



Full wwPDB X-ray Structure Validation Report

Feb 28, 2014 – 04:17 PM GMT

PDB ID : 3CCQ
Title : Structure of Anisomycin resistant 50S Ribosomal Subunit: 23S rRNA mutation A2488U
Authors : Blaha, G.; Gurel, G.
Deposited on : 2008-02-26
Resolution : 2.90 Å(reported)

This is a full wwPDB validation report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

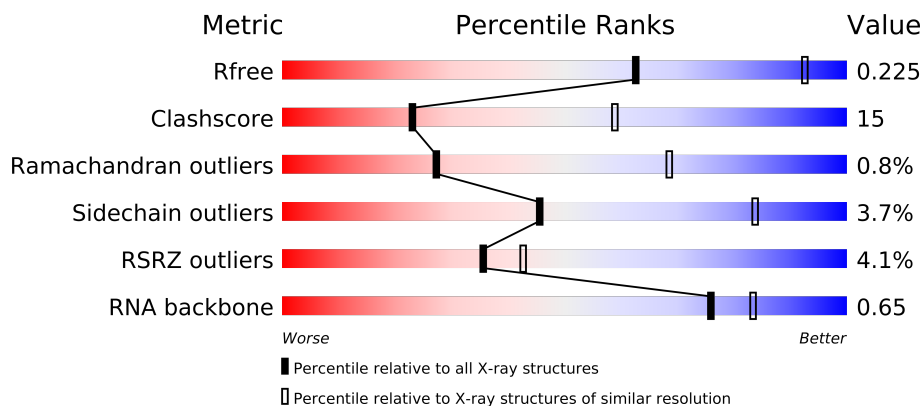
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

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}	66092	1053 (2.90-2.90)
Clashscore	79885	1326 (2.90-2.90)
Ramachandran outliers	78287	1290 (2.90-2.90)
Sidechain outliers	78261	1292 (2.90-2.90)
RSRZ outliers	66119	1054 (2.90-2.90)
RNA backbone	1838	1055 (3.40-2.40)

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 ≥ 3 , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	240	
2	B	338	
3	C	246	
4	D	177	
5	E	178	
6	F	120	
7	G	348	
8	H	177	
9	I	162	
10	J	145	
11	K	132	

Continued on next page...

Continued from previous page...

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

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
32	MG	0	8003	-	X
32	MG	0	8009	-	X
32	MG	0	8014	-	X
32	MG	0	8017	-	X
32	MG	0	8018	-	X
32	MG	0	8022	-	X
32	MG	0	8029	-	X
32	MG	0	8030	-	X
32	MG	0	8033	-	X
32	MG	0	8039	-	X
32	MG	0	8047	-	X
32	MG	0	8048	-	X
32	MG	0	8049	-	X
32	MG	0	8061	-	X
32	MG	0	8063	-	X
32	MG	0	8066	-	X
32	MG	0	8069	-	X

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Geometry	Electron density
32	MG	0	8071	-	X
32	MG	0	8072	-	X
32	MG	0	8073	-	X
32	MG	0	8078	-	X
32	MG	0	8081	-	X
32	MG	0	8082	-	X
32	MG	0	8085	-	X
32	MG	0	8089	-	X
32	MG	A	8051	-	X
33	K	0	8401	-	X
33	K	0	8402	-	X
34	NA	0	8505	-	X
34	NA	0	8509	-	X
34	NA	0	8511	-	X
34	NA	0	8513	-	X
34	NA	0	8516	-	X
34	NA	0	8518	-	X
34	NA	0	8519	-	X
34	NA	0	8521	-	X
34	NA	0	8522	-	X
34	NA	0	8524	-	X
34	NA	0	8525	-	X
34	NA	0	8527	-	X
34	NA	0	8528	-	X
34	NA	0	8530	-	X
34	NA	0	8534	-	X
34	NA	0	8535	-	X
34	NA	0	8536	-	X
34	NA	0	8541	-	X
34	NA	0	8542	-	X
34	NA	0	8544	-	X
34	NA	0	8545	-	X
34	NA	0	8546	-	X
34	NA	0	8547	-	X
34	NA	0	8548	-	X
34	NA	0	8549	-	X
34	NA	0	8550	-	X
34	NA	0	8551	-	X
34	NA	0	8553	-	X
34	NA	0	8554	-	X
34	NA	0	8555	-	X
34	NA	0	8556	-	X

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Geometry	Electron density
34	NA	0	8559	-	X
34	NA	0	8560	-	X
34	NA	0	8561	-	X
34	NA	0	8562	-	X
34	NA	0	8563	-	X
34	NA	0	8564	-	X
34	NA	0	8565	-	X
34	NA	0	8566	-	X
34	NA	0	8567	-	X
34	NA	0	8568	-	X
34	NA	0	8571	-	X
34	NA	0	8573	-	X
34	NA	0	8574	-	X
34	NA	9	8572	-	X
34	NA	B	8552	-	X
34	NA	R	8575	-	X
34	NA	S	8510	-	X
35	CL	0	8822	-	X
35	CL	B	8819	-	X
36	SR	0	8903	-	X
36	SR	0	8905	-	X
36	SR	0	8906	-	X
36	SR	0	8909	-	X
36	SR	0	8914	-	X
36	SR	0	8921	-	X
36	SR	0	8922	-	X
36	SR	0	8926	-	X
36	SR	0	8934	-	X
36	SR	0	8937	-	X
36	SR	0	8947	-	X
36	SR	0	8949	-	X
36	SR	0	8959	-	X
36	SR	0	8962	-	X
36	SR	0	8963	-	X
36	SR	0	8976	-	X
36	SR	0	8981	-	X
36	SR	0	8982	-	X
36	SR	0	8983	-	X
36	SR	0	8986	-	X
36	SR	0	8992	-	X
36	SR	0	8994	-	X
36	SR	0	8996	-	X

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Geometry	Electron density
36	SR	0	8997	-	X
36	SR	0	9002	-	X
36	SR	0	9004	-	X
36	SR	0	9006	-	X
36	SR	0	9007	-	X
36	SR	9	8980	-	X
36	SR	B	8987	-	X

2 Entry composition

There are 38 unique types of molecules in this entry. The entry contains 99120 atoms, of which 0 are hydrogen and 0 are deuterium.

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
			59018	26348	10870	19055	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	65	Total Na 65 65	0	0
34	J	1	Total Na 1 1	0	0
34	Q	1	Total Na 1 1	0	0
34	B	1	Total Na 1 1	0	0
34	C	1	Total Na 1 1	0	0
34	R	2	Total Na 2 2	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	9	Total Cl 9 9	0	0
35	J	3	Total Cl 3 3	0	0
35	Q	1	Total Cl 1 1	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

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
35	Y	1	Total 1	Cl 1	0	0
35	L	1	Total 1	Cl 1	0	0
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	93	Total 93	Sr 93	0	0
36	1	2	Total 2	Sr 2	0	0
36	B	2	Total 2	Sr 2	0	0
36	3	2	Total 2	Sr 2	0	0
36	A	3	Total 3	Sr 3	0	0
36	R	1	Total 1	Sr 1	0	0
36	9	3	Total 3	Sr 3	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

Continued on next page...

Continued from previous page...

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

- Molecule 38 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
38	0	5950	Total	O	0	0
			5950	5950		
38	9	148	Total	O	0	0
			148	148		
38	A	112	Total	O	0	0
			112	112		
38	B	142	Total	O	0	0
			142	142		
38	C	168	Total	O	0	0
			168	168		
38	D	45	Total	O	0	0
			45	45		
38	E	42	Total	O	0	0
			42	42		
38	F	26	Total	O	0	0
			26	26		
38	G	17	Total	O	0	0
			17	17		
38	H	65	Total	O	0	0
			65	65		
38	I	5	Total	O	0	0
			5	5		
38	J	56	Total	O	0	0
			56	56		
38	K	60	Total	O	0	0
			60	60		
38	L	82	Total	O	0	0
			82	82		
38	M	123	Total	O	0	0
			123	123		
38	N	59	Total	O	0	0
			59	59		
38	O	47	Total	O	0	0
			47	47		
38	P	59	Total	O	0	0
			59	59		

Continued on next page...

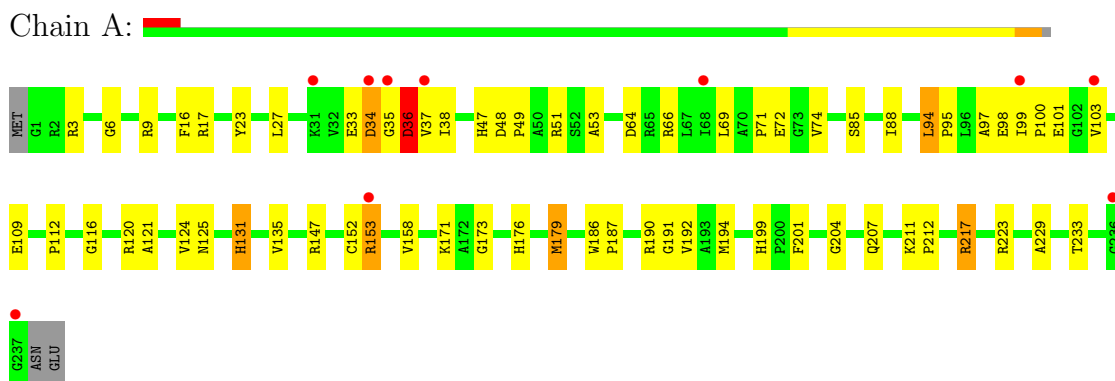
Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
38	Q	47	Total 47	O 47	0	0
38	R	76	Total 76	O 76	0	0
38	S	33	Total 33	O 33	0	0
38	T	36	Total 36	O 36	0	0
38	U	26	Total 26	O 26	0	0
38	V	12	Total 12	O 12	0	0
38	W	66	Total 66	O 66	0	0
38	X	28	Total 28	O 28	0	0
38	Y	97	Total 97	O 97	0	0
38	Z	31	Total 31	O 31	0	0
38	1	54	Total 54	O 54	0	0
38	2	43	Total 43	O 43	0	0
38	3	68	Total 68	O 68	0	0

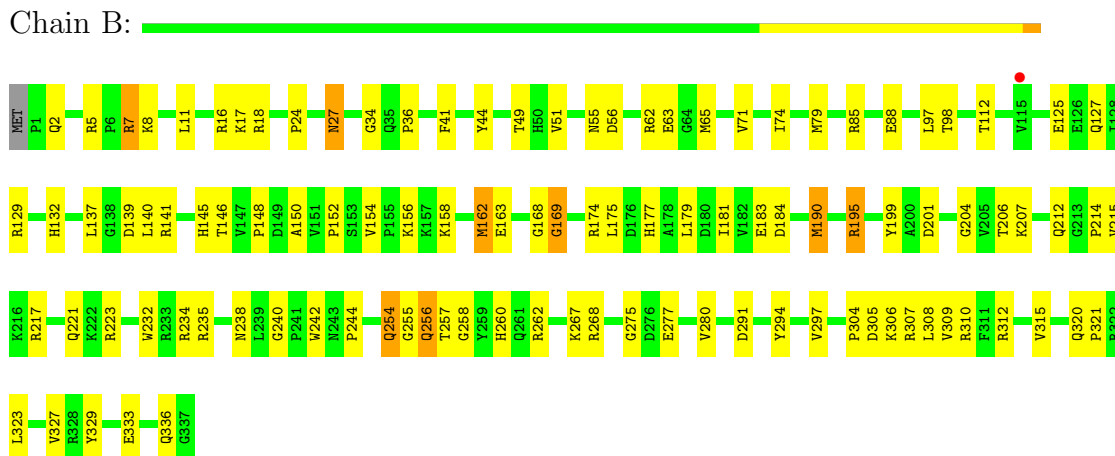
3 Residue-property plots

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.

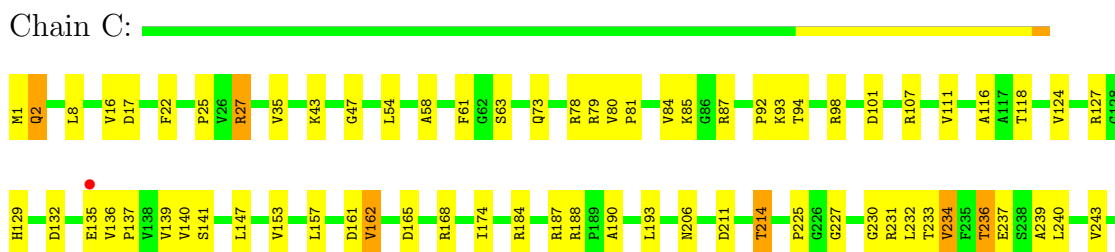
- Molecule 1: 50S ribosomal protein L2P



- Molecule 2: 50S ribosomal protein L3P



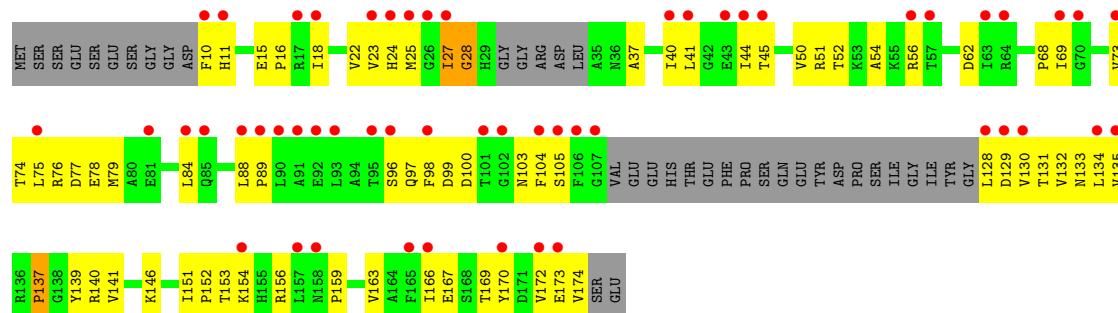
- Molecule 3: 50S ribosomal protein L4P



R246

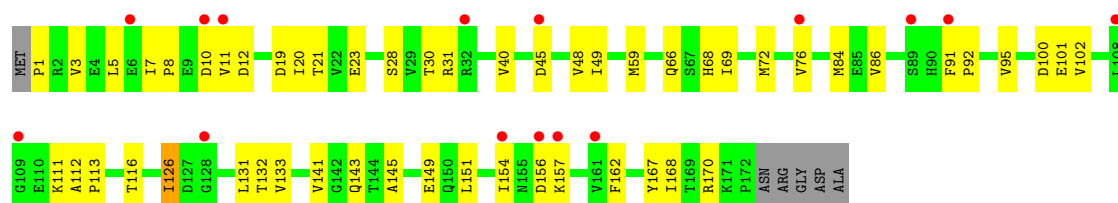
- Molecule 4: 50S ribosomal protein L5P

Chain D:



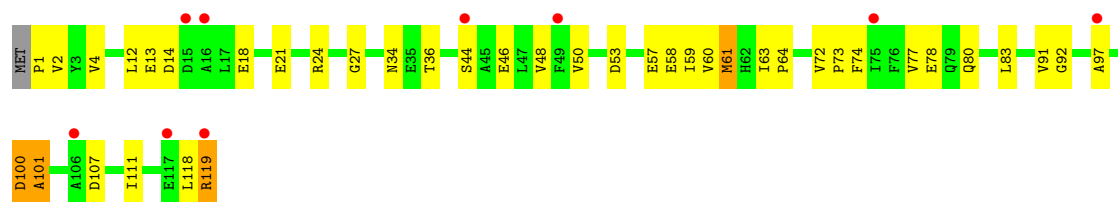
- Molecule 5: 50S ribosomal protein L6P

Chain E:



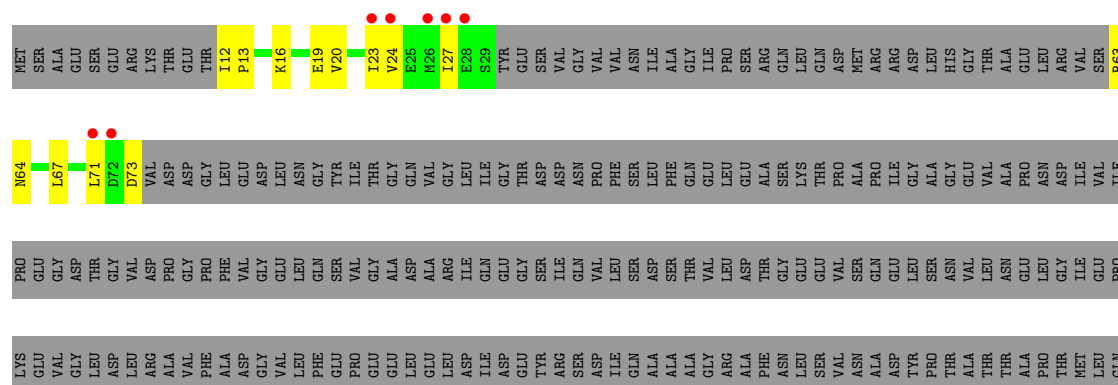
- Molecule 6: 50S ribosomal protein L7Ae

Chain F:

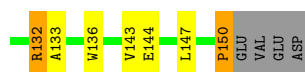


- Molecule 7: 50S ribosomal protein L10E

Chain G:







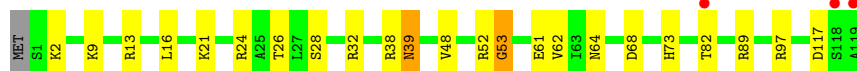
- Molecule 19: 50S ribosomal protein L23P

Chain S:



- Molecule 20: 50S ribosomal protein L24P

Chain T:



- Molecule 21: 50S ribosomal protein L24e

Chain U:



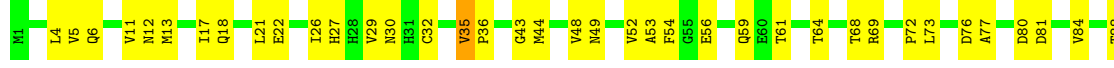
- Molecule 22: 50S ribosomal protein L29P

Chain V:



- Molecule 23: 50S ribosomal protein L30P

Chain W:



- Molecule 24: 50S ribosomal protein L31e

Chain X:



- Molecule 25: 50S ribosomal protein L32e

Chain Y:

MET ALA ASP ASN GLU GLU ASP VAL GLU ALA GLU TYR THR LEU THR ASP ILE SER GLY VAL GLY PRO SER LYS ALA GLU SER LEU ARG GLU ALA GLY PHE SER VAL ASP VAL ARG GLY ALA ASP GLN SER ALA LEU ALA ASP VAL SER GLY ILE GLY ASN LEU

ALA ALA ARG ILE LYS ALA ASP VAL GLY ASN GLU VAL GLU SER THR GLU THR ALA GLY VAL GLN GLY THR GLY GLY GLY GLY VAL T995 A99 P107 R115 K125 P126 Q127 F128 N129 R130 Q131 D132 H133 H134 T141 S142 W143 R144 S151

R154 T163 R169 S170 V174 R175 G176 K177 G181 F182 R186 V187 H188 H189 D192 T200 E201 A202 V203 R204 R212 R216 I217 E218 E219 E220 Y233 Y234 Y236 V236 VAL SER GLU

- Molecule 26: 50S ribosomal protein L37Ae

Chain Z:

MET SER PRO ARG ALA ARG GLU PRO ASN LEU GLY LEU LEU TRP PRO LEU GLY GLN THR THR MET ALA SER LYS SER GLY LYS THR GLY S94 S95 F38 G39 A40 G43 R44 V45 S46 R47 R48 R49 V50 E54 S55 E56 M57 N58 E59 D60 H61 C66 G67

E68 D69 R70 V71 D72 R73 D74 G75 G76 G77 I78 C81 S82 Y83 C84 D85 G90 S106 ILE ARG ALA LEU SER GLU ASP GLU

- Molecule 27: 50S ribosomal protein L37e

Chain 1:

MET T1 Q8 G9 K10 K11 K12 H16 R20 R21 R22 C22 K25 H28 K31 K32 C37 G38 F39 S42 E56

- Molecule 28: 50S ribosomal protein L39e

Chain 2:

MET G1 K2 K5 K8 K9 L11 M18 P22 V25 K28 R31 K35 K38 R39 R40 H41 R42 R43 R44 R45 T47 D48 E49

- Molecule 29: 50S ribosomal protein L44E

Chain 3:

M1 Q2 M3 P4 N8 C11 N15 H20 V25 G28 R29 Q30 N43 K60 P61 K68 Y69 R70 C71 G72 E73 A77 W83 F90 Q91 E92

- Molecule 30: 23S RIBOSOMAL RNA

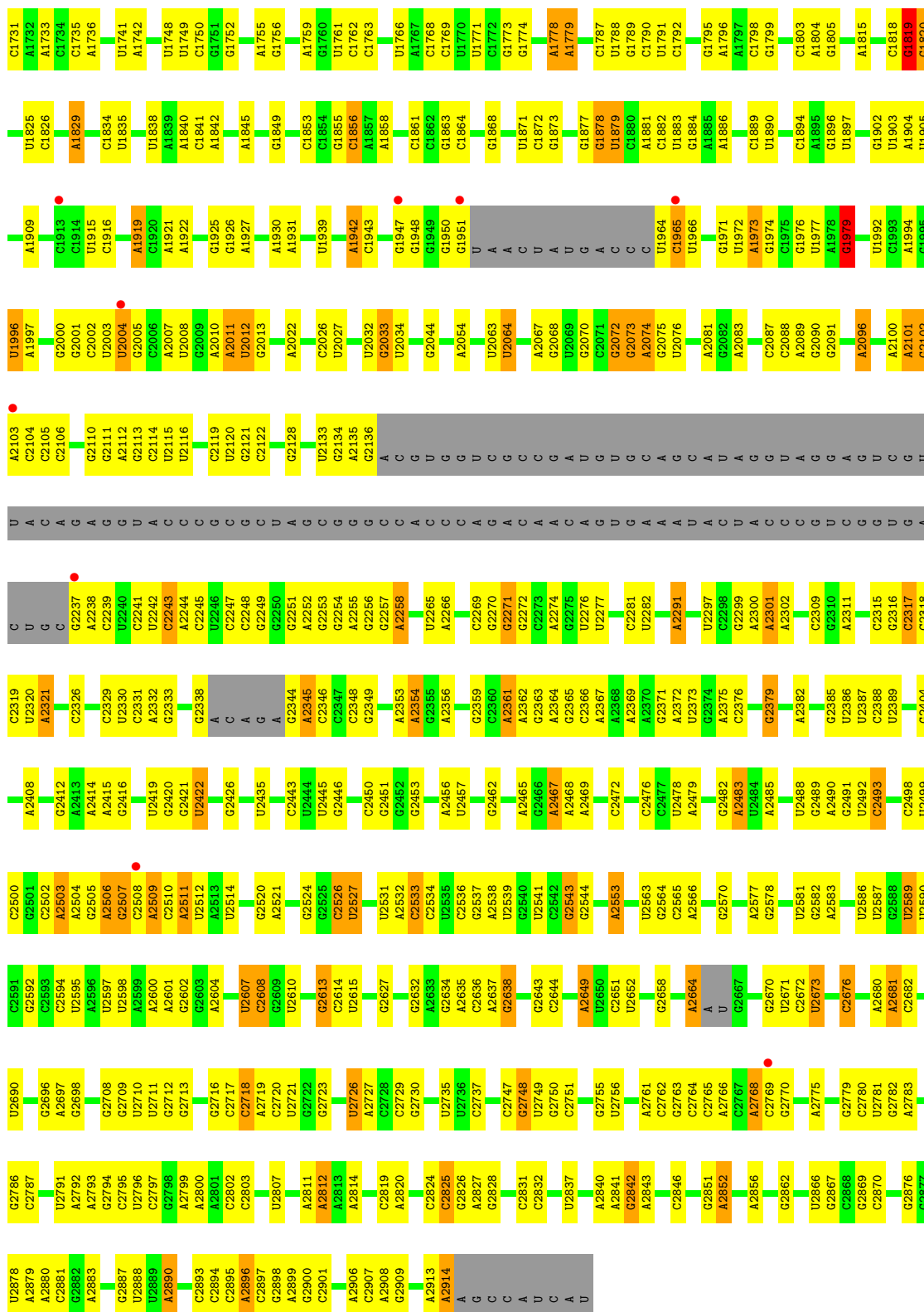
Chain 0:

G U G G C C A U10 A11 U12 G13 G17 C18 G23 G24 A25 U26 U27 C31 A37 G38 G39 G47 A48 G51 A52 G56 A60 G61 G62 U63 G64 G65 G66 A67 U68 A69 A70 G71 G74 U75 G81 G85 A86 C87 G88 G89

A90 G91 G92 C93 A98 A99 C100 G105 A111 U107 U108 G111 G112 A113 A114 U115 A119 A120 U121 C122 U123 C124 U125 C U128 A129 C130 A131 C136 U137 G138 C139 G140 C141 A151 A152 C153 C154 C155 U68 A69 A70 G71 G74 U75 G81 G85 A86 C87 G88 G89

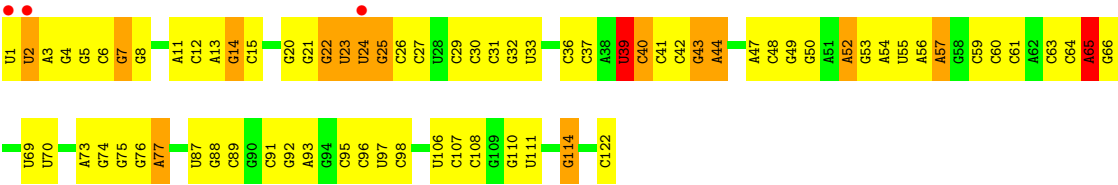
U172 A177 U178 G182 G185 A186 A189 G190 A191 A192 G196 A198 U202 G203 A204 U205 A212 G213 U214 G219 G220 G221 A222 G223 U224 C228 G229 A232 G237 C238 C239 C240 A241 G249 G250 U253 C254 A255 C256 G257 A151 A152 C153 C154 C155 U68 A69 A70 G71 G74 U75 G81 G85 A86 C87 G88 G89





• Molecule 31: 5S RIBOSOMAL RNA

Chain 9:



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	212.33Å 299.62Å 575.24Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.90 85.65 – 2.41	Depositor EDS
% Data completeness (in resolution range)	98.1 (30.00-2.90) 98.2 (85.65-2.41)	Depositor EDS
R_{merge}	0.17	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.00 (at 2.40Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.186 , 0.233 0.184 , 0.225	Depositor DCC
R_{free} test set	3844 reflections (0.99%)	DCC
Wilson B-factor (Å ²)	61.2	Xtriage
Anisotropy	0.153	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 49.6	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	1 of 667142 reflections (0.000%)	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	99120	wwPDB-VP
Average B, all atoms (Å ²)	60.0	wwPDB-VP

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

¹Intensities estimated from amplitudes.

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	0.33	0/1786	0.64	0/2408
2	B	0.34	0/2690	0.65	0/3652
3	C	0.36	0/1885	0.62	0/2552
4	D	0.32	0/1111	0.56	1/1498 (0.1%)
5	E	0.33	0/1382	0.57	0/1880
6	F	0.35	0/901	0.57	0/1224
7	G	0.33	0/241	0.51	0/324
8	H	0.33	0/1302	0.63	0/1743
9	I	0.30	0/526	0.50	0/716
10	J	0.36	0/1136	0.61	0/1530
11	K	0.34	0/1004	0.66	0/1351
12	L	0.35	0/1130	0.64	0/1509
13	M	0.36	0/1582	0.61	0/2116
14	N	0.30	0/1474	0.61	0/1999
15	O	0.35	0/874	0.59	0/1181
16	P	0.33	0/1147	0.53	0/1528
17	Q	0.34	0/749	0.65	0/1005
18	R	1.26	7/1172 (0.6%)	1.09	6/1578 (0.4%)
19	S	0.33	0/648	0.54	0/875
20	T	0.32	0/958	0.64	0/1289
21	U	0.32	0/417	0.57	0/562
22	V	0.32	0/502	0.54	0/675
23	W	0.36	0/1219	0.63	0/1655
24	X	0.35	0/664	0.60	0/895
25	Y	0.37	0/1146	0.62	0/1536
26	Z	0.36	0/584	0.63	0/781
27	1	0.39	0/438	0.62	0/578
28	2	0.34	0/401	0.58	0/529
29	3	0.37	0/771	0.57	0/1024
30	0	0.39	0/65954	0.68	9/102862 (0.0%)
31	9	0.33	0/2904	0.68	1/4526 (0.0%)
All	All	0.40	7/98698 (0.0%)	0.67	17/147581 (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	32
31	9	0	3
All	All	1	36

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	R	150	PRO	CB-CG	27.45	2.87	1.50
18	R	150	PRO	CA-C	-18.11	1.16	1.52
18	R	150	PRO	CG-CD	13.90	1.96	1.50
18	R	150	PRO	C-O	11.92	1.47	1.23
18	R	150	PRO	N-CA	11.35	1.66	1.47
18	R	150	PRO	N-CD	10.74	1.62	1.47
18	R	150	PRO	CA-CB	7.56	1.68	1.53

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	R	150	PRO	CB-CA-C	-22.47	55.81	112.00
18	R	150	PRO	N-CA-C	-19.38	61.71	112.10
18	R	150	PRO	CA-N-CD	12.28	128.89	111.70
18	R	150	PRO	N-CA-CB	10.98	116.47	103.30
18	R	150	PRO	CA-C-O	-8.52	99.75	120.20
31	9	39	U	N1-C1'-C2'	6.32	122.22	114.00
18	R	150	PRO	CA-CB-CG	-6.13	92.34	104.00
30	0	1592	G	N9-C1'-C2'	6.12	121.95	114.00
30	0	1504	A	C1'-O4'-C4'	-5.86	105.21	109.90
30	0	1504	A	N9-C1'-C2'	5.70	121.41	114.00
30	0	871	G	C5'-C4'-O4'	-5.36	102.67	109.10
30	0	1120	U	C5'-C4'-C3'	-5.35	107.45	116.00
30	0	841	A	C1'-O4'-C4'	-5.30	105.66	109.90
30	0	2726	U	N1-C1'-C2'	5.24	120.81	114.00
30	0	1819	G	C5'-C4'-C3'	5.05	124.07	116.00
30	0	2301	A	N9-C1'-C2'	5.01	120.52	114.00
4	D	170	TYR	N-CA-C	5.01	124.53	111.00

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
18	R	150	PRO	CA

All (36) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
30	0	1078	A	Sidechain
30	0	1080	C	Sidechain
30	0	1309	U	Sidechain
30	0	1327	G	Sidechain
30	0	1417	G	Sidechain
30	0	1592	G	Sidechain
30	0	1684	A	Sidechain
30	0	1829	A	Sidechain
30	0	1863	G	Sidechain
30	0	1877	G	Sidechain
30	0	1878	G	Sidechain
30	0	1979	G	Sidechain
30	0	202	U	Sidechain
30	0	205	U	Sidechain
30	0	221	G	Sidechain
30	0	2492	U	Sidechain
30	0	2493	C	Sidechain
30	0	2503	A	Sidechain
30	0	2506	A	Sidechain
30	0	2543	G	Sidechain
30	0	2607	U	Sidechain
30	0	2632	G	Sidechain
30	0	2673	U	Sidechain
30	0	2842	G	Sidechain
30	0	396	U	Sidechain
30	0	470	U	Sidechain
30	0	48	A	Sidechain
30	0	482	G	Sidechain
30	0	518	G	Sidechain
30	0	619	U	Sidechain
30	0	817	G	Sidechain
30	0	818	A	Sidechain
31	9	39	U	Sidechain
31	9	65	A	Sidechain
31	9	87	U	Sidechain
23	W	90	TYR	Sidechain

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1753	0	1766	66	0
2	B	2625	0	2533	94	0
3	C	1860	0	1813	53	0
4	D	1094	0	1085	52	0
5	E	1357	0	1266	36	0
6	F	890	0	843	30	0
7	G	240	0	231	11	0
8	H	1282	0	1292	41	0
9	I	519	0	500	21	0
10	J	1120	0	1098	38	0
11	K	994	0	1027	39	0
12	L	1118	0	1076	33	0
13	M	1558	0	1573	59	0
14	N	1445	0	1401	54	0
15	O	865	0	873	18	0
16	P	1136	0	1123	30	0
17	Q	735	0	729	26	0
18	R	1149	0	1122	32	0
19	S	641	0	605	10	0
20	T	950	0	924	22	0
21	U	410	0	364	17	0
22	V	499	0	511	17	0
23	W	1196	0	1137	66	0
24	X	654	0	653	22	0
25	Y	1130	0	1133	33	0
26	Z	573	0	531	21	0
27	1	431	0	426	21	0
28	2	396	0	413	21	0
29	3	755	0	728	17	0
30	0	59018	0	29809	1329	0
31	9	2599	0	1325	97	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

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
32	K	1	0	0	0	0
32	T	1	0	0	0	0
32	Y	1	0	0	0	0
33	0	2	0	0	0	0
34	0	65	0	0	0	0
34	9	2	0	0	0	0
34	B	1	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	2	0	0	0	0
34	S	1	0	0	0	0
35	0	9	0	0	3	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	1	0
35	N	1	0	0	1	0
35	O	1	0	0	0	0
35	Q	1	0	0	0	0
35	R	1	0	0	0	0
35	Y	1	0	0	0	0
36	0	93	0	0	0	0
36	1	2	0	0	0	0
36	3	2	0	0	0	0
36	9	3	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
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	5950	0	0	203	0
38	1	54	0	0	3	0
38	2	43	0	0	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
38	3	68	0	0	6	0
38	9	148	0	0	9	0
38	A	112	0	0	5	0
38	B	142	0	0	14	0
38	C	168	0	0	13	0
38	D	45	0	0	4	0
38	E	42	0	0	4	0
38	F	26	0	0	1	0
38	G	17	0	0	1	0
38	H	65	0	0	5	0
38	I	5	0	0	0	0
38	J	56	0	0	2	0
38	K	60	0	0	5	0
38	L	82	0	0	8	0
38	M	123	0	0	2	0
38	N	59	0	0	3	0
38	O	47	0	0	4	0
38	P	59	0	0	2	0
38	Q	47	0	0	2	0
38	R	76	0	0	1	0
38	S	33	0	0	0	0
38	T	36	0	0	4	0
38	U	26	0	0	2	0
38	V	12	0	0	1	0
38	W	66	0	0	6	0
38	X	28	0	0	3	0
38	Y	97	0	0	7	0
38	Z	31	0	0	4	0
All	All	99120	0	59910	2191	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 15.

All (2191) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
18:R:150:PRO:CG	18:R:150:PRO:CD	1.96	1.44
30:0:871:G:C8	30:0:871:G:H5'	1.75	1.21
14:N:37:ARG:NH1	31:9:6:C:H5''	1.62	1.12
31:9:56:A:H2'	31:9:57:A:H5''	1.21	1.11
30:0:1160:G:C5'	30:0:1161:A:H5'	1.79	1.11
30:0:1160:G:H5'	30:0:1161:A:C5'	1.83	1.09
30:0:871:G:H8	30:0:871:G:H5'	1.00	1.08

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
30:0:545:G:H8	30:0:545:G:H5'	1.12	1.08
18:R:150:PRO:CG	18:R:150:PRO:C	2.22	1.07
30:0:1474:C:H6	30:0:1474:C:H5'	1.19	1.07
30:0:1559:A:H1'	38:0:5888:HOH:O	1.54	1.07
13:M:171:ARG:HD3	30:0:156:C:H5''	1.38	1.04
30:0:69:A:H5'	30:0:69:A:C8	1.93	1.03
10:J:82:THR:HG23	30:0:1242:A:H5'	1.38	1.02
30:0:1474:C:C6	30:0:1474:C:H5'	1.96	1.01
4:D:154:LYS:HD2	4:D:154:LYS:H	1.26	1.01
30:0:1666:C:O2'	30:0:1667:A:H5''	1.62	0.99
30:0:2717:C:C2'	30:0:2718:C:H5''	1.93	0.99
31:9:76:G:H3'	31:9:77:A:H5''	1.41	0.98
30:0:69:A:H5'	30:0:69:A:H8	1.28	0.97
30:0:871:G:H8	30:0:871:G:C5'	1.78	0.96
30:0:1205:U:H2'	30:0:1206:U:C5'	1.96	0.96
30:0:1116:U:O2'	30:0:1118:A:H2	1.47	0.96
30:0:2717:C:H2'	30:0:2718:C:H5''	1.45	0.96
30:0:2812:A:H2	30:0:2814:A:H62	1.02	0.95
30:0:1603:A:H5'	30:0:1605:G:O4'	1.66	0.95
30:0:545:G:C8	30:0:545:G:H5'	2.00	0.95
30:0:870:G:H2'	30:0:871:G:H5''	1.47	0.95
30:0:1165:G:H21	30:0:1173:A:H5''	1.30	0.95
15:O:3:THR:HG22	30:0:656:G:H5'	1.45	0.95
30:0:877:G:H5'	30:0:878:G:OP1	1.67	0.94
30:0:2291:A:C8	30:0:2309:C:H5'	2.03	0.94
30:0:2316:G:H5''	38:0:6122:HOH:O	1.66	0.94
30:0:1666:C:C2'	30:0:1667:A:H5''	1.97	0.93
30:0:542:A:H5'	30:0:542:A:H8	1.30	0.93
3:C:236:THR:HG22	3:C:239:ALA:H	1.31	0.92
30:0:1206:U:H5'	30:0:1206:U:H6	1.34	0.92
30:0:2506:A:HO2'	30:0:2507:G:H8	1.10	0.92
30:0:381:G:H5''	38:0:4327:HOH:O	1.68	0.92
30:0:2502:C:C2'	30:0:2503:A:H5'	2.00	0.92
11:K:10:GLN:H	11:K:10:GLN:HE21	0.97	0.92
30:0:182:G:H5'	38:0:5177:HOH:O	1.68	0.92
16:P:115:SER:H	16:P:118:GLN:HE21	0.99	0.92
30:0:2502:C:H2'	30:0:2503:A:H5'	1.50	0.91
31:9:56:A:C2'	31:9:57:A:H5''	2.00	0.91
30:0:1160:G:H5'	30:0:1161:A:H5'	0.94	0.91
13:M:99:ARG:HD2	13:M:167:GLY:HA2	1.51	0.91
30:0:2908:A:H2'	30:0:2909:G:O4'	1.69	0.90
30:0:1187:U:HO2'	30:0:1189:A:H2	1.11	0.90

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
30:0:2526:C:H5'	30:0:2526:C:H6	1.36	0.90
10:J:52:GLN:NE2	30:0:1119:G:H2'	1.85	0.90
30:0:1835:U:H5	30:0:1840:A:N7	1.70	0.90
2:B:221:GLN:HE22	11:K:42:ASN:HD22	1.17	0.90
30:0:2004:U:H4'	38:0:5326:HOH:O	1.70	0.90
30:0:1701:A:H4'	30:0:1702:U:H5''	1.51	0.89
30:0:1184:C:H1'	38:0:7505:HOH:O	1.70	0.89
6:F:91:VAL:HG12	6:F:92:GLY:H	1.34	0.89
30:0:2526:C:H5'	30:0:2526:C:C6	2.07	0.89
31:9:29:C:H2'	31:9:30:C:H5'	1.55	0.89
30:0:506:G:H22	30:0:509:A:C5'	1.86	0.89
30:0:282:C:H1'	30:0:368:C:N4	1.86	0.89
26:Z:70:ARG:HD2	26:Z:83:TYR:HB2	1.55	0.88
30:0:1189:A:H1'	30:0:1209:C:O4'	1.74	0.88
38:B:9099:HOH:O	30:0:2672:C:H1'	1.72	0.88
30:0:541:C:H2'	30:0:542:A:H5''	1.56	0.88
30:0:541:C:C2'	30:0:542:A:H5''	2.05	0.87
2:B:238:ASN:HD22	2:B:240:GLY:H	1.20	0.87
30:0:31:C:H2'	38:0:7724:HOH:O	1.73	0.87
30:0:1372:A:H3'	38:0:7228:HOH:O	1.74	0.87
30:0:2769:C:C2'	30:0:2770:G:H5'	2.05	0.87
30:0:2111:G:H1'	38:0:9054:HOH:O	1.75	0.87
30:0:214:U:H5'	38:0:6171:HOH:O	1.74	0.86
30:0:1205:U:H2'	30:0:1206:U:H5''	1.57	0.86
30:0:1183:C:H2'	38:0:6275:HOH:O	1.76	0.86
30:0:1165:G:N2	30:0:1173:A:H5''	1.89	0.86
31:9:14:G:H5'	31:9:14:G:H8	1.41	0.86
2:B:162:MET:HE3	2:B:308:LEU:HD21	1.56	0.86
30:0:2586:U:H3	30:0:2592:G:H22	1.16	0.85
2:B:36:PRO:HA	2:B:168:GLY:HA3	1.59	0.85
24:X:37:LEU:HD13	24:X:85:VAL:HG21	1.57	0.85
30:0:1165:G:H1'	30:0:1174:A:H1'	1.58	0.84
30:0:506:G:H22	30:0:509:A:H5'	1.42	0.84
15:O:3:THR:CG2	30:0:656:G:H5'	2.07	0.84
30:0:2010:A:H2'	38:0:5984:HOH:O	1.77	0.84
14:N:83:LEU:HD13	14:N:175:LEU:HD23	1.58	0.83
13:M:95:LYS:HE2	30:0:157:G:H4'	1.59	0.83
3:C:127:ARG:NH2	3:C:225:PRO:HG2	1.94	0.83
11:K:39:GLY:HA2	38:0:5241:HOH:O	1.79	0.83
30:0:1667:A:H8	30:0:1667:A:H5'	1.44	0.82
30:0:1118:A:H3'	30:0:1118:A:C8	2.13	0.82
23:W:137:GLN:HE21	23:W:141:HIS:HE1	1.24	0.82

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
30:0:2073:G:H5''	38:0:3833:HOH:O	1.80	0.81
9:I:111:LEU:HD23	30:0:1163:G:H4'	1.60	0.81
30:0:1205:U:H2'	30:0:1206:U:H5'	1.62	0.81
8:H:59:GLN:NE2	8:H:129:ARG:HE	1.78	0.81
30:0:1118:A:H3'	30:0:1118:A:H8	1.46	0.80
10:J:52:GLN:HE22	30:0:1119:G:H2'	1.46	0.80
30:0:559:U:H5'	30:0:559:U:H6	1.46	0.80
30:0:1666:C:H2'	30:0:1667:A:C5'	2.12	0.80
30:0:871:G:C8	30:0:871:G:C5'	2.57	0.79
30:0:1201:C:H2'	30:0:1202:A:H5'	1.65	0.79
30:0:282:C:O2'	30:0:283:U:H5'	1.81	0.79
30:0:2769:C:H2'	30:0:2770:G:H5'	1.62	0.79
30:0:2766:A:H5'	38:0:9567:HOH:O	1.81	0.79
2:B:212:GLN:HB2	2:B:257:THR:HG21	1.63	0.79
30:0:1377:C:H6	30:0:1377:C:H5'	1.48	0.79
30:0:1300:G:H1'	38:0:4692:HOH:O	1.81	0.78
30:0:1119:G:N2	30:0:1246:A:C2	2.51	0.78
3:C:139:VAL:HG13	38:C:8646:HOH:O	1.83	0.78
2:B:74:ILE:HD13	2:B:309:VAL:HG21	1.64	0.78
30:0:2748:G:H5'	38:0:7581:HOH:O	1.83	0.78
30:0:10:U:H6	30:0:10:U:H3'	1.49	0.78
30:0:1942:A:H5'	38:0:7387:HOH:O	1.82	0.78
11:K:10:GLN:H	11:K:10:GLN:NE2	1.79	0.78
23:W:4:LEU:HD23	23:W:54:PHE:HB3	1.65	0.78
20:T:9:LYS:HE3	20:T:13:ARG:NH1	1.99	0.78
30:0:308:U:H5'	30:0:309:C:OP1	1.84	0.77
30:0:2103:A:H62	30:0:2538:A:H8	1.32	0.77
30:0:541:C:H2'	30:0:542:A:C5'	2.14	0.77
30:0:396:U:H1'	38:0:7666:HOH:O	1.83	0.77
23:W:88:THR:HB	38:W:6679:HOH:O	1.84	0.77
16:P:115:SER:H	16:P:118:GLN:NE2	1.81	0.77
30:0:2491:G:H1'	38:0:6907:HOH:O	1.86	0.76
26:Z:60:ASP:HB3	26:Z:69:ASP:HB3	1.68	0.76
30:0:1474:C:C5'	30:0:1474:C:H6	1.98	0.76
30:0:2533:C:H5'	30:0:2533:C:H6	1.50	0.76
30:0:870:G:C2'	30:0:871:G:H5''	2.13	0.76
30:0:2420:G:O2'	30:0:2421:G:H5'	1.86	0.76
28:2:43:ARG:HH22	30:0:1684:A:H1'	1.48	0.76
30:0:1205:U:C2'	30:0:1206:U:H5''	2.15	0.76
31:9:2:U:OP2	31:9:3:A:H5'	1.85	0.76
31:9:92:G:H2'	31:9:93:A:C8	2.21	0.76
30:0:558:C:C2'	30:0:559:U:H5''	2.16	0.75

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
26:Z:61:HIS:HB2	26:Z:71:VAL:HB	1.66	0.75
22:V:1:THR:HG23	22:V:2:VAL:H	1.51	0.75
30:0:2256:G:O2'	30:0:2257:G:H5'	1.85	0.75
30:0:2256:G:C2'	30:0:2257:G:H5'	2.16	0.75
30:0:1451:C:H5'	30:0:1505:U:C5	2.21	0.75
30:0:1632:A:H2'	30:0:1633:C:H5'	1.69	0.75
30:0:2717:C:O2'	30:0:2718:C:H5''	1.86	0.75
1:A:199:HIS:HD2	1:A:201:PHE:H	1.33	0.75
30:0:558:C:O2'	30:0:559:U:H5''	1.87	0.75
30:0:2787:C:H5	38:0:4643:HOH:O	1.69	0.75
5:E:116:THR:HG22	5:E:151:LEU:HD22	1.69	0.75
30:0:681:G:N3	30:0:681:G:H5'	2.02	0.75
30:0:1603:A:H5''	30:0:1605:G:H5'	1.68	0.74
5:E:143:GLN:HE21	30:0:2780:C:H1'	1.52	0.74
14:N:113:SER:HB2	38:N:8852:HOH:O	1.87	0.74
30:0:1878:G:H1'	38:0:6151:HOH:O	1.87	0.74
14:N:144:GLY:O	14:N:147:ILE:HG22	1.87	0.74
2:B:179:LEU:O	2:B:183:GLU:HG2	1.86	0.74
6:F:58:GLU:HB3	13:M:8:ILE:HG23	1.69	0.74
30:0:821:U:H3'	38:0:3779:HOH:O	1.87	0.74
30:0:2135:A:O2'	30:0:2136:G:H5'	1.86	0.74
30:0:1187:U:O2'	30:0:1189:A:H2	1.71	0.74
30:0:1116:U:H3	30:0:1246:A:H62	1.36	0.74
30:0:2103:A:HO2'	30:0:2104:C:H6	1.36	0.74
5:E:100:ASP:HB2	38:E:2789:HOH:O	1.86	0.74
2:B:98:THR:HG22	30:0:2820:A:OP1	1.88	0.74
30:0:283:U:H5	30:0:284:C:N3	1.86	0.73
30:0:107:U:H2'	30:0:108:U:H5'	1.70	0.73
19:S:51:GLN:HE21	19:S:53:ASN:HD21	1.33	0.73
38:C:8660:HOH:O	30:0:2100:A:H5'	1.87	0.73
30:0:2426:G:H1'	38:0:6122:HOH:O	1.88	0.73
30:0:2768:A:O2'	30:0:2769:C:H5'	1.88	0.73
30:0:12:U:H2'	30:0:13:G:H5'	1.69	0.73
13:M:171:ARG:CD	30:0:156:C:H5''	2.16	0.73
30:0:1183:C:N4	30:0:1184:C:H41	1.85	0.73
30:0:1835:U:C5	30:0:1840:A:N7	2.55	0.73
2:B:336:GLN:O	30:0:2862:G:H4'	1.88	0.73
24:X:61:ARG:HH12	24:X:67:PRO:HD3	1.54	0.73
30:0:1666:C:C2'	30:0:1667:A:C5'	2.67	0.72
30:0:1166:A:H61	30:0:1180:U:H3	1.37	0.72
30:0:1182:C:H1'	30:0:1192:A:H8	1.54	0.72
30:0:1701:A:H5'	38:0:6316:HOH:O	1.89	0.72

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
30:0:1741:U:H5'	30:0:1742:A:OP1	1.89	0.72
29:3:70:ARG:HG2	29:3:77:ALA:HB2	1.70	0.72
30:0:2506:A:O2'	30:0:2507:G:H8	1.72	0.72
1:A:35:GLY:O	1:A:36:ASP:HB3	1.87	0.72
30:0:1189:A:H3'	38:0:7717:HOH:O	1.89	0.72
22:V:12:THR:HG22	22:V:15:GLU:HG3	1.72	0.72
30:0:2637:A:H5'	38:0:9282:HOH:O	1.88	0.72
22:V:1:THR:HB	30:0:93:C:H5''	1.72	0.72
6:F:63:ILE:HB	6:F:64:PRO:HD3	1.70	0.72
30:0:2896:A:H5''	38:0:6129:HOH:O	1.90	0.72
10:J:70:PHE:CE1	30:0:2676:C:H4'	2.25	0.72
11:K:10:GLN:N	11:K:10:GLN:HE21	1.81	0.71
31:9:14:G:H5'	31:9:14:G:C8	2.24	0.71
11:K:14:LYS:HB2	11:K:45:PRO:HG2	1.71	0.71
14:N:11:ARG:HD3	31:9:114:G:O6	1.90	0.71
24:X:71:ARG:HD3	38:X:2171:HOH:O	1.89	0.71
30:0:2102:G:H5'	30:0:2538:A:C2	2.24	0.71
30:0:1973:A:H5'	30:0:1973:A:H8	1.54	0.71
31:9:54:A:O2'	31:9:55:U:H5'	1.91	0.71
30:0:542:A:H5'	30:0:542:A:C8	2.20	0.71
4:D:25:MET:HE3	4:D:37:ALA:HB1	1.72	0.71
30:0:564:G:H1'	38:0:6343:HOH:O	1.91	0.71
1:A:211:LYS:HB2	38:A:9077:HOH:O	1.90	0.71
30:0:10:U:C6	30:0:10:U:H3'	2.26	0.71
20:T:61:GLU:HG2	38:T:3851:HOH:O	1.90	0.71
30:0:1187:U:H2'	38:0:6936:HOH:O	1.91	0.70
5:E:143:GLN:NE2	30:0:2779:G:H21	1.89	0.70
4:D:105:SER:OG	30:0:2338:G:H1'	1.89	0.70
23:W:88:THR:HG22	23:W:89:ASP:H	1.56	0.70
31:9:23:U:O2'	31:9:24:U:H4'	1.91	0.70
30:0:2578:G:H5'	30:0:2578:G:H8	1.57	0.70
38:Y:8860:HOH:O	35:0:8817:CL:CL	2.46	0.70
23:W:88:THR:HG23	23:W:110:GLN:HB3	1.73	0.70
30:0:2256:G:H2'	30:0:2257:G:H5'	1.73	0.70
3:C:1:MET:HG2	3:C:2:GLN:H	1.55	0.70
30:0:1205:U:C2'	30:0:1206:U:C5'	2.69	0.70
30:0:2781:U:C2'	30:0:2782:G:H5'	2.21	0.70
30:0:2756:U:H3	30:0:2896:A:H2	1.37	0.70
31:9:64:C:H2'	31:9:65:A:H5'	1.74	0.70
11:K:98:VAL:CG1	11:K:102:GLU:HA	2.21	0.70
6:F:91:VAL:HG12	6:F:92:GLY:N	2.07	0.70
30:0:567:U:H5''	38:0:6437:HOH:O	1.90	0.70

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
4:D:103:ASN:HD22	4:D:134:LEU:H	1.39	0.70
30:0:545:G:H8	30:0:545:G:C5'	2.00	0.69
3:C:162:VAL:HG22	3:C:232:LEU:HD21	1.73	0.69
17:Q:11:ARG:HD3	38:0:6291:HOH:O	1.92	0.69
30:0:1058:A:H2'	30:0:1060:C:H5''	1.74	0.69
30:0:1174:A:C5	30:0:1201:C:H4'	2.27	0.69
30:0:794:U:H3	30:0:819:A:H61	1.40	0.69
30:0:1666:C:H2'	30:0:1667:A:H5'	1.75	0.69
30:0:1377:C:H1'	38:0:9044:HOH:O	1.91	0.69
30:0:960:G:H3'	30:0:960:G:N3	2.07	0.69
1:A:223:ARG:HH22	30:0:2271:G:P	2.16	0.69
30:0:847:C:H4'	38:0:3762:HOH:O	1.92	0.69
30:0:1525:G:H5'	30:0:1526:A:OP2	1.93	0.69
14:N:37:ARG:HH12	31:9:6:C:H5''	1.51	0.69
11:K:74:VAL:HG12	11:K:75:ARG:HG3	1.75	0.69
13:M:164:THR:HG22	13:M:167:GLY:H	1.58	0.69
2:B:206:THR:HG21	30:0:2716:G:H5''	1.74	0.69
30:0:821:U:H5''	38:0:3057:HOH:O	1.93	0.68
30:0:1118:A:H62	30:0:1244:U:H3	1.39	0.68
30:0:2852:A:H5''	38:0:5254:HOH:O	1.93	0.68
13:M:102:GLU:OE1	13:M:164:THR:HG21	1.94	0.68
30:0:2769:C:H2'	30:0:2770:G:C5'	2.23	0.68
22:V:50:ARG:HH12	30:0:56:G:H5''	1.59	0.68
30:0:271:C:H41	30:0:378:A:H2	1.40	0.68
30:0:1701:A:H4'	30:0:1702:U:C5'	2.20	0.68
11:K:98:VAL:HG13	11:K:102:GLU:HA	1.74	0.68
30:0:2851:G:O2'	30:0:2852:A:H5'	1.92	0.68
23:W:21:LEU:HD21	23:W:48:VAL:HG11	1.75	0.68
23:W:137:GLN:HE21	23:W:141:HIS:CE1	2.11	0.68
30:0:1595:G:O2'	30:0:1596:U:H5'	1.92	0.68
30:0:2635:A:O2'	30:0:2636:C:H5'	1.94	0.68
10:J:19:MET:HE3	10:J:132:LEU:HD21	1.75	0.68
25:Y:169:ARG:HD2	30:0:1328:A:OP1	1.93	0.68
18:R:150:PRO:O	18:R:150:PRO:CG	2.41	0.68
2:B:97:LEU:HD22	2:B:127:GLN:HE21	1.57	0.68
35:0:8813:CL:CL	38:0:4692:HOH:O	2.48	0.68
30:0:1132:A:N6	30:0:1229:C:H2'	2.09	0.68
1:A:135:VAL:HG11	1:A:147:ARG:NH2	2.09	0.68
18:R:96:VAL:HG13	18:R:106:GLY:HA3	1.76	0.68
11:K:81:ARG:HB2	11:K:87:ARG:HH11	1.59	0.67
30:0:559:U:H5'	30:0:559:U:C6	2.29	0.67
30:0:69:A:H8	30:0:69:A:C5'	2.06	0.67

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
30:0:506:G:H22	30:0:509:A:H5''	1.58	0.67
23:W:84:VAL:HG12	38:W:6679:HOH:O	1.95	0.67
1:A:153:ARG:HH11	1:A:153:ARG:HB2	1.58	0.67
25:Y:212:ARG:HD2	38:Y:8904:HOH:O	1.94	0.67
30:0:2812:A:C2	30:0:2814:A:N6	2.58	0.67
8:H:155:ARG:NH1	30:0:2503:A:H5''	2.09	0.67
8:H:30:LYS:H	8:H:62:HIS:HD2	1.39	0.67
31:9:22:G:H5'	31:9:23:U:OP1	1.95	0.67
30:0:380:A:H2'	38:0:7265:HOH:O	1.93	0.67
30:0:2317:C:C6	38:0:6122:HOH:O	2.46	0.67
14:N:80:SER:HB2	38:N:8833:HOH:O	1.94	0.67
30:0:671:A:O2'	30:0:672:G:H2'	1.94	0.67
16:P:117:SER:HB3	30:0:1593:C:OP1	1.94	0.67
30:0:1279:U:O2	30:0:1279:U:H2'	1.95	0.67
30:0:1183:C:O2	30:0:1183:C:H2'	1.93	0.67
8:H:59:GLN:HE21	8:H:129:ARG:HE	1.41	0.67
5:E:133:VAL:HG12	5:E:141:VAL:HG13	1.76	0.67
1:A:211:LYS:HB3	1:A:212:PRO:HD2	1.77	0.66
1:A:199:HIS:CD2	1:A:201:PHE:H	2.12	0.66
3:C:236:THR:HG22	3:C:239:ALA:N	2.08	0.66
23:W:4:LEU:HD22	23:W:52:VAL:HG21	1.76	0.66
30:0:1159:G:H21	30:0:1189:A:H8	1.43	0.66
23:W:137:GLN:NE2	23:W:141:HIS:HE1	1.94	0.66
30:0:2781:U:O2'	30:0:2782:G:H5'	1.96	0.66
2:B:5:ARG:HH11	2:B:8:LYS:HE2	1.61	0.66
12:L:39:GLU:HG2	30:0:926:A:H4'	1.76	0.66
28:2:41:HIS:HD2	28:2:44:ARG:H	1.42	0.66
30:0:2256:G:H2'	30:0:2257:G:C5'	2.25	0.66
31:9:64:C:C2'	31:9:65:A:H5'	2.26	0.66
10:J:82:THR:CG2	30:0:1242:A:H5'	2.21	0.66
11:K:74:VAL:HG11	11:K:113:ILE:HG12	1.76	0.66
30:0:2781:U:H2'	30:0:2782:G:H5'	1.76	0.66
28:2:18:ASN:HD21	28:2:40:ARG:H	1.41	0.66
31:9:7:G:H5'	38:9:9100:HOH:O	1.96	0.66
25:Y:204:ARG:HH22	30:0:553:G:P	2.18	0.66
21:U:46:ALA:HB1	21:U:52:THR:HG21	1.78	0.66
30:0:1189:A:H1'	30:0:1209:C:C1'	2.25	0.66
30:0:1377:C:H5'	30:0:1377:C:C6	2.31	0.66
4:D:103:ASN:ND2	4:D:134:LEU:H	1.92	0.66
30:0:2001:G:O2'	30:0:2002:C:H5'	1.96	0.66
18:R:99:ALA:HB1	18:R:109:MET:HE1	1.76	0.66
30:0:2251:G:H2'	30:0:2252:A:C8	2.30	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
30:0:2769:C:O2'	30:0:2770:G:H5'	1.96	0.65
30:0:558:C:H2'	30:0:559:U:C5'	2.26	0.65
30:0:1118:A:C8	30:0:1118:A:C3'	2.77	0.65
8:H:72:ALA:HB2	8:H:156:ALA:HB2	1.78	0.65
30:0:1524:U:OP1	30:0:1524:U:H4'	1.96	0.65
30:0:2768:A:H2'	30:0:2769:C:O4'	1.96	0.65
30:0:1634:G:H3'	38:0:3903:HOH:O	1.96	0.65
30:0:603:A:H5''	30:0:604:G:OP1	1.97	0.65
3:C:174:ILE:HD11	30:0:338:C:H4'	1.78	0.65
30:0:2827:A:H2'	30:0:2828:G:O4'	1.97	0.65
30:0:1441:G:O2'	30:0:1442:A:H5'	1.97	0.65
30:0:2507:G:H2'	30:0:2510:C:H42	1.62	0.65
30:0:1972:U:H2'	30:0:1973:A:C5'	2.26	0.65
30:0:2613:G:O2'	30:0:2614:C:H5'	1.97	0.65
6:F:21:GLU:O	6:F:24:ARG:HG2	1.97	0.65
15:O:42:GLU:HB2	38:O:2176:HOH:O	1.96	0.65
30:0:635:A:H2'	30:0:636:G:H5''	1.78	0.65
16:P:55:LYS:HG2	16:P:56:GLY:N	2.12	0.65
10:J:88:PRO:HD3	30:0:1104:C:H4'	1.77	0.65
14:N:37:ARG:NH1	31:9:6:C:C5'	2.51	0.65
27:1:20:ARG:HG2	30:0:111:C:O2'	1.97	0.65
30:0:1632:A:C2'	30:0:1633:C:H5'	2.27	0.64
30:0:2005:G:OP2	30:0:2005:G:H3'	1.97	0.64
30:0:485:A:N3	30:0:487:G:H5''	2.12	0.64
30:0:2281:C:H2'	30:0:2282:U:H5'	1.80	0.64
30:0:1834:C:H2'	30:0:1840:A:N6	2.11	0.64
30:0:283:U:C5	30:0:284:C:N3	2.65	0.64
12:L:39:GLU:HG2	30:0:926:A:C4'	2.27	0.64
38:T:2217:HOH:O	30:0:317:A:H5'	1.97	0.64
30:0:1667:A:C8	30:0:1667:A:H5'	2.29	0.64
30:0:2717:C:H2'	30:0:2718:C:C5'	2.22	0.64
30:0:1185:U:H2'	30:0:1186:C:C6	2.33	0.64
30:0:283:U:H5	30:0:284:C:C2	2.15	0.64
8:H:30:LYS:H	8:H:62:HIS:CD2	2.14	0.64
30:0:363:C:O2'	30:0:364:U:H5'	1.97	0.64
30:0:613:C:H2'	30:0:614:U:H6	1.62	0.64
14:N:12:ARG:HD3	14:N:18:THR:OG1	1.97	0.64
21:U:17:THR:HG22	21:U:18:GLY:N	2.13	0.64
30:0:272:A:H5'	30:0:273:G:OP2	1.97	0.64
8:H:168:VAL:HG13	38:H:213:HOH:O	1.98	0.64
30:0:2563:U:H2'	30:0:2565:C:O5'	1.98	0.64
30:0:2638:G:H5'	38:0:4946:HOH:O	1.98	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
30:0:2371:G:H5'	38:0:5029:HOH:O	1.98	0.64
21:U:17:THR:HG22	21:U:18:GLY:H	1.62	0.64
3:C:184:ARG:NH2	30:0:450:C:OP1	2.31	0.64
30:0:644:G:N3	30:0:644:G:H5'	2.13	0.64
30:0:952:G:H4'	38:0:4042:HOH:O	1.97	0.63
30:0:333:G:O2'	30:0:334:G:H5'	1.97	0.63
30:0:1603:A:C5'	30:0:1605:G:H5'	2.27	0.63
2:B:162:MET:HG3	2:B:310:ARG:HD3	1.80	0.63
30:0:2748:G:H2'	38:0:7581:HOH:O	1.98	0.63
30:0:1596:U:H2'	30:0:1598:A:OP2	1.99	0.63
30:0:2404:G:H5''	38:0:5231:HOH:O	1.97	0.63
18:R:128:ARG:NH2	30:0:2054:A:N3	2.46	0.63
23:W:72:PRO:HG2	23:W:77:ALA:HB3	1.80	0.63
30:0:2718:C:H6	30:0:2718:C:H5'	1.63	0.63
30:0:2610:U:H4'	38:0:9484:HOH:O	1.99	0.63
30:0:2344:G:N3	30:0:2344:G:H2'	2.14	0.63
30:0:420:U:H2'	30:0:421:C:C6	2.33	0.63
30:0:544:G:H2'	30:0:545:G:H5''	1.81	0.63
30:0:1166:A:P	30:0:1174:A:H4'	2.38	0.63
2:B:238:ASN:HD22	2:B:240:GLY:N	1.93	0.63
16:P:115:SER:N	16:P:118:GLN:HE21	1.84	0.63
30:0:1189:A:O2'	30:0:1208:C:H2'	1.98	0.63
5:E:143:GLN:NE2	30:0:2780:C:H1'	2.13	0.63
11:K:81:ARG:HB2	11:K:87:ARG:NH1	2.14	0.63
14:N:7:LYS:HE3	17:Q:21:ARG:O	1.99	0.63
30:0:1206:U:C5'	30:0:1206:U:H6	2.10	0.63
30:0:1200:A:H3'	38:0:5774:HOH:O	1.99	0.63
3:C:140:VAL:HB	38:C:8649:HOH:O	1.98	0.63
30:0:10:U:C3'	30:0:10:U:C6	2.82	0.63
22:V:50:ARG:NH1	30:0:56:G:H5''	2.13	0.63
30:0:2281:C:C2'	30:0:2282:U:H5'	2.29	0.63
2:B:307:ARG:HG3	2:B:307:ARG:HH11	1.64	0.63
12:L:133:VAL:HA	38:L:8871:HOH:O	1.99	0.63
30:0:1942:A:H3'	38:0:7387:HOH:O	1.98	0.62
27:1:16:HIS:HD2	30:0:470:U:O2'	1.81	0.62
30:0:1182:C:H1'	30:0:1192:A:C8	2.34	0.62
30:0:2781:U:H2'	30:0:2782:G:C5'	2.29	0.62
1:A:121:ALA:O	1:A:124:VAL:HG22	1.98	0.62
30:0:2502:C:H2'	30:0:2503:A:C5'	2.28	0.62
30:0:138:U:OP2	30:0:139:C:H5	1.82	0.62
10:J:127:ILE:HG22	35:J:8801:CL:CL	2.36	0.62
30:0:2472:C:O2'	30:0:2634:G:H4'	1.99	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
30:0:420:U:H2'	30:0:421:C:H6	1.64	0.62
3:C:236:THR:HG21	38:C:8573:HOH:O	2.00	0.62
30:0:559:U:C5	30:0:560:U:C5	2.88	0.62
3:C:27:ARG:NH2	30:0:657:G:OP1	2.32	0.62
30:0:2241:C:O2'	30:0:2242:U:H5'	2.00	0.62
23:W:6:GLN:HB2	23:W:26:ILE:HD11	1.81	0.62
4:D:22:VAL:HG22	4:D:74:THR:HG22	1.81	0.62
30:0:1351:G:H1'	38:0:4064:HOH:O	1.98	0.62
24:X:43:VAL:HG12	24:X:44:ASP:H	1.63	0.62
28:2:41:HIS:H	28:2:45:ASN:HD22	1.46	0.62
2:B:320:GLN:HE21	2:B:321:PRO:HD2	1.65	0.62
30:0:1477:C:H5'	30:0:1868:G:C5'	2.30	0.62
1:A:191:GLY:HA2	1:A:194:MET:CE	2.30	0.62
20:T:26:THR:HG23	20:T:97:ARG:HG3	1.82	0.62
28:2:2:LYS:HG3	30:0:1486:A:C5	2.34	0.62
30:0:107:U:C2'	30:0:108:U:H5'	2.29	0.62
30:0:2372:A:H2'	30:0:2373:U:H6	1.65	0.62
29:3:25:VAL:HG22	29:3:68:LYS:HG3	1.80	0.62
25:Y:189:ASN:HA	25:Y:217:ILE:HD11	1.82	0.61
2:B:18:ARG:HG3	2:B:256:GLN:HG3	1.82	0.61
30:0:2643:G:H5''	38:0:3937:HOH:O	1.99	0.61
3:C:129:HIS:CE1	3:C:231:ARG:HA	2.35	0.61
21:U:56:ARG:HD2	38:0:6278:HOH:O	1.98	0.61
30:0:958:G:O2'	30:0:959:C:H5'	2.01	0.61
30:0:2802:C:H2'	30:0:2803:C:C6	2.35	0.61
30:0:196:G:H2'	38:0:6690:HOH:O	2.00	0.61
30:0:2509:A:OP2	30:0:2510:C:H5	1.82	0.61
30:0:1972:U:H2'	30:0:1973:A:H5''	1.80	0.61
30:0:1015:C:H2'	30:0:1016:U:H6	1.65	0.61
30:0:407:A:H3'	38:0:4471:HOH:O	2.00	0.61
31:9:29:C:C2'	31:9:30:C:H5'	2.27	0.61
30:0:308:U:C4	30:0:342:C:H1'	2.36	0.61
23:W:80:ASP:O	23:W:84:VAL:HG23	1.99	0.61
12:L:136:ALA:HB3	38:L:8871:HOH:O	2.00	0.61
11:K:63:GLU:HG2	38:K:6344:HOH:O	2.00	0.61
30:0:705:C:H2'	30:0:705:C:O2	2.01	0.61
30:0:1183:C:H42	30:0:1184:C:H41	1.47	0.61
18:R:99:ALA:HB1	18:R:109:MET:CE	2.31	0.61
30:0:1174:A:C6	30:0:1201:C:H4'	2.36	0.61
2:B:7:ARG:HG2	2:B:7:ARG:HH11	1.66	0.61
2:B:201:ASP:HB2	2:B:312:ARG:HD2	1.82	0.61
27:1:1:THR:HA	38:1:435:HOH:O	2.00	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
12:L:30:ARG:HD3	30:0:164:G:H4'	1.82	0.61
14:N:11:ARG:HG3	14:N:14:ARG:NH1	2.15	0.61
31:9:39:U:H3'	31:9:40:C:H5''	1.83	0.61
16:P:91:LYS:O	16:P:95:GLU:HG3	2.00	0.61
30:0:1165:G:N2	30:0:1173:A:C5'	2.63	0.61
30:0:1972:U:C2'	30:0:1973:A:H5''	2.31	0.61
27:1:28:HIS:HE1	30:0:776:A:OP1	1.84	0.61
30:0:510:U:H6	38:0:7477:HOH:O	1.83	0.60
29:3:15:ASN:O	30:0:2408:A:H4'	2.01	0.60
31:9:39:U:H1'	31:9:44:A:H61	1.65	0.60
22:V:39:ALA:N	22:V:40:PRO:HD2	2.14	0.60
30:0:544:G:C2'	30:0:545:G:H5''	2.31	0.60
8:H:6:ALA:HA	8:H:61:ARG:HH12	1.67	0.60
4:D:135:VAL:HG21	4:D:139:TYR:CD1	2.36	0.60
30:0:2768:A:H5''	38:0:4438:HOH:O	2.00	0.60
30:0:1819:G:H5'	38:0:5835:HOH:O	2.01	0.60
30:0:1379:A:H1'	38:0:9696:HOH:O	2.01	0.60
30:0:69:A:C8	30:0:69:A:C5'	2.78	0.60
30:0:1116:U:C2'	30:0:1118:A:H2	2.14	0.60
30:0:31:C:H4'	38:0:7464:HOH:O	2.00	0.60
30:0:407:A:H5'	38:0:6054:HOH:O	2.00	0.60
30:0:2787:C:C5	38:0:4643:HOH:O	2.49	0.60
19:S:55:GLN:NE2	30:0:1446:U:H2'	2.17	0.60
30:0:285:A:H2'	30:0:286:U:O4'	2.01	0.60
1:A:47:HIS:HD2	30:0:1654:U:H2'	1.66	0.60
30:0:2581:U:H1'	38:0:4486:HOH:O	2.01	0.60
30:0:363:C:H1'	38:0:5301:HOH:O	2.01	0.60
18:R:8:ALA:HB1	18:R:13:THR:HG21	1.82	0.60
25:Y:187:VAL:HG22	25:Y:192:ASP:HB3	1.84	0.60
2:B:258:GLY:H	2:B:260:HIS:CE1	2.19	0.60
20:T:9:LYS:HE3	20:T:13:ARG:CZ	2.32	0.60
30:0:960:G:N3	30:0:960:G:C2'	2.65	0.60
11:K:74:VAL:CG1	11:K:113:ILE:HG12	2.32	0.60
30:0:2893:C:O2'	30:0:2894:C:H5'	2.02	0.60
30:0:164:G:H3'	38:0:3650:HOH:O	2.02	0.60
30:0:853:C:H3'	38:0:4563:HOH:O	2.01	0.60
30:0:2103:A:O2'	30:0:2104:C:H6	1.85	0.59
10:J:75:PRO:HG2	10:J:105:LEU:HD21	1.83	0.59
30:0:2453:G:H3'	38:0:5945:HOH:O	2.01	0.59
25:Y:216:ARG:HD2	38:Y:8873:HOH:O	2.02	0.59
30:0:2637:A:H4'	38:0:4946:HOH:O	2.02	0.59
30:0:2134:G:N2	30:0:2242:U:C2	2.70	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
24:X:76:ARG:HH11	24:X:76:ARG:HG3	1.66	0.59
30:0:941:G:C5	30:0:942:U:C4	2.91	0.59
19:S:17:ASP:HB3	19:S:23:LYS:HB2	1.83	0.59
3:C:233:THR:HG22	3:C:234:VAL:H	1.67	0.59
12:L:56:LYS:HE3	30:0:2443:C:H1'	1.84	0.59
13:M:86:GLN:NE2	30:0:2274:A:H1'	2.17	0.59
10:J:18:ILE:HD13	30:0:1244:U:OP1	2.01	0.59
2:B:162:MET:CE	2:B:308:LEU:HD21	2.32	0.59
17:Q:25:PRO:HB2	38:9:9079:HOH:O	2.01	0.59
30:0:2795:C:O2'	30:0:2796:U:H5'	2.02	0.59
30:0:2361:A:H8	30:0:2361:A:H5'	1.68	0.59
6:F:58:GLU:CD	13:M:27:ARG:HH22	2.05	0.59
30:0:821:U:H2'	30:0:822:C:H6	1.67	0.59
30:0:2372:A:H2'	30:0:2373:U:C6	2.37	0.59
30:0:1819:G:H2'	30:0:1820:G:C5'	2.32	0.59
5:E:49:ILE:HD11	5:E:69:ILE:HD12	1.85	0.59
30:0:1527:A:H1'	30:0:1528:A:C8	2.37	0.59
30:0:1249:U:H2'	30:0:1250:C:C6	2.36	0.59
15:O:24:ALA:HB3	30:0:710:G:OP1	2.02	0.59
13:M:99:ARG:HE	13:M:170:ASN:HD22	1.49	0.59
11:K:45:PRO:HB2	38:K:7169:HOH:O	2.01	0.59
30:0:1625:U:H4'	38:0:4676:HOH:O	2.03	0.59
2:B:234:ARG:HG3	30:0:1735:C:OP2	2.02	0.59
30:0:1202:A:H2'	30:0:1203:G:O4'	2.03	0.59
30:0:2073:G:OP2	30:0:2490:A:H5'	2.01	0.59
8:H:174:LEU:HD21	30:0:1220:U:H4'	1.83	0.59
21:U:6:CYS:HB2	21:U:32:CYS:HB3	1.85	0.59
30:0:1603:A:H5'	30:0:1605:G:C4'	2.33	0.59
30:0:2756:U:N3	30:0:2896:A:H2	2.01	0.59
30:0:905:C:H3'	38:0:5207:HOH:O	2.02	0.59
30:0:2265:U:H2'	30:0:2266:A:C8	2.37	0.59
4:D:54:ALA:HB2	4:D:69:ILE:HD12	1.84	0.59
30:0:513:A:N3	38:0:3665:HOH:O	2.32	0.59
30:0:2846:C:H4'	38:0:5100:HOH:O	2.03	0.59
30:0:1116:U:HO2'	30:0:1118:A:H2	0.68	0.59
30:0:2756:U:N3	30:0:2896:A:C2	2.67	0.59
11:K:87:ARG:HG3	30:0:2721:U:H4'	1.85	0.59
29:3:60:LYS:HG3	29:3:61:PRO:HD2	1.83	0.59
30:0:1120:U:H5'	30:0:1121:G:OP2	2.03	0.59
2:B:141:ARG:HD2	2:B:163:GLU:OE2	2.03	0.59
30:0:137:U:H2'	30:0:139:C:C5	2.38	0.58
1:A:191:GLY:HA2	1:A:194:MET:HE3	1.84	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
30:0:2539:U:H1'	38:0:7825:HOH:O	2.02	0.58
30:0:737:A:H2'	30:0:738:G:O4'	2.02	0.58
14:N:37:ARG:HH11	31:9:6:C:H5''	1.61	0.58
30:0:2526:C:C6	30:0:2526:C:C5'	2.85	0.58
2:B:215:VAL:HB	38:B:9087:HOH:O	2.02	0.58
30:0:2607:U:H4'	38:0:9447:HOH:O	2.03	0.58
29:3:73:GLU:HB3	38:3:9052:HOH:O	2.02	0.58
3:C:236:THR:CG2	3:C:239:ALA:H	2.10	0.58
26:Z:81:CYS:SG	26:Z:83:TYR:HB3	2.43	0.58
5:E:143:GLN:HE22	30:0:2779:G:H21	1.48	0.58
2:B:145:HIS:HD2	2:B:146:THR:O	1.87	0.58
10:J:76:ASP:HA	38:J:5907:HOH:O	2.03	0.58
1:A:23:TYR:HB2	30:0:1872:C:C5	2.38	0.58
30:0:1641:A:H2'	30:0:1642:A:H5'	1.85	0.58
30:0:282:C:O2'	30:0:283:U:C5'	2.52	0.58
30:0:368:C:H2'	30:0:369:G:H5'	1.85	0.58
29:3:70:ARG:HB3	38:3:9064:HOH:O	2.03	0.58
10:J:107:ASN:HD22	10:J:109:TYR:H	1.50	0.58
30:0:304:G:H1'	30:0:347:A:N6	2.18	0.58
8:H:48:VAL:HA	8:H:170:ARG:O	2.02	0.58
2:B:212:GLN:HB2	2:B:257:THR:CG2	2.32	0.58
30:0:1919:A:H4'	38:0:4867:HOH:O	2.03	0.58
30:0:960:G:H4'	38:0:7470:HOH:O	2.03	0.58
30:0:1291:A:H2	38:0:5311:HOH:O	1.86	0.58
30:0:899:C:H5'	38:0:3211:HOH:O	2.03	0.58
12:L:67:ARG:HB2	12:L:112:GLY:HA3	1.85	0.58
30:0:638:C:H2'	30:0:639:A:C8	2.39	0.58
30:0:185:G:H4'	30:0:186:A:OP1	2.02	0.58
30:0:1701:A:H5''	30:0:1702:U:H3'	1.85	0.58
2:B:36:PRO:HG3	2:B:169:GLY:H	1.69	0.58
3:C:2:GLN:HB3	38:C:8583:HOH:O	2.03	0.58
20:T:52:ARG:HD2	30:0:317:A:H5''	1.85	0.58
28:2:2:LYS:HG3	30:0:1486:A:C4	2.39	0.58
3:C:58:ALA:HA	3:C:73:GLN:HE21	1.69	0.58
3:C:101:ASP:HB2	30:0:750:A:O3'	2.04	0.58
26:Z:40:ALA:HA	30:0:1773:G:C8	2.38	0.58
28:2:11:LEU:HD22	30:0:1417:G:O2'	2.04	0.58
13:M:30:GLU:O	13:M:34:GLU:HG3	2.04	0.58
30:0:1206:U:H5'	30:0:1206:U:C6	2.26	0.58
9:I:107:LYS:HB3	9:I:110:ASP:HB2	1.85	0.58
14:N:141:ARG:NH2	31:9:48:C:H4'	2.19	0.58
30:0:1507:C:H4'	38:0:3609:HOH:O	2.03	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
30:0:2670:G:O2'	30:0:2671:U:H5'	2.03	0.58
30:0:877:G:C5'	30:0:878:G:OP1	2.48	0.58
30:0:2802:C:H2'	30:0:2803:C:H6	1.66	0.58
9:I:73:LEU:HD12	9:I:107:LYS:NZ	2.19	0.58
1:A:100:PRO:HG2	1:A:103:VAL:HG21	1.84	0.58
2:B:112:THR:HG23	2:B:158:LYS:NZ	2.18	0.58
30:0:17:G:H2'	30:0:18:C:H6	1.68	0.58
30:0:2842:G:H2'	30:0:2843:A:H5'	1.85	0.58
5:E:84:MET:HG2	5:E:168:ILE:HA	1.86	0.58
2:B:207:LYS:HG3	30:0:2717:C:OP1	2.04	0.58
27:1:25:LYS:HD2	28:2:49:GLU:H	1.68	0.58
17:Q:19:ARG:HH21	31:9:11:A:P	2.27	0.58
30:0:2510:C:H5'	30:0:2511:A:OP2	2.04	0.57
30:0:2445:U:H2'	30:0:2446:G:C8	2.39	0.57
2:B:256:GLN:HG2	38:B:9121:HOH:O	2.04	0.57
7:G:64:ASN:HD22	7:G:64:ASN:N	2.02	0.57
14:N:61:ALA:HB3	14:N:88:ALA:HB2	1.85	0.57
30:0:2356:A:H5'	38:0:5655:HOH:O	2.03	0.57
7:G:16:LYS:O	7:G:20:VAL:HG23	2.03	0.57
12:L:6:ARG:HD3	30:0:1299:G:O6	2.03	0.57
30:0:2755:G:H1'	38:0:4691:HOH:O	2.03	0.57
2:B:5:ARG:NH1	2:B:8:LYS:HE2	2.19	0.57
31:9:39:U:H1'	31:9:44:A:N6	2.18	0.57
30:0:2238:A:O2'	30:0:2239:C:H5'	2.03	0.57
30:0:297:U:H1'	38:0:3945:HOH:O	2.04	0.57
30:0:441:A:H1'	30:0:442:A:N7	2.20	0.57
30:0:812:A:H1'	38:0:3967:HOH:O	2.03	0.57
30:0:2004:U:H2'	30:0:2004:U:O2	2.04	0.57
30:0:1741:U:O2'	30:0:2723:G:H4'	2.04	0.57
29:3:48:ASN:HD21	30:0:2468:A:H61	1.50	0.57
23:W:44:MET:CE	30:0:944:G:H21	2.17	0.57
30:0:1795:G:H2'	30:0:1796:A:O4'	2.04	0.57
30:0:2505:G:O2'	30:0:2506:A:H5'	2.05	0.57
30:0:1278:A:H4'	30:0:1279:U:C4	2.40	0.57
30:0:232:A:H4'	38:0:6113:HOH:O	2.05	0.57
30:0:558:C:H2'	30:0:559:U:H5''	1.84	0.57
19:S:77:VAL:O	19:S:80:ARG:HG2	2.05	0.57
30:0:1167:G:H2'	30:0:1168:C:O4'	2.04	0.57
30:0:820:G:O2'	30:0:856:G:H4'	2.03	0.57
23:W:52:VAL:HG22	23:W:53:ALA:H	1.68	0.57
31:9:39:U:HO2'	31:9:42:C:H5	1.53	0.57
30:0:558:C:C2'	30:0:559:U:C5'	2.83	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
12:L:41:HIS:CD2	30:0:926:A:O2'	2.58	0.57
30:0:945:U:H2'	30:0:946:C:H6	1.70	0.57
30:0:2597:U:H2'	30:0:2598:U:H5'	1.87	0.57
30:0:1538:C:O2'	30:0:1539:U:H5'	2.05	0.57
30:0:2589:U:H2'	30:0:2590:U:C6	2.40	0.57
30:0:168:C:O5'	30:0:168:C:H6	1.88	0.57
10:J:70:PHE:HE1	30:0:2676:C:H4'	1.68	0.57
30:0:2291:A:N9	30:0:2309:C:H5'	2.19	0.57
30:0:483:C:C4	30:0:484:A:C6	2.93	0.57
14:N:24:LEU:HD13	17:Q:26:PRO:HB3	1.86	0.57
30:0:292:G:H2'	30:0:358:G:N2	2.20	0.57
1:A:51:ARG:NH1	1:A:120:ARG:O	2.38	0.57
30:0:1205:U:O2'	30:0:1206:U:H5''	2.05	0.56
38:C:8559:HOH:O	30:0:338:C:H5''	2.04	0.56
30:0:287:C:H42	30:0:365:G:H1	1.53	0.56
23:W:125:HIS:HD2	23:W:127:GLY:H	1.53	0.56
30:0:1214:G:H4'	38:0:4759:HOH:O	2.03	0.56
30:0:125:U:H2'	38:0:3775:HOH:O	2.04	0.56
31:9:55:U:H4'	31:9:56:A:C8	2.40	0.56
14:N:147:ILE:HD12	38:9:9089:HOH:O	2.04	0.56
30:0:2720:C:H3'	38:0:6454:HOH:O	2.05	0.56
30:0:119:A:H2'	30:0:120:A:H5''	1.87	0.56
30:0:334:G:C5	30:0:335:U:C5	2.94	0.56
30:0:1528:A:H2'	30:0:1529:G:O4'	2.05	0.56
30:0:17:G:H2'	30:0:18:C:C6	2.40	0.56
30:0:945:U:H2'	30:0:946:C:C6	2.40	0.56
25:Y:126:PRO:HG2	25:Y:128:PHE:CE1	2.40	0.56
16:P:64:GLU:HG2	38:P:2495:HOH:O	2.05	0.56
10:J:69:TYR:CE1	30:0:2081:A:H4'	2.40	0.56
23:W:139:GLY:O	23:W:141:HIS:HD2	1.87	0.56
8:H:15:PRO:HG3	30:0:1053:G:OP1	2.06	0.56
30:0:1342:C:C2'	30:0:1343:C:H5'	2.35	0.56
25:Y:115:ARG:HH21	30:0:1266:U:H4'	1.71	0.56
25:Y:235:GLU:H	25:Y:235:GLU:CD	2.08	0.56
30:0:1181:A:C2	30:0:1192:A:C8	2.94	0.56
2:B:297:VAL:HB	38:B:9075:HOH:O	2.05	0.56
30:0:2252:A:C5	30:0:2253:G:H1'	2.40	0.56
30:0:136:C:H2'	30:0:137:U:O4'	2.05	0.56
1:A:47:HIS:CD2	30:0:1654:U:H2'	2.41	0.56
18:R:39:THR:HG23	18:R:107:GLU:O	2.04	0.56
8:H:69:ARG:HD3	38:H:232:HOH:O	2.06	0.56
30:0:1679:C:H5'	38:0:9330:HOH:O	2.05	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
13:M:64:ARG:HD2	38:M:8878:HOH:O	2.04	0.56
12:L:143:THR:HG22	12:L:144:ASP:N	2.21	0.56
11:K:130:MET:SD	21:U:25:ASP:O	2.64	0.56
30:0:1903:U:O2'	30:0:1904:A:N7	2.39	0.56
31:9:49:G:H2'	31:9:50:G:O4'	2.06	0.56
11:K:118:ALA:HA	11:K:125:ALA:HB2	1.88	0.56
6:F:50:VAL:HG13	6:F:60:VAL:HG11	1.87	0.56
5:E:149:GLU:HG3	5:E:167:TYR:HA	1.86	0.56
31:9:63:C:O2'	31:9:64:C:H5'	2.06	0.56
21:U:9:CYS:HA	21:U:52:THR:CG2	2.36	0.56
2:B:294:TYR:HE2	38:B:9114:HOH:O	1.89	0.56
7:G:20:VAL:O	7:G:24:VAL:HG23	2.06	0.56
31:9:36:C:C5	31:9:37:C:C5	2.94	0.56
23:W:48:VAL:HG12	23:W:52:VAL:HB	1.87	0.55
30:0:396:U:O2'	30:0:418:C:H4'	2.05	0.55
30:0:2253:G:O2'	30:0:2254:G:H5'	2.06	0.55
4:D:172:VAL:HG12	4:D:173:GLU:H	1.70	0.55
7:G:12:ILE:HG23	38:0:5477:HOH:O	2.07	0.55
30:0:1198:U:H1'	30:0:1201:C:H5	1.71	0.55
30:0:1183:C:N3	30:0:1184:C:C5	2.74	0.55
30:0:283:U:C5	30:0:284:C:C2	2.93	0.55
30:0:960:G:C3'	30:0:960:G:N3	2.70	0.55
30:0:1768:C:H2'	30:0:1769:C:O4'	2.06	0.55
30:0:1664:A:H8	30:0:1664:A:OP1	1.89	0.55
3:C:236:THR:HA	38:C:8649:HOH:O	2.05	0.55
30:0:2419:U:H5''	30:0:2420:G:H5'	1.89	0.55
10:J:19:MET:HE1	10:J:79:PHE:HA	1.89	0.55
14:N:141:ARG:HH21	31:9:48:C:H4'	1.72	0.55
30:0:2608:C:H2'	38:0:3579:HOH:O	2.06	0.55
3:C:47:GLY:HA2	3:C:92:PRO:HB2	1.87	0.55
9:I:111:LEU:CD2	30:0:1163:G:H4'	2.35	0.55
14:N:11:ARG:HG3	14:N:14:ARG:HH12	1.71	0.55
30:0:65:C:O2'	30:0:66:G:H5'	2.06	0.55
11:K:32:ILE:HD11	11:K:56:SER:HB3	1.88	0.55
8:H:22:TYR:CZ	30:0:1007:A:H2'	2.41	0.55
30:0:628:1MA:H4'	38:0:3149:HOH:O	2.06	0.55
6:F:77:VAL:HG21	6:F:83:LEU:HD13	1.88	0.55
30:0:2509:A:C2	30:0:2510:C:H1'	2.42	0.55
30:0:558:C:H2'	30:0:559:U:H5'	1.89	0.55
12:L:22:ARG:HG2	38:0:3241:HOH:O	2.05	0.55
30:0:2478:U:O2'	30:0:2479:A:H5'	2.06	0.55
30:0:1666:C:H2'	30:0:1667:A:H5''	1.71	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
30:0:2908:A:O5'	30:0:2908:A:H8	1.89	0.55
30:0:2353:A:H4'	30:0:2354:A:O5'	2.06	0.55
38:O:1484:HOH:O	30:0:710:G:H1'	2.06	0.55
30:0:1787:C:H4'	30:0:2883:A:O4'	2.07	0.55
2:B:62:ARG:HA	2:B:65:MET:CE	2.36	0.55
30:0:1159:G:H1	30:0:1208:C:H42	1.54	0.55
30:0:567:U:C5'	38:0:6437:HOH:O	2.50	0.55
30:0:960:G:H2'	30:0:960:G:N3	2.22	0.55
30:0:2565:C:H4'	38:0:4851:HOH:O	2.06	0.55
8:H:6:ALA:HA	8:H:61:ARG:NH1	2.21	0.55
25:Y:130:ARG:HB2	25:Y:142:SER:O	2.07	0.55
30:0:2320:U:H4'	30:0:2321:A:O4'	2.07	0.55
30:0:1127:C:C5	30:0:1128:U:C4	2.95	0.55
12:L:36:ASP:HB2	38:L:8836:HOH:O	2.07	0.55
23:W:154:ARG:NH1	30:0:588:G:O6	2.40	0.55
30:0:2896:A:N3	30:0:2896:A:H2'	2.22	0.55
30:0:1120:U:H5''	30:0:1120:U:C6	2.42	0.55
30:0:89:G:H4'	38:0:4779:HOH:O	2.05	0.55
30:0:2249:G:C2	30:0:2253:G:C6	2.95	0.55
30:0:1819:G:H2'	30:0:1820:G:H4'	1.89	0.55
16:P:87:ARG:HG2	38:0:5970:HOH:O	2.07	0.55
30:0:1838:U:H3'	38:0:5544:HOH:O	2.07	0.55
30:0:1474:C:C5'	30:0:1474:C:C6	2.79	0.54
31:9:76:G:C3'	31:9:77:A:H5''	2.27	0.54
30:0:1118:A:H8	30:0:1119:G:H5''	1.73	0.54
30:0:1066:U:H2'	30:0:1067:A:C8	2.41	0.54
1:A:109:GLU:HG2	1:A:116:GLY:H	1.72	0.54
3:C:174:ILE:CD1	30:0:338:C:H4'	2.36	0.54
24:X:43:VAL:HG11	24:X:82:GLU:HA	1.88	0.54
30:0:1750:C:H5''	38:0:3673:HOH:O	2.07	0.54
9:I:112:LEU:CD1	30:0:1162:G:H1'	2.37	0.54
27:1:9:GLY:HA2	30:0:1687:C:O2	2.07	0.54
22:V:64:GLY:O	22:V:65:ASP:HB2	2.06	0.54
23:W:142:ASP:HB3	23:W:145:GLY:H	1.71	0.54
2:B:221:GLN:HE22	11:K:42:ASN:ND2	1.98	0.54
27:1:16:HIS:HE1	30:0:775:G:OP1	1.91	0.54
16:P:80:ARG:HG2	16:P:87:ARG:CZ	2.37	0.54
38:Z:8707:HOH:O	30:0:1886:A:H4'	2.06	0.54
23:W:64:THR:O	23:W:68:THR:HG22	2.06	0.54
30:0:876:A:N3	30:0:876:A:H2'	2.23	0.54
4:D:141:VAL:HG21	31:9:57:A:H8	1.72	0.54
8:H:59:GLN:HE21	8:H:129:ARG:NE	2.05	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
30:0:1016:U:H1'	38:0:3664:HOH:O	2.06	0.54
29:3:11:CYS:HB2	29:3:20:HIS:CE1	2.42	0.54
2:B:305:ASP:O	2:B:306:LYS:HB2	2.08	0.54
30:0:2387:U:H2'	30:0:2388:C:C6	2.42	0.54
2:B:275:GLY:O	2:B:291:ASP:HA	2.07	0.54
30:0:138:U:OP1	30:0:259:G:H5'	2.07	0.54
31:9:12:C:H5'	31:9:70:U:O4'	2.06	0.54
13:M:66:SER:HB3	13:M:128:TRP:CD1	2.42	0.54
24:X:23:HIS:HE1	30:0:2044:G:OP1	1.89	0.54
15:O:105:ASN:HD21	15:O:109:SER:N	2.05	0.54
20:T:68:ASP:HB2	38:0:5678:HOH:O	2.08	0.54
30:0:962:C:H2'	30:0:963:C:H5'	1.89	0.54
30:0:711:G:C2	30:0:718:C:C2	2.96	0.54
23:W:88:THR:HG22	23:W:90:TYR:HD1	1.72	0.54
31:9:1:U:O3'	31:9:3:A:H5''	2.07	0.54
30:0:2271:G:N3	30:0:2271:G:H2'	2.22	0.54
13:M:159:VAL:HG12	35:M:8818:CL:CL	2.45	0.54
26:Z:75:GLY:HA3	38:Z:8717:HOH:O	2.06	0.54
31:9:3:A:N6	31:9:22:G:H1'	2.22	0.54
30:0:2414:A:H2'	30:0:2415:A:C8	2.43	0.54
23:W:13:MET:HE1	23:W:18:GLN:HA	1.88	0.54
8:H:87:LYS:NZ	8:H:87:LYS:HB2	2.23	0.54
30:0:1205:U:H5	38:0:4451:HOH:O	1.91	0.54
13:M:24:GLN:NE2	13:M:27:ARG:HH11	2.06	0.54
30:0:1342:C:O2'	30:0:1343:C:H5'	2.07	0.54
9:I:97:VAL:HG12	9:I:101:LYS:HE3	1.90	0.54
30:0:2880:A:H2'	30:0:2881:C:H5'	1.89	0.54
4:D:18:ILE:HD13	4:D:84:LEU:HD12	1.89	0.54
30:0:567:U:H5''	38:0:5308:HOH:O	2.08	0.54
30:0:1926:G:H2'	30:0:1927:A:C8	2.42	0.54
19:S:11:THR:H	19:S:14:ALA:HB3	1.73	0.54
30:0:1624:A:H5'	30:0:1626:A:O4'	2.07	0.54
30:0:1450:C:H5''	38:0:9624:HOH:O	2.08	0.54
24:X:72:VAL:HG22	24:X:85:VAL:HG12	1.90	0.53
16:P:7:LYS:HD3	16:P:21:VAL:HG22	1.90	0.53
30:0:1137:G:H1'	38:0:3888:HOH:O	2.07	0.53
24:X:30:MET:HE1	24:X:58:ALA:HB3	1.90	0.53
2:B:254:GLN:HG2	2:B:255:GLY:N	2.23	0.53
30:0:1201:C:C2'	30:0:1202:A:H5'	2.37	0.53
30:0:1973:A:H5'	30:0:1973:A:C8	2.41	0.53
30:0:2697:A:H2'	30:0:2698:G:O4'	2.08	0.53
30:0:1766:U:O2	30:0:1778:A:H5'	2.08	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:17:ARG:HD2	38:A:9005:HOH:O	2.07	0.53
17:Q:15:LYS:HD3	30:0:2364:A:H5''	1.89	0.53
31:9:1:U:O3'	31:9:3:A:C5'	2.57	0.53
30:0:644:G:H1'	38:0:6440:HOH:O	2.08	0.53
30:0:1304:U:H2'	30:0:1305:C:C6	2.43	0.53
30:0:121:U:H2'	38:0:9854:HOH:O	2.08	0.53
30:0:682:A:H2'	30:0:683:G:O4'	2.08	0.53
4:D:141:VAL:HG21	31:9:57:A:C8	2.43	0.53
30:0:280:C:H2'	30:0:281:U:O4'	2.07	0.53
30:0:2102:G:C5'	30:0:2538:A:C2	2.91	0.53
30:0:2445:U:H2'	30:0:2446:G:H8	1.72	0.53
30:0:700:A:H5''	30:0:701:U:H5'	1.91	0.53
2:B:154:VAL:HG12	2:B:156:LYS:HG2	1.89	0.53
19:S:37:VAL:O	19:S:41:VAL:HG23	2.08	0.53
30:0:2311:A:H3'	38:0:7716:HOH:O	2.07	0.53
30:0:2354:A:C2	30:0:2367:A:C8	2.97	0.53
30:0:2002:C:H2'	30:0:2003:U:H5'	1.90	0.53
28:2:22:PRO:HG2	28:2:25:VAL:HG23	1.90	0.53
23:W:5:VAL:HG11	23:W:153:MET:CE	2.39	0.53
30:0:482:G:H4'	30:0:508:A:N1	2.24	0.53
14:N:139:TRP:HA	14:N:139:TRP:CE3	2.44	0.53
30:0:1562:C:N4	38:0:5888:HOH:O	2.41	0.53
30:0:407:A:H2'	30:0:408:A:C8	2.44	0.53
27:1:42:SER:HB2	38:1:354:HOH:O	2.08	0.53
30:0:1714:C:O2'	30:0:1715:C:H5'	2.09	0.53
3:C:127:ARG:HD3	3:C:129:HIS:HE1	1.73	0.53
30:0:559:U:C5'	30:0:559:U:H6	2.20	0.53
17:Q:42:LYS:HE2	30:0:952:G:OP1	2.09	0.53
8:H:6:ALA:HB3	30:0:2521:A:OP2	2.09	0.53
4:D:23:VAL:HG21	4:D:45:THR:HG21	1.90	0.53
26:Z:66:CYS:SG	26:Z:67:GLY:N	2.82	0.53
30:0:2764:C:O2'	30:0:2765:C:H5'	2.08	0.53
30:0:2256:G:C2'	30:0:2257:G:C5'	2.86	0.53
30:0:1495:C:H1'	30:0:1573:A:H1'	1.91	0.53
25:Y:141:THR:HG23	38:Y:8892:HOH:O	2.08	0.53
14:N:86:LEU:HD12	14:N:125:ALA:HB2	1.91	0.53
13:M:188:ARG:NH1	30:0:154:C:H3'	2.23	0.53
1:A:190:ARG:NH1	30:0:1845:A:OP2	2.42	0.53
25:Y:132:ASP:OD2	30:0:621:C:H5'	2.08	0.53
8:H:26:ILE:HA	8:H:123:ILE:HG21	1.91	0.53
1:A:192:VAL:CG1	1:A:207:GLN:HB3	2.39	0.53
30:0:1060:C:H6	30:0:1060:C:H5'	1.72	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
10:J:107:ASN:C	10:J:107:ASN:HD22	2.13	0.53
16:P:115:SER:OG	16:P:118:GLN:HG3	2.09	0.52
30:0:603:A:H1'	30:0:605:C:C2	2.43	0.52
14:N:48:VAL:CG1	14:N:55:ASP:HB3	2.39	0.52
30:0:1183:C:C2	30:0:1184:C:C5	2.97	0.52
31:9:13:A:O2'	31:9:14:G:H5''	2.10	0.52
1:A:36:ASP:O	1:A:38:ILE:N	2.41	0.52
30:0:138:U:C5	30:0:140:G:O6	2.62	0.52
30:0:704:C:H2'	30:0:705:C:H6	1.74	0.52
1:A:99:ILE:O	1:A:131:HIS:HE1	1.92	0.52
30:0:2509:A:H2'	30:0:2510:C:O4'	2.09	0.52
30:0:282:C:O2'	30:0:283:U:H4'	2.09	0.52
4:D:134:LEU:HD11	4:D:166:ILE:HD11	1.91	0.52
30:0:1014:A:H2'	30:0:1015:C:H5'	1.92	0.52
30:0:304:G:H1'	30:0:347:A:H61	1.73	0.52
13:M:134:ILE:HG23	13:M:141:ILE:HD13	1.92	0.52
18:R:114:VAL:HA	18:R:144:GLU:O	2.09	0.52
18:R:18:LEU:HB2	18:R:143:VAL:CG1	2.40	0.52
30:0:2359:G:H3'	38:0:5709:HOH:O	2.09	0.52
20:T:28:SER:O	20:T:32:ARG:HG3	2.08	0.52
23:W:88:THR:HG22	23:W:89:ASP:N	2.23	0.52
17:Q:21:ARG:HH12	30:0:2353:A:H1'	1.74	0.52
31:9:42:C:H5'	31:9:43:G:OP2	2.09	0.52
5:E:3:VAL:HG22	5:E:49:ILE:HB	1.91	0.52
30:0:2265:U:H2'	30:0:2266:A:H8	1.75	0.52
7:G:19:GLU:O	7:G:23:ILE:HG13	2.09	0.52
3:C:25:PRO:HG2	38:C:8521:HOH:O	2.08	0.52
18:R:150:PRO:CG	18:R:150:PRO:CB	2.87	0.52
14:N:33:ARG:NH2	31:9:6:C:O2'	2.43	0.52
30:0:1180:U:O2'	30:0:1181:A:H5'	2.10	0.52
30:0:138:U:OP2	30:0:139:C:C5	2.62	0.52
30:0:1724:U:H5''	38:0:3739:HOH:O	2.09	0.52
6:F:13:GLU:OE2	6:F:78:GLU:HG2	2.09	0.52
30:0:1289:C:O2'	30:0:1290:G:H5'	2.09	0.52
4:D:154:LYS:HD2	4:D:154:LYS:N	2.10	0.52
30:0:1185:U:H5'	38:0:7505:HOH:O	2.08	0.52
2:B:267:LYS:HD3	38:0:9567:HOH:O	2.09	0.52
30:0:1249:U:H2'	30:0:1250:C:H6	1.75	0.52
4:D:28:GLY:HA2	4:D:69:ILE:HG23	1.92	0.52
5:E:5:LEU:HD21	5:E:66:GLN:HG3	1.91	0.52
30:0:2072:G:C6	30:0:2533:C:H1'	2.45	0.52
4:D:25:MET:CE	4:D:37:ALA:HB1	2.39	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
30:0:1477:C:H5'	30:0:1868:G:H5'	1.91	0.52
30:0:298:C:H1'	38:0:3853:HOH:O	2.09	0.52
30:0:661:G:C5	30:0:686:A:C2	2.98	0.52
30:0:204:A:H2'	30:0:205:U:H5'	1.92	0.52
30:0:2840:A:H3'	38:0:7686:HOH:O	2.09	0.52
30:0:1175:G:O2'	30:0:1193:A:H2'	2.09	0.52
30:0:1878:G:O2'	30:0:1879:U:C6	2.59	0.52
6:F:2:VAL:HG22	6:F:57:GLU:OE1	2.09	0.52
30:0:1972:U:H2'	30:0:1973:A:H5'	1.91	0.52
13:M:188:ARG:HD3	30:0:155:C:OP2	2.09	0.52
30:0:2604:A:H4'	38:0:7644:HOH:O	2.09	0.52
1:A:217:ARG:HG2	1:A:229:ALA:HB2	1.91	0.52
12:L:121:ILE:HG12	12:L:141:GLU:HB2	1.92	0.52
30:0:2498:C:O2'	30:0:2499:U:H5'	2.09	0.52
30:0:2526:C:O2'	30:0:2527:U:H5'	2.10	0.52
18:R:18:LEU:HB2	18:R:143:VAL:HG12	1.92	0.52
7:G:23:ILE:O	7:G:27:ILE:HG13	2.09	0.52
3:C:16:VAL:HG12	3:C:17:ASP:H	1.73	0.52
5:E:154:ILE:HD11	5:E:157:LYS:HE2	1.92	0.52
30:0:545:G:C8	30:0:545:G:C5'	2.83	0.52
30:0:821:U:H2'	30:0:822:C:C6	2.45	0.52
30:0:734:U:O2'	30:0:736:A:N7	2.37	0.52
17:Q:95:GLU:HA	30:0:949:U:H4'	1.92	0.52
4:D:128:LEU:HB2	38:D:6007:HOH:O	2.08	0.52
30:0:999:C:O2'	30:0:1000:C:H5'	2.10	0.52
30:0:1419:U:H2'	30:0:1685:A:C2	2.45	0.51
30:0:1675:C:H3'	38:0:7847:HOH:O	2.10	0.51
1:A:33:GLU:O	1:A:34:ASP:HB2	2.09	0.51
15:O:37:ARG:HD2	30:0:656:G:OP2	2.09	0.51
2:B:212:GLN:HA	30:0:1733:A:H4'	1.92	0.51
30:0:334:G:C6	30:0:335:U:C4	2.98	0.51
30:0:137:U:OP1	30:0:259:G:O2'	2.28	0.51
15:O:7:LEU:HD22	38:O:5650:HOH:O	2.10	0.51
30:0:2083:A:H3'	38:0:7617:HOH:O	2.10	0.51
30:0:2637:A:OP1	30:0:2637:A:H3'	2.10	0.51
13:M:34:GLU:HB3	13:M:38:GLU:HG3	1.91	0.51
30:0:1393:A:H2'	30:0:1394:C:C6	2.46	0.51
18:R:14:ALA:HB3	18:R:147:LEU:HB2	1.93	0.51
30:0:652:G:H8	38:0:3020:HOH:O	1.93	0.51
30:0:432:G:O2'	30:0:433:C:H5'	2.10	0.51
27:1:16:HIS:CD2	30:0:470:U:O2'	2.63	0.51
8:H:27:PRO:HD3	8:H:123:ILE:HG22	1.91	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
30:0:2493:C:O2	30:0:2493:C:H2'	2.10	0.51
26:Z:76:THR:HG21	30:0:1652:C:H4'	1.91	0.51
30:0:1307:A:H2'	30:0:1308:A:C8	2.46	0.51
30:0:346:U:H4'	38:0:6881:HOH:O	2.10	0.51
26:Z:57:MET:SD	26:Z:73:ARG:HD2	2.51	0.51
30:0:1181:A:H2'	30:0:1182:C:H5'	1.93	0.51
2:B:221:GLN:NE2	11:K:42:ASN:HD22	1.96	0.51
24:X:85:VAL:HG12	24:X:86:GLU:N	2.26	0.51
27:1:8:GLN:HE22	27:1:11:LYS:NZ	2.07	0.51
4:D:62:ASP:HA	38:D:4233:HOH:O	2.10	0.51
30:0:1422:U:H2'	30:0:1423:C:C6	2.46	0.51
31:9:95:C:O2'	31:9:96:C:H5'	2.11	0.51
30:0:466:A:H2'	30:0:467:G:O4'	2.10	0.51
20:T:24:ARG:HH21	20:T:39:ASN:HD22	1.59	0.51
31:9:3:A:OP2	31:9:25:G:N2	2.43	0.51
30:0:553:G:H5'	38:0:3506:HOH:O	2.11	0.51
30:0:120:A:H2'	30:0:120:A:N3	2.26	0.51
30:0:1477:C:O2'	30:0:1478:U:H5'	2.10	0.51
16:P:7:LYS:HG2	16:P:23:PHE:CE2	2.46	0.51
30:0:2329:C:O2'	30:0:2330:U:H5'	2.10	0.51
5:E:21:THR:HG23	5:E:30:THR:OG1	2.11	0.51
30:0:2105:C:H2'	30:0:2106:C:C6	2.45	0.51
30:0:281:U:H2'	30:0:282:C:O4'	2.10	0.51
30:0:282:C:H2'	30:0:283:U:O4'	2.10	0.51
28:2:10:ARG:NH2	30:0:121:U:OP2	2.42	0.51
28:2:38:LYS:HE3	38:0:4239:HOH:O	2.10	0.51
18:R:40:ALA:O	18:R:44:VAL:HG23	2.11	0.51
30:0:1056:U:H2'	30:0:1057:A:O4'	2.11	0.51
10:J:42:GLU:O	10:J:131:THR:HG23	2.11	0.51
30:0:2826:G:C6	30:0:2913:A:N6	2.78	0.51
23:W:81:ASP:OD1	23:W:92:ASP:HB2	2.11	0.51
30:0:1166:A:C6	30:0:1181:A:C2	2.99	0.51
30:0:1181:A:C2'	30:0:1182:C:H5'	2.40	0.51
23:W:13:MET:CE	23:W:17:ILE:HG22	2.41	0.51
30:0:764:C:H2'	30:0:765:G:O4'	2.11	0.51
2:B:223:ARG:HG3	2:B:232:TRP:O	2.10	0.51
30:0:694:A:H2'	30:0:695:C:H5'	1.91	0.51
30:0:1183:C:O2	30:0:1183:C:C2'	2.59	0.51
30:0:1209:C:H2'	30:0:1210:G:H8	1.76	0.51
23:W:80:ASP:HB2	38:W:3312:HOH:O	2.11	0.51
30:0:2786:G:H5''	38:0:4643:HOH:O	2.10	0.51
30:0:951:A:C2'	30:0:952:G:H5'	2.40	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
30:0:2894:C:O2'	30:0:2895:C:H5'	2.11	0.51
18:R:39:THR:HG22	18:R:42:GLU:H	1.75	0.51
31:9:55:U:H4'	31:9:56:A:H8	1.76	0.51
28:2:41:HIS:CD2	28:2:44:ARG:H	2.26	0.51
25:Y:174:VAL:HG23	25:Y:177:LYS:HD2	1.93	0.51
30:0:90:A:H2'	30:0:91:G:O4'	2.11	0.51
30:0:1131:G:C6	30:0:1230:A:C4	2.99	0.51
30:0:255:A:C5	30:0:256:C:C5	2.98	0.51
30:0:255:A:H2'	30:0:256:C:H6	1.76	0.51
38:C:8567:HOH:O	20:T:2:LYS:HE2	2.10	0.51
30:0:172:U:H5'	38:0:4171:HOH:O	2.11	0.51
3:C:63:SER:OG	30:0:2101:A:H2'	2.11	0.51
9:I:114:TYR:CD1	9:I:114:TYR:N	2.80	0.50
23:W:5:VAL:HG11	23:W:153:MET:HE1	1.92	0.50
30:0:305:A:C5	30:0:329:A:C2	2.99	0.50
1:A:173:GLY:O	1:A:176:HIS:HB3	2.10	0.50
27:1:10:LYS:HG3	38:1:2979:HOH:O	2.10	0.50
30:0:2553:A:H2'	30:0:2553:A:N3	2.25	0.50
31:9:29:C:H2'	31:9:30:C:C5'	2.36	0.50
30:0:282:C:O2'	30:0:283:U:C4'	2.59	0.50
6:F:61:MET:HB3	13:M:19:GLN:OE1	2.11	0.50
30:0:512:G:O3'	30:0:513:A:H8	1.93	0.50
1:A:192:VAL:HG12	1:A:207:GLN:HB3	1.93	0.50
30:0:1657:A:H2'	30:0:1658:A:C8	2.46	0.50
30:0:2269:C:C2'	30:0:2270:G:H5'	2.40	0.50
1:A:33:GLU:CD	1:A:33:GLU:H	2.14	0.50
2:B:41:PHE:CZ	2:B:79:MET:HG3	2.46	0.50
30:0:1594:C:O2'	30:0:1607:A:H4'	2.11	0.50
30:0:398:U:H2'	30:0:399:C:C6	2.47	0.50
14:N:37:ARG:NH1	31:9:6:C:OP1	2.44	0.50
6:F:91:VAL:CG1	6:F:92:GLY:H	2.16	0.50
10:J:19:MET:HE3	10:J:132:LEU:HD11	1.92	0.50
21:U:6:CYS:HA	21:U:13:ILE:HD11	1.94	0.50
30:0:1515:A:H2'	30:0:1516:U:C6	2.46	0.50
31:9:75:G:H1	31:9:106:U:H3	1.59	0.50
30:0:23:G:H1'	30:0:520:A:N6	2.26	0.50
31:9:54:A:C2	31:9:55:U:N3	2.80	0.50
13:M:9:ARG:HD2	30:0:380:A:OP2	2.11	0.50
30:0:2589:U:H2'	30:0:2590:U:H6	1.76	0.50
30:0:1903:U:O2'	30:0:1904:A:C8	2.63	0.50
5:E:7:ILE:HG22	5:E:45:ASP:O	2.10	0.50
31:9:59:C:H6	31:9:59:C:O5'	1.94	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
4:D:159:PRO:O	4:D:163:VAL:HG23	2.12	0.50
30:0:10:U:O4	30:0:532:A:OP2	2.30	0.50
30:0:602:A:O2'	30:0:605:C:H4'	2.11	0.50
30:0:1015:C:H2'	30:0:1016:U:C6	2.47	0.50
8:H:19:ARG:HH12	30:0:1008:C:H5''	1.76	0.50
26:Z:50:VAL:O	26:Z:54:GLU:HG3	2.11	0.50
30:0:814:G:H4'	38:0:3140:HOH:O	2.11	0.50
7:G:63:ARG:NH1	30:0:1151:G:OP1	2.45	0.50
20:T:38:ARG:NH1	38:0:6719:HOH:O	2.45	0.50
30:0:2878:U:H2'	30:0:2879:A:O4'	2.12	0.50
11:K:20:CYS:HB2	11:K:29:LEU:HG	1.94	0.50
16:P:14:LEU:HD13	16:P:51:ALA:HB2	1.93	0.50
30:0:1883:U:C2'	30:0:1884:G:H5'	2.42	0.50
30:0:11:A:N3	30:0:11:A:H2'	2.26	0.50
30:0:1588:G:C6	30:0:1589:G:N1	2.80	0.50
31:9:1:U:H4'	31:9:3:A:OP1	2.12	0.50
30:0:2842:G:C2'	30:0:2843:A:H5'	2.41	0.50
30:0:1186:C:N4	30:0:1187:U:C4	2.80	0.50
30:0:1840:A:H4'	30:0:1841:C:O5'	2.12	0.50
30:0:319:A:H4'	30:0:338:C:C4	2.47	0.50
14:N:67:ALA:HA	14:N:71:TRP:HB3	1.93	0.50
30:0:2898:G:O2'	30:0:2899:A:H5'	2.11	0.50
30:0:1947:G:N2	30:0:1966:U:C2	2.80	0.50
30:0:1520:G:H2'	30:0:1521:C:C6	2.46	0.50
30:0:1170:U:H2'	30:0:1172:G:OP2	2.12	0.50
30:0:1759:A:N3	30:0:1818:C:H2'	2.27	0.50
23:W:125:HIS:CE1	30:0:1097:A:H5''	2.47	0.49
30:0:1377:C:H6	30:0:1377:C:C5'	2.19	0.49
2:B:307:ARG:HG3	2:B:307:ARG:NH1	2.26	0.49
10:J:74:ARG:HH11	10:J:74:ARG:HB3	1.76	0.49
30:0:1896:G:C6	30:0:1897:U:C4	3.00	0.49
11:K:4:LEU:HD22	11:K:116:GLU:HB3	1.93	0.49
24:X:43:VAL:HG12	24:X:44:ASP:N	2.26	0.49
12:L:143:THR:HG22	12:L:144:ASP:H	1.78	0.49
30:0:711:G:O2'	30:0:712:C:H5'	2.12	0.49
14:N:5:ARG:HG3	14:N:5:ARG:HH11	1.77	0.49
30:0:1350:U:H5''	38:0:5143:HOH:O	2.11	0.49
30:0:923:A:H2'	38:0:5697:HOH:O	2.12	0.49
23:W:119:HIS:HE1	38:0:9559:HOH:O	1.95	0.49
30:0:2415:A:H2'	30:0:2416:G:H5'	1.94	0.49
1:A:217:ARG:NH2	30:0:1853:C:O2'	2.46	0.49
31:9:107:C:O2'	31:9:108:C:H5'	2.11	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
30:0:1947:G:H2'	30:0:1948:G:H8	1.77	0.49
13:M:75:ARG:HH11	30:0:1864:C:H5	1.59	0.49
30:0:735:C:C5	30:0:736:A:C4	2.99	0.49
9:I:73:LEU:HD12	9:I:107:LYS:HZ1	1.77	0.49
30:0:920:C:H5''	30:0:921:G:O5'	2.13	0.49
30:0:861:A:H4'	30:0:1697:G:H4'	1.94	0.49
30:0:2638:G:H1'	38:0:7796:HOH:O	2.11	0.49
30:0:2134:G:C6	30:0:2258:A:C8	3.01	0.49
1:A:51:ARG:HB2	38:A:9061:HOH:O	2.11	0.49
24:X:21:PRO:HG2	24:X:24:LYS:HD3	1.95	0.49
30:0:1947:G:H2'	30:0:1948:G:C8	2.47	0.49
30:0:939:A:C2	30:0:1027:G:N3	2.81	0.49
30:0:1221:G:C8	38:0:6014:HOH:O	2.55	0.49
27:1:21:ARG:HD2	27:1:37:CYS:SG	2.53	0.49
30:0:2276:U:H2'	30:0:2277:U:C6	2.47	0.49
16:P:61:ARG:NH2	30:0:2737:C:OP2	2.37	0.49
30:0:2651:C:H2'	30:0:2652:U:O4'	2.12	0.49
23:W:125:HIS:CD2	23:W:127:GLY:H	2.31	0.49
31:9:2:U:P	31:9:3:A:H5'	2.52	0.49
30:0:1878:G:O2'	30:0:1879:U:P	2.71	0.49
10:J:75:PRO:HG2	10:J:105:LEU:CD2	2.42	0.49
30:0:2345:A:H3'	30:0:2346:C:C6	2.46	0.49
30:0:1119:G:H22	30:0:1246:A:H2	1.51	0.49
9:I:114:TYR:HD1	9:I:114:TYR:N	2.10	0.49
30:0:370:G:O2'	30:0:371:U:H5'	2.12	0.49
27:1:20:ARG:HH21	30:0:120:A:H5'	1.77	0.49
2:B:17:LYS:O	2:B:260:HIS:HD2	1.94	0.49
3:C:233:THR:HG22	3:C:234:VAL:N	2.26	0.49
30:0:291:C:H2'	30:0:292:G:O4'	2.12	0.49
14:N:159:TYR:HE1	31:9:50:G:H5''	1.78	0.49
30:0:711:G:C2'	30:0:712:C:H5'	2.42	0.49
16:P:54:LYS:HB2	30:0:1717:A:H5''	1.94	0.49
30:0:2385:G:H2'	30:0:2386:U:C6	2.47	0.49
15:O:32:ARG:HD3	15:O:32:ARG:O	2.12	0.49
25:Y:186:ARG:HG2	25:Y:186:ARG:HH11	1.77	0.49
24:X:66:THR:HG23	24:X:67:PRO:HD2	1.95	0.49
17:Q:18:PRO:O	17:Q:21:ARG:HB2	2.12	0.49
30:0:958:G:H2'	30:0:959:C:C6	2.48	0.49
30:0:941:G:C6	30:0:942:U:C4	3.01	0.49
30:0:185:G:H4'	30:0:186:A:H4'	1.93	0.49
30:0:1298:U:H2'	30:0:1299:G:C8	2.48	0.49
9:I:130:LEU:HD22	30:0:1167:G:H4'	1.95	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
8:H:32:ALA:HB3	8:H:69:ARG:HH12	1.78	0.49
30:0:256:C:H2'	30:0:257:G:O4'	2.12	0.49
30:0:699:C:C2	30:0:743:G:N2	2.81	0.49
17:Q:53:HIS:CD2	30:0:2389:U:H4'	2.47	0.49
30:0:806:A:H2'	30:0:807:A:O4'	2.13	0.49
13:M:99:ARG:HD2	13:M:167:GLY:CA	2.35	0.49
30:0:1118:A:C8	30:0:1119:G:H5''	2.48	0.49
1:A:135:VAL:HG21	1:A:147:ARG:HB3	1.94	0.49
12:L:41:HIS:HD2	30:0:926:A:O2'	1.95	0.49
31:9:49:G:O2'	31:9:50:G:H5'	2.13	0.49
30:0:1849:G:H1'	30:0:2011:A:N1	2.28	0.49
30:0:1755:A:H2'	30:0:1756:G:O4'	2.12	0.49
8:H:100:GLU:HB3	8:H:124:VAL:HG11	1.94	0.49
29:3:3:MET:O	29:3:90:PHE:HA	2.12	0.49
30:0:1268:C:H2'	30:0:1269:G:H8	1.77	0.49
30:0:1667:A:H2'	30:0:1668:U:C6	2.48	0.49
30:0:182:G:H5''	38:0:3730:HOH:O	2.13	0.49
30:0:2103:A:N7	30:0:2538:A:N7	2.60	0.49
21:U:56:ARG:NH2	30:0:2890:A:H1'	2.28	0.49
30:0:2064:U:H5'	30:0:2652:U:H4'	1.95	0.49
30:0:699:C:H6	30:0:744:G:O4'	1.96	0.49
30:0:522:U:O2'	30:0:1366:C:H5'	2.13	0.49
30:0:1158:G:O2'	30:0:1159:G:H5'	2.13	0.48
24:X:74:ALA:HB2	24:X:85:VAL:HG13	1.95	0.48
30:0:876:A:N3	30:0:876:A:C2'	2.76	0.48
9:I:101:LYS:O	9:I:105:GLU:HG3	2.12	0.48
2:B:41:PHE:HA	2:B:79:MET:HE2	1.94	0.48
28:2:39:ARG:HG2	38:2:3143:HOH:O	2.13	0.48
14:N:132:ASN:O	14:N:135:VAL:HG12	2.13	0.48
30:0:299:U:H5'	38:0:7377:HOH:O	2.12	0.48
30:0:1909:A:N1	30:0:2128:G:H1'	2.27	0.48
31:9:91:C:H2'	31:9:92:G:O4'	2.13	0.48
13:M:23:LEU:HD13	13:M:27:ARG:NH2	2.28	0.48
11:K:34:VAL:HG22	11:K:47:ALA:HB2	1.94	0.48
1:A:94:LEU:N	1:A:94:LEU:HD23	2.28	0.48
16:P:1:THR:O	30:0:1396:C:H1'	2.13	0.48
10:J:5:GLU:HA	38:J:1652:HOH:O	2.11	0.48
8:H:64:SER:OG	30:0:2520:G:H5'	2.13	0.48
12:L:18:HIS:HD2	30:0:902:G:N7	2.12	0.48
12:L:138:GLY:HA3	38:L:8853:HOH:O	2.13	0.48
30:0:369:G:O2'	30:0:370:G:H5'	2.13	0.48
30:0:2534:C:H1'	38:0:3502:HOH:O	2.12	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
30:0:2768:A:N3	30:0:2768:A:H3'	2.27	0.48
2:B:262:ARG:HG3	30:0:2716:G:H5'	1.95	0.48
30:0:1634:G:H2'	30:0:1635:U:C6	2.48	0.48
30:0:958:G:H2'	30:0:959:C:H6	1.77	0.48
30:0:1778:A:H2'	30:0:1779:A:H5'	1.94	0.48
30:0:652:G:H5''	38:0:3020:HOH:O	2.12	0.48
22:V:56:ILE:O	22:V:60:GLN:HG3	2.14	0.48
13:M:99:ARG:CD	13:M:167:GLY:HA2	2.34	0.48
23:W:125:HIS:HE1	38:W:3071:HOH:O	1.95	0.48
30:0:2032:U:H2'	30:0:2033:G:C5'	2.43	0.48
30:0:2851:G:C2'	30:0:2852:A:H5'	2.44	0.48
30:0:1592:G:O2'	30:0:1593:C:O5'	2.30	0.48
22:V:55:ARG:O	22:V:59:ILE:HG12	2.13	0.48
31:9:54:A:C2'	31:9:55:U:H5'	2.43	0.48
30:0:2315:C:O2'	30:0:2316:G:H5'	2.13	0.48
2:B:217:ARG:HG3	2:B:257:THR:HG22	1.95	0.48
30:0:1972:U:C2'	30:0:1973:A:C5'	2.91	0.48
4:D:25:MET:SD	4:D:40:ILE:HD11	2.53	0.48
4:D:99:ASP:HB3	4:D:103:ASN:H	1.79	0.48
30:0:1625:U:H3'	30:0:1625:U:H6	1.79	0.48
9:I:126:THR:O	9:I:130:LEU:HG	2.14	0.48
30:0:2899:A:O2'	30:0:2900:G:H5'	2.13	0.48
30:0:2900:G:H2'	30:0:2901:C:O4'	2.13	0.48
31:9:31:C:H2'	31:9:32:G:O4'	2.14	0.48
18:R:47:LEU:HB2	18:R:89:LEU:HD21	1.95	0.48
30:0:2906:A:H5'	30:0:2907:C:O4'	2.14	0.48
30:0:1615:A:H5'	38:0:4195:HOH:O	2.13	0.48
30:0:1183:C:H42	30:0:1184:C:N4	2.11	0.48
30:0:368:C:C2'	30:0:369:G:H5'	2.43	0.48
30:0:736:A:H2'	30:0:737:A:O4'	2.14	0.48
25:Y:142:SER:OG	30:0:1331:G:OP2	2.31	0.48
4:D:10:PHE:CG	4:D:11:HIS:N	2.81	0.48
13:M:99:ARG:HE	13:M:170:ASN:ND2	2.10	0.48
23:W:125:HIS:HB2	23:W:137:GLN:HG2	1.94	0.48
30:0:241:A:C2	30:0:378:A:H4'	2.49	0.48
11:K:87:ARG:NH1	38:K:4066:HOH:O	2.46	0.48
8:H:30:LYS:N	8:H:62:HIS:HD2	2.10	0.48
19:S:33:SER:O	19:S:37:VAL:HG23	2.12	0.48
30:0:318:U:H5'	30:0:339:A:C2	2.49	0.48
25:Y:170:SER:OG	25:Y:175:ARG:HG3	2.13	0.48
14:N:154:LEU:C	14:N:156:GLU:H	2.16	0.48
3:C:132:ASP:HB2	3:C:161:ASP:HB3	1.95	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
23:W:130:HIS:O	23:W:136:GLY:HA3	2.13	0.48
30:0:2488:U:O2'	30:0:2489:G:H5'	2.14	0.48
30:0:1173:A:C2	30:0:1177:A:C8	3.02	0.48
30:0:2505:G:C2'	30:0:2506:A:H5'	2.44	0.48
30:0:2672:C:O2'	30:0:2673:U:H5'	2.14	0.48
2:B:310:ARG:HD2	38:B:9112:HOH:O	2.14	0.48
30:0:559:U:C3'	30:0:559:U:C6	2.97	0.48
30:0:1592:G:H2'	30:0:1593:C:H6	1.78	0.48
30:0:2133:U:H4'	30:0:2134:G:C5'	2.44	0.48
30:0:1221:G:H8	38:0:6014:HOH:O	1.94	0.48
30:0:843:A:C2	30:0:846:A:C8	3.02	0.48
30:0:1692:C:H2'	38:0:9867:HOH:O	2.12	0.48
2:B:44:TYR:OH	2:B:148:PRO:HG3	2.13	0.48
30:0:633:C:O2'	30:0:634:G:H5'	2.14	0.48
30:0:2718:C:H5'	30:0:2718:C:C6	2.46	0.48
30:0:1198:U:C6	30:0:1200:A:OP2	2.67	0.48
30:0:484:A:N1	30:0:506:G:H4'	2.29	0.48
30:0:281:U:O2'	30:0:282:C:H5'	2.14	0.48
30:0:2781:U:C2'	30:0:2782:G:C5'	2.91	0.48
23:W:122:ARG:NH2	38:0:6437:HOH:O	2.46	0.48
30:0:334:G:C4	30:0:335:U:C6	3.02	0.48
30:0:660:A:H4'	30:0:661:G:O5'	2.14	0.48
2:B:79:MET:HE1	38:B:9092:HOH:O	2.12	0.48
22:V:4:HIS:HB3	38:V:6622:HOH:O	2.13	0.48
30:0:128:A:O2'	30:0:129:A:H5'	2.14	0.48
30:0:1790:C:H2'	30:0:1791:U:H6	1.78	0.48
38:K:992:HOH:O	30:0:2583:A:H5'	2.13	0.48
3:C:188:ARG:HD3	38:C:8563:HOH:O	2.13	0.48
30:0:2649:A:H5'	30:0:2649:A:H8	1.79	0.48
30:0:1206:U:H2'	30:0:1207:A:O4'	2.14	0.47
30:0:2526:C:H6	30:0:2526:C:C5'	2.18	0.47
4:D:173:GLU:HG3	4:D:174:VAL:HG23	1.96	0.47
30:0:861:A:C4'	30:0:1697:G:H4'	2.44	0.47
15:O:25:VAL:HG12	30:0:709:G:O2'	2.14	0.47
30:0:727:G:H3'	30:0:728:C:H6	1.79	0.47
30:0:559:U:H2'	30:0:560:U:O4'	2.15	0.47
1:A:36:ASP:HB2	1:A:85:SER:H	1.79	0.47
31:9:7:G:C5'	38:9:9100:HOH:O	2.58	0.47
30:0:1634:G:H2'	30:0:1635:U:H6	1.79	0.47
10:J:107:ASN:ND2	10:J:109:TYR:H	2.11	0.47
4:D:23:VAL:HG21	4:D:45:THR:CG2	2.44	0.47
2:B:41:PHE:HB3	2:B:190:MET:HE3	1.95	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
30:0:699:C:C2	30:0:744:G:C2	3.02	0.47
20:T:82:THR:HA	38:0:3998:HOH:O	2.12	0.47
30:0:1855:G:H4'	30:0:1856:C:O5'	2.13	0.47
2:B:280:VAL:HG13	2:B:333:GLU:O	2.13	0.47
30:0:571:C:H6	30:0:571:C:O5'	1.97	0.47
2:B:85:ARG:NH1	38:B:9099:HOH:O	2.47	0.47
10:J:70:PHE:CD1	30:0:2676:C:H4'	2.49	0.47
30:0:1497:G:H4'	30:0:1627:G:O2'	2.14	0.47
15:O:39:THR:HB	38:0:4627:HOH:O	2.14	0.47
25:Y:107:PRO:HB3	25:Y:182:PHE:CD2	2.50	0.47
30:0:619:U:H3'	38:0:3287:HOH:O	2.13	0.47
30:0:816:G:C6	30:0:817:G:N1	2.83	0.47
31:9:76:G:H3'	31:9:77:A:C5'	2.30	0.47
23:W:21:LEU:HD21	23:W:48:VAL:CG1	2.43	0.47
30:0:12:U:C2'	30:0:13:G:H5'	2.40	0.47
2:B:312:ARG:HD3	2:B:315:VAL:HG13	1.95	0.47
30:0:638:C:H2'	30:0:639:A:H8	1.78	0.47
30:0:963:C:O2	30:0:1005:A:N1	2.47	0.47
30:0:1172:G:H1'	38:0:4992:HOH:O	2.14	0.47
27:1:22:CYS:HB3	27:1:37:CYS:SG	2.55	0.47
30:0:1217:G:C2	30:0:1218:U:C2	3.03	0.47
16:P:103:THR:HA	16:P:106:ARG:NH2	2.29	0.47
2:B:27:ASN:H	2:B:27:ASN:HD22	1.63	0.47
30:0:1154:A:H2'	30:0:1155:G:C8	2.49	0.47
30:0:2467:A:H8	38:0:7512:HOH:O	1.97	0.47
30:0:350:G:O2'	30:0:351:A:H5'	2.13	0.47
30:0:724:G:O2'	30:0:725:C:H5'	2.14	0.47
30:0:541:C:C2'	30:0:542:A:C5'	2.81	0.47
31:9:1:U:H5''	31:9:3:A:OP1	2.15	0.47
30:0:1878:G:C1'	38:0:6151:HOH:O	2.51	0.47
30:0:1636:G:O2'	30:0:1637:A:H5'	2.13	0.47
30:0:2614:C:O2'	30:0:2615:U:H5'	2.14	0.47
2:B:307:ARG:HB3	38:B:9117:HOH:O	2.15	0.47
30:0:297:U:H2'	30:0:298:C:C6	2.49	0.47
30:0:255:A:H2'	30:0:256:C:O4'	2.14	0.47
30:0:1856:C:H5'	30:0:1858:A:O4'	2.15	0.47
30:0:74:G:H2'	30:0:75:U:C6	2.49	0.47
6:F:34:ASN:HA	13:M:4:ALA:HB2	1.95	0.47
30:0:2577:A:H5'	38:0:7788:HOH:O	2.14	0.47
1:A:64:ASP:OD2	1:A:66:ARG:HD2	2.15	0.47
30:0:968:G:C2	30:0:1001:U:O2	2.67	0.47
30:0:2121:G:O2'	30:0:2122:C:H5'	2.14	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
30:0:1587:U:H2'	30:0:1588:G:O4'	2.14	0.47
30:0:2524:G:H21	30:0:2526:C:N4	2.12	0.47
30:0:2769:C:H2'	30:0:2770:G:O4'	2.15	0.47
30:0:2842:G:H2'	30:0:2843:A:C5'	2.44	0.47
16:P:59:ARG:O	16:P:63:ARG:HG3	2.15	0.47
13:M:28:GLN:O	13:M:32:ARG:HG3	2.15	0.47
16:P:16:VAL:CG1	16:P:20:ARG:HB2	2.45	0.47
20:T:62:VAL:N	38:T:3851:HOH:O	2.47	0.47
23:W:122:ARG:NH2	38:0:5308:HOH:O	2.48	0.47
1:A:223:ARG:NH2	30:0:2271:G:OP1	2.45	0.47
30:0:736:A:H5''	38:0:4282:HOH:O	2.14	0.47
2:B:242:TRP:CZ2	30:0:2607:U:C4	3.02	0.47
5:E:145:ALA:HB1	5:E:168:ILE:CD1	2.45	0.47
30:0:2587:OMU:O3'	30:0:2587:OMU:HM22	2.15	0.47
30:0:1925:G:O2'	30:0:1926:G:H5'	2.15	0.47
2:B:41:PHE:HB3	2:B:190:MET:CE	2.44	0.47
30:0:1268:C:O2'	30:0:1269:G:H5'	2.15	0.47
30:0:2649:A:H5'	30:0:2649:A:C8	2.50	0.47
6:F:36:THR:HG23	6:F:97:ALA:HB2	1.97	0.47
30:0:1339:G:C6	30:0:1340:G:N1	2.83	0.47
10:J:90:LYS:HB2	35:J:8802:CL:CL	2.51	0.47
3:C:153:VAL:O	3:C:157:LEU:HG	2.15	0.47
11:K:66:ARG:HH22	30:0:1994:A:P	2.37	0.47
30:0:27:U:H5	38:0:5910:HOH:O	1.96	0.47
30:0:758:A:H2'	30:0:759:C:O4'	2.15	0.47
30:0:772:G:H2'	30:0:773:A:O4'	2.15	0.47
2:B:244:PRO:HB3	30:0:1234:U:N3	2.29	0.47
30:0:1803:C:H2'	30:0:1804:A:C8	2.50	0.47
24:X:78:GLU:HB3	38:X:5564:HOH:O	2.15	0.47
31:9:5:G:O2'	31:9:6:C:H5'	2.15	0.47
30:0:1183:C:N3	30:0:1184:C:N4	2.62	0.47
27:1:28:HIS:O	27:1:32:LYS:N	2.47	0.47
30:0:2326:C:H4'	30:0:2412:G:C4'	2.45	0.47
30:0:70:A:H4'	30:0:71:G:O5'	2.15	0.47
31:9:52:A:O2'	31:9:53:G:H5'	2.15	0.47
30:0:24:G:N2	30:0:518:G:H1'	2.30	0.47
3:C:87:ARG:NH2	30:0:894:A:C2	2.83	0.47
5:E:11:VAL:HG12	5:E:12:ASP:N	2.30	0.47
30:0:1204:C:H2'	30:0:1205:U:O4'	2.15	0.47
30:0:2133:U:H4'	30:0:2134:G:H5'	1.96	0.47
18:R:18:LEU:HG	18:R:91:LEU:HD13	1.97	0.47
22:V:44:GLY:O	22:V:48:GLU:HG2	2.15	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
30:0:834:G:H3'	30:0:835:U:H4'	1.97	0.47
30:0:862:U:H2'	30:0:863:G:H8	1.80	0.47
18:R:29:LYS:HE2	30:0:524:A:C5'	2.45	0.47
2:B:139:ASP:HB2	38:B:8997:HOH:O	2.14	0.47
31:9:33:U:H2'	38:9:9066:HOH:O	2.15	0.47
1:A:112:PRO:HD3	1:A:152:CYS:SG	2.55	0.47
6:F:46:GLU:OE1	6:F:100:ASP:HA	2.15	0.47
30:0:625:U:H5''	30:0:1044:C:N4	2.30	0.47
30:0:1181:A:N1	30:0:1192:A:O2'	2.42	0.47
23:W:4:LEU:O	23:W:32:CYS:HA	2.15	0.47
30:0:1641:A:C2'	30:0:1642:A:H5'	2.45	0.47
2:B:62:ARG:HA	2:B:65:MET:HE2	1.97	0.47
30:0:790:A:H1'	30:0:1710:A:H2'	1.97	0.47
30:0:595:U:H2'	30:0:596:C:H6	1.80	0.47
30:0:383:A:H2'	30:0:384:G:O4'	2.15	0.47
13:M:184:ARG:HG3	13:M:185:PRO:HA	1.97	0.47
13:M:123:ASP:OD1	13:M:126:GLN:HG2	2.15	0.47
30:0:1622:G:H2'	30:0:1623:C:H5'	1.97	0.47
14:N:4:PRO:HG3	31:9:69:U:OP1	2.15	0.47
30:0:1116:U:C2'	30:0:1118:A:C2	2.92	0.46
30:0:1589:G:N2	30:0:1605:G:H1'	2.29	0.46
3:C:236:THR:HG22	3:C:239:ALA:CB	2.45	0.46
30:0:2533:C:C6	30:0:2533:C:H5'	2.39	0.46
30:0:737:A:H8	30:0:737:A:O5'	1.98	0.46
1:A:186:TRP:CG	1:A:187:PRO:HA	2.50	0.46
30:0:153:C:O2	30:0:439:A:H2	1.98	0.46
15:O:29:VAL:HG11	15:O:98:LEU:HD21	1.96	0.46
30:0:1196:C:C2	30:0:1197:G:C8	3.03	0.46
30:0:541:C:O2'	30:0:542:A:H5''	2.15	0.46
30:0:2511:A:H2'	30:0:2512:U:O4'	2.15	0.46
30:0:284:C:H6	30:0:284:C:OP2	1.98	0.46
30:0:1819:G:H2'	30:0:1820:G:C4'	2.45	0.46
30:0:2587:OMU:H2'	30:0:2589:U:H5''	1.96	0.46
23:W:13:MET:HE3	23:W:17:ILE:HG22	1.95	0.46
10:J:130:VAL:HG12	10:J:131:THR:N	2.30	0.46
16:P:120:ARG:HD2	30:0:1594:C:OP2	2.16	0.46
30:0:920:C:H4'	30:0:921:G:C2	2.49	0.46
30:0:2791:U:H1'	30:0:2792:A:H5''	1.96	0.46
4:D:77:ASP:HB3	4:D:78:GLU:H	1.55	0.46
31:9:110:G:C6	31:9:111:U:C5	3.03	0.46
30:0:1666:C:HO2'	30:0:1667:A:H5''	1.72	0.46
30:0:2361:A:H2'	30:0:2362:A:O4'	2.15	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:62:ARG:HA	2:B:65:MET:HE3	1.97	0.46
1:A:101:GLU:OE2	1:A:131:HIS:HB2	2.15	0.46
30:0:2269:C:H2'	30:0:2270:G:H5'	1.96	0.46
25:Y:99:ALA:HB2	25:Y:233:TYR:CZ	2.50	0.46
23:W:35:VAL:HA	23:W:36:PRO:HD3	1.80	0.46
30:0:515:C:H5''	38:0:5665:HOH:O	2.13	0.46
30:0:2089:A:O2'	30:0:2090:G:H5'	2.15	0.46
30:0:1706:G:C6	30:0:1707:G:C6	3.04	0.46
30:0:264:G:H1'	30:0:265:U:H5	1.80	0.46
30:0:506:G:N2	30:0:509:A:H5'	2.21	0.46
4:D:129:ASP:OD1	30:0:2338:G:H2'	2.16	0.46
10:J:19:MET:CE	10:J:132:LEU:HD11	2.45	0.46
11:K:87:ARG:NH2	30:0:2720:C:O2	2.49	0.46
30:0:2000:G:O2'	30:0:2001:G:H5'	2.15	0.46
2:B:112:THR:HG23	2:B:158:LYS:HZ2	1.80	0.46
30:0:204:A:C2'	30:0:205:U:H5'	2.45	0.46
30:0:1948:G:H1	30:0:1964:U:H3	1.63	0.46
30:0:1966:U:H6	30:0:1966:U:O5'	1.99	0.46
30:0:128:A:H3'	30:0:128:A:C8	2.50	0.46
30:0:105:G:O2'	30:0:106:A:H5'	2.15	0.46
2:B:125:GLU:O	2:B:129:ARG:HG3	2.15	0.46
30:0:890:C:O2'	30:0:891:G:H5'	2.16	0.46
30:0:254:C:O2	30:0:254:C:H2'	2.14	0.46
30:0:2506:A:N6	30:0:2511:A:O2'	2.49	0.46
23:W:43:GLY:HA3	30:0:945:U:O2'	2.15	0.46
30:0:2326:C:H4'	30:0:2412:G:H4'	1.97	0.46
30:0:1581:A:C5	30:0:1582:C:C5	3.03	0.46
1:A:71:PRO:HD2	1:A:74:VAL:HG21	1.98	0.46
30:0:300:U:C4	30:0:301:C:C5	3.03	0.46
30:0:419:A:H1'	30:0:1921:A:C2	2.51	0.46
16:P:88:GLN:HE22	30:0:1799:G:H21	1.63	0.46
12:L:148:GLU:HA	38:L:8870:HOH:O	2.14	0.46
6:F:101:ALA:HA	38:F:5413:HOH:O	2.15	0.46
2:B:177:HIS:O	2:B:181:ILE:HG13	2.15	0.46
13:M:72:ALA:HB2	13:M:93:ARG:HG2	1.97	0.46
23:W:139:GLY:O	23:W:141:HIS:CD2	2.66	0.46
30:0:1543:G:N1	30:0:1641:A:OP2	2.35	0.46
30:0:441:A:H8	30:0:441:A:O5'	1.97	0.46
11:K:118:ALA:CA	11:K:125:ALA:HB2	2.45	0.46
30:0:129:A:O2'	30:0:131:A:OP1	2.33	0.46
30:0:2775:A:C6	30:0:2799:A:C8	3.04	0.46
23:W:73:LEU:HA	23:W:73:LEU:HD12	1.85	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
30:0:1588:G:C6	30:0:1589:G:C6	3.04	0.46
13:M:86:GLN:HE22	30:0:2274:A:H1'	1.79	0.46
30:0:2658:G:H4'	30:0:2842:G:C8	2.51	0.46
30:0:1393:A:N1	30:0:1725:C:O2'	2.39	0.46
15:O:35:LYS:HD3	38:0:4627:HOH:O	2.15	0.46
2:B:214:PRO:HD2	38:0:9083:HOH:O	2.14	0.46
3:C:214:THR:HG23	38:C:8635:HOH:O	2.16	0.46
30:0:1321:A:H2'	30:0:1322:G:C8	2.51	0.46
30:0:2115:U:H2'	30:0:2116:U:C6	2.51	0.46
15:O:38:ARG:NH1	38:O:7674:HOH:O	2.49	0.46
30:0:1156:C:O5'	30:0:1156:C:H6	1.99	0.46
30:0:1115:U:O2'	30:0:1116:U:H5'	2.15	0.46
30:0:1586:G:O2'	30:0:1587:U:H5'	2.16	0.46
30:0:1973:A:H2'	30:0:1974:G:O4'	2.15	0.46
30:0:2252:A:C6	30:0:2253:G:H1'	2.51	0.46
30:0:1130:U:H2'	30:0:1131:G:O4'	2.16	0.46
1:A:6:GLY:O	30:0:1861:C:H4'	2.15	0.46
9:I:78:ALA:HB1	9:I:93:ALA:HB1	1.96	0.46
30:0:2366:C:O5'	30:0:2366:C:H6	1.99	0.46
31:9:20:G:O2'	31:9:21:G:H5'	2.16	0.46
23:W:119:HIS:CD2	23:W:120:PRO:HD2	2.50	0.46
30:0:2385:G:H2'	30:0:2386:U:H6	1.81	0.46
30:0:2710:U:H2'	30:0:2711:U:C6	2.50	0.46
25:Y:133:HIS:HD2	38:Y:8884:HOH:O	1.98	0.46
30:0:2112:A:H2'	30:0:2113:G:C8	2.50	0.46
30:0:2301:A:H5'	30:0:2302:A:H5'	1.97	0.46
14:N:110:THR:HB	14:N:113:SER:OG	2.16	0.46
30:0:567:U:O2'	30:0:568:G:H5'	2.15	0.46
30:0:1598:A:N6	35:0:8815:CL:CL	2.86	0.46
23:W:26:ILE:HB	38:W:5420:HOH:O	2.15	0.46
22:V:39:ALA:C	22:V:41:GLU:H	2.20	0.46
30:0:440:C:H2'	30:0:441:A:C8	2.51	0.46
30:0:999:C:H2'	30:0:1000:C:O4'	2.16	0.46
30:0:1930:A:H2'	30:0:1931:A:C8	2.51	0.46
30:0:1445:G:N2	30:0:1678:A:H1'	2.31	0.46
4:D:131:THR:HG21	30:0:2348:C:H1'	1.96	0.46
16:P:73:HIS:HE1	30:0:1789:G:O6	1.98	0.46
30:0:417:G:P	38:0:7458:HOH:O	2.73	0.46
4:D:75:LEU:HD22	4:D:79:MET:HB3	1.98	0.46
10:J:54:VAL:HG11	10:J:138:THR:HG21	1.98	0.46
2:B:140:LEU:HD12	2:B:174:ARG:HG3	1.97	0.46
30:0:2831:C:C2'	30:0:2832:C:H5'	2.46	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
18:R:82:GLU:HG3	18:R:83:LYS:N	2.30	0.46
1:A:95:PRO:HA	1:A:153:ARG:HA	1.97	0.45
9:I:112:LEU:HG	30:0:1162:G:O2'	2.15	0.45
30:0:253:U:H1'	30:0:256:C:H41	1.80	0.45
26:Z:46:SER:O	26:Z:50:VAL:HG23	2.16	0.45
30:0:1169:U:C5	30:0:1170:U:C4	3.03	0.45
28:2:28:LYS:O	30:0:87:C:H2'	2.16	0.45
6:F:53:ASP:OD1	6:F:80:GLN:HB2	2.17	0.45
30:0:1456:C:H2'	30:0:1457:U:C6	2.50	0.45
30:0:2299:G:C6	30:0:2300:A:C6	3.05	0.45
30:0:282:C:H1'	30:0:368:C:H41	1.74	0.45
23:W:88:THR:HG21	23:W:96:LEU:HD13	1.98	0.45
13:M:90:ARG:NH2	30:0:2266:A:OP2	2.49	0.45
30:0:2604:A:H5'	38:0:5810:HOH:O	2.16	0.45
25:Y:177:LYS:HD3	25:Y:181:GLY:O	2.17	0.45
30:0:1896:G:C5	30:0:1897:U:C5	3.04	0.45
30:0:861:A:H4'	30:0:1697:G:C4'	2.47	0.45
30:0:1669:G:O2'	30:0:1670:A:H5'	2.16	0.45
30:0:123:U:O2'	30:0:124:C:H5'	2.16	0.45
23:W:56:GLU:O	23:W:143:THR:HG23	2.16	0.45
16:P:36:THR:O	16:P:39:ASP:HB2	2.16	0.45
30:0:851:C:O2	30:0:2022:A:H2	1.99	0.45
30:0:2869:G:H2'	30:0:2870:C:C6	2.51	0.45
14:N:37:ARG:HD3	35:N:8807:CL:CL	2.54	0.45
30:0:1188:A:C5	30:0:1189:A:C2	3.03	0.45
30:0:2712:G:O2'	30:0:2713:G:H5'	2.16	0.45
20:T:26:THR:HA	20:T:39:ASN:HB3	1.98	0.45
30:0:2421:G:H4'	38:0:4797:HOH:O	2.16	0.45
30:0:1314:U:H5''	30:0:1316:G:O4'	2.16	0.45
31:9:39:U:C2'	31:9:40:C:OP1	2.65	0.45
4:D:76:ARG:NE	31:9:44:A:O4'	2.49	0.45
22:V:39:ALA:N	22:V:40:PRO:CD	2.80	0.45
30:0:1788:U:C2	30:0:1805:G:N2	2.84	0.45
1:A:109:GLU:HG2	1:A:116:GLY:N	2.30	0.45
1:A:217:ARG:HH11	1:A:217:ARG:HG3	1.79	0.45
3:C:206:ASN:HB2	30:0:329:A:OP2	2.16	0.45
15:O:32:ARG:HE	15:O:35:LYS:HD2	1.81	0.45
30:0:2664:A:H8	30:0:2664:A:OP1	1.99	0.45
30:0:1309:U:O2'	30:0:1310:U:H5'	2.16	0.45
30:0:1506:U:H5'	30:0:1506:U:H6	1.82	0.45
14:N:44:ARG:HG3	14:N:45:ALA:N	2.32	0.45
3:C:93:LYS:O	3:C:98:ARG:NH2	2.49	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
8:H:52:LEU:HB3	8:H:137:PHE:HB2	1.99	0.45
30:0:1189:A:C3'	38:0:7717:HOH:O	2.59	0.45
17:Q:40:HIS:HE1	30:0:949:U:O2'	1.99	0.45
30:0:1790:C:H2'	30:0:1791:U:C6	2.51	0.45
31:9:110:G:C5	31:9:111:U:C5	3.04	0.45
30:0:397:A:O2'	30:0:417:G:N3	2.39	0.45
30:0:2594:C:O2'	30:0:2595:U:H5'	2.16	0.45
30:0:228:C:H2'	30:0:229:G:H5'	1.98	0.45
30:0:1116:U:H2'	30:0:1118:A:C2	2.52	0.45
9:I:121:LYS:HB3	30:0:1184:C:H4'	1.97	0.45
3:C:129:HIS:HE1	3:C:231:ARG:HA	1.78	0.45
11:K:81:ARG:HD3	11:K:87:ARG:NH1	2.31	0.45
16:P:55:LYS:HD3	30:0:1716:A:H4'	1.97	0.45
18:R:128:ARG:HH12	30:0:840:U:H2'	1.80	0.45
23:W:6:GLN:CB	23:W:26:ILE:HD11	2.45	0.45
30:0:482:G:O4'	30:0:511:A:C2	2.70	0.45
4:D:23:VAL:HG12	4:D:130:VAL:HG22	1.98	0.45
30:0:1002:G:H2'	30:0:1003:U:O5'	2.17	0.45
30:0:1398:G:O2'	30:0:1399:A:H5'	2.16	0.45
28:2:8:LYS:NZ	30:0:1677:U:OP2	2.43	0.45
30:0:2332:A:H5'	30:0:2333:G:OP2	2.17	0.45
30:0:955:A:C2	30:0:1013:A:C4	3.05	0.45
30:0:1563:G:H4'	38:0:4241:HOH:O	2.16	0.45
30:0:158:A:C2'	30:0:159:G:H5'	2.47	0.45
3:C:236:THR:H	3:C:239:ALA:HB3	1.80	0.45
17:Q:11:ARG:HG3	30:0:2363:G:O2'	2.16	0.45
13:M:179:GLY:O	30:0:399:C:H5'	2.17	0.45
30:0:1964:U:C2	30:0:1965:C:C5	3.05	0.45
30:0:228:C:C2'	30:0:229:G:H5'	2.46	0.45
30:0:1023:C:H2'	30:0:1024:G:O4'	2.16	0.45
9:I:87:PRO:HG3	38:0:7157:HOH:O	2.17	0.45
30:0:1503:U:H2'	30:0:1504:A:O4'	2.16	0.45
3:C:35:VAL:HG21	3:C:227:GLY:HA2	1.98	0.45
6:F:72:VAL:HA	6:F:73:PRO:HD3	1.87	0.45
2:B:162:MET:HE2	2:B:310:ARG:HD3	1.99	0.45
12:L:30:ARG:HD2	30:0:164:G:H5''	1.99	0.45
24:X:30:MET:HG2	30:0:1384:C:H5'	1.98	0.45
31:9:60:C:H2'	31:9:61:C:H6	1.81	0.45
25:Y:99:ALA:HB2	25:Y:233:TYR:CE2	2.51	0.45
30:0:1921:A:O2'	30:0:1922:A:H5'	2.17	0.45
23:W:29:VAL:O	23:W:30:ASN:HB2	2.16	0.45
30:0:685:C:O2	30:0:748:C:H4'	2.17	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
30:0:559:U:H3'	30:0:559:U:C6	2.52	0.45
30:0:2251:G:H2'	30:0:2252:A:H8	1.79	0.45
30:0:1573:A:N7	30:0:1574:C:C2	2.85	0.45
30:0:2793:A:H2'	30:0:2794:G:H5'	1.98	0.45
19:S:6:LYS:HB2	19:S:27:ALA:O	2.17	0.45
38:3:9030:HOH:O	30:0:2382:A:H5'	2.16	0.45
14:N:41:LYS:HD3	38:9:9060:HOH:O	2.17	0.45
4:D:15:GLU:HA	4:D:16:PRO:HD3	1.78	0.45
30:0:2316:G:OP1	30:0:2317:C:H1'	2.16	0.45
3:C:127:ARG:HD3	3:C:129:HIS:CE1	2.52	0.45
30:0:2419:U:H5''	30:0:2420:G:C5'	2.46	0.45
23:W:69:ARG:HD2	23:W:117:ARG:O	2.16	0.45
30:0:962:C:C2'	30:0:963:C:H5'	2.47	0.45
28:2:22:PRO:HG2	28:2:25:VAL:CG2	2.47	0.45
30:0:2897:C:O2'	30:0:2898:G:H5'	2.17	0.45
17:Q:3:SER:HB3	38:Q:5998:HOH:O	2.16	0.45
14:N:169:PRO:O	14:N:172:PHE:HB3	2.17	0.45
2:B:199:TYR:HE2	2:B:268:ARG:HB2	1.82	0.45
26:Z:45:VAL:HG12	38:Z:8714:HOH:O	2.17	0.45
5:E:10:ASP:HA	38:E:6017:HOH:O	2.17	0.45
10:J:52:GLN:HE22	30:0:1119:G:H8	1.65	0.45
30:0:1700:C:H5''	30:0:1701:A:OP2	2.16	0.45
23:W:119:HIS:CG	38:0:5308:HOH:O	2.69	0.45
30:0:2002:C:C2'	30:0:2003:U:H5'	2.46	0.45
30:0:1120:U:H6	30:0:1120:U:H5''	1.81	0.45
29:3:11:CYS:HB2	29:3:20:HIS:HE1	1.81	0.45
30:0:1268:C:H2'	30:0:1269:G:C8	2.51	0.45
9:I:108:HIS:H	9:I:109:PRO:HD2	1.82	0.45
5:E:23:GLU:HG2	5:E:28:SER:HB3	1.98	0.45
30:0:249:G:O2'	30:0:250:C:H5'	2.17	0.45
30:0:1209:C:O2'	30:0:1210:G:H5'	2.16	0.44
23:W:88:THR:HG22	23:W:90:TYR:CD1	2.50	0.44
8:H:61:ARG:HG3	8:H:61:ARG:HH11	1.83	0.44
12:L:53:ARG:NH2	12:L:57:VAL:HG12	2.31	0.44
30:0:1904:A:H2'	30:0:1905:U:O4'	2.17	0.44
23:W:68:THR:HG23	23:W:69:ARG:HG2	1.99	0.44
30:0:2831:C:H2'	30:0:2832:C:H5'	1.98	0.44
4:D:140:ARG:HH11	4:D:140:ARG:HG3	1.82	0.44
30:0:62:C:C4	30:0:63:U:C4	3.05	0.44
30:0:81:G:N3	30:0:98:A:C2	2.85	0.44
13:M:6:SER:O	13:M:10:ASP:HB2	2.17	0.44
14:N:43:VAL:HG13	14:N:118:ILE:HD11	1.98	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
30:0:2070:G:H2'	30:0:2072:G:OP1	2.17	0.44
30:0:2103:A:N6	30:0:2538:A:H8	2.09	0.44
30:0:1524:U:H5''	30:0:1524:U:C6	2.52	0.44
27:1:28:HIS:CD2	27:1:31:LYS:HG3	2.52	0.44
30:0:812:A:H2'	30:0:813:C:C6	2.52	0.44
30:0:920:C:H4'	30:0:921:G:N2	2.32	0.44
3:C:54:LEU:HD23	3:C:79:ARG:HG3	1.99	0.44
30:0:177:A:H2'	30:0:178:U:O4'	2.16	0.44
30:0:2072:G:H3'	30:0:2073:G:C5'	2.47	0.44
26:Z:61:HIS:O	26:Z:69:ASP:HA	2.18	0.44
28:2:43:ARG:NH2	30:0:1684:A:H1'	2.25	0.44
14:N:25:ARG:HG2	30:0:2416:G:O2'	2.17	0.44
30:0:1626:A:H2'	30:0:1627:G:C5'	2.48	0.44
30:0:2329:C:H2'	30:0:2330:U:C6	2.52	0.44
31:9:59:C:C4	31:9:60:C:N4	2.86	0.44
5:E:72:MET:O	5:E:76:VAL:HG22	2.18	0.44
11:K:89:LYS:HE2	21:U:19:THR:HG21	2.00	0.44
31:9:97:U:O2'	31:9:98:C:H5'	2.18	0.44
30:0:2297:U:H1'	38:0:5197:HOH:O	2.17	0.44
21:U:37:GLU:HB3	38:U:408:HOH:O	2.18	0.44
1:A:212:PRO:HA	30:0:1943:C:O4'	2.18	0.44
1:A:204:GLY:N	30:0:2634:G:OP2	2.51	0.44
24:X:47:ALA:HB1	24:X:82:GLU:HB3	2.00	0.44
1:A:88:ILE:HD13	1:A:100:PRO:HD3	1.99	0.44
5:E:19:ASP:HA	5:E:31:ARG:O	2.17	0.44
30:0:130:C:H2'	38:0:3168:HOH:O	2.17	0.44
30:0:1712:A:H2'	30:0:1713:G:O4'	2.18	0.44
3:C:168:ARG:NH2	3:C:190:ALA:O	2.51	0.44
30:0:1190:G:H2'	38:0:4068:HOH:O	2.15	0.44
7:G:67:LEU:O	7:G:71:LEU:HG	2.18	0.44
13:M:167:GLY:O	13:M:171:ARG:HG3	2.17	0.44
30:0:506:G:N2	30:0:509:A:H5''	2.30	0.44
30:0:559:U:C4	30:0:560:U:C4	3.06	0.44
30:0:2104:C:O2	30:0:2485:A:N1	2.50	0.44
23:W:90:TYR:N	23:W:90:TYR:CD1	2.85	0.44
30:0:2135:A:C2'	30:0:2136:G:H5'	2.47	0.44
30:0:1592:G:H2'	30:0:1593:C:C6	2.52	0.44
30:0:1523:G:H2'	30:0:1524:U:O4'	2.17	0.44
7:G:64:ASN:N	7:G:64:ASN:ND2	2.66	0.44
1:A:171:LYS:HB2	30:0:820:G:C5	2.53	0.44
30:0:1902:G:O2'	30:0:1903:U:H5'	2.17	0.44
26:Z:78:ILE:HD12	38:Z:8717:HOH:O	2.18	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
30:0:1947:G:N2	30:0:1965:C:O2	2.50	0.44
30:0:1447:U:H3'	30:0:1506:U:O2	2.18	0.44
10:J:39:VAL:HG13	10:J:106:GLY:O	2.17	0.44
30:0:858:U:H2'	30:0:859:C:C6	2.52	0.44
30:0:677:C:O2'	30:0:678:G:H5'	2.17	0.44
5:E:20:ILE:HD11	5:E:40:VAL:HG11	1.99	0.44
12:L:43:HIS:HD2	38:L:8827:HOH:O	2.00	0.44
30:0:1173:A:H3'	38:0:4358:HOH:O	2.16	0.44
30:0:1166:A:OP1	30:0:1174:A:H4'	2.17	0.44
30:0:1182:C:C1'	30:0:1192:A:C8	3.01	0.44
30:0:735:C:H5	30:0:736:A:C4	2.36	0.44
29:3:48:ASN:ND2	30:0:169:A:H1'	2.33	0.44
11:K:125:ALA:C	11:K:127:ALA:H	2.21	0.44
14:N:139:TRP:HA	14:N:139:TRP:HE3	1.81	0.44
30:0:255:A:C4	30:0:256:C:C6	3.06	0.44
30:0:128:A:C8	30:0:128:A:C3'	3.01	0.44
30:0:594:C:C4	30:0:595:U:C4	3.06	0.44
5:E:170:ARG:NH2	38:E:4761:HOH:O	2.50	0.44
30:0:113:A:OP2	30:0:114:A:H2'	2.17	0.44
4:D:41:LEU:HA	4:D:44:ILE:HG22	1.99	0.44
30:0:295:C:H2'	30:0:296:G:O4'	2.18	0.44
30:0:39:G:N2	30:0:444:C:C2	2.86	0.44
30:0:1825:U:O2'	30:0:1826:C:H5'	2.18	0.44
30:0:645:U:O2	30:0:761:A:H2	2.00	0.44
30:0:1052:G:H2'	30:0:1052:G:N3	2.31	0.44
20:T:28:SER:HA	20:T:97:ARG:HD3	2.00	0.44
1:A:199:HIS:HE1	30:0:1881:A:OP1	2.01	0.44
30:0:1318:A:H4'	30:0:1343:C:H4'	2.00	0.44
1:A:179:MET:HG2	1:A:186:TRP:CB	2.48	0.44
1:A:94:LEU:HD12	1:A:98:GLU:HB2	2.00	0.44
30:0:1503:U:C2'	30:0:1504:A:H5'	2.48	0.44
24:X:25:ARG:HD2	38:X:5356:HOH:O	2.16	0.44
30:0:1226:G:H5'	38:0:4543:HOH:O	2.18	0.44
30:0:2087:C:O2'	30:0:2088:C:H5'	2.18	0.44
13:M:80:GLY:O	13:M:81:ARG:HD2	2.17	0.44
30:0:1180:U:H2'	30:0:1181:A:O4'	2.18	0.44
30:0:307:G:H3'	38:0:6719:HOH:O	2.18	0.44
31:9:2:U:H4'	38:9:9103:HOH:O	2.18	0.44
11:K:98:VAL:HG11	11:K:102:GLU:HA	1.98	0.44
18:R:104:PHE:HB3	18:R:109:MET:HE1	2.00	0.44
2:B:304:PRO:HD2	2:B:307:ARG:NE	2.33	0.44
30:0:734:U:H2'	30:0:736:A:OP2	2.18	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
12:L:113:GLN:O	30:0:700:A:N6	2.47	0.44
15:O:105:ASN:HD21	15:O:109:SER:H	1.65	0.44
8:H:39:LYS:HD2	30:0:969:G:H5'	1.98	0.44
30:0:1882:C:H2'	30:0:1883:U:H6	1.83	0.44
30:0:729:C:C2	30:0:743:G:C2	3.06	0.44
30:0:1553:C:O5'	30:0:1553:C:H6	2.00	0.44
30:0:1135:G:H5'	38:0:5953:HOH:O	2.17	0.44
30:0:696:C:O2'	30:0:697:G:H5'	2.17	0.44
5:E:112:ALA:HA	5:E:113:PRO:HD3	1.85	0.44
6:F:1:PRO:H3	6:F:4:VAL:HG23	1.83	0.44
30:0:2533:C:O2'	30:0:2534:C:H5'	2.18	0.44
30:0:2256:G:C6	30:0:2257:G:C4	3.05	0.44
8:H:29:SER:HA	8:H:62:HIS:HD2	1.82	0.44
30:0:1279:U:O2	30:0:1279:U:C2'	2.64	0.44
30:0:812:A:H2'	30:0:813:C:O4'	2.17	0.44
26:Z:66:CYS:SG	26:Z:68:GLU:HB2	2.58	0.44
4:D:52:THR:HG21	30:0:2346:C:O2'	2.17	0.44
30:0:935:G:O2'	30:0:936:C:H5'	2.18	0.44
6:F:59:ILE:HD13	30:0:263:U:O4'	2.17	0.44
4:D:167:GLU:C	4:D:169:THR:H	2.21	0.44
30:0:2914:A:H5''	30:0:2914:A:H8	1.83	0.44
30:0:553:G:O4'	30:0:1325:G:H5'	2.18	0.43
1:A:191:GLY:HA2	1:A:194:MET:HE2	1.99	0.43
30:0:2796:U:H2'	30:0:2797:C:O5'	2.18	0.43
30:0:1342:C:H2'	30:0:1343:C:H5'	2.00	0.43
24:X:23:HIS:CD2	24:X:24:LYS:HG3	2.53	0.43
30:0:1444:G:O2'	30:0:1445:G:H5'	2.18	0.43
14:N:143:ARG:HG2	14:N:172:PHE:CD2	2.52	0.43
8:H:139:ALA:HB3	8:H:149:VAL:HG21	2.00	0.43
30:0:1386:G:O2'	30:0:1387:G:H5'	2.18	0.43
13:M:47:ASP:CG	13:M:48:LYS:N	2.71	0.43
30:0:629:A:H2'	30:0:630:A:O4'	2.18	0.43
15:O:47:ARG:HG3	15:O:47:ARG:HH11	1.82	0.43
30:0:544:G:C3'	30:0:545:G:H5''	2.46	0.43
30:0:2717:C:C2'	30:0:2718:C:C5'	2.81	0.43
30:0:282:C:C2'	30:0:283:U:H5'	2.47	0.43
17:Q:26:PRO:O	17:Q:30:VAL:HG23	2.17	0.43
17:Q:28:ARG:HG2	38:9:9079:HOH:O	2.17	0.43
12:L:71:GLU:HG2	30:0:700:A:C2	2.54	0.43
1:A:48:ASP:HB3	38:A:9061:HOH:O	2.18	0.43
30:0:238:C:H4'	30:0:287:C:OP1	2.18	0.43
5:E:8:PRO:HB2	5:E:11:VAL:HG23	1.99	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
30:0:2332:A:H3'	30:0:2333:G:H8	1.83	0.43
30:0:696:C:O2'	30:0:731:U:OP1	2.35	0.43
15:O:44:ASN:OD1	15:O:65:LEU:HB2	2.18	0.43
16:P:100:ALA:HA	38:0:5526:HOH:O	2.17	0.43
30:0:1705:C:O2	30:0:2735:U:H5''	2.18	0.43
30:0:2761:A:C4	30:0:2763:G:C8	3.06	0.43
30:0:1181:A:H2'	30:0:1182:C:C5'	2.49	0.43
20:T:52:ARG:O	30:0:317:A:OP1	2.36	0.43
25:Y:126:PRO:HG2	25:Y:128:PHE:CZ	2.53	0.43
16:P:7:LYS:HD3	16:P:21:VAL:CG2	2.47	0.43
2:B:232:TRP:CD1	2:B:235:ARG:HD2	2.52	0.43
9:I:120:ALA:O	9:I:124:VAL:HG23	2.18	0.43
30:0:312:U:C2	30:0:320:G:N2	2.87	0.43
24:X:34:ARG:NH1	24:X:48:VAL:O	2.51	0.43
30:0:1098:A:H2'	30:0:1099:G:O4'	2.18	0.43
20:T:53:GLY:HA3	38:T:6384:HOH:O	2.19	0.43
30:0:483:C:N4	30:0:484:A:C6	2.87	0.43
30:0:1889:C:O2'	30:0:1890:U:H5'	2.18	0.43
30:0:2491:G:H5'	38:0:9387:HOH:O	2.19	0.43
6:F:57:GLU:O	6:F:61:MET:HG3	2.18	0.43
1:A:36:ASP:CB	1:A:85:SER:H	2.31	0.43
30:0:815:U:O2'	30:0:1598:A:H4'	2.19	0.43
23:W:44:MET:HE2	30:0:944:G:H21	1.83	0.43
13:M:188:ARG:HH11	30:0:154:C:H3'	1.82	0.43
1:A:187:PRO:HB2	30:0:1845:A:O3'	2.19	0.43
30:0:1622:G:C2'	30:0:1623:C:H5'	2.48	0.43
30:0:300:U:C2	30:0:301:C:C6	3.06	0.43
24:X:15:ARG:HH22	30:0:2856:A:P	2.41	0.43
2:B:329:TYR:CE2	21:U:15:PRO:HG2	2.53	0.43
17:Q:45:PRO:O	30:0:2365:G:H4'	2.18	0.43
30:0:912:A:C4	30:0:1294:A:C2	3.05	0.43
10:J:60:ARG:NH2	30:0:1242:A:OP2	2.45	0.43
2:B:162:MET:CE	2:B:310:ARG:HD3	2.48	0.43
30:0:2421:G:H3'	30:0:2422:U:C5'	2.48	0.43
30:0:2819:C:H2'	30:0:2820:A:C8	2.53	0.43
29:3:70:ARG:HD3	38:3:9064:HOH:O	2.18	0.43
4:D:103:ASN:ND2	4:D:133:ASN:HA	2.33	0.43
18:R:104:PHE:CB	18:R:109:MET:HE1	2.48	0.43
14:N:7:LYS:HB3	17:Q:21:ARG:NH2	2.33	0.43
25:Y:144:ARG:NE	38:Y:8914:HOH:O	2.52	0.43
30:0:962:C:H5''	38:0:4933:HOH:O	2.19	0.43
13:M:147:LEU:O	13:M:150:ILE:HG22	2.18	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
30:0:2247:C:O2'	30:0:2248:C:H5'	2.18	0.43
13:M:158:ARG:HB2	13:M:163:LEU:HB2	2.01	0.43
30:0:844:A:C6	30:0:882:A:C5	3.06	0.43
30:0:213:G:N2	30:0:225:G:H2'	2.34	0.43
23:W:88:THR:CG2	23:W:90:TYR:HD1	2.32	0.43
30:0:2727:A:N1	30:0:2756:U:C2	2.87	0.43
17:Q:25:PRO:HA	17:Q:26:PRO:HD3	1.79	0.43
30:0:1735:C:O2'	30:0:1736:A:H5'	2.18	0.43
27:1:25:LYS:O	27:1:25:LYS:HG2	2.19	0.43
12:L:6:ARG:NH1	30:0:1299:G:N7	2.67	0.43
30:0:2869:G:H5'	38:0:5515:HOH:O	2.18	0.43
23:W:134:GLU:OE2	31:9:97:U:H1'	2.19	0.43
30:0:1482:A:H1'	38:0:9428:HOH:O	2.18	0.43
30:0:653:U:H2'	30:0:654:A:C8	2.53	0.43
30:0:1842:A:C4	30:0:1979:G:C6	3.06	0.43
30:0:2566:A:C2	30:0:2696:G:O4'	2.71	0.43
1:A:9:ARG:HG2	1:A:16:PHE:CD2	2.54	0.43
30:0:451:C:O2'	30:0:452:G:H5'	2.18	0.43
30:0:2812:A:H2	30:0:2814:A:N6	1.86	0.43
30:0:1165:G:H1'	30:0:1174:A:O2'	2.19	0.43
30:0:1184:C:O2'	30:0:1185:U:OP2	2.33	0.43
30:0:1684:A:O2'	30:0:1685:A:H5''	2.18	0.43
31:9:1:U:C4'	31:9:3:A:OP1	2.67	0.43
5:E:101:GLU:HB2	5:E:116:THR:O	2.18	0.43
11:K:74:VAL:HG13	11:K:113:ILE:HG23	2.01	0.43
28:2:40:ARG:HD2	28:2:47:THR:HG22	1.99	0.43
30:0:1524:U:H5''	30:0:1524:U:H6	1.84	0.43
30:0:1477:C:C5'	30:0:1868:G:H5''	2.48	0.43
30:0:2664:A:C8	30:0:2664:A:OP1	2.72	0.43
30:0:629:A:C2	30:0:2074:A:C2	3.07	0.43
13:M:193:LYS:HB3	30:0:392:U:H4'	2.00	0.43
29:3:28:GLY:HA3	30:0:2435:U:OP1	2.18	0.43
30:0:2075:G:C6	30:0:2076:U:C4	3.07	0.43
30:0:1248:A:H3'	38:0:7547:HOH:O	2.17	0.43
31:9:88:G:N2	31:9:89:C:C2	2.87	0.43
18:R:124:GLY:HA3	18:R:136:TRP:O	2.18	0.43
30:0:191:A:C4	30:0:237:G:N7	2.87	0.43
10:J:75:PRO:HD3	10:J:136:SER:OG	2.19	0.43
30:0:111:C:H2'	30:0:112:G:O4'	2.18	0.43
12:L:143:THR:HG21	38:L:8839:HOH:O	2.17	0.43
30:0:1882:C:H2'	30:0:1883:U:C6	2.53	0.43
30:0:1482:A:O2'	30:0:1483:C:H5'	2.18	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
30:0:1545:C:H2'	30:0:1546:G:O4'	2.18	0.43
8:H:46:TYR:HA	8:H:47:PRO:HD3	1.82	0.43
30:0:1157:C:O2'	30:0:1158:G:H5'	2.18	0.43
11:K:41:LYS:HA	30:0:2582:G:O3'	2.19	0.43
30:0:212:A:O3'	30:0:213:G:H4'	2.19	0.43
30:0:2255:A:O2'	30:0:2256:G:H5'	2.18	0.43
13:M:24:GLN:NE2	13:M:27:ARG:NH1	2.67	0.43
30:0:1132:A:H61	30:0:1229:C:H2'	1.83	0.43
30:0:1819:G:H2'	30:0:1820:G:H5'	2.01	0.43
30:0:2096:A:H2'	30:0:2539:U:O4'	2.19	0.43
25:Y:125:LYS:HB2	25:Y:126:PRO:HD2	2.00	0.43
30:0:1883:U:H5'	30:0:2012:U:OP2	2.18	0.43
5:E:40:VAL:HA	5:E:48:VAL:O	2.19	0.43
30:0:47:G:N3	30:0:114:A:C2	2.87	0.43
30:0:2456:A:H2'	30:0:2457:U:C6	2.54	0.43
30:0:1176:C:N4	38:0:9957:HOH:O	2.52	0.43
26:Z:43:GLY:O	26:Z:47:ARG:HG2	2.19	0.43
30:0:1815:A:H4'	30:0:2751:C:O4'	2.19	0.43
30:0:722:G:H22	30:0:938:G:P	2.42	0.43
6:F:48:VAL:CG2	6:F:74:PHE:HB3	2.48	0.43
30:0:2482:G:H4'	30:0:2483:A:C5'	2.48	0.43
30:0:1029:U:O2'	30:0:1273:C:OP1	2.33	0.43
31:9:2:U:OP2	31:9:2:U:H4'	2.19	0.43
6:F:57:GLU:HB2	13:M:23:LEU:HD11	1.99	0.43
14:N:11:ARG:NH1	31:9:8:G:O6	2.52	0.43
21:U:17:THR:CG2	21:U:18:GLY:N	2.82	0.43
30:0:169:A:H5''	38:0:9693:HOH:O	2.18	0.43
30:0:1787:C:O2'	30:0:1788:U:H5'	2.19	0.43
30:0:1520:G:C6	30:0:1521:C:N4	2.87	0.43
30:0:790:A:H2'	30:0:791:A:O4'	2.19	0.43
2:B:148:PRO:HD2	38:B:9048:HOH:O	2.19	0.43
6:F:27:GLY:HA3	6:F:101:ALA:O	2.18	0.43
14:N:164:ASP:OD2	14:N:168:LEU:HG	2.19	0.43
30:0:2729:C:O2'	30:0:2730:G:H5'	2.19	0.43
14:N:116:PHE:HB3	14:N:136:LEU:HD23	2.00	0.43
8:H:65:LEU:HD12	8:H:65:LEU:HA	1.84	0.43
31:9:14:G:O2'	31:9:15:C:H5'	2.19	0.42
30:0:2756:U:H1'	38:0:5024:HOH:O	2.19	0.42
30:0:1315:G:H4'	30:0:1316:G:OP2	2.19	0.42
30:0:365:G:C6	30:0:366:U:C4	3.07	0.42
30:0:1787:C:C4'	30:0:2883:A:O4'	2.67	0.42
30:0:1521:C:H2'	30:0:1522:A:H8	1.84	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
30:0:1044:C:H5''	38:0:9030:HOH:O	2.18	0.42
30:0:1706:G:C5	30:0:1707:G:C6	3.06	0.42
1:A:6:GLY:HA3	38:0:4633:HOH:O	2.19	0.42
18:R:82:GLU:O	18:R:86:LYS:HG3	2.19	0.42
30:0:1894:C:N4	30:0:1939:U:H2'	2.33	0.42
30:0:2866:U:H4'	30:0:2867:G:H5'	2.01	0.42
30:0:85:C:H3'	30:0:86:A:H2'	2.01	0.42
30:0:162:C:H2'	30:0:163:U:H5'	2.01	0.42
30:0:2026:C:O2'	30:0:2027:U:H5'	2.19	0.42
30:0:1189:A:H1'	30:0:1209:C:H1'	2.01	0.42
30:0:1741:U:C4	30:0:2033:G:C8	3.06	0.42
30:0:907:A:H2'	30:0:908:A:C8	2.53	0.42
30:0:1976:G:O2'	30:0:1977:U:H5'	2.19	0.42
2:B:112:THR:HG23	2:B:158:LYS:HZ1	1.84	0.42
30:0:366:U:H2'	30:0:367:G:O4'	2.19	0.42
7:G:12:ILE:N	7:G:13:PRO:HD3	2.35	0.42
2:B:232:TRP:HD1	2:B:235:ARG:HD2	1.83	0.42
30:0:2783:A:H5''	38:0:5252:HOH:O	2.19	0.42
3:C:107:ARG:O	3:C:111:VAL:HG23	2.19	0.42
19:S:10:VAL:HG11	22:V:36:ALA:HA	2.00	0.42
30:0:1603:A:C8	30:0:1605:G:C2	3.07	0.42
4:D:76:ARG:NH1	31:9:42:C:O2	2.49	0.42
29:3:71:CYS:SG	38:3:9052:HOH:O	2.61	0.42
30:0:255:A:H2'	30:0:256:C:C6	2.54	0.42
10:J:74:ARG:O	10:J:78:ILE:HG13	2.19	0.42
15:O:65:LEU:HD13	30:0:746:A:C6	2.54	0.42
30:0:844:A:C6	30:0:882:A:C6	3.07	0.42
26:Z:84:CYS:O	26:Z:85:ASP:HB2	2.19	0.42
30:0:1381:A:N3	30:0:1382:G:H1'	2.34	0.42
5:E:68:HIS:CE1	38:0:6506:HOH:O	2.72	0.42
4:D:104:PHE:CE2	4:D:132:VAL:HB	2.54	0.42
3:C:22:PHE:HA	3:C:116:ALA:HA	2.00	0.42
14:N:108:SER:HA	14:N:109:PRO:HD3	1.82	0.42
30:0:2506:A:O2'	30:0:2507:G:P	2.78	0.42
8:H:158:ASN:ND2	30:0:2502:C:H4'	2.35	0.42
30:0:2780:C:C4	30:0:2781:U:C4	3.08	0.42
30:0:590:A:H2'	30:0:591:A:H5'	2.01	0.42
30:0:2244:A:C4	30:0:2258:A:C2	3.08	0.42
30:0:2414:A:N1	30:0:2415:A:C6	2.87	0.42
1:A:97:ALA:HA	1:A:131:HIS:NE2	2.33	0.42
17:Q:94:GLN:O	17:Q:95:GLU:HB2	2.19	0.42
30:0:26:U:H3'	38:0:5910:HOH:O	2.18	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
18:R:29:LYS:HE2	30:0:524:A:H5'	2.01	0.42
2:B:51:VAL:HG23	2:B:329:TYR:O	2.20	0.42
20:T:64:ASN:HB3	20:T:73:HIS:HB2	2.01	0.42
14:N:73:ALA:HB1	14:N:74:PRO:CD	2.49	0.42
30:0:1681:G:H4'	30:0:1682:A:N3	2.34	0.42
16:P:143:ALA:HA	38:P:5521:HOH:O	2.18	0.42
4:D:156:ARG:NH1	38:D:5234:HOH:O	2.51	0.42
18:R:98:ASN:HD21	30:0:500:G:H21	1.66	0.42
4:D:146:LYS:NZ	14:N:107:ASN:ND2	2.67	0.42
8:H:157:TYR:C	8:H:157:TYR:CD1	2.93	0.42
14:N:37:ARG:HH11	31:9:6:C:C5'	2.28	0.42
13:M:164:THR:CG2	13:M:165:GLY:N	2.82	0.42
31:9:1:U:O3'	31:9:3:A:OP1	2.37	0.42
30:0:2727:A:C5	30:0:2756:U:C4	3.07	0.42
11:K:14:LYS:CB	11:K:45:PRO:HG2	2.43	0.42
23:W:115:THR:HG23	38:W:5420:HOH:O	2.18	0.42
1:A:53:ALA:HB3	38:A:9061:HOH:O	2.18	0.42
30:0:255:A:C5	30:0:256:C:C4	3.08	0.42
31:9:74:G:C6	31:9:75:G:N7	2.87	0.42
30:0:1964:U:O2	30:0:1964:U:H2'	2.18	0.42
30:0:858:U:H2'	30:0:859:C:H6	1.84	0.42
30:0:583:C:H2'	30:0:584:U:H6	1.85	0.42
30:0:2708:G:H2'	30:0:2709:G:O4'	2.19	0.42
3:C:193:LEU:HA	3:C:211:ASP:O	2.20	0.42
5:E:162:PHE:CD1	5:E:162:PHE:N	2.88	0.42
4:D:137:PRO:O	31:9:30:C:OP1	2.37	0.42
22:V:12:THR:HG23	22:V:14:ALA:H	1.85	0.42
30:0:960:G:C8	38:0:5997:HOH:O	2.57	0.42
17:Q:19:ARG:HH22	31:9:11:A:H3'	1.84	0.42
31:9:106:U:O2'	31:9:107:C:H5'	2.20	0.42
30:0:1791:U:O2'	30:0:1792:C:H5'	2.20	0.42
30:0:595:U:O2'	30:0:596:C:H5'	2.20	0.42
21:U:50:GLU:HB2	30:0:2866:U:C5	2.55	0.42
30:0:1748:U:C5	30:0:1749:U:C5	3.08	0.42
13:M:187:LEU:CD2	13:M:194:GLY:HA3	2.49	0.42
30:0:445:U:O2'	30:0:446:G:H5'	2.19	0.42
29:3:91:GLN:O	29:3:92:GLU:HB2	2.19	0.42
30:0:1185:U:C5'	38:0:7505:HOH:O	2.66	0.42
2:B:217:ARG:CD	2:B:257:THR:HG22	2.50	0.42
20:T:32:ARG:NH1	20:T:38:ARG:HH12	2.18	0.42
30:0:1878:G:H5'	38:0:4379:HOH:O	2.19	0.42
30:0:2637:A:C5'	38:0:9282:HOH:O	2.57	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
4:D:40:ILE:HG23	38:D:5583:HOH:O	2.20	0.42
4:D:27:ILE:HB	4:D:69:ILE:O	2.20	0.42
4:D:23:VAL:CG2	4:D:73:VAL:HB	2.50	0.42
30:0:699:C:H2'	30:0:744:G:N3	2.34	0.42
4:D:151:ILE:HB	4:D:156:ARG:HE	1.85	0.42
30:0:2450:C:C2'	30:0:2451:G:O5'	2.67	0.42
30:0:1063:G:H8	38:0:9865:HOH:O	2.02	0.42
30:0:800:G:H2'	30:0:801:U:C6	2.55	0.42
30:0:1555:G:H4'	30:0:1630:A:H2	1.85	0.42
2:B:55:ASN:HB3	2:B:63:GLU:HA	2.00	0.42
14:N:33:ARG:NH1	14:N:103:ASP:OD2	2.51	0.42
13:M:171:ARG:NH2	30:0:189:A:OP1	2.52	0.42
30:0:1119:G:N2	30:0:1246:A:H2	2.10	0.42
31:9:3:A:H2	31:9:21:G:N3	2.18	0.42
30:0:1878:G:O2'	30:0:1879:U:OP2	2.37	0.42
30:0:2135:A:O4'	30:0:2243:C:N4	2.53	0.42
30:0:907:A:H2'	30:0:908:A:H8	1.85	0.42
1:A:153:ARG:CB	1:A:153:ARG:HH11	2.28	0.42
8:H:31:ILE:HG23	38:H:232:HOH:O	2.19	0.42
1:A:217:ARG:CG	1:A:217:ARG:HH11	2.32	0.42
7:G:63:ARG:N	38:G:2569:HOH:O	2.53	0.42
17:Q:55:ARG:HD2	38:Q:2875:HOH:O	2.19	0.42
16:P:41:ARG:NH2	30:0:1500:U:OP2	2.51	0.42
30:0:336:G:H5'	38:0:7404:HOH:O	2.20	0.42
25:Y:134:HIS:HE1	30:0:538:C:OP2	2.02	0.42
6:F:107:ASP:O	6:F:111:ILE:HG13	2.19	0.42
30:0:907:A:H4'	30:0:1328:A:C2	2.54	0.42
30:0:1477:C:H5'	30:0:1868:G:H5''	1.99	0.42
30:0:1167:G:O2'	30:0:1168:C:H5'	2.20	0.42
30:0:1178:G:C6	30:0:1179:C:N4	2.87	0.42
30:0:1343:C:H2'	30:0:1344:G:O5'	2.20	0.42
27:1:8:GLN:HE22	27:1:11:LYS:HZ2	1.68	0.42
30:0:1515:A:H2'	30:0:1516:U:H6	1.83	0.42
30:0:939:A:H2	30:0:1027:G:N3	2.16	0.42
30:0:807:A:C6	30:0:808:A:C6	3.07	0.42
30:0:2113:G:C6	30:0:2114:C:C4	3.08	0.42
21:U:33:SER:O	21:U:37:GLU:HG3	2.18	0.42
30:0:1762:C:H2'	30:0:1763:C:H6	1.84	0.42
30:0:947:U:O2'	30:0:948:G:H5'	2.20	0.42
14:N:171:HIS:CE1	38:N:8858:HOH:O	2.71	0.42
30:0:2007:A:N3	30:0:2627:G:O2'	2.48	0.42
13:M:61:ILE:HG22	13:M:62:VAL:N	2.35	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:C:129:HIS:HD2	3:C:165:ASP:OD2	2.03	0.42
30:0:2765:C:H2'	30:0:2766:A:C8	2.54	0.42
30:0:470:U:H2'	30:0:471:G:O4'	2.20	0.42
8:H:123:ILE:HD12	8:H:123:ILE:N	2.35	0.42
30:0:920:C:H5'	30:0:921:G:C4	2.55	0.42
30:0:1992:U:H2'	30:0:1994:A:OP2	2.19	0.42
18:R:17:MET:HE3	18:R:19:ARG:NH2	2.35	0.42
31:9:26:C:H2'	31:9:27:C:C6	2.55	0.42
30:0:382:U:O2'	30:0:430:A:H1'	2.19	0.42
4:D:88:LEU:N	4:D:89:PRO:CD	2.83	0.42
30:0:1433:G:O2'	30:0:1434:A:H5'	2.20	0.42
5:E:95:VAL:HG11	5:E:131:LEU:HD11	2.02	0.42
30:0:536:A:H4'	38:0:5552:HOH:O	2.18	0.42
27:1:12:ASN:O	30:0:1415:G:H5'	2.19	0.42
30:0:2502:C:O2'	30:0:2503:A:H5'	2.17	0.41
30:0:213:G:O2'	30:0:214:U:OP2	2.38	0.41
2:B:162:MET:HG3	2:B:310:ARG:NH1	2.35	0.41
13:M:58:GLN:NE2	30:0:259:G:H21	2.17	0.41
12:L:57:VAL:HG21	30:0:2443:C:H5'	2.02	0.41
30:0:152:A:H1'	30:0:440:C:O2'	2.21	0.41
1:A:94:LEU:HG	1:A:99:ILE:CD1	2.50	0.41
2:B:27:ASN:HD21	30:0:2807:U:P	2.43	0.41
30:0:2112:A:H2'	30:0:2113:G:H8	1.85	0.41
4:D:146:LYS:NZ	14:N:107:ASN:HD21	2.18	0.41
3:C:8:LEU:HD13	3:C:147:LEU:HD21	2.01	0.41
1:A:72:GLU:HG3	26:Z:90:GLY:HA2	2.01	0.41
6:F:14:ASP:O	6:F:18:GLU:HG3	2.20	0.41
30:0:1950:G:H2'	30:0:1951:G:C8	2.55	0.41
4:D:51:ARG:HH11	4:D:68:PRO:HB3	1.84	0.41
8:H:99:ARG:NH1	30:0:1055:G:OP2	2.53	0.41
11:K:78:LYS:HA	11:K:79:PRO:HD3	1.94	0.41
6:F:118:LEU:O	6:F:119:ARG:HB3	2.20	0.41
14:N:26:LEU:HA	14:N:26:LEU:HD12	1.93	0.41
30:0:1667:A:C2	30:0:1668:U:C2	3.07	0.41
30:0:1890:U:H4'	30:0:2010:A:C6	2.55	0.41
31:9:24:U:H3'	31:9:25:G:C5'	2.51	0.41
6:F:58:GLU:HA	6:F:61:MET:HG3	2.01	0.41
2:B:88:GLU:HB3	2:B:97:LEU:HG	2.01	0.41
30:0:1524:U:C5'	30:0:1524:U:H6	2.33	0.41
12:L:57:VAL:HG12	12:L:57:VAL:O	2.20	0.41
25:Y:144:ARG:NH1	30:0:905:C:OP1	2.54	0.41
12:L:67:ARG:O	12:L:71:GLU:HG3	2.20	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
30:0:969:G:H1	30:0:999:C:N4	2.18	0.41
30:0:1883:U:H2'	30:0:1884:G:H5'	2.02	0.41
30:0:158:A:H2'	30:0:159:G:H5'	2.02	0.41
10:J:39:VAL:HG12	10:J:40:ASN:ND2	2.35	0.41
18:R:9:ASP:HA	18:R:10:PRO:HD2	1.91	0.41
3:C:61:PHE:HB3	38:C:8643:HOH:O	2.20	0.41
30:0:1409:G:H5'	38:0:3732:HOH:O	2.20	0.41
30:0:1871:U:O4'	30:0:1873:G:C8	2.73	0.41
30:0:1414:A:H2	38:0:4921:HOH:O	2.03	0.41
3:C:118:THR:HG22	3:C:137:PRO:HB3	2.00	0.41
10:J:45:VAL:HG11	10:J:121:LEU:HD22	2.02	0.41
30:0:526:U:H2'	30:0:527:U:C6	2.55	0.41
13:M:46:LEU:HG	38:M:8913:HOH:O	2.20	0.41
13:M:49:ALA:C	13:M:54:TYR:HB3	2.40	0.41
23:W:11:VAL:O	23:W:12:ASN:HB2	2.19	0.41
30:0:51:G:O2'	30:0:52:A:H5'	2.20	0.41
30:0:539:G:H2'	30:0:540:A:C8	2.55	0.41
30:0:2245:C:H6	30:0:2245:C:O5'	2.02	0.41
30:0:1119:G:C5	30:0:1243:C:C4	3.08	0.41
30:0:2506:A:O2'	30:0:2507:G:O5'	2.38	0.41
30:0:372:A:H2'	30:0:373:G:C8	2.55	0.41
20:T:21:LYS:HA	20:T:24:ARG:HG3	2.03	0.41
13:M:24:GLN:HE22	13:M:27:ARG:HH11	1.67	0.41
25:Y:212:ARG:HB2	30:0:1315:G:C4	2.55	0.41
30:0:2344:G:N7	38:0:4937:HOH:O	2.49	0.41
25:Y:189:ASN:HD22	25:Y:189:ASN:C	2.23	0.41
30:0:1015:C:O5'	30:0:1015:C:H6	2.02	0.41
30:0:2379:G:N7	30:0:2408:A:N1	2.67	0.41
30:0:2598:U:O2	30:0:2600:A:H8	2.03	0.41
8:H:66:GLU:HA	38:H:232:HOH:O	2.19	0.41
30:0:2330:U:H4'	30:0:2331:C:OP1	2.20	0.41
30:0:708:A:H2'	30:0:709:G:O4'	2.20	0.41
5:E:95:VAL:O	5:E:126:ILE:HD12	2.20	0.41
30:0:2500:C:H1'	38:0:4674:HOH:O	2.20	0.41
30:0:2508:C:H2'	38:0:6793:HOH:O	2.19	0.41
25:Y:151:SER:HB3	25:Y:154:ARG:CB	2.50	0.41
12:L:125:PHE:CE1	12:L:140:VAL:HG13	2.55	0.41
18:R:59:PHE:O	18:R:63:ASN:HB3	2.20	0.41
30:0:2512:U:H4'	30:0:2514:U:O4	2.20	0.41
11:K:41:LYS:O	11:K:42:ASN:HB2	2.20	0.41
11:K:34:VAL:HB	38:K:7169:HOH:O	2.20	0.41
30:0:1058:A:H2'	30:0:1060:C:C5'	2.48	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
30:0:485:A:O2'	30:0:487:G:H5'	2.19	0.41
30:0:735:C:C5	30:0:736:A:N3	2.89	0.41
30:0:1213:C:O2'	30:0:1214:G:H5'	2.21	0.41
30:0:2269:C:H2'	30:0:2270:G:C5'	2.50	0.41
30:0:2011:A:H4'	30:0:2012:U:O5'	2.20	0.41
30:0:2791:U:H4'	30:0:2792:A:OP1	2.20	0.41
2:B:24:PRO:CG	2:B:204:GLY:HA2	2.50	0.41
30:0:393:G:C6	30:0:394:G:C6	3.08	0.41
30:0:2237:G:H1'	38:0:4871:HOH:O	2.20	0.41
30:0:1427:A:O2'	30:0:1428:C:H5'	2.20	0.41
30:0:2375:A:H2'	30:0:2376:C:C6	2.56	0.41
30:0:1603:A:C5'	30:0:1605:G:O4'	2.53	0.41
30:0:284:C:C6	30:0:284:C:OP2	2.73	0.41
2:B:74:ILE:HG13	38:B:9075:HOH:O	2.20	0.41
30:0:1132:A:H2'	30:0:1133:A:C8	2.56	0.41
30:0:1976:G:H1'	30:0:2005:G:N2	2.36	0.41
13:M:133:LEU:O	13:M:134:ILE:HD13	2.21	0.41
31:9:73:A:N1	31:9:108:C:O2	2.54	0.41
30:0:1883:U:O2'	30:0:1884:G:H5'	2.20	0.41
30:0:1522:A:C2	30:0:1665:G:C6	3.09	0.41
30:0:699:C:C6	30:0:744:G:O4'	2.73	0.41
25:Y:182:PHE:HD2	25:Y:200:THR:O	2.03	0.41
2:B:51:VAL:CG2	2:B:327:VAL:HG13	2.50	0.41
30:0:1748:U:C4	30:0:1749:U:C4	3.09	0.41
30:0:1488:U:H4'	30:0:1489:G:OP1	2.21	0.41
30:0:491:C:O2'	30:0:492:C:H5'	2.21	0.41
30:0:2067:A:H2'	30:0:2068:G:O4'	2.20	0.41
1:A:125:ASN:HB3	1:A:158:VAL:HG12	2.02	0.41
23:W:108:ARG:HE	23:W:114:PRO:HG3	1.85	0.41
30:0:1388:U:H2'	30:0:1389:G:O4'	2.20	0.41
4:D:96:SER:C	4:D:98:PHE:H	2.24	0.41
3:C:140:VAL:HG12	3:C:141:SER:N	2.35	0.41
30:0:284:C:H4'	30:0:285:A:H8	1.85	0.41
31:9:2:U:C4'	38:9:9103:HOH:O	2.67	0.41
3:C:184:ARG:HD2	30:0:1306:U:H5''	2.01	0.41
30:0:259:G:O2'	30:0:260:C:H5'	2.20	0.41
2:B:7:ARG:CG	2:B:7:ARG:HH11	2.31	0.41
25:Y:216:ARG:NH1	38:Y:8834:HOH:O	2.53	0.41
30:0:2478:U:H2'	30:0:2479:A:C8	2.55	0.41
30:0:1926:G:H2'	30:0:1927:A:H8	1.84	0.41
30:0:523:C:H2'	30:0:524:A:C8	2.56	0.41
30:0:300:U:N3	30:0:301:C:C5	2.88	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
30:0:1761:U:H2'	30:0:1762:C:C6	2.55	0.41
13:M:139:PRO:HA	13:M:142:GLN:HB2	2.03	0.41
29:3:30:GLN:NE2	38:3:9046:HOH:O	2.51	0.41
30:0:1319:G:H1'	38:0:4701:HOH:O	2.19	0.41
9:I:91:PHE:HD2	9:I:131:GLY:HA2	1.85	0.41
12:L:117:GLU:HG2	38:L:8860:HOH:O	2.20	0.41
30:0:240:C:O2	30:0:240:C:H2'	2.21	0.41
31:9:5:G:C2'	31:9:6:C:H5'	2.50	0.41
4:D:154:LYS:H	4:D:154:LYS:CD	2.09	0.41
30:0:1206:U:C3'	30:0:1206:U:C6	3.04	0.41
30:0:2421:G:H3'	30:0:2422:U:H5''	2.02	0.41
30:0:1523:G:C6	30:0:1524:U:C4	3.09	0.41
10:J:127:ILE:O	10:J:127:ILE:HG12	2.21	0.41
30:0:853:C:H2'	30:0:854:G:O4'	2.21	0.41
30:0:1662:C:H2'	30:0:1663:G:O4'	2.21	0.41
30:0:1417:G:N3	30:0:1417:G:H2'	2.35	0.41
30:0:2597:U:C2'	30:0:2598:U:H5'	2.50	0.41
30:0:64:G:H2'	30:0:65:C:O4'	2.21	0.41
30:0:2878:U:OP1	30:0:2878:U:H6	2.03	0.41
24:X:78:GLU:HG2	24:X:79:GLU:H	1.86	0.41
2:B:137:LEU:HD21	2:B:140:LEU:HD21	2.03	0.41
5:E:111:LYS:HE3	30:0:2690:U:H4'	2.02	0.41
10:J:47:THR:O	10:J:53:ILE:HD11	2.21	0.41
30:0:541:C:H2'	30:0:542:A:H5'	1.95	0.41
9:I:114:TYR:HE1	30:0:1186:C:H4'	1.85	0.41
6:F:91:VAL:CG1	6:F:92:GLY:N	2.78	0.41
26:Z:70:ARG:CD	26:Z:83:TYR:HB2	2.36	0.41
1:A:212:PRO:HB2	38:0:4373:HOH:O	2.20	0.41
30:0:1265:G:H1'	38:0:5020:HOH:O	2.21	0.41
30:0:466:A:C2	30:0:476:A:C4	3.09	0.41
30:0:862:U:H2'	30:0:863:G:C8	2.56	0.41
30:0:2090:G:H2'	30:0:2091:G:C8	2.55	0.41
30:0:123:U:H5'	38:0:6689:HOH:O	2.20	0.41
9:I:108:HIS:N	9:I:109:PRO:HD2	2.35	0.41
26:Z:35:SER:HB3	26:Z:47:ARG:HB2	2.03	0.41
30:0:1762:C:H2'	30:0:1763:C:C6	2.56	0.41
30:0:1576:G:H2'	30:0:1577:U:O4'	2.21	0.41
30:0:60:A:C2	30:0:61:G:C8	3.09	0.41
23:W:59:GLN:NE2	23:W:97:ALA:HB3	2.36	0.41
3:C:84:VAL:HG12	3:C:85:LYS:HG2	2.02	0.41
17:Q:66:LYS:HB2	17:Q:70:ALA:O	2.21	0.41
5:E:91:PHE:HA	5:E:92:PRO:HD3	1.87	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
30:0:1589:G:H22	30:0:1605:G:H1'	1.85	0.41
30:0:2511:A:H4'	38:0:5487:HOH:O	2.21	0.41
30:0:1632:A:C3'	30:0:1633:C:H5'	2.51	0.41
30:0:1878:G:C4'	38:0:6151:HOH:O	2.69	0.41
22:V:12:THR:HB	22:V:15:GLU:OE2	2.20	0.41
1:A:211:LYS:HB3	1:A:212:PRO:CD	2.49	0.41
23:W:122:ARG:HH11	23:W:122:ARG:HG3	1.85	0.41
10:J:75:PRO:HB3	10:J:132:LEU:HB3	2.02	0.41
10:J:132:LEU:HA	10:J:132:LEU:HD23	1.92	0.41
30:0:1592:G:O2'	30:0:1593:C:O4'	2.32	0.41
2:B:307:ARG:HG3	30:0:2837:U:O2	2.21	0.41
30:0:1486:A:H4'	30:0:1487:A:OP2	2.20	0.41
30:0:1250:C:O2'	30:0:1251:C:H5'	2.20	0.41
30:0:711:G:N2	30:0:718:C:C2	2.89	0.41
30:0:2063:U:O4	30:0:2083:A:H2	2.03	0.41
20:T:2:LYS:HG2	30:0:447:A:OP1	2.21	0.41
29:3:3:MET:HG3	29:3:4:PRO:HD2	2.03	0.41
13:M:61:ILE:N	13:M:61:ILE:HD12	2.36	0.41
23:W:11:VAL:HG11	30:0:1086:A:C6	2.56	0.41
12:L:11:ARG:O	30:0:903:U:C2	2.73	0.41
28:2:5:LYS:O	28:2:9:LYS:HG3	2.21	0.41
5:E:132:THR:HB	38:E:2227:HOH:O	2.21	0.41
13:M:65:VAL:HG21	13:M:105:ALA:HB2	2.03	0.41
2:B:195:ARG:HG2	2:B:323:LEU:HD22	2.03	0.41
2:B:150:ALA:O	2:B:152:PRO:HD3	2.21	0.41
30:0:2543:G:H2'	30:0:2544:G:O4'	2.21	0.41
19:S:57:THR:HG22	19:S:58:MET:N	2.35	0.41
23:W:61:THR:HG23	23:W:151:GLU:HG3	2.03	0.41
21:U:44:ARG:HB3	38:U:3805:HOH:O	2.21	0.41
31:9:76:G:O5'	31:9:76:G:H8	2.04	0.41
30:0:1119:G:N2	30:0:1246:A:N1	2.68	0.41
30:0:2712:G:H5'	38:0:5241:HOH:O	2.19	0.41
1:A:233:THR:HB	30:0:1942:A:H5''	2.03	0.41
31:9:93:A:H8	31:9:93:A:O5'	2.04	0.41
30:0:1525:G:OP1	30:0:1525:G:H4'	2.21	0.41
30:0:2361:A:H2'	30:0:2362:A:C8	2.55	0.41
30:0:1771:U:O2'	30:0:1773:G:N7	2.53	0.41
30:0:1167:G:H1	30:0:1179:C:H42	1.69	0.41
1:A:48:ASP:HA	1:A:49:PRO:HD3	1.89	0.41
14:N:154:LEU:O	14:N:155:GLU:HB3	2.21	0.41
12:L:145:LEU:O	12:L:148:GLU:HG3	2.21	0.41
30:0:2088:C:H1'	30:0:2841:A:C2	2.56	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
30:0:2680:A:O2'	30:0:2681:A:C4	2.72	0.41
30:0:2887:G:H2'	30:0:2888:U:O4'	2.20	0.41
17:Q:34:ASP:O	17:Q:37:GLU:HB2	2.21	0.41
12:L:32:ASP:HB3	30:0:222:A:H5''	2.03	0.41
18:R:33:ARG:NH2	38:R:8935:HOH:O	2.54	0.41
30:0:2824:C:H5''	30:0:2825:C:H5'	2.02	0.41
30:0:2318:C:H2'	30:0:2319:C:H6	1.86	0.41
30:0:613:C:C2	30:0:614:U:C5	3.09	0.40
30:0:371:U:H2'	30:0:372:A:H8	1.85	0.40
30:0:1635:U:O2'	30:0:1636:G:H5'	2.19	0.40
28:2:11:LEU:HA	28:2:11:LEU:HD23	1.91	0.40
30:0:1265:G:C5	30:0:1266:U:C5	3.09	0.40
27:1:21:ARG:HD2	27:1:39:PHE:HB2	2.03	0.40
22:V:42:ASN:O	22:V:44:GLY:N	2.55	0.40
13:M:138:HIS:O	13:M:142:GLN:HG3	2.21	0.40
30:0:932:U:O2'	30:0:1296:A:H1'	2.21	0.40
30:0:488:U:H2'	38:0:4016:HOH:O	2.21	0.40
14:N:34:LEU:HD22	14:N:129:ILE:HD13	2.02	0.40
3:C:80:VAL:HA	3:C:81:PRO:HD3	1.88	0.40
30:0:2531:U:O2'	30:0:2532:A:H5'	2.21	0.40
17:Q:64:GLU:HG3	17:Q:74:ASP:OD2	2.21	0.40
13:M:164:THR:HG22	13:M:166:ALA:N	2.36	0.40
14:N:1:ALA:HB2	31:9:14:G:O2'	2.21	0.40
30:0:2010:A:C2'	38:0:5984:HOH:O	2.51	0.40
30:0:1505:U:H4'	38:0:5200:HOH:O	2.22	0.40
30:0:1632:A:H2'	30:0:1633:C:C5'	2.46	0.40
30:0:2716:G:H1'	38:0:3037:HOH:O	2.21	0.40
30:0:1838:U:O2'	30:0:2644:C:H5'	2.21	0.40
30:0:1573:A:H2'	30:0:1574:C:O4'	2.21	0.40
30:0:154:C:H2'	30:0:155:C:H6	1.86	0.40
8:H:100:GLU:HG2	8:H:102:LYS:HB3	2.03	0.40
30:0:634:G:O2'	30:0:1358:A:OP1	2.36	0.40
30:0:625:U:H5'	38:0:3194:HOH:O	2.20	0.40
30:0:2348:C:O2'	30:0:2349:G:H5'	2.21	0.40
30:0:1413:A:H2'	30:0:1414:A:O4'	2.20	0.40
3:C:124:VAL:HA	3:C:230:GLY:O	2.21	0.40
30:0:1252:A:H2'	30:0:1253:C:O4'	2.21	0.40
30:0:2119:C:O2'	30:0:2120:U:H5'	2.22	0.40
25:Y:219:GLU:HG3	25:Y:220:GLU:N	2.36	0.40
30:0:1202:A:C2'	30:0:1203:G:H5'	2.52	0.40
30:0:613:C:H2'	30:0:614:U:C6	2.49	0.40
30:0:2765:C:H2'	30:0:2766:A:H8	1.86	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
31:9:47:A:C2	31:9:48:C:C2	3.09	0.40
27:1:25:LYS:HD2	28:2:48:ASP:HA	2.03	0.40
25:Y:182:PHE:CG	25:Y:202:ALA:HB2	2.57	0.40
30:0:2467:A:H3'	38:0:5475:HOH:O	2.22	0.40
23:W:22:GLU:HG2	23:W:27:HIS:CD2	2.56	0.40
5:E:1:PRO:HG2	5:E:59:MET:SD	2.61	0.40
30:0:1511:U:O2'	30:0:1512:G:H5'	2.22	0.40
2:B:16:ARG:NH2	38:B:9021:HOH:O	2.49	0.40
30:0:622:G:O2'	30:0:623:U:H5'	2.21	0.40
3:C:43:LYS:HG2	30:0:449:A:N7	2.36	0.40
21:U:20:MET:CG	21:U:28:THR:HG23	2.51	0.40
18:R:132:ARG:HG2	18:R:133:ALA:N	2.36	0.40
13:M:176:LYS:HB3	13:M:176:LYS:HE2	1.95	0.40
30:0:1588:G:C5	30:0:1589:G:C6	3.09	0.40
30:0:1603:A:C5'	30:0:1605:G:C5'	2.98	0.40
20:T:97:ARG:NH2	30:0:309:C:OP1	2.54	0.40
5:E:116:THR:CG2	5:E:151:LEU:HD22	2.43	0.40
8:H:6:ALA:HB3	30:0:2521:A:P	2.61	0.40
2:B:141:ARG:N	38:B:9047:HOH:O	2.54	0.40
30:0:2598:U:O2	30:0:2600:A:C8	2.74	0.40
16:P:2:ASP:OD1	30:0:1396:C:H4'	2.21	0.40
30:0:596:C:H2'	30:0:597:A:C8	2.56	0.40
16:P:81:LYS:HB3	30:0:1707:G:O3'	2.21	0.40
30:0:645:U:H2'	30:0:646:G:C8	2.56	0.40
4:D:151:ILE:HA	4:D:152:PRO:HD3	1.95	0.40
30:0:1576:G:H2'	30:0:1577:U:C6	2.56	0.40
30:0:222:A:H2'	30:0:223:G:O4'	2.21	0.40
30:0:1565:C:H2'	30:0:1566:C:H6	1.86	0.40
30:0:1996:U:O2'	30:0:1997:A:H5'	2.21	0.40
30:0:37:A:H2'	30:0:38:G:C8	2.57	0.40
30:0:1915:U:O2'	30:0:1916:C:H5'	2.22	0.40
17:Q:16:ASN:HD22	17:Q:16:ASN:HA	1.71	0.40
8:H:155:ARG:NE	38:H:198:HOH:O	2.54	0.40
30:0:1188:A:C6	30:0:1189:A:C6	3.09	0.40
26:Z:70:ARG:NH2	30:0:1602:C:OP2	2.53	0.40
30:0:535:G:C5	30:0:2063:U:C4	3.09	0.40
14:N:44:ARG:NH1	31:9:4:G:H21	2.20	0.40
6:F:59:ILE:CD1	30:0:263:U:C2	3.04	0.40
8:H:74:ARG:NH1	30:0:2504:A:H4'	2.36	0.40
3:C:135:GLU:HB3	38:C:8576:HOH:O	2.22	0.40
20:T:16:LEU:HB2	30:0:100:C:H4'	2.03	0.40
11:K:64:MET:HA	11:K:67:GLN:HE21	1.87	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	235/240 (98%)	213 (91%)	18 (8%)	4 (2%)	14	45
2	B	335/338 (99%)	309 (92%)	22 (7%)	4 (1%)	19	57
3	C	244/246 (99%)	222 (91%)	22 (9%)	0	100	100
4	D	134/177 (76%)	107 (80%)	22 (16%)	5 (4%)	5	20
5	E	170/178 (96%)	156 (92%)	14 (8%)	0	100	100
6	F	117/120 (98%)	104 (89%)	9 (8%)	4 (3%)	6	23
7	G	25/348 (7%)	23 (92%)	2 (8%)	0	100	100
8	H	156/177 (88%)	145 (93%)	11 (7%)	0	100	100
9	I	68/162 (42%)	54 (79%)	13 (19%)	1 (2%)	15	50
10	J	140/145 (97%)	132 (94%)	8 (6%)	0	100	100
11	K	130/132 (98%)	124 (95%)	6 (5%)	0	100	100
12	L	141/165 (86%)	124 (88%)	14 (10%)	3 (2%)	11	39
13	M	192/196 (98%)	182 (95%)	10 (5%)	0	100	100
14	N	184/187 (98%)	169 (92%)	11 (6%)	4 (2%)	10	37
15	O	113/116 (97%)	108 (96%)	5 (4%)	0	100	100
16	P	141/149 (95%)	138 (98%)	3 (2%)	0	100	100
17	Q	93/96 (97%)	89 (96%)	4 (4%)	0	100	100
18	R	148/155 (96%)	137 (93%)	11 (7%)	0	100	100
19	S	79/85 (93%)	72 (91%)	7 (9%)	0	100	100
20	T	117/120 (98%)	107 (92%)	9 (8%)	1 (1%)	25	66
21	U	51/67 (76%)	48 (94%)	3 (6%)	0	100	100
22	V	63/71 (89%)	58 (92%)	3 (5%)	2 (3%)	6	25
23	W	152/154 (99%)	145 (95%)	6 (4%)	1 (1%)	30	72
24	X	80/92 (87%)	71 (89%)	8 (10%)	1 (1%)	18	54

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
25	Y	140/241 (58%)	140 (100%)	0	0	100	100
26	Z	71/116 (61%)	62 (87%)	8 (11%)	1 (1%)	16	52
27	1	54/57 (95%)	51 (94%)	3 (6%)	0	100	100
28	2	42/50 (84%)	37 (88%)	5 (12%)	0	100	100
29	3	90/92 (98%)	89 (99%)	1 (1%)	0	100	100
All	All	3705/4472 (83%)	3416 (92%)	258 (7%)	31 (1%)	27	68

All (31) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	27	LEU
1	A	36	ASP
1	A	37	VAL
6	F	101	ALA
14	N	154	LEU
14	N	183	ASP
14	N	184	ILE
1	A	34	ASP
4	D	27	ILE
6	F	44	SER
24	X	70	ILE
4	D	97	GLN
12	L	149	ARG
14	N	139	TRP
26	Z	44	ARG
2	B	2	GLN
2	B	184	ASP
4	D	56	ARG
6	F	100	ASP
12	L	80	ASP
22	V	43	PRO
6	F	61	MET
9	I	83	GLY
20	T	53	GLY
23	W	49	ASN
12	L	82	ALA
2	B	34	GLY
2	B	169	GLY
4	D	28	GLY
4	D	137	PRO

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
22	V	40	PRO

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	179/182 (98%)	171 (96%)	8 (4%)	38	77
2	B	282/283 (100%)	268 (95%)	14 (5%)	34	73
3	C	193/193 (100%)	180 (93%)	13 (7%)	23	56
4	D	117/148 (79%)	113 (97%)	4 (3%)	49	86
5	E	152/156 (97%)	148 (97%)	4 (3%)	59	90
6	F	93/94 (99%)	91 (98%)	2 (2%)	64	92
7	G	27/282 (10%)	26 (96%)	1 (4%)	45	84
8	H	134/145 (92%)	128 (96%)	6 (4%)	38	77
9	I	58/130 (45%)	56 (97%)	2 (3%)	49	86
10	J	118/121 (98%)	110 (93%)	8 (7%)	22	55
11	K	106/106 (100%)	103 (97%)	3 (3%)	56	90
12	L	113/127 (89%)	108 (96%)	5 (4%)	39	77
13	M	158/160 (99%)	151 (96%)	7 (4%)	39	77
14	N	149/150 (99%)	147 (99%)	2 (1%)	80	96
15	O	93/94 (99%)	92 (99%)	1 (1%)	84	97
16	P	113/117 (97%)	111 (98%)	2 (2%)	71	94
17	Q	79/80 (99%)	75 (95%)	4 (5%)	33	72
18	R	117/122 (96%)	112 (96%)	5 (4%)	40	78
19	S	71/74 (96%)	71 (100%)	0	100	100
20	T	105/106 (99%)	101 (96%)	4 (4%)	44	83
21	U	44/53 (83%)	42 (96%)	2 (4%)	38	77
22	V	51/57 (90%)	48 (94%)	3 (6%)	28	64
23	W	130/130 (100%)	127 (98%)	3 (2%)	63	92
24	X	66/74 (89%)	63 (96%)	3 (4%)	38	77

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
25	Y	120/196 (61%)	116 (97%)	4 (3%)	50	87
26	Z	60/94 (64%)	59 (98%)	1 (2%)	73	94
27	1	46/47 (98%)	46 (100%)	0	100	100
28	2	42/46 (91%)	41 (98%)	1 (2%)	61	91
29	3	79/79 (100%)	78 (99%)	1 (1%)	80	96
All	All	3095/3646 (85%)	2982 (96%)	113 (4%)	45	84

All (113) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	ARG
1	A	36	ASP
1	A	69	LEU
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	56	ASP
2	B	71	VAL
2	B	132	HIS
2	B	162	MET
2	B	175	LEU
2	B	190	MET
2	B	195	ARG
2	B	254	GLN
2	B	256	GLN
2	B	277	GLU
3	C	2	GLN
3	C	27	ARG
3	C	78	ARG
3	C	94	THR
3	C	136	VAL
3	C	162	VAL
3	C	187	ARG
3	C	214	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	C	234	VAL
3	C	236	THR
3	C	237	GLU
3	C	240	LEU
3	C	243	VAL
4	D	24	HIS
4	D	50	VAL
4	D	100	ASP
4	D	153	THR
5	E	86	VAL
5	E	102	VAL
5	E	126	ILE
5	E	156	ASP
6	F	12	LEU
6	F	119	ARG
7	G	73	ASP
8	H	21	GLU
8	H	65	LEU
8	H	87	LYS
8	H	91	ARG
8	H	157	TYR
8	H	173	GLU
9	I	110	ASP
9	I	114	TYR
10	J	45	VAL
10	J	46	ILE
10	J	52	GLN
10	J	74	ARG
10	J	79	PHE
10	J	107	ASN
10	J	127	ILE
10	J	131	THR
11	K	7	ASP
11	K	10	GLN
11	K	55	VAL
12	L	32	ASP
12	L	35	ARG
12	L	43	HIS
12	L	101	ASP
12	L	104	ASP
13	M	46	LEU
13	M	68	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
13	M	93	ARG
13	M	99	ARG
13	M	116	ASN
13	M	130	GLU
13	M	164	THR
14	N	26	LEU
14	N	138	ASP
15	O	67	SER
16	P	91	LYS
16	P	98	ILE
17	Q	16	ASN
17	Q	18	PRO
17	Q	20	ASP
17	Q	57	ASP
18	R	13	THR
18	R	39	THR
18	R	119	VAL
18	R	123	GLN
18	R	132	ARG
20	T	39	ASN
20	T	48	VAL
20	T	89	ARG
20	T	117	ASP
21	U	52	THR
21	U	53	ASP
22	V	12	THR
22	V	22	ASP
22	V	65	ASP
23	W	35	VAL
23	W	76	ASP
23	W	146	ILE
24	X	27	ASP
24	X	46	ASP
24	X	88	GLU
25	Y	163	THR
25	Y	186	ARG
25	Y	189	ASN
25	Y	203	VAL
26	Z	106	SER
28	2	18	ASN
29	3	3	MET

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (77) such

sidechains are listed below:

Mol	Chain	Res	Type
1	A	199	HIS
2	B	27	ASN
2	B	127	GLN
2	B	145	HIS
2	B	221	GLN
2	B	238	ASN
2	B	260	HIS
2	B	320	GLN
3	C	2	GLN
3	C	39	GLN
3	C	73	GLN
3	C	129	HIS
3	C	151	GLN
4	D	103	ASN
5	E	74	HIS
5	E	119	HIS
5	E	143	GLN
7	G	17	GLN
7	G	64	ASN
8	H	34	HIS
8	H	59	GLN
8	H	62	HIS
8	H	158	ASN
9	I	106	GLN
10	J	52	GLN
10	J	107	ASN
10	J	126	ASN
11	K	10	GLN
11	K	44	HIS
11	K	67	GLN
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	53	ASN
14	N	93	GLN
14	N	107	ASN
16	P	50	GLN
16	P	66	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
16	P	73	HIS
16	P	88	GLN
16	P	118	GLN
17	Q	40	HIS
18	R	94	ASN
18	R	98	ASN
18	R	113	HIS
18	R	117	HIS
19	S	9	HIS
19	S	44	GLN
19	S	53	ASN
20	T	39	ASN
21	U	39	ASN
21	U	48	ASN
22	V	4	HIS
22	V	34	GLN
22	V	60	GLN
23	W	2	HIS
23	W	27	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	149	GLN
25	Y	189	ASN
27	1	8	GLN
27	1	16	HIS
27	1	28	HIS
28	2	18	ASN
28	2	37	HIS
28	2	41	HIS
28	2	45	ASN
29	3	48	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
30	0	2745/2923 (93%)	242 (8%)	22 (0%)
31	9	121/122 (99%)	18 (14%)	1 (0%)

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
All	All	2866/3045 (94%)	260 (9%)	23 (0%)

All (260) 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
30	0	114	A
30	0	115	U
30	0	130	C
30	0	131	A
30	0	138	U
30	0	139	C
30	0	141	C
30	0	151	A
30	0	166	A
30	0	186	A
30	0	191	A
30	0	192	A
30	0	198	A
30	0	204	A
30	0	219	G
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	337	A
30	0	358	G
30	0	368	C
30	0	381	G
30	0	417	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
30	0	461	C
30	0	487	G
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
30	0	553	G
30	0	559	U
30	0	581	G
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	702	G
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	882	A
30	0	885	G
30	0	898	G
30	0	905	C
30	0	920	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
30	0	921	G
30	0	953	G
30	0	960	G
30	0	961	A
30	0	1006	A
30	0	1008	C
30	0	1015	C
30	0	1029	U
30	0	1045	G
30	0	1059	G
30	0	1060	C
30	0	1072	G
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	1151	G
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	1357	A
30	0	1360	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
30	0	1377	C
30	0	1378	G
30	0	1407	A
30	0	1409	G
30	0	1474	C
30	0	1492	A
30	0	1505	U
30	0	1506	U
30	0	1524	U
30	0	1525	G
30	0	1526	A
30	0	1528	A
30	0	1535	G
30	0	1559	A
30	0	1592	G
30	0	1625	U
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	1730	G
30	0	1731	C
30	0	1752	G
30	0	1774	G
30	0	1778	A
30	0	1779	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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
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
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	2469	A
30	0	2476	C
30	0	2483	A
30	0	2507	G
30	0	2509	A
30	0	2511	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
30	0	2526	C
30	0	2527	U
30	0	2533	C
30	0	2537	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	2613	G
30	0	2638	G
30	0	2649	A
30	0	2664	A
30	0	2676	C
30	0	2681	A
30	0	2682	C
30	0	2718	C
30	0	2719	A
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	2914	A
31	9	2	U
31	9	7	G
31	9	14	G
31	9	22	G
31	9	23	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
31	9	24	U
31	9	25	G
31	9	39	U
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 (23) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
30	0	69	A
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	1237	U
30	0	1246	A
30	0	1352	A
30	0	1377	C
30	0	1474	C
30	0	1506	U
30	0	1692	C
30	0	2467	A
30	0	2526	C
30	0	2536	C
30	0	2649	A
30	0	2681	A
30	0	2718	C
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	20,22,23	0.72	1 (5%)	24,31,34	0.73	0
30	OMG	0	2588	30	24,26,27	0.84	1 (4%)	32,38,41	5.05	3 (9%)
30	UR3	0	2619	30	20,22,23	0.73	0	23,32,35	0.87	0
30	PSU	0	2621	30	19,21,22	1.11	3 (15%)	23,30,33	1.10	2 (8%)
30	1MA	0	628	30	23,25,26	0.85	0	32,37,40	0.94	1 (3%)

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	-	0/8/27/28	0/2/2/2
30	OMG	0	2588	30	-	0/10/27/28	0/1/3/3
30	UR3	0	2619	30	-	0/6/25/26	0/2/2/2
30	PSU	0	2621	30	-	0/8/25/26	0/2/2/2
30	1MA	0	628	30	-	1/8/25/26	0/1/3/3

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	0	2621	PSU	C2-N1	2.73	1.42	1.37
30	0	2588	OMG	P-OP1	2.32	1.49	1.46
30	0	2621	PSU	C6-N1	2.24	1.34	1.32
30	0	2587	OMU	P-OP1	2.11	1.49	1.46
30	0	2621	PSU	P-OP1	2.04	1.49	1.46

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	0	2588	OMG	C6-C5-N7	-28.00	130.37	134.14
30	0	628	1MA	C2-N3-C4	-3.29	110.61	116.23
30	0	2588	OMG	C6-N1-C2	3.26	125.21	119.51
30	0	2621	PSU	C5-C4-N3	-2.26	114.74	118.86
30	0	2588	OMG	C2-N3-C4	-2.24	111.94	115.09
30	0	2621	PSU	C5-C1'-C2'	-2.10	111.90	115.61

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
30	0	628	1MA	C2'-C1'-N9-C8

There are no ring outliers.

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

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.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	237/240 (98%)	-0.18	10 (4%) 35 41	34, 56, 94, 116	0
2	B	337/338 (99%)	-0.50	1 (0%) 91 95	34, 58, 89, 99	0
3	C	246/246 (100%)	-0.38	1 (0%) 90 94	32, 51, 75, 87	0
4	D	140/177 (79%)	1.64	53 (37%) 1 0	69, 106, 134, 144	0
5	E	172/178 (96%)	0.24	15 (8%) 10 13	49, 73, 97, 102	0
6	F	119/120 (99%)	0.14	9 (7%) 14 17	52, 76, 109, 124	0
7	G	29/348 (8%)	0.98	7 (24%) 1 2	79, 103, 110, 113	0
8	H	160/177 (90%)	-0.16	5 (3%) 47 55	53, 73, 107, 111	0
9	I	70/162 (43%)	3.42	44 (62%) 0 0	137, 155, 173, 175	0
10	J	142/145 (97%)	-0.56	0 100 100	43, 57, 77, 99	0
11	K	132/132 (100%)	-0.33	5 (3%) 38 45	39, 54, 79, 83	0
12	L	145/165 (87%)	0.48	11 (7%) 14 17	32, 71, 123, 134	0
13	M	194/196 (98%)	-0.53	1 (0%) 88 93	35, 49, 64, 71	0
14	N	186/187 (99%)	0.02	15 (8%) 12 15	51, 74, 121, 131	0
15	O	115/116 (99%)	-0.49	0 100 100	44, 61, 78, 85	0
16	P	143/149 (95%)	-0.32	1 (0%) 84 90	47, 61, 74, 83	0
17	Q	95/96 (98%)	-0.54	0 100 100	44, 55, 72, 85	0
18	R	150/155 (96%)	-0.47	0 100 100	37, 51, 73, 84	0
19	S	81/85 (95%)	-0.06	2 (2%) 54 64	49, 64, 87, 97	0
20	T	119/120 (99%)	-0.24	3 (2%) 54 64	42, 62, 92, 121	0
21	U	53/67 (79%)	0.10	1 (1%) 64 72	51, 64, 83, 91	0
22	V	65/71 (91%)	0.97	12 (18%) 2 3	53, 76, 130, 134	0
23	W	154/154 (100%)	-0.75	0 100 100	41, 56, 74, 88	0
24	X	82/92 (89%)	-0.14	3 (3%) 39 47	49, 66, 91, 108	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
25	Y	142/241 (58%)	-0.66	1 (0%) 84 90	34, 48, 72, 94	0
26	Z	73/116 (62%)	0.50	10 (13%) 4 5	59, 77, 92, 101	0
27	1	56/57 (98%)	-0.50	0 100 100	33, 39, 48, 56	0
28	2	46/50 (92%)	-0.20	1 (2%) 59 67	41, 69, 102, 114	0
29	3	92/92 (100%)	-0.17	2 (2%) 59 67	43, 65, 78, 91	0
30	0	2754/2923 (94%)	-0.23	54 (1%) 62 71	28, 51, 95, 171	0
31	9	122/122 (100%)	-0.18	3 (2%) 54 64	45, 72, 95, 154	0
All	All	6651/7517 (88%)	-0.15	270 (4%) 35 43	28, 57, 106, 175	0

All (270) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
31	9	1	U	13.5
9	I	71	ALA	13.1
9	I	74	ILE	12.4
22	V	1	THR	12.2
9	I	80	PHE	9.8
22	V	43	PRO	9.8
9	I	72	GLU	9.4
9	I	82	THR	8.1
14	N	166	ALA	8.1
9	I	70	THR	7.9
9	I	132	VAL	7.9
9	I	79	GLY	7.7
12	L	60	GLU	7.3
9	I	83	GLY	7.1
9	I	128	THR	7.1
9	I	88	GLN	6.9
26	Z	35	SER	6.8
30	0	735	C	6.5
9	I	81	GLU	6.4
4	D	63	ILE	6.2
20	T	119	ALA	5.7
4	D	69	ILE	5.5
9	I	92	VAL	5.5
9	I	112	LEU	5.5
7	G	27	ILE	5.5
26	Z	46	SER	5.4
4	D	26	GLY	5.3
14	N	147	ILE	5.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
30	0	1169	U	5.2
1	A	37	VAL	5.2
4	D	10	PHE	5.1
4	D	85	GLN	5.1
4	D	18	ILE	5.0
14	N	138	ASP	5.0
4	D	44	ILE	4.9
9	I	93	ALA	4.9
22	V	39	ALA	4.8
9	I	91	PHE	4.6
4	D	90	LEU	4.6
30	0	1170	U	4.6
22	V	40	PRO	4.6
4	D	128	LEU	4.5
9	I	97	VAL	4.5
30	0	1172	G	4.5
9	I	69	PRO	4.5
4	D	57	THR	4.5
9	I	111	LEU	4.5
1	A	35	GLY	4.5
9	I	131	GLY	4.5
4	D	27	ILE	4.5
5	E	108	LEU	4.5
4	D	25	MET	4.4
12	L	106	VAL	4.4
30	0	970	U	4.4
9	I	75	LYS	4.4
9	I	84	SER	4.3
30	0	1168	C	4.2
12	L	99	GLU	4.2
4	D	93	LEU	4.2
8	H	158	ASN	4.2
26	Z	58	ASN	4.2
4	D	107	GLY	4.1
4	D	23	VAL	4.1
6	F	106	ALA	4.1
31	9	2	U	4.1
4	D	70	GLY	4.0
4	D	75	LEU	4.0
4	D	134	LEU	4.0
30	0	1192	A	4.0
9	I	66	GLY	4.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
30	0	1190	G	4.0
30	0	1207	A	4.0
4	D	89	PRO	3.9
30	0	2237	G	3.9
9	I	129	SER	3.9
16	P	67	LYS	3.9
30	0	1181	A	3.9
30	0	138	U	3.9
9	I	130	LEU	3.9
4	D	104	PHE	3.9
22	V	46	ILE	3.9
4	D	92	GLU	3.9
4	D	130	VAL	3.8
30	0	1171	A	3.8
14	N	75	THR	3.8
4	D	40	ILE	3.8
5	E	157	LYS	3.8
5	E	154	ILE	3.8
9	I	86	GLU	3.7
22	V	52	ALA	3.7
12	L	105	TYR	3.6
4	D	106	PHE	3.6
9	I	127	CYS	3.6
30	0	1166	A	3.6
14	N	165	ALA	3.5
26	Z	50	VAL	3.5
22	V	51	LYS	3.5
20	T	118	SER	3.5
9	I	109	PRO	3.4
5	E	10	ASP	3.4
9	I	76	ASP	3.4
4	D	41	LEU	3.4
9	I	113	SER	3.4
4	D	165	PHE	3.4
9	I	133	THR	3.4
31	9	24	U	3.4
30	0	1175	G	3.4
30	0	1164	U	3.3
30	0	1174	A	3.3
4	D	172	VAL	3.3
5	E	45	ASP	3.3
30	0	1173	A	3.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
30	0	1193	A	3.2
12	L	100	ALA	3.2
30	0	1195	G	3.1
5	E	156	ASP	3.1
4	D	24	HIS	3.1
5	E	109	GLY	3.1
30	0	282	C	3.1
30	0	1208	C	3.1
4	D	135	VAL	3.1
24	X	10	VAL	3.0
5	E	11	VAL	3.0
22	V	44	GLY	3.0
5	E	6	GLU	3.0
22	V	48	GLU	3.0
4	D	98	PHE	3.0
4	D	102	GLY	2.9
4	D	154	LYS	2.9
30	0	1167	G	2.9
26	Z	45	VAL	2.9
30	0	1163	G	2.9
4	D	88	LEU	2.9
4	D	17	ARG	2.9
7	G	26	MET	2.9
4	D	73	VAL	2.9
12	L	62	ALA	2.9
30	0	1177	A	2.8
5	E	161	VAL	2.8
7	G	28	GLU	2.8
9	I	94	ASP	2.8
26	Z	55	SER	2.8
22	V	2	VAL	2.8
30	0	1165	G	2.8
30	0	736	A	2.8
30	0	1191	A	2.8
4	D	11	HIS	2.8
14	N	158	LEU	2.8
1	A	237	GLY	2.8
8	H	40	GLN	2.8
4	D	43	GLU	2.8
6	F	49	PHE	2.8
1	A	236	GLY	2.8
9	I	104	ALA	2.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
30	0	999	C	2.7
28	2	39	ARG	2.7
11	K	129	THR	2.7
30	0	1206	U	2.7
4	D	101	THR	2.7
5	E	76	VAL	2.7
4	D	173	GLU	2.7
30	0	1199	A	2.6
4	D	45	THR	2.6
4	D	129	ASP	2.6
30	0	1202	A	2.6
1	A	99	ILE	2.6
11	K	132	VAL	2.6
6	F	119	ARG	2.6
1	A	31	LYS	2.6
6	F	44	SER	2.6
14	N	134	ASP	2.6
5	E	89	SER	2.6
4	D	81	GLU	2.6
25	Y	235	GLU	2.6
11	K	108	GLU	2.5
14	N	113	SER	2.5
9	I	126	THR	2.5
9	I	73	LEU	2.5
19	S	81	ILE	2.5
30	0	1161	A	2.5
9	I	99	GLN	2.5
30	0	1162	G	2.5
30	0	1176	C	2.5
4	D	166	ILE	2.5
30	0	1947	G	2.5
26	Z	44	ARG	2.5
26	Z	49	ARG	2.4
30	0	1182	C	2.4
30	0	1198	U	2.4
11	K	118	ALA	2.4
5	E	128	GLY	2.4
14	N	159	TYR	2.4
12	L	66	VAL	2.4
9	I	87	PRO	2.4
30	0	280	C	2.4
11	K	125	ALA	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
19	S	76	GLU	2.4
9	I	100	VAL	2.4
6	F	15	ASP	2.4
7	G	23	ILE	2.4
6	F	117	GLU	2.4
22	V	3	LEU	2.4
9	I	78	ALA	2.4
4	D	64	ARG	2.3
13	M	194	GLY	2.3
24	X	80	GLU	2.3
9	I	108	HIS	2.3
20	T	82	THR	2.3
4	D	157	LEU	2.3
26	Z	34	SER	2.3
4	D	91	ALA	2.3
1	A	103	VAL	2.3
9	I	125	GLY	2.3
30	0	1189	A	2.3
9	I	103	ILE	2.3
12	L	130	ARG	2.3
3	C	135	GLU	2.2
4	D	95	THR	2.2
12	L	59	GLU	2.2
6	F	16	ALA	2.2
30	0	2004	U	2.2
30	0	130	C	2.2
30	0	2508	C	2.2
14	N	155	GLU	2.2
30	0	969	G	2.2
22	V	49	LEU	2.2
30	0	1178	G	2.2
4	D	105	SER	2.2
5	E	91	PHE	2.2
26	Z	38	PHE	2.2
30	0	2769	C	2.2
9	I	67	VAL	2.1
4	D	96	SER	2.1
30	0	1200	A	2.1
6	F	97	ALA	2.1
1	A	34	ASP	2.1
29	3	83	TRP	2.1
4	D	170	TYR	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
6	F	75	ILE	2.1
14	N	140	GLN	2.1
4	D	56	ARG	2.1
21	U	47	ARG	2.1
4	D	84	LEU	2.1
9	I	110	ASP	2.1
14	N	137	ALA	2.1
30	0	1180	U	2.1
30	0	1913	C	2.1
7	G	71	LEU	2.1
2	B	115	VAL	2.1
14	N	145	ALA	2.1
4	D	158	ASN	2.1
29	3	8	ASN	2.1
1	A	153	ARG	2.1
8	H	39	LYS	2.1
14	N	149	GLU	2.1
8	H	42	ASP	2.0
30	0	1951	G	2.0
12	L	149	ARG	2.0
7	G	24	VAL	2.0
12	L	80	ASP	2.0
5	E	32	ARG	2.0
30	0	1965	C	2.0
30	0	1194	A	2.0
30	0	2103	A	2.0
7	G	72	ASP	2.0
1	A	68	ILE	2.0
14	N	152	GLU	2.0
24	X	88	GLU	2.0
30	0	10	U	2.0
8	H	86	TYR	2.0

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

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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q < 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
30	UR3	0	2619	21/22	0.14	1.23	42,44,47,47	0
30	OMG	0	2588	24/25	0.13	0.72	36,39,42,43	0
30	1MA	0	628	23/24	0.17	0.49	33,37,38,39	0
30	OMU	0	2587	21/22	0.12	-0.21	38,40,44,45	0
30	PSU	0	2621	20/21	0.15	-0.75	34,35,47,48	0

6.3 Carbohydrates

There are no carbohydrates in this entry.

6.4 Ligands

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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
36	SR	0	9006	1/1	1.82	3413.00	200,200,200,200	0
34	NA	0	8509	1/1	1.24	164.24	85,85,85,85	0
36	SR	0	8982	1/1	1.94	154.42	200,200,200,200	0
36	SR	0	8996	1/1	0.74	126.61	200,200,200,200	0
36	SR	0	8994	1/1	0.82	125.75	200,200,200,200	0
36	SR	0	9007	1/1	0.94	102.57	200,200,200,200	0
34	NA	0	8505	1/1	1.08	78.69	48,48,48,48	0
34	NA	0	8562	1/1	1.15	69.64	78,78,78,78	0
34	NA	0	8565	1/1	0.55	61.89	79,79,79,79	0
34	NA	0	8549	1/1	0.87	59.99	52,52,52,52	0
34	NA	0	8547	1/1	0.72	59.47	80,80,80,80	0
36	SR	0	8997	1/1	0.71	57.66	200,200,200,200	0
33	K	0	8401	1/1	0.96	55.00	128,128,128,128	0
34	NA	0	8550	1/1	1.28	54.87	57,57,57,57	0
34	NA	0	8553	1/1	0.87	53.50	65,65,65,65	0
34	NA	0	8560	1/1	0.81	44.25	101,101,101,101	0
34	NA	0	8545	1/1	0.61	43.53	47,47,47,47	0
34	NA	B	8552	1/1	0.50	33.19	83,83,83,83	0
34	NA	0	8535	1/1	0.52	31.52	61,61,61,61	0
32	MG	0	8039	1/1	0.37	28.48	76,76,76,76	0
34	NA	0	8536	1/1	0.23	28.39	61,61,61,61	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å ²)	Q<0.9
34	NA	0	8551	1/1	0.81	26.07	52,52,52,52	0
34	NA	0	8522	1/1	0.75	24.98	79,79,79,79	0
34	NA	0	8564	1/1	0.31	23.69	68,68,68,68	0
36	SR	0	8963	1/1	0.14	23.00	112,112,112,112	0
32	MG	0	8073	1/1	0.31	22.14	73,73,73,73	0
34	NA	0	8513	1/1	0.46	21.11	54,54,54,54	0
34	NA	0	8573	1/1	0.43	20.48	73,73,73,73	0
34	NA	0	8559	1/1	0.30	20.37	91,91,91,91	0
34	NA	0	8567	1/1	0.56	19.99	76,76,76,76	0
34	NA	0	8521	1/1	0.50	19.51	61,61,61,61	0
32	MG	0	8085	1/1	0.44	18.50	97,97,97,97	0
34	NA	9	8572	1/1	0.81	17.53	81,81,81,81	0
34	NA	0	8544	1/1	0.18	17.25	67,67,67,67	0
34	NA	0	8548	1/1	0.22	16.54	58,58,58,58	0
34	NA	0	8555	1/1	0.52	16.48	75,75,75,75	0
35	CL	0	8822	1/1	0.31	15.46	81,81,81,81	0
36	SR	0	8962	1/1	0.30	15.36	169,169,169,169	0
34	NA	0	8554	1/1	0.83	15.32	65,65,65,65	0
33	K	0	8402	1/1	0.46	15.17	76,76,76,76	0
34	NA	0	8525	1/1	0.23	14.87	92,92,92,92	0
34	NA	0	8528	1/1	0.60	14.82	66,66,66,66	0
32	MG	0	8081	1/1	0.24	14.41	73,73,73,73	0
36	SR	0	8947	1/1	0.43	13.74	200,200,200,200	0
34	NA	0	8524	1/1	0.26	13.50	58,58,58,58	0
36	SR	0	8959	1/1	0.26	13.20	163,163,163,163	0
36	SR	0	8986	1/1	0.39	13.16	200,200,200,200	0
34	NA	0	8527	1/1	0.31	11.05	71,71,71,71	0
36	SR	0	8914	1/1	0.27	10.32	120,120,120,120	0
36	SR	0	8922	1/1	0.39	10.30	161,161,161,161	0
36	SR	B	8987	1/1	0.49	9.93	200,200,200,200	0
32	MG	0	8089	1/1	0.22	9.90	72,72,72,72	0
34	NA	0	8518	1/1	0.43	9.75	88,88,88,88	0
34	NA	0	8519	1/1	0.25	9.63	43,43,43,43	0
32	MG	0	8030	1/1	0.27	9.57	68,68,68,68	0
34	NA	0	8563	1/1	0.40	9.42	88,88,88,88	0
32	MG	0	8082	1/1	0.59	9.36	89,89,89,89	0
34	NA	S	8510	1/1	0.46	9.28	64,64,64,64	0
34	NA	0	8534	1/1	0.27	9.21	44,44,44,44	0
34	NA	0	8556	1/1	0.85	9.15	64,64,64,64	0
32	MG	0	8049	1/1	0.31	9.13	69,69,69,69	0
34	NA	0	8566	1/1	0.35	9.03	64,64,64,64	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
32	MG	0	8022	1/1	0.22	8.44	44,44,44,44	0
36	SR	0	8903	1/1	0.18	7.72	59,59,59,59	0
34	NA	0	8516	1/1	0.17	7.65	45,45,45,45	0
32	MG	0	8047	1/1	0.27	7.41	51,51,51,51	0
32	MG	A	8051	1/1	0.71	7.37	70,70,70,70	0
34	NA	0	8571	1/1	0.18	7.37	76,76,76,76	0
34	NA	0	8561	1/1	0.24	7.28	68,68,68,68	0
32	MG	0	8029	1/1	0.17	6.96	49,49,49,49	0
36	SR	0	8934	1/1	0.27	6.92	134,134,134,134	0
36	SR	0	8976	1/1	0.30	6.75	194,194,194,194	0
32	MG	0	8018	1/1	0.21	6.60	40,40,40,40	0
36	SR	0	8905	1/1	0.25	6.49	61,61,61,61	0
34	NA	0	8568	1/1	0.39	6.49	52,52,52,52	0
36	SR	0	8992	1/1	0.20	6.47	136,136,136,136	0
36	SR	0	8949	1/1	0.16	6.37	122,122,122,122	0
32	MG	0	8009	1/1	0.24	6.33	36,36,36,36	0
34	NA	R	8575	1/1	0.27	6.26	99,99,99,99	0
34	NA	0	8541	1/1	0.21	6.22	75,75,75,75	0
32	MG	0	8033	1/1	0.16	5.84	55,55,55,55	0
36	SR	9	8980	1/1	0.21	5.82	175,175,175,175	0
34	NA	0	8511	1/1	0.30	5.68	69,69,69,69	0
34	NA	0	8542	1/1	0.36	5.64	49,49,49,49	0
34	NA	0	8530	1/1	0.37	5.63	59,59,59,59	0
32	MG	0	8014	1/1	0.22	5.61	33,33,33,33	0
36	SR	0	8926	1/1	0.16	5.57	108,108,108,108	0
36	SR	0	9002	1/1	0.15	5.28	177,177,177,177	0
34	NA	0	8546	1/1	0.28	5.14	65,65,65,65	0
34	NA	0	8574	1/1	0.20	5.12	59,59,59,59	0
32	MG	0	8078	1/1	0.25	5.09	69,69,69,69	0
36	SR	0	8981	1/1	0.21	4.80	178,178,178,178	0
32	MG	0	8072	1/1	0.19	4.58	63,63,63,63	0
32	MG	0	8071	1/1	0.17	4.55	72,72,72,72	0
36	SR	0	8983	1/1	0.19	4.32	170,170,170,170	0
32	MG	0	8017	1/1	0.18	3.78	52,52,52,52	0
36	SR	0	8937	1/1	0.21	3.67	112,112,112,112	0
32	MG	0	8069	1/1	0.32	3.42	73,73,73,73	0
32	MG	0	8066	1/1	0.17	3.29	70,70,70,70	0
36	SR	0	9004	1/1	0.32	2.89	200,200,200,200	0
36	SR	0	8909	1/1	0.14	2.41	88,88,88,88	0
32	MG	0	8063	1/1	0.14	2.41	80,80,80,80	0
32	MG	0	8048	1/1	0.18	2.30	33,33,33,33	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å ²)	Q<0.9
36	SR	0	8921	1/1	0.14	2.25	96,96,96,96	0
32	MG	0	8003	1/1	0.20	2.21	45,45,45,45	0
35	CL	B	8819	1/1	0.17	2.20	58,58,58,58	0
32	MG	0	8061	1/1	0.17	2.17	37,37,37,37	0
36	SR	0	8906	1/1	0.21	2.05	64,64,64,64	0
32	MG	0	8084	1/1	0.15	1.94	33,33,33,33	0
32	MG	0	8036	1/1	0.11	1.88	56,56,56,56	0
35	CL	R	8806	1/1	0.16	1.85	57,57,57,57	0
32	MG	0	8019	1/1	0.17	1.82	28,28,28,28	0
32	MG	0	8028	1/1	0.14	1.81	26,26,26,26	0
36	SR	0	8904	1/1	0.15	1.65	65,65,65,65	0
36	SR	0	8998	1/1	0.18	1.44	173,173,173,173	0
32	MG	K	8054	1/1	0.17	1.40	46,46,46,46	0
32	MG	0	8045	1/1	0.14	1.30	44,44,44,44	0
32	MG	0	8037	1/1	0.14	1.26	88,88,88,88	0
36	SR	0	8918	1/1	0.15	1.25	80,80,80,80	0
32	MG	0	8064	1/1	0.18	1.15	44,44,44,44	0
32	MG	0	8088	1/1	0.19	1.09	52,52,52,52	0
35	CL	J	8802	1/1	0.19	1.04	75,75,75,75	0
36	SR	0	8955	1/1	0.11	1.04	199,199,199,199	0
36	SR	A	8929	1/1	0.17	0.97	144,144,144,144	0
32	MG	0	8011	1/1	0.20	0.97	25,25,25,25	0
32	MG	0	8041	1/1	0.15	0.79	29,29,29,29	0
36	SR	0	8907	1/1	0.14	0.75	56,56,56,56	0
32	MG	0	8015	1/1	0.13	0.74	30,30,30,30	0
34	NA	0	8502	1/1	0.12	0.68	66,66,66,66	0
36	SR	0	9001	1/1	0.11	0.68	173,173,173,173	0
34	NA	0	8533	1/1	0.14	0.68	55,55,55,55	0
36	SR	0	8989	1/1	0.15	0.67	168,168,168,168	0
35	CL	0	8814	1/1	0.16	0.61	72,72,72,72	0
32	MG	0	8027	1/1	0.12	0.54	51,51,51,51	0
36	SR	0	8933	1/1	0.11	0.54	139,139,139,139	0
36	SR	R	8912	1/1	0.15	0.48	92,92,92,92	0
36	SR	0	8946	1/1	0.16	0.47	123,123,123,123	0
32	MG	0	8005	1/1	0.20	0.45	35,35,35,35	0
34	NA	M	8539	1/1	0.14	0.42	34,34,34,34	0
36	SR	0	8924	1/1	0.12	0.42	154,154,154,154	0
34	NA	0	8515	1/1	0.19	0.39	41,41,41,41	0
36	SR	0	8985	1/1	0.12	0.33	134,134,134,134	0
34	NA	J	8538	1/1	0.18	0.17	56,56,56,56	0
36	SR	0	8965	1/1	0.11	0.17	132,132,132,132	0
32	MG	0	8010	1/1	0.21	0.02	45,45,45,45	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å ²)	Q<0.9
36	SR	0	8966	1/1	0.10	0.00	107,107,107,107	0
32	MG	0	8040	1/1	0.12	-0.02	96,96,96,96	0
32	MG	0	8038	1/1	0.20	-0.04	70,70,70,70	0
36	SR	0	9008	1/1	0.15	-0.06	95,95,95,95	0
35	CL	0	8817	1/1	0.12	-0.13	67,67,67,67	0
34	NA	0	8569	1/1	0.15	-0.16	48,48,48,48	0
34	NA	0	8514	1/1	0.17	-0.17	56,56,56,56	0
34	NA	0	8504	1/1	0.15	-0.17	44,44,44,44	0
37	CD	Z	8703	1/1	0.12	-0.27	75,75,75,75	0
32	MG	0	8053	1/1	0.14	-0.28	47,47,47,47	0
35	CL	J	8801	1/1	0.10	-0.34	79,79,79,79	0
35	CL	0	8816	1/1	0.12	-0.41	79,79,79,79	0
32	MG	0	8046	1/1	0.13	-0.41	43,43,43,43	0
36	SR	0	8957	1/1	0.11	-0.45	195,195,195,195	0
32	MG	0	8004	1/1	0.13	-0.46	32,32,32,32	0
36	SR	0	8972	1/1	0.14	-0.52	146,146,146,146	0
36	SR	0	8967	1/1	0.10	-0.53	133,133,133,133	0
36	SR	0	8964	1/1	0.09	-0.53	131,131,131,131	0
34	NA	C	8503	1/1	0.15	-0.60	36,36,36,36	0
32	MG	0	8090	1/1	0.14	-0.62	65,65,65,65	0
36	SR	0	8936	1/1	0.11	-0.63	94,94,94,94	0
34	NA	0	8506	1/1	0.11	-0.71	64,64,64,64	0
36	SR	0	8927	1/1	0.11	-0.74	153,153,153,153	0
34	NA	0	8526	1/1	0.11	-0.83	47,47,47,47	0
36	SR	3	8932	1/1	0.11	-0.85	76,76,76,76	0
37	CD	1	8702	1/1	0.11	-0.88	67,67,67,67	0
36	SR	3	8999	1/1	0.10	-0.89	110,110,110,110	0
35	CL	J	8821	1/1	0.11	-0.89	67,67,67,67	0
32	MG	0	8002	1/1	0.14	-0.94	36,36,36,36	0
35	CL	0	8813	1/1	0.10	-0.94	66,66,66,66	0
34	NA	0	8520	1/1	0.07	-1.00	49,49,49,49	0
34	NA	0	8558	1/1	0.13	-1.01	49,49,49,49	0
32	MG	0	8067	1/1	0.12	-1.04	40,40,40,40	0
37	CD	3	8704	1/1	0.09	-1.04	74,74,74,74	0
36	SR	0	8993	1/1	0.07	-1.05	176,176,176,176	0
36	SR	0	8939	1/1	0.09	-1.07	149,149,149,149	0
34	NA	Q	8540	1/1	0.12	-1.07	64,64,64,64	0
36	SR	0	8979	1/1	0.10	-1.08	200,200,200,200	0
36	SR	0	8935	1/1	0.09	-1.10	79,79,79,79	0
32	MG	0	8083	1/1	0.08	-1.15	60,60,60,60	0
35	CL	N	8807	1/1	0.09	-1.23	69,69,69,69	0
35	CL	A	8809	1/1	0.12	-1.24	80,80,80,80	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
32	MG	0	8058	1/1	0.08	-1.28	22,22,22,22	0
36	SR	0	8956	1/1	0.05	-1.31	155,155,155,155	0
36	SR	0	8944	1/1	0.10	-1.32	169,169,169,169	0
34	NA	0	8523	1/1	0.10	-1.35	50,50,50,50	0
36	SR	0	8968	1/1	0.07	-1.35	160,160,160,160	0
35	CL	L	8810	1/1	0.10	-1.41	68,68,68,68	0
36	SR	0	8990	1/1	0.10	-1.42	139,139,139,139	0
32	MG	0	8043	1/1	0.06	-1.42	52,52,52,52	0
32	MG	0	8060	1/1	0.07	-1.45	53,53,53,53	0
32	MG	T	8057	1/1	0.11	-1.50	60,60,60,60	0
32	MG	0	8065	1/1	0.10	-1.54	57,57,57,57	0
36	SR	0	8975	1/1	0.10	-1.59	130,130,130,130	0
36	SR	1	8952	1/1	0.13	-1.62	89,89,89,89	0
36	SR	0	8902	1/1	0.14	-1.66	66,66,66,66	0
35	CL	O	8808	1/1	0.09	-1.66	70,70,70,70	0
32	MG	B	8042	1/1	0.06	-1.66	44,44,44,44	0
36	SR	1	8913	1/1	0.12	-1.68	95,95,95,95	0
36	SR	0	8911	1/1	0.08	-1.70	85,85,85,85	0
34	NA	0	8537	1/1	0.08	-1.70	38,38,38,38	0
36	SR	F	9005	1/1	0.06	-1.71	133,133,133,133	0
37	CD	U	8701	1/1	0.09	-1.72	63,63,63,63	0
32	MG	0	8056	1/1	0.12	-1.79	47,47,47,47	0
32	MG	0	8008	1/1	0.10	-1.87	28,28,28,28	0
36	SR	0	8954	1/1	0.09	-1.90	109,109,109,109	0
35	CL	0	8815	1/1	0.09	-1.91	77,77,77,77	0
35	CL	Q	8811	1/1	0.12	-1.93	82,82,82,82	0
32	MG	0	8023	1/1	0.09	-1.97	37,37,37,37	0
32	MG	0	8050	1/1	0.07	-1.97	32,32,32,32	0
36	SR	0	8953	1/1	0.12	-2.01	144,144,144,144	0
34	NA	9	8543	1/1	0.08	-2.06	74,74,74,74	0
34	NA	R	8532	1/1	0.09	-2.11	58,58,58,58	0
32	MG	0	8034	1/1	0.14	-2.17	46,46,46,46	0
36	SR	0	8969	1/1	0.08	-2.19	159,159,159,159	0
35	CL	M	8818	1/1	0.08	-2.25	40,40,40,40	0
32	MG	0	8025	1/1	0.11	-2.32	37,37,37,37	0
36	SR	0	8908	1/1	0.07	-2.35	116,116,116,116	0
32	MG	0	8044	1/1	0.09	-2.37	50,50,50,50	0
36	SR	A	8977	1/1	0.05	-2.39	160,160,160,160	0
32	MG	0	8007	1/1	0.11	-2.45	32,32,32,32	0
36	SR	0	8974	1/1	0.17	-2.45	165,165,165,165	0
32	MG	0	8021	1/1	0.05	-2.48	40,40,40,40	0
35	CL	0	8803	1/1	0.09	-2.51	58,58,58,58	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
36	SR	A	8930	1/1	0.05	-2.57	97,97,97,97	0
36	SR	9	8978	1/1	0.07	-2.61	135,135,135,135	0
36	SR	0	8917	1/1	0.06	-2.61	107,107,107,107	0
32	MG	0	8001	1/1	0.11	-2.68	33,33,33,33	0
35	CL	3	8804	1/1	0.06	-2.69	63,63,63,63	0
32	MG	0	8070	1/1	0.10	-2.73	46,46,46,46	0
36	SR	0	8958	1/1	0.05	-2.74	122,122,122,122	0
34	NA	0	8557	1/1	0.05	-2.77	53,53,53,53	0
36	SR	0	8943	1/1	0.05	-2.81	124,124,124,124	0
32	MG	0	8062	1/1	0.11	-2.86	59,59,59,59	0
36	SR	0	8960	1/1	0.07	-2.86	141,141,141,141	0
34	NA	0	8570	1/1	0.07	-2.88	52,52,52,52	0
32	MG	0	8052	1/1	0.08	-2.92	56,56,56,56	0
35	CL	0	8812	1/1	0.06	-2.94	58,58,58,58	0
36	SR	0	8951	1/1	0.04	-2.96	148,148,148,148	0
32	MG	0	8068	1/1	0.09	-2.96	51,51,51,51	0
32	MG	0	8016	1/1	0.11	-2.99	48,48,48,48	0
32	MG	Y	8086	1/1	0.07	-3.01	44,44,44,44	0
35	CL	0	8805	1/1	0.05	-3.05	67,67,67,67	0
32	MG	0	8087	1/1	0.10	-3.15	51,51,51,51	0
34	NA	0	8529	1/1	0.06	-3.17	39,39,39,39	0
36	SR	0	8940	1/1	0.06	-3.18	97,97,97,97	0
32	MG	0	8079	1/1	0.08	-3.18	51,51,51,51	0
36	SR	0	8991	1/1	0.07	-3.23	199,199,199,199	0
34	NA	0	8512	1/1	0.13	-3.24	52,52,52,52	0
37	CD	O	8705	1/1	0.05	-3.28	118,118,118,118	0
36	SR	0	8942	1/1	0.09	-3.29	122,122,122,122	0
36	SR	0	8920	1/1	0.07	-3.36	135,135,135,135	0
32	MG	0	8020	1/1	0.07	-3.41	40,40,40,40	0
36	SR	0	8919	1/1	0.11	-3.47	170,170,170,170	0
32	MG	0	8075	1/1	0.07	-3.75	42,42,42,42	0
36	SR	0	8915	1/1	0.08	-3.79	121,121,121,121	0
36	SR	0	8928	1/1	0.06	-3.83	135,135,135,135	0
36	SR	0	8923	1/1	0.07	-3.89	101,101,101,101	0
32	MG	9	8074	1/1	0.08	-3.95	86,86,86,86	0
36	SR	0	8948	1/1	0.09	-3.95	92,92,92,92	0
35	CL	Y	8820	1/1	0.06	-3.96	48,48,48,48	0
36	SR	0	8931	1/1	0.07	-3.98	113,113,113,113	0
32	MG	0	8031	1/1	0.07	-3.98	62,62,62,62	0
36	SR	0	8984	1/1	0.06	-4.08	121,121,121,121	0
32	MG	0	8013	1/1	0.04	-4.26	25,25,25,25	0
32	MG	0	8026	1/1	0.08	-4.40	35,35,35,35	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
36	SR	S	8961	1/1	0.06	-4.45	121,121,121,121	0
32	MG	0	8035	1/1	0.07	-4.47	54,54,54,54	0
36	SR	0	8973	1/1	0.06	-4.68	130,130,130,130	0
32	MG	0	8055	1/1	0.09	-4.71	53,53,53,53	0
32	MG	0	8077	1/1	0.03	-4.86	45,45,45,45	0
36	SR	9	9003	1/1	0.05	-5.02	171,171,171,171	0
34	NA	0	8507	1/1	0.07	-5.20	37,37,37,37	0
36	SR	0	8941	1/1	0.11	-5.34	108,108,108,108	0
32	MG	0	8093	1/1	0.08	-5.39	42,42,42,42	0
36	SR	0	8938	1/1	0.02	-5.53	147,147,147,147	0
36	SR	0	8995	1/1	0.10	-5.56	136,136,136,136	0
36	SR	0	8910	1/1	0.05	-5.56	100,100,100,100	0
36	SR	0	8945	1/1	0.06	-5.62	106,106,106,106	0
34	NA	0	8508	1/1	0.05	-5.64	35,35,35,35	0
32	MG	0	8076	1/1	0.07	-5.93	40,40,40,40	0
36	SR	B	8950	1/1	0.08	-6.22	116,116,116,116	0
32	MG	0	8059	1/1	0.07	-6.25	57,57,57,57	0
32	MG	0	8006	1/1	0.07	-6.35	32,32,32,32	0
36	SR	0	8970	1/1	0.01	-6.55	123,123,123,123	0
34	NA	0	8517	1/1	0.06	-6.70	31,31,31,31	0
32	MG	0	8012	1/1	0.09	-6.80	18,18,18,18	0
32	MG	0	8091	1/1	0.03	-7.50	57,57,57,57	0
36	SR	0	8925	1/1	0.06	-8.55	86,86,86,86	0
32	MG	0	8080	1/1	0.03	-8.87	75,75,75,75	0
34	NA	0	8501	1/1	0.07	-9.09	40,40,40,40	0
34	NA	0	8531	1/1	0.05	-9.36	40,40,40,40	0
36	SR	0	8988	1/1	0.06	-10.67	158,158,158,158	0
36	SR	0	9000	1/1	0.04	-10.78	176,176,176,176	0
36	SR	0	8916	1/1	0.03	-11.34	120,120,120,120	0
32	MG	0	8032	1/1	0.05	-12.45	44,44,44,44	0
32	MG	0	8092	1/1	0.10	-13.00	53,53,53,53	0
36	SR	0	8901	1/1	0.07	-13.72	91,91,91,91	0
32	MG	0	8024	1/1	0.09	-15.60	49,49,49,49	0
36	SR	0	8971	1/1	0.07	-39.00	171,171,171,171	0

6.5 Other polymers ⓘ

There are no such residues in this entry.