:2561:C:OP1	8:E:153:ARG:NH2	2.46	0.48
4:A:32:VAL:HG22	4:A:38:ILE:HG13	1.95	0.48
4:A:105:VAL:HG11	4:A:154:ALA:CB	2.43	0.48
6:C:236:THR:HG21	38:C:9175:HOH:O	2.13	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:L:125:PHE:CZ	14:L:140:VAL:HG13	2.47	0.48
24:V:58:THR:O	24:V:62:GLU:HG3	2.13	0.48
30:2:22:PRO:HG2	30:2:25:VAL:CG2	2.42	0.48
1:0:558:C:H2'	1:0:559:U:C5'	2.41	0.48
1:0:1878:G:O2'	1:0:1879:U:C6	2.64	0.48
1:0:2362:A:H2'	1:0:2363:G:C8	2.48	0.48
7:D:163:VAL:HA	38:D:6326:HOH:O	2.13	0.48
8:E:20:ILE:HD11	8:E:40:VAL:CG1	2.44	0.48
9:F:99:THR:HG23	9:F:99:THR:O	2.13	0.48
11:H:154:TYR:C	11:H:154:TYR:HD1	2.22	0.48
21:S:57:THR:C	21:S:59:ASP:H	2.22	0.48
27:Y:155:ARG:NH1	38:Y:8147:HOH:O	2.47	0.48
27:Y:187:VAL:HG23	27:Y:192:ASP:HB3	1.92	0.48
1:0:319:A:H4'	1:0:338:C:C5	2.49	0.48
1:0:1168:C:H4'	38:I:5128:HOH:O	2.13	0.48
1:0:2015:A:H2'	1:0:2016:U:O4'	2.13	0.48
1:0:2541:U:H4'	1:0:2542:C:OP1	2.13	0.48
1:0:2898:G:H4'	5:B:288:GLY:HA2	1.95	0.48
2:9:3012:C:H5'	2:9:3070:U:O4'	2.12	0.48
6:C:102:LEU:HD12	38:C:9117:HOH:O	2.14	0.48
14:L:133:VAL:HB	38:L:9357:HOH:O	2.13	0.48
16:N:73:ALA:HB1	16:N:74:PRO:CD	2.43	0.48
19:Q:30:VAL:HG12	19:Q:30:VAL:O	2.13	0.48
22:T:24:ARG:NH2	22:T:39:ASN:HD22	2.12	0.48
1:0:1352:A:N1	6:C:48:SER:HB3	2.28	0.48
1:0:2478:U:O2'	1:0:2479:A:H5'	2.14	0.48
1:0:2783:A:H2'	1:0:2784:A:C8	2.49	0.48
8:E:16:ASP:O	8:E:17:HIS:HB2	2.13	0.48
11:H:9:ILE:HG12	11:H:56:GLN:CG	2.44	0.48
12:J:52:GLN:HG3	12:J:53:ILE:H	1.77	0.48
14:L:130:ARG:O	14:L:131:GLU:C	2.57	0.48
16:N:163:PHE:O	16:N:164:ASP:CG	2.56	0.48
24:V:11:MET:HB3	24:V:15:GLU:HB2	1.94	0.48
26:X:12:ILE:HB	26:X:70:ILE:HG22	1.95	0.48
1:0:1849:G:H1'	1:0:2011:A:N1	2.28	0.48
1:0:2269:C:C2'	1:0:2270:G:H5'	2.43	0.48
11:H:36:LYS:HA	11:H:84:LYS:HZ1	1.78	0.48
13:K:9:THR:O	13:K:10:GLN:C	2.57	0.48
21:S:53:ASN:HD22	21:S:53:ASN:N	2.09	0.48
25:W:3:ALA:O	25:W:54:PHE:HA	2.14	0.48
1:0:157:G:H4'	15:M:95:LYS:CE	2.43	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:396:U:OP2	31:3:38:ARG:HD2	2.13	0.47
1:0:832:U:H2'	1:0:833:G:C8	2.49	0.47
1:0:1568:G:O2'	1:0:1569:U:H5'	2.14	0.47
1:0:1942:A:H3'	38:0:7527:HOH:O	2.15	0.47
1:0:2472:C:O2'	1:0:2634:G:H4'	2.13	0.47
1:0:2846:C:H4'	5:B:156:LYS:HB3	1.96	0.47
5:B:72:THR:HB	38:B:9406:HOH:O	2.13	0.47
6:C:7:ASP:C	6:C:9:ASP:H	2.22	0.47
7:D:153:THR:HA	7:D:156:ARG:CG	2.43	0.47
7:D:159:PRO:O	7:D:162:ALA:HB3	2.14	0.47
17:O:45:LEU:HD12	17:O:88:LYS:HD2	1.95	0.47
31:3:16:GLU:HG3	31:3:18:GLN:HE21	1.79	0.47
1:0:1634:G:H2'	1:0:1635:U:C6	2.49	0.47
7:D:169:THR:C	7:D:170:TYR:HD1	2.22	0.47
8:E:132:THR:HB	38:E:2227:HOH:O	2.15	0.47
18:P:20:ARG:NH1	18:P:54:LYS:HD3	2.28	0.47
27:Y:151:SER:HB3	27:Y:154:ARG:CB	2.44	0.47
28:Z:81:ARG:O	28:Z:82:SER:C	2.56	0.47
1:0:558:C:C2'	1:0:559:U:C5'	2.92	0.47
1:0:1307:A:H2'	1:0:1308:A:C8	2.49	0.47
1:0:1940:C:H4'	38:0:7527:HOH:O	2.13	0.47
16:N:152:GLU:C	16:N:154:LEU:N	2.70	0.47
20:R:119:VAL:O	20:R:119:VAL:HG12	2.14	0.47
22:T:71:VAL:HG12	22:T:72:ILE:N	2.28	0.47
1:0:343:C:O2'	1:0:344:C:H5'	2.14	0.47
1:0:1120:U:H5'	1:0:1120:U:C6	2.40	0.47
1:0:1613:C:H2'	1:0:1614:G:O4'	2.14	0.47
1:0:2694:A:H4'	8:E:91:PHE:CE1	2.48	0.47
2:9:3028:U:H2'	2:9:3029:C:C6	2.48	0.47
7:D:135:VAL:HG22	7:D:136:ARG:H	1.79	0.47
15:M:48:LYS:HE3	15:M:52:GLN:NE2	2.29	0.47
32:I:133:THR:N	38:I:5371:HOH:O	2.47	0.47
1:0:621:C:H5'	27:Y:132:ASP:OD2	2.15	0.47
1:0:1825:U:O2'	1:0:1826:C:H5'	2.14	0.47
2:9:3114:G:H2'	2:9:3115:C:C6	2.50	0.47
4:A:211:LYS:NZ	38:A:9413:HOH:O	2.46	0.47
5:B:141:ARG:HG2	5:B:165:ARG:HA	1.97	0.47
7:D:138:GLY:N	38:D:7597:HOH:O	2.47	0.47
24:V:39:ALA:O	24:V:41:GLU:N	2.42	0.47
25:W:125:HIS:HE1	38:W:3071:HOH:O	1.97	0.47
32:I:129:VAL:HG13	32:I:139:ILE:CD1	2.41	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:731:U:H2'	1:0:732:C:C6	2.50	0.47
1:0:944:G:H21	25:W:44:MET:HE2	1.80	0.47
1:0:1925:G:O2'	1:0:1926:G:H5'	2.15	0.47
1:0:2379:G:H5'	1:0:2381:C:O4'	2.14	0.47
7:D:28:GLY:CA	7:D:69:ILE:HG23	2.42	0.47
7:D:58:VAL:HG12	7:D:60:GLU:HG2	1.96	0.47
8:E:37:ASP:OD1	12:J:125:SER:HB3	2.14	0.47
13:K:132:VAL:HG11	23:U:22:VAL:HG22	1.96	0.47
14:L:145:LEU:O	14:L:145:LEU:HD23	2.15	0.47
18:P:103:THR:O	18:P:106:ARG:HB3	2.15	0.47
28:Z:19:GLY:O	28:Z:23:ARG:HG2	2.15	0.47
1:0:1010:C:H4'	16:N:4:PRO:HB2	1.97	0.47
1:0:1427:A:H61	1:0:1440:U:C1'	2.27	0.47
1:0:1677:U:OP2	30:2:8:LYS:NZ	2.46	0.47
1:0:2547:C:OP2	5:B:5:ARG:NH1	2.47	0.47
1:0:2694:A:H4'	8:E:91:PHE:HE1	1.80	0.47
38:0:4353:HOH:O	5:B:27:ASN:HB2	2.14	0.47
4:A:192:VAL:HG13	38:A:9354:HOH:O	2.15	0.47
7:D:35:ALA:C	7:D:37:ALA:N	2.71	0.47
11:H:169:GLY:C	11:H:170:ASN:HD22	2.23	0.47
15:M:134:ILE:CG2	15:M:141:ILE:HD13	2.45	0.47
16:N:37:ARG:CZ	38:N:9334:HOH:O	2.62	0.47
21:S:42:GLU:HG2	21:S:49:VAL:HG23	1.95	0.47
22:T:73:HIS:CD2	22:T:88:PRO:HG3	2.49	0.47
28:Z:33:MET:SD	28:Z:49:ARG:HD2	2.54	0.47
30:2:40:ARG:HD2	30:2:47:THR:HG22	1.95	0.47
31:3:69:TYR:HB2	31:3:78:HIS:CE1	2.49	0.47
32:I:92:PRO:O	32:I:94:GLU:HG3	2.14	0.47
32:I:132:CYS:O	32:I:135:LEU:N	2.47	0.47
1:0:705:C:O2	1:0:705:C:H2'	2.15	0.47
1:0:1118:A:H8	1:0:1119:G:H5''	1.79	0.47
1:0:1462:C:H2'	1:0:1463:A:H8	1.78	0.47
1:0:1503:U:H2'	1:0:1504:A:O4'	2.15	0.47
1:0:1730:G:H5'	1:0:1731:C:H5	1.78	0.47
1:0:1890:U:H4'	1:0:2010:A:C6	2.50	0.47
4:A:36:ASP:HB2	4:A:84:VAL:N	2.30	0.47
4:A:217:ARG:CG	4:A:217:ARG:NH1	2.77	0.47
6:C:5:ILE:HD11	6:C:16:VAL:CG2	2.45	0.47
6:C:76:ARG:HH11	6:C:76:ARG:CG	2.28	0.47
13:K:99:ASP:OD1	13:K:101:ASN:N	2.43	0.47
1:0:394:G:H1	15:M:181:GLU:CD	2.23	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:945:U:O2'	25:W:43:GLY:HA3	2.14	0.47
1:0:1701:A:H5''	1:0:1702:U:H3'	1.97	0.47
1:0:2869:G:H2'	1:0:2870:C:C6	2.50	0.47
2:9:3001:U:O3'	2:9:3003:A:H5'	2.14	0.47
2:9:3029:C:C2'	2:9:3030:C:H5'	2.44	0.47
2:9:3076:G:C3'	2:9:3077:A:H5''	2.36	0.47
5:B:279:THR:OG1	5:B:290:VAL:HB	2.14	0.47
6:C:20:ASP:O	6:C:23:GLU:HB2	2.15	0.47
8:E:97:VAL:HG12	38:E:4191:HOH:O	2.15	0.47
9:F:56:PRO:HG2	15:M:44:THR:HA	1.95	0.47
12:J:74:ARG:HH12	12:J:76:ASP:HB2	1.76	0.47
1:0:284:C:H4'	1:0:285:A:O5'	2.15	0.47
1:0:659:A:N1	17:O:42:GLU:OE2	2.48	0.47
1:0:952:G:N3	1:0:2302:A:H2'	2.30	0.47
1:0:2668:G:H2'	1:0:2669:U:H6	1.77	0.47
1:0:2748:G:H2'	38:0:7705:HOH:O	2.15	0.47
2:9:3056:A:H1'	7:D:14:ARG:HG2	1.97	0.47
2:9:3107:C:H5	38:9:3167:HOH:O	1.97	0.47
4:A:48:ASP:HB3	38:A:9401:HOH:O	2.15	0.47
5:B:210:GLY:HA2	5:B:256:GLN:HE22	1.80	0.47
7:D:91:ALA:HB1	38:D:5198:HOH:O	2.15	0.47
8:E:84:MET:HG2	8:E:168:ILE:HD13	1.97	0.47
9:F:50:VAL:CG1	9:F:60:VAL:HG11	2.45	0.47
9:F:61:MET:HB3	15:M:19:GLN:OE1	2.14	0.47
16:N:5:ARG:HG3	19:Q:18:PRO:CB	2.44	0.47
1:0:100:C:H4'	22:T:16:LEU:HB2	1.98	0.46
1:0:947:U:H2'	1:0:948:G:C8	2.50	0.46
1:0:1419:U:H2'	1:0:1685:A:C2	2.51	0.46
1:0:1787:C:OP1	18:P:68:LYS:HE2	2.15	0.46
1:0:2545:U:OP2	5:B:2:GLN:HG2	2.14	0.46
2:9:3013:A:N3	16:N:14:ARG:NH2	2.57	0.46
5:B:41:PHE:HB3	5:B:190:MET:CE	2.45	0.46
9:F:4:VAL:HG13	9:F:76:PHE:CE1	2.50	0.46
9:F:37:THR:O	9:F:41:GLU:HG3	2.14	0.46
17:O:47:ARG:HA	17:O:50:ARG:NH1	2.30	0.46
20:R:61:GLN:CD	38:R:9341:HOH:O	2.58	0.46
20:R:113:HIS:O	20:R:145:LEU:HD12	2.15	0.46
21:S:57:THR:CG2	21:S:58:MET:N	2.78	0.46
30:2:10:ARG:HD2	30:2:49:GLU:OE2	2.15	0.46
1:0:352:A:H2'	1:0:353:G:C8	2.49	0.46
1:0:1162:G:H1'	32:I:117:LEU:CD1	2.37	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1285:U:H4'	25:W:74:GLU:OE1	2.15	0.46
10:G:71:LEU:C	10:G:73:ASP:N	2.73	0.46
11:H:66:ARG:HD3	38:H:9177:HOH:O	2.14	0.46
11:H:162:ARG:HD3	38:H:9180:HOH:O	2.14	0.46
13:K:81:ARG:HD3	13:K:87:ARG:CZ	2.45	0.46
20:R:19:ARG:HA	20:R:142:ASP:OD1	2.15	0.46
31:3:54:LYS:NZ	38:3:9328:HOH:O	2.47	0.46
1:0:669:G:O2'	1:0:670:G:H5'	2.16	0.46
1:0:1434:A:H2'	1:0:1436:C:C5	2.50	0.46
1:0:2534:C:H1'	38:0:3787:HOH:O	2.14	0.46
1:0:2840:A:H3'	38:0:7810:HOH:O	2.14	0.46
4:A:164:ARG:NE	38:A:9383:HOH:O	2.47	0.46
6:C:4:THR:HA	6:C:15:GLU:HB3	1.96	0.46
6:C:76:ARG:HH11	6:C:76:ARG:HG2	1.81	0.46
7:D:18:ILE:HD13	7:D:84:LEU:CD1	2.45	0.46
15:M:164:THR:HG23	15:M:166:ALA:N	2.30	0.46
16:N:69:TYR:CE2	16:N:184:ILE:HD11	2.51	0.46
26:X:10:VAL:HG12	26:X:11:THR:N	2.29	0.46
1:0:466:A:H2'	1:0:467:G:O4'	2.15	0.46
1:0:1187:U:H2'	38:0:7102:HOH:O	2.16	0.46
1:0:1759:A:N3	1:0:1818:C:H2'	2.31	0.46
1:0:2591:C:H2'	1:0:2592:G:O4'	2.15	0.46
1:0:2820:A:H2'	1:0:2821:C:C6	2.51	0.46
5:B:24:PRO:HG2	5:B:204:GLY:HA2	1.98	0.46
5:B:30:PRO:HB2	5:B:39:GLN:NE2	2.29	0.46
5:B:66:GLU:OE1	5:B:328:ARG:HD2	2.15	0.46
6:C:166:ILE:CD1	6:C:207:LEU:HD13	2.45	0.46
13:K:87:ARG:NH1	38:K:4066:HOH:O	2.48	0.46
14:L:35:ARG:O	14:L:40:PHE:HA	2.15	0.46
16:N:164:ASP:OD1	16:N:167:ASP:HA	2.15	0.46
17:O:39:THR:O	17:O:115:ARG:NH2	2.48	0.46
17:O:96:VAL:HG12	17:O:97:SER:N	2.30	0.46
18:P:101:GLN:HG3	38:P:164:HOH:O	2.16	0.46
20:R:30:ALA:HA	20:R:33:ARG:HH12	1.81	0.46
31:3:72:GLY:HA2	38:3:9373:HOH:O	2.15	0.46
1:0:20:G:H21	20:R:117:HIS:HD2	1.62	0.46
1:0:259:G:H21	15:M:58:GLN:NE2	2.14	0.46
1:0:308:U:C4	1:0:342:C:H1'	2.51	0.46
1:0:506:G:H22	1:0:509:A:H5''	1.79	0.46
1:0:945:U:H2'	1:0:946:C:H6	1.80	0.46
1:0:1521:C:H2'	1:0:1522:A:H8	1.80	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:G:67:LEU:O	10:G:71:LEU:HG	2.16	0.46
15:M:139:PRO:O	15:M:143:ASN:ND2	2.49	0.46
23:U:6:CYS:HB2	23:U:32:CYS:HB3	1.97	0.46
32:I:132:CYS:O	32:I:134:SER:N	2.49	0.46
1:O:166:A:N7	14:L:25:GLY:HA2	2.30	0.46
1:O:226:A:H1'	1:O:393:G:C5	2.50	0.46
1:O:853:C:H2'	1:O:854:G:O4'	2.15	0.46
1:O:1058:A:H2'	1:O:1060:C:C5'	2.43	0.46
1:O:1185:U:H5'	38:O:7636:HOH:O	2.16	0.46
1:O:1329:A:N1	36:O:9313:CL:CL	2.85	0.46
1:O:1545:C:H2'	1:O:1546:G:O4'	2.16	0.46
1:O:1603:A:H5'	1:O:1605:G:C4'	2.45	0.46
1:O:1919:A:H5'	38:O:6245:HOH:O	2.16	0.46
1:O:2421:G:H4'	38:O:5056:HOH:O	2.15	0.46
2:9:3014:G:O2'	16:N:1:ALA:HB2	2.15	0.46
7:D:173:GLU:O	7:D:174:VAL:C	2.58	0.46
15:M:61:ILE:HG22	15:M:62:VAL:N	2.31	0.46
15:M:159:VAL:HG13	15:M:160:PHE:N	2.30	0.46
16:N:34:LEU:HD22	16:N:129:ILE:HD13	1.97	0.46
26:X:43:VAL:CG1	26:X:47:ALA:HB3	2.45	0.46
29:1:28:HIS:HD2	29:1:30:LYS:H	1.62	0.46
32:I:132:CYS:C	32:I:134:SER:N	2.72	0.46
1:O:74:A:H2'	1:O:75:U:C6	2.51	0.46
1:O:522:U:O2'	1:O:1366:C:H5'	2.15	0.46
1:O:820:G:H5'	1:O:821:U:H5'	1.96	0.46
1:O:821:U:H2'	1:O:822:C:H6	1.80	0.46
1:O:1804:A:H2'	1:O:1805:G:H8	1.80	0.46
1:O:2521:A:OP2	11:H:3:ALA:HB3	2.15	0.46
1:O:2715:G:N2	5:B:264:GLU:OE1	2.45	0.46
1:O:2900:G:H2'	1:O:2901:C:O4'	2.16	0.46
38:9:3472:HOH:O	16:N:41:LYS:HD3	2.15	0.46
6:C:88:SER:O	6:C:91:PRO:HD3	2.15	0.46
7:D:25:MET:HE1	7:D:37:ALA:O	2.15	0.46
9:F:56:PRO:CG	15:M:44:THR:HA	2.45	0.46
14:L:17:SER:C	14:L:19:LYS:N	2.74	0.46
16:N:82:TYR:C	16:N:82:TYR:CD2	2.94	0.46
32:I:123:ASN:HA	32:I:126:LYS:CD	2.46	0.46
1:O:911:G:H5'	1:O:932:U:OP1	2.16	0.46
1:O:1385:G:O3'	26:X:49:ARG:NH1	2.49	0.46
1:O:1517:U:C2	1:O:1670:G:N2	2.84	0.46
6:C:12:THR:HB	38:C:9244:HOH:O	2.15	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:C:182:ARG:HD2	6:C:184:ARG:HH12	1.81	0.46
12:J:131:THR:HB	12:J:134:GLU:OE1	2.15	0.46
13:K:23:ASN:HD21	13:K:107:THR:HB	1.81	0.46
1:O:497:A:H2'	1:O:498:A:C5'	2.46	0.46
2:9:3049:G:H2'	2:9:3050:G:O4'	2.15	0.46
4:A:188:ASN:HA	38:A:9363:HOH:O	2.16	0.46
5:B:62:ARG:CA	5:B:65:MET:HE3	2.45	0.46
6:C:93:LYS:O	6:C:98:ARG:NH2	2.49	0.46
6:C:129:HIS:CE1	6:C:231:ARG:HA	2.50	0.46
7:D:67:ASP:O	7:D:69:ILE:HG13	2.16	0.46
11:H:78:GLY:C	11:H:80:GLU:H	2.24	0.46
11:H:114:ARG:O	11:H:115:ALA:C	2.59	0.46
12:J:108:PRO:HG2	12:J:109:TYR:CD1	2.51	0.46
16:N:34:LEU:HD13	16:N:47:LEU:HD21	1.97	0.46
18:P:15:ASP:O	18:P:16:VAL:HG23	2.16	0.46
26:X:27:ASP:OD2	26:X:27:ASP:N	2.48	0.46
31:3:42:ARG:HH11	31:3:42:ARG:HG3	1.80	0.46
1:O:671:A:O2'	1:O:672:G:H2'	2.16	0.46
1:O:960:G:N3	1:O:960:G:C2'	2.79	0.46
1:O:1072:G:P	27:Y:154:ARG:HH22	2.39	0.46
1:O:2338:G:OP1	7:D:97:GLN:HG2	2.15	0.46
4:A:96:LEU:HD22	4:A:128:LEU:HD13	1.97	0.46
5:B:56:ASP:OD1	5:B:322:ARG:HB3	2.15	0.46
5:B:195:ARG:N	5:B:198:GLU:OE1	2.50	0.46
7:D:25:MET:CE	7:D:37:ALA:HB1	2.45	0.46
7:D:64:ARG:CD	7:D:67:ASP:HB3	2.46	0.46
10:G:23:ILE:HD13	10:G:67:LEU:HD23	1.97	0.46
11:H:84:LYS:NZ	11:H:84:LYS:HB2	2.31	0.46
12:J:133:GLY:O	12:J:137:GLU:HG3	2.16	0.46
13:K:7:ASP:OD2	13:K:81:ARG:NH2	2.49	0.46
16:N:154:LEU:C	16:N:156:GLU:H	2.22	0.46
22:T:88:PRO:O	22:T:90:PRO:HD3	2.16	0.46
25:W:64:THR:O	25:W:68:THR:HG22	2.16	0.46
25:W:131:PRO:HD2	25:W:134:GLU:OE1	2.15	0.46
25:W:154:ARG:HE	25:W:154:ARG:HB3	1.53	0.46
29:1:25:LYS:HD2	30:2:48:ASP:CA	2.45	0.46
1:O:1184:C:O2'	1:O:1185:U:OP2	2.24	0.45
1:O:2420:G:O2'	1:O:2421:G:H5'	2.17	0.45
4:A:70:ALA:HA	4:A:71:PRO:HD3	1.80	0.45
5:B:314:ALA:HB3	5:B:317:PRO:HG3	1.98	0.45
9:F:1:PRO:HB2	38:F:5897:HOH:O	2.16	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:H:9:ILE:HG12	11:H:56:GLN:HG3	1.98	0.45
14:L:10:SER:O	14:L:11:ARG:HB3	2.16	0.45
17:O:45:LEU:CD1	17:O:88:LYS:HD2	2.45	0.45
28:Z:60:CYS:O	28:Z:61:ASP:HB2	2.17	0.45
29:1:28:HIS:CE1	29:1:31:LYS:HE2	2.51	0.45
29:1:45:ARG:NH2	38:1:9232:HOH:O	2.43	0.45
1:0:316:A:N3	1:0:336:G:O2'	2.45	0.45
1:0:553:G:O2'	27:Y:179:PRO:HG3	2.16	0.45
1:0:1666:C:C2'	1:0:1667:A:C5'	2.94	0.45
6:C:19:PRO:CB	6:C:244:ALA:HB2	2.45	0.45
11:H:38:LYS:HE2	11:H:42:ASP:HB2	1.97	0.45
11:H:58:ARG:HG3	11:H:58:ARG:NH1	2.27	0.45
11:H:171:ALA:HA	38:H:9168:HOH:O	2.17	0.45
13:K:66:ARG:HD3	38:K:2777:HOH:O	2.16	0.45
14:L:143:THR:CG2	14:L:144:ASP:N	2.79	0.45
15:M:122:GLN:HG3	15:M:122:GLN:O	2.15	0.45
25:W:38:THR:HG22	38:W:3580:HOH:O	2.16	0.45
32:I:92:PRO:C	32:I:94:GLU:N	2.74	0.45
1:0:2506:A:H1'	38:0:4035:HOH:O	2.15	0.45
13:K:6:ALA:HB2	13:K:116:GLU:HG2	1.98	0.45
19:Q:94:GLN:O	19:Q:95:GLU:HB2	2.16	0.45
19:Q:94:GLN:HG2	19:Q:95:GLU:OE1	2.17	0.45
22:T:40:VAL:HG23	22:T:119:ALA:C	2.41	0.45
1:0:86:A:C2	30:2:25:VAL:HG13	2.51	0.45
1:0:285:A:C2	1:0:368:C:H4'	2.51	0.45
1:0:1406:A:H4'	1:0:1407:A:C5'	2.46	0.45
4:A:36:ASP:HB2	4:A:83:GLY:C	2.41	0.45
5:B:149:ASP:HB2	38:B:9379:HOH:O	2.15	0.45
6:C:200:PRO:HB3	6:C:212:VAL:HG23	1.97	0.45
7:D:101:THR:O	7:D:157:LEU:HB3	2.16	0.45
16:N:43:VAL:CG1	16:N:118:ILE:HD11	2.44	0.45
19:Q:25:PRO:HA	19:Q:26:PRO:HD3	1.83	0.45
22:T:20:HIS:ND1	22:T:41:ARG:NE	2.60	0.45
31:3:3:MET:O	31:3:90:PHE:HA	2.16	0.45
1:0:35:U:H5'	6:C:47:GLY:O	2.17	0.45
1:0:1155:G:H2'	1:0:1156:C:C6	2.52	0.45
1:0:1641:A:H2'	1:0:1642:A:C5'	2.45	0.45
1:0:2404:G:OP1	19:Q:68:GLY:HA3	2.16	0.45
1:0:2589:U:H2'	1:0:2590:U:C6	2.51	0.45
2:9:3020:G:O2'	2:9:3021:G:H5'	2.16	0.45
2:9:3052:A:H2'	2:9:3053:G:O4'	2.17	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:7:ARG:HD3	5:B:9:GLY:O	2.16	0.45
6:C:236:THR:O	6:C:239:ALA:N	2.50	0.45
14:L:34:GLY:HA3	14:L:38:HIS:CE1	2.51	0.45
16:N:44:ARG:HG3	16:N:45:ALA:N	2.32	0.45
16:N:67:ALA:O	16:N:69:TYR:N	2.50	0.45
17:O:32:ARG:HH21	17:O:35:LYS:HD2	1.81	0.45
20:R:30:ALA:HA	20:R:33:ARG:NH1	2.31	0.45
25:W:65:VAL:HA	25:W:68:THR:CG2	2.46	0.45
1:O:710:G:O2'	1:O:711:G:H5'	2.16	0.45
5:B:82:VAL:HG12	5:B:101:TRP:CE3	2.51	0.45
5:B:145:HIS:HA	5:B:160:ASP:O	2.17	0.45
5:B:320:GLN:NE2	5:B:321:PRO:CD	2.79	0.45
14:L:126:SER:O	14:L:127:GLU:C	2.57	0.45
15:M:32:ARG:NH2	38:M:9391:HOH:O	2.49	0.45
18:P:45:ASP:C	18:P:47:GLY:H	2.24	0.45
26:X:36:HIS:CE1	26:X:40:HIS:CD2	3.05	0.45
32:I:93:GLN:HA	32:I:96:PHE:CE2	2.45	0.45
1:O:1185:U:O2'	1:O:1186:C:H5'	2.17	0.45
1:O:1279:U:O2	1:O:1279:U:H2'	2.17	0.45
1:O:1298:U:H2'	1:O:1299:G:C8	2.51	0.45
1:O:2050:G:H5''	20:R:80:TYR:O	2.17	0.45
2:9:3056:A:C3'	2:9:3057:A:H5''	2.45	0.45
4:A:8:ARG:NH1	38:A:9349:HOH:O	2.45	0.45
4:A:103:VAL:O	4:A:105:VAL:HG23	2.16	0.45
5:B:313:PRO:O	5:B:314:ALA:C	2.59	0.45
6:C:138:VAL:O	6:C:234:VAL:HA	2.16	0.45
14:L:65:ASP:CG	14:L:111:ALA:HB3	2.41	0.45
17:O:32:ARG:HG2	38:O:2336:HOH:O	2.16	0.45
17:O:44:ASN:OD1	17:O:65:LEU:HB2	2.17	0.45
19:Q:64:GLU:OE1	19:Q:64:GLU:HA	2.17	0.45
25:W:4:LEU:HD23	25:W:4:LEU:HA	1.75	0.45
1:O:1573:A:H2'	1:O:1574:C:O4'	2.16	0.45
1:O:1874:U:P	4:A:51:ARG:HD2	2.57	0.45
1:O:2039:A:OP2	5:B:234:ARG:NH2	2.50	0.45
1:O:2045:G:H2'	1:O:2046:G:O4'	2.17	0.45
1:O:2424:U:H1'	19:Q:7:LEU:HD12	1.99	0.45
1:O:2781:U:H1'	8:E:139:GLU:OE2	2.16	0.45
1:O:2812:A:C2	1:O:2814:A:N6	2.72	0.45
5:B:248:ARG:NH2	38:B:9325:HOH:O	2.49	0.45
12:J:75:PRO:HD3	12:J:136:SER:OG	2.16	0.45
14:L:89:PHE:CD1	14:L:89:PHE:N	2.84	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:L:97:VAL:O	14:L:100:ALA:HB2	2.16	0.45
19:Q:32:GLU:HA	19:Q:71:TYR:OH	2.17	0.45
20:R:39:THR:O	20:R:40:ALA:C	2.59	0.45
1:O:1666:C:H2'	1:O:1667:A:C5'	2.46	0.45
1:O:1730:G:C5'	1:O:1731:C:H6	2.30	0.45
1:O:1790:C:H2'	1:O:1791:U:C6	2.50	0.45
1:O:1855:G:H4'	1:O:1856:C:O5'	2.16	0.45
6:C:218:VAL:HG12	38:C:9228:HOH:O	2.16	0.45
7:D:15:GLU:HA	7:D:16:PRO:HD3	1.83	0.45
7:D:167:GLU:OE2	7:D:173:GLU:HG2	2.17	0.45
9:F:48:VAL:HG12	9:F:97:ALA:HB2	1.99	0.45
15:M:61:ILE:CG2	15:M:62:VAL:N	2.80	0.45
16:N:163:PHE:O	16:N:164:ASP:OD1	2.35	0.45
19:Q:10:THR:O	19:Q:11:ARG:C	2.60	0.45
20:R:33:ARG:NH1	38:R:9344:HOH:O	2.49	0.45
21:S:52:VAL:HG22	21:S:66:VAL:HG13	1.98	0.45
26:X:43:VAL:CG1	26:X:44:ASP:N	2.79	0.45
32:I:113:HIS:NE2	32:I:121:LEU:HD22	2.32	0.45
1:O:21:G:H5''	20:R:1:GLY:O	2.17	0.45
1:O:222:A:H2'	1:O:223:G:O4'	2.17	0.45
1:O:746:A:C6	17:O:65:LEU:HD13	2.52	0.45
1:O:902:G:N7	14:L:18:HIS:CD2	2.83	0.45
1:O:1185:U:H2'	1:O:1186:C:C6	2.51	0.45
1:O:1293:U:O2'	27:Y:149:GLN:NE2	2.46	0.45
1:O:1425:G:O2'	1:O:1426:C:H5'	2.17	0.45
4:A:53:ALA:HB1	4:A:54:PRO:HD2	1.99	0.45
7:D:170:TYR:CD1	7:D:170:TYR:N	2.85	0.45
10:G:64:ASN:ND2	10:G:64:ASN:H	2.15	0.45
20:R:113:HIS:HE1	20:R:144:GLU:CD	2.25	0.45
22:T:64:ASN:HB3	22:T:73:HIS:HB2	1.98	0.45
31:3:31:THR:HB	31:3:33:MET:HE3	1.98	0.45
1:O:1098:A:H2'	1:O:1099:G:O4'	2.17	0.44
1:O:2404:G:OP1	19:Q:69:ASP:N	2.46	0.44
38:O:6984:HOH:O	16:N:5:ARG:HB2	2.17	0.44
2:9:3035:C:H5''	38:9:4078:HOH:O	2.16	0.44
5:B:137:LEU:HD21	5:B:140:LEU:HD21	1.98	0.44
6:C:115:LEU:CD2	6:C:243:VAL:HG13	2.45	0.44
6:C:132:ASP:HB2	6:C:161:ASP:HB3	1.98	0.44
9:F:28:ALA:CB	9:F:99:THR:HG23	2.47	0.44
13:K:110:LYS:O	13:K:111:GLY:O	2.34	0.44
19:Q:37:GLU:OE1	19:Q:93:ARG:NE	2.49	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:W:110:GLN:NE2	25:W:110:GLN:HA	2.32	0.44
1:0:170:U:H2'	1:0:171:C:H5'	1.99	0.44
1:0:303:C:H2'	1:0:304:G:O4'	2.17	0.44
1:0:558:C:C2'	1:0:559:U:H5''	2.46	0.44
1:0:694:A:H4'	1:0:2441:U:OP1	2.18	0.44
1:0:877:G:H1'	38:0:9479:HOH:O	2.17	0.44
1:0:949:U:O2'	19:Q:40:HIS:HE1	2.00	0.44
1:0:1209:C:H2'	1:0:1210:G:H8	1.82	0.44
1:0:1486:A:C5	30:2:2:LYS:HG3	2.52	0.44
1:0:2699:A:H2'	1:0:2700:G:O4'	2.16	0.44
9:F:48:VAL:CG2	9:F:74:PHE:HB3	2.47	0.44
13:K:68:VAL:O	13:K:68:VAL:HG12	2.17	0.44
22:T:18:GLU:O	22:T:21:LYS:HE2	2.17	0.44
31:3:69:TYR:CE1	31:3:80:ARG:HD2	2.52	0.44
1:0:1205:U:C2'	1:0:1206:U:C5'	2.95	0.44
1:0:1496:G:H5'	1:0:1572:A:H1'	1.98	0.44
1:0:1589:G:N2	1:0:1605:G:H1'	2.33	0.44
1:0:1803:C:H2'	1:0:1804:A:C8	2.52	0.44
1:0:2044:G:OP1	26:X:23:HIS:HE1	2.00	0.44
1:0:2301:A:H5''	1:0:2302:A:H5'	1.98	0.44
38:0:4497:HOH:O	13:K:2:GLU:HA	2.17	0.44
2:9:3002:U:P	2:9:3003:A:H5'	2.58	0.44
4:A:33:GLU:OE1	4:A:33:GLU:N	2.47	0.44
5:B:207:LYS:HG2	5:B:304:PRO:HB3	1.99	0.44
11:H:170:ASN:N	11:H:170:ASN:ND2	2.66	0.44
12:J:42:GLU:O	12:J:131:THR:HG23	2.18	0.44
16:N:115:VAL:HG23	16:N:116:PHE:N	2.31	0.44
17:O:26:TRP:HA	17:O:26:TRP:CE3	2.53	0.44
18:P:142:ASP:O	18:P:143:ALA:O	2.35	0.44
1:0:162:C:H2'	1:0:163:U:H5'	2.00	0.44
1:0:299:U:H5'	38:0:7516:HOH:O	2.16	0.44
1:0:604:G:H2'	38:0:7912:HOH:O	2.17	0.44
1:0:827:A:H2'	1:0:828:G:O4'	2.17	0.44
1:0:920:C:H5'	1:0:921:G:C4	2.53	0.44
1:0:1398:G:O2'	1:0:1399:A:H5'	2.18	0.44
1:0:1477:C:H5'	1:0:1868:G:H5''	2.00	0.44
1:0:2781:U:C2'	1:0:2782:G:H5'	2.47	0.44
1:0:2795:C:O2'	1:0:2796:U:H5'	2.18	0.44
6:C:103:ASN:HB3	38:C:9109:HOH:O	2.18	0.44
13:K:96:VAL:HG21	13:K:109:LEU:HD22	1.99	0.44
16:N:179:LEU:HD23	16:N:184:ILE:HD12	1.99	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:T:14:ALA:HA	22:T:15:PRO:HD3	1.87	0.44
22:T:41:ARG:NH1	22:T:42:VAL:O	2.51	0.44
32:I:89:SER:HB3	32:I:97:VAL:HG23	1.98	0.44
1:O:290:C:O2'	1:O:291:C:H5'	2.17	0.44
1:O:794:U:H3	1:O:819:A:H61	1.66	0.44
1:O:958:G:H2'	1:O:959:C:C6	2.53	0.44
1:O:1131:G:C6	1:O:1230:A:C4	3.05	0.44
4:A:199:HIS:HD2	4:A:201:PHE:H	1.65	0.44
4:A:212:PRO:HB2	38:A:9357:HOH:O	2.17	0.44
5:B:102:THR:CG2	5:B:182:VAL:HG12	2.48	0.44
5:B:125:GLU:OE2	5:B:129:ARG:NH1	2.51	0.44
7:D:25:MET:HE1	7:D:37:ALA:HB1	1.99	0.44
17:O:32:ARG:HH21	17:O:35:LYS:CD	2.31	0.44
18:P:38:GLU:HA	18:P:41:ARG:HH11	1.82	0.44
31:3:25:VAL:HG13	31:3:68:LYS:HE3	2.00	0.44
1:O:484:A:N1	1:O:506:G:H4'	2.33	0.44
1:O:825:U:H5''	1:O:826:U:OP1	2.18	0.44
1:O:1119:G:C8	12:J:52:GLN:NE2	2.85	0.44
1:O:2092:G:H2'	1:O:2613:G:OP1	2.18	0.44
1:O:2271:G:N3	1:O:2271:G:H2'	2.33	0.44
4:A:87:GLU:HB3	38:A:9415:HOH:O	2.16	0.44
5:B:175:LEU:O	5:B:175:LEU:HD23	2.18	0.44
6:C:19:PRO:HB3	6:C:244:ALA:HB2	2.00	0.44
24:V:31:ARG:NE	38:V:2682:HOH:O	2.51	0.44
25:W:6:GLN:HA	25:W:52:VAL:HG23	1.99	0.44
32:I:99:ASP:O	32:I:100:LEU:HG	2.18	0.44
1:O:106:A:H2'	1:O:107:U:O4'	2.18	0.44
1:O:1525:G:H5'	1:O:1526:A:OP2	2.17	0.44
1:O:2670:G:O2'	1:O:2671:U:H5'	2.17	0.44
1:O:2769:C:H2'	1:O:2770:G:C5'	2.48	0.44
38:O:5004:HOH:O	16:N:21:HIS:HD2	2.01	0.44
2:9:3053:G:O2'	2:9:3054:A:H5'	2.18	0.44
4:A:36:ASP:O	4:A:38:ILE:N	2.50	0.44
5:B:310:ARG:HB3	38:B:9444:HOH:O	2.16	0.44
15:M:159:VAL:HG12	36:M:9318:CL:CL	2.54	0.44
16:N:37:ARG:NH2	38:N:9334:HOH:O	2.51	0.44
20:R:82:GLU:HG3	20:R:83:LYS:N	2.32	0.44
20:R:100:ASP:C	20:R:102:GLN:N	2.74	0.44
22:T:78:THR:HB	22:T:87:VAL:O	2.18	0.44
24:V:12:THR:HG23	24:V:14:ALA:H	1.83	0.44
29:1:8:GLN:HE22	29:1:11:LYS:HZ1	1.60	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:1:8:GLN:NE2	29:1:11:LYS:HZ2	2.11	0.44
1:0:64:G:H2'	1:0:65:C:O4'	2.18	0.44
1:0:1135:G:H5'	38:0:6173:HOH:O	2.18	0.44
1:0:2112:A:H2'	1:0:2113:G:C8	2.53	0.44
1:0:2312:G:H2'	1:0:2313:C:H5'	1.99	0.44
1:0:2314:G:C2'	1:0:2315:C:H5'	2.47	0.44
1:0:2451:G:O2'	31:3:38:ARG:NH2	2.51	0.44
6:C:19:PRO:HG2	6:C:22:PHE:CE1	2.53	0.44
6:C:54:LEU:HD23	6:C:79:ARG:HG3	1.98	0.44
13:K:113:ILE:HD12	13:K:128:ALA:HB2	2.00	0.44
16:N:147:ILE:HG23	16:N:148:ALA:N	2.33	0.44
19:Q:32:GLU:O	19:Q:93:ARG:NH2	2.51	0.44
1:0:820:G:C5	4:A:171:LYS:HB2	2.53	0.44
1:0:1334:C:H2'	1:0:1335:C:H6	1.83	0.44
1:0:1596:U:H2'	1:0:1598:A:OP2	2.17	0.44
1:0:1711:A:O2'	1:0:1712:A:H5'	2.18	0.44
1:0:2467:A:O2'	1:0:2468:A:H2'	2.17	0.44
4:A:165:THR:O	4:A:165:THR:HG22	2.17	0.44
4:A:192:VAL:HB	38:A:9387:HOH:O	2.18	0.44
5:B:84:LEU:HD13	5:B:84:LEU:C	2.43	0.44
13:K:118:ALA:C	13:K:120:ARG:N	2.76	0.44
14:L:91:VAL:HB	38:L:9358:HOH:O	2.17	0.44
1:0:445:U:H2'	1:0:446:G:H8	1.82	0.43
1:0:794:U:H2'	1:0:795:G:H5'	2.00	0.43
1:0:816:G:C6	1:0:817:G:N1	2.86	0.43
1:0:941:G:C5	1:0:942:U:C4	3.06	0.43
1:0:2326:U:H4'	1:0:2412:G:H4'	2.00	0.43
38:0:4890:HOH:O	17:O:35:LYS:HD3	2.18	0.43
6:C:84:VAL:O	6:C:85:LYS:HB2	2.17	0.43
8:E:107:PHE:CE1	8:E:152:THR:HB	2.52	0.43
8:E:145:ALA:HB1	8:E:168:ILE:CD1	2.47	0.43
14:L:134:GLU:HG3	38:L:9357:HOH:O	2.18	0.43
15:M:68:ARG:O	15:M:68:ARG:HD3	2.17	0.43
16:N:42:HIS:CG	16:N:62:HIS:HE1	2.36	0.43
16:N:62:HIS:O	16:N:65:ASP:OD1	2.35	0.43
16:N:86:LEU:HD21	16:N:180:LEU:CD1	2.48	0.43
16:N:86:LEU:O	16:N:90:LEU:HG	2.18	0.43
16:N:127:LEU:HB2	38:N:9356:HOH:O	2.17	0.43
17:O:38:ARG:NH1	38:O:7674:HOH:O	2.51	0.43
23:U:14:GLU:OE1	23:U:15:PRO:HD2	2.17	0.43
23:U:25:ASP:OD2	23:U:25:ASP:C	2.61	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:X:76:ARG:NH1	26:X:76:ARG:CG	2.74	0.43
1:O:474:C:O3'	6:C:73:LEU:HD21	2.17	0.43
1:O:757:C:OP1	14:L:27:ARG:HD2	2.16	0.43
1:O:2050:G:OP1	20:R:79:ARG:HB3	2.18	0.43
6:C:236:THR:HA	38:C:9252:HOH:O	2.18	0.43
7:D:76:ARG:O	7:D:77:ASP:HB2	2.18	0.43
14:L:93:VAL:HG12	14:L:97:VAL:HG23	2.00	0.43
16:N:71:TRP:HE3	16:N:175:LEU:HD22	1.82	0.43
18:P:59:ARG:NH2	18:P:66:GLN:NE2	2.62	0.43
20:R:18:LEU:HG	20:R:91:LEU:HD13	1.99	0.43
26:X:74:ALA:HB2	26:X:85:VAL:HG13	1.99	0.43
1:O:1850:U:H2'	1:O:1851:G:C8	2.53	0.43
4:A:128:LEU:HG	38:A:9366:HOH:O	2.18	0.43
5:B:109:LEU:CG	5:B:113:LEU:HD12	2.49	0.43
6:C:49:ASP:HB3	6:C:52:ALA:HB2	1.99	0.43
8:E:20:ILE:HD12	8:E:33:LEU:HD12	2.00	0.43
11:H:9:ILE:HG23	11:H:126:ARG:NE	2.33	0.43
11:H:59:HIS:HA	11:H:62:LEU:HD23	1.98	0.43
11:H:146:VAL:HG22	38:H:9174:HOH:O	2.19	0.43
14:L:21:ARG:N	38:L:9330:HOH:O	2.51	0.43
14:L:121:ILE:HA	14:L:141:GLU:O	2.18	0.43
18:P:27:ARG:O	18:P:31:ILE:HG13	2.18	0.43
22:T:48:VAL:HG13	22:T:97:ARG:C	2.44	0.43
26:X:43:VAL:HG12	26:X:47:ALA:HB3	2.00	0.43
27:Y:187:VAL:HG12	27:Y:205:ILE:HA	2.00	0.43
30:2:35:ARG:HB2	38:2:2691:HOH:O	2.18	0.43
32:I:110:GLU:HA	32:I:113:HIS:NE2	2.34	0.43
1:O:136:C:P	15:M:39:ARG:HH22	2.42	0.43
1:O:541:C:O2'	1:O:542:A:H5''	2.19	0.43
1:O:690:G:H4'	1:O:741:C:O2	2.19	0.43
1:O:1375:A:C2'	1:O:1376:G:H5'	2.48	0.43
1:O:1768:C:H2'	1:O:1769:C:H5'	2.00	0.43
6:C:5:ILE:HG23	38:C:9234:HOH:O	2.18	0.43
6:C:79:ARG:O	6:C:87:ARG:HG2	2.17	0.43
6:C:184:ARG:NE	38:C:9216:HOH:O	2.51	0.43
7:D:49:PRO:HA	7:D:73:VAL:HG22	2.00	0.43
7:D:52:THR:HB	7:D:70:GLY:C	2.43	0.43
9:F:36:THR:O	9:F:40:ILE:HG13	2.19	0.43
11:H:43:TYR:HA	11:H:44:PRO:HD3	1.76	0.43
17:O:26:TRP:HA	17:O:26:TRP:HE3	1.82	0.43
24:V:7:GLU:O	24:V:11:MET:HG3	2.18	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:W:65:VAL:HG12	25:W:116:LEU:HD13	1.99	0.43
31:3:65:THR:CG2	31:3:67:LEU:HG	2.48	0.43
1:0:922:A:N7	1:0:2281:C:H5'	2.33	0.43
1:0:2719:A:C2	5:B:70:PRO:HG3	2.53	0.43
5:B:13:PHE:N	38:B:9416:HOH:O	2.47	0.43
5:B:147:VAL:HG12	5:B:147:VAL:O	2.19	0.43
6:C:19:PRO:HD2	6:C:240:LEU:CD2	2.49	0.43
8:E:47:VAL:HG11	8:E:69:ILE:HD13	2.01	0.43
9:F:34:ASN:HA	15:M:4:ALA:HB2	2.01	0.43
25:W:88:THR:CG2	25:W:89:ASP:H	2.22	0.43
30:2:40:ARG:HG3	30:2:45:ASN:CB	2.48	0.43
1:0:244:C:OP2	9:F:38:LYS:HE3	2.19	0.43
1:0:661:G:C5	1:0:686:A:C2	3.07	0.43
1:0:737:A:H2'	1:0:738:G:O4'	2.18	0.43
1:0:1398:G:H2'	1:0:1399:A:C8	2.53	0.43
1:0:1772:C:H5'	1:0:1773:G:C5	2.53	0.43
1:0:2754:G:H2'	1:0:2755:G:O4'	2.18	0.43
1:0:2781:U:H2'	1:0:2782:G:H5'	1.99	0.43
1:0:2909:G:H2'	1:0:2910:A:C8	2.52	0.43
5:B:148:PRO:HD2	38:B:9379:HOH:O	2.18	0.43
8:E:93:MET:HE2	8:E:107:PHE:CD1	2.54	0.43
13:K:29:LEU:HB3	13:K:55:VAL:CG1	2.42	0.43
13:K:49:LEU:HA	13:K:73:VAL:HG12	2.00	0.43
15:M:184:ARG:HG3	15:M:185:PRO:HA	2.01	0.43
20:R:119:VAL:HG21	20:R:142:ASP:CG	2.43	0.43
26:X:21:PRO:HG2	26:X:24:LYS:HD3	1.99	0.43
1:0:363:A:O2'	1:0:364:C:H5'	2.18	0.43
1:0:1151:G:OP2	10:G:65:THR:HG21	2.19	0.43
4:A:194:MET:HE1	38:A:9315:HOH:O	2.19	0.43
5:B:26:PHE:HE1	38:B:9444:HOH:O	2.00	0.43
8:E:3:VAL:CG2	8:E:49:ILE:HB	2.44	0.43
8:E:77:THR:OG1	8:E:78:GLU:N	2.48	0.43
8:E:81:GLU:O	8:E:172:PRO:HD3	2.18	0.43
25:W:146:ILE:HG23	25:W:150:LEU:HD12	2.00	0.43
26:X:12:ILE:HB	26:X:70:ILE:CG2	2.48	0.43
1:0:204:A:C2'	1:0:205:U:H5'	2.49	0.43
1:0:470:U:O2'	29:1:16:HIS:CD2	2.68	0.43
1:0:635:A:H2'	1:0:636:G:H5''	2.01	0.43
1:0:766:A:H5'	38:0:4926:HOH:O	2.18	0.43
1:0:1007:A:H2'	11:H:19:TYR:CZ	2.54	0.43
1:0:1174:A:C5	1:0:1201:C:H4'	2.53	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1594:C:O2'	1:0:1607:A:H4'	2.19	0.43
1:0:1852:A:H4'	4:A:230:SER:HB2	2.00	0.43
1:0:2241:C:H2'	1:0:2242:U:H6	1.81	0.43
1:0:2264:A:H2'	1:0:2265:U:C6	2.54	0.43
1:0:2382:A:H5'	38:0:5017:HOH:O	2.18	0.43
1:0:2531:U:O2'	1:0:2532:A:H5'	2.19	0.43
4:A:35:GLY:O	4:A:36:ASP:CB	2.67	0.43
6:C:162:VAL:CG1	6:C:192:ILE:HD11	2.49	0.43
7:D:58:VAL:HB	7:D:62:ASP:HB3	2.01	0.43
8:E:132:THR:HG23	8:E:132:THR:O	2.19	0.43
9:F:48:VAL:HG23	9:F:74:PHE:CB	2.49	0.43
11:H:112:GLY:N	38:H:9185:HOH:O	2.52	0.43
12:J:130:VAL:HG12	12:J:131:THR:H	1.84	0.43
13:K:72:VAL:O	13:K:95:ALA:HA	2.18	0.43
25:W:1:MET:N	25:W:103:GLU:OE2	2.47	0.43
1:0:677:C:O2'	1:0:678:G:H5'	2.18	0.43
1:0:1943:C:O4'	4:A:212:PRO:HA	2.18	0.43
38:0:3098:HOH:O	13:K:39:GLY:HA3	2.18	0.43
4:A:140:LEU:HB3	4:A:141:PRO:HD2	2.00	0.43
7:D:140:ARG:O	7:D:144:ARG:HG2	2.19	0.43
16:N:62:HIS:HB3	16:N:65:ASP:OD1	2.19	0.43
17:O:47:ARG:HG3	17:O:47:ARG:NH1	2.32	0.43
25:W:54:PHE:CZ	25:W:140:LYS:HB2	2.54	0.43
27:Y:144:ARG:HG3	27:Y:144:ARG:HH11	1.84	0.43
32:I:113:HIS:N	32:I:114:PRO:HD2	2.33	0.43
1:0:10:U:O4	1:0:532:A:OP2	2.37	0.43
1:0:553:G:P	27:Y:204:ARG:NH2	2.89	0.43
1:0:1080:C:O5'	1:0:1080:C:H6	2.01	0.43
1:0:1123:A:C6	1:0:1238:C:H5'	2.54	0.43
1:0:2070:G:H2'	1:0:2072:G:OP1	2.18	0.43
1:0:2785:C:H4'	1:0:2786:G:OP2	2.18	0.43
5:B:103:ASP:HB2	38:B:9395:HOH:O	2.19	0.43
5:B:217:ARG:CD	5:B:257:THR:HG22	2.49	0.43
6:C:107:ARG:HB3	6:C:107:ARG:CZ	2.49	0.43
8:E:156:ASP:OD2	8:E:157:LYS:NZ	2.46	0.43
25:W:73:LEU:HD12	25:W:73:LEU:HA	1.76	0.43
28:Z:56:GLN:HG3	28:Z:62:TYR:O	2.19	0.43
1:0:177:A:H2'	1:0:178:U:O4'	2.18	0.42
1:0:288:A:H61	1:0:364:C:H42	1.67	0.42
1:0:1095:U:O2	25:W:120:PRO:HG2	2.19	0.42
1:0:1603:A:H5''	1:0:1605:G:H5'	2.00	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1617:C:C4	1:0:1643:C:H4'	2.54	0.42
1:0:1675:C:H5''	30:2:5:LYS:HD2	2.01	0.42
1:0:2265:U:H2'	1:0:2266:A:H8	1.84	0.42
1:0:2791:U:H1'	1:0:2792:A:H5''	2.00	0.42
4:A:123:GLY:HA3	4:A:162:GLY:HA2	2.01	0.42
5:B:66:GLU:HG2	38:B:9443:HOH:O	2.18	0.42
6:C:5:ILE:HA	6:C:139:VAL:HG12	2.01	0.42
6:C:37:ALA:O	6:C:41:ASN:ND2	2.51	0.42
7:D:11:HIS:CG	7:D:12:GLU:N	2.87	0.42
20:R:114:VAL:HA	20:R:144:GLU:O	2.19	0.42
24:V:12:THR:O	24:V:13:PRO:C	2.62	0.42
31:3:75:GLY:HA2	38:3:9358:HOH:O	2.18	0.42
1:0:451:C:C2'	1:0:452:G:H5'	2.49	0.42
1:0:1236:A:C8	12:J:63:ILE:HD11	2.53	0.42
1:0:1829:A:H5''	38:0:3377:HOH:O	2.18	0.42
1:0:2489:G:H1'	38:0:7457:HOH:O	2.19	0.42
5:B:154:VAL:HA	5:B:155:PRO:HD3	1.84	0.42
13:K:14:LYS:HD2	13:K:45:PRO:HG3	2.01	0.42
20:R:100:ASP:C	20:R:102:GLN:H	2.26	0.42
27:Y:144:ARG:HH11	27:Y:144:ARG:CG	2.32	0.42
28:Z:60:CYS:SG	28:Z:62:TYR:HB2	2.59	0.42
1:0:23:G:H1'	1:0:520:A:N6	2.35	0.42
1:0:907:A:H4'	1:0:1328:A:C2	2.54	0.42
1:0:1051:C:H2'	1:0:1052:G:O4'	2.20	0.42
1:0:1306:U:OP1	6:C:184:ARG:HD2	2.19	0.42
1:0:1903:U:O2'	1:0:1904:A:N7	2.50	0.42
1:0:2326:U:H4'	1:0:2412:G:C4'	2.49	0.42
1:0:2869:G:H2'	1:0:2870:C:H6	1.84	0.42
13:K:28:GLU:HB3	13:K:59:LYS:HB2	2.02	0.42
17:O:26:TRP:HB2	38:O:3062:HOH:O	2.18	0.42
18:P:45:ASP:C	18:P:47:GLY:N	2.77	0.42
20:R:39:THR:HB	20:R:42:GLU:CG	2.48	0.42
1:0:297:U:H2'	1:0:298:C:H6	1.84	0.42
1:0:1158:G:O2'	1:0:1159:G:H5'	2.20	0.42
1:0:1299:G:H5'	38:0:4362:HOH:O	2.19	0.42
1:0:1603:A:C5'	1:0:1605:G:H5'	2.50	0.42
1:0:2434:A:O3'	31:3:28:GLY:HA3	2.19	0.42
1:0:2664:A:H8	1:0:2664:A:OP1	2.02	0.42
1:0:2809:G:H2'	1:0:2810:G:O4'	2.19	0.42
2:9:3047:A:C2	2:9:3048:C:C2	3.07	0.42
4:A:65:ARG:O	4:A:66:ARG:HG3	2.18	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:199:HIS:HD2	4:A:201:PHE:HB2	1.85	0.42
7:D:40:ILE:HG23	38:D:5583:HOH:O	2.18	0.42
14:L:57:VAL:O	14:L:57:VAL:HG12	2.19	0.42
16:N:151:ASP:HB3	38:N:9328:HOH:O	2.19	0.42
21:S:58:MET:SD	30:2:8:LYS:HE3	2.59	0.42
21:S:76:GLU:HB3	38:S:9143:HOH:O	2.19	0.42
25:W:19:ASP:O	25:W:23:MET:HG3	2.19	0.42
1:0:95:A:H5''	1:0:97:G:O4'	2.19	0.42
1:0:292:G:H2'	1:0:358:G:N2	2.34	0.42
1:0:2269:C:H2'	1:0:2270:G:C5'	2.48	0.42
1:0:2672:C:O2'	1:0:2673:U:H5'	2.20	0.42
2:9:3007:G:H5'	38:N:9346:HOH:O	2.18	0.42
3:4:74:C:C2'	3:4:75:C:H5'	2.49	0.42
8:E:86:VAL:CG1	8:E:129:GLU:HA	2.48	0.42
8:E:112:ALA:HA	8:E:113:PRO:HD3	1.88	0.42
8:E:137:ASP:OD1	8:E:137:ASP:C	2.62	0.42
9:F:28:ALA:HB3	9:F:99:THR:O	2.19	0.42
16:N:12:ARG:HD3	16:N:18:THR:OG1	2.20	0.42
23:U:20:MET:HE2	23:U:30:HIS:CE1	2.54	0.42
25:W:122:ARG:HH11	25:W:122:ARG:CG	2.33	0.42
32:I:112:LYS:O	32:I:113:HIS:C	2.63	0.42
1:0:156:C:H5''	15:M:171:ARG:CD	2.27	0.42
1:0:245:C:H2'	1:0:246:G:H5'	2.02	0.42
1:0:1201:C:C2'	1:0:1202:A:H5'	2.46	0.42
1:0:1676:G:O2'	1:0:1677:U:H5'	2.20	0.42
1:0:2323:G:H5'	38:0:7221:HOH:O	2.19	0.42
1:0:2443:C:O3'	14:L:56:LYS:HE3	2.20	0.42
5:B:175:LEU:C	5:B:175:LEU:CD2	2.93	0.42
5:B:195:ARG:HG2	5:B:323:LEU:HD22	2.02	0.42
6:C:21:VAL:C	6:C:23:GLU:H	2.28	0.42
6:C:164:ALA:O	6:C:167:ASP:HB2	2.20	0.42
7:D:20:LYS:HA	7:D:75:LEU:O	2.20	0.42
7:D:41:LEU:HA	7:D:44:ILE:CG2	2.48	0.42
7:D:55:LYS:O	7:D:56:ARG:HB2	2.19	0.42
11:H:139:ASN:O	11:H:141:GLU:N	2.52	0.42
13:K:34:VAL:HG21	13:K:46:LYS:O	2.20	0.42
20:R:25:PHE:CZ	20:R:29:LYS:HE2	2.55	0.42
25:W:29:VAL:O	25:W:30:ASN:HB2	2.19	0.42
1:0:111:C:H2'	1:0:112:G:O4'	2.20	0.42
1:0:517:U:H1'	38:0:7742:HOH:O	2.17	0.42
1:0:794:U:C2'	1:0:795:G:H5'	2.50	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1025:C:H5'	25:W:23:MET:O	2.20	0.42
1:0:1166:A:H2'	1:0:1166:A:N3	2.35	0.42
1:0:1314:U:H5''	1:0:1316:G:O4'	2.19	0.42
1:0:1631:A:H2'	1:0:1632:A:C8	2.54	0.42
1:0:1979:G:H2'	38:0:3589:HOH:O	2.19	0.42
1:0:2064:U:H5'	1:0:2652:U:O3'	2.20	0.42
1:0:2541:U:H3'	1:0:2541:U:H6	1.84	0.42
1:0:2638:G:H1'	38:0:4856:HOH:O	2.19	0.42
1:0:2824:C:H5''	1:0:2825:C:H5'	2.00	0.42
5:B:17:LYS:O	5:B:260:HIS:CD2	2.73	0.42
5:B:195:ARG:CG	5:B:323:LEU:HD22	2.50	0.42
5:B:238:ASN:ND2	5:B:240:GLY:N	2.56	0.42
6:C:187:ARG:NH2	38:C:9164:HOH:O	2.51	0.42
7:D:64:ARG:HG2	7:D:67:ASP:HB3	2.02	0.42
10:G:12:ILE:N	10:G:13:PRO:HD3	2.34	0.42
21:S:6:LYS:O	21:S:7:HIS:HB3	2.20	0.42
24:V:42:ASN:N	24:V:43:PRO:HD3	2.34	0.42
24:V:60:GLN:O	24:V:65:ASP:N	2.47	0.42
25:W:13:MET:HE1	25:W:21:LEU:HD12	2.02	0.42
32:I:112:LYS:HB3	32:I:116:LEU:HG	2.02	0.42
1:0:39:G:N2	1:0:444:C:C2	2.88	0.42
1:0:472:A:H5'	29:1:35:SER:OG	2.19	0.42
1:0:656:G:H3'	17:O:37:ARG:HH12	1.84	0.42
1:0:947:U:O2'	1:0:948:G:H5'	2.19	0.42
1:0:2506:A:O2'	1:0:2507:G:P	2.78	0.42
1:0:2728:C:H4'	1:0:2894:C:HO2'	1.85	0.42
38:0:6519:HOH:O	27:Y:158:LYS:HD3	2.19	0.42
4:A:51:ARG:HB2	38:A:9401:HOH:O	2.19	0.42
5:B:86:ALA:HA	38:B:9378:HOH:O	2.19	0.42
11:H:69:ALA:HB2	11:H:153:ALA:HB2	2.02	0.42
15:M:115:LEU:HD13	15:M:116:ASN:HB2	2.02	0.42
18:P:10:ALA:HA	18:P:13:VAL:CG1	2.50	0.42
18:P:115:SER:OG	18:P:118:GLN:CG	2.68	0.42
19:Q:75:ILE:CD1	19:Q:84:ILE:HD11	2.50	0.42
27:Y:187:VAL:HB	38:Y:8158:HOH:O	2.19	0.42
1:0:1878:G:O2'	1:0:1879:U:OP2	2.37	0.42
1:0:2425:A:H5'	1:0:2426:G:OP2	2.20	0.42
5:B:104:GLU:HG3	38:B:9395:HOH:O	2.20	0.42
14:L:24:ALA:HB2	14:L:30:ARG:HD2	2.02	0.42
26:X:70:ILE:O	26:X:70:ILE:HG23	2.20	0.42
30:2:49:GLU:HB2	38:2:719:HOH:O	2.20	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:195:C:H2'	1:0:196:G:H5'	2.02	0.42
1:0:462:A:C8	30:2:37:HIS:CE1	3.08	0.42
1:0:611:U:H2'	1:0:612:U:C6	2.55	0.42
1:0:790:A:H1'	1:0:1710:A:H2'	2.02	0.42
1:0:1562:C:N4	38:0:6115:HOH:O	2.51	0.42
1:0:1878:G:O2'	1:0:1879:U:P	2.78	0.42
38:0:9421:HOH:O	5:B:229:ARG:HD2	2.20	0.42
4:A:95:PRO:HG2	4:A:98:GLU:HG2	2.02	0.42
6:C:115:LEU:HD12	6:C:115:LEU:HA	1.92	0.42
8:E:101:GLU:HB3	8:E:117:THR:HA	2.01	0.42
14:L:53:ARG:NH2	14:L:57:VAL:HG12	2.35	0.42
21:S:39:ASP:HB3	21:S:43:GLU:OE2	2.20	0.42
22:T:3:GLN:HA	22:T:4:PRO:HD3	1.88	0.42
22:T:37:GLN:OE1	22:T:118:SER:HA	2.19	0.42
1:0:249:G:H1'	1:0:265:U:O2	2.20	0.41
1:0:1242:A:OP2	12:J:60:ARG:NH2	2.49	0.41
1:0:1921:A:C6	1:0:1922:A:C2	3.08	0.41
1:0:2642:G:H2'	1:0:2643:G:O4'	2.20	0.41
4:A:99:ILE:O	4:A:131:HIS:CE1	2.72	0.41
5:B:146:THR:C	5:B:148:PRO:HD3	2.45	0.41
14:L:143:THR:HG22	14:L:144:ASP:H	1.83	0.41
15:M:47:ASP:CG	15:M:48:LYS:H	2.28	0.41
16:N:71:TRP:CE3	16:N:175:LEU:HD22	2.55	0.41
21:S:29:ASP:CG	21:S:31:ARG:NH1	2.78	0.41
22:T:12:ARG:O	22:T:19:ARG:NH2	2.53	0.41
22:T:49:GLU:HB3	22:T:59:GLU:HG3	2.02	0.41
25:W:141:HIS:HB2	25:W:146:ILE:HG12	2.02	0.41
28:Z:22:SER:O	28:Z:26:VAL:HG23	2.19	0.41
31:3:11:CYS:HB2	31:3:20:HIS:CE1	2.55	0.41
1:0:711:G:C2	1:0:718:C:C2	3.08	0.41
1:0:806:A:H2'	1:0:807:A:O4'	2.20	0.41
1:0:886:A:OP2	1:0:2113:G:H5'	2.20	0.41
1:0:1163:G:H5''	32:I:115:ASP:HB3	2.03	0.41
1:0:1192:A:N6	32:I:134:SER:CB	2.82	0.41
1:0:2003:U:H4'	1:0:2004:U:H5	1.85	0.41
1:0:2515:C:H2'	1:0:2516:G:O4'	2.20	0.41
1:0:2780:C:H2'	1:0:2781:U:C6	2.56	0.41
2:9:3096:C:O2'	2:9:3097:U:H5'	2.21	0.41
5:B:82:VAL:HG12	5:B:82:VAL:O	2.19	0.41
6:C:51:TYR:CE2	29:1:53:LYS:HB3	2.55	0.41
7:D:22:VAL:HA	7:D:73:VAL:O	2.19	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:D:169:THR:O	7:D:169:THR:HG22	2.19	0.41
9:F:91:VAL:CG1	9:F:92:GLY:H	2.15	0.41
11:H:76:GLU:O	11:H:77:LEU:HD23	2.20	0.41
16:N:50:LEU:HD12	16:N:55:ASP:OD1	2.20	0.41
18:P:131:PHE:CD1	18:P:137:LEU:HD13	2.56	0.41
21:S:29:ASP:OD1	21:S:31:ARG:NH1	2.53	0.41
24:V:49:LEU:O	24:V:53:ILE:HG13	2.20	0.41
28:Z:67:GLY:N	28:Z:70:LYS:O	2.52	0.41
29:1:21:ARG:HD2	29:1:37:CYS:SG	2.59	0.41
1:0:664:U:O4	1:0:681:G:H5''	2.19	0.41
1:0:1474:C:H6	1:0:1474:C:C5'	2.20	0.41
1:0:1481:G:H2'	1:0:1482:A:O4'	2.21	0.41
1:0:2676:C:H4'	12:J:70:PHE:HE1	1.85	0.41
2:9:3095:C:O2'	2:9:3096:C:H5'	2.20	0.41
4:A:36:ASP:HA	4:A:83:GLY:HA3	2.01	0.41
5:B:51:VAL:HG23	5:B:330:VAL:HG22	2.01	0.41
5:B:205:VAL:O	5:B:307:ARG:NE	2.53	0.41
5:B:280:VAL:HG13	5:B:333:GLU:O	2.19	0.41
6:C:165:ASP:O	6:C:168:ARG:HB3	2.19	0.41
7:D:153:THR:O	7:D:156:ARG:HB2	2.20	0.41
8:E:68:HIS:O	8:E:72:MET:HG3	2.19	0.41
13:K:41:LYS:O	13:K:42:ASN:HB2	2.20	0.41
14:L:66:VAL:HG23	14:L:67:ARG:N	2.35	0.41
20:R:114:VAL:HB	20:R:145:LEU:HD13	2.01	0.41
24:V:1:THR:C	24:V:3:LEU:N	2.78	0.41
26:X:44:ASP:HB3	26:X:46:ASP:OD2	2.20	0.41
26:X:72:VAL:HG22	26:X:85:VAL:CG1	2.45	0.41
1:0:200:U:H2'	38:0:3736:HOH:O	2.20	0.41
1:0:559:U:O2'	1:0:560:C:H5'	2.20	0.41
1:0:815:U:O2'	1:0:1598:A:H4'	2.20	0.41
1:0:1041:U:H4'	1:0:1295:G:H5'	2.03	0.41
1:0:1343:C:H2'	1:0:1344:G:O5'	2.20	0.41
1:0:1414:A:H2'	1:0:1415:G:O4'	2.20	0.41
1:0:1730:G:H5''	1:0:1731:C:C6	2.54	0.41
1:0:1764:C:H2'	1:0:1765:G:O4'	2.20	0.41
1:0:1945:G:O2'	1:0:1946:C:H5'	2.20	0.41
1:0:2363:G:O2'	19:Q:11:ARG:HG3	2.20	0.41
2:9:3049:G:C2'	2:9:3050:G:H5'	2.51	0.41
2:9:3088:G:OP1	25:W:130:HIS:NE2	2.49	0.41
4:A:93:THR:HG23	4:A:154:ALA:O	2.21	0.41
5:B:33:ASP:O	5:B:34:GLY:O	2.38	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:C:123:LEU:HD23	6:C:123:LEU:HA	1.94	0.41
7:D:59:GLY:C	7:D:61:PHE:H	2.29	0.41
22:T:48:VAL:O	22:T:59:GLU:HG2	2.20	0.41
25:W:6:GLN:HG2	25:W:29:VAL:HA	2.01	0.41
27:Y:189:ASN:HD22	27:Y:192:ASP:H	1.67	0.41
1:O:88:G:H5'	1:O:88:G:C8	2.53	0.41
1:O:656:G:H5'	17:O:3:THR:HB	2.02	0.41
1:O:1056:U:H2'	1:O:1057:A:O4'	2.20	0.41
1:O:1477:C:H4'	1:O:1868:G:H5''	2.01	0.41
1:O:2252:A:H2'	1:O:2253:G:H5'	2.02	0.41
1:O:2474:A:N6	3:4:176:DA:OP2	2.53	0.41
1:O:2712:G:H5'	38:K:4183:HOH:O	2.21	0.41
1:O:2766:A:O2'	1:O:2767:C:H5'	2.20	0.41
38:O:5775:HOH:O	5:B:298:LYS:HD3	2.19	0.41
4:A:134:ASN:O	4:A:150:PRO:HD3	2.20	0.41
4:A:195:ASN:O	4:A:196:ALA:C	2.64	0.41
5:B:195:ARG:O	5:B:196:ALA:C	2.62	0.41
6:C:7:ASP:OD1	6:C:11:ASN:O	2.37	0.41
6:C:140:VAL:HG12	6:C:141:SER:N	2.34	0.41
8:E:84:MET:HE2	8:E:133:VAL:HG23	2.01	0.41
8:E:88:TYR:CD1	8:E:88:TYR:C	2.98	0.41
12:J:70:PHE:CD2	12:J:70:PHE:O	2.74	0.41
13:K:109:LEU:HD13	13:K:113:ILE:CD1	2.51	0.41
15:M:50:ARG:N	15:M:54:TYR:HB3	2.34	0.41
20:R:79:ARG:C	20:R:81:PRO:HD3	2.44	0.41
20:R:122:GLN:HB3	20:R:138:SER:HB2	2.03	0.41
1:O:711:G:H1'	38:O:7290:HOH:O	2.20	0.41
1:O:870:G:C3'	1:O:871:G:H5''	2.50	0.41
1:O:947:U:H2'	1:O:948:G:H8	1.83	0.41
1:O:1188:A:C6	1:O:1189:A:C6	3.09	0.41
1:O:1755:A:H2'	1:O:1756:G:O4'	2.20	0.41
1:O:1773:G:N2	1:O:1774:G:C8	2.88	0.41
1:O:1838:U:O2'	1:O:2644:C:H5'	2.21	0.41
1:O:2436:U:H5'	31:3:68:LYS:HE2	2.01	0.41
1:O:2781:U:H2'	1:O:2782:G:C5'	2.51	0.41
4:A:76:VAL:CG2	28:Z:63:LYS:HB3	2.49	0.41
5:B:5:ARG:HA	5:B:6:PRO:HD3	1.97	0.41
5:B:27:ASN:HB3	38:B:9425:HOH:O	2.20	0.41
5:B:224:LYS:HA	5:B:224:LYS:HD3	1.93	0.41
5:B:280:VAL:HG13	5:B:334:SER:HA	2.03	0.41
7:D:41:LEU:CA	7:D:44:ILE:HG22	2.48	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:E:35:TYR:HA	12:J:127:ILE:CD1	2.48	0.41
9:F:63:ILE:HB	9:F:64:PRO:CD	2.47	0.41
26:X:78:GLU:CG	26:X:79:GLU:H	2.27	0.41
27:Y:184:GLU:CD	27:Y:204:ARG:HH11	2.28	0.41
27:Y:197:ASP:C	27:Y:197:ASP:OD1	2.63	0.41
1:0:212:A:O4'	1:0:214:U:C6	2.74	0.41
1:0:695:C:H2'	1:0:696:C:C6	2.56	0.41
1:0:820:G:O2'	1:0:856:G:H4'	2.21	0.41
1:0:844:A:C6	1:0:882:A:C5	3.09	0.41
1:0:876:A:N3	1:0:876:A:H2'	2.36	0.41
1:0:1328:A:C8	27:Y:169:ARG:HD3	2.56	0.41
1:0:1717:A:H5''	18:P:54:LYS:HB2	2.03	0.41
1:0:1915:U:O2'	1:0:1916:C:H5'	2.20	0.41
1:0:1937:U:O2'	1:0:1938:G:H5'	2.20	0.41
1:0:2090:G:H2'	1:0:2091:G:C8	2.55	0.41
2:9:3011:A:O2'	2:9:3012:C:H3'	2.21	0.41
2:9:3057:A:C8	7:D:141:VAL:HG21	2.56	0.41
4:A:66:ARG:CB	4:A:66:ARG:NH1	2.84	0.41
4:A:173:GLY:O	4:A:176:HIS:HB3	2.21	0.41
10:G:71:LEU:C	10:G:73:ASP:H	2.29	0.41
11:H:27:LYS:H	11:H:59:HIS:CD2	2.32	0.41
20:R:26:LYS:HB3	20:R:62:HIS:CD2	2.56	0.41
23:U:20:MET:CG	23:U:28:THR:HG23	2.51	0.41
26:X:74:ALA:CB	26:X:85:VAL:HG22	2.51	0.41
28:Z:80:ARG:O	28:Z:81:ARG:O	2.39	0.41
1:0:47:G:N3	1:0:114:A:C2	2.89	0.41
1:0:350:C:O2'	1:0:351:G:H5'	2.21	0.41
1:0:903:U:O4	14:L:18:HIS:HB2	2.21	0.41
1:0:1333:U:H2'	1:0:1334:C:H6	1.86	0.41
1:0:1439:C:H6	1:0:1439:C:O5'	2.04	0.41
1:0:1659:A:H2'	1:0:1660:G:O4'	2.20	0.41
1:0:2416:G:O2'	16:N:25:ARG:HG2	2.21	0.41
4:A:194:MET:CE	4:A:199:HIS:HB2	2.31	0.41
4:A:200:PRO:HD3	38:A:9319:HOH:O	2.21	0.41
5:B:182:VAL:O	5:B:183:GLU:C	2.64	0.41
6:C:76:ARG:CG	6:C:76:ARG:NH1	2.81	0.41
6:C:140:VAL:CG1	6:C:141:SER:N	2.84	0.41
7:D:44:ILE:HG23	7:D:45:THR:HG23	2.02	0.41
26:X:61:ARG:HH12	26:X:67:PRO:HD3	1.84	0.41
27:Y:106:THR:CG2	27:Y:107:PRO:HD2	2.51	0.41
1:0:318:C:H5'	1:0:339:A:C4	2.55	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:638:C:H2'	1:0:639:A:H8	1.85	0.41
1:0:697:G:H4'	1:0:730:G:O3'	2.21	0.41
1:0:764:C:OP1	6:C:87:ARG:NH1	2.54	0.41
1:0:930:C:N3	1:0:1040:A:N6	2.68	0.41
1:0:1313:A:H5'	27:Y:208:LYS:O	2.21	0.41
1:0:1321:A:H2'	1:0:1322:G:C8	2.56	0.41
1:0:1406:A:H5'	1:0:1407:A:C8	2.56	0.41
1:0:1477:C:O2'	1:0:1478:U:H5'	2.21	0.41
1:0:1543:G:N1	1:0:1641:A:OP2	2.39	0.41
1:0:1654:U:H2'	4:A:47:HIS:CD2	2.54	0.41
1:0:1747:A:C8	13:K:44:LEU:HD13	2.56	0.41
1:0:1811:A:H2'	1:0:1812:G:H5'	2.01	0.41
1:0:1820:G:C6	1:0:2030:A:C2	3.09	0.41
1:0:1839:A:H5'	1:0:2643:G:H4'	2.02	0.41
1:0:2403:C:H2'	1:0:2404:G:O5'	2.20	0.41
1:0:2435:U:OP1	31:3:28:GLY:HA3	2.20	0.41
1:0:2626:C:H2'	1:0:2627:G:C8	2.56	0.41
1:0:2724:U:O5'	1:0:2724:U:H6	2.03	0.41
2:9:3003:A:H2	2:9:3021:G:N3	2.19	0.41
2:9:3039:U:H3'	2:9:3040:C:H5''	2.02	0.41
5:B:7:ARG:HH11	5:B:7:ARG:CG	2.33	0.41
5:B:33:ASP:HB3	5:B:34:GLY:H	1.76	0.41
5:B:225:GLY:HA3	38:B:9367:HOH:O	2.21	0.41
7:D:96:SER:C	7:D:98:PHE:H	2.29	0.41
7:D:172:VAL:HG12	7:D:173:GLU:N	2.35	0.41
8:E:12:ASP:HA	38:E:1750:HOH:O	2.19	0.41
8:E:81:GLU:HA	8:E:133:VAL:O	2.21	0.41
11:H:88:ARG:HG2	11:H:133:LEU:O	2.20	0.41
13:K:90:PHE:CD1	13:K:90:PHE:N	2.89	0.41
16:N:47:LEU:HD13	16:N:97:VAL:HG11	2.02	0.41
16:N:93:GLN:HG2	38:N:9356:HOH:O	2.21	0.41
20:R:12:THR:HG22	20:R:149:GLU:OE1	2.21	0.41
20:R:27:HIS:O	20:R:31:ILE:HG13	2.21	0.41
22:T:48:VAL:CG1	22:T:96:VAL:HG22	2.50	0.41
23:U:9:CYS:O	23:U:52:THR:HG23	2.20	0.41
24:V:1:THR:O	24:V:4:HIS:CE1	2.74	0.41
24:V:4:HIS:O	24:V:8:ILE:HG13	2.20	0.41
26:X:9:VAL:HG22	26:X:88:GLU:OE2	2.20	0.41
26:X:61:ARG:NH1	26:X:67:PRO:HD3	2.36	0.41
28:Z:28:GLU:O	28:Z:29:ILE:C	2.63	0.41
29:1:25:LYS:HE2	38:1:9262:HOH:O	2.20	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:29:C:O2'	1:0:30:U:H5'	2.21	0.41
1:0:185:G:H4'	1:0:186:A:H4'	2.03	0.41
1:0:396:U:P	31:3:38:ARG:HH11	2.44	0.41
1:0:414:C:H5'	38:0:9961:HOH:O	2.20	0.41
1:0:1130:U:H4'	38:0:6364:HOH:O	2.20	0.41
1:0:1173:A:H4'	1:0:1174:A:C8	2.56	0.41
1:0:1471:A:H2'	1:0:1472:C:C6	2.55	0.41
1:0:2705:U:O2'	1:0:2706:A:H5'	2.20	0.41
1:0:2880:A:H2'	1:0:2881:C:H5'	2.03	0.41
2:9:3061:C:H2'	2:9:3062:A:H8	1.85	0.41
4:A:215:ILE:HG13	4:A:216:SER:N	2.36	0.41
5:B:55:ASN:HB3	5:B:64:GLY:H	1.85	0.41
6:C:19:PRO:HD2	6:C:240:LEU:HD21	2.03	0.41
7:D:24:HIS:HB2	7:D:71:ALA:O	2.21	0.41
7:D:154:LYS:H	7:D:154:LYS:CD	2.09	0.41
9:F:49:PHE:CD1	9:F:49:PHE:N	2.89	0.41
15:M:99:ARG:HE	15:M:170:ASN:ND2	2.19	0.41
17:O:50:ARG:HD2	17:O:51:TYR:CE1	2.56	0.41
25:W:1:MET:N	25:W:37:GLU:HG3	2.36	0.41
25:W:92:ASP:N	25:W:92:ASP:OD1	2.54	0.41
26:X:76:ARG:O	26:X:77:PHE:HB3	2.20	0.41
1:0:1705:C:C5'	18:P:59:ARG:HH12	2.34	0.40
1:0:1969:A:N7	1:0:1970:G:C6	2.89	0.40
1:0:2408:A:H4'	31:3:15:ASN:O	2.21	0.40
4:A:1:GLY:HA2	4:A:197:VAL:HG23	2.02	0.40
4:A:211:LYS:CB	38:A:9412:HOH:O	2.68	0.40
5:B:57:GLU:HA	5:B:58:PRO:HD2	1.96	0.40
5:B:175:LEU:HD23	5:B:175:LEU:C	2.46	0.40
6:C:21:VAL:HG23	6:C:22:PHE:CD1	2.56	0.40
9:F:102:GLY:O	9:F:103:GLU:HB2	2.21	0.40
19:Q:16:ASN:HD22	19:Q:16:ASN:HA	1.70	0.40
28:Z:20:ARG:O	28:Z:21:VAL:C	2.62	0.40
1:0:354:A:H2'	1:0:355:C:C6	2.56	0.40
1:0:450:C:OP1	6:C:184:ARG:NH2	2.55	0.40
1:0:803:C:O2'	1:0:804:C:H5'	2.21	0.40
1:0:1160:G:O2'	1:0:1190:G:H1'	2.21	0.40
1:0:1268:C:O2'	27:Y:169:ARG:HB2	2.22	0.40
1:0:1477:C:H5'	1:0:1868:G:C5'	2.51	0.40
1:0:1634:G:H2'	1:0:1635:U:H6	1.86	0.40
1:0:2047:C:H5'	38:0:3119:HOH:O	2.20	0.40
1:0:2072:G:N2	38:0:7076:HOH:O	2.46	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:2072:G:C6	1:0:2533:C:H1'	2.57	0.40
1:0:2503:A:OP1	11:H:151:ARG:NH2	2.50	0.40
4:A:112:PRO:HD3	4:A:152:CYS:SG	2.61	0.40
5:B:51:VAL:HG23	5:B:329:TYR:O	2.21	0.40
5:B:132:HIS:CE1	5:B:171:VAL:CG2	3.05	0.40
5:B:321:PRO:HA	38:B:9454:HOH:O	2.21	0.40
6:C:191:SER:OG	6:C:192:ILE:N	2.54	0.40
7:D:94:ALA:HB3	7:D:97:GLN:NE2	2.35	0.40
8:E:154:ILE:HD11	8:E:157:LYS:HE2	2.03	0.40
9:F:13:GLU:OE2	9:F:78:GLU:HG2	2.21	0.40
11:H:66:ARG:HB3	38:H:9177:HOH:O	2.21	0.40
11:H:164:ASP:OD1	11:H:164:ASP:C	2.65	0.40
11:H:167:PRO:O	11:H:168:ALA:CB	2.67	0.40
15:M:99:ARG:HE	15:M:170:ASN:HD22	1.69	0.40
18:P:103:THR:O	18:P:107:GLU:HG3	2.21	0.40
21:S:29:ASP:OD1	21:S:31:ARG:HG3	2.21	0.40
24:V:12:THR:H	24:V:15:GLU:HB2	1.86	0.40
25:W:69:ARG:HD2	25:W:117:ARG:O	2.21	0.40
27:Y:141:THR:HG23	38:Y:8175:HOH:O	2.19	0.40
1:0:308:U:H5'	22:T:97:ARG:NH2	2.37	0.40
1:0:622:G:P	27:Y:148:GLY:HA3	2.60	0.40
1:0:860:U:H2'	1:0:861:A:C8	2.56	0.40
1:0:1118:A:C8	1:0:1119:G:H5''	2.56	0.40
1:0:1819:G:H2'	1:0:1820:G:C4'	2.48	0.40
1:0:2105:C:H2'	1:0:2106:C:C6	2.56	0.40
1:0:2281:C:C2'	1:0:2282:U:H5'	2.50	0.40
1:0:2710:U:H1'	38:O:7786:HOH:O	2.21	0.40
1:0:2906:A:H5'	1:0:2907:C:O4'	2.21	0.40
4:A:32:VAL:O	4:A:33:GLU:C	2.63	0.40
4:A:48:ASP:HA	4:A:49:PRO:HD3	1.82	0.40
5:B:54:VAL:O	5:B:55:ASN:C	2.64	0.40
13:K:98:VAL:CG1	13:K:99:ASP:N	2.85	0.40
13:K:118:ALA:O	13:K:120:ARG:N	2.54	0.40
15:M:67:VAL:HB	15:M:97:ILE:HG23	2.04	0.40
16:N:108:SER:HA	16:N:109:PRO:HD3	1.79	0.40
17:O:80:ASP:OD1	17:O:81:PHE:N	2.54	0.40
18:P:13:VAL:HG11	18:P:40:VAL:CG1	2.51	0.40
26:X:41:PHE:CZ	26:X:74:ALA:HB3	2.57	0.40
27:Y:189:ASN:C	27:Y:189:ASN:ND2	2.72	0.40
27:Y:205:ILE:O	27:Y:206:ALA:C	2.63	0.40
31:3:91:GLN:O	31:3:92:GLU:HB2	2.21	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:318:C:H5'	1:0:339:A:C2	2.57	0.40
1:0:475:G:C5'	6:C:73:LEU:HD23	2.52	0.40
1:0:536:A:H3'	38:0:5321:HOH:O	2.21	0.40
1:0:581:G:O2'	1:0:582:C:H5'	2.21	0.40
1:0:694:A:C2'	1:0:695:C:H5'	2.51	0.40
1:0:1375:A:H2'	1:0:1376:G:H5'	2.03	0.40
1:0:1556:G:O2'	1:0:1557:G:H5'	2.21	0.40
1:0:1783:A:O2'	1:0:1784:U:H5'	2.20	0.40
1:0:2089:A:O2'	1:0:2090:G:H5'	2.21	0.40
1:0:2729:C:O2'	1:0:2730:G:H5'	2.22	0.40
5:B:24:PRO:CG	5:B:204:GLY:HA2	2.51	0.40
5:B:87:TYR:CE2	5:B:96:PRO:HG3	2.56	0.40
5:B:223:ARG:HG3	5:B:232:TRP:O	2.22	0.40
7:D:13:MET:CA	7:D:137:PRO:HG2	2.51	0.40
8:E:154:ILE:HG13	8:E:156:ASP:OD1	2.21	0.40
9:F:39:SER:HB3	9:F:45:ALA:HB2	2.04	0.40
9:F:57:GLU:O	9:F:61:MET:HG3	2.22	0.40
11:H:27:LYS:N	11:H:59:HIS:HD2	2.14	0.40
12:J:74:ARG:HH12	12:J:76:ASP:CB	2.34	0.40
12:J:107:ASN:C	12:J:107:ASN:ND2	2.75	0.40
15:M:164:THR:HG23	15:M:166:ALA:H	1.85	0.40
16:N:138:ASP:O	16:N:139:TRP:C	2.63	0.40
1:0:68:U:O2'	1:0:69:A:H5''	2.22	0.40
1:0:1066:U:H2'	1:0:1067:A:C8	2.57	0.40
1:0:1311:G:C2	1:0:1312:G:C8	3.09	0.40
1:0:1388:U:H2'	1:0:1389:G:O4'	2.22	0.40
1:0:1391:G:H2'	1:0:1392:A:H5'	2.03	0.40
1:0:2667:G:H1'	1:0:2914:A:N3	2.36	0.40
4:A:19:PRO:O	4:A:20:SER:C	2.65	0.40
4:A:109:GLU:HG2	4:A:116:GLY:H	1.85	0.40
4:A:125:ASN:HB3	4:A:158:VAL:HG12	2.03	0.40
6:C:157:LEU:HD11	6:C:194:PHE:HZ	1.85	0.40
7:D:57:THR:CG2	7:D:63:ILE:HG22	2.49	0.40
7:D:166:ILE:O	7:D:167:GLU:C	2.62	0.40
9:F:26:THR:CG2	9:F:102:GLY:HA3	2.52	0.40
15:M:24:GLN:HE22	15:M:27:ARG:HH11	1.67	0.40
16:N:139:TRP:CZ2	16:N:176:ARG:NH1	2.90	0.40
18:P:98:ILE:HD12	18:P:102:ARG:NE	2.37	0.40
26:X:12:ILE:HD13	26:X:36:HIS:CE1	2.56	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	A	235/240 (98%)	205 (87%)	28 (12%)	2 (1%)	14	35
5	B	335/338 (99%)	303 (90%)	27 (8%)	5 (2%)	8	22
6	C	244/246 (99%)	223 (91%)	20 (8%)	1 (0%)	30	54
7	D	134/177 (76%)	94 (70%)	34 (25%)	6 (4%)	2	4
8	E	170/178 (96%)	161 (95%)	7 (4%)	2 (1%)	10	27
9	F	117/120 (98%)	101 (86%)	13 (11%)	3 (3%)	4	11
10	G	25/348 (7%)	24 (96%)	1 (4%)	0	100	100
11	H	156/171 (91%)	144 (92%)	7 (4%)	5 (3%)	3	7
12	J	140/145 (97%)	128 (91%)	10 (7%)	2 (1%)	9	23
13	K	130/132 (98%)	116 (89%)	12 (9%)	2 (2%)	8	22
14	L	141/165 (86%)	118 (84%)	23 (16%)	0	100	100
15	M	192/194 (99%)	178 (93%)	13 (7%)	1 (0%)	24	48
16	N	184/187 (98%)	167 (91%)	12 (6%)	5 (3%)	4	10
17	O	113/116 (97%)	107 (95%)	6 (5%)	0	100	100
18	P	141/149 (95%)	131 (93%)	9 (6%)	1 (1%)	18	41
19	Q	93/96 (97%)	90 (97%)	3 (3%)	0	100	100
20	R	148/155 (96%)	133 (90%)	14 (10%)	1 (1%)	18	41
21	S	79/85 (93%)	75 (95%)	4 (5%)	0	100	100
22	T	117/120 (98%)	108 (92%)	8 (7%)	1 (1%)	14	35
23	U	51/66 (77%)	47 (92%)	3 (6%)	1 (2%)	6	16
24	V	63/71 (89%)	55 (87%)	7 (11%)	1 (2%)	7	20
25	W	152/154 (99%)	144 (95%)	6 (4%)	2 (1%)	9	25
26	X	80/92 (87%)	72 (90%)	7 (9%)	1 (1%)	9	25
27	Y	140/241 (58%)	134 (96%)	6 (4%)	0	100	100
28	Z	71/83 (86%)	57 (80%)	9 (13%)	5 (7%)	1	1

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
29	1	54/57 (95%)	53 (98%)	1 (2%)	0	100	100
30	2	42/50 (84%)	40 (95%)	2 (5%)	0	100	100
31	3	90/92 (98%)	85 (94%)	5 (6%)	0	100	100
32	I	68/162 (42%)	55 (81%)	11 (16%)	2 (3%)	3	9
All	All	3705/4430 (84%)	3348 (90%)	308 (8%)	49 (1%)	9	25

All (49) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
7	D	27	ILE
7	D	137	PRO
7	D	173	GLU
9	F	101	ALA
11	H	140	VAL
11	H	166	SER
11	H	168	ALA
16	N	154	LEU
28	Z	42	CYS
28	Z	81	ARG
5	B	34	GLY
6	C	8	LEU
7	D	65	GLU
7	D	138	GLY
12	J	5	GLU
13	K	111	GLY
16	N	139	TRP
24	V	43	PRO
4	A	34	ASP
5	B	139	ASP
5	B	184	ASP
11	H	16	ARG
12	J	89	HIS
16	N	68	GLU
16	N	164	ASP
18	P	116	SER
25	W	49	ASN
25	W	77	ALA
26	X	87	ALA
28	Z	41	ASN
32	I	76	ALA
32	I	133	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
5	B	185	GLY
8	E	17	HIS
9	F	44	SER
13	K	119	GLN
28	Z	43	GLY
4	A	37	VAL
7	D	28	GLY
23	U	7	ASP
28	Z	28	GLU
8	E	44	GLY
9	F	64	PRO
11	H	79	GLU
22	T	53	GLY
5	B	2	GLN
15	M	88	VAL
20	R	81	PRO
16	N	74	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	A	179/182 (98%)	167 (93%)	12 (7%)	15	36
5	B	282/283 (100%)	262 (93%)	20 (7%)	13	33
6	C	193/193 (100%)	179 (93%)	14 (7%)	13	32
7	D	117/148 (79%)	113 (97%)	4 (3%)	32	62
8	E	152/156 (97%)	148 (97%)	4 (3%)	40	70
9	F	93/94 (99%)	92 (99%)	1 (1%)	65	85
10	G	27/283 (10%)	26 (96%)	1 (4%)	30	59
11	H	132/138 (96%)	125 (95%)	7 (5%)	20	46
12	J	118/121 (98%)	111 (94%)	7 (6%)	18	42
13	K	106/106 (100%)	103 (97%)	3 (3%)	38	68
14	L	113/127 (89%)	110 (97%)	3 (3%)	39	69

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
15	M	158/158 (100%)	153 (97%)	5 (3%)	34	64
16	N	149/150 (99%)	144 (97%)	5 (3%)	32	62
17	O	93/94 (99%)	89 (96%)	4 (4%)	26	54
18	P	113/117 (97%)	108 (96%)	5 (4%)	25	53
19	Q	79/80 (99%)	76 (96%)	3 (4%)	29	58
20	R	117/122 (96%)	112 (96%)	5 (4%)	26	54
21	S	71/74 (96%)	70 (99%)	1 (1%)	59	82
22	T	105/106 (99%)	99 (94%)	6 (6%)	18	43
23	U	44/52 (85%)	44 (100%)	0	100	100
24	V	51/57 (90%)	51 (100%)	0	100	100
25	W	130/130 (100%)	123 (95%)	7 (5%)	20	45
26	X	66/74 (89%)	59 (89%)	7 (11%)	6	17
27	Y	120/196 (61%)	114 (95%)	6 (5%)	22	48
28	Z	60/68 (88%)	59 (98%)	1 (2%)	53	79
29	1	46/47 (98%)	46 (100%)	0	100	100
30	2	42/46 (91%)	42 (100%)	0	100	100
31	3	79/79 (100%)	79 (100%)	0	100	100
32	I	58/130 (45%)	58 (100%)	0	100	100
All	All	3093/3611 (86%)	2962 (96%)	131 (4%)	26	55

All (131) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	A	3	ARG
4	A	33	GLU
4	A	36	ASP
4	A	66	ARG
4	A	69	LEU
4	A	94	LEU
4	A	120	ARG
4	A	131	HIS
4	A	153	ARG
4	A	175	LYS
4	A	206	ARG
4	A	217	ARG
5	B	7	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
5	B	11	LEU
5	B	27	ASN
5	B	49	THR
5	B	63	GLU
5	B	97	LEU
5	B	98	THR
5	B	140	LEU
5	B	175	LEU
5	B	190	MET
5	B	195	ARG
5	B	234	ARG
5	B	245	SER
5	B	251	VAL
5	B	254	GLN
5	B	256	GLN
5	B	257	THR
5	B	264	GLU
5	B	304	PRO
5	B	307	ARG
6	C	2	GLN
6	C	27	ARG
6	C	76	ARG
6	C	91	PRO
6	C	94	THR
6	C	115	LEU
6	C	136	VAL
6	C	162	VAL
6	C	187	ARG
6	C	214	THR
6	C	223	LEU
6	C	234	VAL
6	C	236	THR
6	C	240	LEU
7	D	24	HIS
7	D	133	ASN
7	D	136	ARG
7	D	137	PRO
8	E	7	ILE
8	E	15	GLN
8	E	86	VAL
8	E	102	VAL
9	F	46	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
10	G	64	ASN
11	H	18	GLU
11	H	30	GLN
11	H	84	LYS
11	H	88	ARG
11	H	111	ASP
11	H	132	GLN
11	H	154	TYR
12	J	45	VAL
12	J	46	ILE
12	J	52	GLN
12	J	74	ARG
12	J	127	ILE
12	J	130	VAL
12	J	131	THR
13	K	7	ASP
13	K	10	GLN
13	K	49	LEU
14	L	35	ARG
14	L	102	ASP
14	L	117	GLU
15	M	46	LEU
15	M	93	ARG
15	M	99	ARG
15	M	130	GLU
15	M	164	THR
16	N	26	LEU
16	N	47	LEU
16	N	50	LEU
16	N	139	TRP
16	N	152	GLU
17	O	3	THR
17	O	43	VAL
17	O	69	VAL
17	O	98	LEU
18	P	13	VAL
18	P	21	VAL
18	P	52	LYS
18	P	91	LYS
18	P	98	ILE
19	Q	11	ARG
19	Q	16	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
19	Q	57	ASP
20	R	13	THR
20	R	39	THR
20	R	82	GLU
20	R	132	ARG
20	R	143	VAL
21	S	71	ASP
22	T	23	VAL
22	T	26	THR
22	T	39	ASN
22	T	75	GLU
22	T	96	VAL
22	T	112	LEU
25	W	26	ILE
25	W	45	VAL
25	W	52	VAL
25	W	73	LEU
25	W	142	ASP
25	W	146	ILE
25	W	154	ARG
26	X	15	ARG
26	X	27	ASP
26	X	46	ASP
26	X	66	THR
26	X	72	VAL
26	X	82	GLU
26	X	85	VAL
27	Y	154	ARG
27	Y	163	THR
27	Y	189	ASN
27	Y	200	THR
27	Y	203	VAL
27	Y	235	GLU
28	Z	13	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (107) such sidechains are listed below:

Mol	Chain	Res	Type
4	A	29	HIS
4	A	47	HIS
4	A	199	HIS
4	A	218	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
5	B	2	GLN
5	B	27	ASN
5	B	145	HIS
5	B	230	GLN
5	B	238	ASN
5	B	243	ASN
5	B	256	GLN
5	B	260	HIS
5	B	318	ASN
5	B	320	GLN
5	B	332	ASN
6	C	2	GLN
6	C	39	GLN
6	C	67	GLN
6	C	129	HIS
6	C	163	HIS
7	D	97	GLN
7	D	133	ASN
8	E	74	HIS
8	E	106	ASN
8	E	119	HIS
8	E	143	GLN
9	F	80	GLN
10	G	64	ASN
11	H	31	HIS
11	H	56	GLN
11	H	59	HIS
11	H	70	ASN
11	H	72	HIS
11	H	128	GLN
11	H	132	GLN
12	J	29	GLN
12	J	52	GLN
12	J	107	ASN
13	K	10	GLN
13	K	67	GLN
14	L	18	HIS
14	L	41	HIS
14	L	42	ASN
14	L	58	GLN
15	M	24	GLN
15	M	52	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
15	M	58	GLN
15	M	137	ASN
15	M	143	ASN
15	M	170	ASN
16	N	22	GLN
16	N	40	ASN
16	N	107	ASN
17	O	100	GLN
18	P	50	GLN
18	P	66	GLN
18	P	118	GLN
19	Q	16	ASN
19	Q	40	HIS
20	R	22	GLN
20	R	61	GLN
20	R	62	HIS
20	R	94	ASN
20	R	98	ASN
20	R	113	HIS
20	R	117	HIS
21	S	9	HIS
21	S	25	GLN
21	S	53	ASN
21	S	55	GLN
21	S	56	ASN
22	T	11	GLN
22	T	39	ASN
22	T	43	ASN
22	T	73	HIS
23	U	39	ASN
24	V	34	GLN
24	V	60	GLN
25	W	14	HIS
25	W	28	HIS
25	W	87	HIS
25	W	110	GLN
25	W	119	HIS
25	W	125	HIS
25	W	141	HIS
26	X	36	HIS
27	Y	119	GLN
27	Y	121	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
27	Y	133	HIS
27	Y	134	HIS
27	Y	149	GLN
27	Y	153	GLN
27	Y	189	ASN
28	Z	37	HIS
29	1	8	GLN
29	1	16	HIS
29	1	28	HIS
30	2	16	ASN
30	2	18	ASN
30	2	41	HIS
30	2	45	ASN
31	3	2	GLN
31	3	8	ASN
31	3	15	ASN
31	3	30	GLN
31	3	48	ASN
32	I	111	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	0	2745/2922 (93%)	243 (8%)	34 (1%)
2	9	121/122 (99%)	17 (14%)	1 (0%)
3	4	1/8 (12%)	0	0
All	All	2867/3052 (93%)	260 (9%)	35 (1%)

All (260) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	0	31	C
1	0	60	A
1	0	67	A
1	0	69	A
1	0	70	A
1	0	71	G
1	0	87	C
1	0	88	G
1	0	114	A
1	0	115	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	0	120	A
1	0	130	C
1	0	141	C
1	0	151	A
1	0	166	A
1	0	169	A
1	0	170	U
1	0	186	A
1	0	191	A
1	0	192	A
1	0	200	U
1	0	219	G
1	0	237	G
1	0	271	C
1	0	272	A
1	0	273	G
1	0	283	U
1	0	284	C
1	0	285	A
1	0	308	U
1	0	309	C
1	0	331	A
1	0	336	G
1	0	337	A
1	0	345	G
1	0	358	G
1	0	381	G
1	0	397	A
1	0	417	G
1	0	461	C
1	0	487	G
1	0	498	A
1	0	510	U
1	0	511	A
1	0	514	G
1	0	516	A
1	0	537	G
1	0	538	C
1	0	539	G
1	0	542	A
1	0	545	G
1	0	553	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	0	559	U
1	0	581	G
1	0	588	G
1	0	604	G
1	0	605	C
1	0	620	A
1	0	630	A
1	0	632	A
1	0	644	G
1	0	660	A
1	0	688	A
1	0	698	A
1	0	701	U
1	0	759	C
1	0	777	U
1	0	809	G
1	0	821	U
1	0	835	U
1	0	840	U
1	0	857	A
1	0	858	U
1	0	868	G
1	0	869	G
1	0	871	G
1	0	872	U
1	0	875	A
1	0	877	G
1	0	878	G
1	0	884	C
1	0	885	G
1	0	898	G
1	0	905	C
1	0	920	C
1	0	921	G
1	0	923	A
1	0	953	G
1	0	960	G
1	0	961	A
1	0	1006	A
1	0	1008	C
1	0	1029	U
1	0	1045	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	0	1059	G
1	0	1060	C
1	0	1072	G
1	0	1081	A
1	0	1088	A
1	0	1109	U
1	0	1110	G
1	0	1119	G
1	0	1120	U
1	0	1130	U
1	0	1137	G
1	0	1164	U
1	0	1165	G
1	0	1166	A
1	0	1174	A
1	0	1175	G
1	0	1185	U
1	0	1193	A
1	0	1206	U
1	0	1208	C
1	0	1216	G
1	0	1237	U
1	0	1238	C
1	0	1239	G
1	0	1279	U
1	0	1289	C
1	0	1342	C
1	0	1353	C
1	0	1360	C
1	0	1377	C
1	0	1378	G
1	0	1407	A
1	0	1451	C
1	0	1474	C
1	0	1485	A
1	0	1505	U
1	0	1506	U
1	0	1524	U
1	0	1525	G
1	0	1526	A
1	0	1528	A
1	0	1563	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	0	1564	C
1	0	1592	G
1	0	1625	U
1	0	1626	A
1	0	1633	C
1	0	1634	G
1	0	1656	A
1	0	1667	A
1	0	1682	A
1	0	1684	A
1	0	1685	A
1	0	1692	C
1	0	1701	A
1	0	1722	U
1	0	1723	G
1	0	1725	C
1	0	1731	C
1	0	1752	G
1	0	1778	A
1	0	1798	C
1	0	1819	G
1	0	1820	G
1	0	1829	A
1	0	1856	C
1	0	1879	U
1	0	1919	A
1	0	1942	A
1	0	1943	C
1	0	1971	G
1	0	1973	A
1	0	1978	A
1	0	1980	U
1	0	1996	U
1	0	2004	U
1	0	2008	U
1	0	2011	A
1	0	2012	U
1	0	2013	G
1	0	2033	G
1	0	2034	U
1	0	2064	U
1	0	2072	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	0	2073	G
1	0	2074	A
1	0	2096	A
1	0	2101	A
1	0	2102	G
1	0	2110	G
1	0	2243	C
1	0	2258	A
1	0	2271	G
1	0	2272	G
1	0	2291	A
1	0	2317	C
1	0	2321	A
1	0	2332	A
1	0	2354	A
1	0	2361	A
1	0	2369	A
1	0	2379	G
1	0	2422	U
1	0	2462	G
1	0	2467	A
1	0	2469	A
1	0	2476	C
1	0	2480	G
1	0	2483	A
1	0	2507	G
1	0	2509	A
1	0	2511	A
1	0	2533	C
1	0	2537	G
1	0	2541	U
1	0	2542	C
1	0	2553	A
1	0	2564	G
1	0	2589	U
1	0	2601	A
1	0	2602	G
1	0	2608	C
1	0	2613	G
1	0	2637	A
1	0	2649	A
1	0	2650	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	0	2664	A
1	0	2681	A
1	0	2682	C
1	0	2718	C
1	0	2719	A
1	0	2726	U
1	0	2747	C
1	0	2748	G
1	0	2749	U
1	0	2750	G
1	0	2762	C
1	0	2768	A
1	0	2786	G
1	0	2792	A
1	0	2800	A
1	0	2811	A
1	0	2825	C
1	0	2850	C
1	0	2876	G
1	0	2890	A
1	0	2896	A
1	0	2903	C
1	0	2914	A
2	9	3002	U
2	9	3007	G
2	9	3014	G
2	9	3022	G
2	9	3023	U
2	9	3024	U
2	9	3025	G
2	9	3040	C
2	9	3041	C
2	9	3043	G
2	9	3044	A
2	9	3052	A
2	9	3057	A
2	9	3066	G
2	9	3077	A
2	9	3114	G
2	9	3122	C

All (35) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	0	69	A
1	0	129	A
1	0	169	A
1	0	338	C
1	0	603	A
1	0	604	G
1	0	699	C
1	0	834	G
1	0	857	A
1	0	869	G
1	0	871	G
1	0	877	G
1	0	898	G
1	0	1080	C
1	0	1237	U
1	0	1246	A
1	0	1352	A
1	0	1377	C
1	0	1450	C
1	0	1506	U
1	0	1563	G
1	0	1692	C
1	0	1730	G
1	0	1856	C
1	0	1942	A
1	0	1979	G
1	0	2011	A
1	0	2313	C
1	0	2467	A
1	0	2536	C
1	0	2541	U
1	0	2649	A
1	0	2718	C
1	0	2791	U
2	9	3065	A

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

6 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond

length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	OMG	0	2588	1,3	23,26,27	0.32	0	32,38,41	0.36	0
1	UR3	0	2619	1	19,22,23	0.36	0	26,32,35	0.69	1 (3%)
1	OMU	0	2587	1	19,22,23	0.29	0	25,31,34	0.38	0
3	5AA	4	76	1,3	23,26,27	0.44	0	29,38,41	0.82	2 (6%)
1	PSU	0	2621	1	18,21,22	1.64	2 (11%)	21,30,33	1.38	3 (14%)
1	1MA	0	628	1	21,25,26	0.74	1 (4%)	30,37,40	0.86	2 (6%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	OMG	0	2588	1,3	-	1/9/27/28	0/3/3/3
1	UR3	0	2619	1	-	0/7/25/26	0/2/2/2
1	OMU	0	2587	1	-	0/9/27/28	0/2/2/2
3	5AA	4	76	1,3	-	0/11/29/30	0/3/3/3
1	PSU	0	2621	1	-	0/7/25/26	0/2/2/2
1	1MA	0	628	1	-	2/7/25/26	0/3/3/3

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	0	2621	PSU	C2-N1	5.34	1.43	1.36
1	0	2621	PSU	C6-C5	3.43	1.39	1.35
1	0	628	1MA	C6-N6	2.57	1.34	1.28

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	0	2621	PSU	C6-C5-C4	3.40	120.47	118.17
1	0	2621	PSU	C6-N1-C2	-3.37	119.57	122.69
3	4	76	5AA	C2-N1-C6	2.95	119.04	111.83
1	0	628	1MA	N1-C2-N3	2.88	129.42	126.00
1	0	2621	PSU	O2-C2-N1	2.81	125.68	122.79
1	0	2619	UR3	C4-N3-C2	2.65	126.71	124.58
3	4	76	5AA	C9-N6-C6	2.23	126.20	120.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	0	628	1MA	CM1-N1-C6	2.23	123.60	120.15

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	0	628	1MA	C2'-C1'-N9-C8
1	0	2588	OMG	C3'-C2'-O2'-CM2
1	0	628	1MA	C2'-C1'-N9-C4

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	0	2619	UR3	1	0
1	0	2587	OMU	2	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 233 ligands modelled in this entry, 233 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	0	2749/2922 (94%)	-0.45	34 (1%) 76 75	29, 51, 94, 161	0
2	9	122/122 (100%)	-0.07	5 (4%) 41 37	39, 62, 91, 152	0
3	4	5/8 (62%)	-0.68	0 100 100	41, 43, 47, 47	0
4	A	237/240 (98%)	0.16	6 (2%) 58 55	33, 57, 95, 119	0
5	B	337/338 (99%)	0.15	4 (1%) 76 75	29, 57, 80, 94	0
6	C	246/246 (100%)	0.12	4 (1%) 70 68	27, 53, 75, 84	0
7	D	140/177 (79%)	1.40	35 (25%) 2 1	58, 101, 127, 137	0
8	E	172/178 (96%)	0.44	9 (5%) 33 29	47, 67, 87, 93	0
9	F	119/120 (99%)	0.79	5 (4%) 40 37	60, 82, 104, 119	0
10	G	29/348 (8%)	0.94	3 (10%) 12 10	65, 90, 102, 105	0
11	H	160/171 (93%)	0.21	5 (3%) 51 48	41, 59, 90, 99	0
12	J	142/145 (97%)	0.08	3 (2%) 63 61	37, 52, 72, 90	0
13	K	132/132 (100%)	0.25	3 (2%) 61 58	34, 56, 77, 87	0
14	L	145/165 (87%)	0.69	21 (14%) 6 5	30, 72, 118, 132	0
15	M	194/194 (100%)	0.02	1 (0%) 87 86	34, 50, 67, 74	0
16	N	186/187 (99%)	0.61	12 (6%) 25 22	38, 66, 115, 121	0
17	O	115/116 (99%)	0.31	2 (1%) 69 67	45, 61, 77, 85	0
18	P	143/149 (95%)	0.43	6 (4%) 40 37	45, 60, 77, 85	0
19	Q	95/96 (98%)	-0.08	2 (2%) 63 61	40, 48, 60, 75	0
20	R	150/155 (96%)	-0.19	0 100 100	37, 48, 68, 75	0
21	S	81/85 (95%)	0.27	2 (2%) 58 55	49, 67, 85, 94	0
22	T	119/120 (99%)	0.39	7 (5%) 28 25	46, 63, 91, 110	0
23	U	53/66 (80%)	0.18	1 (1%) 66 63	43, 57, 74, 84	0
24	V	65/71 (91%)	1.30	16 (24%) 2 1	63, 86, 117, 121	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
25	W	154/154 (100%)	-0.10	0 100 100	39, 50, 67, 76	0
26	X	82/92 (89%)	0.28	5 (6%) 27 24	45, 59, 77, 94	0
27	Y	142/241 (58%)	0.05	3 (2%) 63 61	30, 49, 71, 86	0
28	Z	73/83 (87%)	0.48	5 (6%) 23 20	44, 63, 77, 97	0
29	1	56/57 (98%)	-0.48	0 100 100	33, 40, 46, 54	0
30	2	46/50 (92%)	0.79	7 (15%) 5 4	41, 65, 97, 109	0
31	3	92/92 (100%)	0.18	2 (2%) 62 59	37, 59, 73, 84	0
32	I	70/162 (43%)	2.11	31 (44%) 0 0	99, 121, 143, 145	0
All	All	6651/7482 (88%)	-0.00	239 (3%) 46 42	27, 56, 102, 161	0

All (239) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
32	I	133	THR	9.7
24	V	1	THR	7.1
7	D	10	PHE	6.1
16	N	168	LEU	5.4
24	V	2	VAL	5.2
2	9	3023	U	5.2
30	2	49	GLU	5.2
15	M	194	ALA	5.1
2	9	3001	U	4.9
32	I	96	PHE	4.9
14	L	82	ALA	4.8
24	V	39	ALA	4.8
7	D	63	ILE	4.8
7	D	90	LEU	4.8
24	V	40	PRO	4.6
1	0	10	U	4.6
7	D	174	VAL	4.5
8	E	45	ASP	4.4
7	D	107	GLY	4.4
1	0	138	U	4.3
1	0	1171	A	4.3
32	I	138	THR	4.2
7	D	88	LEU	4.1
32	I	93	GLN	3.9
24	V	43	PRO	3.9
14	L	99	GLU	3.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
26	X	88	GLU	3.9
32	I	90	GLY	3.8
1	0	1173	A	3.8
28	Z	82	SER	3.8
28	Z	10	ARG	3.8
18	P	143	ALA	3.7
32	I	118	SER	3.7
4	A	37	VAL	3.6
2	9	3002	U	3.6
32	I	137	VAL	3.6
5	B	1	PRO	3.5
2	9	3024	U	3.4
7	D	128	LEU	3.4
16	N	154	LEU	3.4
14	L	81	VAL	3.4
22	T	1	SER	3.4
24	V	45	ARG	3.4
14	L	148	GLU	3.4
16	N	169	PRO	3.3
22	T	119	ALA	3.3
32	I	76	ALA	3.3
1	0	1279	U	3.3
11	H	112	GLY	3.3
14	L	150	GLN	3.2
4	A	237	GLY	3.2
32	I	106	LYS	3.2
32	I	113	HIS	3.2
7	D	104	PHE	3.2
32	I	100	LEU	3.2
7	D	87	ALA	3.2
19	Q	95	GLU	3.1
32	I	102	VAL	3.1
1	0	2344	G	3.1
32	I	135	LEU	3.1
32	I	139	ILE	3.1
32	I	119	TYR	3.1
30	2	35	ARG	3.1
14	L	83	GLU	3.1
11	H	40	ALA	3.1
14	L	75	LEU	3.0
1	0	1524	U	3.0
7	D	55	LYS	3.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
24	V	38	GLY	3.0
10	G	12	ILE	3.0
7	D	106	PHE	3.0
27	Y	235	GLU	3.0
1	0	2345	A	3.0
30	2	37	HIS	3.0
16	N	167	ASP	3.0
16	N	148	ALA	3.0
17	O	23	GLY	2.9
8	E	53	GLU	2.9
1	0	128	A	2.9
7	D	17	ARG	2.9
8	E	10	ASP	2.9
10	G	27	ILE	2.9
7	D	135	VAL	2.9
7	D	171	ASP	2.8
24	V	36	ALA	2.8
7	D	11	HIS	2.8
4	A	36	ASP	2.8
8	E	156	ASP	2.8
11	H	111	ASP	2.8
14	L	105	TYR	2.8
7	D	130	VAL	2.8
7	D	105	SER	2.8
31	3	62	THR	2.8
11	H	168	ALA	2.8
16	N	165	ALA	2.8
1	0	2254	G	2.8
27	Y	216	ARG	2.8
7	D	93	LEU	2.7
32	I	129	VAL	2.7
31	3	41	GLU	2.7
32	I	85	PHE	2.7
32	I	87	THR	2.7
1	0	2769	C	2.7
8	E	154	ILE	2.7
18	P	35	ILE	2.7
13	K	63	GLU	2.7
7	D	57	THR	2.7
12	J	4	ALA	2.7
32	I	105	VAL	2.7
13	K	119	GLN	2.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	0	1561	U	2.6
32	I	117	LEU	2.6
14	L	130	ARG	2.6
8	E	170	ARG	2.6
7	D	172	VAL	2.6
26	X	83	ALA	2.6
14	L	104	ASP	2.6
14	L	78	ALA	2.6
24	V	42	ASN	2.6
22	T	118	SER	2.6
5	B	74	ILE	2.6
32	I	78	LEU	2.6
7	D	19	GLU	2.6
1	0	1964	U	2.6
7	D	61	PHE	2.6
32	I	79	ILE	2.5
22	T	18	GLU	2.5
32	I	88	GLY	2.5
7	D	21	VAL	2.5
16	N	166	ALA	2.5
9	F	47	LEU	2.5
16	N	158	LEU	2.5
1	0	1525	G	2.5
26	X	85	VAL	2.5
1	0	960	G	2.5
32	I	121	LEU	2.5
14	L	124	ASP	2.5
6	C	135	GLU	2.5
7	D	12	GLU	2.5
24	V	44	GLY	2.5
24	V	47	LYS	2.4
1	0	1202	A	2.4
7	D	129	ASP	2.4
24	V	41	GLU	2.4
8	E	172	PRO	2.4
14	L	89	PHE	2.4
26	X	87	ALA	2.4
7	D	44	ILE	2.4
7	D	134	LEU	2.4
32	I	120	ASP	2.4
1	0	1172	G	2.4
1	0	735	C	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
24	V	35	ALA	2.4
32	I	132	CYS	2.4
1	0	1175	G	2.4
9	F	90	GLU	2.4
4	A	211	LYS	2.4
7	D	59	GLY	2.4
14	L	55	GLN	2.4
28	Z	24	ARG	2.4
32	I	109	ALA	2.4
1	0	2250	G	2.3
8	E	126	ILE	2.3
1	0	272	A	2.3
7	D	101	THR	2.3
30	2	47	THR	2.3
14	L	102	ASP	2.3
30	2	31	ARG	2.3
7	D	166	ILE	2.3
12	J	76	ASP	2.3
16	N	164	ASP	2.3
10	G	63	ARG	2.3
30	2	39	ARG	2.3
7	D	35	ALA	2.3
13	K	6	ALA	2.3
2	9	3025	G	2.3
14	L	44	GLU	2.3
9	F	1	PRO	2.3
1	0	1199	A	2.3
1	0	1130	U	2.2
17	O	24	ALA	2.2
21	S	81	ILE	2.2
14	L	60	GLU	2.2
6	C	132	ASP	2.2
24	V	3	LEU	2.2
32	I	72	VAL	2.2
4	A	31	LYS	2.2
6	C	184	ARG	2.2
14	L	36	ASP	2.2
22	T	114	SER	2.2
4	A	27	LEU	2.2
14	L	100	ALA	2.2
9	F	103	GLU	2.2
22	T	41	ARG	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
16	N	157	PRO	2.2
22	T	112	LEU	2.2
1	0	1184	C	2.2
7	D	69	ILE	2.2
32	I	82	GLU	2.2
19	Q	92	ARG	2.2
1	0	2103	A	2.2
21	S	44	GLN	2.2
16	N	134	ASP	2.2
32	I	99	ASP	2.2
12	J	70	PHE	2.2
18	P	77	ALA	2.1
7	D	131	THR	2.1
28	Z	20	ARG	2.1
1	0	2136	G	2.1
11	H	32	LYS	2.1
1	0	1161	A	2.1
1	0	1170	U	2.1
27	Y	108	ASP	2.1
14	L	149	ARG	2.1
28	Z	25	ARG	2.1
30	2	44	ARG	2.1
6	C	118	THR	2.1
23	U	52	THR	2.1
1	0	2237	G	2.1
14	L	146	GLY	2.1
24	V	37	GLY	2.1
1	0	1176	C	2.1
5	B	51	VAL	2.1
24	V	46	ILE	2.1
16	N	163	PHE	2.1
1	0	1559	A	2.1
18	P	29	GLY	2.1
7	D	170	TYR	2.1
18	P	58	SER	2.0
32	I	126	LYS	2.0
8	E	5	LEU	2.0
1	0	1929	G	2.0
26	X	65	ASN	2.0
7	D	18	ILE	2.0
9	F	98	VAL	2.0
18	P	16	VAL	2.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
5	B	57	GLU	2.0
1	0	1204	C	2.0
1	0	1177	A	2.0

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	5AA	4	76	24/25	0.97	0.07	38,44,48,48	0
1	OMU	0	2587	21/22	0.98	0.06	35,37,39,42	0
1	OMG	0	2588	24/25	0.98	0.06	32,36,39,40	0
1	UR3	0	2619	21/22	0.98	0.07	32,39,41,42	0
1	PSU	0	2621	20/21	0.98	0.05	30,33,37,38	0
1	1MA	0	628	23/24	0.98	0.05	29,32,34,36	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
35	NA	0	9184	1/1	0.49	0.23	96,96,96,96	0
35	NA	9	9151	1/1	0.57	0.20	87,87,87,87	0
35	NA	R	9186	1/1	0.59	0.40	84,84,84,84	0
35	NA	0	9182	1/1	0.69	0.25	84,84,84,84	0
35	NA	0	9129	1/1	0.71	0.14	65,65,65,65	0
35	NA	S	9112	1/1	0.74	0.23	75,75,75,75	0
37	CD	O	9205	1/1	0.76	0.33	200,200,200,200	0
35	NA	0	9177	1/1	0.78	0.36	73,73,73,73	0
35	NA	0	9166	1/1	0.82	0.23	68,68,68,68	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
35	NA	0	9170	1/1	0.82	0.69	97,97,97,97	0
35	NA	0	9124	1/1	0.82	0.36	67,67,67,67	0
33	MG	0	8082	1/1	0.84	0.17	65,65,65,65	0
33	MG	0	8046	1/1	0.84	0.10	54,54,54,54	0
33	MG	0	8024	1/1	0.85	0.27	83,83,83,83	0
35	NA	0	9126	1/1	0.85	0.12	44,44,44,44	0
33	MG	9	8095	1/1	0.86	0.22	75,75,75,75	0
33	MG	0	8094	1/1	0.86	0.20	86,86,86,86	0
35	NA	0	9157	1/1	0.86	0.15	69,69,69,69	0
35	NA	0	9169	1/1	0.87	0.34	79,79,79,79	0
35	NA	0	9185	1/1	0.87	0.32	54,54,54,54	0
35	NA	0	9168	1/1	0.87	0.17	56,56,56,56	0
35	NA	0	9150	1/1	0.88	0.14	48,48,48,48	0
33	MG	0	8092	1/1	0.88	0.24	115,115,115,115	0
35	NA	0	9171	1/1	0.89	0.27	64,64,64,64	0
33	MG	0	8090	1/1	0.89	0.19	69,69,69,69	0
36	CL	0	9315	1/1	0.89	0.17	84,84,84,84	0
33	MG	0	8111	1/1	0.89	0.16	77,77,77,77	0
33	MG	0	8047	1/1	0.90	0.24	78,78,78,78	0
35	NA	0	9165	1/1	0.90	0.15	42,42,42,42	0
33	MG	0	8049	1/1	0.90	0.18	80,80,80,80	0
35	NA	0	9152	1/1	0.90	0.29	65,65,65,65	0
35	NA	0	9163	1/1	0.91	0.22	63,63,63,63	0
33	MG	0	8041	1/1	0.91	0.09	72,72,72,72	0
35	NA	0	9102	1/1	0.91	0.09	44,44,44,44	0
36	CL	A	9309	1/1	0.91	0.18	77,77,77,77	0
35	NA	0	9111	1/1	0.91	0.12	59,59,59,59	0
35	NA	0	9133	1/1	0.92	0.13	32,32,32,32	0
33	MG	0	8087	1/1	0.92	0.12	54,54,54,54	0
33	MG	0	8098	1/1	0.92	0.17	40,40,40,40	0
33	MG	0	8093	1/1	0.92	0.07	52,52,52,52	0
35	NA	C	9104	1/1	0.92	0.07	41,41,41,41	0
35	NA	0	9167	1/1	0.93	0.08	47,47,47,47	0
35	NA	0	9107	1/1	0.93	0.07	50,50,50,50	0
35	NA	0	9113	1/1	0.93	0.07	66,66,66,66	0
35	NA	0	9158	1/1	0.93	0.23	84,84,84,84	0
35	NA	0	9162	1/1	0.93	0.18	72,72,72,72	0
35	NA	0	9114	1/1	0.93	0.14	51,51,51,51	0
36	CL	0	9322	1/1	0.93	0.38	92,92,92,92	0
35	NA	0	9140	1/1	0.93	0.07	45,45,45,45	0
35	NA	0	9110	1/1	0.93	0.08	38,38,38,38	0
35	NA	0	9135	1/1	0.94	0.12	50,50,50,50	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
34	K	0	9001	1/1	0.94	0.33	74,74,74,74	0
35	NA	0	9173	1/1	0.94	0.06	58,58,58,58	0
35	NA	0	9175	1/1	0.94	0.23	56,56,56,56	0
33	MG	0	8089	1/1	0.94	0.07	60,60,60,60	0
33	MG	0	8050	1/1	0.94	0.05	61,61,61,61	0
35	NA	0	9108	1/1	0.94	0.10	61,61,61,61	0
33	MG	0	8099	1/1	0.94	0.09	63,63,63,63	0
35	NA	0	9161	1/1	0.94	0.14	56,56,56,56	0
35	NA	9	9183	1/1	0.94	0.07	49,49,49,49	0
33	MG	0	8101	1/1	0.94	0.17	74,74,74,74	0
33	MG	0	8102	1/1	0.94	0.07	67,67,67,67	0
33	MG	0	8104	1/1	0.94	0.11	73,73,73,73	0
33	MG	0	8106	1/1	0.94	0.06	63,63,63,63	0
33	MG	0	8085	1/1	0.94	0.14	74,74,74,74	0
33	MG	0	8057	1/1	0.94	0.06	45,45,45,45	0
33	MG	T	8073	1/1	0.94	0.06	66,66,66,66	0
35	NA	0	9155	1/1	0.95	0.20	78,78,78,78	0
33	MG	0	8072	1/1	0.95	0.11	55,55,55,55	0
35	NA	0	9101	1/1	0.95	0.10	47,47,47,47	0
35	NA	0	9160	1/1	0.95	0.15	49,49,49,49	0
35	NA	0	9125	1/1	0.95	0.13	69,69,69,69	0
33	MG	0	8097	1/1	0.95	0.06	40,40,40,40	0
35	NA	L	9180	1/1	0.95	0.16	72,72,72,72	0
33	MG	0	8108	1/1	0.95	0.16	75,75,75,75	0
35	NA	0	9174	1/1	0.95	0.23	64,64,64,64	0
36	CL	0	9305	1/1	0.95	0.10	71,71,71,71	0
35	NA	0	9164	1/1	0.95	0.10	55,55,55,55	0
35	NA	0	9176	1/1	0.95	0.13	42,42,42,42	0
35	NA	0	9154	1/1	0.95	0.15	38,38,38,38	0
36	CL	3	9304	1/1	0.95	0.08	70,70,70,70	0
35	NA	0	9179	1/1	0.95	0.10	57,57,57,57	0
33	MG	0	8042	1/1	0.96	0.06	39,39,39,39	0
33	MG	0	8051	1/1	0.96	0.05	61,61,61,61	0
35	NA	0	9156	1/1	0.96	0.12	51,51,51,51	0
35	NA	0	9115	1/1	0.96	0.06	39,39,39,39	0
35	NA	0	9118	1/1	0.96	0.07	47,47,47,47	0
35	NA	0	9159	1/1	0.96	0.12	56,56,56,56	0
35	NA	0	9121	1/1	0.96	0.14	58,58,58,58	0
33	MG	0	8043	1/1	0.96	0.06	53,53,53,53	0
34	K	0	9003	1/1	0.96	0.17	66,66,66,66	0
33	MG	0	8063	1/1	0.96	0.08	84,84,84,84	0
35	NA	0	9127	1/1	0.96	0.05	35,35,35,35	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
33	MG	0	8064	1/1	0.96	0.04	33,33,33,33	0
35	NA	M	9147	1/1	0.96	0.07	33,33,33,33	0
35	NA	Q	9148	1/1	0.96	0.15	43,43,43,43	0
35	NA	R	9137	1/1	0.96	0.08	50,50,50,50	0
35	NA	0	9106	1/1	0.96	0.38	51,51,51,51	0
35	NA	0	9134	1/1	0.96	0.14	37,37,37,37	0
33	MG	0	8048	1/1	0.96	0.08	62,62,62,62	0
33	MG	0	8081	1/1	0.96	0.08	54,54,54,54	0
36	CL	0	9320	1/1	0.96	0.08	48,48,48,48	0
35	NA	0	9144	1/1	0.96	0.05	27,27,27,27	0
33	MG	0	8044	1/1	0.96	0.11	49,49,49,49	0
36	CL	J	9302	1/1	0.96	0.07	61,61,61,61	0
36	CL	L	9310	1/1	0.96	0.08	61,61,61,61	0
35	NA	0	9172	1/1	0.96	0.11	61,61,61,61	0
33	MG	0	8112	1/1	0.96	0.08	47,47,47,47	0
33	MG	0	8117	1/1	0.97	0.06	40,40,40,40	0
35	NA	0	9131	1/1	0.97	0.06	36,36,36,36	0
35	NA	0	9132	1/1	0.97	0.07	35,35,35,35	0
35	NA	0	9103	1/1	0.97	0.07	39,39,39,39	0
35	NA	0	9116	1/1	0.97	0.06	36,36,36,36	0
35	NA	A	9145	1/1	0.97	0.05	45,45,45,45	0
35	NA	0	9117	1/1	0.97	0.07	46,46,46,46	0
35	NA	H	9109	1/1	0.97	0.08	36,36,36,36	0
35	NA	H	9122	1/1	0.97	0.10	59,59,59,59	0
35	NA	0	9136	1/1	0.97	0.10	56,56,56,56	0
33	MG	0	8088	1/1	0.97	0.05	36,36,36,36	0
35	NA	0	9141	1/1	0.97	0.06	47,47,47,47	0
35	NA	0	9142	1/1	0.97	0.13	53,53,53,53	0
35	NA	R	9138	1/1	0.97	0.05	61,61,61,61	0
35	NA	0	9119	1/1	0.97	0.06	36,36,36,36	0
35	NA	0	9149	1/1	0.97	0.06	42,42,42,42	0
35	NA	0	9120	1/1	0.97	0.06	43,43,43,43	0
36	CL	0	9313	1/1	0.97	0.10	61,61,61,61	0
33	MG	K	8069	1/1	0.97	0.05	49,49,49,49	0
35	NA	0	9153	1/1	0.97	0.04	25,25,25,25	0
35	NA	0	9123	1/1	0.97	0.07	43,43,43,43	0
33	MG	0	8075	1/1	0.97	0.05	43,43,43,43	0
36	CL	J	9301	1/1	0.97	0.11	73,73,73,73	0
33	MG	0	8103	1/1	0.97	0.10	81,81,81,81	0
33	MG	0	8076	1/1	0.97	0.04	70,70,70,70	0
36	CL	N	9307	1/1	0.97	0.07	66,66,66,66	0
33	MG	0	8114	1/1	0.97	0.09	56,56,56,56	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
35	NA	0	9181	1/1	0.97	0.10	48,48,48,48	0
37	CD	3	9204	1/1	0.97	0.05	66,66,66,66	0
33	MG	0	8096	1/1	0.98	0.08	51,51,51,51	0
33	MG	0	8116	1/1	0.98	0.08	47,47,47,47	0
33	MG	0	8060	1/1	0.98	0.13	49,49,49,49	0
33	MG	0	8062	1/1	0.98	0.06	57,57,57,57	0
33	MG	A	8065	1/1	0.98	0.09	52,52,52,52	0
33	MG	0	8083	1/1	0.98	0.04	42,42,42,42	0
35	NA	0	9143	1/1	0.98	0.06	36,36,36,36	0
33	MG	0	8100	1/1	0.98	0.07	82,82,82,82	0
33	MG	Y	8109	1/1	0.98	0.05	39,39,39,39	0
33	MG	3	8078	1/1	0.98	0.03	55,55,55,55	0
33	MG	0	8014	1/1	0.98	0.04	41,41,41,41	0
33	MG	0	8045	1/1	0.98	0.08	62,62,62,62	0
36	CL	0	9314	1/1	0.98	0.05	53,53,53,53	0
33	MG	0	8067	1/1	0.98	0.07	46,46,46,46	0
36	CL	0	9316	1/1	0.98	0.14	61,61,61,61	0
36	CL	0	9317	1/1	0.98	0.07	64,64,64,64	0
33	MG	0	8071	1/1	0.98	0.07	72,72,72,72	0
35	NA	0	9178	1/1	0.98	0.07	57,57,57,57	0
33	MG	0	8053	1/1	0.98	0.09	58,58,58,58	0
36	CL	B	9319	1/1	0.98	0.09	60,60,60,60	0
35	NA	0	9105	1/1	0.98	0.03	39,39,39,39	0
35	NA	0	9128	1/1	0.98	0.05	35,35,35,35	0
36	CL	K	9312	1/1	0.98	0.06	55,55,55,55	0
33	MG	0	8054	1/1	0.98	0.04	39,39,39,39	0
36	CL	M	9318	1/1	0.98	0.04	50,50,50,50	0
35	NA	0	9130	1/1	0.98	0.08	44,44,44,44	0
36	CL	O	9308	1/1	0.98	0.13	81,81,81,81	0
36	CL	R	9306	1/1	0.98	0.06	48,48,48,48	0
33	MG	0	8023	1/1	0.98	0.09	48,48,48,48	0
33	MG	0	8080	1/1	0.98	0.08	46,46,46,46	0
33	MG	0	8113	1/1	0.98	0.04	45,45,45,45	0
35	NA	J	9146	1/1	0.99	0.02	35,35,35,35	0
33	MG	0	8020	1/1	0.99	0.03	24,24,24,24	0
33	MG	0	8012	1/1	0.99	0.04	32,32,32,32	0
33	MG	0	8068	1/1	0.99	0.02	59,59,59,59	0
34	K	0	9002	1/1	0.99	0.13	54,54,54,54	0
33	MG	0	8070	1/1	0.99	0.04	45,45,45,45	0
33	MG	0	8003	1/1	0.99	0.03	40,40,40,40	0
33	MG	0	8027	1/1	0.99	0.05	55,55,55,55	0
36	CL	0	9303	1/1	0.99	0.07	64,64,64,64	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
33	MG	0	8028	1/1	0.99	0.03	44,44,44,44	0
36	CL	0	9311	1/1	0.99	0.04	52,52,52,52	0
33	MG	0	8030	1/1	0.99	0.05	26,26,26,26	0
33	MG	0	8032	1/1	0.99	0.08	35,35,35,35	0
35	NA	0	9139	1/1	0.99	0.07	22,22,22,22	0
33	MG	0	8034	1/1	0.99	0.03	32,32,32,32	0
33	MG	0	8037	1/1	0.99	0.03	44,44,44,44	0
33	MG	0	8039	1/1	0.99	0.05	51,51,51,51	0
33	MG	0	8110	1/1	0.99	0.06	40,40,40,40	0
33	MG	0	8084	1/1	0.99	0.03	51,51,51,51	0
33	MG	0	8040	1/1	0.99	0.07	52,52,52,52	0
33	MG	0	8086	1/1	0.99	0.03	47,47,47,47	0
33	MG	0	8058	1/1	0.99	0.03	57,57,57,57	0
36	CL	J	9321	1/1	0.99	0.04	54,54,54,54	0
33	MG	0	8059	1/1	0.99	0.05	44,44,44,44	0
33	MG	0	8016	1/1	0.99	0.07	44,44,44,44	0
33	MG	9	8052	1/1	0.99	0.04	47,47,47,47	0
33	MG	0	8061	1/1	0.99	0.02	45,45,45,45	0
33	MG	0	8091	1/1	0.99	0.04	57,57,57,57	0
33	MG	A	8066	1/1	0.99	0.03	66,66,66,66	0
33	MG	B	8055	1/1	0.99	0.06	52,52,52,52	0
33	MG	0	8017	1/1	0.99	0.06	33,33,33,33	0
33	MG	0	8019	1/1	0.99	0.04	38,38,38,38	0
33	MG	0	8056	1/1	1.00	0.02	51,51,51,51	0
33	MG	0	8031	1/1	1.00	0.02	37,37,37,37	0
33	MG	0	8013	1/1	1.00	0.03	41,41,41,41	0
33	MG	0	8033	1/1	1.00	0.03	32,32,32,32	0
33	MG	0	8001	1/1	1.00	0.02	38,38,38,38	0
33	MG	0	8035	1/1	1.00	0.04	51,51,51,51	0
33	MG	0	8036	1/1	1.00	0.01	35,35,35,35	0
33	MG	0	8015	1/1	1.00	0.03	31,31,31,31	0
33	MG	0	8038	1/1	1.00	0.02	26,26,26,26	0
33	MG	0	8004	1/1	1.00	0.03	27,27,27,27	0
33	MG	0	8005	1/1	1.00	0.04	37,37,37,37	0
33	MG	0	8018	1/1	1.00	0.05	47,47,47,47	0
33	MG	0	8006	1/1	1.00	0.02	33,33,33,33	0
33	MG	0	8007	1/1	1.00	0.02	24,24,24,24	0
33	MG	0	8074	1/1	1.00	0.04	40,40,40,40	0
33	MG	0	8021	1/1	1.00	0.04	30,30,30,30	0
33	MG	0	8022	1/1	1.00	0.02	35,35,35,35	0
33	MG	0	8107	1/1	1.00	0.04	38,38,38,38	0
33	MG	0	8077	1/1	1.00	0.02	35,35,35,35	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
33	MG	0	8079	1/1	1.00	0.04	38,38,38,38	0
33	MG	0	8008	1/1	1.00	0.03	37,37,37,37	0
33	MG	0	8009	1/1	1.00	0.02	35,35,35,35	0
33	MG	0	8025	1/1	1.00	0.03	35,35,35,35	0
33	MG	0	8026	1/1	1.00	0.04	31,31,31,31	0
33	MG	0	8115	1/1	1.00	0.04	49,49,49,49	0
33	MG	0	8010	1/1	1.00	0.01	29,29,29,29	0
33	MG	0	8011	1/1	1.00	0.07	23,23,23,23	0
33	MG	0	8118	1/1	1.00	0.02	40,40,40,40	0
33	MG	0	8029	1/1	1.00	0.02	36,36,36,36	0
37	CD	U	9201	1/1	1.00	0.01	69,69,69,69	0
37	CD	Z	9203	1/1	1.00	0.02	68,68,68,68	0
37	CD	1	9202	1/1	1.00	0.06	68,68,68,68	0
33	MG	0	8002	1/1	1.00	0.04	39,39,39,39	0

6.5 Other polymers [i](#)

There are no such residues in this entry.