



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 07:58 AM GMT

PDB ID : 3CCV  
Title : Structure of Anisomycin resistant 50S Ribosomal Subunit: 23S rRNA mutation G2616A  
Authors : Blaha, G.; Gurel, G.  
Deposited on : 2008-02-26  
Resolution : 2.90 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](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

---

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

MolProbity : 4.02b-467  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

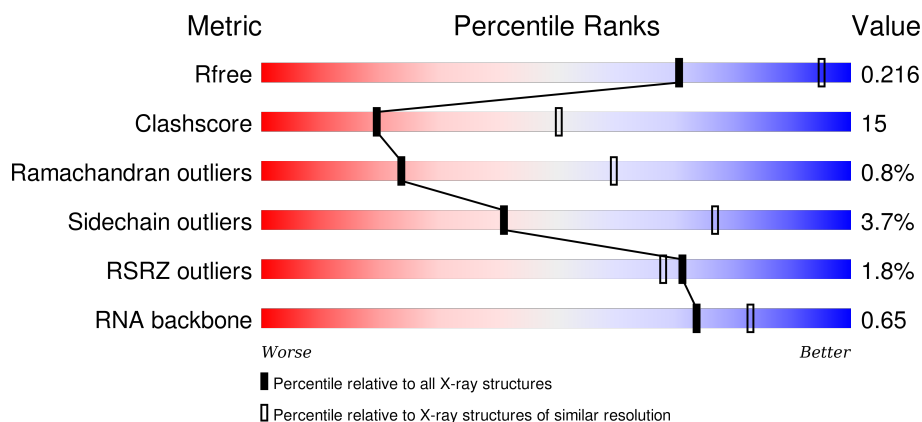
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.90 Å.

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



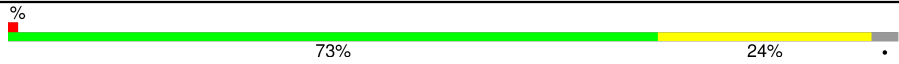

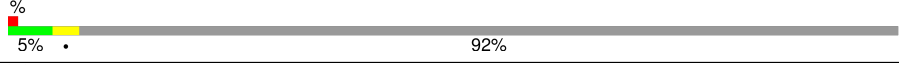

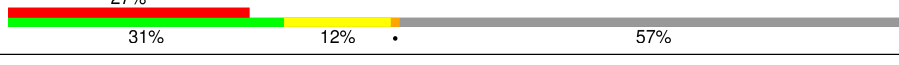
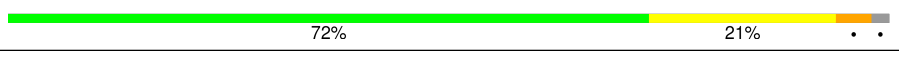
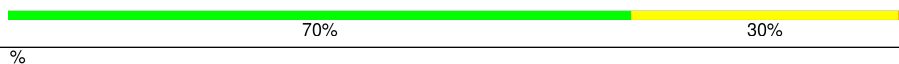

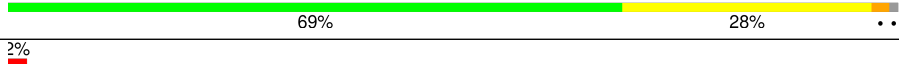


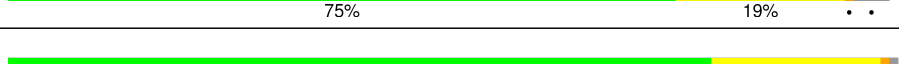
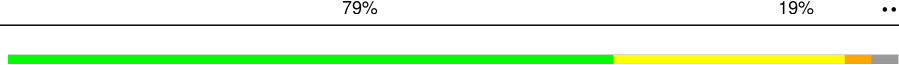
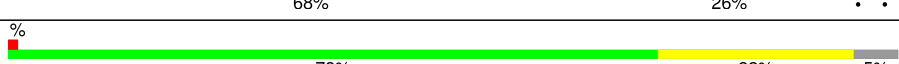


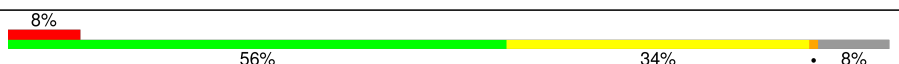
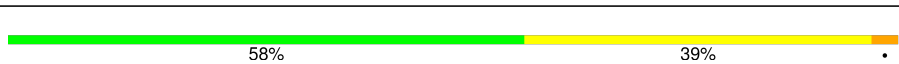
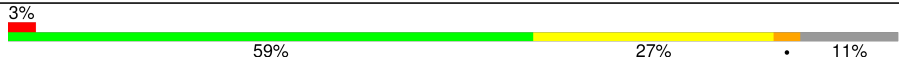
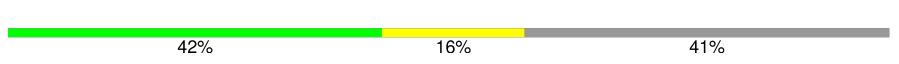
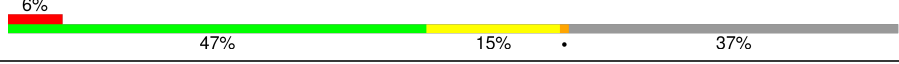
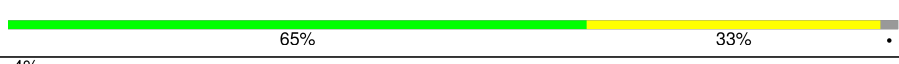
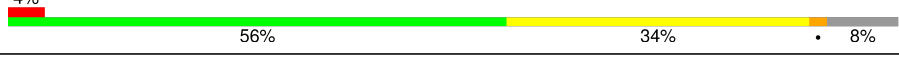


Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	91344	1451 (2.90-2.90)
Clashscore	102246	1668 (2.90-2.90)
Ramachandran outliers	100387	1630 (2.90-2.90)
Sidechain outliers	100360	1632 (2.90-2.90)
RSRZ outliers	91569	1456 (2.90-2.90)
RNA backbone	2183	1093 (3.30-2.50)

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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	240	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 16%, orange 0%, yellow 68%, green 28%, grey 0%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> <span>16%</span> <span>68%</span> <span>28%</span> <span>• •</span> </div> </div>
2	B	338	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, yellow 64%, green 32%, orange 0%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> <span>64%</span> <span>32%</span> <span>•</span> </div> </div>
3	C	246	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, yellow 70%, green 28%, orange 0%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> <span>70%</span> <span>28%</span> <span>•</span> </div> </div>
4	D	177	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 16%, orange 0%, yellow 50%, green 27%, grey 21%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> <span>16%</span> <span>50%</span> <span>27%</span> <span>•</span> <span>21%</span> </div> </div>

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Length	Quality of chain
5	E	178	
6	F	120	
7	G	348	
8	H	177	
9	I	162	
10	J	145	
11	K	132	
12	L	165	
13	M	196	
14	N	187	
15	O	116	
16	P	149	
17	Q	96	
18	R	155	
19	S	85	
20	T	120	
21	U	67	
22	V	71	
23	W	154	
24	X	92	
25	Y	241	
26	Z	116	
27	1	57	
28	2	50	
29	3	92	

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Length	Quality of chain
30	0	2923	
31	9	122	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
32	MG	0	8003	-	-	-	X
32	MG	0	8004	-	-	-	X
32	MG	0	8006	-	-	-	X
32	MG	0	8009	-	-	-	X
32	MG	0	8014	-	-	-	X
32	MG	0	8016	-	-	-	X
32	MG	0	8028	-	-	-	X
32	MG	0	8041	-	-	-	X
32	MG	0	8047	-	-	-	X
32	MG	0	8084	-	-	-	X
32	MG	A	8051	-	-	-	X
34	NA	0	8507	-	-	-	X
34	NA	0	8512	-	-	-	X
34	NA	0	8517	-	-	-	X
34	NA	0	8521	-	-	-	X
34	NA	0	8527	-	-	-	X
34	NA	0	8528	-	-	-	X
34	NA	0	8530	-	-	-	X
34	NA	0	8535	-	-	-	X
34	NA	0	8537	-	-	-	X
34	NA	0	8542	-	-	-	X
34	NA	0	8546	-	-	-	X
34	NA	0	8547	-	-	-	X
34	NA	0	8552	-	-	-	X
34	NA	0	8553	-	-	-	X
34	NA	0	8555	-	-	-	X
34	NA	0	8556	-	-	-	X
34	NA	0	8557	-	-	-	X
34	NA	0	8558	-	-	-	X
34	NA	0	8559	-	-	-	X
34	NA	0	8560	-	-	-	X
34	NA	0	8562	-	-	-	X
34	NA	0	8563	-	-	-	X

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
34	NA	0	8564	-	-	-	X
34	NA	0	8565	-	-	-	X
34	NA	0	8568	-	-	-	X
34	NA	0	8575	-	-	-	X
34	NA	9	8572	-	-	-	X
35	CL	J	8801	-	-	X	-
36	SR	0	8903	-	-	-	X
36	SR	0	8904	-	-	-	X
36	SR	0	8969	-	-	-	X
36	SR	0	8986	-	-	-	X
36	SR	B	8987	-	-	-	X
36	SR	R	8912	-	-	-	X

## 2 Entry composition

There are 38 unique types of molecules in this entry. The entry contains 99121 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 protein called 50S ribosomal protein L2P.

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

- Molecule 2 is a protein called 50S ribosomal protein L3P.

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

- Molecule 3 is a protein called 50S ribosomal protein L4P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	246	Total	C	N	O	S	0	0	0
			1860	1130	345	384	1			

- Molecule 4 is a protein called 50S ribosomal protein L5P.

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

- Molecule 5 is a protein called 50S ribosomal protein L6P.

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

- Molecule 6 is a protein called 50S ribosomal protein L7Ae.

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

- Molecule 7 is a protein called 50S ribosomal protein L10E.

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

- Molecule 8 is a protein called 50S ribosomal protein L10e.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	H	160	Total	C	N	O	S	0	0	0
			1282	798	240	238	6			

- Molecule 9 is a protein called 50S ribosomal protein L11P.

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

- Molecule 10 is a protein called 50S ribosomal protein L13P.

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

- Molecule 11 is a protein called 50S ribosomal protein L14P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	K	132	Total	C	N	O	S	0	0	0
			994	609	189	192	4			

- Molecule 12 is a protein called 50S ribosomal protein L15P.

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

- Molecule 13 is a protein called 50S ribosomal protein L15e.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	M	194	Total	C	N	O	S	0	0	0
			1558	943	333	281	1			

- Molecule 14 is a protein called 50S ribosomal protein L18P.

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

- Molecule 15 is a protein called 50S ribosomal protein L18e.

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

- Molecule 16 is a protein called 50S ribosomal protein L19e.

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

- Molecule 17 is a protein called 50S ribosomal protein L21e.

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

- Molecule 18 is a protein called 50S ribosomal protein L22P.

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

- Molecule 19 is a protein called 50S ribosomal protein L23P.

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

- Molecule 20 is a protein called 50S ribosomal protein L24P.

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

- Molecule 21 is a protein called 50S ribosomal protein L24e.



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

- Molecule 22 is a protein called 50S ribosomal protein L29P.

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

- Molecule 23 is a protein called 50S ribosomal protein L30P.

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

- Molecule 24 is a protein called 50S ribosomal protein L31e.

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

- Molecule 25 is a protein called 50S ribosomal protein L32e.

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

- Molecule 26 is a protein called 50S ribosomal protein L37Ae.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	Z	73	Total	C	N	O	S	0	0	0
			573	343	113	112	5			

- Molecule 27 is a protein called 50S ribosomal protein L37e.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
27	1	56	Total	C	N	O	S	0	0	0
			431	258	86	83	4			

- Molecule 28 is a protein called 50S ribosomal protein L39e.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
28	2	46	Total	C	N	O	S	0	0	0
			396	239	89	67	1			

- Molecule 29 is a protein called 50S ribosomal protein L44E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
29	3	92	Total	C	N	O	S	0	0	0
			755	458	153	137	7			

- Molecule 30 is a RNA chain called 23S RIBOSOMAL RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
30	0	2754	Total	C	N	O	P	0	0	0
			59019	26349	10873	19052	2745			

- Molecule 31 is a RNA chain called 5S RIBOSOMAL RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
31	9	122	Total	C	N	O	P	0	0	0
			2599	1160	471	847	121			

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
32	0	87	Total	Mg	0	0
			87	87		
32	Y	1	Total	Mg	0	0
			1	1		
32	K	1	Total	Mg	0	0
			1	1		
32	B	1	Total	Mg	0	0
			1	1		
32	A	1	Total	Mg	0	0
			1	1		
32	T	1	Total	Mg	0	0
			1	1		
32	9	1	Total	Mg	0	0
			1	1		

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

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

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
34	0	67	Total Na 67 67	0	0
34	J	1	Total Na 1 1	0	0
34	Q	1	Total Na 1 1	0	0
34	C	1	Total Na 1 1	0	0
34	R	1	Total Na 1 1	0	0
34	9	2	Total Na 2 2	0	0
34	S	1	Total Na 1 1	0	0
34	M	1	Total Na 1 1	0	0

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
35	0	10	Total Cl 10 10	0	0
35	J	3	Total Cl 3 3	0	0
35	B	1	Total Cl 1 1	0	0
35	A	1	Total Cl 1 1	0	0
35	N	1	Total Cl 1 1	0	0
35	O	1	Total Cl 1 1	0	0
35	R	1	Total Cl 1 1	0	0
35	Y	1	Total Cl 1 1	0	0
35	L	1	Total Cl 1 1	0	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
35	3	1	Total 1	Cl 1	0	0
35	M	1	Total 1	Cl 1	0	0

- Molecule 36 is STRONTIUM ION (three-letter code: SR) (formula: Sr).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
36	0	94	Total 94	Sr 94	0	0
36	Y	1	Total 1	Sr 1	0	0
36	B	2	Total 2	Sr 2	0	0
36	1	2	Total 2	Sr 2	0	0
36	A	3	Total 3	Sr 3	0	0
36	3	1	Total 1	Sr 1	0	0
36	R	1	Total 1	Sr 1	0	0
36	9	2	Total 2	Sr 2	0	0
36	S	1	Total 1	Sr 1	0	0
36	F	1	Total 1	Sr 1	0	0

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

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

- Molecule 38 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
38	0	5910	Total 5910	O 5910	0	0
38	9	142	Total 142	O 142	0	0
38	A	112	Total 112	O 112	0	0
38	B	149	Total 149	O 149	0	0
38	C	185	Total 185	O 185	0	0
38	D	49	Total 49	O 49	0	0
38	E	45	Total 45	O 45	0	0
38	F	26	Total 26	O 26	0	0
38	G	17	Total 17	O 17	0	0
38	H	67	Total 67	O 67	0	0
38	I	8	Total 8	O 8	0	0
38	J	51	Total 51	O 51	0	0
38	K	51	Total 51	O 51	0	0
38	L	89	Total 89	O 89	0	0
38	M	133	Total 133	O 133	0	0
38	N	61	Total 61	O 61	0	0
38	O	39	Total 39	O 39	0	0
38	P	62	Total 62	O 62	0	0
38	Q	45	Total 45	O 45	0	0
38	R	81	Total 81	O 81	0	0
38	S	32	Total 32	O 32	0	0

*Continued on next page...*

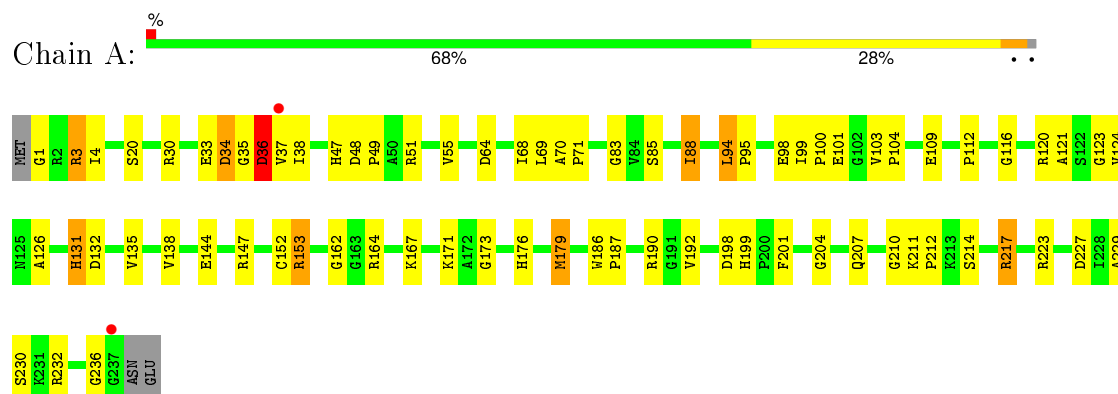
*Continued from previous page...*

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
38	T	35	Total 35	O 35	0	0
38	U	29	Total 29	O 29	0	0
38	V	15	Total 15	O 15	0	0
38	W	67	Total 67	O 67	0	0
38	X	26	Total 26	O 26	0	0
38	Y	98	Total 98	O 98	0	0
38	Z	32	Total 32	O 32	0	0
38	1	54	Total 54	O 54	0	0
38	2	44	Total 44	O 44	0	0
38	3	69	Total 69	O 69	0	0

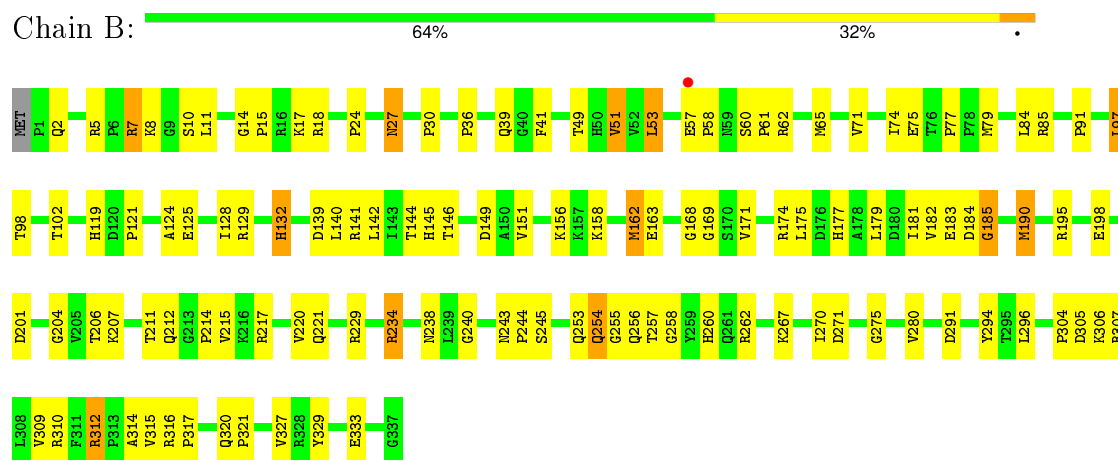
### 3 Residue-property plots

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

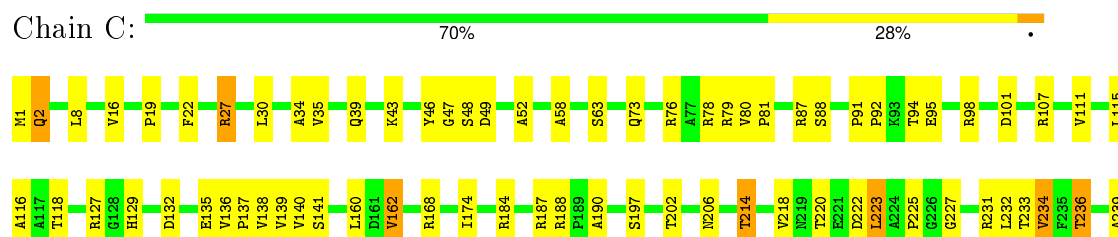
- Molecule 1: 50S ribosomal protein L2P



- Molecule 2: 50S ribosomal protein L3P



- Molecule 3: 50S ribosomal protein L4P

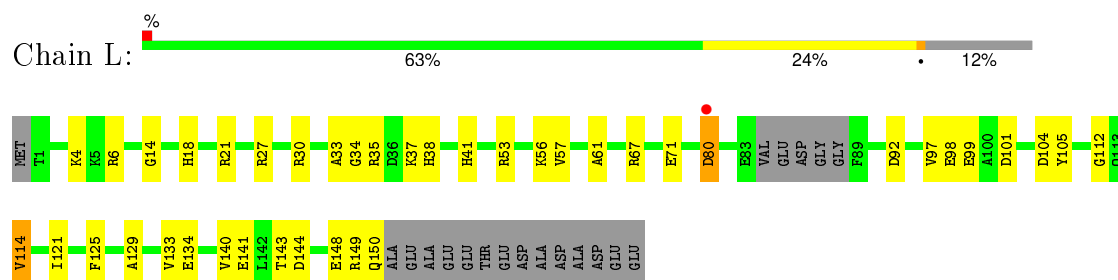




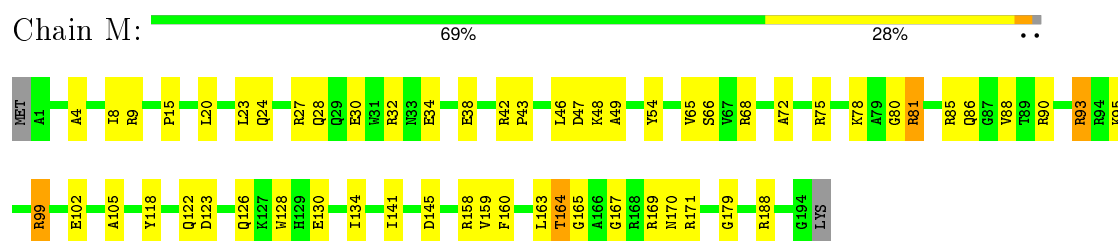




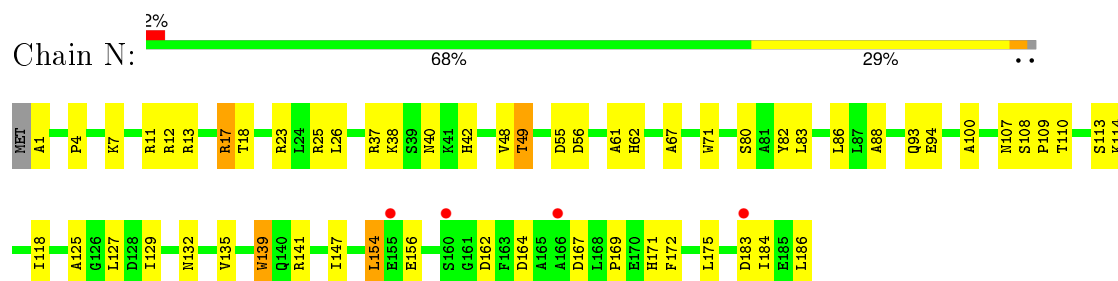
- Molecule 12: 50S ribosomal protein L15P



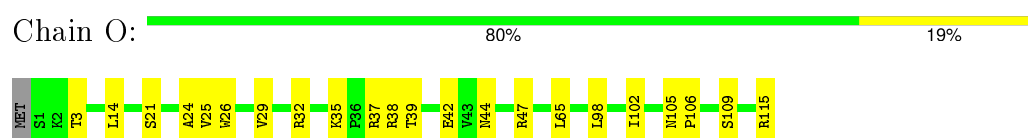
- Molecule 13: 50S ribosomal protein L15e



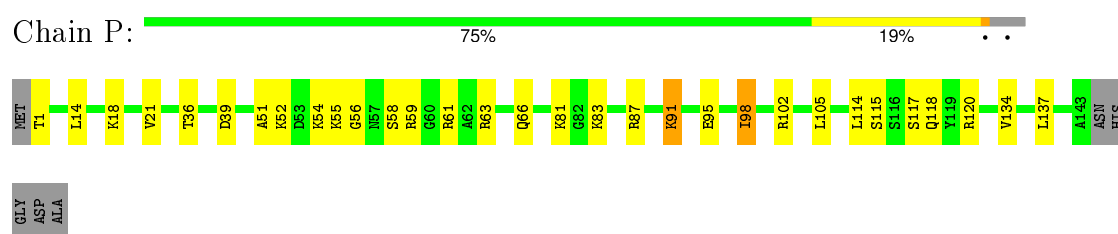
- Molecule 14: 50S ribosomal protein L18P



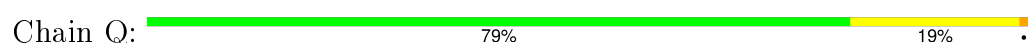
- Molecule 15: 50S ribosomal protein L18e



- Molecule 16: 50S ribosomal protein L19e

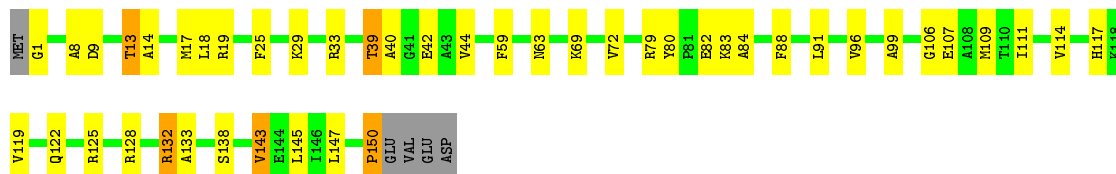


- Molecule 17: 50S ribosomal protein L21e





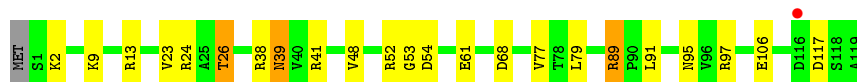
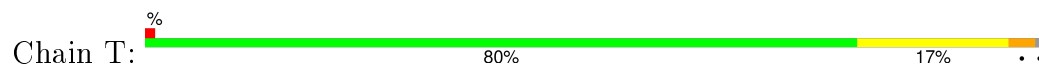
- Molecule 18: 50S ribosomal protein L22P



- Molecule 19: 50S ribosomal protein L23P



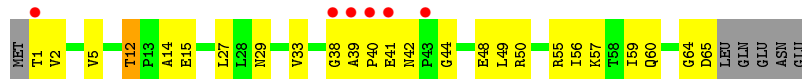
- Molecule 20: 50S ribosomal protein L24P



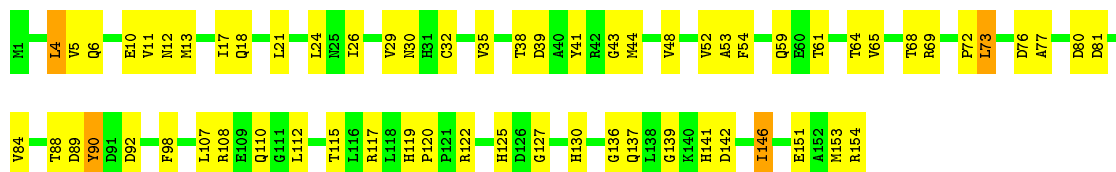
- Molecule 21: 50S ribosomal protein L24e



- Molecule 22: 50S ribosomal protein L29P



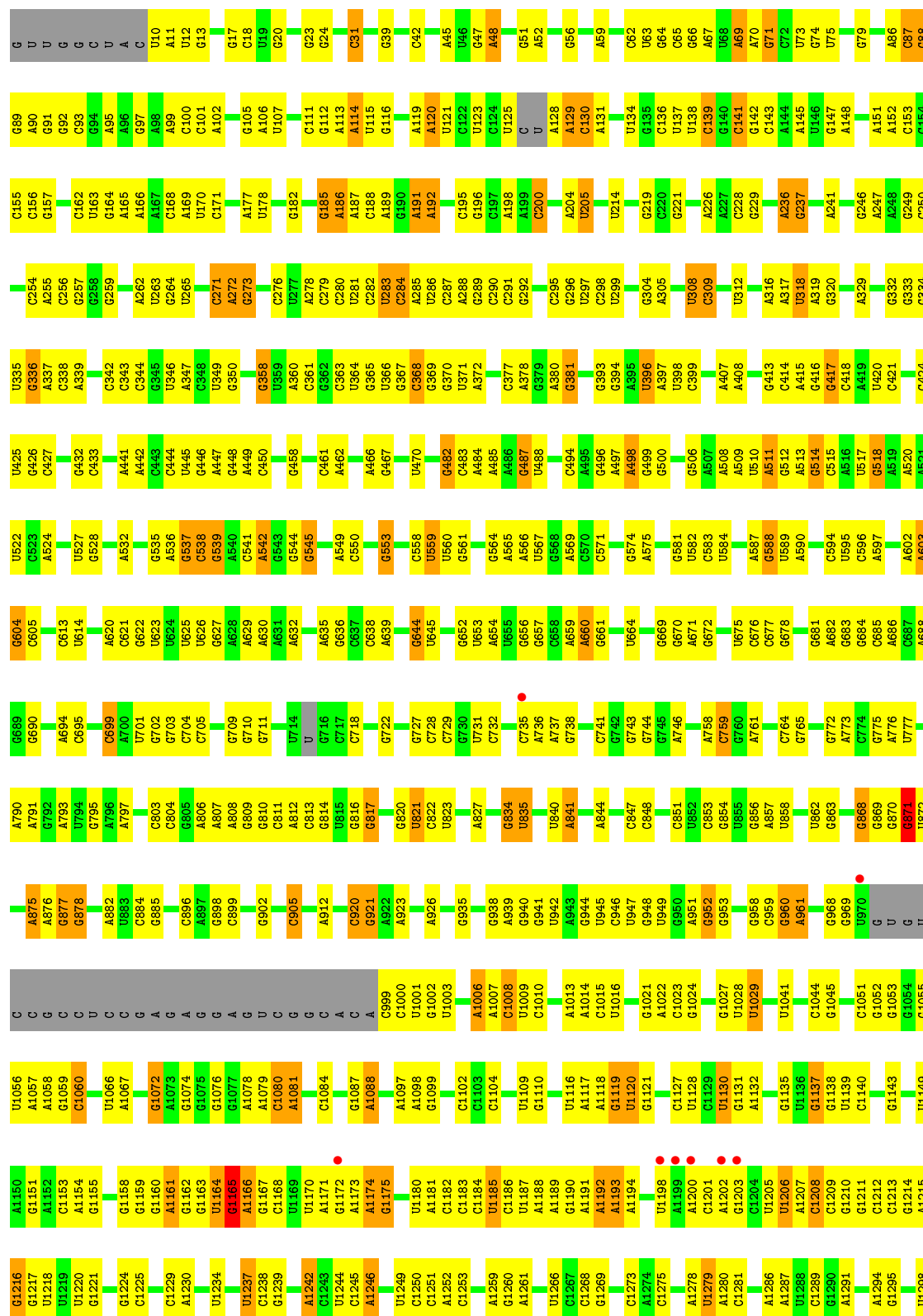
- Molecule 23: 50S ribosomal protein L30P



- |    |    |    |  |     |  |     |  |     |  |     |  |     |  |     |  |     |     |     |  |     |  |     |     |  |     |     |     |  |     |     |     |  |     |     |     |  |
|----|----|----|--|-----|--|-----|--|-----|--|-----|--|-----|--|-----|--|-----|-----|-----|--|-----|--|-----|-----|--|-----|-----|-----|--|-----|-----|-----|--|-----|-----|-----|--|
| M1 | Q2 | M3 |  | G11 |  | M15 |  | H20 |  | V25 |  | G28 |  | R38 |  | N48 | D49 | G50 |  | P56 |  | K60 | P61 |  | K68 | V69 | R70 |  | H78 | L79 | R80 |  | F90 | Q91 | E92 |  |
|----|----|----|--|-----|--|-----|--|-----|--|-----|--|-----|--|-----|--|-----|-----|-----|--|-----|--|-----|-----|--|-----|-----|-----|--|-----|-----|-----|--|-----|-----|-----|--|

● Molecule 30: 23S RIBOSOMAL RNA

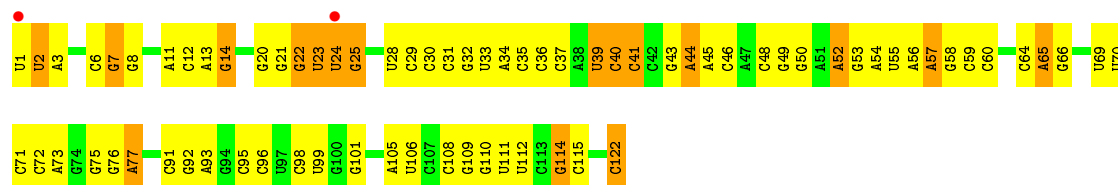
Chain 0: 



WORLDWIDE  
**PDB**  
PROTEIN DATA BANK



• Molecule 31: 5S RIBOSOMAL RNA



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	211.75Å 299.01Å 574.48Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.99 – 2.90 85.44 – 2.40	Depositor EDS
% Data completeness (in resolution range)	93.5 (49.99-2.90) 93.6 (85.44-2.40)	Depositor EDS
$R_{merge}$	0.14	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	0.00 (at 2.40Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, $R_{free}$	0.175 , 0.225 0.170 , 0.216	Depositor DCC
$R_{free}$ test set	3894 reflections (1.07%)	DCC
Wilson B-factor (Å <sup>2</sup> )	47.7	Xtriage
Anisotropy	0.289	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 73.5	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 667149 reflections	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	99121	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	53.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.43% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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: MG, OMG, CL, SR, NA, K, CD, OMU, UR3, 1MA, 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	A	0.32	0/1786	0.64	0/2408
2	B	0.32	0/2690	0.65	0/3652
3	C	0.36	0/1885	0.63	0/2552
4	D	0.33	0/1111	0.56	0/1498
5	E	0.33	0/1382	0.57	0/1880
6	F	0.33	0/901	0.57	0/1224
7	G	0.32	0/241	0.49	0/324
8	H	0.34	0/1302	0.65	0/1743
9	I	0.29	0/526	0.50	0/716
10	J	0.36	0/1136	0.60	0/1530
11	K	0.36	0/1004	0.68	0/1351
12	L	0.35	0/1130	0.66	0/1509
13	M	0.34	0/1582	0.62	0/2116
14	N	0.30	0/1474	0.63	0/1999
15	O	0.34	0/874	0.59	0/1181
16	P	0.32	0/1147	0.51	0/1528
17	Q	0.34	0/749	0.67	0/1005
18	R	1.26	7/1172 (0.6%)	1.10	6/1578 (0.4%)
19	S	0.33	0/648	0.57	0/875
20	T	0.33	0/958	0.64	0/1289
21	U	0.33	0/417	0.56	0/562
22	V	0.32	0/502	0.53	0/675
23	W	0.35	0/1219	0.62	0/1655
24	X	0.34	0/664	0.59	0/895
25	Y	0.35	0/1146	0.61	0/1536
26	Z	0.36	0/584	0.61	0/781
27	1	0.39	0/438	0.60	0/578
28	2	0.33	0/401	0.56	0/529
29	3	0.34	0/771	0.56	0/1024
30	0	0.38	0/65956	0.69	13/102865 (0.0%)
31	9	0.32	0/2904	0.68	1/4526 (0.0%)
All	All	0.39	7/98700 (0.0%)	0.67	20/147584 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
18	R	1	0
23	W	0	1
30	0	0	29
All	All	1	30

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	R	150	PRO	CB-CG	27.44	2.87	1.50
18	R	150	PRO	CA-C	-18.09	1.16	1.52
18	R	150	PRO	CG-CD	13.93	1.96	1.50
18	R	150	PRO	C-O	11.89	1.47	1.23
18	R	150	PRO	N-CA	11.37	1.66	1.47
18	R	150	PRO	N-CD	10.70	1.62	1.47
18	R	150	PRO	CA-CB	7.62	1.68	1.53

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	R	150	PRO	CB-CA-C	-22.52	55.71	112.00
18	R	150	PRO	N-CA-C	-19.33	61.85	112.10
18	R	150	PRO	CA-N-CD	12.27	128.87	111.70
18	R	150	PRO	N-CA-CB	11.00	116.50	103.30
18	R	150	PRO	CA-C-O	-8.51	99.79	120.20
18	R	150	PRO	CA-CB-CG	-6.15	92.32	104.00
30	0	1942	A	C5'-C4'-C3'	6.08	125.73	116.00
30	0	2316	G	C5'-C4'-C3'	-5.93	106.52	116.00
31	9	39	U	N1-C1'-C2'	5.87	121.63	114.00
30	0	1504	A	N9-C1'-C2'	5.86	121.62	114.00
30	0	1504	A	C1'-O4'-C4'	-5.83	105.24	109.90
30	0	1120	U	C5'-C4'-C3'	-5.56	107.11	116.00
30	0	2726	U	N1-C1'-C2'	5.45	121.08	114.00
30	0	871	G	C5'-C4'-O4'	-5.44	102.57	109.10
30	0	2313	C	C5'-C4'-O4'	5.34	115.51	109.10
30	0	1165	G	C1'-O4'-C4'	-5.32	105.64	109.90
30	0	2467	A	C1'-O4'-C4'	-5.22	105.72	109.90
30	0	1592	G	N9-C1'-C2'	5.21	120.78	114.00
30	0	1829	A	N9-C1'-C2'	-5.19	106.29	112.00

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	0	841	A	C1'-O4'-C4'	-5.16	105.77	109.90

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
18	R	150	PRO	CA

All (30) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
30	0	1078	A	Sidechain
30	0	1237	U	Sidechain
30	0	1430	G	Sidechain
30	0	1819	G	Sidechain
30	0	1829	A	Sidechain
30	0	1863	G	Sidechain
30	0	1877	G	Sidechain
30	0	1878	G	Sidechain
30	0	205	U	Sidechain
30	0	221	G	Sidechain
30	0	2308	U	Sidechain
30	0	2313	C	Sidechain
30	0	246	G	Sidechain
30	0	2465	A	Sidechain
30	0	2493	C	Sidechain
30	0	2503	A	Sidechain
30	0	2506	A	Sidechain
30	0	2607	U	Sidechain
30	0	2673	U	Sidechain
30	0	2842	G	Sidechain
30	0	396	U	Sidechain
30	0	458	G	Sidechain
30	0	48	A	Sidechain
30	0	482	G	Sidechain
30	0	518	G	Sidechain
30	0	795	G	Sidechain
30	0	817	G	Sidechain
30	0	868	G	Sidechain
30	0	952	G	Sidechain
23	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	A	1753	0	1766	74	0
2	B	2625	0	2532	108	0
3	C	1860	0	1813	56	0
4	D	1094	0	1085	38	0
5	E	1357	0	1266	34	0
6	F	890	0	843	28	0
7	G	240	0	231	9	0
8	H	1282	0	1292	39	0
9	I	519	0	500	20	0
10	J	1120	0	1098	43	0
11	K	994	0	1027	40	0
12	L	1118	0	1076	37	0
13	M	1558	0	1573	52	0
14	N	1445	0	1401	54	0
15	O	865	0	873	23	0
16	P	1136	0	1123	25	0
17	Q	735	0	729	18	0
18	R	1149	0	1122	40	0
19	S	641	0	605	14	0
20	T	950	0	924	22	0
21	U	410	0	364	16	0
22	V	499	0	511	20	0
23	W	1196	0	1137	66	0
24	X	654	0	653	23	0
25	Y	1130	0	1133	40	0
26	Z	573	0	531	15	0
27	1	431	0	426	25	0
28	2	396	0	413	18	0
29	3	755	0	728	15	0
30	0	59019	0	29809	1374	0
31	9	2599	0	1325	96	0
32	0	87	0	0	0	0
32	9	1	0	0	0	0
32	A	1	0	0	0	0
32	B	1	0	0	0	0
32	K	1	0	0	0	0
32	T	1	0	0	0	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
32	Y	1	0	0	0	0
33	0	2	0	0	0	0
34	0	67	0	0	0	0
34	9	2	0	0	0	0
34	C	1	0	0	0	0
34	J	1	0	0	0	0
34	M	1	0	0	0	0
34	Q	1	0	0	0	0
34	R	1	0	0	0	0
34	S	1	0	0	0	0
35	0	10	0	0	1	0
35	3	1	0	0	0	0
35	A	1	0	0	0	0
35	B	1	0	0	0	0
35	J	3	0	0	2	0
35	L	1	0	0	0	0
35	M	1	0	0	0	0
35	N	1	0	0	0	0
35	O	1	0	0	0	0
35	R	1	0	0	0	0
35	Y	1	0	0	0	0
36	0	94	0	0	0	0
36	1	2	0	0	0	0
36	3	1	0	0	0	0
36	9	2	0	0	0	0
36	A	3	0	0	0	0
36	B	2	0	0	0	0
36	F	1	0	0	0	0
36	R	1	0	0	0	0
36	S	1	0	0	0	0
36	Y	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	5910	0	0	205	0
38	1	54	0	0	6	0
38	2	44	0	0	1	0
38	3	69	0	0	2	0
38	9	142	0	0	10	0
38	A	112	0	0	7	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
38	B	149	0	0	13	0
38	C	185	0	0	17	0
38	D	49	0	0	4	0
38	E	45	0	0	4	0
38	F	26	0	0	3	0
38	G	17	0	0	0	0
38	H	67	0	0	4	0
38	I	8	0	0	1	0
38	J	51	0	0	2	0
38	K	51	0	0	2	0
38	L	89	0	0	8	0
38	M	133	0	0	4	0
38	N	61	0	0	7	0
38	O	39	0	0	3	0
38	P	62	0	0	1	0
38	Q	45	0	0	2	0
38	R	81	0	0	3	0
38	S	32	0	0	3	0
38	T	35	0	0	3	0
38	U	29	0	0	2	0
38	V	15	0	0	2	0
38	W	67	0	0	6	0
38	X	26	0	0	4	0
38	Y	98	0	0	5	0
38	Z	32	0	0	1	0
All	All	99121	0	59909	2240	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 15.

All (2240) 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)
18:R:150:PRO:CG	18:R:150:PRO:CD	1.96	1.43
30:0:1160:G:C5'	30:0:1161:A:H5'	1.74	1.18
30:0:871:G:C8	30:0:871:G:H5'	1.80	1.15
30:0:1160:G:H5'	30:0:1161:A:C5'	1.74	1.15
30:0:871:G:H8	30:0:871:G:H5'	1.07	1.11
14:N:37:ARG:NH1	31:9:6:C:H5''	1.63	1.09
30:0:1559:A:H1'	38:0:5862:HOH:O	1.53	1.08
18:R:150:PRO:CG	18:R:150:PRO:C	2.22	1.08

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:1205:U:H2'	30:0:1206:U:H5''	1.31	1.07
30:0:2717:C:C2'	30:0:2718:C:H5''	1.84	1.07
30:0:1701:A:H4'	30:0:1702:U:H5''	1.38	1.05
30:0:2717:C:H2'	30:0:2718:C:H5''	1.34	1.05
31:9:56:A:C2'	31:9:57:A:H5''	1.86	1.05
31:9:56:A:H2'	31:9:57:A:H5''	1.08	1.03
15:O:3:THR:HG22	30:0:656:G:H5'	1.37	1.02
30:0:2291:A:C8	30:0:2309:C:H5'	1.95	1.02
31:9:76:G:H3'	31:9:77:A:H5''	1.41	1.00
10:J:82:THR:HG23	30:0:1242:A:H5'	1.41	0.98
30:0:1666:C:O2'	30:0:1667:A:H5''	1.64	0.98
30:0:282:C:H1'	30:0:368:C:N4	1.79	0.98
30:0:1474:C:H6	30:0:1474:C:H5'	1.29	0.97
30:0:545:G:H8	30:0:545:G:H5'	1.24	0.97
13:M:171:ARG:HD3	30:0:156:C:H5''	1.44	0.96
30:0:1187:U:HO2'	30:0:1189:A:H2	0.98	0.96
30:0:870:G:H2'	30:0:871:G:H5''	1.48	0.95
30:0:1625:U:H4'	38:0:4666:HOH:O	1.67	0.95
30:0:871:G:H8	30:0:871:G:C5'	1.81	0.94
11:K:10:GLN:H	11:K:10:GLN:HE21	1.06	0.93
4:D:154:LYS:HD2	4:D:154:LYS:H	1.34	0.93
30:0:1205:U:H2'	30:0:1206:U:C5'	1.99	0.93
10:J:52:GLN:NE2	30:0:1119:G:H2'	1.82	0.92
30:0:2812:A:H2	30:0:2814:A:H62	1.11	0.92
30:0:1116:U:O2'	30:0:1118:A:H2	1.51	0.92
30:0:542:A:H5'	30:0:542:A:H8	1.35	0.92
23:W:137:GLN:HE21	23:W:141:HIS:HE1	1.10	0.92
11:K:29:LEU:HB3	11:K:55:VAL:HG11	1.49	0.92
30:0:506:G:H22	30:0:509:A:C5'	1.82	0.92
3:C:236:THR:HG22	3:C:239:ALA:H	1.31	0.91
30:0:2010:A:H2'	38:0:5957:HOH:O	1.69	0.91
30:0:2533:C:H5'	30:0:2533:C:H6	1.34	0.90
30:0:1184:C:H1'	38:0:7462:HOH:O	1.71	0.90
30:0:69:A:H5'	30:0:69:A:C8	2.07	0.90
23:W:6:GLN:HB2	23:W:26:ILE:HD11	1.54	0.90
30:0:1603:A:H5'	30:0:1605:G:O4'	1.71	0.90
30:0:877:G:H5'	30:0:878:G:OP1	1.72	0.90
16:P:115:SER:H	16:P:118:GLN:HE21	1.18	0.90
15:O:3:THR:CG2	30:0:656:G:H5'	2.02	0.89
30:0:381:G:H5''	38:0:4318:HOH:O	1.72	0.89
30:0:853:C:H3'	38:0:4550:HOH:O	1.72	0.89

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:2908:A:H2'	30:0:2909:G:O4'	1.73	0.89
30:0:1474:C:C6	30:0:1474:C:H5'	2.09	0.88
30:0:282:C:O2'	30:0:283:U:H5'	1.73	0.88
30:0:2541:U:H5'	30:0:2541:U:H6	1.37	0.88
30:0:541:C:H2'	30:0:542:A:H5''	1.55	0.88
8:H:59:GLN:HE21	8:H:129:ARG:HE	1.18	0.88
30:0:272:A:H3'	38:0:7525:HOH:O	1.74	0.88
30:0:541:C:C2'	30:0:542:A:H5''	2.04	0.88
30:0:69:A:H5'	30:0:69:A:H8	1.39	0.87
30:0:1878:G:H1'	38:0:6119:HOH:O	1.74	0.87
30:0:2783:A:H3'	38:0:5234:HOH:O	1.75	0.87
2:B:238:ASN:HD22	2:B:240:GLY:H	1.22	0.87
30:0:1667:A:H8	30:0:1667:A:H5'	1.39	0.86
13:M:99:ARG:HD2	13:M:167:GLY:HA2	1.57	0.86
30:0:1835:U:H5	30:0:1840:A:N7	1.74	0.86
30:0:1118:A:H3'	30:0:1118:A:H8	1.39	0.86
18:R:99:ALA:HB1	18:R:109:MET:HE1	1.58	0.85
30:0:2644:C:O2'	30:0:2645:U:H5'	1.76	0.85
24:X:37:LEU:HD13	24:X:85:VAL:HG21	1.58	0.85
2:B:36:PRO:HA	2:B:168:GLY:HA3	1.58	0.85
30:0:1205:U:C2'	30:0:1206:U:H5''	2.06	0.85
1:A:211:LYS:HB3	1:A:212:PRO:HD2	1.59	0.85
30:0:1979:G:H2'	38:0:3289:HOH:O	1.73	0.85
28:2:18:ASN:HD21	28:2:40:ARG:H	1.24	0.84
30:0:1118:A:H3'	30:0:1118:A:C8	2.11	0.84
14:N:37:ARG:HH12	31:9:6:C:H5''	1.43	0.84
30:0:1666:C:C2'	30:0:1667:A:H5''	2.07	0.84
30:0:2506:A:O2'	30:0:2507:G:H8	1.59	0.84
30:0:1372:A:H3'	38:0:7186:HOH:O	1.78	0.84
3:C:1:MET:HG2	3:C:2:GLN:H	1.42	0.84
31:9:92:G:H2'	31:9:93:A:C8	2.13	0.84
30:0:2769:C:C2'	30:0:2770:G:H5'	2.08	0.84
30:0:1183:C:N4	30:0:1184:C:H41	1.76	0.83
30:0:182:G:H5'	38:0:5160:HOH:O	1.79	0.83
31:9:29:C:H2'	31:9:30:C:H5'	1.60	0.83
30:0:2635:A:O2'	30:0:2636:C:H5'	1.79	0.83
14:N:83:LEU:HD13	14:N:175:LEU:HD23	1.59	0.83
30:0:559:U:H5'	30:0:559:U:H6	1.43	0.83
30:0:506:G:H22	30:0:509:A:H5'	1.44	0.82
30:0:1119:G:H22	30:0:1246:A:H2	1.25	0.82
23:W:88:THR:HB	38:W:6679:HOH:O	1.78	0.82

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:221:GLN:HE22	11:K:42:ASN:HD22	1.25	0.82
30:0:1701:A:H5'	38:0:6284:HOH:O	1.80	0.82
30:0:545:G:C8	30:0:545:G:H5'	2.12	0.82
1:A:94:LEU:HD12	1:A:98:GLU:HB2	1.62	0.81
30:0:2586:U:H3	30:0:2592:G:H22	1.26	0.81
31:9:14:G:H5'	31:9:14:G:H8	1.45	0.81
11:K:39:GLY:HA2	38:0:5223:HOH:O	1.79	0.81
30:0:2502:C:C2'	30:0:2503:A:H5'	2.11	0.81
18:R:8:ALA:HB1	18:R:13:THR:HG21	1.63	0.81
30:0:2502:C:H2'	30:0:2503:A:H5'	1.61	0.81
30:0:2506:A:HO2'	30:0:2507:G:H8	0.83	0.81
2:B:201:ASP:HB2	2:B:312:ARG:HD2	1.62	0.81
30:0:1119:G:N2	30:0:1246:A:C2	2.48	0.80
30:0:1175:G:H1'	30:0:1193:A:H2'	1.63	0.80
10:J:52:GLN:HE22	30:0:1119:G:H2'	1.46	0.80
8:H:59:GLN:NE2	8:H:129:ARG:HE	1.77	0.80
30:0:2896:A:H5''	38:0:6099:HOH:O	1.81	0.80
30:0:363:C:H1'	38:0:5282:HOH:O	1.82	0.80
30:0:1206:U:H6	30:0:1206:U:H5'	1.45	0.80
30:0:283:U:H5	30:0:284:C:N3	1.79	0.80
30:0:1160:G:H5'	30:0:1161:A:H5'	0.87	0.80
28:2:41:HIS:H	28:2:45:ASN:HD22	1.29	0.80
30:0:1973:A:H8	30:0:1973:A:H5'	1.45	0.80
30:0:603:A:H5''	30:0:604:G:OP1	1.81	0.80
30:0:1603:A:H5''	30:0:1605:G:H5'	1.63	0.79
30:0:541:C:H2'	30:0:542:A:C5'	2.12	0.79
23:W:72:PRO:HG2	23:W:77:ALA:HB3	1.64	0.79
10:J:70:PHE:CE1	30:0:2676:C:H4'	2.17	0.78
30:0:281:U:O2'	30:0:282:C:H5'	1.83	0.78
27:1:1:THR:HA	38:0:9358:HOH:O	1.83	0.78
30:0:2644:C:H2'	38:0:4596:HOH:O	1.83	0.78
14:N:113:SER:HB2	38:N:8855:HOH:O	1.82	0.78
15:O:47:ARG:HG3	15:O:47:ARG:HH11	1.47	0.78
21:U:9:CYS:HA	21:U:52:THR:HG22	1.64	0.78
30:0:1183:C:H42	30:0:1184:C:H41	1.32	0.78
30:0:2795:C:O2'	30:0:2796:U:H5'	1.83	0.78
3:C:115:LEU:HD13	3:C:223:LEU:HD21	1.63	0.78
30:0:1189:A:H1'	30:0:1209:C:O4'	1.84	0.78
23:W:84:VAL:HG12	38:W:6679:HOH:O	1.84	0.78
30:0:236:A:H4'	30:0:237:G:H5'	1.66	0.78
30:0:558:C:O2'	30:0:559:U:H5''	1.84	0.77

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:2748:G:H5'	38:0:7537:HOH:O	1.83	0.77
30:0:1300:G:H1'	38:0:4684:HOH:O	1.83	0.77
16:P:117:SER:HB3	30:0:1593:C:OP1	1.84	0.77
30:0:1116:U:H3	30:0:1246:A:H62	1.31	0.77
30:0:2769:C:O2'	30:0:2770:G:H5'	1.83	0.77
2:B:179:LEU:O	2:B:183:GLU:HG2	1.84	0.77
12:L:133:VAL:HA	38:L:8876:HOH:O	1.84	0.77
30:0:871:G:C8	30:0:871:G:C5'	2.60	0.77
30:0:1183:C:H2'	38:0:6244:HOH:O	1.85	0.77
10:J:127:ILE:HG22	35:J:8801:CL:CL	2.22	0.77
31:9:49:G:H5''	38:9:9087:HOH:O	1.84	0.77
30:0:2578:G:H5'	30:0:2578:G:H8	1.51	0.76
2:B:206:THR:HG21	30:0:2716:G:H5''	1.68	0.76
29:3:25:VAL:HG22	29:3:68:LYS:HG3	1.65	0.76
14:N:141:ARG:HH21	31:9:48:C:H4'	1.50	0.76
30:0:1209:C:H2'	30:0:1210:G:H8	1.51	0.76
30:0:192:A:H5'	38:0:7639:HOH:O	1.86	0.76
8:H:29:SER:HA	8:H:62:HIS:HD2	1.50	0.76
30:0:2533:C:C6	30:0:2533:C:H5'	2.20	0.75
23:W:4:LEU:HD23	23:W:54:PHE:HB3	1.69	0.75
30:0:2748:G:H1'	38:0:7896:HOH:O	1.85	0.75
30:0:567:U:H5''	38:0:5289:HOH:O	1.87	0.75
30:0:1189:A:H1'	30:0:1209:C:C1'	2.15	0.75
30:0:506:G:H22	30:0:509:A:H5''	1.51	0.75
30:0:847:C:H4'	38:0:3748:HOH:O	1.87	0.75
30:0:1790:C:H2'	30:0:1791:U:H6	1.52	0.75
11:K:98:VAL:CG1	11:K:102:GLU:HA	2.15	0.74
30:0:1701:A:H4'	30:0:1702:U:C5'	2.17	0.74
30:0:1120:U:H5'	30:0:1121:G:OP2	1.86	0.74
1:A:35:GLY:O	1:A:36:ASP:HB3	1.86	0.74
30:0:558:C:C2'	30:0:559:U:H5''	2.17	0.74
30:0:1666:C:H2'	30:0:1667:A:C5'	2.16	0.74
30:0:2487:C:H5	38:0:4889:HOH:O	1.71	0.74
3:C:127:ARG:NH2	3:C:225:PRO:HG2	2.03	0.74
30:0:1080:C:H4'	30:0:1081:A:OP1	1.87	0.74
13:M:102:GLU:OE1	13:M:164:THR:HG21	1.88	0.74
30:0:870:G:C2'	30:0:871:G:H5''	2.16	0.74
30:0:2717:C:H2'	30:0:2718:C:C5'	2.14	0.74
30:0:2637:A:H4'	38:0:6063:HOH:O	1.87	0.74
30:0:544:G:H2'	30:0:545:G:H5''	1.70	0.73
23:W:21:LEU:HD21	23:W:48:VAL:HG11	1.70	0.73

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:1441:G:O2'	30:0:1442:A:H5'	1.88	0.73
26:Z:61:HIS:HB2	26:Z:71:VAL:HB	1.70	0.73
30:0:1189:A:H3'	38:0:7676:HOH:O	1.86	0.73
3:C:47:GLY:HA2	3:C:92:PRO:HB2	1.71	0.73
30:0:2541:U:H5'	30:0:2541:U:C6	2.23	0.73
30:0:2787:C:H5	38:0:4633:HOH:O	1.72	0.73
30:0:2717:C:O2'	30:0:2718:C:H5''	1.89	0.73
30:0:1641:A:H2'	30:0:1642:A:H5'	1.69	0.73
30:0:1666:C:H2'	30:0:1667:A:H5'	1.71	0.73
30:0:2679:G:H2'	30:0:2681:A:OP2	1.89	0.73
30:0:2524:G:H21	30:0:2526:C:N4	1.86	0.73
14:N:49:THR:HG22	14:N:56:ASP:HB2	1.70	0.73
30:0:1701:A:H5''	30:0:1702:U:H3'	1.71	0.73
26:Z:60:ASP:HB3	26:Z:69:ASP:HB3	1.70	0.73
22:V:1:THR:HG23	22:V:2:VAL:H	1.54	0.73
30:0:271:C:H41	30:0:378:A:H2	1.33	0.73
30:0:2420:G:O2'	30:0:2421:G:H5'	1.88	0.73
30:0:396:U:H1'	38:0:7622:HOH:O	1.88	0.72
30:0:1118:A:H62	30:0:1244:U:H3	1.36	0.72
30:0:1525:G:H5'	30:0:1526:A:OP2	1.89	0.72
11:K:118:ALA:HA	11:K:125:ALA:HB2	1.71	0.72
30:0:2102:G:H2'	38:0:7763:HOH:O	1.87	0.72
4:D:103:ASN:ND2	4:D:134:LEU:H	1.88	0.72
30:0:827:A:H1'	38:0:6214:HOH:O	1.89	0.72
30:0:2254:G:H1'	38:0:5534:HOH:O	1.89	0.72
30:0:2644:C:HO2'	30:0:2645:U:H6	1.36	0.71
30:0:1632:A:H2'	30:0:1633:C:H5'	1.72	0.71
30:0:1441:G:H1'	38:0:7761:HOH:O	1.90	0.71
18:R:25:PHE:CE2	18:R:29:LYS:HE2	2.25	0.71
30:0:280:C:H2'	30:0:281:U:O4'	1.91	0.71
30:0:2769:C:H2'	30:0:2770:G:H5'	1.73	0.71
3:C:139:VAL:HG13	38:C:8659:HOH:O	1.90	0.71
13:M:95:LYS:HE2	30:0:157:G:H4'	1.73	0.71
30:0:281:U:H2'	30:0:282:C:O4'	1.91	0.71
30:0:2491:G:H1'	38:0:6868:HOH:O	1.90	0.70
30:0:2577:A:H8	38:0:9598:HOH:O	1.74	0.70
30:0:31:C:H4'	38:0:7421:HOH:O	1.91	0.70
30:0:1730:G:H5'	30:0:1731:C:C5	2.27	0.70
30:0:2505:G:O2'	30:0:2506:A:H5'	1.92	0.70
30:0:2756:U:H3	30:0:2896:A:H2	1.35	0.70
4:D:105:SER:OG	30:0:2338:G:H1'	1.90	0.70

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:134:ILE:HG23	13:M:141:ILE:HD13	1.74	0.70
5:E:100:ASP:HB2	38:E:2789:HOH:O	1.92	0.70
30:0:2812:A:H1'	38:0:5787:HOH:O	1.92	0.70
28:2:43:ARG:HH22	30:0:1684:A:H1'	1.57	0.70
30:0:2073:G:OP2	30:0:2490:A:H5'	1.92	0.70
1:A:51:ARG:HB2	38:A:9063:HOH:O	1.91	0.70
13:M:171:ARG:CD	30:0:156:C:H5''	2.20	0.69
30:0:1838:U:O2'	30:0:2644:C:H5'	1.92	0.69
26:Z:81:CYS:SG	26:Z:83:TYR:HB3	2.32	0.69
11:K:14:LYS:HB2	11:K:45:PRO:HG2	1.74	0.69
38:C:8676:HOH:O	30:0:2100:A:H5'	1.92	0.69
30:0:2135:A:O2'	30:0:2136:G:H5'	1.92	0.69
2:B:212:GLN:HB2	2:B:257:THR:HG21	1.74	0.69
30:0:285:A:H2'	30:0:286:U:O4'	1.92	0.69
30:0:2004:U:H4'	38:0:5307:HOH:O	1.92	0.69
30:0:1634:G:H3'	38:0:3891:HOH:O	1.93	0.69
23:W:137:GLN:HE21	23:W:141:HIS:CE1	2.03	0.69
30:0:558:C:H2'	30:0:559:U:C5'	2.23	0.69
30:0:681:G:N3	30:0:681:G:H5'	2.08	0.69
30:0:2670:G:O2'	30:0:2671:U:H5'	1.92	0.69
30:0:1666:C:C2'	30:0:1667:A:C5'	2.70	0.69
30:0:1451:C:H5'	30:0:1505:U:C5	2.28	0.69
24:X:61:ARG:HH12	24:X:67:PRO:HD3	1.57	0.69
30:0:1377:C:H6	30:0:1377:C:H5'	1.58	0.69
23:W:137:GLN:NE2	23:W:141:HIS:HE1	1.88	0.69
30:0:1835:U:C5	30:0:1840:A:N7	2.59	0.69
21:U:56:ARG:NH2	30:0:2890:A:H1'	2.08	0.68
10:J:19:MET:HE3	10:J:132:LEU:HD21	1.73	0.68
30:0:2563:U:H2'	30:0:2565:C:O5'	1.93	0.68
24:X:78:GLU:HB3	38:X:5564:HOH:O	1.94	0.68
30:0:1667:A:C8	30:0:1667:A:H5'	2.27	0.68
16:P:115:SER:H	16:P:118:GLN:NE2	1.88	0.68
30:0:960:G:H2'	30:0:960:G:N3	2.09	0.68
30:0:2851:G:O2'	30:0:2852:A:H5'	1.94	0.68
30:0:2005:G:H3'	30:0:2005:G:OP2	1.94	0.68
1:A:135:VAL:HG11	1:A:147:ARG:NH2	2.08	0.68
30:0:812:A:H1'	38:0:3955:HOH:O	1.93	0.68
21:U:47:ARG:HG3	38:U:4381:HOH:O	1.94	0.68
18:R:18:LEU:HB2	18:R:143:VAL:HG13	1.76	0.68
30:0:138:U:H5''	30:0:139:C:OP2	1.94	0.68
1:A:199:HIS:HD2	1:A:201:PHE:H	1.41	0.68

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:2111:G:H1'	38:0:9049:HOH:O	1.93	0.68
23:W:48:VAL:HG12	23:W:52:VAL:HB	1.75	0.68
30:0:564:G:H1'	38:0:6310:HOH:O	1.92	0.68
30:0:1528:A:H2'	30:0:1529:G:O4'	1.94	0.68
20:T:2:LYS:HG2	30:0:447:A:OP1	1.93	0.68
30:0:2659:U:H5''	38:0:4123:HOH:O	1.93	0.68
30:0:1730:G:H5''	30:0:1731:C:H6	1.59	0.67
4:D:28:GLY:HA2	4:D:69:ILE:HG23	1.75	0.67
30:0:2827:A:H2'	30:0:2828:G:O4'	1.94	0.67
24:X:76:ARG:HH11	24:X:76:ARG:HG3	1.60	0.67
1:A:88:ILE:HD13	1:A:100:PRO:HD3	1.74	0.67
11:K:87:ARG:HG3	30:0:2721:U:H4'	1.76	0.67
18:R:150:PRO:O	18:R:150:PRO:CG	2.42	0.67
30:0:1562:C:O2	30:0:1562:C:H2'	1.94	0.67
30:0:1182:C:H1'	30:0:1192:A:H8	1.60	0.67
3:C:236:THR:HA	38:C:8662:HOH:O	1.95	0.67
30:0:299:U:H5'	38:0:7336:HOH:O	1.93	0.67
14:N:37:ARG:NH1	31:9:6:C:C5'	2.52	0.67
3:C:236:THR:HG22	3:C:239:ALA:N	2.09	0.67
30:0:544:G:C2'	30:0:545:G:H5''	2.24	0.67
23:W:80:ASP:O	23:W:84:VAL:HG23	1.94	0.67
30:0:130:C:H2'	38:0:3158:HOH:O	1.95	0.67
29:3:48:ASN:HD21	30:0:2468:A:H61	1.43	0.67
31:9:75:G:H1	31:9:106:U:H3	1.42	0.67
10:J:18:ILE:HD13	30:0:1244:U:OP1	1.95	0.67
30:0:2852:A:H5''	38:0:5236:HOH:O	1.94	0.67
30:0:292:G:H2'	30:0:358:G:N2	2.10	0.66
5:E:116:THR:HG22	5:E:151:LEU:HD22	1.77	0.66
3:C:27:ARG:NH2	30:0:657:G:OP1	2.29	0.66
9:I:86:GLU:HG2	30:0:1180:U:H4'	1.76	0.66
30:0:1159:G:H21	30:0:1189:A:H8	1.42	0.66
22:V:42:ASN:HB3	38:V:7247:HOH:O	1.95	0.66
25:Y:169:ARG:HD2	30:0:1328:A:OP1	1.95	0.66
30:0:2524:G:H21	30:0:2526:C:H41	1.44	0.66
30:0:1189:A:O2'	30:0:1208:C:H2'	1.96	0.66
30:0:848:C:H5'	38:0:7271:HOH:O	1.94	0.66
35:0:8813:CL:CL	38:0:4684:HOH:O	2.51	0.66
22:V:57:LYS:HA	22:V:60:GLN:HE21	1.59	0.66
31:9:23:U:O2'	31:9:24:U:H4'	1.96	0.66
1:A:47:HIS:HD2	30:0:1654:U:H2'	1.60	0.66
30:0:1118:A:C8	30:0:1118:A:C3'	2.75	0.66

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:N:110:THR:HB	14:N:113:SER:OG	1.95	0.66
30:0:1834:C:H2'	30:0:1840:A:N6	2.10	0.66
31:9:92:G:H2'	31:9:93:A:H8	1.61	0.65
26:Z:34:SER:HA	30:0:797:A:H5'	1.76	0.65
30:0:441:A:H1'	30:0:442:A:N7	2.12	0.65
30:0:2812:A:C2	30:0:2814:A:N6	2.62	0.65
10:J:70:PHE:HE1	30:0:2676:C:H4'	1.61	0.65
23:W:59:GLN:HE22	23:W:98:PHE:HB2	1.62	0.65
14:N:38:LYS:HE2	14:N:107:ASN:ND2	2.11	0.65
13:M:164:THR:HG22	13:M:167:GLY:H	1.59	0.65
14:N:86:LEU:HD12	14:N:125:ALA:HB2	1.78	0.65
30:0:482:G:H4'	30:0:508:A:N1	2.12	0.65
30:0:2755:G:H1'	38:0:4683:HOH:O	1.97	0.65
3:C:140:VAL:HB	38:C:8662:HOH:O	1.97	0.65
1:A:100:PRO:HG2	1:A:103:VAL:HG21	1.78	0.65
30:0:2878:U:H2'	30:0:2879:A:O4'	1.96	0.65
6:F:96:ALA:HA	38:F:3111:HOH:O	1.96	0.65
5:E:20:ILE:HD11	5:E:40:VAL:HG11	1.79	0.65
30:0:2769:C:H2'	30:0:2770:G:C5'	2.25	0.65
30:0:2748:G:H2'	38:0:7537:HOH:O	1.96	0.65
31:9:14:G:H5'	31:9:14:G:C8	2.30	0.65
2:B:217:ARG:HG3	2:B:257:THR:HG22	1.79	0.65
30:0:841:A:H5''	38:0:6907:HOH:O	1.96	0.65
30:0:1741:U:H5'	30:0:1742:A:OP1	1.96	0.65
30:0:1477:C:H5'	30:0:1868:G:C5'	2.27	0.65
30:0:2559:C:H4'	38:0:7254:HOH:O	1.97	0.65
6:F:63:ILE:HB	6:F:64:PRO:HD3	1.78	0.65
30:0:1278:A:H4'	30:0:1279:U:C4	2.32	0.65
30:0:558:C:H2'	30:0:559:U:H5'	1.79	0.64
30:0:2756:U:N3	30:0:2896:A:H2	1.95	0.64
30:0:1649:G:H1'	38:0:5533:HOH:O	1.97	0.64
30:0:2768:A:H2'	30:0:2769:C:O4'	1.96	0.64
30:0:711:G:H1'	38:0:7093:HOH:O	1.96	0.64
3:C:184:ARG:NH2	30:0:450:C:OP1	2.30	0.64
12:L:57:VAL:HG21	30:0:2443:C:H5'	1.80	0.64
19:S:43:GLU:HB3	38:S:8989:HOH:O	1.97	0.64
2:B:307:ARG:HG3	2:B:307:ARG:HH11	1.61	0.64
30:0:308:U:H5'	30:0:309:C:OP1	1.96	0.64
10:J:41:ALA:HB3	38:J:5907:HOH:O	1.96	0.64
4:D:25:MET:HE3	4:D:37:ALA:HB1	1.77	0.64
30:0:2256:G:O2'	30:0:2257:G:H5'	1.98	0.64

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:1166:A:H61	30:0:1180:U:H3	1.45	0.64
23:W:26:ILE:HB	38:W:5420:HOH:O	1.96	0.64
30:0:1741:U:O2'	30:0:2723:G:H4'	1.98	0.64
30:0:2894:C:O2'	30:0:2895:C:H5'	1.98	0.64
2:B:98:THR:HG22	30:0:2820:A:OP1	1.98	0.64
38:Z:8707:HOH:O	30:0:1886:A:H4'	1.97	0.64
12:L:114:VAL:HG11	38:L:8876:HOH:O	1.97	0.64
12:L:56:LYS:HE3	30:0:2443:C:H1'	1.80	0.64
2:B:41:PHE:HA	2:B:79:MET:HE2	1.80	0.64
9:I:73:LEU:HD12	9:I:107:LYS:NZ	2.13	0.64
4:D:135:VAL:HG21	4:D:139:TYR:CD1	2.33	0.64
3:C:129:HIS:CE1	3:C:231:ARG:HA	2.33	0.64
10:J:82:THR:CG2	30:0:1242:A:H5'	2.21	0.64
30:0:1603:A:C5'	30:0:1605:G:H5'	2.28	0.64
24:X:74:ALA:HB2	24:X:85:VAL:HG13	1.80	0.64
30:0:559:U:H5'	30:0:559:U:C6	2.29	0.64
11:K:66:ARG:HH22	30:0:1994:A:P	2.21	0.64
10:J:69:TYR:CE1	30:0:2081:A:H4'	2.33	0.63
4:D:23:VAL:HG22	4:D:73:VAL:HB	1.80	0.63
30:0:1790:C:H2'	30:0:1791:U:C6	2.32	0.63
3:C:174:ILE:HD11	30:0:338:C:H4'	1.80	0.63
30:0:1183:C:N3	30:0:1184:C:C5	2.67	0.63
2:B:320:GLN:HE21	2:B:321:PRO:HD2	1.63	0.63
31:9:49:G:H2'	31:9:50:G:O4'	1.98	0.63
11:K:74:VAL:CG1	11:K:113:ILE:HG12	2.28	0.63
20:T:24:ARG:HH21	20:T:39:ASN:HD22	1.46	0.63
13:M:86:GLN:NE2	30:0:2274:A:H1'	2.14	0.63
12:L:18:HIS:HD2	30:0:902:G:N7	1.97	0.63
30:0:542:A:C8	30:0:542:A:H5'	2.24	0.63
30:0:1187:U:H2'	38:0:6893:HOH:O	1.99	0.63
30:0:1189:A:H1'	30:0:1209:C:H1'	1.79	0.63
30:0:71:G:H8	38:0:3908:HOH:O	1.81	0.63
30:0:123:U:H5'	38:0:6657:HOH:O	1.97	0.63
38:N:8844:HOH:O	31:9:7:G:H5'	1.98	0.63
30:0:247:A:H2'	38:0:3920:HOH:O	1.99	0.63
2:B:254:GLN:HG2	2:B:255:GLY:N	2.14	0.63
5:E:137:ASP:O	5:E:141:VAL:HG23	1.99	0.63
17:Q:25:PRO:HB2	38:Q:4350:HOH:O	1.99	0.62
30:0:2345:A:H3'	30:0:2346:C:C6	2.34	0.62
9:I:126:THR:O	9:I:130:LEU:HG	1.99	0.62
30:0:1973:A:H5'	30:0:1973:A:C8	2.32	0.62

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:2637:A:H5'	38:0:4930:HOH:O	1.99	0.62
30:0:200:C:H2'	38:0:3440:HOH:O	1.97	0.62
30:0:2426:G:H1'	38:0:6092:HOH:O	1.98	0.62
30:0:1632:A:C2'	30:0:1633:C:H5'	2.29	0.62
3:C:174:ILE:CD1	30:0:338:C:H4'	2.30	0.62
30:0:2481:G:H5''	38:0:4543:HOH:O	1.98	0.62
30:0:1249:U:H2'	30:0:1250:C:C6	2.34	0.62
25:Y:187:VAL:HG23	25:Y:192:ASP:CB	2.29	0.62
4:D:159:PRO:O	4:D:163:VAL:HG23	2.00	0.62
30:0:371:U:H2'	30:0:372:A:H8	1.65	0.62
30:0:2320:U:H4'	30:0:2321:A:O4'	1.99	0.62
30:0:2478:U:O2'	30:0:2479:A:H5'	1.99	0.62
23:W:6:GLN:CB	23:W:26:ILE:HD11	2.27	0.62
30:0:1730:G:C5'	30:0:1731:C:C6	2.82	0.62
28:2:35:ARG:HB2	38:2:2691:HOH:O	1.98	0.62
30:0:583:C:H2'	30:0:584:U:H6	1.64	0.62
30:0:1132:A:N6	30:0:1229:C:H2'	2.14	0.62
15:O:25:VAL:HG12	30:0:709:G:O2'	1.99	0.62
11:K:98:VAL:HG13	11:K:102:GLU:HA	1.81	0.62
30:0:960:G:N3	30:0:960:G:C2'	2.63	0.62
8:H:59:GLN:HE21	8:H:129:ARG:NE	1.95	0.62
30:0:2541:U:H6	30:0:2541:U:C5'	2.09	0.61
30:0:2644:C:O2'	30:0:2645:U:H6	1.83	0.61
30:0:1942:A:H3'	38:0:7346:HOH:O	1.99	0.61
30:0:363:C:O2'	30:0:364:U:H5'	2.00	0.61
6:F:91:VAL:HG12	6:F:92:GLY:N	2.15	0.61
16:P:59:ARG:HH22	16:P:66:GLN:NE2	1.98	0.61
31:9:39:U:H1'	31:9:44:A:H61	1.65	0.61
19:S:17:ASP:HB3	19:S:23:LYS:HB2	1.81	0.61
31:9:58:G:C8	31:9:59:C:C5	2.88	0.61
10:J:131:THR:HB	10:J:134:GLU:HG3	1.81	0.61
9:I:130:LEU:HD22	30:0:1167:G:H4'	1.82	0.61
30:0:2241:C:O2'	30:0:2242:U:H5'	2.00	0.61
5:E:91:PHE:HE1	30:0:2694:A:H4'	1.63	0.61
14:N:67:ALA:HA	14:N:71:TRP:HB3	1.80	0.61
1:A:192:VAL:CG1	1:A:207:GLN:HB3	2.29	0.61
30:0:2768:A:O2'	30:0:2769:C:H5'	2.00	0.61
8:H:19:ARG:HH12	30:0:1008:C:H5''	1.64	0.61
30:0:1172:G:H1'	38:0:4974:HOH:O	2.01	0.61
30:0:635:A:H2'	30:0:636:G:H5''	1.82	0.61
30:0:1474:C:C5'	30:0:1474:C:H6	2.07	0.61

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:72:ALA:HB2	13:M:93:ARG:HG2	1.81	0.61
23:W:4:LEU:CD2	23:W:54:PHE:HB3	2.31	0.61
1:A:109:GLU:HG2	1:A:116:GLY:H	1.65	0.61
30:0:1185:U:H5'	38:0:7462:HOH:O	1.99	0.61
11:K:10:GLN:N	11:K:10:GLN:HE21	1.89	0.61
30:0:558:C:C2'	30:0:559:U:C5'	2.79	0.61
23:W:88:THR:HG23	23:W:110:GLN:HB3	1.81	0.61
30:0:2604:A:H5'	38:0:5788:HOH:O	2.01	0.61
4:D:22:VAL:HG22	4:D:74:THR:HG22	1.83	0.61
29:3:15:ASN:O	30:0:2408:A:H4'	2.01	0.61
3:C:1:MET:HG2	3:C:2:GLN:N	2.15	0.61
30:0:407:A:H5'	38:0:6024:HOH:O	2.00	0.61
11:K:49:LEU:HD23	11:K:80:ILE:HD13	1.83	0.61
1:A:36:ASP:O	1:A:38:ILE:N	2.33	0.61
12:L:6:ARG:HD3	30:0:1299:G:O6	1.99	0.61
20:T:61:GLU:HG2	38:T:3851:HOH:O	1.98	0.61
5:E:143:GLN:HE21	30:0:2780:C:H1'	1.66	0.61
30:0:1202:A:C2'	30:0:1203:G:H5'	2.31	0.60
23:W:125:HIS:HE1	38:W:3071:HOH:O	1.84	0.60
30:0:1377:C:H5'	30:0:1377:C:C6	2.36	0.60
26:Z:34:SER:CB	30:0:797:A:H4'	2.30	0.60
30:0:2781:U:C2'	30:0:2782:G:H5'	2.31	0.60
30:0:514:G:H4'	38:0:5644:HOH:O	2.00	0.60
17:Q:21:ARG:HH12	30:0:2353:A:H1'	1.66	0.60
27:1:8:GLN:HE22	27:1:11:LYS:NZ	1.98	0.60
30:0:969:G:H1	30:0:999:C:N4	1.98	0.60
23:W:141:HIS:HB2	23:W:146:ILE:HG12	1.84	0.60
5:E:91:PHE:CE1	30:0:2694:A:H4'	2.36	0.60
30:0:644:G:N3	30:0:644:G:H5'	2.16	0.60
30:0:2414:A:H2'	30:0:2415:A:C8	2.35	0.60
9:I:112:LEU:HD11	30:0:1162:G:H1'	1.83	0.60
4:D:173:GLU:HG3	4:D:174:VAL:HG23	1.84	0.60
30:0:1819:G:H2'	30:0:1820:G:H4'	1.81	0.60
1:A:199:HIS:CD2	1:A:201:PHE:H	2.18	0.60
30:0:120:A:H2'	30:0:120:A:N3	2.16	0.60
17:Q:15:LYS:HD3	30:0:2364:A:H5''	1.83	0.60
25:Y:204:ARG:HH22	30:0:553:G:P	2.25	0.60
30:0:1202:A:O2'	30:0:1203:G:H5'	2.01	0.60
30:0:1730:G:H5''	30:0:1731:C:C6	2.36	0.60
10:J:39:VAL:HG22	10:J:106:GLY:O	2.01	0.60
30:0:920:C:H5''	30:0:921:G:O5'	2.02	0.60

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:1342:C:C2'	30:0:1343:C:H5'	2.30	0.60
30:0:625:U:H5''	30:0:1044:C:N4	2.16	0.60
2:B:71:VAL:HG11	2:B:296:LEU:HB3	1.81	0.60
14:N:7:LYS:HE3	17:Q:21:ARG:O	2.01	0.60
30:0:746:A:H5'	38:0:5514:HOH:O	2.02	0.60
26:Z:40:ALA:HA	30:0:1773:G:C8	2.37	0.60
2:B:141:ARG:HD2	2:B:163:GLU:OE2	2.02	0.60
18:R:39:THR:HG22	18:R:42:GLU:H	1.67	0.60
27:1:21:ARG:HD2	27:1:37:CYS:SG	2.41	0.60
14:N:40:ASN:ND2	31:9:28:U:H5''	2.17	0.60
14:N:48:VAL:CG1	14:N:55:ASP:HB3	2.32	0.60
30:0:1393:A:H2'	30:0:1394:C:C6	2.37	0.60
30:0:2869:G:H2'	30:0:2870:C:C6	2.36	0.60
18:R:128:ARG:NH2	30:0:2054:A:N3	2.50	0.59
30:0:669:G:O2'	30:0:670:G:H5'	2.02	0.59
27:1:16:HIS:HD2	30:0:470:U:O2'	1.83	0.59
30:0:2524:G:N2	30:0:2526:C:H41	2.00	0.59
30:0:31:C:H2'	38:0:7684:HOH:O	2.02	0.59
30:0:515:C:H5''	38:0:5644:HOH:O	2.01	0.59
30:0:283:U:C5	30:0:284:C:N3	2.67	0.59
2:B:74:ILE:HD13	2:B:309:VAL:HG21	1.83	0.59
30:0:1457:U:H5	38:0:7872:HOH:O	1.84	0.59
20:T:9:LYS:HD3	38:0:3750:HOH:O	2.02	0.59
30:0:128:A:O2'	30:0:129:A:H5'	2.02	0.59
18:R:39:THR:HG23	18:R:107:GLU:O	2.02	0.59
12:L:41:HIS:CD2	30:0:926:A:O2'	2.56	0.59
8:H:72:ALA:HB2	8:H:156:ALA:HB2	1.84	0.59
9:I:120:ALA:O	9:I:124:VAL:HG23	2.02	0.59
30:0:2498:C:O2'	30:0:2499:U:H5'	2.02	0.59
30:0:2756:U:N3	30:0:2896:A:C2	2.63	0.59
30:0:1425:G:O2'	30:0:1426:C:H5'	2.02	0.59
2:B:156:LYS:HB3	30:0:2846:C:H4'	1.84	0.59
30:0:2403:C:H5'	38:0:6025:HOH:O	2.02	0.59
2:B:36:PRO:HG3	2:B:169:GLY:H	1.67	0.59
31:9:13:A:O2'	31:9:14:G:H5''	2.03	0.59
13:M:24:GLN:NE2	13:M:27:ARG:HH11	2.01	0.59
30:0:1183:C:H42	30:0:1184:C:N4	2.00	0.59
18:R:99:ALA:HB1	18:R:109:MET:CE	2.30	0.59
2:B:51:VAL:HG13	2:B:53:LEU:HD13	1.83	0.59
30:0:1268:C:O2'	30:0:1269:G:H5'	2.01	0.59
12:L:134:GLU:HG3	38:L:8857:HOH:O	2.03	0.59

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:2505:G:C2'	30:0:2506:A:H5'	2.33	0.59
1:A:99:ILE:O	1:A:131:HIS:HE1	1.86	0.59
30:0:2419:U:H5''	30:0:2420:G:H5'	1.83	0.59
30:0:1426:C:H2'	38:0:9591:HOH:O	2.03	0.59
22:V:12:THR:HG22	22:V:15:GLU:HG3	1.84	0.59
10:J:70:PHE:CD1	30:0:2676:C:H4'	2.38	0.59
20:T:9:LYS:HB2	38:0:7421:HOH:O	2.01	0.59
2:B:294:TYR:HE2	38:B:9117:HOH:O	1.85	0.59
31:9:2:U:OP2	31:9:3:A:H5'	2.03	0.58
27:1:28:HIS:HE1	30:0:776:A:OP1	1.86	0.58
30:0:807:A:O2'	30:0:808:A:H5'	2.03	0.58
30:0:2637:A:C5'	38:0:4930:HOH:O	2.50	0.58
20:T:9:LYS:HE3	20:T:13:ARG:NH1	2.18	0.58
30:0:2781:U:H2'	30:0:2782:G:H5'	1.84	0.58
30:0:2344:G:N3	30:0:2344:G:H2'	2.18	0.58
30:0:2900:G:H2'	30:0:2901:C:O4'	2.03	0.58
18:R:29:LYS:HD3	30:0:524:A:H5''	1.85	0.58
1:A:48:ASP:HB3	38:A:9063:HOH:O	2.02	0.58
11:K:8:VAL:HG13	11:K:80:ILE:HG22	1.84	0.58
6:F:58:GLU:CD	13:M:27:ARG:HH22	2.06	0.58
30:0:1201:C:H5''	38:0:6233:HOH:O	2.02	0.58
11:K:32:ILE:HD11	11:K:56:SER:HB3	1.84	0.58
23:W:52:VAL:HG22	23:W:53:ALA:H	1.68	0.58
31:9:1:U:H5''	31:9:3:A:OP1	2.03	0.58
22:V:44:GLY:HA3	30:0:92:G:H4'	1.85	0.58
30:0:1942:A:O2'	30:0:1943:C:H5'	2.03	0.58
30:0:1230:A:OP1	30:0:1230:A:H8	1.85	0.58
15:O:42:GLU:HB2	38:O:2176:HOH:O	2.02	0.58
14:N:11:ARG:HD3	31:9:114:G:O6	2.03	0.58
2:B:312:ARG:HD3	2:B:315:VAL:HG13	1.85	0.58
4:D:25:MET:HE2	4:D:41:LEU:HG	1.85	0.58
30:0:485:A:N3	30:0:487:G:H5''	2.19	0.58
30:0:2335:C:H2'	30:0:2336:G:C8	2.38	0.58
30:0:2533:C:H6	30:0:2533:C:C5'	2.12	0.58
14:N:141:ARG:NH2	31:9:48:C:H4'	2.19	0.58
18:R:18:LEU:HG	18:R:91:LEU:HD13	1.86	0.58
30:0:1649:G:O2'	30:0:1650:C:H5'	2.04	0.58
30:0:1211:G:H2'	30:0:1212:C:H6	1.69	0.58
12:L:30:ARG:HD3	30:0:164:G:H4'	1.86	0.58
2:B:162:MET:CE	2:B:310:ARG:HD3	2.33	0.58
20:T:41:ARG:HG2	20:T:41:ARG:HH11	1.66	0.58

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:1015:C:H2'	30:0:1016:U:H6	1.67	0.58
14:N:61:ALA:HB3	14:N:88:ALA:HB2	1.85	0.58
30:0:2802:C:H2'	30:0:2803:C:H6	1.68	0.58
30:0:2445:U:H2'	30:0:2446:G:C8	2.39	0.58
13:M:179:GLY:O	30:0:399:C:H5'	2.04	0.58
1:A:212:PRO:HB2	38:A:9024:HOH:O	2.04	0.58
30:0:2032:U:H2'	30:0:2033:G:C5'	2.34	0.58
13:M:163:LEU:HD21	30:0:188:C:H5''	1.86	0.58
2:B:145:HIS:HD2	2:B:146:THR:O	1.87	0.58
30:0:1165:G:O2'	30:0:1174:A:H1'	2.04	0.57
30:0:1207:A:C8	30:0:1208:C:C5	2.92	0.57
30:0:1856:C:H5'	30:0:1858:A:O4'	2.04	0.57
1:A:55:VAL:HG23	1:A:68:ILE:O	2.04	0.57
30:0:1947:G:N2	30:0:1966:U:C2	2.71	0.57
30:0:1596:U:H2'	30:0:1598:A:OP2	2.03	0.57
9:I:110:ASP:O	30:0:1163:G:H5'	2.04	0.57
30:0:1181:A:H2'	30:0:1182:C:H5'	1.86	0.57
30:0:1819:G:H2'	30:0:1820:G:C5'	2.34	0.57
30:0:1015:C:H2'	30:0:1016:U:C6	2.39	0.57
30:0:2472:C:O2'	30:0:2634:G:H4'	2.03	0.57
30:0:705:C:H2'	30:0:705:C:O2	2.04	0.57
30:0:1903:U:O2'	30:0:1904:A:N7	2.38	0.57
30:0:2851:G:C2'	30:0:2852:A:H5'	2.34	0.57
30:0:1477:C:O2'	30:0:1478:U:H5'	2.04	0.57
30:0:1307:A:H2'	30:0:1308:A:C8	2.39	0.57
6:F:34:ASN:HA	13:M:4:ALA:HB2	1.86	0.57
21:U:17:THR:HG22	21:U:18:GLY:N	2.18	0.57
30:0:1463:U:H2'	30:0:1464:C:C6	2.39	0.57
22:V:1:THR:HB	30:0:93:C:H5''	1.86	0.57
22:V:38:GLY:O	22:V:41:GLU:HG3	2.05	0.57
30:0:2251:G:H2'	30:0:2252:A:C8	2.40	0.57
30:0:2415:A:H2'	30:0:2416:G:H5'	1.86	0.57
30:0:255:A:H2'	30:0:256:C:H6	1.68	0.57
30:0:264:G:H1'	30:0:265:U:H5	1.70	0.57
2:B:125:GLU:O	2:B:129:ARG:HG3	2.04	0.57
30:0:2689:A:H2'	30:0:2690:U:H5'	1.87	0.57
30:0:1138:G:H4'	38:0:5706:HOH:O	2.03	0.57
30:0:876:A:N3	30:0:876:A:H2'	2.19	0.57
30:0:1588:G:C6	30:0:1589:G:N1	2.73	0.57
1:A:47:HIS:CD2	30:0:1654:U:H2'	2.39	0.57
9:I:130:LEU:CD2	30:0:1167:G:H4'	2.35	0.57

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:941:G:C5	30:0:942:U:C4	2.93	0.57
30:0:1174:A:C5	30:0:1201:C:H4'	2.39	0.57
30:0:2291:A:N9	30:0:2309:C:H5'	2.19	0.57
30:0:1603:A:H5'	30:0:1605:G:C4'	2.34	0.57
30:0:2509:A:H2'	30:0:2510:C:O4'	2.05	0.57
38:B:9100:HOH:O	30:0:2672:C:H1'	2.05	0.57
18:R:18:LEU:HB2	18:R:143:VAL:CG1	2.34	0.57
30:0:2134:G:N2	30:0:2242:U:C2	2.73	0.57
30:0:1044:C:H5''	38:0:9025:HOH:O	2.05	0.57
1:A:121:ALA:O	1:A:124:VAL:HG22	2.05	0.57
30:0:823:U:H3'	38:0:4446:HOH:O	2.03	0.57
31:9:22:G:H5'	31:9:23:U:OP1	2.05	0.57
2:B:140:LEU:HA	38:B:9048:HOH:O	2.05	0.57
30:0:694:A:H2'	30:0:695:C:H5'	1.86	0.57
16:P:54:LYS:HB2	30:0:1717:A:H5''	1.87	0.57
30:0:834:G:H3'	30:0:835:U:H4'	1.87	0.56
5:E:132:THR:HB	38:E:2227:HOH:O	2.05	0.56
30:0:821:U:H3'	38:0:3765:HOH:O	2.05	0.56
30:0:821:U:H2'	30:0:822:C:H6	1.70	0.56
30:0:2710:U:H1'	38:0:7616:HOH:O	2.04	0.56
3:C:188:ARG:HD3	38:C:8564:HOH:O	2.05	0.56
31:9:29:C:C2'	31:9:30:C:H5'	2.33	0.56
30:0:1641:A:C2'	30:0:1642:A:H5'	2.35	0.56
4:D:25:MET:CE	4:D:37:ALA:HB1	2.35	0.56
9:I:112:LEU:CD1	30:0:1162:G:H1'	2.34	0.56
30:0:952:G:N3	30:0:2302:A:H2'	2.20	0.56
30:0:671:A:O2'	30:0:672:G:H2'	2.05	0.56
30:0:1135:G:H5'	38:0:5927:HOH:O	2.05	0.56
10:J:74:ARG:O	10:J:78:ILE:HG12	2.05	0.56
17:Q:19:ARG:HH21	31:9:11:A:P	2.27	0.56
23:W:88:THR:HG22	23:W:90:TYR:HD1	1.69	0.56
30:0:308:U:C4	30:0:342:C:H1'	2.41	0.56
17:Q:28:ARG:HG2	38:Q:4350:HOH:O	2.04	0.56
30:0:1160:G:O2'	30:0:1190:G:H1'	2.06	0.56
30:0:1279:U:O2	30:0:1279:U:H2'	2.05	0.56
5:E:143:GLN:NE2	30:0:2779:G:H21	2.04	0.56
27:I:20:ARG:HG2	30:0:111:C:O2'	2.06	0.56
30:0:316:A:N3	30:0:336:G:O2'	2.37	0.56
8:H:26:ILE:HA	8:H:123:ILE:HG21	1.87	0.56
30:0:2256:G:H2'	30:0:2257:G:C5'	2.35	0.56
25:Y:187:VAL:HG23	25:Y:192:ASP:HB2	1.87	0.56

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:9:76:G:C3'	31:9:77:A:H5''	2.28	0.56
23:W:139:GLY:O	23:W:141:HIS:HD2	1.89	0.56
9:I:108:HIS:H	9:I:109:PRO:HD2	1.71	0.56
24:X:23:HIS:HE1	30:0:2044:G:OP1	1.88	0.56
30:0:10:U:O4	30:0:532:A:OP2	2.23	0.56
30:0:282:C:O2'	30:0:283:U:C5'	2.50	0.56
23:W:125:HIS:NE2	30:0:1097:A:H5''	2.21	0.56
30:0:1592:G:H2'	30:0:1593:C:C6	2.41	0.56
1:A:36:ASP:HB2	1:A:85:SER:H	1.71	0.56
3:C:129:HIS:HE1	3:C:231:ARG:HA	1.71	0.56
17:Q:26:PRO:O	17:Q:30:VAL:HG23	2.05	0.56
30:0:2880:A:H2'	30:0:2881:C:H5'	1.88	0.56
30:0:1768:C:H2'	30:0:1769:C:O4'	2.06	0.56
6:F:39:SER:HB3	6:F:45:ALA:HB2	1.88	0.56
14:N:37:ARG:NH1	31:9:6:C:OP1	2.38	0.56
13:M:99:ARG:CD	13:M:167:GLY:HA2	2.33	0.56
2:B:85:ARG:NH1	38:B:9100:HOH:O	2.39	0.56
14:N:169:PRO:O	14:N:172:PHE:HB3	2.06	0.56
31:9:64:C:C2'	31:9:65:A:H5'	2.36	0.56
28:2:8:LYS:NZ	30:0:1677:U:OP2	2.37	0.56
24:X:43:VAL:HG11	24:X:82:GLU:HA	1.88	0.56
30:0:1118:A:H8	30:0:1119:G:H5''	1.71	0.55
30:0:816:G:C6	30:0:817:G:N1	2.74	0.55
31:9:64:C:H2'	31:9:65:A:H5'	1.88	0.55
30:0:2703:A:H2'	30:0:2704:C:H6	1.71	0.55
2:B:27:ASN:H	2:B:27:ASN:HD22	1.54	0.55
19:S:76:GLU:HB3	38:S:8991:HOH:O	2.05	0.55
30:0:1163:G:H1	30:0:1184:C:N4	2.03	0.55
30:0:1588:G:C6	30:0:1589:G:C6	2.94	0.55
30:0:2645:U:OP2	30:0:2645:U:C6	2.60	0.55
30:0:2802:C:H2'	30:0:2803:C:C6	2.41	0.55
30:0:1595:G:O2'	30:0:1596:U:H5'	2.06	0.55
30:0:2269:C:C2'	30:0:2270:G:H5'	2.37	0.55
8:H:48:VAL:HA	8:H:170:ARG:O	2.05	0.55
30:0:1119:G:N2	30:0:1246:A:H2	1.97	0.55
30:0:1477:C:H5'	30:0:1868:G:H5''	1.88	0.55
30:0:2256:G:C2'	30:0:2257:G:H5'	2.35	0.55
28:2:10:ARG:NH2	30:0:121:U:OP2	2.40	0.55
30:0:1878:G:O2'	30:0:1879:U:C6	2.58	0.55
23:W:88:THR:HG22	23:W:89:ASP:H	1.71	0.55
31:9:39:U:H3'	31:9:40:C:H5''	1.88	0.55

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:407:A:H3'	38:0:4460:HOH:O	2.06	0.55
5:E:84:MET:HG2	5:E:168:ILE:HA	1.88	0.55
30:0:735:C:H2'	30:0:736:A:H5'	1.87	0.55
18:R:96:VAL:HG13	18:R:106:GLY:HA3	1.88	0.55
30:0:652:G:H8	38:0:3009:HOH:O	1.89	0.55
9:I:111:LEU:HD23	30:0:1163:G:H4'	1.88	0.55
30:0:272:A:H5'	30:0:273:G:OP2	2.07	0.55
30:0:1377:C:C5'	30:0:1377:C:H6	2.18	0.55
2:B:234:ARG:HG3	30:0:1735:C:OP2	2.06	0.55
30:0:2626:C:H2'	30:0:2627:G:C8	2.42	0.55
1:A:33:GLU:CD	1:A:33:GLU:H	2.10	0.55
30:0:810:G:H2'	30:0:811:C:C6	2.42	0.55
2:B:275:GLY:O	2:B:291:ASP:HA	2.07	0.55
4:D:154:LYS:HD2	4:D:154:LYS:N	2.15	0.55
30:0:877:G:C5'	30:0:878:G:OP1	2.52	0.55
28:2:18:ASN:ND2	28:2:40:ARG:H	2.01	0.55
23:W:88:THR:HG23	23:W:110:GLN:HE21	1.71	0.55
31:9:49:G:O2'	31:9:50:G:H5'	2.07	0.55
31:9:39:U:H1'	31:9:44:A:N6	2.21	0.55
27:1:46:ARG:HA	38:1:8971:HOH:O	2.05	0.55
31:9:12:C:H5'	31:9:70:U:O4'	2.06	0.55
30:0:581:G:O2'	30:0:582:U:H5'	2.06	0.55
1:A:223:ARG:HD2	30:0:2272:G:OP1	2.07	0.55
22:V:50:ARG:HH12	30:0:56:G:H5''	1.70	0.55
38:O:7674:HOH:O	30:0:935:G:H5'	2.05	0.55
13:M:99:ARG:HD2	13:M:167:GLY:CA	2.35	0.55
31:9:91:C:H2'	31:9:92:G:O4'	2.07	0.55
31:9:28:U:H2'	31:9:29:C:C6	2.41	0.55
30:0:2502:C:H2'	30:0:2503:A:C5'	2.36	0.55
23:W:38:THR:HG22	23:W:39:ASP:N	2.22	0.55
17:Q:40:HIS:HE1	30:0:949:U:O2'	1.90	0.55
30:0:1174:A:C6	30:0:1201:C:H4'	2.42	0.54
30:0:1209:C:H2'	30:0:1210:G:C8	2.36	0.54
30:0:271:C:C2	30:0:273:G:O4'	2.60	0.54
30:0:567:U:H5''	38:0:6401:HOH:O	2.06	0.54
31:9:1:U:H4'	31:9:3:A:OP1	2.07	0.54
22:V:50:ARG:NH1	30:0:56:G:H5''	2.22	0.54
30:0:2697:A:H2'	30:0:2698:G:O4'	2.07	0.54
13:M:34:GLU:HB3	13:M:38:GLU:HG3	1.89	0.54
6:F:2:VAL:HG22	6:F:57:GLU:OE1	2.07	0.54
30:0:2718:C:H6	30:0:2718:C:H5'	1.73	0.54

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:O:47:ARG:HG3	15:O:47:ARG:NH1	2.19	0.54
2:B:162:MET:HE3	2:B:310:ARG:HD3	1.89	0.54
30:0:204:A:H2'	30:0:205:U:H5'	1.88	0.54
30:0:2616:A:H4'	30:0:2617:G:OP1	2.06	0.54
30:0:1291:A:H2	38:0:5292:HOH:O	1.89	0.54
1:A:135:VAL:HG21	1:A:147:ARG:HB3	1.89	0.54
30:0:1172:G:H5''	38:0:7257:HOH:O	2.07	0.54
30:0:999:C:O2'	30:0:1000:C:H5'	2.07	0.54
27:1:9:GLY:HA2	30:0:1687:C:O2	2.07	0.54
23:W:154:ARG:NH1	30:0:588:G:O6	2.40	0.54
21:U:9:CYS:HA	21:U:52:THR:CG2	2.35	0.54
30:0:2564:G:OP2	30:0:2565:C:H5''	2.06	0.54
21:U:17:THR:HG22	21:U:18:GLY:H	1.72	0.54
30:0:1484:G:H2'	38:0:9103:HOH:O	2.08	0.54
13:M:99:ARG:HE	13:M:170:ASN:HD22	1.55	0.54
2:B:304:PRO:HD2	2:B:307:ARG:NE	2.22	0.54
11:K:27:ARG:HD2	38:K:3442:HOH:O	2.07	0.54
17:Q:7:LEU:HD12	30:0:2424:U:H1'	1.89	0.54
2:B:267:LYS:HD3	38:0:9562:HOH:O	2.06	0.54
30:0:1559:A:OP2	30:0:1559:A:H8	1.88	0.54
30:0:1175:G:H1'	30:0:1193:A:C2'	2.36	0.54
14:N:80:SER:HB2	38:N:8833:HOH:O	2.07	0.54
30:0:1766:U:O2	30:0:1778:A:H5'	2.08	0.54
8:H:168:VAL:HG13	38:H:213:HOH:O	2.08	0.54
15:O:37:ARG:HD2	30:0:656:G:OP2	2.08	0.54
2:B:79:MET:HE1	38:B:9092:HOH:O	2.07	0.54
30:0:65:C:O2'	30:0:66:G:H5'	2.07	0.54
18:R:14:ALA:HB3	18:R:147:LEU:HB2	1.89	0.54
30:0:1183:C:C2	30:0:1184:C:C5	2.96	0.54
21:U:46:ALA:HB1	21:U:52:THR:HG21	1.89	0.54
27:1:37:CYS:SG	27:1:39:PHE:HB2	2.48	0.54
30:0:1131:G:C6	30:0:1230:A:C4	2.96	0.54
5:E:154:ILE:HD11	5:E:157:LYS:HE2	1.90	0.54
30:0:958:G:H2'	30:0:959:C:C6	2.42	0.54
19:S:33:SER:O	19:S:37:VAL:HG23	2.08	0.54
2:B:211:THR:HG23	30:0:2840:A:OP1	2.08	0.54
8:H:64:SER:OG	30:0:2520:G:H5'	2.07	0.54
5:E:10:ASP:HA	38:E:6017:HOH:O	2.06	0.54
6:F:58:GLU:HB3	13:M:8:ILE:HG23	1.90	0.54
30:0:2269:C:O2'	30:0:2270:G:H5'	2.07	0.54
14:N:132:ASN:O	14:N:135:VAL:HG12	2.08	0.54

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:20:VAL:O	7:G:24:VAL:HG23	2.08	0.54
31:9:34:A:H2'	31:9:35:C:O4'	2.08	0.53
30:0:420:U:H2'	30:0:421:C:C6	2.44	0.53
30:0:549:A:O2'	30:0:550:C:H5'	2.08	0.53
30:0:2070:G:H2'	30:0:2072:G:OP1	2.08	0.53
30:0:1730:G:H5'	30:0:1731:C:H5	1.73	0.53
31:9:1:U:O3'	31:9:3:A:H5''	2.08	0.53
30:0:2345:A:H3'	30:0:2346:C:H6	1.71	0.53
13:M:23:LEU:HD13	13:M:27:ARG:NH2	2.23	0.53
30:0:2705:U:H2'	30:0:2706:A:C8	2.43	0.53
30:0:961:A:H4'	38:0:6768:HOH:O	2.07	0.53
30:0:90:A:H2'	30:0:91:G:O4'	2.08	0.53
13:M:28:GLN:O	13:M:32:ARG:HG3	2.08	0.53
8:H:61:ARG:HG3	8:H:61:ARG:HH11	1.73	0.53
23:W:125:HIS:HB2	23:W:137:GLN:HG2	1.90	0.53
30:0:1505:U:H1'	38:0:7584:HOH:O	2.07	0.53
2:B:41:PHE:HB3	2:B:190:MET:HE3	1.89	0.53
30:0:255:A:H2'	30:0:256:C:C6	2.44	0.53
22:V:55:ARG:O	22:V:59:ILE:HG12	2.08	0.53
3:C:95:GLU:HG3	38:C:8688:HOH:O	2.07	0.53
5:E:68:HIS:O	5:E:72:MET:HG3	2.09	0.53
11:K:4:LEU:HD22	11:K:116:GLU:HB3	1.90	0.53
30:0:2826:G:C6	30:0:2913:A:N6	2.75	0.53
30:0:1615:A:H5'	38:0:4180:HOH:O	2.09	0.53
30:0:1622:G:H2'	30:0:1623:C:H5'	1.90	0.53
10:J:19:MET:HE3	10:J:132:LEU:HD11	1.89	0.53
14:N:114:LYS:O	14:N:118:ILE:HG13	2.07	0.53
12:L:41:HIS:HD2	30:0:926:A:O2'	1.90	0.53
8:H:27:PRO:HD3	8:H:123:ILE:HG22	1.91	0.53
8:H:174:LEU:HD21	30:0:1220:U:H4'	1.89	0.53
13:M:188:ARG:HD3	30:0:155:C:OP2	2.08	0.53
30:0:297:U:H2'	30:0:298:C:C6	2.43	0.53
30:0:484:A:N1	30:0:506:G:H4'	2.23	0.53
30:0:1838:U:H3'	38:0:5521:HOH:O	2.09	0.53
31:9:20:G:O2'	31:9:21:G:H5'	2.08	0.53
30:0:2597:U:H2'	30:0:2598:U:H5'	1.90	0.53
30:0:318:U:H5'	30:0:339:A:C2	2.44	0.53
30:0:2243:C:H5''	38:0:3745:HOH:O	2.07	0.53
23:W:35:VAL:HG23	23:W:41:TYR:CD2	2.43	0.53
30:0:281:U:C2'	30:0:282:C:H5'	2.39	0.53
30:0:1878:G:O2'	30:0:1879:U:P	2.67	0.53

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:7:ARG:HG2	2:B:7:ARG:HH11	1.72	0.53
8:H:6:ALA:HB3	30:0:2521:A:OP2	2.09	0.53
30:0:2371:G:H5'	38:0:5010:HOH:O	2.07	0.53
13:M:164:THR:HB	38:M:8819:HOH:O	2.08	0.53
30:0:1972:U:H2'	30:0:1973:A:C5'	2.38	0.53
30:0:1592:G:H2'	30:0:1593:C:H6	1.71	0.53
31:9:24:U:H3'	31:9:25:G:C5'	2.39	0.53
30:0:319:A:H4'	30:0:338:C:C4	2.44	0.53
30:0:1483:C:O2'	30:0:1484:G:H5'	2.09	0.53
5:E:69:ILE:HA	5:E:72:MET:CE	2.39	0.53
30:0:1921:A:O2'	30:0:1922:A:H5'	2.09	0.53
28:2:28:LYS:O	30:0:87:C:H2'	2.09	0.53
30:0:506:G:N2	30:0:509:A:H5''	2.22	0.53
14:N:38:LYS:HE2	14:N:107:ASN:HD21	1.72	0.53
30:0:256:C:H2'	30:0:257:G:O4'	2.09	0.53
30:0:2301:A:H5''	30:0:2302:A:H5'	1.91	0.53
30:0:1202:A:H2'	30:0:1203:G:C5'	2.39	0.53
28:2:41:HIS:HD2	28:2:44:ARG:H	1.56	0.53
15:O:44:ASN:OD1	15:O:65:LEU:HB2	2.07	0.53
30:0:1795:G:H2'	30:0:1796:A:O4'	2.09	0.53
30:0:522:U:O2'	30:0:1366:C:H5'	2.08	0.53
30:0:396:U:O2'	30:0:418:C:H4'	2.08	0.52
30:0:1342:C:H2'	30:0:1343:C:H5'	1.91	0.52
27:1:45:ARG:NH2	38:1:8976:HOH:O	2.38	0.52
22:V:39:ALA:N	22:V:40:PRO:HD2	2.24	0.52
30:0:413:G:H2'	30:0:414:C:C6	2.44	0.52
30:0:1535:G:H2'	30:0:1536:C:C6	2.44	0.52
3:C:63:SER:OG	30:0:2101:A:H2'	2.09	0.52
30:0:1201:C:H2'	30:0:1202:A:H5'	1.91	0.52
30:0:1603:A:C5'	30:0:1605:G:O4'	2.53	0.52
30:0:1878:G:C1'	38:0:6119:HOH:O	2.42	0.52
30:0:2507:G:H2'	30:0:2510:C:H42	1.74	0.52
12:L:37:LYS:HE2	30:0:2466:G:OP2	2.09	0.52
9:I:121:LYS:HB3	30:0:1184:C:H4'	1.90	0.52
23:W:4:LEU:HD22	23:W:52:VAL:HG21	1.90	0.52
3:C:2:GLN:HB3	38:C:8534:HOH:O	2.09	0.52
30:0:1268:C:H2'	30:0:1269:G:H8	1.75	0.52
28:2:22:PRO:HG2	28:2:25:VAL:HG23	1.90	0.52
30:0:1213:C:O2'	30:0:1214:G:H5'	2.10	0.52
22:V:64:GLY:O	22:V:65:ASP:HB2	2.08	0.52
3:C:218:VAL:HG12	38:C:8634:HOH:O	2.08	0.52

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:Y:134:HIS:HE1	30:0:538:C:OP2	1.92	0.52
8:H:69:ARG:HD3	38:H:233:HOH:O	2.10	0.52
31:9:56:A:H2'	31:9:57:A:C5'	2.05	0.52
30:0:613:C:H2'	30:0:614:U:H6	1.75	0.52
28:2:40:ARG:HD2	28:2:47:THR:HG22	1.91	0.52
1:A:101:GLU:OE2	1:A:131:HIS:HB2	2.10	0.52
30:0:1855:G:H4'	30:0:1856:C:O5'	2.09	0.52
5:E:3:VAL:HG22	5:E:49:ILE:HB	1.90	0.52
18:R:33:ARG:NH1	38:R:8946:HOH:O	2.43	0.52
13:M:75:ARG:HH11	30:0:1864:C:H5	1.56	0.52
30:0:1183:C:O2	30:0:1183:C:H2'	2.08	0.52
30:0:137:U:H2'	30:0:139:C:C5	2.45	0.52
1:A:186:TRP:CG	1:A:187:PRO:HA	2.45	0.52
30:0:2300:A:H4'	30:0:2301:A:O5'	2.10	0.52
14:N:93:GLN:HE21	14:N:93:GLN:HA	1.74	0.52
25:Y:235:GLU:H	25:Y:235:GLU:CD	2.11	0.52
30:0:1679:C:H5'	38:0:9325:HOH:O	2.08	0.52
30:0:2613:G:O2'	30:0:2614:C:H5'	2.09	0.52
30:0:2433:A:H2'	30:0:2434:A:C8	2.44	0.52
30:0:1497:G:H4'	30:0:1627:G:O2'	2.09	0.52
5:E:80:TRP:O	5:E:134:SER:HA	2.09	0.52
23:W:119:HIS:HD2	23:W:120:PRO:O	1.93	0.52
3:C:162:VAL:HG22	3:C:232:LEU:HD21	1.89	0.52
30:0:2445:U:H2'	30:0:2446:G:H8	1.74	0.52
13:M:30:GLU:O	13:M:34:GLU:HG3	2.10	0.52
25:Y:146:PRO:O	25:Y:154:ARG:HG3	2.10	0.52
12:L:148:GLU:HA	38:L:8875:HOH:O	2.08	0.52
30:0:2469:A:H1'	38:0:3237:HOH:O	2.08	0.52
2:B:238:ASN:HD22	2:B:240:GLY:N	2.00	0.52
30:0:603:A:H1'	30:0:605:C:C2	2.44	0.52
30:0:2256:G:H2'	30:0:2257:G:H5'	1.92	0.52
2:B:320:GLN:NE2	2:B:321:PRO:HD2	2.24	0.52
5:E:143:GLN:NE2	30:0:2780:C:H1'	2.25	0.52
30:0:2781:U:O2'	30:0:2782:G:H5'	2.08	0.52
27:1:8:GLN:HE22	27:1:11:LYS:HZ2	1.58	0.52
30:0:1342:C:O2'	30:0:1343:C:H5'	2.09	0.52
3:C:107:ARG:O	3:C:111:VAL:HG23	2.10	0.52
2:B:8:LYS:HG3	2:B:220:VAL:HG12	1.92	0.52
30:0:1309:U:O2'	30:0:1310:U:H5'	2.10	0.52
25:Y:170:SER:OG	25:Y:175:ARG:HG3	2.09	0.52
18:R:117:HIS:HD2	30:0:20:G:H21	1.56	0.52

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:T:38:ARG:NH1	38:T:6217:HOH:O	2.42	0.52
30:0:1202:A:H2'	30:0:1203:G:H5'	1.91	0.52
11:K:98:VAL:HG11	11:K:102:GLU:HA	1.88	0.52
30:0:1527:A:H1'	30:0:1528:A:C8	2.45	0.52
4:D:52:THR:HG21	30:0:2346:C:O2'	2.10	0.52
2:B:271:ASP:HB3	2:B:296:LEU:HD12	1.91	0.52
16:P:58:SER:HB3	38:0:5627:HOH:O	2.10	0.52
25:Y:142:SER:OG	30:0:1331:G:OP2	2.27	0.52
31:9:52:A:O2'	31:9:53:G:H5'	2.10	0.52
31:9:110:G:C5	31:9:111:U:C5	2.97	0.52
30:0:905:C:H3'	38:0:5190:HOH:O	2.08	0.52
30:0:2587:OMU:H2'	30:0:2589:U:H5''	1.92	0.52
30:0:645:U:O2	30:0:761:A:H2	1.92	0.52
30:0:1207:A:C8	30:0:1208:C:C6	2.98	0.52
2:B:207:LYS:HG3	30:0:2717:C:OP1	2.10	0.52
16:P:115:SER:N	16:P:118:GLN:HE21	1.97	0.52
30:0:559:U:H6	30:0:559:U:C5'	2.17	0.52
21:U:9:CYS:CA	21:U:52:THR:HG22	2.39	0.52
30:0:1477:C:C5'	30:0:1868:G:H5''	2.39	0.52
2:B:158:LYS:HD3	30:0:2846:C:OP1	2.10	0.52
1:A:171:LYS:HB2	30:0:820:G:C5	2.45	0.52
30:0:2269:C:H2'	30:0:2270:G:C5'	2.40	0.52
6:F:57:GLU:O	6:F:61:MET:HG3	2.09	0.52
12:L:143:THR:HG21	38:L:8841:HOH:O	2.09	0.52
30:0:2836:G:H1'	38:0:6838:HOH:O	2.09	0.52
30:0:1825:U:O2'	30:0:1826:C:H5'	2.10	0.52
9:I:69:PRO:HA	30:0:1164:U:OP1	2.10	0.52
30:0:2072:G:C6	30:0:2533:C:H1'	2.45	0.52
2:B:41:PHE:HB3	2:B:190:MET:CE	2.40	0.52
30:0:2781:U:H2'	30:0:2782:G:C5'	2.39	0.52
24:X:43:VAL:HG12	24:X:44:ASP:N	2.25	0.52
30:0:538:C:H5''	30:0:539:G:C8	2.45	0.52
30:0:1857:A:H5''	38:0:6701:HOH:O	2.10	0.52
18:R:40:ALA:O	18:R:44:VAL:HG23	2.10	0.52
30:0:177:A:H2'	30:0:178:U:O4'	2.09	0.52
30:0:1636:G:O2'	30:0:1637:A:H5'	2.09	0.52
15:O:3:THR:HG22	30:0:656:G:C5'	2.26	0.51
30:0:1589:G:H4'	38:0:6857:HOH:O	2.10	0.51
30:0:2830:U:O2'	30:0:2831:C:H5'	2.09	0.51
30:0:1419:U:H2'	30:0:1685:A:C2	2.45	0.51
4:D:65:GLU:HA	38:D:6752:HOH:O	2.09	0.51

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:912:A:C4	30:0:1294:A:C2	2.97	0.51
30:0:12:U:H2'	30:0:13:G:H5'	1.92	0.51
30:0:1165:G:H4'	30:0:1174:A:O2'	2.10	0.51
30:0:1762:C:H2'	30:0:1763:C:H6	1.76	0.51
30:0:497:A:H2'	30:0:498:A:C5'	2.41	0.51
30:0:24:G:N2	30:0:518:G:H1'	2.25	0.51
30:0:1058:A:H2'	30:0:1060:C:H5''	1.91	0.51
11:K:82:ARG:NH2	11:K:115:ARG:HG2	2.26	0.51
30:0:1188:A:C6	30:0:1189:A:C6	2.98	0.51
30:0:558:C:H2'	30:0:559:U:H5''	1.87	0.51
1:A:51:ARG:NH1	1:A:120:ARG:O	2.43	0.51
31:9:52:A:H2'	31:9:53:G:O4'	2.09	0.51
30:0:661:G:C5	30:0:686:A:C2	2.99	0.51
27:1:25:LYS:HD2	28:2:48:ASP:HA	1.92	0.51
30:0:2435:U:H1'	38:0:5428:HOH:O	2.11	0.51
1:A:210:GLY:HA3	38:A:9046:HOH:O	2.08	0.51
30:0:304:G:H1'	30:0:347:A:N6	2.25	0.51
30:0:2064:U:H5'	30:0:2652:U:H4'	1.93	0.51
29:3:70:ARG:HB3	38:3:8997:HOH:O	2.09	0.51
30:0:1976:G:H1'	30:0:2005:G:N2	2.26	0.51
11:K:74:VAL:HG11	11:K:113:ILE:HG12	1.91	0.51
30:0:119:A:H2'	30:0:120:A:H5''	1.92	0.51
30:0:2689:A:C2'	30:0:2690:U:H5'	2.39	0.51
20:T:68:ASP:HB2	38:0:5658:HOH:O	2.10	0.51
30:0:1565:C:O2'	30:0:1566:C:H5'	2.10	0.51
23:W:21:LEU:HD21	23:W:48:VAL:CG1	2.39	0.51
30:0:64:G:H2'	30:0:65:C:O4'	2.11	0.51
8:H:32:ALA:HB3	8:H:69:ARG:HH12	1.76	0.51
30:0:380:A:H2'	38:0:7225:HOH:O	2.10	0.51
29:3:3:MET:O	29:3:90:PHE:HA	2.10	0.51
30:0:2421:G:H3'	30:0:2422:U:H5''	1.92	0.51
30:0:2421:G:H3'	30:0:2422:U:C5'	2.40	0.51
30:0:204:A:C2'	30:0:205:U:H5'	2.40	0.51
5:E:69:ILE:HA	5:E:72:MET:HE2	1.91	0.51
30:0:677:C:O2'	30:0:678:G:H5'	2.10	0.51
4:D:58:VAL:CG1	4:D:60:GLU:HG2	2.40	0.51
30:0:42:C:H1'	38:0:4676:HOH:O	2.10	0.51
24:X:85:VAL:HG12	24:X:86:GLU:N	2.26	0.51
30:0:1730:G:C5'	30:0:1731:C:H6	2.23	0.51
8:H:61:ARG:HG3	38:0:4972:HOH:O	2.10	0.51
25:Y:133:HIS:HD2	38:Y:9065:HOH:O	1.93	0.51

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:26:VAL:HG13	10:J:36:VAL:HG11	1.93	0.51
2:B:212:GLN:HA	30:0:1733:A:H4'	1.91	0.51
6:F:50:VAL:HG13	6:F:60:VAL:HG11	1.92	0.51
20:T:97:ARG:NH2	30:0:309:C:OP1	2.44	0.51
30:0:407:A:H8	38:0:4460:HOH:O	1.94	0.51
30:0:537:G:O4'	30:0:538:C:C5	2.64	0.51
30:0:589:U:H2'	30:0:590:A:H8	1.75	0.51
18:R:59:PHE:O	18:R:63:ASN:HB3	2.11	0.51
30:0:2105:C:H2'	30:0:2106:C:C6	2.46	0.51
30:0:1925:G:O2'	30:0:1926:G:H5'	2.11	0.51
30:0:1622:G:C2'	30:0:1623:C:H5'	2.41	0.51
3:C:214:THR:HG23	38:C:8648:HOH:O	2.10	0.51
7:G:12:ILE:HG23	38:0:5457:HOH:O	2.09	0.51
8:H:22:TYR:CZ	30:0:1007:A:H2'	2.46	0.51
14:N:110:THR:HB	14:N:113:SER:HG	1.74	0.51
23:W:119:HIS:HE1	38:0:9554:HOH:O	1.93	0.51
30:0:1819:G:H2'	30:0:1820:G:C4'	2.41	0.51
30:0:1482:A:O2'	30:0:1483:C:H5'	2.11	0.51
7:G:64:ASN:N	7:G:64:ASN:HD22	2.09	0.51
30:0:1252:A:H2'	30:0:1253:C:O4'	2.11	0.51
12:L:92:ASP:HA	12:L:121:ILE:HB	1.91	0.51
30:0:1205:U:C2'	30:0:1206:U:C5'	2.77	0.50
30:0:2717:C:C2'	30:0:2718:C:C5'	2.75	0.50
30:0:567:U:C5'	38:0:6401:HOH:O	2.59	0.50
25:Y:187:VAL:HG23	25:Y:192:ASP:HB3	1.92	0.50
12:L:143:THR:HG22	12:L:144:ASP:N	2.27	0.50
30:0:1321:A:H2'	30:0:1322:G:C8	2.47	0.50
2:B:5:ARG:NH2	30:0:2548:C:OP2	2.44	0.50
16:P:83:LYS:HG2	30:0:793:A:H5''	1.93	0.50
30:0:1173:A:H4'	30:0:1174:A:C8	2.45	0.50
30:0:1191:A:C2	30:0:1207:A:C2	2.99	0.50
30:0:2769:C:H2'	30:0:2770:G:O4'	2.11	0.50
30:0:1684:A:O2'	30:0:1685:A:H5''	2.12	0.50
30:0:1778:A:H2'	30:0:1779:A:H5'	1.92	0.50
30:0:1762:C:O2'	30:0:1763:C:H5'	2.12	0.50
13:M:90:ARG:NH2	30:0:2266:A:OP2	2.44	0.50
30:0:939:A:N1	30:0:1027:G:O2'	2.40	0.50
30:0:1386:G:O2'	30:0:1387:G:H5'	2.12	0.50
2:B:132:HIS:NE2	2:B:171:VAL:HG23	2.27	0.50
30:0:1915:U:O2'	30:0:1916:C:H5'	2.11	0.50
25:Y:212:ARG:HD2	38:Y:9085:HOH:O	2.09	0.50

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:1158:G:O2'	30:0:1159:G:H5'	2.11	0.50
30:0:1667:A:H2'	30:0:1668:U:C6	2.45	0.50
4:D:103:ASN:HD22	4:D:134:LEU:H	1.59	0.50
30:0:711:G:C2	30:0:718:C:C2	3.00	0.50
30:0:940:G:C5	30:0:1027:G:C2	3.00	0.50
12:L:97:VAL:HG12	12:L:98:GLU:O	2.12	0.50
1:A:112:PRO:HD3	1:A:152:CYS:SG	2.51	0.50
6:F:53:ASP:OD1	6:F:80:GLN:HB2	2.11	0.50
29:3:60:LYS:HG3	29:3:61:PRO:HD2	1.92	0.50
30:0:2385:G:H2'	30:0:2386:U:C6	2.47	0.50
2:B:102:THR:HG21	2:B:182:VAL:O	2.11	0.50
21:U:6:CYS:HB2	21:U:32:CYS:HB3	1.93	0.50
2:B:62:ARG:HA	2:B:65:MET:CE	2.41	0.50
30:0:1187:U:O2'	30:0:1189:A:H2	1.79	0.50
31:9:3:A:H2	31:9:21:G:N3	2.09	0.50
15:O:25:VAL:HG23	15:O:26:TRP:N	2.27	0.50
30:0:1130:U:H2'	30:0:1131:G:O4'	2.11	0.50
30:0:2250:G:N2	30:0:2251:G:H1'	2.27	0.50
30:0:735:C:C2'	30:0:736:A:H5'	2.41	0.50
21:U:39:ASN:ND2	21:U:44:ARG:HH11	2.08	0.50
30:0:1304:U:H2'	30:0:1305:C:C6	2.46	0.50
23:W:43:GLY:HA3	30:0:945:U:O2'	2.11	0.50
30:0:2089:A:O2'	30:0:2090:G:H5'	2.11	0.50
30:0:2667:G:H1'	30:0:2914:A:N3	2.26	0.50
38:M:8837:HOH:O	30:0:169:A:H5''	2.12	0.50
18:R:132:ARG:HG2	18:R:133:ALA:N	2.24	0.50
30:0:2584:G:H4'	38:0:7115:HOH:O	2.10	0.50
18:R:150:PRO:CG	18:R:150:PRO:CB	2.87	0.50
30:0:282:C:H1'	30:0:368:C:H41	1.71	0.50
30:0:559:U:C5	30:0:560:U:C5	3.00	0.50
30:0:2724:U:H2'	30:0:2725:G:O4'	2.11	0.50
30:0:17:G:H2'	30:0:18:C:C6	2.47	0.50
3:C:22:PHE:HA	3:C:116:ALA:HA	1.92	0.50
9:I:89:GLU:OE2	30:0:1181:A:H5'	2.11	0.50
31:9:55:U:H5'	38:9:9135:HOH:O	2.11	0.50
30:0:69:A:C8	30:0:69:A:C5'	2.90	0.50
10:J:19:MET:CE	10:J:132:LEU:HD11	2.41	0.50
1:A:33:GLU:O	1:A:34:ASP:HB2	2.10	0.50
17:Q:95:GLU:HA	30:0:949:U:H4'	1.93	0.50
25:Y:151:SER:HB3	25:Y:154:ARG:HB2	1.92	0.50
3:C:79:ARG:O	3:C:87:ARG:HG2	2.11	0.50

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:1333:U:H2'	30:0:1334:C:C6	2.47	0.50
30:0:332:G:O2'	30:0:333:G:H5'	2.12	0.50
26:Z:34:SER:HB3	30:0:797:A:H4'	1.93	0.50
1:A:109:GLU:HG2	1:A:116:GLY:N	2.26	0.50
10:J:107:ASN:HD22	10:J:109:TYR:H	1.58	0.50
30:0:2710:U:H2'	30:0:2711:U:C6	2.46	0.50
5:E:154:ILE:HD11	5:E:157:LYS:HB2	1.92	0.50
30:0:1200:A:H3'	38:0:5754:HOH:O	2.11	0.50
30:0:1422:U:H2'	30:0:1423:C:C6	2.47	0.50
30:0:2372:A:H2'	30:0:2373:U:H6	1.77	0.50
12:L:67:ARG:HB2	12:L:112:GLY:HA3	1.93	0.50
30:0:1170:U:H2'	30:0:1172:G:OP2	2.11	0.50
30:0:920:C:H4'	30:0:921:G:C2	2.45	0.50
30:0:2252:A:C5	30:0:2253:G:H1'	2.47	0.50
30:0:1762:C:H2'	30:0:1763:C:C6	2.47	0.50
30:0:1380:U:H5'	38:0:9218:HOH:O	2.12	0.50
30:0:638:C:H2'	30:0:639:A:C8	2.47	0.50
31:9:24:U:H3'	31:9:25:G:H5'	1.94	0.50
22:V:12:THR:HG23	22:V:14:ALA:H	1.77	0.50
30:0:876:A:N3	30:0:876:A:C2'	2.75	0.50
2:B:258:GLY:H	2:B:260:HIS:CE1	2.29	0.50
31:9:55:U:H4'	31:9:56:A:C8	2.47	0.49
11:K:55:VAL:HG12	11:K:56:SER:N	2.27	0.49
30:0:136:C:H2'	30:0:137:U:O4'	2.12	0.49
6:F:91:VAL:HG11	30:0:262:A:OP2	2.11	0.49
11:K:49:LEU:CD2	11:K:80:ILE:HD13	2.42	0.49
30:0:2871:G:H2'	30:0:2872:U:C6	2.47	0.49
23:W:13:MET:HE3	23:W:17:ILE:HG22	1.93	0.49
4:D:50:VAL:HG13	31:9:41:C:O4'	2.12	0.49
30:0:1165:G:O2'	30:0:1174:A:C1'	2.60	0.49
30:0:1211:G:H2'	30:0:1212:C:C6	2.47	0.49
30:0:488:U:H2'	38:0:4004:HOH:O	2.12	0.49
8:H:34:HIS:HD2	8:H:90:LEU:O	1.95	0.49
12:L:34:GLY:HA3	12:L:38:HIS:CE1	2.46	0.49
30:0:2534:C:H1'	38:0:3491:HOH:O	2.11	0.49
23:W:61:THR:HG23	23:W:151:GLU:HG3	1.94	0.49
30:0:1186:C:N4	30:0:1187:U:C4	2.81	0.49
30:0:559:U:H2'	30:0:560:U:O4'	2.12	0.49
18:R:9:ASP:O	18:R:13:THR:HB	2.11	0.49
18:R:18:LEU:HD12	18:R:143:VAL:CG1	2.42	0.49
4:D:76:ARG:NE	31:9:44:A:O4'	2.44	0.49

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:91:PRO:HA	10:J:144:THR:OG1	2.12	0.49
30:0:790:A:H1'	30:0:1710:A:H2'	1.94	0.49
6:F:13:GLU:OE2	6:F:78:GLU:HG2	2.13	0.49
25:Y:115:ARG:HH21	30:0:1266:U:H4'	1.76	0.49
38:R:8953:HOH:O	30:0:1370:G:H5''	2.12	0.49
13:M:99:ARG:HE	13:M:170:ASN:ND2	2.10	0.49
30:0:69:A:H8	30:0:69:A:C5'	2.17	0.49
14:N:71:TRP:CE3	14:N:175:LEU:HD22	2.47	0.49
30:0:1972:U:C2'	30:0:1973:A:H5''	2.42	0.49
18:R:128:ARG:NH2	30:0:2054:A:C2	2.80	0.49
30:0:1309:U:C2'	30:0:1310:U:H5'	2.43	0.49
30:0:1524:U:OP1	30:0:1524:U:H4'	2.12	0.49
30:0:947:U:O2'	30:0:948:G:H5'	2.13	0.49
8:H:39:LYS:HA	8:H:87:LYS:NZ	2.27	0.49
2:B:244:PRO:HB3	30:0:1234:U:N3	2.27	0.49
30:0:1515:A:H2'	30:0:1516:U:C6	2.48	0.49
30:0:1286:A:H5''	30:0:1287:A:OP1	2.13	0.49
30:0:1193:A:C2	30:0:1194:A:N6	2.80	0.49
30:0:483:C:C4	30:0:484:A:C6	3.01	0.49
14:N:1:ALA:HB2	31:9:14:G:O2'	2.13	0.49
5:E:139:GLU:OE2	30:0:2781:U:H1'	2.13	0.49
30:0:968:G:C2	30:0:1001:U:O2	2.66	0.49
30:0:2326:C:H4'	30:0:2412:G:C4'	2.43	0.49
24:X:30:MET:HG2	30:0:1384:C:H5'	1.94	0.49
30:0:1119:G:N2	30:0:1246:A:N1	2.60	0.49
1:A:211:LYS:HB3	1:A:212:PRO:CD	2.38	0.49
30:0:1278:A:H2'	30:0:1280:A:C8	2.48	0.49
30:0:920:C:H5'	30:0:921:G:C4	2.48	0.49
30:0:1245:C:O5'	30:0:1245:C:H6	1.96	0.49
30:0:1056:U:H2'	30:0:1057:A:O4'	2.12	0.49
5:E:126:ILE:HB	5:E:131:LEU:HD23	1.94	0.49
31:9:56:A:C3'	31:9:57:A:H5''	2.42	0.49
30:0:2541:U:O2'	30:0:2542:C:H5'	2.13	0.49
30:0:371:U:H2'	30:0:372:A:C8	2.47	0.49
30:0:2269:C:H2'	30:0:2270:G:H5'	1.94	0.49
2:B:17:LYS:O	2:B:260:HIS:HD2	1.95	0.49
11:K:34:VAL:HG22	11:K:47:ALA:HB2	1.94	0.49
30:0:899:C:H5'	38:0:3199:HOH:O	2.13	0.49
30:0:1706:G:H1'	30:0:1712:A:H61	1.78	0.49
19:S:57:THR:HG22	19:S:58:MET:N	2.28	0.49
11:K:130:MET:SD	21:U:25:ASP:O	2.70	0.49

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:1909:A:N1	30:0:2128:G:H1'	2.27	0.49
9:I:73:LEU:HD12	9:I:107:LYS:HZ1	1.76	0.49
14:N:12:ARG:HD3	14:N:18:THR:OG1	2.13	0.49
1:A:179:MET:HG2	1:A:186:TRP:CB	2.43	0.49
30:0:2869:G:H2'	30:0:2870:C:H6	1.78	0.49
14:N:17:ARG:HH11	14:N:17:ARG:HB3	1.78	0.49
30:0:1849:G:H1'	30:0:2011:A:N1	2.28	0.49
8:H:15:PRO:HG3	30:0:1053:G:OP1	2.12	0.49
6:F:107:ASP:O	6:F:111:ILE:HG13	2.12	0.49
1:A:94:LEU:HG	1:A:99:ILE:CD1	2.43	0.49
2:B:262:ARG:HG3	30:0:2716:G:H5'	1.94	0.49
3:C:127:ARG:CZ	3:C:225:PRO:HG2	2.42	0.49
25:Y:169:ARG:HD3	30:0:1328:A:C8	2.47	0.49
2:B:307:ARG:HG3	2:B:307:ARG:NH1	2.28	0.49
15:O:24:ALA:HB3	30:0:710:G:OP1	2.13	0.49
1:A:190:ARG:NH2	1:A:207:GLN:OE1	2.45	0.49
30:0:2121:G:O2'	30:0:2122:C:H5'	2.13	0.49
30:0:2512:U:H4'	30:0:2514:U:O4	2.12	0.49
2:B:206:THR:HG21	30:0:2716:G:C5'	2.40	0.49
30:0:2271:G:N3	30:0:2271:G:H2'	2.28	0.49
30:0:226:A:H1'	30:0:393:G:C5	2.48	0.49
30:0:1506:U:H6	30:0:1506:U:H5'	1.77	0.49
30:0:1066:U:H2'	30:0:1067:A:C8	2.48	0.49
20:T:53:GLY:HA3	38:0:6800:HOH:O	2.12	0.49
14:N:4:PRO:HG3	31:9:69:U:OP1	2.13	0.49
3:C:34:ALA:HB3	3:C:220:THR:HG21	1.94	0.49
13:M:78:LYS:HD3	38:0:7679:HOH:O	2.13	0.49
13:M:167:GLY:O	13:M:171:ARG:HG3	2.13	0.48
30:0:1118:A:C8	30:0:1119:G:H5''	2.48	0.48
30:0:2645:U:H1'	38:0:9305:HOH:O	2.13	0.48
30:0:191:A:C4	30:0:237:G:N7	2.81	0.48
30:0:2836:G:H5''	38:0:5165:HOH:O	2.12	0.48
19:S:57:THR:HG23	38:S:8979:HOH:O	2.11	0.48
30:0:2664:A:OP1	30:0:2664:A:H8	1.96	0.48
19:S:11:THR:H	19:S:14:ALA:HB3	1.77	0.48
30:0:1545:C:H2'	30:0:1546:G:O4'	2.13	0.48
30:0:1116:U:O2'	30:0:1118:A:C2	2.39	0.48
30:0:1972:U:H2'	30:0:1973:A:H5''	1.94	0.48
31:9:3:A:OP2	31:9:25:G:N2	2.45	0.48
30:0:1477:C:H5'	30:0:1868:G:H5'	1.94	0.48
30:0:2379:G:N7	30:0:2408:A:N1	2.61	0.48

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:2326:C:H4'	30:0:2412:G:H4'	1.95	0.48
30:0:1447:U:H3'	30:0:1506:U:O2	2.13	0.48
3:C:58:ALA:HA	3:C:73:GLN:HE21	1.78	0.48
30:0:2329:C:O2'	30:0:2330:U:H5'	2.13	0.48
17:Q:53:HIS:CD2	30:0:2389:U:H4'	2.48	0.48
4:D:141:VAL:HG21	31:9:57:A:H8	1.78	0.48
23:W:4:LEU:O	23:W:32:CYS:HA	2.13	0.48
30:0:2102:G:H1'	30:0:2103:A:N7	2.29	0.48
30:0:447:A:O2'	30:0:448:G:H5'	2.13	0.48
30:0:10:U:C4	30:0:532:A:C8	3.01	0.48
30:0:1013:A:H1'	38:0:9158:HOH:O	2.13	0.48
30:0:2816:A:H5''	30:0:2817:G:H5'	1.96	0.48
30:0:59:A:H5'	38:0:4330:HOH:O	2.12	0.48
3:C:43:LYS:HG2	30:0:449:A:N7	2.28	0.48
30:0:1185:U:H2'	30:0:1186:C:C6	2.48	0.48
30:0:1667:A:C2	30:0:1668:U:C2	3.02	0.48
23:W:139:GLY:O	23:W:141:HIS:CD2	2.66	0.48
30:0:1589:G:N2	30:0:1605:G:H1'	2.27	0.48
16:P:115:SER:OG	16:P:118:GLN:HG3	2.13	0.48
30:0:2420:G:H2'	30:0:2421:G:H8	1.79	0.48
10:J:74:ARG:HB3	10:J:74:ARG:HH11	1.77	0.48
12:L:34:GLY:HA2	38:0:5408:HOH:O	2.12	0.48
2:B:139:ASP:HB2	38:B:8995:HOH:O	2.12	0.48
13:M:171:ARG:NH2	30:0:189:A:OP1	2.47	0.48
30:0:541:C:O2'	30:0:542:A:H5''	2.14	0.48
23:W:88:THR:HG22	23:W:90:TYR:CD1	2.48	0.48
1:A:95:PRO:HG2	1:A:98:GLU:HG2	1.96	0.48
30:0:2493:C:O2	30:0:2493:C:H2'	2.13	0.48
2:B:119:HIS:O	2:B:121:PRO:HD3	2.13	0.48
30:0:699:C:H6	30:0:744:G:O4'	1.96	0.48
30:0:228:C:H2'	30:0:229:G:H5'	1.94	0.48
6:F:30:LYS:HE2	6:F:99:THR:HG21	1.94	0.48
30:0:1520:G:C6	30:0:1521:C:N4	2.82	0.48
30:0:1522:A:C2	30:0:1665:G:C6	3.02	0.48
30:0:2374:G:H2'	30:0:2375:A:C8	2.48	0.48
30:0:2372:A:H2'	30:0:2373:U:C6	2.48	0.48
16:P:1:THR:O	30:0:1396:C:H1'	2.14	0.48
30:0:499:G:O2'	30:0:500:G:H5'	2.13	0.48
30:0:536:A:H3'	38:0:5049:HOH:O	2.14	0.48
30:0:1029:U:O2'	30:0:1273:C:OP1	2.27	0.48
20:T:106:GLU:HG3	38:T:4913:HOH:O	2.13	0.48

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:101:GLU:HB2	5:E:116:THR:O	2.14	0.48
30:0:834:G:H4'	30:0:835:U:OP2	2.13	0.48
27:1:45:ARG:HB3	38:1:8967:HOH:O	2.14	0.48
30:0:1594:C:O2'	30:0:1607:A:H4'	2.13	0.48
30:0:346:U:H4'	38:0:6842:HOH:O	2.13	0.48
30:0:2387:U:H2'	30:0:2388:C:C6	2.48	0.48
1:A:1:GLY:HA2	30:0:2114:C:OP1	2.13	0.48
30:0:1739:G:O2'	30:0:1740:U:H5'	2.13	0.48
30:0:291:C:H2'	30:0:292:G:O4'	2.14	0.48
31:9:1:U:C4'	31:9:3:A:OP1	2.60	0.48
30:0:1130:U:H5'	38:0:7668:HOH:O	2.13	0.48
30:0:1314:U:H5''	30:0:1316:G:O4'	2.13	0.48
31:9:45:A:C5	31:9:46:C:C5	3.02	0.48
30:0:312:U:C2	30:0:320:G:N2	2.82	0.48
1:A:3:ARG:HD3	30:0:870:G:OP2	2.13	0.48
30:0:545:G:H8	30:0:545:G:C5'	2.12	0.48
30:0:289:G:O2'	30:0:290:C:H5'	2.14	0.48
30:0:2255:A:O2'	30:0:2256:G:H5'	2.14	0.48
30:0:304:G:H1'	30:0:347:A:H61	1.78	0.48
1:A:126:ALA:HB1	1:A:138:VAL:CG1	2.44	0.48
6:F:36:THR:HG23	6:F:97:ALA:HB2	1.94	0.48
16:P:98:ILE:HD12	16:P:102:ARG:NE	2.29	0.48
30:0:1593:C:H1'	38:0:6105:HOH:O	2.14	0.48
10:J:107:ASN:C	10:J:107:ASN:HD22	2.16	0.48
30:0:625:U:H3'	38:0:3250:HOH:O	2.13	0.48
30:0:820:G:H5'	30:0:821:U:H5'	1.95	0.48
30:0:2840:A:H3'	38:0:7643:HOH:O	2.13	0.48
28:2:22:PRO:HG2	28:2:25:VAL:CG2	2.44	0.48
30:0:2090:G:H2'	30:0:2091:G:C8	2.48	0.48
30:0:1423:C:O2'	30:0:1424:A:H5'	2.14	0.48
23:W:68:THR:HG23	23:W:69:ARG:HG2	1.96	0.48
27:1:12:ASN:O	30:0:1415:G:H5'	2.14	0.48
30:0:466:A:H2'	30:0:467:G:O4'	2.13	0.48
30:0:541:C:C2'	30:0:542:A:C5'	2.79	0.47
23:W:122:ARG:NH2	38:0:5289:HOH:O	2.46	0.47
30:0:736:A:H2'	30:0:737:A:O4'	2.14	0.47
31:9:110:G:C6	31:9:111:U:C5	3.02	0.47
30:0:106:A:H2'	30:0:107:U:O4'	2.14	0.47
30:0:1028:U:H1'	38:0:3639:HOH:O	2.14	0.47
25:Y:132:ASP:OD2	30:0:621:C:H5'	2.14	0.47
30:0:559:U:C3'	30:0:559:U:C6	2.97	0.47

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:602:A:O2'	30:0:605:C:H4'	2.13	0.47
4:D:103:ASN:ND2	4:D:133:ASN:HA	2.29	0.47
30:0:1787:C:H4'	30:0:2883:A:O4'	2.14	0.47
4:D:51:ARG:NH1	4:D:68:PRO:HB3	2.29	0.47
16:P:87:ARG:HG2	38:P:185:HOH:O	2.14	0.47
30:0:722:G:H22	30:0:938:G:P	2.37	0.47
30:0:185:G:O3'	30:0:186:A:H4'	2.14	0.47
30:0:1181:A:H2'	30:0:1182:C:C5'	2.44	0.47
30:0:1181:A:C2'	30:0:1182:C:H5'	2.43	0.47
30:0:2541:U:H3'	38:0:9060:HOH:O	2.14	0.47
8:H:158:ASN:ND2	30:0:2502:C:H4'	2.30	0.47
30:0:1562:C:O2	30:0:1562:C:C2'	2.61	0.47
30:0:2134:G:C6	30:0:2258:A:C8	3.02	0.47
30:0:1456:C:H2'	30:0:1457:U:C6	2.49	0.47
22:V:12:THR:HG22	22:V:15:GLU:H	1.77	0.47
30:0:2032:U:O2'	30:0:2033:G:H5''	2.14	0.47
30:0:2266:A:H2'	30:0:2267:G:C8	2.49	0.47
30:0:946:C:O2'	30:0:947:U:H5'	2.14	0.47
14:N:100:ALA:O	14:N:129:ILE:HG23	2.13	0.47
6:F:59:ILE:CD1	30:0:263:U:C2	2.98	0.47
25:Y:126:PRO:HG2	25:Y:128:PHE:CE1	2.49	0.47
30:0:1890:U:H4'	30:0:2010:A:C6	2.50	0.47
30:0:1588:G:C5	30:0:1589:G:C6	3.03	0.47
2:B:41:PHE:CZ	2:B:79:MET:HG3	2.50	0.47
30:0:968:G:O2'	30:0:969:G:H5'	2.14	0.47
31:9:71:C:H2'	31:9:72:C:H6	1.79	0.47
30:0:1183:C:N3	30:0:1184:C:N4	2.62	0.47
30:0:1206:U:H2'	30:0:1207:A:O4'	2.14	0.47
30:0:2712:G:O2'	30:0:2713:G:H5'	2.14	0.47
30:0:2000:G:O2'	30:0:2001:G:H5'	2.15	0.47
30:0:2001:G:O2'	30:0:2002:C:H5'	2.14	0.47
31:9:65:A:N6	31:9:112:U:C6	2.82	0.47
8:H:31:ILE:HD11	8:H:65:LEU:HD23	1.96	0.47
23:W:64:THR:O	23:W:68:THR:HG22	2.14	0.47
30:0:168:C:O5'	30:0:168:C:H6	1.97	0.47
30:0:305:A:C5	30:0:329:A:C2	3.03	0.47
30:0:1137:G:H1'	38:0:3876:HOH:O	2.14	0.47
1:A:217:ARG:HG2	1:A:229:ALA:HB2	1.96	0.47
25:Y:210:GLY:H	30:0:1313:A:H5''	1.78	0.47
30:0:138:U:OP2	30:0:139:C:H5	1.98	0.47
11:K:81:ARG:HD3	11:K:87:ARG:NH2	2.30	0.47

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:2335:C:H2'	30:0:2336:G:H8	1.78	0.47
30:0:1406:A:H4'	30:0:1407:A:H5''	1.96	0.47
30:0:1153:C:N3	30:0:2786:G:O6	2.48	0.47
30:0:1823:G:O2'	30:0:1824:C:H5'	2.14	0.47
30:0:283:U:C5	30:0:284:C:C4	3.03	0.47
11:K:29:LEU:HB3	11:K:55:VAL:CG1	2.32	0.47
30:0:560:U:H2'	30:0:561:G:H8	1.79	0.47
11:K:41:LYS:O	11:K:42:ASN:HB2	2.15	0.47
26:Z:70:ARG:HD3	26:Z:83:TYR:HB2	1.95	0.47
20:T:26:THR:HA	20:T:39:ASN:HB3	1.95	0.47
11:K:74:VAL:HG12	11:K:75:ARG:HG3	1.95	0.47
16:P:59:ARG:O	16:P:63:ARG:HG3	2.15	0.47
30:0:969:G:H1	30:0:999:C:H42	1.61	0.47
29:3:28:GLY:HA3	30:0:2435:U:OP1	2.15	0.47
21:U:44:ARG:HB3	38:U:3805:HOH:O	2.13	0.47
25:Y:136:LYS:HE2	25:Y:138:ARG:NH1	2.28	0.47
30:0:2871:G:H2'	30:0:2872:U:H6	1.79	0.47
23:W:13:MET:HE1	23:W:18:GLN:HA	1.95	0.47
1:A:217:ARG:NH2	30:0:1853:C:O2'	2.48	0.47
30:0:2239:C:O2'	30:0:2240:U:H5'	2.14	0.47
30:0:1400:C:O2'	30:0:1401:G:H5'	2.15	0.47
30:0:2361:A:H2'	30:0:2362:A:C8	2.49	0.47
30:0:527:U:H2'	30:0:528:G:C8	2.49	0.47
30:0:2074:A:H2'	38:0:3533:HOH:O	2.14	0.47
30:0:2649:A:H5'	30:0:2649:A:C8	2.50	0.47
19:S:77:VAL:O	19:S:80:ARG:HG2	2.15	0.47
30:0:844:A:C6	30:0:882:A:C6	3.03	0.47
30:0:814:G:H4'	38:0:3130:HOH:O	2.15	0.47
30:0:1548:U:O2'	30:0:1549:C:H5'	2.14	0.47
30:0:853:C:H2'	30:0:854:G:O4'	2.14	0.47
30:0:2506:A:N6	30:0:2511:A:O2'	2.43	0.47
2:B:221:GLN:HE22	11:K:42:ASN:ND2	2.04	0.47
30:0:1904:A:H2'	30:0:1905:U:O4'	2.15	0.47
30:0:810:G:H2'	30:0:811:C:H6	1.79	0.47
30:0:249:G:O2'	30:0:250:C:H5'	2.15	0.47
18:R:122:GLN:HB3	18:R:138:SER:HB2	1.95	0.47
30:0:1942:A:H2'	30:0:1943:C:H6	1.79	0.47
10:J:127:ILE:CG2	35:J:8801:CL:CL	2.96	0.47
14:N:147:ILE:HB	38:9:9087:HOH:O	2.15	0.47
30:0:1377:C:H1'	38:0:9039:HOH:O	2.15	0.47
30:0:290:C:O2'	30:0:291:C:H5'	2.14	0.47

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:1014:A:H2'	30:0:1015:C:H5'	1.96	0.47
25:Y:144:ARG:CZ	38:Y:9096:HOH:O	2.62	0.47
2:B:212:GLN:HB2	2:B:257:THR:CG2	2.44	0.47
2:B:144:THR:HB	38:B:9092:HOH:O	2.14	0.47
11:K:113:ILE:HD12	11:K:128:ALA:HB2	1.96	0.47
10:J:6:PHE:HB3	10:J:109:TYR:OH	2.15	0.47
27:1:28:HIS:CD2	27:1:31:LYS:HG3	2.50	0.47
30:0:2649:A:H5'	30:0:2649:A:H8	1.79	0.47
14:N:139:TRP:CE3	14:N:139:TRP:HA	2.50	0.47
30:0:1970:G:H2'	30:0:1970:G:N3	2.30	0.47
14:N:162:ASP:HA	38:N:8830:HOH:O	2.15	0.47
16:P:114:LEU:HA	16:P:118:GLN:NE2	2.30	0.46
30:0:364:U:H2'	30:0:365:G:O4'	2.15	0.46
31:9:3:A:C2	31:9:21:G:N3	2.83	0.46
10:J:131:THR:HG22	10:J:133:GLY:N	2.30	0.46
12:L:27:ARG:HH21	12:L:30:ARG:HG2	1.80	0.46
30:0:17:G:H2'	30:0:18:C:H6	1.79	0.46
30:0:254:C:O2	30:0:254:C:H2'	2.14	0.46
30:0:1149:U:C5	30:0:1215:A:C5	3.04	0.46
16:P:91:LYS:O	16:P:95:GLU:HG3	2.15	0.46
3:C:168:ARG:NH2	3:C:190:ALA:O	2.48	0.46
30:0:1760:G:H5'	30:0:1818:C:O2'	2.15	0.46
31:9:76:G:H3'	31:9:77:A:C5'	2.28	0.46
25:Y:189:ASN:ND2	25:Y:192:ASP:H	2.13	0.46
27:1:16:HIS:HE1	30:0:775:G:OP1	1.98	0.46
27:1:42:SER:HB2	38:1:8956:HOH:O	2.14	0.46
18:R:111:ILE:HG23	18:R:145:LEU:CD1	2.46	0.46
30:0:1379:A:H1'	38:0:9689:HOH:O	2.15	0.46
30:0:1244:U:H4'	30:0:1246:A:O4'	2.16	0.46
30:0:1940:C:H4'	38:0:7346:HOH:O	2.16	0.46
26:Z:70:ARG:CD	26:Z:83:TYR:HB2	2.45	0.46
31:9:1:U:O3'	31:9:3:A:C5'	2.63	0.46
30:0:1820:G:C6	30:0:2030:A:C2	3.04	0.46
15:O:65:LEU:HD13	30:0:746:A:C6	2.51	0.46
12:L:30:ARG:NH2	38:L:8823:HOH:O	2.44	0.46
23:W:13:MET:CE	23:W:17:ILE:HG22	2.46	0.46
13:M:169:ARG:NH2	38:M:8849:HOH:O	2.48	0.46
30:0:162:C:H2'	30:0:163:U:H5'	1.97	0.46
30:0:2858:U:H2'	30:0:2859:C:O4'	2.15	0.46
30:0:2578:G:C8	30:0:2578:G:H5'	2.39	0.46
27:1:16:HIS:CD2	30:0:470:U:O2'	2.67	0.46

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:1268:C:H2'	30:0:1269:G:C8	2.50	0.46
30:0:1921:A:C6	30:0:1922:A:C2	3.04	0.46
30:0:2064:U:H4'	30:0:2653:A:OP1	2.14	0.46
30:0:764:C:H2'	30:0:765:G:O4'	2.15	0.46
25:Y:117:LEU:HA	25:Y:174:VAL:HG11	1.98	0.46
30:0:95:A:H5''	30:0:97:G:O4'	2.14	0.46
30:0:1511:U:O2'	30:0:1512:G:H5'	2.15	0.46
30:0:152:A:H2'	30:0:153:C:C6	2.50	0.46
30:0:2783:A:H2'	30:0:2784:A:C8	2.50	0.46
27:1:1:THR:HB	38:0:7140:HOH:O	2.15	0.46
1:A:36:ASP:CB	1:A:85:SER:H	2.29	0.46
30:0:2420:G:H2'	30:0:2421:G:C8	2.51	0.46
31:9:58:G:H3'	31:9:59:C:C6	2.49	0.46
30:0:255:A:C5	30:0:256:C:C4	3.04	0.46
15:O:38:ARG:NH1	38:O:7674:HOH:O	2.48	0.46
30:0:2839:C:H2'	30:0:2840:A:H5''	1.96	0.46
3:C:39:GLN:O	3:C:43:LYS:HD3	2.16	0.46
1:A:70:ALA:HA	1:A:71:PRO:HD3	1.79	0.46
30:0:1021:G:O2'	30:0:1022:A:H5'	2.16	0.46
31:9:33:U:H2'	38:9:9066:HOH:O	2.15	0.46
30:0:89:G:H4'	38:0:4766:HOH:O	2.16	0.46
10:J:54:VAL:HG11	10:J:138:THR:HG21	1.96	0.46
30:0:1339:G:C6	30:0:1340:G:N1	2.84	0.46
24:X:71:ARG:HD3	38:X:2171:HOH:O	2.16	0.46
30:0:282:C:C2'	30:0:283:U:H5'	2.45	0.46
23:W:125:HIS:CE1	30:0:1097:A:H5''	2.51	0.46
28:2:44:ARG:HD3	38:0:6937:HOH:O	2.15	0.46
30:0:1845:A:O2'	30:0:1846:U:H5'	2.15	0.46
30:0:2617:G:H2'	30:0:2617:G:N3	2.30	0.46
3:C:19:PRO:HG2	3:C:22:PHE:CE1	2.50	0.46
30:0:125:U:H2'	38:0:3761:HOH:O	2.15	0.46
3:C:132:ASP:HB3	38:C:8567:HOH:O	2.16	0.46
30:0:1087:G:H4'	30:0:1088:A:OP1	2.15	0.46
2:B:280:VAL:HG13	2:B:333:GLU:O	2.16	0.46
30:0:1166:A:N3	30:0:1166:A:H2'	2.31	0.46
30:0:1878:G:O2'	30:0:1879:U:OP2	2.33	0.46
30:0:1840:A:H4'	30:0:1841:C:O5'	2.16	0.46
3:C:46:TYR:CE1	30:0:450:C:H4'	2.50	0.46
4:D:52:THR:CG2	30:0:2346:C:H4'	2.45	0.46
30:0:407:A:H2'	30:0:408:A:C8	2.51	0.46
30:0:1044:C:H5	38:0:6604:HOH:O	1.98	0.46

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:704:C:H2'	30:0:705:C:H6	1.81	0.46
7:G:16:LYS:O	7:G:20:VAL:HG23	2.16	0.46
2:B:260:HIS:HE1	38:0:5167:HOH:O	1.97	0.46
2:B:314:ALA:HB3	2:B:317:PRO:HG3	1.98	0.46
16:P:61:ARG:NH2	30:0:2737:C:OP2	2.48	0.46
24:X:85:VAL:HG12	24:X:86:GLU:H	1.80	0.46
30:0:1730:G:C5'	30:0:1731:C:C5	2.95	0.46
10:J:75:PRO:HG2	10:J:105:LEU:HD21	1.98	0.46
5:E:143:GLN:HE22	30:0:2779:G:H21	1.63	0.46
30:0:2353:A:H4'	30:0:2354:A:O5'	2.16	0.46
30:0:2032:U:H2'	30:0:2033:G:H5'	1.97	0.46
23:W:10:GLU:HB2	23:W:18:GLN:NE2	2.31	0.46
19:S:45:TYR:O	19:S:80:ARG:NH2	2.49	0.46
13:M:159:VAL:HG13	13:M:160:PHE:N	2.31	0.46
3:C:48:SER:HB3	30:0:1352:A:N1	2.31	0.46
13:M:81:ARG:HG3	13:M:85:ARG:HB2	1.97	0.46
13:M:65:VAL:HG21	13:M:105:ALA:HB2	1.98	0.46
30:0:1834:C:H2'	30:0:1840:A:H62	1.81	0.46
11:K:74:VAL:HG13	11:K:113:ILE:HG12	1.98	0.46
19:S:56:ASN:O	28:2:8:LYS:NZ	2.47	0.46
13:M:145:ASP:HB2	38:M:8864:HOH:O	2.15	0.46
30:0:862:U:H2'	30:0:863:G:H8	1.80	0.46
30:0:772:G:H2'	30:0:773:A:O4'	2.16	0.46
30:0:1052:G:H2'	30:0:1052:G:N3	2.30	0.46
3:C:197:SER:HB3	38:C:8579:HOH:O	2.16	0.46
30:0:2002:C:H2'	30:0:2003:U:H5'	1.97	0.46
30:0:2250:G:H2'	30:0:2251:G:O4'	2.16	0.46
30:0:699:C:H2'	30:0:744:G:N3	2.31	0.46
30:0:571:C:H6	30:0:571:C:O5'	1.99	0.46
30:0:2594:C:O2'	30:0:2595:U:H5'	2.16	0.46
14:N:94:GLU:HG3	14:N:186:LEU:HD12	1.98	0.46
31:9:36:C:C5	31:9:37:C:C5	3.04	0.46
2:B:329:TYR:CE2	21:U:15:PRO:HG2	2.51	0.46
30:0:2906:A:H5'	30:0:2907:C:O4'	2.16	0.46
30:0:424:C:H2'	30:0:425:U:C6	2.51	0.46
3:C:233:THR:HG22	3:C:234:VAL:N	2.31	0.46
30:0:2505:G:H2'	30:0:2506:A:H5'	1.97	0.45
1:A:94:LEU:HG	1:A:99:ILE:HD11	1.97	0.45
3:C:27:ARG:HG2	3:C:30:LEU:HG	1.98	0.45
10:J:75:PRO:HG2	10:J:105:LEU:CD2	2.45	0.45
12:L:18:HIS:CD2	30:0:902:G:N7	2.82	0.45

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:9:58:G:H3'	31:9:59:C:C5	2.51	0.45
10:J:39:VAL:HG22	10:J:107:ASN:HA	1.98	0.45
1:A:223:ARG:NH1	30:0:2270:G:H4'	2.31	0.45
8:H:91:ARG:O	30:0:1003:U:H4'	2.16	0.45
4:D:75:LEU:HD22	4:D:79:MET:HB3	1.98	0.45
7:G:23:ILE:O	7:G:27:ILE:HG13	2.16	0.45
30:0:1154:A:H2'	30:0:1155:G:C8	2.51	0.45
6:F:48:VAL:CG2	6:F:74:PHE:HB3	2.46	0.45
30:0:1181:A:N1	30:0:1192:A:O2'	2.42	0.45
23:W:24:LEU:O	23:W:26:ILE:HG22	2.16	0.45
30:0:559:U:H3'	30:0:559:U:C6	2.51	0.45
30:0:2756:U:C2	30:0:2896:A:H2	2.33	0.45
30:0:1080:C:O5'	30:0:1080:C:H6	1.99	0.45
30:0:1626:A:H2'	30:0:1627:G:C5'	2.47	0.45
13:M:9:ARG:HD2	30:0:380:A:OP2	2.15	0.45
7:G:67:LEU:O	7:G:71:LEU:HG	2.15	0.45
2:B:305:ASP:O	2:B:306:LYS:HB2	2.17	0.45
3:C:118:THR:HG22	3:C:137:PRO:HB3	1.96	0.45
30:0:2473:U:O3'	30:0:2474:A:H3'	2.16	0.45
30:0:2112:A:H2'	30:0:2113:G:C8	2.51	0.45
30:0:1185:U:C5'	38:0:7462:HOH:O	2.62	0.45
2:B:36:PRO:CA	2:B:168:GLY:HA3	2.40	0.45
30:0:2506:A:O2'	30:0:2507:G:O5'	2.35	0.45
30:0:2511:A:H2'	30:0:2512:U:O4'	2.16	0.45
30:0:366:U:H2'	30:0:367:G:O4'	2.16	0.45
12:L:18:HIS:HB3	38:0:9150:HOH:O	2.15	0.45
31:9:114:G:H2'	31:9:115:C:C6	2.52	0.45
30:0:2825:C:H4'	30:0:2826:G:O5'	2.16	0.45
8:H:31:ILE:HG23	38:H:233:HOH:O	2.16	0.45
25:Y:99:ALA:HB2	25:Y:233:TYR:CZ	2.51	0.45
10:J:88:PRO:HD3	30:0:1104:C:H4'	1.98	0.45
11:K:114:ALA:HB3	11:K:117:VAL:HG23	1.99	0.45
31:9:55:U:H4'	31:9:56:A:H8	1.81	0.45
3:C:129:HIS:CE1	3:C:232:LEU:H	2.35	0.45
30:0:816:G:H5'	30:0:1598:A:H4'	1.98	0.45
2:B:27:ASN:HD21	30:0:2807:U:P	2.39	0.45
19:S:37:VAL:O	19:S:41:VAL:HG23	2.16	0.45
30:0:297:U:H2'	30:0:298:C:H6	1.80	0.45
12:L:67:ARG:O	12:L:71:GLU:HG3	2.17	0.45
30:0:1850:U:H2'	30:0:1851:G:H8	1.80	0.45
30:0:214:U:H5'	38:0:6139:HOH:O	2.15	0.45

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:Y:148:GLY:HA3	30:0:622:G:P	2.56	0.45
30:0:1182:C:C1'	30:0:1192:A:H8	2.28	0.45
10:J:52:GLN:HE22	30:0:1119:G:H8	1.65	0.45
30:0:513:A:N3	38:0:3653:HOH:O	2.36	0.45
30:0:2250:G:C2	30:0:2251:G:H1'	2.50	0.45
20:T:54:ASP:OD2	30:0:316:A:H5'	2.16	0.45
4:D:140:ARG:HG3	4:D:140:ARG:HH11	1.80	0.45
15:O:21:SER:OG	15:O:106:PRO:HB2	2.15	0.45
17:Q:32:GLU:O	17:Q:93:ARG:NH2	2.50	0.45
1:A:164:ARG:NH2	30:0:1877:G:OP1	2.49	0.45
30:0:702:G:O2'	30:0:703:G:H5'	2.16	0.45
30:0:432:G:O2'	30:0:433:C:H5'	2.16	0.45
30:0:2740:G:H2'	30:0:2741:A:O4'	2.16	0.45
25:Y:122:ARG:NH2	38:Y:9019:HOH:O	2.49	0.45
30:0:2644:C:H4'	38:0:9154:HOH:O	2.16	0.45
30:0:1789:G:H2'	30:0:1790:C:O5'	2.16	0.45
10:J:19:MET:HE1	10:J:79:PHE:HA	1.98	0.45
4:D:49:PRO:HA	4:D:73:VAL:HG22	1.99	0.45
30:0:652:G:H2'	30:0:653:U:O4'	2.16	0.45
30:0:101:C:H2'	30:0:102:A:C8	2.51	0.45
13:M:66:SER:HB3	13:M:128:TRP:CD1	2.51	0.45
30:0:2439:C:H5'	38:0:5486:HOH:O	2.17	0.45
30:0:2637:A:H5'	38:0:9275:HOH:O	2.16	0.45
30:0:2415:A:C2'	30:0:2416:G:H5'	2.46	0.45
12:L:30:ARG:HD2	30:0:164:G:H5''	1.99	0.45
30:0:1198:U:C6	30:0:1200:A:OP2	2.70	0.45
18:R:111:ILE:HG23	18:R:145:LEU:HD11	1.99	0.45
20:T:79:LEU:HG	20:T:89:ARG:HB2	1.98	0.45
24:X:25:ARG:HD2	38:X:5356:HOH:O	2.17	0.45
30:0:415:A:O2'	30:0:416:G:H5'	2.17	0.45
30:0:1209:C:C2	30:0:1210:G:C8	3.05	0.45
13:M:164:THR:CG2	13:M:165:GLY:N	2.79	0.45
23:W:122:ARG:HH11	23:W:122:ARG:HG3	1.81	0.45
12:L:57:VAL:HG12	12:L:57:VAL:O	2.17	0.45
6:F:91:VAL:HG12	6:F:92:GLY:H	1.79	0.45
30:0:1015:C:O5'	30:0:1015:C:H6	1.99	0.45
30:0:2032:U:C2'	30:0:2033:G:C5'	2.95	0.45
30:0:2324:G:N2	30:0:2377:U:H1'	2.32	0.45
30:0:113:A:OP2	30:0:114:A:H2'	2.17	0.45
2:B:256:GLN:HG2	38:B:9125:HOH:O	2.16	0.45
30:0:2566:A:C2	30:0:2696:G:O4'	2.70	0.45

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:281:U:HO2'	30:0:282:C:H5'	1.80	0.45
30:0:1117:A:C2	30:0:1244:U:C2	3.05	0.45
23:W:119:HIS:CG	38:0:5289:HOH:O	2.70	0.45
4:D:48:MET:HB3	31:9:41:C:H4'	1.99	0.45
30:0:2361:A:H8	30:0:2361:A:H5'	1.82	0.45
12:L:150:GLN:HB3	38:L:8872:HOH:O	2.16	0.45
30:0:1006:A:N1	30:0:2311:A:H1'	2.31	0.45
30:0:690:G:H4'	30:0:741:C:O2	2.17	0.45
1:A:232:ARG:NH2	1:A:236:GLY:O	2.50	0.45
23:W:11:VAL:O	23:W:12:ASN:HB2	2.17	0.45
14:N:154:LEU:C	14:N:156:GLU:H	2.18	0.45
30:0:587:A:H5''	38:0:7285:HOH:O	2.16	0.45
16:P:36:THR:O	16:P:39:ASP:HB2	2.17	0.45
15:O:35:LYS:HD3	38:0:4615:HOH:O	2.17	0.45
1:A:211:LYS:HB2	38:A:9077:HOH:O	2.16	0.45
30:0:1543:G:N1	30:0:1641:A:OP2	2.40	0.45
1:A:192:VAL:HG12	1:A:207:GLN:HB3	1.99	0.45
30:0:1171:A:H2'	30:0:1172:G:H5'	1.98	0.45
30:0:737:A:H2'	30:0:738:G:O4'	2.17	0.45
2:B:215:VAL:HA	2:B:220:VAL:HG22	1.98	0.45
30:0:629:A:H2'	30:0:630:A:O4'	2.17	0.45
2:B:214:PRO:HD2	38:0:9075:HOH:O	2.15	0.45
2:B:229:ARG:HD2	38:0:9108:HOH:O	2.17	0.45
3:C:49:ASP:HB3	3:C:52:ALA:HB2	1.99	0.45
30:0:1163:G:H2'	30:0:1164:U:C5	2.52	0.44
30:0:1188:A:N6	30:0:1189:A:N6	2.65	0.44
18:R:29:LYS:HD2	38:R:8943:HOH:O	2.16	0.44
9:I:112:LEU:HG	30:0:1162:G:O2'	2.17	0.44
31:9:35:C:H5''	38:9:9076:HOH:O	2.17	0.44
30:0:2114:C:O2'	30:0:2115:U:H5'	2.17	0.44
30:0:105:G:O2'	30:0:106:A:H5'	2.17	0.44
24:X:25:ARG:HD3	24:X:64:ALA:O	2.16	0.44
30:0:2325:U:O2'	30:0:2411:C:H1'	2.16	0.44
30:0:1224:G:H2'	30:0:1225:C:C6	2.51	0.44
2:B:177:HIS:O	2:B:181:ILE:HG13	2.17	0.44
3:C:138:VAL:HG11	3:C:160:LEU:HD13	1.98	0.44
30:0:541:C:H2'	30:0:542:A:H5'	1.91	0.44
30:0:1592:G:O2'	30:0:1593:C:O5'	2.35	0.44
8:H:30:LYS:H	8:H:62:HIS:CD2	2.35	0.44
13:M:134:ILE:CG2	13:M:141:ILE:HD13	2.46	0.44
2:B:217:ARG:CG	2:B:257:THR:HG22	2.47	0.44

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:137:U:OP1	30:0:259:G:O2'	2.33	0.44
30:0:1992:U:H2'	30:0:1994:A:OP2	2.17	0.44
30:0:820:G:O2'	30:0:856:G:H4'	2.18	0.44
27:1:25:LYS:O	27:1:25:LYS:HG2	2.18	0.44
30:0:699:C:C2	30:0:743:G:N2	2.85	0.44
30:0:1398:G:O2'	30:0:1399:A:H5'	2.18	0.44
16:P:55:LYS:HG2	16:P:56:GLY:N	2.31	0.44
24:X:21:PRO:HG2	24:X:24:LYS:HD3	1.99	0.44
12:L:33:ALA:HB3	38:L:8896:HOH:O	2.16	0.44
30:0:1501:A:H4'	38:0:5597:HOH:O	2.17	0.44
30:0:134:U:C2	30:0:145:A:C2	3.06	0.44
12:L:14:GLY:O	30:0:1295:G:H5''	2.17	0.44
30:0:727:G:H3'	30:0:728:C:H6	1.82	0.44
30:0:195:C:H2'	30:0:196:G:H5'	1.99	0.44
30:0:1206:U:C5'	30:0:1206:U:H6	2.22	0.44
30:0:1702:U:H1'	38:0:5772:HOH:O	2.18	0.44
30:0:283:U:H5	30:0:284:C:C4	2.33	0.44
30:0:2509:A:OP2	30:0:2510:C:H5	2.00	0.44
15:O:25:VAL:CG1	30:0:710:G:H5'	2.48	0.44
30:0:660:A:H4'	30:0:661:G:O5'	2.18	0.44
2:B:243:ASN:HA	2:B:244:PRO:C	2.38	0.44
30:0:1583:U:H2'	30:0:1584:C:O4'	2.18	0.44
6:F:101:ALA:HA	38:F:5413:HOH:O	2.16	0.44
30:0:2753:G:O2'	30:0:2754:G:H5'	2.18	0.44
24:X:73:ARG:NH1	24:X:88:GLU:HB2	2.33	0.44
2:B:198:GLU:HA	38:B:9126:HOH:O	2.17	0.44
30:0:1166:A:OP1	30:0:1174:A:H4'	2.16	0.44
30:0:2003:U:H4'	30:0:2004:U:H5	1.83	0.44
30:0:1249:U:H2'	30:0:1250:C:H6	1.79	0.44
30:0:999:C:H2'	30:0:1000:C:O4'	2.17	0.44
2:B:253:GLN:OE1	30:0:2090:G:N2	2.51	0.44
30:0:790:A:H2'	30:0:791:A:O4'	2.18	0.44
25:Y:210:GLY:N	30:0:1313:A:H5''	2.33	0.44
30:0:2245:C:H6	30:0:2245:C:O5'	2.00	0.44
10:J:45:VAL:HG11	10:J:121:LEU:HD22	1.99	0.44
28:2:37:HIS:CE1	30:0:462:A:C8	3.06	0.44
30:0:535:G:C5	30:0:2063:U:C4	3.05	0.44
30:0:295:C:H2'	30:0:296:G:O4'	2.17	0.44
30:0:1714:C:O2'	30:0:1715:C:H5'	2.17	0.44
30:0:2401:A:H2'	30:0:2402:A:C8	2.52	0.44
26:Z:77:GLY:HA2	26:Z:91:GLY:O	2.17	0.44

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:1163:G:N2	38:0:4726:HOH:O	2.49	0.44
30:0:1183:C:H41	30:0:1192:A:P	2.40	0.44
30:0:545:G:C8	30:0:545:G:C5'	2.94	0.44
1:A:199:HIS:HE1	30:0:1881:A:OP1	2.01	0.44
10:J:130:VAL:HG12	10:J:131:THR:N	2.33	0.44
1:A:144:GLU:OE2	30:0:1855:G:H8	2.00	0.44
30:0:694:A:C2'	30:0:695:C:H5'	2.47	0.44
12:L:4:LYS:HE2	30:0:645:U:OP2	2.18	0.44
30:0:73:U:O2'	30:0:74:G:H5'	2.18	0.44
8:H:76:LEU:HD21	8:H:149:VAL:HA	1.98	0.44
3:C:80:VAL:HA	3:C:81:PRO:HD3	1.84	0.44
30:0:1434:A:H2'	30:0:1436:C:C5	2.52	0.44
17:Q:1:PRO:HA	30:0:2299:G:O6	2.17	0.44
30:0:1163:G:C2	30:0:1184:C:N3	2.86	0.44
30:0:1191:A:H2	30:0:1206:U:H3	1.64	0.44
31:9:31:C:H2'	31:9:32:G:O4'	2.18	0.44
26:Z:44:ARG:HB2	30:0:1886:A:O2'	2.18	0.44
11:K:66:ARG:HH12	30:0:1992:U:H3'	1.82	0.44
30:0:2846:C:H4'	38:0:5080:HOH:O	2.18	0.44
16:P:120:ARG:NH1	30:0:1594:C:C5	2.86	0.44
30:0:1755:A:H2'	30:0:1756:G:O4'	2.18	0.44
30:0:758:A:H2'	30:0:759:C:O4'	2.17	0.44
30:0:1871:U:O4'	30:0:1873:G:C8	2.71	0.44
1:A:167:LYS:HB2	26:Z:53:ILE:HD13	1.99	0.44
30:0:1444:G:O2'	30:0:1502:A:N1	2.41	0.44
30:0:1805:G:O2'	30:0:1806:G:H5'	2.17	0.44
9:I:87:PRO:HD2	30:0:1180:U:O2'	2.17	0.44
30:0:241:A:N1	30:0:378:A:H4'	2.33	0.44
30:0:506:G:N2	30:0:509:A:C5'	2.66	0.44
11:K:41:LYS:HA	30:0:2582:G:O3'	2.18	0.44
30:0:1972:U:H2'	30:0:1973:A:H5'	1.99	0.44
30:0:603:A:H4'	30:0:604:G:O5'	2.17	0.44
30:0:2104:C:O2	30:0:2485:A:N1	2.51	0.44
31:9:1:U:C5'	31:9:3:A:OP1	2.65	0.44
30:0:2895:C:H2'	38:0:9570:HOH:O	2.18	0.44
2:B:51:VAL:CG1	2:B:53:LEU:HD13	2.46	0.44
30:0:2064:U:H5'	30:0:2652:U:O3'	2.18	0.44
15:O:32:ARG:HD3	15:O:32:ARG:O	2.17	0.44
29:3:11:CYS:HB2	29:3:20:HIS:CE1	2.52	0.44
2:B:75:GLU:OE2	2:B:151:VAL:HG13	2.18	0.44
25:Y:165:GLU:HB3	38:0:6704:HOH:O	2.17	0.44

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:S:55:GLN:NE2	30:0:1446:U:H2'	2.32	0.44
30:0:1702:U:H5'	38:0:3421:HOH:O	2.16	0.44
1:A:95:PRO:HA	1:A:153:ARG:HA	2.00	0.44
30:0:512:G:O3'	30:0:513:A:H8	2.00	0.44
30:0:1051:C:H2'	30:0:1052:G:O4'	2.18	0.44
14:N:108:SER:HA	14:N:109:PRO:HD3	1.75	0.44
30:0:574:G:O2'	30:0:575:A:H5'	2.18	0.44
30:0:1143:G:C6	30:0:1221:G:C6	3.06	0.44
4:D:62:ASP:HA	38:D:4233:HOH:O	2.18	0.44
7:G:63:ARG:NH1	30:0:1151:G:OP1	2.51	0.44
30:0:731:U:H2'	30:0:732:C:C6	2.53	0.44
8:H:57:THR:HG23	8:H:131:GLN:HA	2.00	0.44
30:0:1116:U:HO2'	30:0:1118:A:H2	0.68	0.44
30:0:2908:A:O5'	30:0:2908:A:H8	2.00	0.44
30:0:2073:G:H5''	38:0:3823:HOH:O	2.17	0.44
13:M:86:GLN:HE22	30:0:2274:A:H1'	1.83	0.44
25:Y:189:ASN:HD22	25:Y:189:ASN:C	2.21	0.44
31:9:39:U:C2'	31:9:40:C:OP1	2.66	0.44
30:0:1819:G:C2'	30:0:1820:G:H5'	2.47	0.44
20:T:23:VAL:HG23	20:T:41:ARG:HG3	1.98	0.44
30:0:2249:G:C2	30:0:2253:G:C6	3.06	0.44
30:0:2328:U:C4	30:0:2329:C:C5	3.06	0.44
9:I:101:LYS:O	9:I:105:GLU:HG3	2.18	0.44
2:B:124:ALA:O	2:B:128:ILE:HG13	2.18	0.44
30:0:494:C:H2'	30:0:496:G:OP2	2.17	0.44
30:0:2891:A:C2	30:0:2892:G:C4	3.06	0.44
30:0:596:C:H2'	30:0:597:A:C8	2.52	0.44
30:0:596:C:H2'	30:0:597:A:H8	1.83	0.44
3:C:16:VAL:HG21	38:C:8641:HOH:O	2.17	0.44
9:I:87:PRO:HB3	38:I:6825:HOH:O	2.18	0.43
30:0:1586:G:O2'	30:0:1587:U:H5'	2.18	0.43
2:B:315:VAL:HG23	2:B:316:ARG:HG2	2.00	0.43
30:0:2896:A:N3	30:0:2896:A:H2'	2.32	0.43
1:A:223:ARG:NH1	38:A:8985:HOH:O	2.50	0.43
30:0:2662:G:N3	30:0:2816:A:H2	2.16	0.43
30:0:276:C:O5'	30:0:276:C:H6	2.01	0.43
30:0:2515:C:H2'	30:0:2516:G:O4'	2.18	0.43
30:0:2544:G:H2'	30:0:2545:U:O4'	2.18	0.43
16:P:81:LYS:HG2	38:0:9538:HOH:O	2.18	0.43
16:P:105:LEU:HD21	16:P:137:LEU:HD11	1.99	0.43
30:0:88:G:H5'	30:0:88:G:H8	1.83	0.43

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:2314:G:C2'	30:0:2315:C:H5'	2.48	0.43
30:0:506:G:N2	30:0:509:A:H5'	2.23	0.43
30:0:2524:G:H5''	38:0:4731:HOH:O	2.18	0.43
30:0:482:G:O4'	30:0:511:A:C2	2.70	0.43
14:N:18:THR:HG21	38:N:8844:HOH:O	2.17	0.43
10:J:131:THR:HG22	10:J:133:GLY:H	1.82	0.43
30:0:2705:U:H2'	30:0:2706:A:H8	1.82	0.43
30:0:1504:A:H5'	38:0:4414:HOH:O	2.18	0.43
30:0:1568:G:O2'	30:0:1569:U:H5'	2.18	0.43
30:0:1797:A:H2'	30:0:1799:G:O5'	2.18	0.43
3:C:88:SER:HB3	3:C:91:PRO:HB3	2.01	0.43
10:J:135:ILE:O	10:J:139:LEU:HG	2.18	0.43
30:0:1996:U:O2'	30:0:1997:A:H5'	2.18	0.43
2:B:24:PRO:HG2	2:B:204:GLY:HA2	2.00	0.43
30:0:1163:G:N2	30:0:1184:C:N3	2.66	0.43
11:K:20:CYS:HB2	11:K:29:LEU:HG	1.99	0.43
23:W:21:LEU:O	23:W:26:ILE:HG23	2.19	0.43
30:0:960:G:H3'	30:0:960:G:N3	2.33	0.43
11:K:74:VAL:HG21	11:K:96:VAL:HG23	1.99	0.43
30:0:1167:G:H2'	30:0:1168:C:O4'	2.18	0.43
30:0:806:A:H2'	30:0:807:A:O4'	2.19	0.43
30:0:398:U:H2'	30:0:399:C:C6	2.53	0.43
30:0:875:A:H5'	30:0:876:A:N7	2.33	0.43
2:B:215:VAL:HB	38:B:9086:HOH:O	2.18	0.43
30:0:2115:U:H2'	30:0:2116:U:C6	2.53	0.43
30:0:629:A:C2	30:0:2074:A:C2	3.06	0.43
8:H:91:ARG:NH1	8:H:138:THR:OG1	2.47	0.43
13:M:123:ASP:OD1	13:M:126:GLN:HG2	2.18	0.43
30:0:2887:G:H2'	30:0:2888:U:C6	2.53	0.43
30:0:675:U:H2'	30:0:676:C:H5'	2.00	0.43
38:3:8961:HOH:O	30:0:2382:A:H5'	2.17	0.43
30:0:1538:C:O2'	30:0:1539:U:H5'	2.17	0.43
2:B:185:GLY:HA2	38:B:9099:HOH:O	2.17	0.43
20:T:52:ARG:O	30:0:317:A:OP1	2.35	0.43
23:W:115:THR:HG23	38:W:5420:HOH:O	2.19	0.43
30:0:2653:A:H2'	30:0:2654:C:C6	2.54	0.43
15:O:105:ASN:HD21	15:O:109:SER:N	2.16	0.43
30:0:2067:A:H2'	30:0:2068:G:O4'	2.18	0.43
30:0:1079:A:H4'	30:0:2078:U:H5'	2.00	0.43
19:S:49:VAL:HG13	19:S:66:VAL:HG13	2.00	0.43
8:H:46:TYR:HA	8:H:47:PRO:HD3	1.81	0.43

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:368:C:H2'	30:0:369:G:H5'	2.00	0.43
30:0:1890:U:H1'	38:0:5957:HOH:O	2.18	0.43
17:Q:25:PRO:HA	17:Q:26:PRO:HD3	1.83	0.43
30:0:255:A:C5	30:0:256:C:C5	3.06	0.43
30:0:2265:U:H2'	30:0:2266:A:C8	2.53	0.43
30:0:1333:U:H2'	30:0:1334:C:H6	1.83	0.43
5:E:126:ILE:HB	5:E:131:LEU:CD2	2.48	0.43
30:0:699:C:C6	30:0:744:G:O4'	2.71	0.43
30:0:2543:G:O3'	30:0:2590:U:H5'	2.19	0.43
30:0:1127:C:C5	30:0:1128:U:C4	3.06	0.43
28:2:5:LYS:O	28:2:9:LYS:HG3	2.18	0.43
30:0:445:U:H2'	30:0:446:G:H8	1.84	0.43
23:W:81:ASP:OD1	23:W:92:ASP:HB2	2.19	0.43
6:F:77:VAL:HG21	6:F:83:LEU:HD13	1.99	0.43
26:Z:55:SER:O	26:Z:59:GLU:HG3	2.17	0.43
30:0:2072:G:N2	38:0:6868:HOH:O	2.51	0.43
14:N:38:LYS:HD2	14:N:114:LYS:HE3	2.01	0.43
4:D:41:LEU:HA	4:D:44:ILE:HG22	2.00	0.43
30:0:1425:G:C2'	30:0:1426:C:H5'	2.48	0.43
30:0:2403:C:H2'	30:0:2404:G:O5'	2.18	0.43
30:0:821:U:H2'	30:0:822:C:C6	2.50	0.43
21:U:6:CYS:HA	21:U:13:ILE:HD11	2.01	0.43
23:W:117:ARG:HD3	30:0:1287:A:O4'	2.19	0.43
30:0:1850:U:O4'	30:0:1941:A:C2	2.71	0.43
16:P:134:VAL:O	16:P:137:LEU:HB3	2.19	0.43
12:L:125:PHE:CE1	12:L:140:VAL:HG13	2.54	0.43
30:0:565:A:C6	30:0:566:A:C6	3.07	0.43
30:0:426:G:H2'	30:0:427:C:O4'	2.18	0.43
31:9:98:C:O2'	31:9:99:U:H5'	2.19	0.43
30:0:1250:C:O2'	30:0:1251:C:H5'	2.18	0.43
6:F:91:VAL:CG1	6:F:92:GLY:N	2.81	0.43
12:L:6:ARG:NH1	30:0:1299:G:N7	2.66	0.43
30:0:1819:G:O2'	30:0:1820:G:H5'	2.18	0.43
30:0:1773:G:N2	30:0:1774:G:C8	2.86	0.43
30:0:807:A:H2'	30:0:808:A:O4'	2.19	0.43
2:B:5:ARG:NH1	30:0:2547:C:OP2	2.52	0.43
25:Y:107:PRO:HB3	25:Y:182:PHE:CD2	2.53	0.43
30:0:1427:A:H61	30:0:1440:U:H1'	1.82	0.43
1:A:123:GLY:HA3	1:A:162:GLY:HA2	1.99	0.43
23:W:130:HIS:O	23:W:136:GLY:HA3	2.18	0.43
30:0:170:U:H2'	30:0:171:C:H5'	1.98	0.43

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:1474:C:C5'	30:0:1474:C:C6	2.90	0.43
30:0:1634:G:H2'	30:0:1635:U:C6	2.53	0.43
24:X:76:ARG:NH1	24:X:76:ARG:HG3	2.31	0.43
31:9:105:A:H2'	31:9:106:U:O4'	2.18	0.43
30:0:2256:G:C2'	30:0:2257:G:C5'	2.97	0.43
26:Z:43:GLY:HA2	30:0:1771:U:O2	2.19	0.43
30:0:163:U:O3'	30:0:896:C:H4'	2.19	0.43
30:0:2543:G:H2'	30:0:2544:G:O4'	2.18	0.43
30:0:684:G:H2'	30:0:685:C:C6	2.54	0.43
23:W:107:LEU:O	23:W:112:LEU:HB2	2.18	0.43
31:9:54:A:C2	31:9:55:U:N3	2.87	0.43
30:0:2661:U:H3	30:0:2812:A:H62	1.65	0.43
30:0:1167:G:C2	30:0:1168:C:C2	3.07	0.43
30:0:1463:U:H2'	30:0:1464:C:H6	1.83	0.43
30:0:111:C:O2'	30:0:112:G:H5'	2.19	0.43
5:E:11:VAL:HG12	5:E:12:ASP:N	2.34	0.43
5:E:19:ASP:HA	5:E:31:ARG:O	2.19	0.43
8:H:49:GLN:HG3	8:H:140:TYR:CE2	2.54	0.43
22:V:29:ASN:O	22:V:33:VAL:HG23	2.18	0.43
30:0:544:G:C3'	30:0:545:G:H5''	2.48	0.43
1:A:101:GLU:HG2	38:A:9034:HOH:O	2.18	0.43
11:K:87:ARG:NH1	38:K:4066:HOH:O	2.47	0.43
22:V:56:ILE:O	22:V:60:GLN:HG3	2.19	0.43
25:Y:189:ASN:ND2	25:Y:192:ASP:N	2.66	0.43
30:0:111:C:C2'	30:0:112:G:H5'	2.49	0.43
24:X:71:ARG:HD2	38:X:7542:HOH:O	2.18	0.43
12:L:33:ALA:HB2	30:0:165:A:H5''	1.99	0.43
30:0:1023:C:O2'	30:0:1024:G:H5'	2.19	0.43
30:0:1517:C:O2	30:0:1670:A:C2	2.72	0.43
30:0:1682:A:H5''	38:0:9456:HOH:O	2.19	0.43
30:0:2079:G:H2'	30:0:2080:G:O4'	2.19	0.43
30:0:2540:G:H5''	38:0:4662:HOH:O	2.19	0.43
30:0:2757:A:H2'	30:0:2758:G:O4'	2.18	0.43
14:N:37:ARG:HH11	31:9:6:C:H5''	1.71	0.42
30:0:2102:G:C2'	38:0:7763:HOH:O	2.59	0.42
10:J:107:ASN:ND2	10:J:109:TYR:H	2.16	0.42
30:0:920:C:H4'	30:0:921:G:N2	2.34	0.42
27:1:28:HIS:HD2	27:1:30:LYS:H	1.65	0.42
30:0:699:C:C2	30:0:744:G:C2	3.06	0.42
7:G:19:GLU:O	7:G:23:ILE:HG13	2.19	0.42
30:0:702:G:C2	30:0:703:G:C8	3.07	0.42

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:1503:U:H2'	30:0:1504:A:O4'	2.19	0.42
26:Z:66:CYS:SG	26:Z:67:GLY:N	2.92	0.42
30:0:2692:G:HO2'	30:0:2693:U:P	2.41	0.42
30:0:1576:G:H2'	30:0:1577:U:O4'	2.19	0.42
30:0:2610:U:H3'	38:0:7521:HOH:O	2.18	0.42
30:0:2668:G:H2'	30:0:2669:U:C6	2.54	0.42
30:0:1461:U:H2'	30:0:1462:C:C6	2.54	0.42
30:0:1166:A:H1'	30:0:1192:A:C2	2.55	0.42
30:0:1181:A:C2	30:0:1192:A:C8	3.06	0.42
23:W:4:LEU:HD13	23:W:52:VAL:HG21	2.01	0.42
18:R:106:GLY:HA2	18:R:109:MET:HE3	2.00	0.42
30:0:2635:A:C2'	30:0:2636:C:H5'	2.49	0.42
29:3:48:ASN:ND2	29:3:50:GLY:H	2.17	0.42
1:A:190:ARG:HD2	30:0:1884:G:O6	2.18	0.42
30:0:512:G:H5''	30:0:515:C:H1'	2.00	0.42
30:0:2054:A:H5'	38:0:4901:HOH:O	2.18	0.42
30:0:705:C:C2'	30:0:705:C:O2	2.67	0.42
30:0:946:C:H2'	30:0:947:U:H6	1.83	0.42
11:K:34:VAL:CG2	11:K:47:ALA:HB2	2.49	0.42
30:0:62:C:C4	30:0:63:U:C4	3.07	0.42
30:0:682:A:H2'	30:0:683:G:O4'	2.18	0.42
30:0:142:G:O2'	30:0:143:C:H5'	2.18	0.42
8:H:99:ARG:NH1	30:0:1055:G:OP2	2.52	0.42
14:N:164:ASP:OD1	14:N:167:ASP:HA	2.19	0.42
30:0:343:C:O2'	30:0:344:C:H5'	2.19	0.42
12:L:61:ALA:HB2	12:L:105:TYR:CZ	2.54	0.42
1:A:4:ILE:HG22	1:A:198:ASP:O	2.19	0.42
30:0:2646:G:C5	30:0:2647:C:C5	3.07	0.42
24:X:72:VAL:HG22	24:X:85:VAL:HG12	2.01	0.42
3:C:46:TYR:CE2	3:C:98:ARG:NH1	2.87	0.42
17:Q:18:PRO:O	17:Q:21:ARG:HB2	2.19	0.42
14:N:132:ASN:HD22	30:0:2413:A:H4'	1.83	0.42
30:0:729:C:C2	30:0:743:G:C2	3.07	0.42
23:W:65:VAL:HA	23:W:68:THR:HG22	2.00	0.42
30:0:2474:A:N7	30:0:2621:PSU:H4'	2.34	0.42
5:E:21:THR:HG23	5:E:30:THR:OG1	2.18	0.42
30:0:2809:G:H2'	30:0:2810:G:O4'	2.20	0.42
31:9:108:C:H2'	31:9:109:G:C8	2.53	0.42
30:0:2657:G:O2'	30:0:2842:G:N7	2.47	0.42
31:9:95:C:O2'	31:9:96:C:H5'	2.20	0.42
3:C:140:VAL:HG12	3:C:141:SER:N	2.34	0.42

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:W:88:THR:CG2	23:W:90:TYR:HD1	2.31	0.42
13:M:93:ARG:HD2	30:0:1470:A:OP1	2.19	0.42
30:0:1298:U:H2'	30:0:1299:G:C8	2.54	0.42
10:J:39:VAL:CG2	10:J:107:ASN:HA	2.49	0.42
2:B:53:LEU:HD21	2:B:270:ILE:HD12	2.00	0.42
30:0:1947:G:H2'	30:0:1948:G:H8	1.84	0.42
8:H:123:ILE:HD12	8:H:123:ILE:N	2.34	0.42
24:X:43:VAL:HG12	24:X:44:ASP:H	1.83	0.42
25:Y:234:VAL:HG12	25:Y:235:GLU:N	2.33	0.42
25:Y:154:ARG:NH2	30:0:1072:G:OP2	2.53	0.42
30:0:622:G:O2'	30:0:623:U:H5'	2.20	0.42
18:R:17:MET:HE3	18:R:19:ARG:NH2	2.34	0.42
25:Y:152:LYS:CB	25:Y:160:LYS:HG3	2.49	0.42
8:H:141:CYS:HB2	38:H:197:HOH:O	2.20	0.42
30:0:349:U:O2'	30:0:350:G:H5'	2.19	0.42
30:0:51:G:O2'	30:0:52:A:H5'	2.20	0.42
14:N:42:HIS:CG	14:N:62:HIS:HE1	2.37	0.42
30:0:48:A:N1	30:0:148:A:O2'	2.43	0.42
14:N:71:TRP:HB2	38:N:8836:HOH:O	2.19	0.42
18:R:18:LEU:HD12	18:R:143:VAL:HG11	2.01	0.42
12:L:53:ARG:NH2	12:L:57:VAL:HG12	2.34	0.42
4:D:135:VAL:HG22	4:D:136:ARG:N	2.34	0.42
30:0:2316:G:H4'	38:0:6092:HOH:O	2.19	0.42
1:A:186:TRP:CD1	1:A:187:PRO:HA	2.55	0.42
30:0:2626:C:H2'	30:0:2627:G:H8	1.84	0.42
25:Y:130:ARG:HB2	25:Y:142:SER:O	2.18	0.42
30:0:1706:G:C6	30:0:1707:G:C6	3.08	0.42
6:F:99:THR:HG23	6:F:99:THR:O	2.19	0.42
30:0:2237:G:H1'	38:0:4856:HOH:O	2.18	0.42
30:0:2429:A:H4'	38:0:7729:HOH:O	2.19	0.42
2:B:84:LEU:HD23	2:B:142:LEU:HD23	2.02	0.42
30:0:1416:G:C2'	30:0:1417:G:H5'	2.50	0.42
3:C:35:VAL:HG21	3:C:227:GLY:HA2	2.01	0.42
30:0:1616:A:H5''	30:0:1617:C:OP1	2.19	0.42
13:M:49:ALA:C	13:M:54:TYR:HB3	2.39	0.42
30:0:39:G:N2	30:0:444:C:C2	2.88	0.42
9:I:118:ASN:HB3	30:0:1185:U:H5''	2.01	0.42
30:0:1973:A:H2'	30:0:1974:G:O4'	2.19	0.42
30:0:567:U:O5'	30:0:567:U:H6	2.03	0.42
1:A:36:ASP:HA	1:A:83:GLY:HA3	2.01	0.42
30:0:2002:C:C2'	30:0:2003:U:H5'	2.49	0.42

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:2004:U:H6	30:0:2004:U:P	2.43	0.42
30:0:664:U:O4	30:0:681:G:H5'	2.20	0.42
30:0:2709:G:N2	38:0:7616:HOH:O	2.51	0.42
30:0:2883:A:H2'	30:0:2884:G:O4'	2.19	0.42
30:0:1850:U:H2'	30:0:1851:G:C8	2.55	0.42
30:0:2751:C:H2'	30:0:2752:C:H6	1.84	0.42
30:0:360:A:H2'	30:0:361:C:O4'	2.19	0.42
30:0:1098:A:H2'	30:0:1099:G:O4'	2.19	0.42
30:0:851:C:O2	30:0:2022:A:H2	2.03	0.42
2:B:60:SER:HA	2:B:61:PRO:HD3	1.87	0.42
30:0:2645:U:O2'	30:0:2646:G:P	2.78	0.42
30:0:1942:A:H2'	30:0:1943:C:C6	2.55	0.42
30:0:236:A:H4'	30:0:237:G:OP1	2.19	0.42
1:A:88:ILE:HG22	1:A:88:ILE:O	2.20	0.42
30:0:128:A:H3'	30:0:128:A:C8	2.54	0.42
30:0:130:C:H5'	38:0:5216:HOH:O	2.19	0.42
30:0:187:A:H3'	30:0:188:C:C6	2.55	0.42
30:0:1058:A:H2'	30:0:1060:C:C5'	2.50	0.42
10:J:22:VAL:O	10:J:26:VAL:HG23	2.20	0.42
2:B:102:THR:HG23	2:B:182:VAL:HG12	2.02	0.42
2:B:258:GLY:HA2	38:0:4005:HOH:O	2.20	0.42
2:B:18:ARG:HG3	2:B:256:GLN:HG3	2.02	0.42
5:E:7:ILE:HG22	5:E:45:ASP:O	2.19	0.42
28:2:2:LYS:HG3	30:0:1486:A:C5	2.54	0.42
30:0:1139:U:H2'	30:0:1140:C:C6	2.54	0.42
30:0:417:G:P	38:0:7414:HOH:O	2.77	0.42
4:D:128:LEU:HB2	38:D:6007:HOH:O	2.20	0.42
13:M:42:ARG:HA	13:M:43:PRO:HD3	1.87	0.42
18:R:84:ALA:O	18:R:88:PHE:HD1	2.02	0.42
30:0:2761:A:C4	30:0:2763:G:C8	3.07	0.42
30:0:1917:G:C6	30:0:1918:U:C4	3.07	0.42
30:0:1191:A:N3	30:0:1207:A:C2	2.87	0.42
3:C:236:THR:HG21	38:C:8579:HOH:O	2.20	0.42
5:E:60:SER:OG	30:0:2784:A:H1'	2.20	0.42
31:9:31:C:C2	31:9:50:G:N2	2.88	0.42
30:0:309:C:O2	30:0:309:C:H2'	2.19	0.42
20:T:24:ARG:HH21	20:T:39:ASN:ND2	2.16	0.42
30:0:1214:G:H4'	38:0:4747:HOH:O	2.19	0.42
30:0:1060:C:H6	30:0:1060:C:H5'	1.85	0.42
25:Y:138:ARG:HD3	30:0:638:C:OP2	2.20	0.42
5:E:11:VAL:HG13	5:E:23:GLU:O	2.19	0.42

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:W:44:MET:CE	30:0:944:G:H21	2.33	0.42
3:C:242:GLU:HB2	38:C:8587:HOH:O	2.19	0.42
30:0:1907:U:O2'	30:0:1908:G:H5'	2.20	0.42
15:O:29:VAL:HG11	15:O:98:LEU:HD21	2.01	0.42
27:1:10:LYS:HG3	38:1:8981:HOH:O	2.19	0.42
30:0:377:C:H5	38:0:3302:HOH:O	2.01	0.42
30:0:1159:G:H1	30:0:1208:C:H42	1.68	0.42
30:0:241:A:C2	30:0:378:A:H4'	2.54	0.42
30:0:1789:G:C2'	30:0:1790:C:O5'	2.68	0.42
1:A:103:VAL:HA	1:A:104:PRO:HD3	1.86	0.42
30:0:1008:C:O2'	30:0:1009:U:H5'	2.20	0.42
30:0:999:C:C2'	30:0:1000:C:H5'	2.49	0.42
30:0:1903:U:O2'	30:0:1904:A:C8	2.68	0.42
3:C:95:GLU:CD	3:C:95:GLU:H	2.23	0.42
30:0:1520:G:C6	30:0:1521:C:C4	3.07	0.42
13:M:80:GLY:O	13:M:81:ARG:HD3	2.20	0.42
30:0:569:A:H5''	30:0:587:A:N1	2.35	0.42
8:H:139:ALA:HB3	8:H:149:VAL:HG21	2.02	0.42
13:M:122:GLN:HB2	13:M:126:GLN:O	2.20	0.42
31:9:73:A:N1	31:9:108:C:O2	2.53	0.42
14:N:82:TYR:CD2	14:N:82:TYR:C	2.93	0.42
13:M:15:PRO:HA	13:M:20:LEU:HD23	2.02	0.42
15:O:39:THR:O	15:O:115:ARG:NH2	2.53	0.42
4:D:167:GLU:C	4:D:169:THR:H	2.23	0.42
30:0:365:G:C6	30:0:366:U:C4	3.08	0.42
22:V:1:THR:CG2	22:V:2:VAL:H	2.25	0.42
30:0:1130:U:H2'	30:0:1131:G:C4'	2.50	0.42
13:M:158:ARG:HB2	13:M:163:LEU:HB2	2.02	0.42
10:J:74:ARG:NH1	10:J:76:ASP:HB2	2.35	0.42
30:0:699:C:C6	30:0:744:G:C4	3.08	0.42
3:C:206:ASN:HB2	30:0:329:A:OP2	2.20	0.42
30:0:2739:A:C6	30:0:2740:G:C5	3.08	0.42
5:E:7:ILE:HA	5:E:8:PRO:HD3	1.95	0.42
30:0:2553:A:H2'	30:0:2553:A:N3	2.35	0.42
25:Y:141:THR:HG23	38:Y:9073:HOH:O	2.19	0.42
23:W:29:VAL:O	23:W:30:ASN:HB2	2.19	0.42
30:0:1494:A:C4	30:0:1495:C:C5	3.08	0.42
14:N:171:HIS:CE1	38:N:8861:HOH:O	2.71	0.42
18:R:69:LYS:HB2	18:R:72:VAL:HG23	2.02	0.42
30:0:1373:G:H4'	38:0:5286:HOH:O	2.20	0.42
30:0:1183:C:N3	30:0:1184:C:C4	2.88	0.41

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:1207:A:N6	38:0:5631:HOH:O	2.53	0.41
30:0:2541:U:H5'	38:0:5398:HOH:O	2.20	0.41
30:0:1878:G:O2'	30:0:1879:U:H6	2.03	0.41
30:0:116:G:H1'	30:0:129:A:N3	2.35	0.41
30:0:2256:G:H2'	30:0:2257:G:O5'	2.19	0.41
30:0:2425:A:H5'	30:0:2426:G:OP2	2.20	0.41
30:0:1771:U:O2'	30:0:1773:G:N7	2.52	0.41
20:T:41:ARG:NH1	20:T:41:ARG:HG2	2.34	0.41
30:0:941:G:C6	30:0:942:U:C4	3.08	0.41
30:0:2616:A:C4'	30:0:2617:G:OP1	2.67	0.41
30:0:2587:OMU:H6	30:0:2587:OMU:O5'	2.19	0.41
30:0:1926:G:H2'	30:0:1927:A:C8	2.55	0.41
30:0:939:A:C2	30:0:1027:G:N3	2.88	0.41
24:X:30:MET:HE1	24:X:58:ALA:HB3	2.02	0.41
30:0:424:C:H2'	30:0:425:U:H6	1.85	0.41
2:B:24:PRO:CG	2:B:204:GLY:HA2	2.49	0.41
6:F:83:LEU:HA	6:F:83:LEU:HD12	1.91	0.41
30:0:1416:G:H2'	30:0:1417:G:H5'	2.01	0.41
30:0:1574:C:H6	30:0:1574:C:O5'	2.03	0.41
2:B:14:GLY:HA2	2:B:15:PRO:C	2.39	0.41
30:0:1375:A:C2'	30:0:1376:G:H5'	2.50	0.41
30:0:45:A:N6	30:0:147:G:C4	2.88	0.41
30:0:1202:A:H2'	30:0:1203:G:O4'	2.20	0.41
30:0:2509:A:OP2	30:0:2510:C:C5	2.73	0.41
30:0:2591:C:H2'	30:0:2592:G:O4'	2.20	0.41
31:9:2:U:C1'	38:9:9099:HOH:O	2.67	0.41
31:9:2:U:H1'	38:9:9099:HOH:O	2.19	0.41
11:K:109:LEU:CD1	11:K:113:ILE:HD11	2.50	0.41
30:0:1001:U:O2'	30:0:1002:G:H5'	2.20	0.41
27:1:28:HIS:CE1	27:1:31:LYS:HE2	2.56	0.41
30:0:803:C:O2'	30:0:804:C:H5'	2.21	0.41
30:0:2611:G:H5'	30:0:2613:G:C8	2.55	0.41
8:H:102:LYS:HD3	8:H:122:LYS:HD3	2.02	0.41
30:0:131:A:OP2	30:0:141:C:H5	2.03	0.41
30:0:2866:U:H4'	30:0:2867:G:H5'	2.01	0.41
30:0:1191:A:H2'	30:0:1193:A:H5'	2.02	0.41
23:W:125:HIS:CD2	23:W:127:GLY:H	2.38	0.41
1:A:212:PRO:HA	30:0:1943:C:O4'	2.19	0.41
25:Y:189:ASN:HD22	25:Y:192:ASP:H	1.67	0.41
14:N:25:ARG:HG2	30:0:2416:G:O2'	2.20	0.41
4:D:58:VAL:HG12	4:D:60:GLU:HG2	2.01	0.41

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:102:THR:CG2	2:B:182:VAL:HG12	2.50	0.41
2:B:62:ARG:HA	2:B:65:MET:HE3	2.02	0.41
30:0:2361:A:H2'	30:0:2362:A:O4'	2.20	0.41
30:0:862:U:H2'	30:0:863:G:C8	2.55	0.41
30:0:2438:G:H2'	30:0:2439:C:C6	2.55	0.41
24:X:73:ARG:HH12	24:X:88:GLU:HB2	1.85	0.41
23:W:73:LEU:HA	23:W:73:LEU:HD12	1.77	0.41
30:0:1391:G:H2'	30:0:1392:A:H5'	2.02	0.41
30:0:1946:C:H2'	30:0:1971:G:C8	2.55	0.41
30:0:2729:C:O2'	30:0:2730:G:H5'	2.19	0.41
30:0:1940:C:H1'	38:0:9375:HOH:O	2.20	0.41
3:C:240:LEU:HB2	38:C:8659:HOH:O	2.20	0.41
20:T:26:THR:HG23	20:T:97:ARG:HG3	2.02	0.41
10:J:75:PRO:HD3	10:J:136:SER:OG	2.20	0.41
22:V:44:GLY:O	22:V:48:GLU:HG2	2.21	0.41
30:0:2880:A:C2'	30:0:2881:C:H5'	2.50	0.41
15:O:38:ARG:HD3	30:0:654:A:OP2	2.20	0.41
17:Q:7:LEU:HD12	30:0:2424:U:C1'	2.50	0.41
14:N:4:PRO:HB2	30:0:1010:C:H4'	2.02	0.41
30:0:1398:G:H2'	30:0:1399:A:C8	2.55	0.41
30:0:1576:G:H2'	30:0:1577:U:C6	2.55	0.41
30:0:1613:C:H2'	30:0:1614:G:O4'	2.20	0.41
29:3:69:TYR:HB2	29:3:78:HIS:CE1	2.55	0.41
30:0:23:G:H1'	30:0:520:A:N6	2.36	0.41
21:U:23:HIS:NE2	21:U:29:THR:OG1	2.41	0.41
14:N:147:ILE:HD12	38:9:9087:HOH:O	2.20	0.41
31:9:2:U:OP2	31:9:2:U:H4'	2.21	0.41
30:0:370:G:N2	30:0:371:U:C2	2.89	0.41
1:A:187:PRO:HB2	30:0:1845:A:O3'	2.20	0.41
18:R:39:THR:HB	18:R:42:GLU:HG3	2.02	0.41
23:W:38:THR:HG22	23:W:39:ASP:H	1.86	0.41
30:0:1327:G:C6	30:0:1331:G:C6	3.09	0.41
30:0:946:C:H2'	30:0:947:U:C6	2.54	0.41
30:0:2737:C:H2'	38:0:6141:HOH:O	2.21	0.41
1:A:214:SER:HA	1:A:227:ASP:O	2.21	0.41
6:F:72:VAL:HA	6:F:73:PRO:HD3	1.86	0.41
30:0:2506:A:H62	30:0:2511:A:HO2'	1.66	0.41
29:3:38:ARG:HD2	30:0:396:U:OP2	2.20	0.41
1:A:48:ASP:HA	1:A:49:PRO:HD3	1.92	0.41
6:F:32:GLY:N	38:F:3111:HOH:O	2.53	0.41
13:M:24:GLN:HA	13:M:24:GLN:NE2	2.35	0.41

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:S:57:THR:C	19:S:59:ASP:H	2.24	0.41
25:Y:145:LYS:O	25:Y:147:ARG:HG2	2.20	0.41
8:H:92:LYS:HG3	8:H:130:VAL:HG22	2.02	0.41
30:0:1311:G:C2	30:0:1312:G:C8	3.08	0.41
30:0:1471:A:H2'	30:0:1472:C:C6	2.55	0.41
30:0:659:A:H5''	38:0:7096:HOH:O	2.19	0.41
30:0:334:G:H2'	30:0:335:U:O4'	2.20	0.41
4:D:88:LEU:HB2	4:D:89:PRO:HD3	2.02	0.41
30:0:1259:A:N1	30:0:1261:A:H1'	2.35	0.41
30:0:2088:C:H1'	30:0:2841:A:N1	2.36	0.41
18:R:80:TYR:O	30:0:2050:G:H5''	2.20	0.41
38:D:7597:HOH:O	31:9:56:A:H2	2.04	0.41
10:J:52:GLN:NE2	30:0:1119:G:H8	2.18	0.41
30:0:2526:C:H3'	30:0:2526:C:H6	1.85	0.41
30:0:2102:G:N2	30:0:2104:C:C6	2.89	0.41
30:0:2480:G:O2'	30:0:2481:G:H5'	2.21	0.41
24:X:43:VAL:HG12	24:X:47:ALA:HB3	2.01	0.41
25:Y:151:SER:HB3	25:Y:154:ARG:CB	2.50	0.41
30:0:517:U:C2'	30:0:518:G:H5'	2.50	0.41
2:B:174:ARG:HA	2:B:177:HIS:HB3	2.03	0.41
29:3:69:TYR:CZ	29:3:80:ARG:HD2	2.55	0.41
8:H:157:TYR:C	8:H:157:TYR:CD1	2.94	0.41
18:R:114:VAL:HG13	18:R:114:VAL:O	2.21	0.41
20:T:77:VAL:HG11	20:T:91:LEU:HD11	2.03	0.41
1:A:20:SER:HB3	30:0:1872:C:H5	1.85	0.41
30:0:99:A:C8	30:0:100:C:C5	3.08	0.41
30:0:2083:A:H3'	38:0:7573:HOH:O	2.20	0.41
17:Q:66:LYS:HB2	17:Q:70:ALA:O	2.20	0.41
30:0:1982:C:H2'	30:0:1983:C:O4'	2.20	0.41
6:F:1:PRO:H3	6:F:4:VAL:HG23	1.86	0.41
11:K:78:LYS:HA	11:K:79:PRO:HD3	1.94	0.41
30:0:1076:G:C2	30:0:1084:C:C2	3.08	0.41
16:P:18:LYS:O	16:P:21:VAL:HG13	2.20	0.41
30:0:2764:C:H2'	30:0:2765:C:H6	1.84	0.41
29:3:91:GLN:O	29:3:92:GLU:HB2	2.20	0.41
30:0:1896:G:C6	30:0:1897:U:C4	3.09	0.41
31:9:1:U:O3'	31:9:3:A:OP1	2.39	0.41
6:F:50:VAL:CG2	6:F:63:ILE:HG21	2.51	0.41
2:B:97:LEU:O	2:B:98:THR:HG23	2.21	0.41
2:B:53:LEU:HD11	2:B:327:VAL:HG22	2.02	0.41
30:0:10:U:O4	30:0:532:A:H8	2.04	0.41

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:1626:A:C2'	30:0:1627:G:H5'	2.51	0.41
30:0:79:G:N2	30:0:97:G:H1'	2.36	0.41
30:0:2607:U:H4'	38:0:9440:HOH:O	2.21	0.41
18:R:1:GLY:HA2	18:R:119:VAL:HG21	2.02	0.41
15:O:14:LEU:CD2	15:O:102:ILE:HD11	2.51	0.41
30:0:626:U:C4	30:0:627:G:C6	3.08	0.41
30:0:278:A:C6	30:0:279:C:C4	3.09	0.41
23:W:80:ASP:HB2	38:W:3312:HOH:O	2.21	0.41
30:0:1632:A:C3'	30:0:1633:C:H5'	2.51	0.41
30:0:812:A:H2'	30:0:813:C:C6	2.55	0.41
30:0:812:A:H2'	30:0:813:C:O4'	2.21	0.41
14:N:38:LYS:HB2	14:N:38:LYS:HE3	1.81	0.41
16:P:59:ARG:HH22	16:P:66:GLN:HE22	1.69	0.41
27:1:28:HIS:O	27:1:32:LYS:N	2.47	0.41
30:0:393:G:C6	30:0:394:G:C6	3.09	0.41
30:0:1406:A:H4'	30:0:1407:A:C5'	2.51	0.41
30:0:196:G:H1'	30:0:198:A:N7	2.35	0.41
4:D:88:LEU:N	4:D:89:PRO:CD	2.83	0.41
15:O:14:LEU:HD23	15:O:102:ILE:HD11	2.03	0.41
5:E:166:VAL:HG12	38:E:3134:HOH:O	2.21	0.41
30:0:1783:A:O2'	30:0:1784:U:H5'	2.21	0.41
2:B:10:SER:HB2	30:0:2714:U:H4'	2.02	0.41
30:0:1552:G:H2'	30:0:1553:C:C6	2.56	0.41
30:0:1275:C:N3	30:0:1281:C:N4	2.69	0.41
30:0:287:C:H2'	30:0:288:A:C8	2.56	0.41
30:0:1964:U:O2	30:0:1964:U:H2'	2.21	0.41
30:0:1445:G:N2	30:0:1678:A:H1'	2.36	0.41
30:0:1074:G:H4'	30:0:1260:G:C6	2.56	0.41
30:0:1184:C:O2'	30:0:1185:U:OP2	2.34	0.41
30:0:1587:U:H2'	30:0:1588:G:O4'	2.21	0.41
30:0:1641:A:H2'	30:0:1642:A:C5'	2.45	0.41
2:B:85:ARG:NH1	30:0:2671:U:O2	2.54	0.41
10:J:105:LEU:HD23	38:J:5907:HOH:O	2.21	0.41
31:9:58:G:N7	31:9:59:C:C4	2.89	0.41
17:Q:50:GLY:HA2	38:0:6025:HOH:O	2.20	0.41
1:A:204:GLY:N	30:0:2634:G:OP2	2.53	0.41
2:B:211:THR:HG21	38:0:7451:HOH:O	2.21	0.41
5:E:49:ILE:HD11	5:E:69:ILE:HD12	2.03	0.41
30:0:1712:A:H2'	30:0:1713:G:O4'	2.20	0.41
30:0:74:G:O2'	30:0:75:U:H5'	2.20	0.41
30:0:2842:G:H2'	30:0:2843:A:H5'	2.02	0.41

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:R:79:ARG:HB3	30:0:2050:G:OP1	2.21	0.41
30:0:1084:C:H6	30:0:1084:C:O5'	2.04	0.41
2:B:57:GLU:HA	2:B:58:PRO:HD2	1.91	0.41
30:0:1930:A:H2'	30:0:1931:A:C8	2.55	0.41
30:0:1743:G:H1'	38:0:4892:HOH:O	2.20	0.41
8:H:100:GLU:HB3	8:H:124:VAL:HG11	2.02	0.41
30:0:594:C:C4	30:0:595:U:C4	3.09	0.41
30:0:2804:C:H2'	30:0:2805:A:O4'	2.21	0.41
14:N:13:ARG:NH1	30:0:2368:A:C6	2.89	0.41
30:0:2277:U:O2'	30:0:2278:U:H5'	2.21	0.41
30:0:1363:G:H2'	30:0:1364:G:C8	2.56	0.41
21:U:33:SER:O	21:U:37:GLU:HG3	2.21	0.41
30:0:2072:G:O2'	30:0:2489:G:N2	2.53	0.40
12:L:129:ALA:O	12:L:133:VAL:HG23	2.21	0.40
29:3:38:ARG:HH11	30:0:396:U:P	2.43	0.40
4:D:25:MET:HE2	4:D:41:LEU:CG	2.50	0.40
1:A:190:ARG:NH1	30:0:1845:A:OP2	2.54	0.40
30:0:2617:G:C2	30:0:2618:G:C8	3.09	0.40
30:0:11:A:H5'	30:0:12:U:OP2	2.20	0.40
3:C:214:THR:HG21	38:C:8608:HOH:O	2.20	0.40
12:L:121:ILE:HG12	12:L:141:GLU:HB2	2.04	0.40
30:0:228:C:C2'	30:0:229:G:H5'	2.51	0.40
30:0:1760:G:C2	30:0:1813:U:O4'	2.74	0.40
30:0:1041:U:H4'	30:0:1295:G:H5'	2.03	0.40
30:0:1917:G:C5	30:0:1918:U:C4	3.09	0.40
22:V:5:VAL:HG23	38:V:2271:HOH:O	2.20	0.40
29:3:79:LEU:HD13	30:0:2457:U:H1'	2.04	0.40
4:D:18:ILE:HD13	4:D:84:LEU:HD12	2.03	0.40
18:R:82:GLU:HG3	18:R:83:LYS:N	2.35	0.40
22:V:27:LEU:HA	22:V:49:LEU:HD13	2.02	0.40
30:0:2712:G:H5'	38:0:5223:HOH:O	2.20	0.40
30:0:2712:G:P	38:0:5223:HOH:O	2.80	0.40
30:0:2820:A:H2'	30:0:2821:C:C6	2.55	0.40
30:0:1819:G:C2'	30:0:1820:G:C5'	2.99	0.40
2:B:310:ARG:HD2	38:B:9115:HOH:O	2.21	0.40
30:0:1014:A:H5''	31:9:101:G:O2'	2.21	0.40
30:0:42:C:H3'	38:0:4165:HOH:O	2.21	0.40
30:0:17:G:O2'	30:0:18:C:H5'	2.20	0.40
30:0:844:A:C6	30:0:882:A:C5	3.08	0.40
30:0:1215:A:O3'	30:0:1216:G:C4'	2.69	0.40
30:0:79:G:H22	30:0:97:G:H1'	1.86	0.40

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:75:GLU:C	2:B:77:PRO:HD3	2.42	0.40
14:N:23:ARG:HH11	14:N:23:ARG:HG2	1.87	0.40
30:0:2791:U:H1'	30:0:2792:A:H5''	2.03	0.40
16:P:14:LEU:HD13	16:P:51:ALA:HB2	2.03	0.40
1:A:173:GLY:O	1:A:176:HIS:HB3	2.21	0.40
2:B:30:PRO:HB2	2:B:39:GLN:NE2	2.36	0.40
30:0:1183:C:O2	30:0:1183:C:C2'	2.70	0.40
1:A:94:LEU:HD12	1:A:98:GLU:CB	2.43	0.40
30:0:2004:U:H2'	30:0:2005:G:OP1	2.22	0.40
30:0:2819:C:H2'	30:0:2820:A:C8	2.55	0.40
30:0:2252:A:H2'	30:0:2253:G:H5'	2.03	0.40
2:B:7:ARG:CG	2:B:7:ARG:HH11	2.35	0.40
14:N:93:GLN:NE2	14:N:93:GLN:HA	2.35	0.40
30:0:1624:A:H5'	30:0:1626:A:O4'	2.20	0.40
30:0:517:U:H2'	30:0:518:G:H5'	2.03	0.40
30:0:47:G:N3	30:0:114:A:C2	2.90	0.40
30:0:1102:C:H5	38:0:3487:HOH:O	2.04	0.40
30:0:2039:A:H4'	30:0:2760:C:O2'	2.22	0.40
30:0:2897:C:H2'	30:0:2898:G:H8	1.85	0.40
3:C:135:GLU:HB3	38:C:8582:HOH:O	2.20	0.40
30:0:2550:U:O2'	30:0:2551:C:H5'	2.20	0.40
13:M:118:TYR:CZ	13:M:130:GLU:HB2	2.56	0.40
23:W:88:THR:HG22	23:W:89:ASP:N	2.34	0.40
1:A:132:ASP:HB3	1:A:135:VAL:H	1.87	0.40
30:0:129:A:H4'	30:0:130:C:OP1	2.21	0.40
31:9:59:C:H2'	31:9:60:C:C6	2.56	0.40
30:0:694:A:H4'	30:0:2441:U:OP1	2.21	0.40
7:G:64:ASN:N	7:G:64:ASN:ND2	2.69	0.40
30:0:1544:U:H2'	30:0:1545:C:H6	1.87	0.40
25:Y:126:PRO:HG2	25:Y:128:PHE:CZ	2.56	0.40
30:0:249:G:H2'	30:0:250:C:H6	1.86	0.40
30:0:101:C:H2'	30:0:102:A:H8	1.87	0.40
20:T:52:ARG:HB2	20:T:95:ASN:HB3	2.02	0.40
30:0:445:U:H2'	30:0:446:G:C8	2.57	0.40
30:0:2758:G:H2'	30:0:2759:C:C6	2.56	0.40
30:0:1139:U:H2'	30:0:1140:C:H6	1.85	0.40
27:1:10:LYS:N	38:1:8981:HOH:O	2.50	0.40
1:A:230:SER:HB2	30:0:1852:A:H4'	2.04	0.40
2:B:245:SER:HB3	30:0:2094:G:H4'	2.02	0.40
13:M:47:ASP:CG	13:M:48:LYS:N	2.75	0.40
31:9:122:C:C6	38:9:9043:HOH:O	2.71	0.40

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:272:A:N1	30:0:369:G:H5''	2.36	0.40
30:0:1116:U:C2'	30:0:1118:A:C2	3.05	0.40
30:0:2491:G:C1'	38:0:6868:HOH:O	2.59	0.40
30:0:1589:G:H22	30:0:1605:G:H1'	1.85	0.40
4:D:146:LYS:NZ	14:N:107:ASN:ND2	2.70	0.40
13:M:24:GLN:HE22	13:M:27:ARG:HH11	1.68	0.40
1:A:171:LYS:HB2	30:0:820:G:C6	2.57	0.40
30:0:951:A:O2'	30:0:952:G:H5'	2.21	0.40
31:9:65:A:C6	31:9:112:U:C5	3.10	0.40
5:E:84:MET:HE1	5:E:148:ILE:HD12	2.04	0.40
30:0:2824:C:H5''	30:0:2825:C:H5'	2.03	0.40
30:0:517:U:H1'	38:0:7571:HOH:O	2.20	0.40
30:0:2327:A:H2'	30:0:2328:U:O4'	2.21	0.40
30:0:1472:C:H6	30:0:1472:C:O5'	2.04	0.40
30:0:1217:G:C2	30:0:1218:U:C2	3.09	0.40
23:W:5:VAL:HG11	23:W:153:MET:CE	2.52	0.40
2:B:149:ASP:HB2	38:B:9049:HOH:O	2.21	0.40
31:9:8:G:H5'	38:9:9103:HOH:O	2.21	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	235/240 (98%)	212 (90%)	19 (8%)	4 (2%)	11	38
2	B	335/338 (99%)	308 (92%)	24 (7%)	3 (1%)	21	57
3	C	244/246 (99%)	228 (93%)	15 (6%)	1 (0%)	39	74
4	D	134/177 (76%)	112 (84%)	18 (13%)	4 (3%)	5	22
5	E	170/178 (96%)	162 (95%)	8 (5%)	0	100	100
6	F	117/120 (98%)	106 (91%)	8 (7%)	3 (3%)	7	26

*Continued on next page...*

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
7	G	25/348 (7%)	24 (96%)	1 (4%)	0	100	100
8	H	156/177 (88%)	144 (92%)	10 (6%)	2 (1%)	15	46
9	I	68/162 (42%)	55 (81%)	11 (16%)	2 (3%)	6	23
10	J	140/145 (97%)	131 (94%)	9 (6%)	0	100	100
11	K	130/132 (98%)	123 (95%)	6 (5%)	1 (1%)	24	60
12	L	141/165 (86%)	126 (89%)	12 (8%)	3 (2%)	9	32
13	M	192/196 (98%)	185 (96%)	6 (3%)	1 (0%)	34	71
14	N	184/187 (98%)	169 (92%)	11 (6%)	4 (2%)	8	31
15	O	113/116 (97%)	109 (96%)	4 (4%)	0	100	100
16	P	141/149 (95%)	138 (98%)	3 (2%)	0	100	100
17	Q	93/96 (97%)	87 (94%)	6 (6%)	0	100	100
18	R	148/155 (96%)	140 (95%)	8 (5%)	0	100	100
19	S	79/85 (93%)	76 (96%)	3 (4%)	0	100	100
20	T	117/120 (98%)	111 (95%)	6 (5%)	0	100	100
21	U	51/67 (76%)	46 (90%)	5 (10%)	0	100	100
22	V	63/71 (89%)	59 (94%)	4 (6%)	0	100	100
23	W	152/154 (99%)	146 (96%)	6 (4%)	0	100	100
24	X	80/92 (87%)	74 (92%)	5 (6%)	1 (1%)	15	46
25	Y	140/241 (58%)	138 (99%)	2 (1%)	0	100	100
26	Z	71/116 (61%)	63 (89%)	7 (10%)	1 (1%)	14	44
27	1	54/57 (95%)	51 (94%)	3 (6%)	0	100	100
28	2	42/50 (84%)	41 (98%)	1 (2%)	0	100	100
29	3	90/92 (98%)	87 (97%)	2 (2%)	1 (1%)	17	51
All	All	3705/4472 (83%)	3451 (93%)	223 (6%)	31 (1%)	24	60

All (31) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	37	VAL
4	D	137	PRO
6	F	101	ALA
14	N	154	LEU
14	N	183	ASP
14	N	184	ILE

Continued on next page...

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	34	ASP
4	D	27	ILE
12	L	80	ASP
12	L	149	ARG
24	X	70	ILE
26	Z	44	ARG
1	A	36	ASP
1	A	88	ILE
2	B	2	GLN
3	C	8	LEU
6	F	100	ASP
8	H	19	ARG
11	K	127	ALA
12	L	21	ARG
14	N	139	TRP
2	B	184	ASP
4	D	56	ARG
2	B	185	GLY
6	F	61	MET
9	I	108	HIS
9	I	83	GLY
29	3	56	PRO
8	H	171	GLY
4	D	28	GLY
13	M	88	VAL

### 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	
1	A	179/182 (98%)	169 (94%)	10 (6%)	26	60
2	B	282/283 (100%)	267 (95%)	15 (5%)	28	63
3	C	193/193 (100%)	177 (92%)	16 (8%)	14	38
4	D	117/148 (79%)	112 (96%)	5 (4%)	35	71
5	E	152/156 (97%)	149 (98%)	3 (2%)	63	88

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
6	F	93/94 (99%)	92 (99%)	1 (1%)	80	95
7	G	27/282 (10%)	26 (96%)	1 (4%)	41	77
8	H	134/145 (92%)	128 (96%)	6 (4%)	34	70
9	I	58/130 (45%)	58 (100%)	0	100	100
10	J	118/121 (98%)	111 (94%)	7 (6%)	24	58
11	K	106/106 (100%)	105 (99%)	1 (1%)	84	96
12	L	113/127 (89%)	107 (95%)	6 (5%)	28	63
13	M	158/160 (99%)	152 (96%)	6 (4%)	40	76
14	N	149/150 (99%)	145 (97%)	4 (3%)	52	84
15	O	93/94 (99%)	93 (100%)	0	100	100
16	P	113/117 (97%)	110 (97%)	3 (3%)	52	84
17	Q	79/80 (99%)	77 (98%)	2 (2%)	55	85
18	R	117/122 (96%)	112 (96%)	5 (4%)	35	71
19	S	71/74 (96%)	71 (100%)	0	100	100
20	T	105/106 (99%)	100 (95%)	5 (5%)	31	67
21	U	44/53 (83%)	43 (98%)	1 (2%)	58	87
22	V	51/57 (90%)	50 (98%)	1 (2%)	63	88
23	W	130/130 (100%)	124 (95%)	6 (5%)	33	69
24	X	66/74 (89%)	59 (89%)	7 (11%)	8	25
25	Y	120/196 (61%)	118 (98%)	2 (2%)	68	91
26	Z	60/94 (64%)	60 (100%)	0	100	100
27	1	46/47 (98%)	46 (100%)	0	100	100
28	2	42/46 (91%)	41 (98%)	1 (2%)	57	86
29	3	79/79 (100%)	78 (99%)	1 (1%)	76	94
All	All	3095/3646 (85%)	2980 (96%)	115 (4%)	41	77

All (115) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	ARG
1	A	30	ARG
1	A	36	ASP
1	A	64	ASP
1	A	69	LEU

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type
1	A	94	LEU
1	A	131	HIS
1	A	153	ARG
1	A	179	MET
1	A	217	ARG
2	B	7	ARG
2	B	11	LEU
2	B	27	ASN
2	B	49	THR
2	B	51	VAL
2	B	53	LEU
2	B	97	LEU
2	B	132	HIS
2	B	162	MET
2	B	175	LEU
2	B	190	MET
2	B	195	ARG
2	B	234	ARG
2	B	254	GLN
2	B	312	ARG
3	C	2	GLN
3	C	27	ARG
3	C	76	ARG
3	C	78	ARG
3	C	94	THR
3	C	101	ASP
3	C	136	VAL
3	C	162	VAL
3	C	187	ARG
3	C	202	THR
3	C	214	THR
3	C	222	ASP
3	C	223	LEU
3	C	234	VAL
3	C	236	THR
3	C	243	VAL
4	D	24	HIS
4	D	50	VAL
4	D	62	ASP
4	D	149	ARG
4	D	153	THR
5	E	16	ASP

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
5	E	155	ASN
5	E	156	ASP
6	F	12	LEU
7	G	73	ASP
8	H	62	HIS
8	H	65	LEU
8	H	87	LYS
8	H	91	ARG
8	H	157	TYR
8	H	173	GLU
10	J	39	VAL
10	J	45	VAL
10	J	46	ILE
10	J	52	GLN
10	J	74	ARG
10	J	79	PHE
10	J	107	ASN
11	K	10	GLN
12	L	35	ARG
12	L	80	ASP
12	L	99	GLU
12	L	101	ASP
12	L	104	ASP
12	L	114	VAL
13	M	46	LEU
13	M	68	ARG
13	M	81	ARG
13	M	93	ARG
13	M	99	ARG
13	M	164	THR
14	N	17	ARG
14	N	26	LEU
14	N	49	THR
14	N	127	LEU
16	P	52	LYS
16	P	91	LYS
16	P	98	ILE
17	Q	11	ARG
17	Q	95	GLU
18	R	13	THR
18	R	39	THR
18	R	125	ARG

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
18	R	132	ARG
18	R	143	VAL
20	T	26	THR
20	T	39	ASN
20	T	48	VAL
20	T	89	ARG
20	T	117	ASP
21	U	52	THR
22	V	12	THR
23	W	4	LEU
23	W	73	LEU
23	W	76	ASP
23	W	108	ARG
23	W	142	ASP
23	W	146	ILE
24	X	12	ILE
24	X	27	ASP
24	X	46	ASP
24	X	72	VAL
24	X	79	GLU
24	X	82	GLU
24	X	88	GLU
25	Y	189	ASN
25	Y	203	VAL
28	2	18	ASN
29	3	56	PRO

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (76) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	47	HIS
1	A	199	HIS
2	B	2	GLN
2	B	27	ASN
2	B	145	HIS
2	B	221	GLN
2	B	238	ASN
2	B	260	HIS
2	B	320	GLN
2	B	332	ASN
3	C	73	GLN
3	C	129	HIS

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
3	C	163	HIS
4	D	103	ASN
4	D	133	ASN
5	E	143	GLN
7	G	64	ASN
8	H	34	HIS
8	H	59	GLN
8	H	62	HIS
9	I	106	GLN
10	J	52	GLN
10	J	107	ASN
11	K	10	GLN
11	K	44	HIS
12	L	18	HIS
12	L	41	HIS
12	L	116	HIS
13	M	24	GLN
13	M	58	GLN
13	M	137	ASN
13	M	170	ASN
14	N	21	HIS
14	N	40	ASN
14	N	93	GLN
14	N	107	ASN
16	P	50	GLN
16	P	66	GLN
16	P	73	HIS
16	P	89	ASN
16	P	118	GLN
17	Q	16	ASN
17	Q	40	HIS
18	R	22	GLN
18	R	61	GLN
18	R	94	ASN
18	R	98	ASN
18	R	113	HIS
18	R	117	HIS
18	R	122	GLN
18	R	123	GLN
19	S	9	HIS
19	S	44	GLN
20	T	39	ASN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
21	U	39	ASN
22	V	60	GLN
23	W	28	HIS
23	W	59	GLN
23	W	87	HIS
23	W	110	GLN
23	W	119	HIS
23	W	125	HIS
23	W	141	HIS
24	X	23	HIS
25	Y	134	HIS
25	Y	189	ASN
26	Z	61	HIS
27	1	8	GLN
27	1	16	HIS
27	1	28	HIS
28	2	16	ASN
28	2	18	ASN
28	2	41	HIS
28	2	45	ASN
29	3	2	GLN
29	3	48	ASN

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
30	0	2745/2923 (93%)	238 (8%)	25 (0%)
31	9	121/122 (99%)	17 (14%)	2 (1%)
All	All	2866/3045 (94%)	255 (8%)	27 (0%)

All (255) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
30	0	31	C
30	0	67	A
30	0	69	A
30	0	70	A
30	0	71	G
30	0	86	A
30	0	87	C
30	0	88	G

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
30	0	114	A
30	0	115	U
30	0	120	A
30	0	130	C
30	0	139	C
30	0	141	C
30	0	151	A
30	0	166	A
30	0	185	G
30	0	186	A
30	0	191	A
30	0	192	A
30	0	200	C
30	0	219	G
30	0	236	A
30	0	237	G
30	0	271	C
30	0	272	A
30	0	273	G
30	0	283	U
30	0	284	C
30	0	308	U
30	0	309	C
30	0	318	U
30	0	336	G
30	0	337	A
30	0	358	G
30	0	368	C
30	0	381	G
30	0	397	A
30	0	417	G
30	0	461	C
30	0	487	G
30	0	498	A
30	0	510	U
30	0	511	A
30	0	514	G
30	0	537	G
30	0	538	C
30	0	539	G
30	0	542	A
30	0	545	G

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
30	0	553	G
30	0	559	U
30	0	588	G
30	0	604	G
30	0	620	A
30	0	632	A
30	0	644	G
30	0	660	A
30	0	688	A
30	0	701	U
30	0	759	C
30	0	777	U
30	0	809	G
30	0	821	U
30	0	835	U
30	0	840	U
30	0	857	A
30	0	858	U
30	0	868	G
30	0	869	G
30	0	871	G
30	0	872	U
30	0	875	A
30	0	877	G
30	0	878	G
30	0	884	C
30	0	885	G
30	0	898	G
30	0	905	C
30	0	920	C
30	0	921	G
30	0	923	A
30	0	953	G
30	0	960	G
30	0	961	A
30	0	1006	A
30	0	1008	C
30	0	1029	U
30	0	1045	G
30	0	1059	G
30	0	1060	C
30	0	1072	G

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
30	0	1081	A
30	0	1088	A
30	0	1109	U
30	0	1110	G
30	0	1119	G
30	0	1130	U
30	0	1137	G
30	0	1161	A
30	0	1164	U
30	0	1165	G
30	0	1166	A
30	0	1174	A
30	0	1175	G
30	0	1185	U
30	0	1192	A
30	0	1193	A
30	0	1206	U
30	0	1208	C
30	0	1216	G
30	0	1237	U
30	0	1238	C
30	0	1239	G
30	0	1242	A
30	0	1279	U
30	0	1289	C
30	0	1331	G
30	0	1342	C
30	0	1353	C
30	0	1360	C
30	0	1377	C
30	0	1378	G
30	0	1407	A
30	0	1409	G
30	0	1474	C
30	0	1505	U
30	0	1506	U
30	0	1524	U
30	0	1525	G
30	0	1526	A
30	0	1559	A
30	0	1592	G
30	0	1625	U

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type
30	0	1626	A
30	0	1634	G
30	0	1656	A
30	0	1667	A
30	0	1682	A
30	0	1684	A
30	0	1685	A
30	0	1692	C
30	0	1701	A
30	0	1722	U
30	0	1723	G
30	0	1725	C
30	0	1731	C
30	0	1752	G
30	0	1778	A
30	0	1798	C
30	0	1819	G
30	0	1820	G
30	0	1829	A
30	0	1856	C
30	0	1879	U
30	0	1919	A
30	0	1942	A
30	0	1965	C
30	0	1971	G
30	0	1973	A
30	0	1979	G
30	0	1996	U
30	0	2004	U
30	0	2008	U
30	0	2011	A
30	0	2012	U
30	0	2013	G
30	0	2033	G
30	0	2034	U
30	0	2064	U
30	0	2072	G
30	0	2073	G
30	0	2074	A
30	0	2096	A
30	0	2101	A
30	0	2102	G

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
30	0	2103	A
30	0	2110	G
30	0	2243	C
30	0	2258	A
30	0	2271	G
30	0	2272	G
30	0	2291	A
30	0	2317	C
30	0	2321	A
30	0	2345	A
30	0	2354	A
30	0	2361	A
30	0	2369	A
30	0	2379	G
30	0	2422	U
30	0	2462	G
30	0	2465	A
30	0	2467	A
30	0	2476	C
30	0	2483	A
30	0	2507	G
30	0	2509	A
30	0	2511	A
30	0	2533	C
30	0	2537	G
30	0	2540	G
30	0	2541	U
30	0	2553	A
30	0	2564	G
30	0	2570	G
30	0	2589	U
30	0	2601	A
30	0	2602	G
30	0	2608	C
30	0	2611	G
30	0	2613	G
30	0	2617	G
30	0	2634	G
30	0	2638	G
30	0	2645	U
30	0	2649	A
30	0	2650	U

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
30	0	2664	A
30	0	2681	A
30	0	2682	C
30	0	2726	U
30	0	2747	C
30	0	2748	G
30	0	2749	U
30	0	2750	G
30	0	2762	C
30	0	2768	A
30	0	2800	A
30	0	2811	A
30	0	2812	A
30	0	2825	C
30	0	2852	A
30	0	2876	G
30	0	2890	A
30	0	2896	A
30	0	2903	C
30	0	2914	A
31	9	2	U
31	9	7	G
31	9	14	G
31	9	22	G
31	9	23	U
31	9	24	U
31	9	25	G
31	9	40	C
31	9	41	C
31	9	43	G
31	9	44	A
31	9	52	A
31	9	57	A
31	9	66	G
31	9	77	A
31	9	114	G
31	9	122	C

All (27) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
30	0	69	A

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
30	0	129	A
30	0	603	A
30	0	644	G
30	0	699	C
30	0	834	G
30	0	857	A
30	0	871	G
30	0	877	G
30	0	1080	C
30	0	1237	U
30	0	1246	A
30	0	1352	A
30	0	1474	C
30	0	1506	U
30	0	1692	C
30	0	1730	G
30	0	2313	C
30	0	2467	A
30	0	2536	C
30	0	2616	A
30	0	2649	A
30	0	2718	C
30	0	2726	U
30	0	2761	A
31	9	43	G
31	9	65	A

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

5 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$
30	OMU	0	2587	30,34	12,22,23	1.02	1 (8%)	19,31,34	3.12	2 (10%)
30	OMG	0	2588	30	17,26,27	1.03	1 (5%)	21,38,41	2.54	3 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
30	UR3	0	2619	30	12,22,23	0.80	1 (8%)	16,32,35	0.72	0
30	PSU	0	2621	30	13,21,22	1.75	2 (15%)	18,30,33	6.10	4 (22%)
30	1MA	0	628	30,34	14,25,26	0.99	1 (7%)	15,37,40	1.19	1 (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
30	OMU	0	2587	30,34	-	0/5/27/28	0/2/2/2
30	OMG	0	2588	30	-	0/5/27/28	0/3/3/3
30	UR3	0	2619	30	-	0/3/25/26	0/2/2/2
30	PSU	0	2621	30	-	0/7/25/26	0/2/2/2
30	1MA	0	628	30,34	-	0/3/25/26	0/3/3/3

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	0	2621	PSU	C5-C1'	-5.44	1.47	1.52
30	0	2619	UR3	C6-C5	-2.07	1.33	1.38
30	0	2587	OMU	C4-N3	2.40	1.37	1.33
30	0	2621	PSU	C4-N3	2.44	1.37	1.33
30	0	628	1MA	C6-N6	2.69	1.34	1.29
30	0	2588	OMG	C6-N1	3.11	1.38	1.33

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	0	2621	PSU	N1-C2-N3	-21.37	114.70	128.33
30	0	2588	OMG	C5-C6-N1	-8.72	111.66	123.59
30	0	628	1MA	C2-N3-C4	-3.67	110.71	116.40
30	0	2587	OMU	C5-C4-N3	-3.25	114.78	123.12
30	0	2588	OMG	N3-C2-N1	-2.36	123.84	127.44
30	0	2621	PSU	C5-C1'-C2'	-2.28	111.48	115.52
30	0	2621	PSU	C6-N1-C2	2.63	119.70	115.47
30	0	2588	OMG	C6-N1-C2	6.72	125.26	115.94
30	0	2587	OMU	C4-N3-C2	12.98	127.00	114.14
30	0	2621	PSU	C4-N3-C2	13.77	127.15	115.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
30	0	2587	OMU	2	0
30	0	2621	PSU	1	0

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 305 ligands modelled in this entry, 305 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 [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	237/240 (98%)	-0.52	2 (0%) 87 86	25, 49, 89, 109	0
2	B	337/338 (99%)	-0.61	1 (0%) 94 94	27, 54, 81, 92	0
3	C	246/246 (100%)	-0.67	0 100 100	22, 42, 65, 77	0
4	D	140/177 (79%)	0.91	28 (20%) 1 1	65, 101, 125, 137	0
5	E	172/178 (96%)	-0.32	1 (0%) 90 89	45, 71, 92, 97	0
6	F	119/120 (99%)	0.01	2 (1%) 73 70	48, 69, 99, 116	0
7	G	29/348 (8%)	0.70	3 (10%) 9 5	76, 95, 103, 106	0
8	H	160/177 (90%)	-0.24	3 (1%) 70 66	41, 59, 97, 103	0
9	I	70/162 (43%)	3.02	44 (62%) 0 0	127, 146, 165, 166	0
10	J	142/145 (97%)	-0.64	0 100 100	38, 51, 72, 91	0
11	K	132/132 (100%)	-0.73	0 100 100	35, 50, 74, 84	0
12	L	145/165 (87%)	-0.16	1 (0%) 89 88	25, 64, 110, 127	0
13	M	194/196 (98%)	-0.75	0 100 100	28, 40, 57, 65	0
14	N	186/187 (99%)	-0.24	4 (2%) 65 60	41, 66, 114, 123	0
15	O	115/116 (99%)	-0.62	0 100 100	34, 53, 72, 76	0
16	P	143/149 (95%)	-0.62	0 100 100	37, 54, 69, 79	0
17	Q	95/96 (98%)	-0.63	0 100 100	36, 46, 62, 76	0
18	R	150/155 (96%)	-0.75	0 100 100	30, 44, 65, 81	0
19	S	81/85 (95%)	-0.51	1 (1%) 81 78	41, 56, 78, 89	0
20	T	119/120 (99%)	-0.48	1 (0%) 87 86	39, 54, 83, 110	0
21	U	53/67 (79%)	-0.62	0 100 100	42, 55, 75, 83	0
22	V	65/71 (91%)	0.31	6 (9%) 11 7	44, 70, 119, 125	0
23	W	154/154 (100%)	-0.58	0 100 100	36, 50, 67, 80	0
24	X	82/92 (89%)	-0.35	3 (3%) 45 38	43, 61, 86, 101	0

*Continued on next page...*

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
25	Y	142/241 (58%)	-0.74	1 (0%) 89 88	24, 42, 67, 88	0
26	Z	73/116 (62%)	0.43	7 (9%) 10 6	55, 77, 92, 98	0
27	1	56/57 (98%)	-0.64	0 100 100	25, 30, 37, 43	0
28	2	46/50 (92%)	-0.27	2 (4%) 39 32	31, 61, 91, 101	0
29	3	92/92 (100%)	-0.29	0 100 100	36, 63, 77, 90	0
30	0	2749/2923 (94%)	-0.59	10 (0%) 93 92	19, 44, 88, 164	0
31	9	122/122 (100%)	-0.65	2 (1%) 74 72	37, 67, 89, 147	0
All	All	6646/7517 (88%)	-0.46	122 (1%) 71 68	19, 51, 100, 166	0

All (122) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
9	I	74	ILE	8.7
9	I	70	THR	7.4
22	V	39	ALA	7.1
22	V	40	PRO	7.1
9	I	72	GLU	6.7
9	I	71	ALA	6.3
26	Z	46	SER	6.2
9	I	108	HIS	6.1
9	I	102	GLN	6.1
9	I	76	ASP	5.8
4	D	57	THR	5.6
4	D	63	ILE	5.6
9	I	93	ALA	5.3
9	I	113	SER	5.3
9	I	104	ALA	5.2
9	I	79	GLY	4.9
9	I	99	GLN	4.8
9	I	112	LEU	4.7
14	N	166	ALA	4.7
9	I	128	THR	4.6
9	I	80	PHE	4.5
9	I	92	VAL	4.5
4	D	90	LEU	4.5
31	9	1	U	4.3
9	I	106	GLN	4.3
9	I	109	PRO	4.3
9	I	100	VAL	4.3
9	I	69	PRO	4.2

Continued on next page...



*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
9	I	66	GLY	4.2
9	I	97	VAL	4.2
4	D	85	GLN	4.2
9	I	83	GLY	4.0
9	I	111	LEU	4.0
4	D	44	ILE	4.0
9	I	91	PHE	3.9
19	S	81	ILE	3.8
9	I	73	LEU	3.6
25	Y	235	GLU	3.6
9	I	67	VAL	3.6
9	I	132	VAL	3.6
22	V	43	PRO	3.5
22	V	1	THR	3.5
4	D	170	TYR	3.5
9	I	82	THR	3.5
9	I	88	GLN	3.5
9	I	110	ASP	3.4
4	D	89	PRO	3.3
9	I	86	GLU	3.3
9	I	78	ALA	3.3
9	I	98	ASP	3.3
26	Z	44	ARG	3.2
9	I	116	LEU	3.2
1	A	37	VAL	3.2
9	I	84	SER	3.2
26	Z	45	VAL	3.1
4	D	75	LEU	3.1
26	Z	58	ASN	3.1
24	X	88	GLU	3.0
28	2	49	GLU	3.0
4	D	18	ILE	3.0
4	D	40	ILE	3.0
30	0	1172	G	3.0
26	Z	50	VAL	3.0
8	H	40	GLN	2.9
4	D	92	GLU	2.9
9	I	103	ILE	2.9
4	D	171	ASP	2.8
9	I	81	GLU	2.8
9	I	75	LYS	2.7
4	D	61	PHE	2.7

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
9	I	105	GLU	2.7
4	D	17	ARG	2.6
30	0	1198	U	2.6
4	D	81	GLU	2.6
6	F	106	ALA	2.6
22	V	38	GLY	2.6
2	B	57	GLU	2.6
26	Z	35	SER	2.5
12	L	80	ASP	2.5
28	2	39	ARG	2.5
1	A	237	GLY	2.5
14	N	155	GLU	2.5
8	H	174	LEU	2.5
31	9	24	U	2.5
4	D	84	LEU	2.4
24	X	80	GLU	2.4
4	D	27	ILE	2.4
14	N	183	ASP	2.4
5	E	100	ASP	2.4
20	T	116	ASP	2.4
9	I	114	TYR	2.4
4	D	26	GLY	2.3
4	D	166	ILE	2.3
4	D	41	LEU	2.3
4	D	134	LEU	2.3
30	0	1199	A	2.3
4	D	88	LEU	2.3
4	D	104	PHE	2.2
8	H	87	LYS	2.2
30	0	1200	A	2.2
4	D	73	VAL	2.2
4	D	45	THR	2.2
6	F	49	PHE	2.2
4	D	69	ILE	2.2
30	0	1202	A	2.2
9	I	121	LYS	2.2
4	D	102	GLY	2.2
14	N	160	SER	2.2
7	G	25	GLU	2.2
7	G	26	MET	2.1
30	0	735	C	2.1
9	I	117	THR	2.1

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
26	Z	69	ASP	2.1
7	G	27	ILE	2.1
9	I	90	ASP	2.1
30	0	1203	G	2.1
4	D	47	GLN	2.1
30	0	970	U	2.1
30	0	2237	G	2.1
24	X	71	ARG	2.1
30	0	2645	U	2.0
22	V	41	GLU	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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> 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	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
30	1MA	0	628	23/24	0.98	0.17	-	28,29,31,32	0
30	OMU	0	2587	21/22	0.98	0.12	-	32,36,38,39	0
30	PSU	0	2621	20/21	0.98	0.14	-	26,30,50,51	0
30	OMG	0	2588	24/25	0.99	0.12	-	30,35,38,40	0
30	UR3	0	2619	21/22	0.98	0.13	-	45,48,53,54	0

## 6.3 Carbohydrates [i](#)

There are no carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> 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	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
34	NA	0	8547	1/1	0.86	1.00	61.22	60,60,60,60	0
34	NA	0	8535	1/1	0.94	0.36	32.30	55,55,55,55	0
34	NA	0	8562	1/1	0.69	0.40	28.92	55,55,55,55	0
34	NA	0	8546	1/1	0.89	0.81	24.84	82,82,82,82	0
34	NA	0	8560	1/1	0.92	0.59	24.79	85,85,85,85	0
34	NA	0	8565	1/1	0.90	0.35	20.42	57,57,57,57	0
36	SR	0	8986	1/1	0.97	0.31	18.92	200,200,200,200	0
34	NA	0	8555	1/1	0.83	0.48	17.03	53,53,53,53	0
34	NA	0	8568	1/1	0.99	0.54	15.93	36,36,36,36	0
34	NA	0	8563	1/1	0.80	0.41	15.83	67,67,67,67	0
34	NA	0	8556	1/1	0.70	0.74	13.57	55,55,55,55	0
34	NA	0	8512	1/1	1.00	0.31	13.33	45,45,45,45	0
34	NA	0	8542	1/1	0.95	0.27	12.66	48,48,48,48	0
32	MG	0	8041	1/1	0.98	0.22	12.29	29,29,29,29	0
36	SR	B	8987	1/1	0.90	0.53	11.48	200,200,200,200	0
34	NA	0	8559	1/1	0.94	0.18	11.32	67,67,67,67	0
34	NA	0	8553	1/1	0.84	0.28	9.54	52,52,52,52	0
34	NA	0	8528	1/1	0.88	0.25	9.14	44,44,44,44	0
34	NA	9	8572	1/1	0.84	0.24	8.90	80,80,80,80	0
34	NA	0	8558	1/1	0.93	0.32	7.85	45,45,45,45	0
36	SR	0	8903	1/1	1.00	0.16	7.17	53,53,53,53	0
34	NA	0	8552	1/1	0.93	0.29	7.15	72,72,72,72	0
32	MG	0	8047	1/1	0.98	0.25	6.77	50,50,50,50	0
32	MG	0	8016	1/1	0.94	0.27	6.05	50,50,50,50	0
32	MG	0	8009	1/1	0.99	0.21	5.64	28,28,28,28	0
34	NA	0	8517	1/1	0.99	0.18	5.25	46,46,46,46	0
36	SR	0	8904	1/1	0.98	0.19	4.60	55,55,55,55	0
34	NA	0	8521	1/1	0.98	0.20	4.43	50,50,50,50	0
36	SR	0	8969	1/1	0.95	0.21	4.40	164,164,164,164	0
34	NA	0	8575	1/1	0.95	0.22	4.39	83,83,83,83	0
34	NA	0	8564	1/1	0.88	0.18	4.10	70,70,70,70	0
34	NA	0	8557	1/1	0.94	0.14	3.78	57,57,57,57	0
36	SR	R	8912	1/1	0.97	0.17	3.62	83,83,83,83	0
32	MG	0	8084	1/1	0.97	0.14	3.07	29,29,29,29	0
32	MG	0	8028	1/1	1.00	0.18	3.03	24,24,24,24	0
34	NA	0	8507	1/1	0.95	0.17	2.97	32,32,32,32	0
32	MG	0	8014	1/1	0.99	0.16	2.93	21,21,21,21	0
32	MG	0	8003	1/1	0.98	0.18	2.91	26,26,26,26	0
32	MG	A	8051	1/1	0.89	0.28	2.58	60,60,60,60	0
34	NA	0	8530	1/1	0.97	0.18	2.47	41,41,41,41	0
34	NA	0	8537	1/1	0.96	0.12	2.34	38,38,38,38	0
32	MG	0	8006	1/1	0.93	0.15	2.28	21,21,21,21	0

Continued on next page...

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
34	NA	0	8527	1/1	0.94	0.16	2.12	47,47,47,47	0
32	MG	0	8004	1/1	0.97	0.18	2.08	25,25,25,25	0
32	MG	0	8045	1/1	1.00	0.12	1.94	35,35,35,35	0
36	SR	0	8944	1/1	0.83	0.12	1.66	175,175,175,175	0
34	NA	0	8515	1/1	0.99	0.20	1.61	35,35,35,35	0
34	NA	0	8504	1/1	0.98	0.17	1.19	31,31,31,31	0
36	SR	0	8992	1/1	0.95	0.14	1.14	133,133,133,133	0
32	MG	0	8008	1/1	0.99	0.13	1.06	24,24,24,24	0
32	MG	0	8062	1/1	0.98	0.17	0.88	44,44,44,44	0
32	MG	0	8088	1/1	0.98	0.15	0.81	32,32,32,32	0
36	SR	0	8926	1/1	0.94	0.11	0.60	122,122,122,122	0
34	NA	0	8520	1/1	0.96	0.12	0.43	40,40,40,40	0
32	MG	0	8021	1/1	0.98	0.11	0.39	32,32,32,32	0
34	NA	0	8534	1/1	0.96	0.23	0.39	64,64,64,64	0
32	MG	B	8042	1/1	0.95	0.12	0.34	44,44,44,44	0
36	SR	3	8932	1/1	0.99	0.14	0.31	74,74,74,74	0
32	MG	0	8025	1/1	0.98	0.13	0.03	27,27,27,27	0
33	K	0	8401	1/1	0.99	0.15	-0.14	93,93,93,93	0
32	MG	0	8001	1/1	0.96	0.13	-0.19	30,30,30,30	0
37	CD	1	8702	1/1	1.00	0.12	-0.20	60,60,60,60	0
34	NA	Q	8540	1/1	0.82	0.11	-0.40	58,58,58,58	0
32	MG	0	8070	1/1	0.99	0.12	-0.43	43,43,43,43	0
36	SR	0	8936	1/1	0.94	0.11	-0.43	91,91,91,91	0
34	NA	M	8539	1/1	0.99	0.10	-0.58	26,26,26,26	0
32	MG	0	8012	1/1	0.97	0.15	-0.62	22,22,22,22	0
34	NA	0	8519	1/1	0.96	0.15	-0.66	39,39,39,39	0
32	MG	0	8050	1/1	0.99	0.13	-0.75	28,28,28,28	0
37	CD	U	8701	1/1	1.00	0.09	-0.98	62,62,62,62	0
32	MG	0	8085	1/1	0.96	0.11	-1.00	80,80,80,80	0
36	SR	F	9005	1/1	0.99	0.07	-1.04	132,132,132,132	0
36	SR	0	8975	1/1	0.82	0.08	-1.07	137,137,137,137	0
36	SR	0	8972	1/1	0.96	0.10	-1.09	127,127,127,127	0
36	SR	0	8947	1/1	0.92	0.13	-1.14	162,162,162,162	0
35	CL	J	8821	1/1	0.97	0.09	-1.15	60,60,60,60	0
36	SR	0	8923	1/1	0.98	0.12	-1.18	87,87,87,87	0
32	MG	K	8054	1/1	0.96	0.12	-1.19	37,37,37,37	0
35	CL	O	8808	1/1	0.91	0.10	-1.27	73,73,73,73	0
36	SR	A	8929	1/1	0.93	0.09	-1.37	130,130,130,130	0
32	MG	0	8010	1/1	0.98	0.14	-1.39	48,48,48,48	0
34	NA	0	8523	1/1	0.97	0.10	-1.42	46,46,46,46	0
34	NA	J	8538	1/1	0.94	0.07	-1.46	43,43,43,43	0
36	SR	0	8943	1/1	0.97	0.08	-1.61	99,99,99,99	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
32	MG	0	8043	1/1	0.99	0.09	-1.65	43,43,43,43	0
35	CL	M	8818	1/1	0.96	0.08	-1.66	44,44,44,44	0
32	MG	0	8058	1/1	0.99	0.08	-1.67	16,16,16,16	0
36	SR	0	8985	1/1	0.88	0.07	-1.73	124,124,124,124	0
32	MG	0	8011	1/1	0.98	0.13	-1.74	23,23,23,23	0
32	MG	0	8002	1/1	0.97	0.12	-1.84	30,30,30,30	0
34	NA	R	8532	1/1	0.97	0.07	-1.85	45,45,45,45	0
36	SR	0	8935	1/1	0.98	0.09	-1.91	80,80,80,80	0
34	NA	0	8533	1/1	0.93	0.09	-1.92	55,55,55,55	0
36	SR	1	8913	1/1	0.98	0.10	-2.06	91,91,91,91	0
37	CD	3	8704	1/1	0.99	0.06	-2.09	76,76,76,76	0
36	SR	A	8930	1/1	0.93	0.05	-2.13	110,110,110,110	0
35	CL	3	8804	1/1	0.96	0.08	-2.16	58,58,58,58	0
35	CL	0	8812	1/1	0.96	0.07	-2.20	45,45,45,45	0
37	CD	Z	8703	1/1	0.99	0.06	-2.33	83,83,83,83	0
36	SR	0	8984	1/1	0.99	0.09	-2.39	114,114,114,114	0
32	MG	T	8057	1/1	0.92	0.08	-2.48	66,66,66,66	0
35	CL	0	8805	1/1	0.95	0.07	-3.44	53,53,53,53	0
32	MG	0	8044	1/1	0.96	0.08	-3.71	45,45,45,45	0
35	CL	B	8819	1/1	0.96	0.10	-3.86	51,51,51,51	0
33	K	0	8402	1/1	0.98	0.08	-4.02	67,67,67,67	0
34	NA	0	8569	1/1	0.95	0.09	-4.25	44,44,44,44	0
32	MG	0	8034	1/1	0.99	0.07	-4.29	38,38,38,38	0
35	CL	0	8815	1/1	0.94	0.07	-4.43	67,67,67,67	0
32	MG	0	8052	1/1	0.99	0.05	-4.59	39,39,39,39	0
32	MG	0	8075	1/1	0.93	0.04	-5.07	39,39,39,39	0
36	SR	0	8910	1/1	0.98	0.06	-5.39	99,99,99,99	0
32	MG	0	8065	1/1	0.97	0.04	-5.46	33,33,33,33	0
35	CL	0	8813	1/1	0.98	0.05	-5.64	46,46,46,46	0
36	SR	0	8970	1/1	0.95	0.02	-5.81	123,123,123,123	0
32	MG	Y	8086	1/1	0.99	0.06	-5.90	35,35,35,35	0
36	SR	0	8949	1/1	0.90	0.07	-6.62	104,104,104,104	0
32	MG	0	8087	1/1	0.99	0.08	-7.92	31,31,31,31	0
32	MG	0	8013	1/1	0.99	0.04	-10.66	21,21,21,21	0
32	MG	0	8069	1/1	0.97	0.20	-	57,57,57,57	0
36	SR	0	8954	1/1	0.97	0.11	-	100,100,100,100	0
36	SR	0	8994	1/1	0.96	0.18	-	192,192,192,192	0
36	SR	0	8993	1/1	0.68	0.08	-	173,173,173,173	0
34	NA	0	8522	1/1	0.95	0.27	-	67,67,67,67	0
32	MG	0	8071	1/1	0.99	0.19	-	50,50,50,50	0
36	SR	0	8956	1/1	0.90	0.08	-	138,138,138,138	0
35	CL	0	8816	1/1	0.99	0.20	-	67,67,67,67	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
32	MG	0	8039	1/1	0.97	0.34	-	67,67,67,67	0
36	SR	0	8958	1/1	0.98	0.10	-	97,97,97,97	0
36	SR	0	8946	1/1	0.99	0.15	-	99,99,99,99	0
36	SR	0	8974	1/1	0.95	0.16	-	158,158,158,158	0
36	SR	0	8948	1/1	0.94	0.11	-	88,88,88,88	0
32	MG	0	8007	1/1	0.96	0.10	-	43,43,43,43	0
36	SR	0	8966	1/1	0.95	0.07	-	100,100,100,100	0
36	SR	0	8998	1/1	0.86	0.12	-	172,172,172,172	0
36	SR	Y	9002	1/1	0.85	0.13	-	188,188,188,188	0
32	MG	0	8038	1/1	0.61	0.09	-	66,66,66,66	0
36	SR	0	8983	1/1	0.94	0.06	-	177,177,177,177	0
34	NA	0	8506	1/1	0.75	0.22	-	63,63,63,63	0
36	SR	0	8965	1/1	0.96	0.08	-	121,121,121,121	0
32	MG	0	8073	1/1	0.96	0.10	-	74,74,74,74	0
32	MG	0	8053	1/1	0.95	0.05	-	38,38,38,38	0
32	MG	0	8060	1/1	0.94	0.10	-	43,43,43,43	0
34	NA	0	8516	1/1	0.89	0.13	-	45,45,45,45	0
32	MG	0	8080	1/1	0.96	0.15	-	66,66,66,66	0
36	SR	0	8999	1/1	0.97	0.06	-	93,93,93,93	0
36	SR	0	8931	1/1	0.93	0.09	-	110,110,110,110	0
32	MG	0	8078	1/1	0.88	0.31	-	76,76,76,76	0
32	MG	0	8030	1/1	0.98	0.36	-	72,72,72,72	0
34	NA	0	8508	1/1	0.85	0.20	-	43,43,43,43	0
36	SR	0	8978	1/1	0.95	0.04	-	119,119,119,119	0
32	MG	0	8049	1/1	0.98	0.22	-	58,58,58,58	0
36	SR	0	8907	1/1	1.00	0.12	-	43,43,43,43	0
36	SR	0	8996	1/1	0.81	0.50	-	200,200,200,200	0
36	SR	0	8981	1/1	0.95	0.12	-	171,171,171,171	0
34	NA	9	8543	1/1	0.97	0.19	-	44,44,44,44	0
32	MG	0	8091	1/1	0.96	0.08	-	51,51,51,51	0
36	SR	9	8980	1/1	0.93	0.09	-	158,158,158,158	0
35	CL	0	8803	1/1	0.95	0.08	-	52,52,52,52	0
34	NA	0	8573	1/1	0.95	0.16	-	61,61,61,61	0
36	SR	0	8906	1/1	0.99	0.19	-	53,53,53,53	0
36	SR	0	8902	1/1	0.99	0.14	-	37,37,37,37	0
34	NA	0	8529	1/1	0.95	0.05	-	39,39,39,39	0
32	MG	0	8066	1/1	0.94	0.29	-	80,80,80,80	0
36	SR	0	8963	1/1	0.95	0.04	-	131,131,131,131	0
32	MG	0	8068	1/1	0.97	0.07	-	52,52,52,52	0
36	SR	0	8990	1/1	0.96	0.16	-	173,173,173,173	0
34	NA	0	8549	1/1	0.85	0.23	-	51,51,51,51	0
36	SR	0	8909	1/1	0.99	0.15	-	86,86,86,86	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
36	SR	0	8921	1/1	0.98	0.12	-	77,77,77,77	0
36	SR	0	8934	1/1	0.93	0.12	-	117,117,117,117	0
32	MG	0	8017	1/1	0.99	0.21	-	23,23,23,23	0
34	NA	0	8524	1/1	0.93	0.19	-	52,52,52,52	0
32	MG	0	8063	1/1	0.87	0.17	-	90,90,90,90	0
32	MG	0	8022	1/1	0.94	0.14	-	31,31,31,31	0
36	SR	0	9001	1/1	0.67	0.18	-	176,176,176,176	0
37	CD	O	8705	1/1	1.00	0.09	-	84,84,84,84	0
32	MG	0	8055	1/1	0.98	0.21	-	30,30,30,30	0
32	MG	0	8064	1/1	0.97	0.11	-	41,41,41,41	0
32	MG	0	8026	1/1	0.98	0.12	-	33,33,33,33	0
35	CL	N	8807	1/1	0.98	0.09	-	71,71,71,71	0
36	SR	0	8941	1/1	0.94	0.15	-	104,104,104,104	0
32	MG	0	8059	1/1	0.80	0.09	-	50,50,50,50	0
32	MG	0	8035	1/1	0.96	0.13	-	43,43,43,43	0
34	NA	0	8566	1/1	0.90	0.35	-	71,71,71,71	0
34	NA	0	8541	1/1	0.96	0.26	-	61,61,61,61	0
34	NA	0	8502	1/1	0.81	0.09	-	51,51,51,51	0
34	NA	0	8545	1/1	0.87	0.17	-	38,38,38,38	0
32	MG	0	8040	1/1	0.99	0.17	-	80,80,80,80	0
35	CL	R	8806	1/1	0.99	0.10	-	47,47,47,47	0
36	SR	0	8953	1/1	0.99	0.19	-	160,160,160,160	0
36	SR	0	8945	1/1	0.96	0.07	-	107,107,107,107	0
32	MG	0	8031	1/1	0.95	0.17	-	57,57,57,57	0
32	MG	0	8019	1/1	0.99	0.15	-	19,19,19,19	0
36	SR	0	8997	1/1	0.94	0.63	-	194,194,194,194	0
34	NA	0	8501	1/1	0.98	0.17	-	33,33,33,33	0
36	SR	0	8982	1/1	0.38	0.71	-	197,197,197,197	0
36	SR	0	8918	1/1	1.00	0.12	-	79,79,79,79	0
34	NA	0	8536	1/1	0.86	0.06	-	47,47,47,47	0
36	SR	0	8989	1/1	0.98	0.07	-	159,159,159,159	0
34	NA	0	8544	1/1	0.96	0.12	-	60,60,60,60	0
32	MG	0	8005	1/1	0.99	0.16	-	31,31,31,31	0
34	NA	0	8550	1/1	0.88	0.22	-	53,53,53,53	0
34	NA	0	8531	1/1	0.95	0.12	-	41,41,41,41	0
36	SR	0	8979	1/1	0.85	0.19	-	198,198,198,198	0
36	SR	0	8955	1/1	0.68	0.12	-	198,198,198,198	0
36	SR	0	8960	1/1	0.94	0.04	-	134,134,134,134	0
32	MG	0	8018	1/1	0.97	0.12	-	27,27,27,27	0
32	MG	0	8081	1/1	0.76	0.15	-	74,74,74,74	0
34	NA	C	8503	1/1	0.94	0.09	-	27,27,27,27	0
34	NA	0	8514	1/1	0.89	0.39	-	48,48,48,48	0

*Continued on next page...*



*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
35	CL	Y	8820	1/1	0.93	0.06	-	40,40,40,40	0
36	SR	0	8928	1/1	0.84	0.08	-	139,139,139,139	0
34	NA	0	8570	1/1	0.89	0.07	-	48,48,48,48	0
36	SR	0	8911	1/1	0.97	0.08	-	75,75,75,75	0
34	NA	0	8511	1/1	0.96	0.12	-	56,56,56,56	0
35	CL	L	8810	1/1	0.96	0.05	-	52,52,52,52	0
34	NA	0	8554	1/1	0.88	0.69	-	69,69,69,69	0
32	MG	0	8079	1/1	0.97	0.16	-	39,39,39,39	0
34	NA	0	8518	1/1	0.92	0.35	-	82,82,82,82	0
36	SR	0	8937	1/1	0.97	0.23	-	102,102,102,102	0
34	NA	S	8510	1/1	0.94	0.06	-	27,27,27,27	0
36	SR	0	8925	1/1	0.99	0.12	-	87,87,87,87	0
34	NA	0	8551	1/1	0.98	0.16	-	38,38,38,38	0
36	SR	0	8915	1/1	0.97	0.09	-	110,110,110,110	0
35	CL	0	8811	1/1	0.98	0.06	-	63,63,63,63	0
32	MG	0	8032	1/1	0.95	0.04	-	44,44,44,44	0
36	SR	0	9006	1/1	0.13	2.35	-	200,200,200,200	0
32	MG	0	8056	1/1	0.92	0.14	-	41,41,41,41	0
36	SR	0	8919	1/1	0.89	0.11	-	178,178,178,178	0
32	MG	0	8067	1/1	0.91	0.27	-	50,50,50,50	0
35	CL	0	8817	1/1	0.98	0.06	-	51,51,51,51	0
36	SR	0	8964	1/1	0.98	0.10	-	124,124,124,124	0
36	SR	0	8933	1/1	0.95	0.13	-	141,141,141,141	0
32	MG	0	8061	1/1	1.00	0.20	-	25,25,25,25	0
36	SR	0	8939	1/1	0.98	0.04	-	145,145,145,145	0
32	MG	0	8072	1/1	0.98	0.18	-	43,43,43,43	0
35	CL	J	8801	1/1	0.94	0.10	-	71,71,71,71	0
36	SR	0	9007	1/1	0.98	0.23	-	191,191,191,191	0
36	SR	B	8950	1/1	0.93	0.15	-	114,114,114,114	0
36	SR	0	8905	1/1	0.98	0.24	-	69,69,69,69	0
36	SR	0	8976	1/1	0.82	0.22	-	194,194,194,194	0
32	MG	0	8048	1/1	0.95	0.17	-	22,22,22,22	0
36	SR	A	8977	1/1	0.89	0.05	-	154,154,154,154	0
36	SR	0	8908	1/1	0.96	0.11	-	83,83,83,83	0
34	NA	0	8561	1/1	0.92	0.78	-	77,77,77,77	0
32	MG	0	8046	1/1	0.95	0.16	-	44,44,44,44	0
36	SR	0	8922	1/1	0.97	0.14	-	155,155,155,155	0
32	MG	0	8090	1/1	0.95	0.17	-	55,55,55,55	0
36	SR	0	8920	1/1	0.91	0.05	-	112,112,112,112	0
32	MG	0	8015	1/1	1.00	0.14	-	31,31,31,31	0
36	SR	0	8967	1/1	0.99	0.02	-	131,131,131,131	0
36	SR	0	8991	1/1	0.81	0.12	-	186,186,186,186	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
36	SR	0	8940	1/1	1.00	0.12	-	78,78,78,78	0
32	MG	0	8093	1/1	0.98	0.05	-	27,27,27,27	0
34	NA	0	8567	1/1	0.80	0.17	-	72,72,72,72	0
36	SR	0	8995	1/1	0.96	0.09	-	136,136,136,136	0
36	SR	0	9008	1/1	0.97	0.12	-	84,84,84,84	0
35	CL	0	8822	1/1	0.97	0.55	-	83,83,83,83	0
36	SR	9	9003	1/1	0.86	0.07	-	171,171,171,171	0
36	SR	0	8901	1/1	0.96	0.07	-	84,84,84,84	0
32	MG	0	8024	1/1	0.95	0.14	-	52,52,52,52	0
36	SR	0	8968	1/1	0.91	0.05	-	161,161,161,161	0
36	SR	1	8952	1/1	1.00	0.12	-	79,79,79,79	0
36	SR	0	8957	1/1	0.82	0.25	-	200,200,200,200	0
32	MG	0	8037	1/1	0.93	0.14	-	59,59,59,59	0
32	MG	0	8089	1/1	0.62	0.07	-	42,42,42,42	0
36	SR	S	8961	1/1	0.88	0.06	-	128,128,128,128	0
36	SR	0	8914	1/1	0.99	0.27	-	121,121,121,121	0
36	SR	0	9004	1/1	0.74	1.12	-	200,200,200,200	0
32	MG	9	8074	1/1	0.96	0.19	-	75,75,75,75	0
35	CL	0	8814	1/1	0.96	0.11	-	50,50,50,50	0
36	SR	0	9000	1/1	0.94	0.06	-	165,165,165,165	0
36	SR	0	8973	1/1	0.95	0.10	-	121,121,121,121	0
36	SR	0	8962	1/1	0.57	0.21	-	155,155,155,155	0
32	MG	0	8023	1/1	1.00	0.14	-	26,26,26,26	0
32	MG	0	8076	1/1	0.95	0.10	-	39,39,39,39	0
35	CL	J	8802	1/1	0.98	0.10	-	66,66,66,66	0
34	NA	0	8505	1/1	0.95	0.72	-	34,34,34,34	0
32	MG	0	8077	1/1	0.96	0.05	-	35,35,35,35	0
36	SR	0	8988	1/1	0.80	0.15	-	162,162,162,162	0
36	SR	0	8942	1/1	0.98	0.07	-	115,115,115,115	0
36	SR	0	8938	1/1	0.93	0.07	-	165,165,165,165	0
36	SR	0	8959	1/1	0.95	0.12	-	159,159,159,159	0
36	SR	0	8927	1/1	0.72	0.08	-	170,170,170,170	0
35	CL	A	8809	1/1	0.97	0.06	-	65,65,65,65	0
32	MG	0	8082	1/1	0.98	0.16	-	73,73,73,73	0
34	NA	0	8548	1/1	0.89	0.11	-	42,42,42,42	0
36	SR	0	8916	1/1	0.99	0.05	-	104,104,104,104	0
32	MG	0	8036	1/1	0.87	0.06	-	46,46,46,46	0
32	MG	0	8033	1/1	0.79	0.06	-	49,49,49,49	0
34	NA	0	8509	1/1	0.75	0.18	-	63,63,63,63	0
34	NA	0	8525	1/1	0.51	0.22	-	83,83,83,83	0
32	MG	0	8083	1/1	0.93	0.09	-	37,37,37,37	0
36	SR	0	8971	1/1	0.84	0.05	-	175,175,175,175	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
36	SR	0	8917	1/1	0.97	0.10	-	111,111,111,111	0
36	SR	0	8924	1/1	0.90	0.17	-	133,133,133,133	0
34	NA	0	8526	1/1	0.92	0.04	-	39,39,39,39	0
32	MG	0	8027	1/1	0.96	0.06	-	31,31,31,31	0
34	NA	0	8574	1/1	0.85	0.38	-	52,52,52,52	0
32	MG	0	8029	1/1	0.98	0.17	-	46,46,46,46	0
36	SR	0	8951	1/1	0.89	0.03	-	144,144,144,144	0
34	NA	0	8571	1/1	0.82	0.09	-	61,61,61,61	0
32	MG	0	8020	1/1	0.99	0.12	-	36,36,36,36	0
34	NA	0	8513	1/1	0.92	0.21	-	42,42,42,42	0
32	MG	0	8092	1/1	0.97	0.08	-	66,66,66,66	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.