



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 28, 2014 – 04:16 PM GMT

PDB ID : 3CCE
Title : Structure of Anisomycin resistant 50S Ribosomal Subunit: 23S rRNA mutation U2535A
Authors : Blaha, G.; Gurel, G.
Deposited on : 2008-02-25
Resolution : 2.75 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>

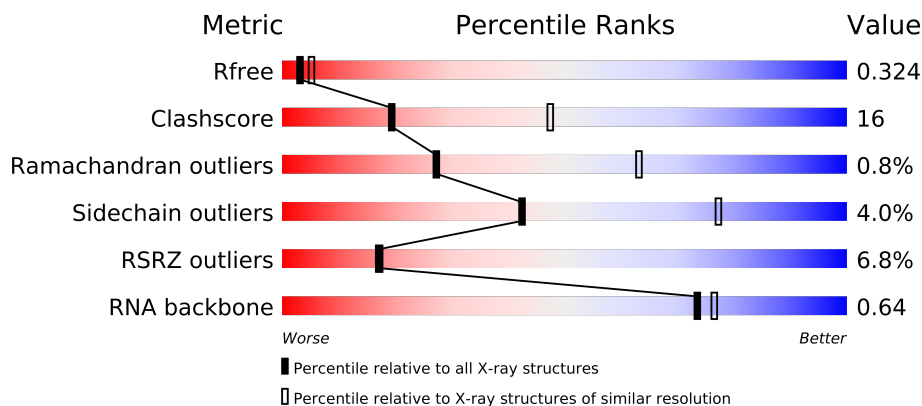
The following versions of software and data (see [references](#)) were used in the production of this report:

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 2.75 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	2406 (2.80-2.72)
Clashscore	79885	2995 (2.80-2.72)
Ramachandran outliers	78287	2941 (2.80-2.72)
Sidechain outliers	78261	2944 (2.80-2.72)
RSRZ outliers	66119	2409 (2.80-2.72)
RNA backbone	1838	1019 (3.26-2.26)

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	8008	-	X
32	MG	0	8015	-	X
32	MG	0	8030	-	X
32	MG	0	8037	-	X
32	MG	0	8038	-	X
32	MG	0	8040	-	X
32	MG	0	8049	-	X
32	MG	0	8061	-	X
32	MG	0	8062	-	X
32	MG	0	8063	-	X
32	MG	0	8068	-	X
32	MG	0	8069	-	X
32	MG	0	8071	-	X
32	MG	0	8072	-	X
32	MG	0	8073	-	X
32	MG	0	8075	-	X
32	MG	0	8076	-	X

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Geometry	Electron density
32	MG	0	8079	-	X
32	MG	0	8082	-	X
32	MG	0	8085	-	X
32	MG	0	8089	-	X
32	MG	0	8090	-	X
32	MG	0	8092	-	X
32	MG	A	8051	-	X
33	K	0	8401	-	X
33	K	0	8402	-	X
34	NA	0	8501	-	X
34	NA	0	8502	-	X
34	NA	0	8504	-	X
34	NA	0	8505	-	X
34	NA	0	8506	-	X
34	NA	0	8507	-	X
34	NA	0	8509	-	X
34	NA	0	8511	-	X
34	NA	0	8512	-	X
34	NA	0	8513	-	X
34	NA	0	8514	-	X
34	NA	0	8516	-	X
34	NA	0	8517	-	X
34	NA	0	8518	-	X
34	NA	0	8519	-	X
34	NA	0	8520	-	X
34	NA	0	8522	-	X
34	NA	0	8523	-	X
34	NA	0	8524	-	X
34	NA	0	8525	-	X
34	NA	0	8526	-	X
34	NA	0	8528	-	X
34	NA	0	8530	-	X
34	NA	0	8533	-	X
34	NA	0	8534	-	X
34	NA	0	8541	-	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	8551	-	X

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Geometry	Electron density
34	NA	0	8552	-	X
34	NA	0	8553	-	X
34	NA	0	8554	-	X
34	NA	0	8556	-	X
34	NA	0	8558	-	X
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	8569	-	X
34	NA	0	8571	-	X
34	NA	0	8573	-	X
34	NA	0	8574	-	X
34	NA	0	8575	-	X
34	NA	Q	8540	-	X
35	CL	0	8814	-	X
35	CL	0	8822	-	X
35	CL	J	8802	-	X
35	CL	R	8806	-	X
36	SR	0	8914	-	X
36	SR	0	8938	-	X
36	SR	0	8947	-	X
36	SR	0	8957	-	X
36	SR	0	8962	-	X
36	SR	0	8967	-	X
36	SR	0	8969	-	X
36	SR	0	8971	-	X
36	SR	0	8972	-	X
36	SR	0	8976	-	X
36	SR	0	8979	-	X
36	SR	0	8982	-	X
36	SR	0	8983	-	X
36	SR	0	8985	-	X
36	SR	0	8988	-	X
36	SR	0	8989	-	X
36	SR	0	8991	-	X
36	SR	0	8994	-	X

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Geometry	Electron density
36	SR	0	8996	-	X
36	SR	0	8997	-	X
36	SR	0	9000	-	X
36	SR	0	9001	-	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 99124 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
			59022	26350	10876	19051	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	86	Total	Mg	0	0
			86	86		
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	2	Total	Mg	0	0
			2	2		
32	T	1	Total	Mg	0	0
			1	1		
32	9	1	Total	Mg	0	0
			1	1		

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

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

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

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

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
35	0	10	Total Cl 10 10	0	0
35	J	3	Total Cl 3 3	0	0
35	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
35	L	1	Total Cl 1 1	0	0

Continued on next page...

Continued from previous page...

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

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
36	0	92	Total 92	Sr 92	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	4	Total 4	Sr 4	0	0
36	S	1	Total 1	Sr 1	0	0
36	F	1	Total 1	Sr 1	0	0

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

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

- Molecule 38 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
38	0	5927	Total 5927	O 5927	0	0
38	9	144	Total 144	O 144	0	0
38	A	118	Total 118	O 118	0	0
38	B	144	Total 144	O 144	0	0
38	C	179	Total 179	O 179	0	0
38	D	46	Total 46	O 46	0	0
38	E	40	Total 40	O 40	0	0
38	F	27	Total 27	O 27	0	0
38	G	19	Total 19	O 19	0	0
38	H	68	Total 68	O 68	0	0
38	I	5	Total 5	O 5	0	0
38	J	55	Total 55	O 55	0	0
38	K	52	Total 52	O 52	0	0
38	L	84	Total 84	O 84	0	0
38	M	127	Total 127	O 127	0	0
38	N	63	Total 63	O 63	0	0
38	O	40	Total 40	O 40	0	0
38	P	61	Total 61	O 61	0	0
38	Q	43	Total 43	O 43	0	0
38	R	84	Total 84	O 84	0	0
38	S	33	Total 33	O 33	0	0
38	T	33	Total 33	O 33	0	0

Continued on next page...

Continued from previous page...

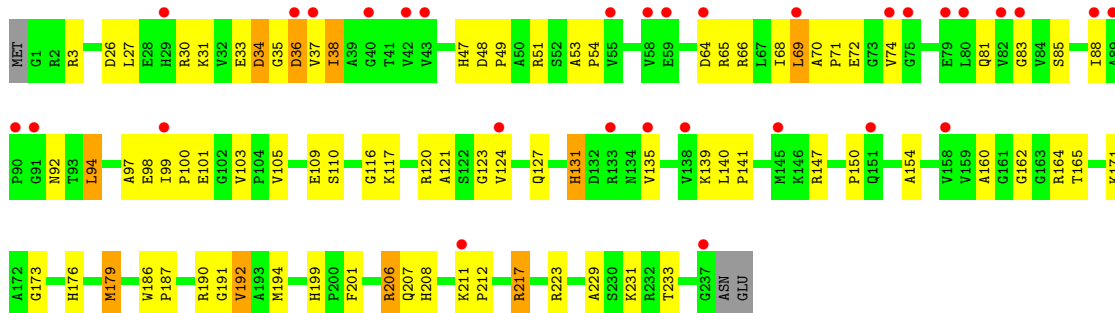
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
38	U	28	Total 28	O 28	0	0
38	V	14	Total 14	O 14	0	0
38	W	67	Total 67	O 67	0	0
38	X	30	Total 30	O 30	0	0
38	Y	100	Total 100	O 100	0	0
38	Z	32	Total 32	O 32	0	0
38	1	55	Total 55	O 55	0	0
38	2	42	Total 42	O 42	0	0
38	3	63	Total 63	O 63	0	0

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.

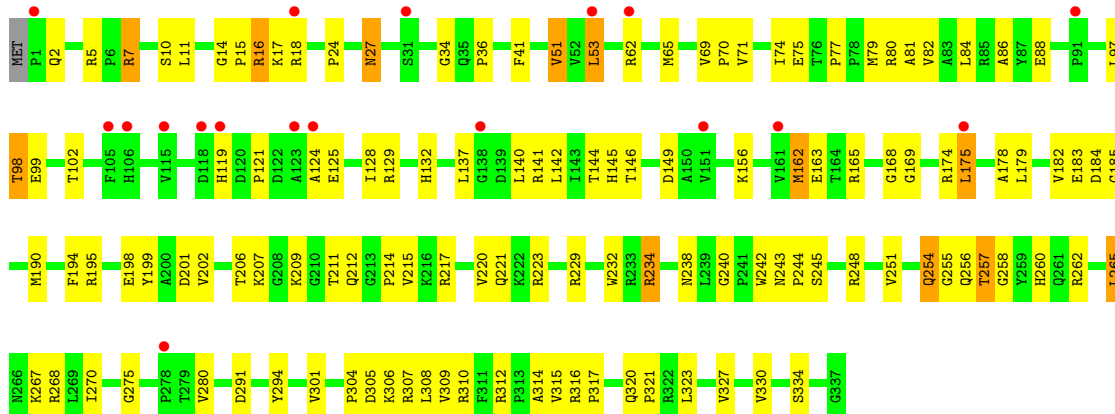
• Molecule 1: 50S ribosomal protein L2P

Chain A: 



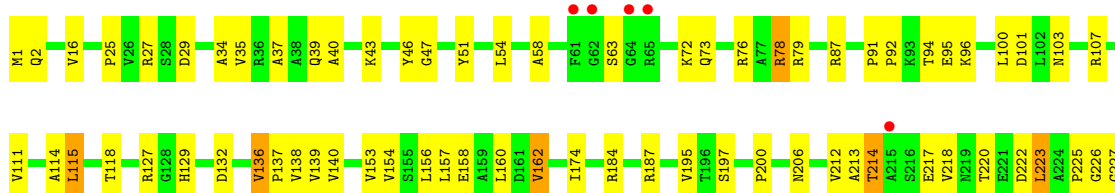
• Molecule 2: 50S ribosomal protein L3P

Chain B: 



• Molecule 3: 50S ribosomal protein L4P

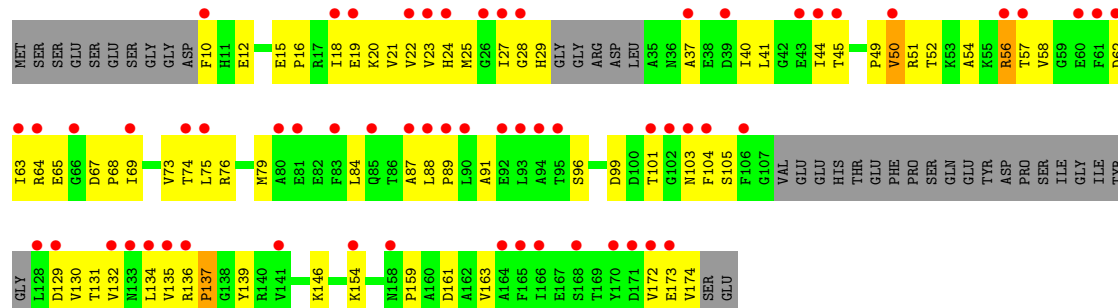
Chain C: 





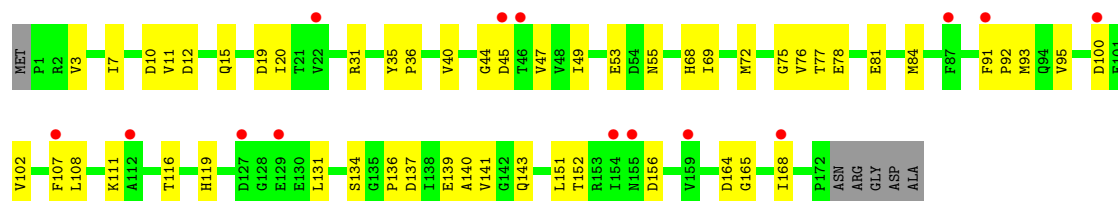
- Molecule 4: 50S ribosomal protein L5P

Chain D:



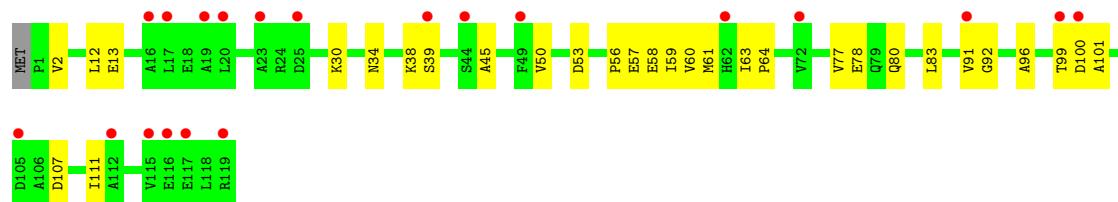
- Molecule 5: 50S ribosomal protein L6P

Chain E:



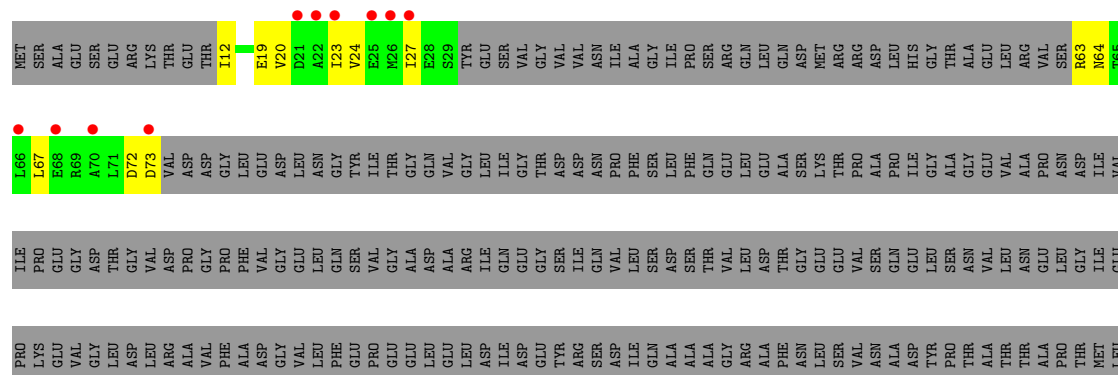
- Molecule 6: 50S ribosomal protein L7Ae

Chain F:



- Molecule 7: 50S ribosomal protein L10E

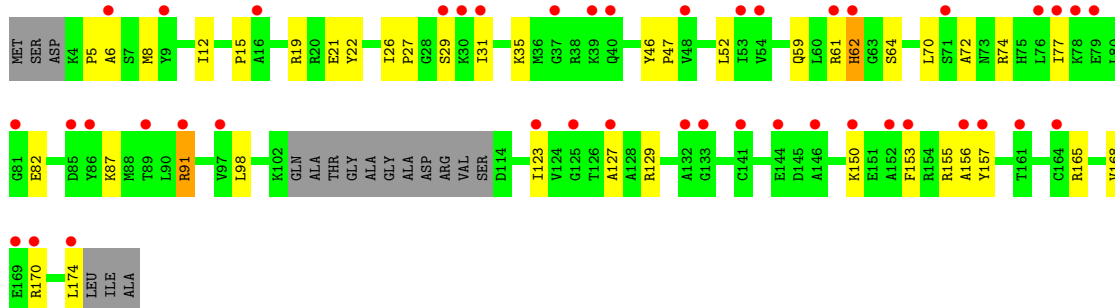
Chain G:



GLU	PRO	THR	ASP	ASP	GLN	ASP	ASP	ASP	THR	ALA	SER	GLU	ASP	ASP	ALA	ALA	GLU	GLU	ALA	ASP	ASP	ASP	ASP	ASP	ASP	GLU	ALA	GLY	ASP	ALA	LEU	GLY	ALA	MET	PHE
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

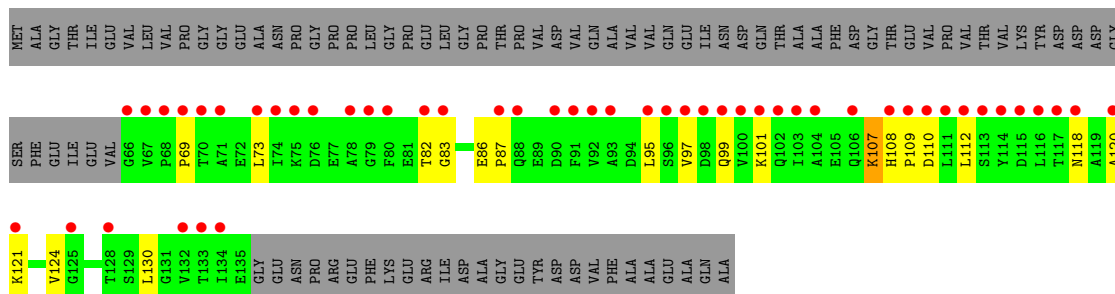
- Molecule 8: 50S ribosomal protein L10e

Chain H:



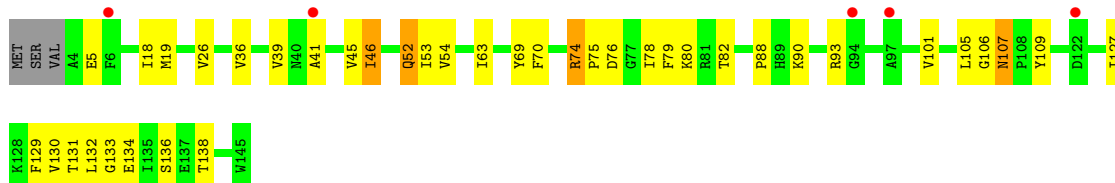
- Molecule 9: 50S ribosomal protein L11P

Chain I:



- Molecule 10: 50S ribosomal protein L13P

Chain J:



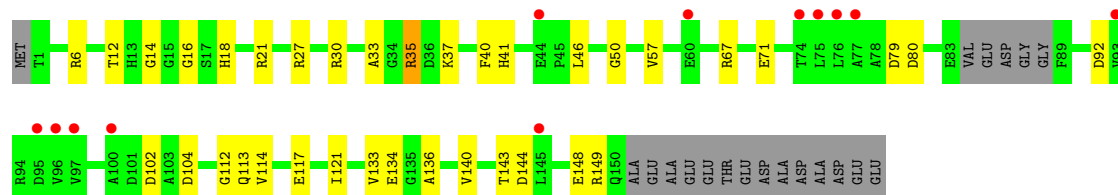
- Molecule 11: 50S ribosomal protein L14P

Chain K:



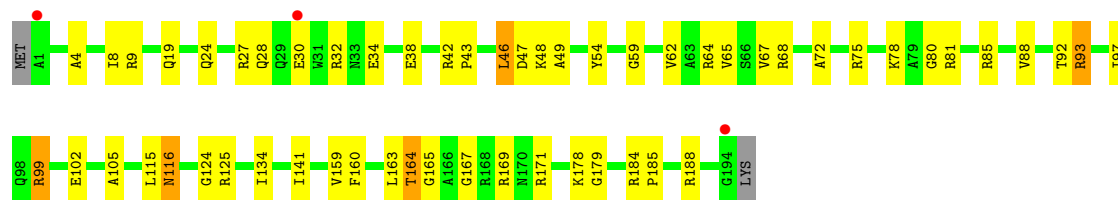
- Molecule 12: 50S ribosomal protein L15P

Chain L:



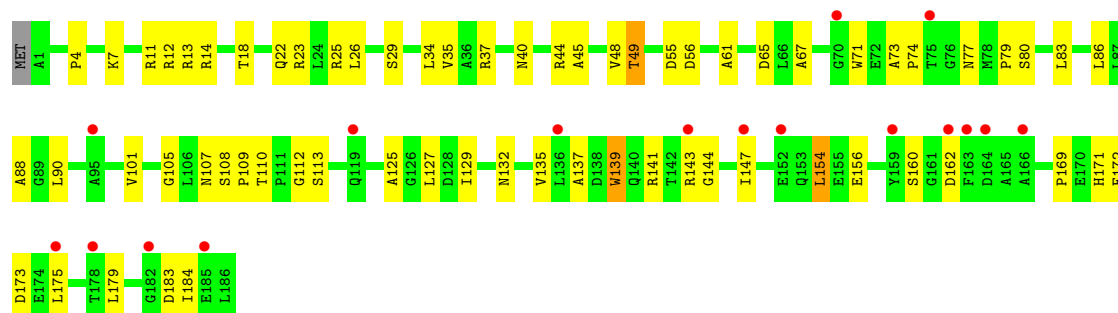
- Molecule 13: 50S ribosomal protein L15e

Chain M:



- Molecule 14: 50S ribosomal protein L18P

Chain N:



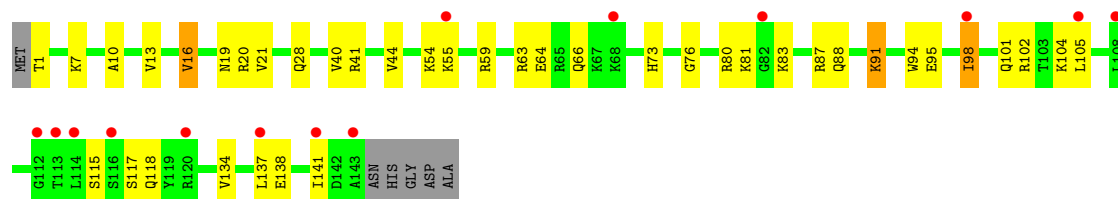
- Molecule 15: 50S ribosomal protein L18e

Chain O:



- Molecule 16: 50S ribosomal protein L19e

Chain P:



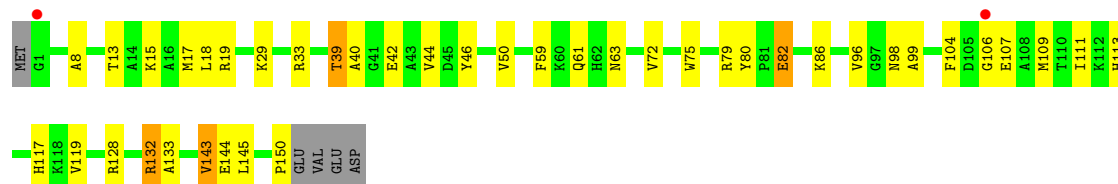
- Molecule 17: 50S ribosomal protein L21e

Chain Q:



- Molecule 18: 50S ribosomal protein L22P

Chain R:



- Molecule 19: 50S ribosomal protein L23P

Chain S:



- Molecule 20: 50S ribosomal protein L24P

Chain T:



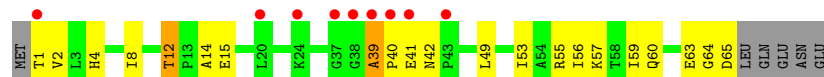
- Molecule 21: 50S ribosomal protein L24e

Chain U:



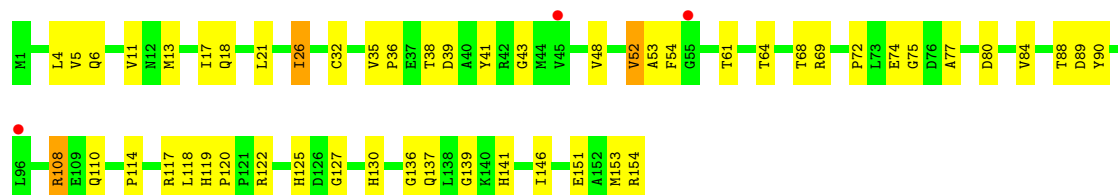
- Molecule 22: 50S ribosomal protein L29P

Chain V:



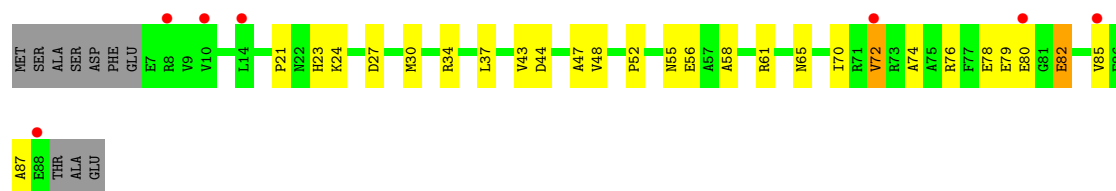
- Molecule 23: 50S ribosomal protein L30P

Chain W:



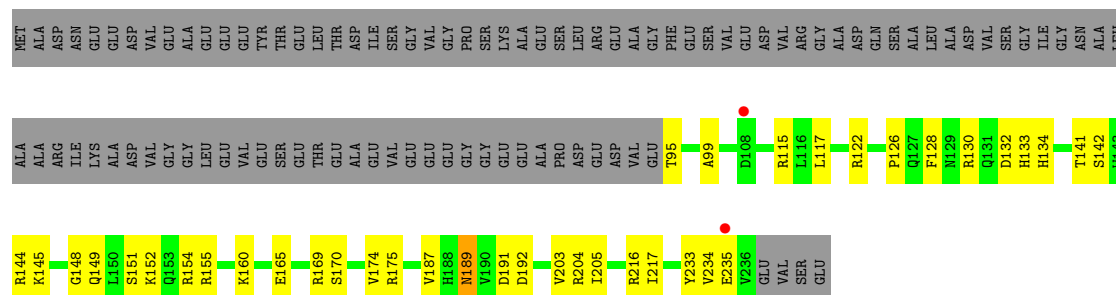
- Molecule 24: 50S ribosomal protein L31e

Chain X:



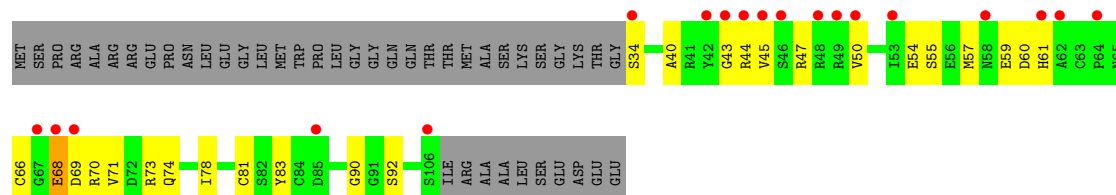
- Molecule 25: 50S ribosomal protein L32e

Chain Y:



- Molecule 26: 50S ribosomal protein L37Ae

Chain Z:



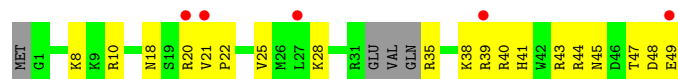
- Molecule 27: 50S ribosomal protein L37e

Chain 1:



- Molecule 28: 50S ribosomal protein L39e

Chain 2:



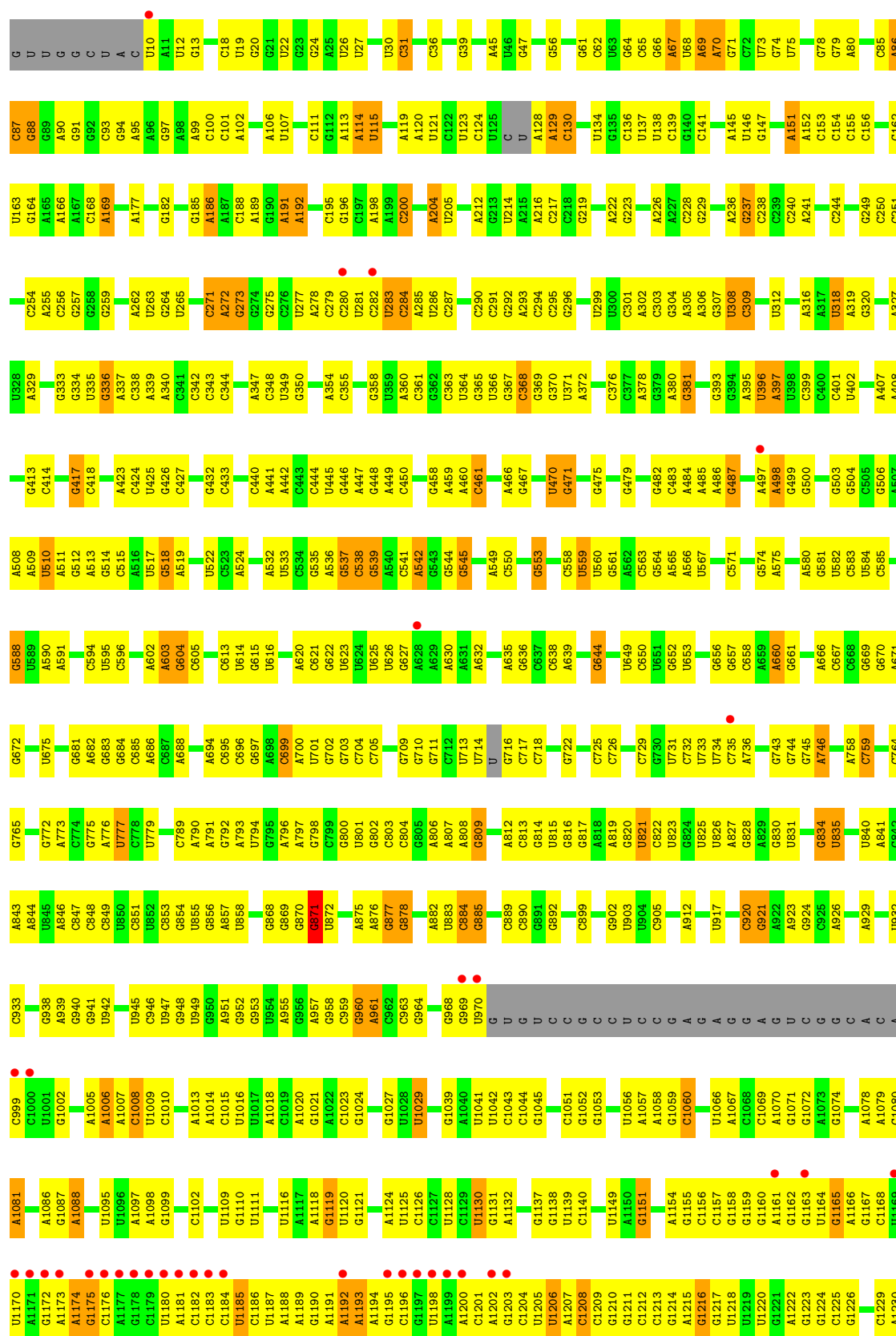
- Molecule 29: 50S ribosomal protein L44E

Chain 3:

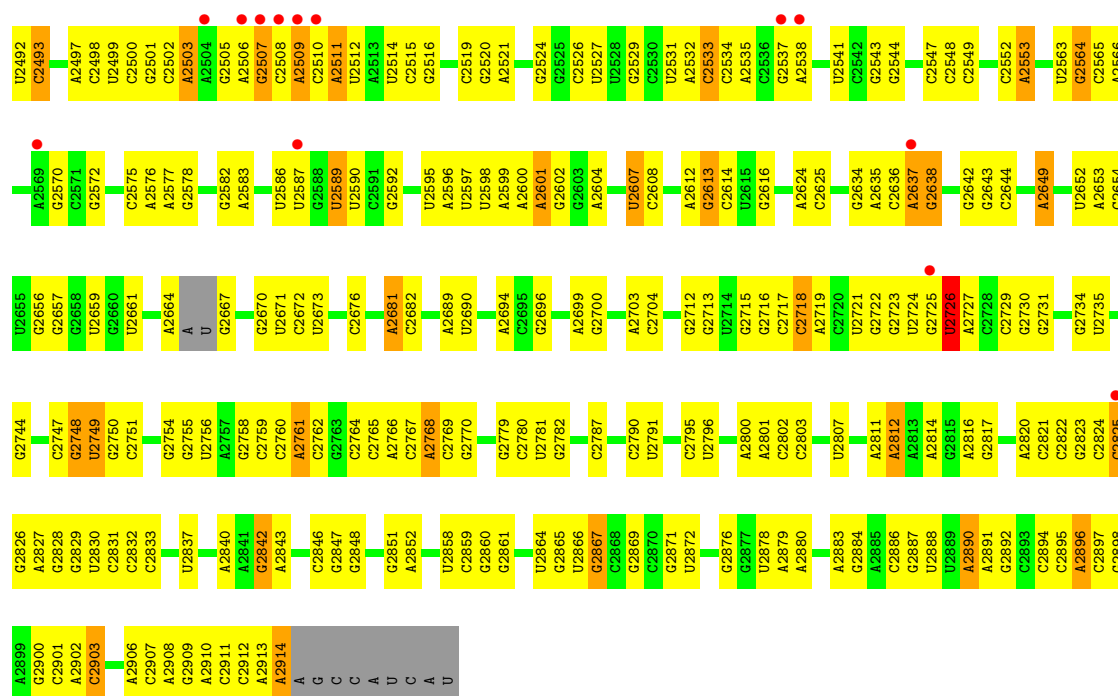


● Molecule 30: 23S RIBOSOMAL RNA

Chain 0:

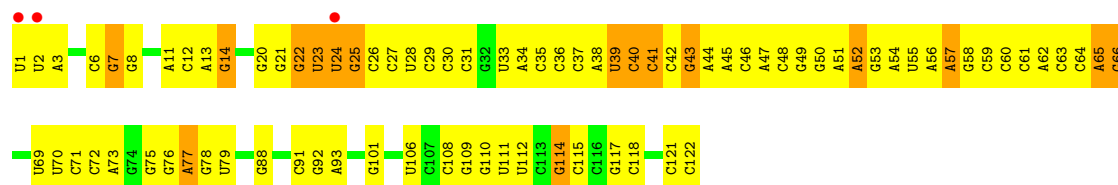


WORLDWIDE
PDB
PROTEIN DATA BANK



• 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	212.83Å 299.90Å 576.01Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.33 – 2.75 85.81 – 2.41	Depositor EDS
% Data completeness (in resolution range)	81.3 (49.33-2.75) 81.1 (85.81-2.41)	Depositor EDS
R_{merge}	0.11	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}	0.183 , 0.232 0.311 , 0.324	Depositor DCC
R_{free} test set	3763 reflections (0.99%)	DCC
Wilson B-factor (Å ²)	45.6	Xtriage
Anisotropy	0.228	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 47.5	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 667164 reflections	Xtriage
F_o, F_c correlation	0.83	EDS
Total number of atoms	99124	wwPDB-VP
Average B, all atoms (Å ²)	52.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.24% 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	0.34	0/1786	0.65	0/2408
2	B	0.33	0/2690	0.64	0/3652
3	C	0.36	0/1885	0.65	0/2552
4	D	0.33	0/1111	0.55	0/1498
5	E	0.33	0/1382	0.56	0/1880
6	F	0.34	0/901	0.57	0/1224
7	G	0.30	0/241	0.50	0/324
8	H	0.35	0/1302	0.61	0/1743
9	I	0.30	0/526	0.50	0/716
10	J	0.34	0/1136	0.59	0/1530
11	K	0.35	0/1004	0.66	0/1351
12	L	0.31	0/1130	0.64	0/1509
13	M	0.34	0/1582	0.63	0/2116
14	N	0.30	0/1474	0.62	0/1999
15	O	0.34	0/874	0.60	0/1181
16	P	0.32	0/1147	0.53	0/1528
17	Q	0.34	0/749	0.65	0/1005
18	R	0.35	0/1172	0.64	0/1578
19	S	0.35	0/648	0.59	0/875
20	T	0.33	0/958	0.62	0/1289
21	U	0.34	0/417	0.57	0/562
22	V	0.31	0/502	0.49	0/675
23	W	0.34	0/1219	0.61	0/1655
24	X	0.34	0/664	0.60	0/895
25	Y	0.36	0/1146	0.62	0/1536
26	Z	0.36	0/584	0.58	0/781
27	1	0.40	0/438	0.63	0/578
28	2	0.34	0/401	0.60	0/529
29	3	0.36	0/771	0.59	0/1024
30	0	0.37	0/65960	0.68	6/102872 (0.0%)
31	9	0.32	0/2904	0.67	1/4526 (0.0%)
All	All	0.36	0/98704	0.66	7/147591 (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
23	W	0	1
30	0	0	26
All	All	0	27

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	0	1819	G	C5'-C4'-C3'	6.12	125.79	116.00
30	0	871	G	C5'-C4'-O4'	-6.04	101.86	109.10
30	0	1504	A	C1'-O4'-C4'	-5.84	105.22	109.90
30	0	1504	A	N9-C1'-C2'	5.53	121.18	114.00
30	0	841	A	C1'-O4'-C4'	-5.34	105.63	109.90
30	0	2726	U	N1-C1'-C2'	5.27	120.85	114.00
31	9	39	U	N1-C1'-C2'	5.25	120.82	114.00

There are no chirality outliers.

All (27) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
30	0	1039	G	Sidechain
30	0	1078	A	Sidechain
30	0	1340	G	Sidechain
30	0	1417	G	Sidechain
30	0	1445	G	Sidechain
30	0	1653	A	Sidechain
30	0	1777	G	Sidechain
30	0	1829	A	Sidechain
30	0	1877	G	Sidechain
30	0	1878	G	Sidechain
30	0	1972	U	Sidechain
30	0	2076	U	Sidechain
30	0	22	U	Sidechain
30	0	2412	G	Sidechain
30	0	2465	A	Sidechain
30	0	2493	C	Sidechain
30	0	2503	A	Sidechain

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
30	0	2552	C	Sidechain
30	0	26	U	Sidechain
30	0	2607	U	Sidechain
30	0	2842	G	Sidechain
30	0	396	U	Sidechain
30	0	458	G	Sidechain
30	0	470	U	Sidechain
30	0	471	G	Sidechain
30	0	518	G	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	80	0
2	B	2625	0	2533	110	0
3	C	1860	0	1813	73	0
4	D	1094	0	1085	56	0
5	E	1357	0	1266	42	0
6	F	890	0	843	23	0
7	G	240	0	231	7	0
8	H	1282	0	1292	33	0
9	I	519	0	500	24	0
10	J	1120	0	1098	36	0
11	K	994	0	1027	37	0
12	L	1118	0	1076	30	0
13	M	1558	0	1573	48	0
14	N	1445	0	1401	61	0
15	O	865	0	873	22	0
16	P	1136	0	1123	36	0
17	Q	735	0	729	20	0
18	R	1149	0	1122	33	0
19	S	641	0	605	13	0
20	T	950	0	924	21	0
21	U	410	0	364	16	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
22	V	499	0	511	16	0
23	W	1196	0	1137	58	0
24	X	654	0	653	21	0
25	Y	1130	0	1133	41	0
26	Z	573	0	531	18	0
27	1	431	0	426	25	0
28	2	396	0	413	21	0
29	3	755	0	729	15	0
30	0	59022	0	29809	1550	0
31	9	2599	0	1325	114	0
32	0	86	0	0	0	0
32	9	1	0	0	0	0
32	A	2	0	0	0	0
32	B	1	0	0	0	0
32	K	1	0	0	0	0
32	T	1	0	0	0	0
32	Y	1	0	0	0	0
33	0	2	0	0	0	0
34	0	67	0	0	0	0
34	9	2	0	0	0	0
34	C	1	0	0	0	0
34	J	1	0	0	0	0
34	M	1	0	0	0	0
34	Q	1	0	0	0	0
34	R	1	0	0	0	0
34	S	1	0	0	0	0
35	0	10	0	0	1	0
35	3	1	0	0	0	0
35	A	1	0	0	0	0
35	B	1	0	0	0	0
35	J	3	0	0	5	0
35	L	1	0	0	0	0
35	M	1	0	0	0	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
36	0	92	0	0	0	0
36	1	2	0	0	0	0
36	3	2	0	0	0	0
36	9	4	0	0	0	0
36	A	3	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	5927	0	0	235	0
38	1	55	0	0	3	0
38	2	42	0	0	3	0
38	3	63	0	0	3	0
38	9	144	0	0	10	0
38	A	118	0	0	7	0
38	B	144	0	0	11	0
38	C	179	0	0	19	0
38	D	46	0	0	4	0
38	E	40	0	0	2	0
38	F	27	0	0	1	0
38	G	19	0	0	0	0
38	H	68	0	0	5	0
38	I	5	0	0	1	0
38	J	55	0	0	2	0
38	K	52	0	0	2	0
38	L	84	0	0	10	0
38	M	127	0	0	5	0
38	N	63	0	0	4	0
38	O	40	0	0	2	0
38	P	61	0	0	1	0
38	Q	43	0	0	1	0
38	R	84	0	0	5	0
38	S	33	0	0	2	0
38	T	33	0	0	2	0
38	U	28	0	0	2	0
38	V	14	0	0	1	0
38	W	67	0	0	5	0
38	X	30	0	0	0	0
38	Y	100	0	0	10	0
38	Z	32	0	0	0	0
All	All	99124	0	59911	2446	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 16.

All (2446) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
14:N:37:ARG:NH1	31:9:6:C:H5''	1.60	1.15
30:0:1160:G:C5'	30:0:1161:A:H5'	1.78	1.11
13:M:171:ARG:HD3	30:0:156:C:H5''	1.32	1.11
30:0:871:G:H8	30:0:871:G:H5'	1.12	1.11
30:0:871:G:C8	30:0:871:G:H5'	1.84	1.11
30:0:2717:C:H2'	30:0:2718:C:H5''	1.33	1.10
30:0:2291:A:C8	30:0:2309:C:H5'	1.87	1.09
30:0:1160:G:H5'	30:0:1161:A:C5'	1.82	1.08
30:0:381:G:H5''	38:0:4322:HOH:O	1.54	1.07
31:9:56:A:H2'	31:9:57:A:H5''	1.38	1.05
30:0:2502:C:H2'	30:0:2503:A:H5'	1.33	1.05
30:0:2502:C:C2'	30:0:2503:A:H5'	1.89	1.01
10:J:82:THR:HG23	30:0:1242:A:H5'	1.39	1.01
30:0:1209:C:H2'	30:0:1210:G:H8	1.19	1.01
31:9:76:G:H3'	31:9:77:A:H5''	1.39	1.01
30:0:282:C:H1'	30:0:368:C:N4	1.77	1.00
30:0:2717:C:C2'	30:0:2718:C:H5''	1.91	0.99
22:V:1:THR:HB	30:0:93:C:H5''	1.42	0.99
16:P:115:SER:H	16:P:118:GLN:HE21	1.08	0.99
30:0:2812:A:H2	30:0:2814:A:H62	1.07	0.98
30:0:1118:A:H3'	30:0:1118:A:H8	1.28	0.98
30:0:1372:A:H3'	38:0:7202:HOH:O	1.64	0.98
15:O:3:THR:HG22	30:0:656:G:H5'	1.45	0.97
30:0:1116:U:H3	30:0:1246:A:H62	1.11	0.96
8:H:59:GLN:HE21	8:H:129:ARG:HE	1.12	0.95
30:0:2908:A:H2'	30:0:2909:G:O4'	1.66	0.95
30:0:545:G:H8	30:0:545:G:H5'	1.30	0.95
30:0:542:A:H5'	30:0:542:A:H8	1.32	0.95
30:0:1160:G:H5'	30:0:1161:A:H5'	0.96	0.94
30:0:1666:C:O2'	30:0:1667:A:H5''	1.67	0.94
11:K:10:GLN:H	11:K:10:GLN:HE21	1.15	0.93
30:0:2769:C:C2'	30:0:2770:G:H5'	1.98	0.93
30:0:2497:A:H1'	30:0:2526:C:N4	1.84	0.93
30:0:1603:A:H5'	30:0:1605:G:O4'	1.68	0.92
30:0:1118:A:H3'	30:0:1118:A:C8	2.04	0.92
30:0:1701:A:H4'	30:0:1702:U:H5''	1.49	0.92
31:9:14:G:H5'	31:9:14:G:H8	1.36	0.91
30:0:1205:U:H2'	30:0:1206:U:H5''	1.52	0.91
30:0:960:G:H3'	30:0:960:G:N3	1.85	0.91
30:0:2812:A:H1'	38:0:5804:HOH:O	1.71	0.91

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
5:E:143:GLN:HE21	30:0:2780:C:H1'	1.34	0.91
30:0:871:G:C5'	30:0:871:G:H8	1.85	0.90
31:9:3:A:N6	31:9:22:G:H1'	1.86	0.90
30:0:870:G:H2'	30:0:871:G:H5''	1.53	0.90
30:0:282:C:O2'	30:0:283:U:H5'	1.71	0.90
2:B:212:GLN:HB2	2:B:257:THR:HG21	1.54	0.89
30:0:1679:C:H5'	38:0:9328:HOH:O	1.72	0.89
24:X:37:LEU:HD13	24:X:85:VAL:HG21	1.55	0.89
30:0:182:G:H5'	38:0:5169:HOH:O	1.72	0.88
30:0:1474:C:H6	30:0:1474:C:H5'	1.36	0.88
30:0:2524:G:N2	30:0:2526:C:H41	1.71	0.88
30:0:1119:G:N2	30:0:1246:A:C2	2.42	0.88
30:0:1666:C:H2'	30:0:1667:A:H5'	1.55	0.87
30:0:2769:C:H2'	30:0:2770:G:H5'	1.55	0.87
30:0:2508:C:H2'	38:0:6774:HOH:O	1.72	0.87
30:0:1118:A:H62	30:0:1244:U:H3	1.23	0.87
8:H:59:GLN:NE2	8:H:129:ARG:HE	1.71	0.87
31:9:56:A:C2'	31:9:57:A:H5''	2.05	0.87
30:0:2506:A:HO2'	30:0:2507:G:H8	1.16	0.87
30:0:2637:A:H5'	38:0:9279:HOH:O	1.74	0.86
30:0:1278:A:H4'	30:0:1279:U:C4	2.10	0.86
15:O:3:THR:CG2	30:0:656:G:H5'	2.05	0.86
30:0:1130:U:H5'	38:0:7684:HOH:O	1.75	0.86
30:0:541:C:C2'	30:0:542:A:H5''	2.05	0.86
2:B:238:ASN:HD22	2:B:240:GLY:H	1.22	0.85
23:W:88:THR:HB	38:W:6679:HOH:O	1.75	0.85
30:0:558:C:C2'	30:0:559:U:H5''	2.06	0.85
31:9:49:G:H5''	38:9:9088:HOH:O	1.75	0.85
30:0:1116:U:HO2'	30:0:1118:A:H2	0.86	0.85
30:0:1119:G:H22	30:0:1246:A:H2	1.19	0.85
30:0:2884:G:H5'	38:0:4133:HOH:O	1.76	0.84
30:0:506:G:H22	30:0:509:A:C5'	1.89	0.84
31:9:54:A:O2'	31:9:55:U:H5'	1.77	0.84
30:0:1451:C:H5'	30:0:1505:U:C5	2.12	0.84
23:W:137:GLN:HE21	23:W:141:HIS:HE1	1.21	0.84
23:W:88:THR:HG22	23:W:89:ASP:H	1.41	0.83
30:0:2586:U:H3	30:0:2592:G:H22	1.23	0.83
30:0:1183:C:H2'	38:0:6259:HOH:O	1.77	0.83
30:0:558:C:O2'	30:0:559:U:H5''	1.79	0.83
30:0:877:G:H5'	30:0:878:G:OP1	1.79	0.82
30:0:282:C:H1'	30:0:368:C:H41	1.41	0.82
30:0:1209:C:H2'	30:0:1210:G:C8	2.10	0.82

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
31:9:92:G:H2'	31:9:93:A:C8	2.14	0.82
15:O:32:ARG:HE	15:O:35:LYS:HD2	1.43	0.82
30:0:2524:G:H21	30:0:2526:C:H41	1.23	0.82
11:K:39:GLY:HA2	38:0:5233:HOH:O	1.79	0.82
4:D:154:LYS:HD2	4:D:154:LYS:H	1.42	0.82
30:0:1835:U:H5	30:0:1840:A:N7	1.76	0.82
30:0:2896:A:H5''	38:0:6114:HOH:O	1.78	0.82
30:0:855:U:H5''	38:0:3639:HOH:O	1.80	0.82
1:A:223:ARG:HH12	30:0:2270:G:H4'	1.44	0.82
30:0:559:U:H5'	30:0:559:U:H6	1.45	0.81
30:0:1741:U:H5'	30:0:1742:A:OP1	1.80	0.81
10:J:75:PRO:HG2	10:J:105:LEU:HD21	1.61	0.81
30:0:2748:G:H2'	38:0:7557:HOH:O	1.78	0.81
23:W:88:THR:HG23	23:W:110:GLN:HB3	1.62	0.81
30:0:1527:A:H1'	30:0:1528:A:C8	2.16	0.81
30:0:2529:G:H3'	38:0:7196:HOH:O	1.80	0.81
30:0:506:G:H22	30:0:509:A:H5''	1.45	0.81
22:V:12:THR:HG22	22:V:15:GLU:HG3	1.61	0.81
17:Q:15:LYS:HD3	30:0:2364:A:H5''	1.62	0.80
30:0:2497:A:H1'	30:0:2526:C:H42	1.46	0.80
30:0:541:C:H2'	30:0:542:A:C5'	2.11	0.80
22:V:1:THR:HG23	22:V:2:VAL:H	1.47	0.80
11:K:29:LEU:HB3	11:K:55:VAL:HG11	1.63	0.80
27:1:25:LYS:HD2	28:2:49:GLU:H	1.47	0.80
30:0:545:G:H5'	30:0:545:G:C8	2.15	0.80
30:0:2505:G:O2'	30:0:2506:A:H5'	1.82	0.80
16:P:117:SER:HB3	30:0:1593:C:OP1	1.82	0.80
30:0:541:C:H2'	30:0:542:A:H5''	1.64	0.79
30:0:2506:A:O2'	30:0:2507:G:H8	1.65	0.79
30:0:2570:G:H5''	38:0:4925:HOH:O	1.82	0.79
3:C:115:LEU:HD13	3:C:223:LEU:HD21	1.63	0.79
23:W:4:LEU:HD23	23:W:54:PHE:HB3	1.64	0.79
14:N:37:ARG:HH11	31:9:6:C:H5''	1.44	0.79
31:9:20:G:H3'	38:9:9054:HOH:O	1.82	0.79
30:0:1878:G:H1'	38:0:6135:HOH:O	1.81	0.79
14:N:83:LEU:HD13	14:N:175:LEU:HD23	1.65	0.79
30:0:1165:G:H21	30:0:1173:A:H5''	1.48	0.78
30:0:2604:A:H5'	38:0:5805:HOH:O	1.83	0.78
2:B:206:THR:HG21	30:0:2716:G:H5''	1.65	0.78
30:0:1856:C:H5'	30:0:1858:A:O4'	1.83	0.78
30:0:567:U:H5''	38:0:6420:HOH:O	1.83	0.78
30:0:1206:U:H5'	30:0:1206:U:H6	1.47	0.78

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
13:M:99:ARG:HD2	13:M:167:GLY:HA2	1.66	0.78
30:0:2635:A:O2'	30:0:2636:C:H5'	1.83	0.78
30:0:2769:C:H2'	30:0:2770:G:C5'	2.14	0.78
14:N:37:ARG:HH12	31:9:6:C:H5''	1.49	0.78
10:J:52:GLN:NE2	30:0:1119:G:H2'	1.99	0.78
13:M:164:THR:HG22	13:M:167:GLY:H	1.46	0.77
30:0:69:A:H5'	30:0:69:A:H8	1.49	0.77
30:0:254:C:H2'	30:0:254:C:O2	1.84	0.77
30:0:2565:C:H4'	38:0:4847:HOH:O	1.84	0.77
30:0:2563:U:H2'	30:0:2565:C:O5'	1.85	0.77
1:A:199:HIS:HD2	1:A:201:PHE:H	1.31	0.77
30:0:1205:U:H2'	30:0:1206:U:C5'	2.13	0.77
16:P:115:SER:H	16:P:118:GLN:NE2	1.83	0.77
30:0:711:G:H1'	38:0:7109:HOH:O	1.84	0.77
30:0:1300:G:H1'	38:0:4697:HOH:O	1.84	0.77
16:P:88:GLN:NE2	30:0:1800:G:H1'	1.98	0.77
3:C:127:ARG:NH2	3:C:225:PRO:HG2	1.99	0.77
30:0:1205:U:C2'	30:0:1206:U:H5''	2.15	0.76
30:0:2812:A:H2	30:0:2814:A:N6	1.83	0.76
30:0:1973:A:H8	30:0:1973:A:H5'	1.49	0.76
29:3:25:VAL:HG22	29:3:68:LYS:HG3	1.67	0.76
30:0:1184:C:H1'	38:0:7483:HOH:O	1.85	0.76
30:0:536:A:H3'	38:0:5057:HOH:O	1.86	0.76
30:0:1342:C:C2'	30:0:1343:C:H5'	2.14	0.76
31:9:14:G:H5'	31:9:14:G:C8	2.18	0.76
30:0:2587:OMU:H5	38:0:7502:HOH:O	1.85	0.76
30:0:1979:G:H2'	38:0:3302:HOH:O	1.85	0.76
30:0:1641:A:H2'	30:0:1642:A:H5'	1.67	0.76
30:0:1185:U:H2'	30:0:1186:C:H6	1.50	0.76
30:0:69:A:H5'	30:0:69:A:C8	2.21	0.76
30:0:1701:A:H5''	30:0:1702:U:H3'	1.68	0.75
30:0:1474:C:C6	30:0:1474:C:H5'	2.20	0.75
30:0:396:U:H1'	38:0:7643:HOH:O	1.86	0.75
26:Z:44:ARG:HH21	30:0:1771:U:H5'	1.52	0.75
18:R:8:ALA:HB1	18:R:13:THR:HG21	1.69	0.75
22:V:39:ALA:H	22:V:40:PRO:HD2	1.51	0.75
23:W:6:GLN:HB2	23:W:26:ILE:HD12	1.69	0.75
30:0:1182:C:H1'	30:0:1192:A:H8	1.51	0.75
1:A:223:ARG:NH1	30:0:2270:G:H4'	2.02	0.75
30:0:282:C:O2	30:0:282:C:H2'	1.85	0.75
30:0:31:C:H2'	38:0:7701:HOH:O	1.86	0.75
30:0:2498:C:O2'	30:0:2499:U:H5'	1.87	0.75

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
30:0:1455:C:H3'	38:0:7887:HOH:O	1.86	0.74
20:T:24:ARG:HH21	20:T:39:ASN:HD22	1.34	0.74
30:0:1919:A:H4'	38:0:4863:HOH:O	1.86	0.74
30:0:2426:G:H1'	38:0:6107:HOH:O	1.87	0.74
30:0:1118:A:C8	30:0:1118:A:C3'	2.69	0.74
14:N:144:GLY:O	14:N:147:ILE:HG22	1.88	0.74
13:M:134:ILE:HG23	13:M:141:ILE:HD13	1.69	0.74
30:0:2456:A:H1'	38:0:6611:HOH:O	1.87	0.74
10:J:131:THR:HB	10:J:134:GLU:HG3	1.70	0.74
31:9:54:A:H2	38:9:9061:HOH:O	1.70	0.74
30:0:582:U:H2'	30:0:583:C:H6	1.53	0.74
14:N:113:SER:HB2	38:N:8854:HOH:O	1.88	0.74
10:J:82:THR:CG2	30:0:1242:A:H5'	2.16	0.73
30:0:2073:G:H5''	38:0:3832:HOH:O	1.88	0.73
30:0:564:G:H1'	38:0:6328:HOH:O	1.86	0.73
30:0:1634:G:H3'	38:0:3900:HOH:O	1.87	0.73
23:W:80:ASP:O	23:W:84:VAL:HG23	1.88	0.73
17:Q:95:GLU:HA	30:0:949:U:H4'	1.71	0.73
18:R:39:THR:HG22	18:R:42:GLU:H	1.53	0.73
30:0:2004:U:H4'	38:0:5318:HOH:O	1.87	0.73
30:0:2851:G:O2'	30:0:2852:A:H5'	1.89	0.73
30:0:542:A:H5'	30:0:542:A:C8	2.21	0.73
28:2:43:ARG:HH22	30:0:1684:A:H1'	1.53	0.73
30:0:1615:A:H4'	38:0:5899:HOH:O	1.88	0.73
21:U:47:ARG:HG3	38:U:4381:HOH:O	1.89	0.73
10:J:127:ILE:HG22	35:J:8801:CL:CL	2.24	0.73
30:0:2524:G:H21	30:0:2526:C:N4	1.85	0.73
30:0:854:G:H5''	38:0:3639:HOH:O	1.88	0.73
30:0:603:A:H5''	30:0:604:G:OP1	1.88	0.73
2:B:18:ARG:HE	2:B:256:GLN:HE21	1.35	0.73
30:0:1060:C:H6	30:0:1060:C:H5'	1.53	0.73
30:0:558:C:H2'	30:0:559:U:C5'	2.19	0.73
9:I:73:LEU:HD12	9:I:107:LYS:NZ	2.04	0.73
30:0:318:U:H5'	30:0:339:A:C2	2.24	0.73
30:0:1157:C:H2'	30:0:1158:G:H8	1.53	0.73
10:J:18:ILE:HD13	30:0:1244:U:OP1	1.89	0.73
30:0:2769:C:O2'	30:0:2770:G:H5'	1.89	0.73
30:0:2420:G:O2'	30:0:2421:G:H5'	1.88	0.73
3:C:78:ARG:HG3	3:C:78:ARG:HH11	1.54	0.73
30:0:1213:C:O2'	30:0:1214:G:H5'	1.89	0.73
3:C:139:VAL:HG13	38:C:8654:HOH:O	1.87	0.73
31:9:55:U:H4'	31:9:56:A:C8	2.24	0.73

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
30:0:1119:G:N2	30:0:1246:A:H2	1.84	0.73
30:0:871:G:C8	30:0:871:G:C5'	2.63	0.72
30:0:1666:C:H2'	30:0:1667:A:C5'	2.19	0.72
30:0:214:U:H5'	38:0:6153:HOH:O	1.88	0.72
31:9:75:G:H1	31:9:106:U:H3	1.37	0.72
30:0:848:C:H5'	38:0:7287:HOH:O	1.89	0.72
30:0:1942:A:H3'	38:0:7363:HOH:O	1.88	0.72
30:0:1942:A:H5'	38:0:7363:HOH:O	1.88	0.72
3:C:1:MET:HG2	3:C:2:GLN:H	1.52	0.72
30:0:2010:A:H2'	38:0:5975:HOH:O	1.90	0.72
23:W:84:VAL:HG12	38:W:6679:HOH:O	1.89	0.72
23:W:21:LEU:HD21	23:W:48:VAL:HG11	1.72	0.72
30:0:1528:A:H2'	30:0:1529:G:O4'	1.88	0.72
30:0:1595:G:O2'	30:0:1596:U:H5'	1.89	0.72
30:0:1964:U:O2	30:0:1964:U:H2'	1.88	0.72
30:0:2787:C:H5	38:0:4647:HOH:O	1.72	0.72
30:0:1603:A:H5''	30:0:1605:G:H5'	1.72	0.72
30:0:1834:C:H2'	30:0:1840:A:N6	2.04	0.72
2:B:258:GLY:H	2:B:260:HIS:CE1	2.08	0.72
25:Y:216:ARG:HD3	38:Y:8139:HOH:O	1.90	0.72
30:0:12:U:H2'	30:0:13:G:H5'	1.72	0.71
30:0:2481:G:H5''	38:0:4556:HOH:O	1.89	0.71
30:0:272:A:H5'	30:0:273:G:OP2	1.89	0.71
30:0:969:G:H1	30:0:999:C:H42	1.38	0.71
30:0:363:C:H1'	38:0:5292:HOH:O	1.90	0.71
13:M:102:GLU:OE1	13:M:164:THR:HG21	1.88	0.71
30:0:603:A:H1'	30:0:605:C:C2	2.25	0.71
22:V:1:THR:CB	30:0:93:C:H5''	2.17	0.71
30:0:2768:A:H2'	30:0:2769:C:O4'	1.90	0.71
30:0:2748:G:H1'	38:0:7912:HOH:O	1.91	0.71
19:S:51:GLN:HE21	19:S:53:ASN:HD21	1.38	0.71
30:0:2533:C:H5'	30:0:2533:C:H6	1.54	0.71
1:A:47:HIS:HD2	30:0:1654:U:H2'	1.56	0.71
14:N:141:ARG:HH12	31:9:35:C:H2'	1.56	0.71
30:0:1701:A:H5'	38:0:6302:HOH:O	1.89	0.71
3:C:162:VAL:HG22	3:C:232:LEU:HD21	1.73	0.71
30:0:870:G:C2'	30:0:871:G:H5''	2.20	0.71
4:D:172:VAL:HG12	4:D:173:GLU:H	1.55	0.71
1:A:72:GLU:HG3	26:Z:90:GLY:HA2	1.72	0.70
2:B:195:ARG:HG2	2:B:323:LEU:HD22	1.72	0.70
31:9:7:G:H5'	38:9:9098:HOH:O	1.91	0.70
30:0:2243:C:H5''	38:0:3756:HOH:O	1.91	0.70

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:192:VAL:CG1	1:A:207:GLN:HB3	2.21	0.70
5:E:81:GLU:HG2	5:E:134:SER:HB3	1.73	0.70
30:0:560:U:H2'	30:0:561:G:H8	1.56	0.70
3:C:140:VAL:HB	38:C:8657:HOH:O	1.91	0.70
30:0:2502:C:H2'	30:0:2503:A:C5'	2.17	0.70
30:0:960:G:C3'	30:0:960:G:N3	2.54	0.70
10:J:70:PHE:CE1	30:0:2676:C:H4'	2.26	0.70
30:0:2453:G:H3'	38:0:5935:HOH:O	1.91	0.70
23:W:72:PRO:HG2	23:W:77:ALA:HB3	1.73	0.70
30:0:1116:U:O2'	30:0:1118:A:H2	1.69	0.70
23:W:6:GLN:HB2	23:W:26:ILE:CD1	2.21	0.70
30:0:1666:C:C2'	30:0:1667:A:C5'	2.70	0.70
31:9:3:A:H61	31:9:22:G:H1'	1.56	0.70
14:N:40:ASN:ND2	31:9:28:U:H5''	2.06	0.70
30:0:2005:G:H3'	30:0:2005:G:OP2	1.91	0.70
30:0:2578:G:H5'	30:0:2578:G:H8	1.56	0.69
30:0:1377:C:H6	30:0:1377:C:H5'	1.57	0.69
30:0:2372:A:H2'	30:0:2373:U:C6	2.27	0.69
2:B:201:ASP:HB2	2:B:312:ARG:HD2	1.75	0.69
30:0:2717:C:H2'	30:0:2718:C:C5'	2.18	0.69
30:0:1701:A:H4'	30:0:1702:U:C5'	2.19	0.69
31:9:13:A:O2'	31:9:14:G:H5''	1.92	0.69
30:0:2073:G:OP2	30:0:2490:A:H5'	1.93	0.69
30:0:401:C:H2'	30:0:402:U:C6	2.27	0.69
30:0:613:C:H2'	30:0:614:U:H6	1.57	0.69
30:0:441:A:H1'	30:0:442:A:N7	2.08	0.69
9:I:110:ASP:O	30:0:1163:G:H5'	1.91	0.69
31:9:36:C:C5	31:9:37:C:C5	2.80	0.69
29:3:70:ARG:HD3	38:3:9059:HOH:O	1.90	0.69
30:0:1441:G:O2'	30:0:1442:A:H5'	1.92	0.69
4:D:135:VAL:HG21	4:D:139:TYR:CD1	2.27	0.69
30:0:625:U:H5''	30:0:1044:C:N4	2.08	0.69
14:N:49:THR:HG22	14:N:56:ASP:HB2	1.75	0.69
30:0:1667:A:H8	30:0:1667:A:H5'	1.57	0.69
30:0:1477:C:H5'	30:0:1868:G:C5'	2.22	0.69
28:2:41:HIS:H	28:2:45:ASN:HD22	1.39	0.69
30:0:271:C:H41	30:0:378:A:H2	1.36	0.69
11:K:74:VAL:HG11	11:K:113:ILE:HG12	1.74	0.69
30:0:249:G:O2'	30:0:250:C:H5'	1.93	0.69
11:K:98:VAL:HG13	11:K:102:GLU:HA	1.74	0.69
30:0:544:G:H2'	30:0:545:G:H5''	1.75	0.68
26:Z:70:ARG:HD3	26:Z:83:TYR:HB2	1.74	0.68

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
30:0:2535:A:H2	38:0:4805:HOH:O	1.75	0.68
31:9:29:C:H2'	31:9:30:C:H5'	1.75	0.68
30:0:2616:G:H1'	38:0:9426:HOH:O	1.93	0.68
30:0:1204:C:H2'	30:0:1205:U:O4'	1.92	0.68
30:0:816:G:C6	30:0:817:G:N1	2.61	0.68
30:0:1730:G:H5'	30:0:1731:C:C5	2.28	0.68
30:0:1819:G:H2'	30:0:1820:G:H4'	1.73	0.68
26:Z:66:CYS:SG	26:Z:68:GLU:HB2	2.33	0.68
1:A:100:PRO:HG2	1:A:103:VAL:HG21	1.73	0.68
13:M:178:LYS:HB2	38:0:6895:HOH:O	1.92	0.68
6:F:63:ILE:HB	6:F:64:PRO:HD3	1.74	0.68
30:0:2768:A:O2'	30:0:2769:C:H5'	1.94	0.68
30:0:1201:C:H2'	30:0:1202:A:H5'	1.75	0.68
30:0:1342:C:H2'	30:0:1343:C:H5'	1.76	0.68
15:O:47:ARG:HG3	15:O:47:ARG:HH11	1.58	0.68
30:0:2812:A:C2	30:0:2814:A:N6	2.58	0.68
14:N:48:VAL:CG1	14:N:55:ASP:HB3	2.24	0.67
11:K:87:ARG:HG3	30:0:2721:U:H4'	1.76	0.67
30:0:1183:C:N4	30:0:1184:C:H41	1.92	0.67
30:0:1191:A:H2'	30:0:1193:A:H5'	1.76	0.67
30:0:2534:C:H1'	38:0:3501:HOH:O	1.95	0.67
30:0:2659:U:H5''	38:0:4130:HOH:O	1.95	0.67
31:9:24:U:H3'	31:9:25:G:H5'	1.77	0.67
30:0:1422:U:H2'	30:0:1423:C:C6	2.29	0.67
8:H:6:ALA:HA	8:H:61:ARG:HH12	1.59	0.67
2:B:207:LYS:HG3	30:0:2717:C:OP1	1.95	0.67
1:A:199:HIS:CD2	1:A:201:PHE:H	2.12	0.67
30:0:308:U:H5'	30:0:309:C:OP1	1.93	0.67
30:0:2703:A:H2'	30:0:2704:C:H6	1.60	0.66
30:0:1165:G:H21	30:0:1173:A:C5'	2.08	0.66
11:K:74:VAL:CG1	11:K:113:ILE:HG12	2.25	0.66
30:0:2485:A:H3'	38:0:4900:HOH:O	1.95	0.66
2:B:41:PHE:CD1	2:B:79:MET:HE2	2.31	0.66
30:0:1185:U:H2'	30:0:1186:C:C6	2.28	0.66
30:0:1603:A:C5'	30:0:1605:G:H5'	2.25	0.66
30:0:559:U:H5'	30:0:559:U:C6	2.29	0.66
18:R:99:ALA:HB1	18:R:109:MET:HE1	1.77	0.66
30:0:1857:A:H5''	38:0:6720:HOH:O	1.94	0.66
27:1:1:THR:HA	38:1:8959:HOH:O	1.94	0.66
31:9:49:G:O2'	31:9:50:G:H5'	1.96	0.66
23:W:21:LEU:HD21	23:W:48:VAL:CG1	2.26	0.66
30:0:1477:C:H5'	30:0:1868:G:H5'	1.77	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
30:0:280:C:H2'	30:0:281:U:O4'	1.96	0.66
30:0:281:U:H2'	30:0:282:C:O4'	1.94	0.66
30:0:582:U:H2'	30:0:583:C:C6	2.31	0.66
30:0:2509:A:H2'	30:0:2510:C:O4'	1.96	0.65
30:0:506:G:H22	30:0:509:A:H5'	1.61	0.65
1:A:192:VAL:HG12	38:A:9055:HOH:O	1.96	0.65
30:0:1855:G:H4'	30:0:1856:C:O5'	1.96	0.65
30:0:969:G:H1	30:0:999:C:N4	1.94	0.65
1:A:94:LEU:HG	1:A:99:ILE:HD11	1.77	0.65
30:0:625:U:H5'	38:0:3191:HOH:O	1.96	0.65
3:C:118:THR:O	3:C:136:VAL:HG13	1.96	0.65
30:0:1157:C:H2'	30:0:1158:G:C8	2.31	0.65
30:0:1189:A:H3'	38:0:7692:HOH:O	1.95	0.65
30:0:1211:G:H2'	30:0:1212:C:H6	1.61	0.65
30:0:1687:C:H3'	38:0:9459:HOH:O	1.94	0.65
1:A:36:ASP:HB2	1:A:85:SER:H	1.60	0.65
30:0:1186:C:H42	30:0:1190:G:H22	1.44	0.65
8:H:168:VAL:HG13	38:H:212:HOH:O	1.95	0.65
18:R:117:HIS:HD2	30:0:20:G:H21	1.45	0.65
22:V:55:ARG:O	22:V:59:ILE:HG12	1.97	0.65
6:F:30:LYS:HE2	6:F:99:THR:HG21	1.79	0.65
30:0:714:U:H4'	38:0:5753:HOH:O	1.95	0.65
30:0:2672:C:H1'	38:0:6699:HOH:O	1.96	0.65
31:9:20:G:O2'	31:9:21:G:H5'	1.97	0.65
30:0:1834:C:H2'	30:0:1840:A:H62	1.61	0.65
30:0:2004:U:O5'	30:0:2004:U:H6	1.80	0.65
11:K:63:GLU:HB2	38:K:6344:HOH:O	1.97	0.65
6:F:77:VAL:HG21	6:F:83:LEU:HD13	1.77	0.65
8:H:29:SER:HA	8:H:62:HIS:HD2	1.61	0.65
30:0:2781:U:H2'	30:0:2782:G:H5'	1.77	0.65
1:A:51:ARG:HB2	38:A:9068:HOH:O	1.97	0.65
30:0:558:C:C2'	30:0:559:U:C5'	2.75	0.64
30:0:1632:A:H2'	30:0:1633:C:H5'	1.79	0.64
30:0:558:C:H2'	30:0:559:U:H5''	1.76	0.64
30:0:1058:A:H2'	30:0:1060:C:H5''	1.79	0.64
4:D:25:MET:SD	4:D:40:ILE:HD11	2.36	0.64
30:0:380:A:H2'	38:0:7242:HOH:O	1.96	0.64
30:0:1666:C:C2'	30:0:1667:A:H5''	2.27	0.64
30:0:1342:C:O2'	30:0:1343:C:H5'	1.98	0.64
30:0:272:A:H3'	38:0:7547:HOH:O	1.96	0.64
31:9:1:U:H4'	31:9:3:A:OP1	1.97	0.64
30:0:595:U:H2'	30:0:596:C:H6	1.63	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
11:K:14:LYS:HB2	11:K:45:PRO:HG2	1.80	0.64
30:0:2894:C:O2'	30:0:2895:C:H5'	1.97	0.64
25:Y:169:ARG:HD2	30:0:1328:A:OP1	1.97	0.64
12:L:41:HIS:HD2	30:0:926:A:O2'	1.79	0.64
18:R:128:ARG:NH2	30:0:2054:A:N3	2.45	0.64
30:0:2361:A:H5''	38:0:9009:HOH:O	1.97	0.64
31:9:64:C:C2'	31:9:65:A:H5'	2.27	0.64
30:0:1175:G:H1'	30:0:1193:A:C8	2.32	0.64
30:0:2824:C:H5''	30:0:2825:C:H5'	1.79	0.64
30:0:1116:U:H3	30:0:1246:A:N6	1.89	0.64
18:R:18:LEU:HB2	18:R:143:VAL:HG13	1.79	0.64
30:0:2781:U:C2'	30:0:2782:G:H5'	2.28	0.64
30:0:1398:G:O2'	30:0:1399:A:H5'	1.98	0.64
15:O:42:GLU:HB2	38:O:2176:HOH:O	1.97	0.64
5:E:100:ASP:HB2	38:E:2789:HOH:O	1.97	0.64
30:0:1180:U:O2'	30:0:1181:A:H5'	1.98	0.63
30:0:544:G:C2'	30:0:545:G:H5''	2.28	0.63
30:0:541:C:C2'	30:0:542:A:C5'	2.74	0.63
28:2:41:HIS:HD2	28:2:44:ARG:H	1.44	0.63
20:T:61:GLU:HG2	38:T:3851:HOH:O	1.97	0.63
30:0:2510:C:H42	30:0:2564:G:H22	1.47	0.63
8:H:72:ALA:HB2	8:H:156:ALA:HB2	1.80	0.63
30:0:1307:A:H2'	30:0:1308:A:C8	2.33	0.63
24:X:74:ALA:HB2	24:X:85:VAL:HG13	1.80	0.63
30:0:1165:G:H4'	30:0:1174:A:O2'	1.98	0.63
30:0:1634:G:H2'	30:0:1635:U:H6	1.63	0.63
30:0:2335:C:H2'	30:0:2336:G:H8	1.64	0.63
2:B:320:GLN:HE21	2:B:321:PRO:HD2	1.62	0.63
25:Y:187:VAL:HG23	25:Y:192:ASP:CB	2.28	0.63
5:E:93:MET:HE1	5:E:165:GLY:H	1.61	0.63
31:9:56:A:C3'	31:9:57:A:H5''	2.29	0.63
30:0:281:U:O2'	30:0:282:C:H5'	1.99	0.63
23:W:13:MET:HE1	23:W:18:GLN:HA	1.80	0.63
3:C:214:THR:HG23	38:C:8640:HOH:O	1.96	0.63
30:0:316:A:N3	30:0:336:G:O2'	2.30	0.63
30:0:236:A:H4'	30:0:237:G:H5'	1.81	0.63
27:1:25:LYS:HD2	28:2:49:GLU:N	2.13	0.63
30:0:1878:G:C1'	38:0:6135:HOH:O	2.43	0.63
30:0:74:G:H2'	30:0:75:U:C6	2.34	0.63
14:N:37:ARG:NH1	31:9:6:C:C5'	2.52	0.63
3:C:27:ARG:NH2	30:0:657:G:OP1	2.31	0.63
30:0:2717:C:O2'	30:0:2718:C:H5''	1.97	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
30:0:541:C:H2'	30:0:542:A:H5'	1.80	0.63
30:0:1278:A:H4'	30:0:1279:U:N3	2.13	0.63
30:0:1377:C:H5'	30:0:1377:C:C6	2.34	0.63
6:F:91:VAL:HG12	6:F:92:GLY:N	2.13	0.63
31:9:33:U:H2'	38:9:9065:HOH:O	1.98	0.63
3:C:218:VAL:HG12	38:C:8628:HOH:O	1.99	0.63
18:R:99:ALA:HB1	18:R:109:MET:CE	2.29	0.62
30:0:694:A:H2'	30:0:695:C:H5'	1.80	0.62
30:0:285:A:H2'	30:0:286:U:O4'	1.98	0.62
14:N:7:LYS:HE3	17:Q:21:ARG:O	1.99	0.62
31:9:64:C:H2'	31:9:65:A:H5'	1.81	0.62
30:0:2071:C:H5'	38:0:9532:HOH:O	1.99	0.62
30:0:533:U:H3'	38:0:3754:HOH:O	1.98	0.62
25:Y:115:ARG:HH21	30:0:1266:U:H4'	1.64	0.62
30:0:2670:G:O2'	30:0:2671:U:H5'	1.99	0.62
3:C:236:THR:HG22	3:C:239:ALA:HB2	1.80	0.62
30:0:2414:A:H2'	30:0:2415:A:C8	2.34	0.62
30:0:2320:U:H4'	30:0:2321:A:O4'	1.99	0.62
3:C:236:THR:HG22	3:C:239:ALA:CB	2.30	0.62
30:0:200:C:H2'	38:0:3449:HOH:O	2.00	0.62
3:C:2:GLN:HB3	38:C:8587:HOH:O	1.98	0.62
30:0:1398:G:H2'	30:0:1399:A:C8	2.34	0.62
30:0:920:C:H4'	30:0:921:G:C2	2.34	0.62
5:E:49:ILE:HD11	5:E:69:ILE:HD12	1.82	0.62
1:A:191:GLY:HA2	1:A:194:MET:HE3	1.81	0.62
2:B:179:LEU:O	2:B:183:GLU:HG2	2.00	0.62
2:B:262:ARG:HG3	30:0:2716:G:H5'	1.82	0.62
30:0:2512:U:H4'	30:0:2514:U:O4	1.99	0.62
27:1:10:LYS:HG3	38:1:8981:HOH:O	2.00	0.62
30:0:162:C:H2'	30:0:163:U:H5'	1.80	0.62
2:B:162:MET:HG3	2:B:310:ARG:HD3	1.82	0.61
31:9:55:U:H4'	31:9:56:A:H8	1.62	0.61
25:Y:187:VAL:HG23	25:Y:192:ASP:HB2	1.82	0.61
30:0:1524:U:H5''	30:0:1524:U:H6	1.63	0.61
30:0:585:C:H5''	38:0:4883:HOH:O	1.99	0.61
30:0:1132:A:N6	30:0:1229:C:H2'	2.16	0.61
30:0:2900:G:H2'	30:0:2901:C:O4'	1.99	0.61
30:0:1654:U:H5''	38:0:7439:HOH:O	1.99	0.61
30:0:1838:U:H3'	38:0:5538:HOH:O	1.98	0.61
5:E:20:ILE:HD11	5:E:40:VAL:HG11	1.83	0.61
30:0:137:U:H2'	30:0:139:C:C5	2.35	0.61
38:C:8669:HOH:O	30:0:2100:A:H5'	1.99	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
30:0:2507:G:H2'	30:0:2510:C:N4	2.15	0.61
9:I:108:HIS:H	9:I:109:PRO:HD2	1.66	0.61
2:B:307:ARG:HH11	2:B:307:ARG:HG3	1.66	0.61
30:0:1350:U:H4'	38:0:5132:HOH:O	2.00	0.61
30:0:1603:A:H5'	30:0:1605:G:C4'	2.30	0.61
30:0:1972:U:H2'	30:0:1973:A:H5''	1.83	0.61
1:A:211:LYS:HB2	38:A:9083:HOH:O	2.00	0.61
30:0:2064:U:H5'	30:0:2652:U:H4'	1.82	0.61
30:0:2908:A:O5'	30:0:2908:A:H8	1.83	0.61
12:L:18:HIS:HD2	30:0:902:G:N7	1.99	0.61
2:B:212:GLN:HB2	2:B:257:THR:CG2	2.28	0.61
30:0:1835:U:C5	30:0:1840:A:N7	2.65	0.61
29:3:48:ASN:HD21	30:0:2468:A:H61	1.48	0.61
12:L:133:VAL:HA	38:L:8873:HOH:O	2.00	0.61
3:C:127:ARG:HD3	3:C:129:HIS:HE1	1.65	0.61
3:C:37:ALA:HA	3:C:100:LEU:HD12	1.82	0.61
30:0:1226:G:H5'	38:0:4541:HOH:O	1.99	0.61
2:B:145:HIS:HD2	2:B:146:THR:O	1.83	0.61
12:L:6:ARG:HD3	30:0:1299:G:O6	2.00	0.61
23:W:4:LEU:HD22	23:W:52:VAL:HG21	1.83	0.61
25:Y:132:ASP:OD2	30:0:621:C:H5'	2.00	0.61
21:U:17:THR:HG22	21:U:18:GLY:N	2.16	0.61
25:Y:235:GLU:H	25:Y:235:GLU:CD	2.04	0.60
2:B:74:ILE:HD13	2:B:309:VAL:HG21	1.82	0.60
2:B:304:PRO:HD2	2:B:307:ARG:NE	2.16	0.60
26:Z:60:ASP:HB3	26:Z:69:ASP:HB3	1.83	0.60
3:C:95:GLU:HG3	38:C:8682:HOH:O	2.00	0.60
30:0:1181:A:C2'	30:0:1182:C:H5'	2.32	0.60
30:0:1741:U:O2'	30:0:2723:G:H4'	2.01	0.60
30:0:401:C:H2'	30:0:402:U:H6	1.64	0.60
30:0:1819:G:H5'	38:0:4725:HOH:O	2.00	0.60
28:2:40:ARG:HD2	28:2:47:THR:HG22	1.83	0.60
3:C:76:ARG:HG2	3:C:78:ARG:NH1	2.15	0.60
30:0:1819:G:H2'	30:0:1820:G:C5'	2.31	0.60
21:U:52:THR:HG22	21:U:54:THR:H	1.66	0.60
30:0:10:U:C4	30:0:532:A:N7	2.70	0.60
20:T:24:ARG:HH21	20:T:39:ASN:ND2	1.98	0.60
30:0:595:U:H2'	30:0:596:C:C6	2.37	0.60
18:R:128:ARG:NH2	30:0:2054:A:C2	2.70	0.60
30:0:1587:U:H2'	30:0:1588:G:O4'	2.02	0.60
30:0:447:A:O2'	30:0:448:G:H5'	2.01	0.60
8:H:155:ARG:NH1	30:0:2503:A:H5''	2.17	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
30:0:558:C:H2'	30:0:559:U:H5'	1.83	0.60
30:0:2372:A:H2'	30:0:2373:U:H6	1.66	0.60
30:0:847:C:H4'	38:0:3759:HOH:O	1.99	0.60
10:J:19:MET:HE1	10:J:132:LEU:HD21	1.83	0.60
29:3:73:GLU:HB3	38:3:9049:HOH:O	2.01	0.60
10:J:26:VAL:HG13	10:J:36:VAL:HG11	1.82	0.60
30:0:541:C:O2'	30:0:542:A:H5''	2.02	0.60
30:0:1202:A:C2'	30:0:1203:G:H5'	2.32	0.60
30:0:396:U:O2'	30:0:418:C:H4'	2.02	0.60
8:H:6:ALA:HA	8:H:61:ARG:NH1	2.17	0.60
30:0:407:A:H2'	30:0:408:A:C8	2.37	0.60
29:3:67:LEU:HD11	29:3:88:LEU:HD21	1.82	0.60
30:0:2281:C:C2'	30:0:2282:U:H5'	2.32	0.60
30:0:282:C:O2'	30:0:283:U:C5'	2.49	0.60
30:0:1583:U:H1'	38:0:9989:HOH:O	2.02	0.60
23:W:21:LEU:HD22	23:W:26:ILE:CD1	2.32	0.60
3:C:238:SER:HB2	38:C:8577:HOH:O	2.01	0.60
21:U:46:ALA:HB1	21:U:52:THR:HG21	1.83	0.60
30:0:130:C:H2'	38:0:3166:HOH:O	2.02	0.60
13:M:179:GLY:O	30:0:399:C:H5'	2.02	0.60
30:0:807:A:O2'	30:0:808:A:H5'	2.01	0.60
13:M:163:LEU:HD21	30:0:188:C:H5''	1.84	0.60
9:I:86:GLU:HG2	30:0:1180:U:H4'	1.83	0.59
7:G:12:ILE:HG23	38:0:5471:HOH:O	2.02	0.59
13:M:164:THR:HG23	13:M:165:GLY:N	2.17	0.59
31:9:47:A:C2	31:9:48:C:C2	2.89	0.59
11:K:98:VAL:CG1	11:K:102:GLU:HA	2.32	0.59
30:0:1676:G:O2'	30:0:1677:U:H5'	2.03	0.59
19:S:55:GLN:NE2	30:0:1446:U:H2'	2.18	0.59
30:0:1172:G:H5''	38:0:7275:HOH:O	2.01	0.59
30:0:1206:U:H2'	30:0:1207:A:O4'	2.01	0.59
2:B:18:ARG:HG3	2:B:256:GLN:HG3	1.82	0.59
2:B:51:VAL:HG23	2:B:330:VAL:HG22	1.83	0.59
30:0:2135:A:O2'	30:0:2136:G:H5'	2.03	0.59
11:K:32:ILE:HD11	11:K:56:SER:HB3	1.84	0.59
30:0:1165:G:N2	30:0:1173:A:H5''	2.15	0.59
30:0:2826:G:C6	30:0:2913:A:N6	2.70	0.59
5:E:68:HIS:O	5:E:72:MET:HG3	2.01	0.59
10:J:45:VAL:HG23	10:J:130:VAL:O	2.00	0.59
4:D:105:SER:OG	30:0:2338:G:H1'	2.03	0.59
4:D:65:GLU:HA	38:D:6752:HOH:O	2.02	0.59
13:M:164:THR:HG22	13:M:167:GLY:N	2.16	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
30:0:2505:G:C2'	30:0:2506:A:H5'	2.32	0.59
31:9:92:G:H2'	31:9:93:A:H8	1.67	0.59
30:0:1524:U:C5'	30:0:1524:U:H6	2.16	0.59
30:0:1766:U:O2	30:0:1778:A:H5'	2.01	0.59
1:A:186:TRP:CG	1:A:187:PRO:HA	2.38	0.59
25:Y:126:PRO:HG2	25:Y:128:PHE:CE1	2.37	0.59
30:0:2748:G:H5'	38:0:7557:HOH:O	2.02	0.59
30:0:1165:G:N2	30:0:1173:A:C5'	2.66	0.59
13:M:125:ARG:HD2	38:M:8893:HOH:O	2.02	0.59
14:N:34:LEU:HD22	14:N:129:ILE:HD13	1.83	0.59
30:0:1042:U:O2'	30:0:1043:C:H5'	2.02	0.59
30:0:424:C:H2'	30:0:425:U:C6	2.38	0.59
3:C:16:VAL:HG21	38:C:8634:HOH:O	2.02	0.59
30:0:482:G:H4'	30:0:508:A:N1	2.18	0.59
10:J:63:ILE:HD11	30:0:1236:A:C8	2.38	0.59
30:0:522:U:O2'	30:0:1366:C:H5'	2.02	0.59
30:0:1641:A:C2'	30:0:1642:A:H5'	2.32	0.59
30:0:853:C:H3'	38:0:4563:HOH:O	2.03	0.59
30:0:1511:U:O2'	30:0:1512:G:H5'	2.03	0.59
30:0:2374:G:H2'	30:0:2375:A:C8	2.37	0.59
30:0:1973:A:H5'	30:0:1973:A:C8	2.36	0.59
16:P:10:ALA:HA	16:P:13:VAL:HG12	1.85	0.59
28:2:39:ARG:HG2	38:2:3143:HOH:O	2.03	0.59
30:0:1790:C:H2'	30:0:1791:U:H6	1.67	0.59
30:0:255:A:H2'	30:0:256:C:C6	2.38	0.59
30:0:2324:G:N2	30:0:2377:U:H1'	2.17	0.59
30:0:368:C:H2'	30:0:369:G:H5'	1.84	0.58
10:J:52:GLN:HE22	30:0:1119:G:H2'	1.67	0.58
27:1:9:GLY:HA2	30:0:1687:C:O2	2.02	0.58
1:A:36:ASP:O	1:A:38:ILE:N	2.36	0.58
30:0:1321:A:H2'	30:0:1322:G:C8	2.38	0.58
30:0:1196:C:N4	30:0:1204:C:H42	2.01	0.58
30:0:2467:A:O2'	30:0:2468:A:H2'	2.02	0.58
30:0:123:U:H5'	38:0:6671:HOH:O	2.03	0.58
8:H:15:PRO:HG3	30:0:1053:G:OP1	2.02	0.58
30:0:1904:A:H2'	30:0:1905:U:O4'	2.03	0.58
1:A:94:LEU:HG	1:A:99:ILE:CD1	2.33	0.58
30:0:2335:C:H2'	30:0:2336:G:C8	2.38	0.58
17:Q:21:ARG:HH12	30:0:2353:A:H1'	1.67	0.58
30:0:10:U:C4	30:0:532:A:C8	2.91	0.58
3:C:79:ARG:O	3:C:87:ARG:HG2	2.03	0.58
30:0:1182:C:C1'	30:0:1192:A:H8	2.16	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
28:2:41:HIS:HB3	28:2:44:ARG:HB2	1.84	0.58
30:0:1170:U:H2'	30:0:1172:G:OP2	2.02	0.58
30:0:2878:U:H2'	30:0:2879:A:O4'	2.02	0.58
30:0:1948:G:H2'	30:0:1949:G:C8	2.39	0.58
11:K:4:LEU:HD22	11:K:116:GLU:HB3	1.85	0.58
30:0:2281:C:H2'	30:0:2282:U:H5'	1.85	0.58
3:C:78:ARG:HG3	3:C:78:ARG:NH1	2.15	0.58
30:0:960:G:H8	38:0:5987:HOH:O	1.85	0.58
30:0:2852:A:H5''	38:0:5246:HOH:O	2.03	0.58
8:H:174:LEU:HD21	30:0:1220:U:H4'	1.85	0.58
1:A:121:ALA:O	1:A:124:VAL:HG22	2.03	0.58
9:I:112:LEU:CD1	30:0:1162:G:H1'	2.34	0.58
30:0:2768:A:H5''	38:0:4434:HOH:O	2.03	0.58
3:C:76:ARG:HG2	3:C:78:ARG:HH12	1.69	0.58
3:C:237:GLU:HG3	38:C:8634:HOH:O	2.04	0.58
12:L:14:GLY:O	30:0:1295:G:H5''	2.03	0.58
30:0:440:C:H2'	30:0:441:A:C8	2.39	0.58
31:9:37:C:H2'	31:9:38:A:H8	1.68	0.58
30:0:1819:G:H2'	30:0:1820:G:C4'	2.34	0.58
25:Y:141:THR:HG23	38:Y:8158:HOH:O	2.03	0.58
24:X:23:HIS:HE1	30:0:2044:G:OP1	1.86	0.58
22:V:64:GLY:O	22:V:65:ASP:HB2	2.04	0.58
14:N:71:TRP:CE3	14:N:175:LEU:HD22	2.38	0.58
13:M:134:ILE:CG2	13:M:141:ILE:HD13	2.34	0.58
30:0:681:G:N3	30:0:681:G:H5'	2.19	0.58
30:0:2820:A:H2'	30:0:2821:C:C6	2.38	0.58
30:0:2643:G:H5''	38:0:3933:HOH:O	2.03	0.58
14:N:141:ARG:NH1	31:9:35:C:H2'	2.18	0.58
23:W:68:THR:HG23	23:W:69:ARG:HG2	1.86	0.58
11:K:20:CYS:HB2	11:K:29:LEU:HG	1.86	0.57
30:0:1947:G:H2'	30:0:1948:G:H8	1.69	0.57
30:0:2760:C:H5''	38:0:5337:HOH:O	2.03	0.57
19:S:76:GLU:HB3	38:S:8992:HOH:O	2.04	0.57
30:0:249:G:N2	30:0:250:C:C2	2.72	0.57
30:0:1730:G:C5'	30:0:1731:C:C6	2.86	0.57
28:2:38:LYS:HE3	38:0:4231:HOH:O	2.04	0.57
2:B:27:ASN:H	2:B:27:ASN:HD22	1.51	0.57
24:X:47:ALA:HB1	24:X:82:GLU:HB3	1.86	0.57
27:1:16:HIS:HD2	30:0:470:U:O2'	1.86	0.57
3:C:174:ILE:HD11	30:0:338:C:H4'	1.85	0.57
2:B:238:ASN:HD22	2:B:240:GLY:N	1.97	0.57
6:F:91:VAL:HG12	6:F:92:GLY:H	1.68	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
30:0:1191:A:C2	30:0:1207:A:C2	2.93	0.57
31:9:76:G:C3'	31:9:77:A:H5''	2.25	0.57
3:C:129:HIS:CE1	3:C:231:ARG:HA	2.38	0.57
30:0:2003:U:HO2'	30:0:2004:U:H5	1.52	0.57
30:0:1965:C:O2'	30:0:1966:U:H5'	2.04	0.57
30:0:395:A:H5''	38:0:3928:HOH:O	2.05	0.57
30:0:2254:G:O2'	30:0:2255:A:H5'	2.04	0.57
30:0:2532:A:H2	38:0:7579:HOH:O	1.87	0.57
30:0:360:A:H2'	30:0:361:C:O4'	2.04	0.57
30:0:185:G:H4'	30:0:186:A:OP1	2.04	0.57
31:9:23:U:O2'	31:9:24:U:H4'	2.05	0.57
31:9:3:A:C8	31:9:26:C:C2	2.93	0.57
38:O:7674:HOH:O	30:0:653:U:H5''	2.05	0.57
13:M:188:ARG:HD3	30:0:155:C:OP2	2.03	0.57
30:0:602:A:O2'	30:0:605:C:H4'	2.04	0.57
30:0:1524:U:OP1	30:0:1524:U:H4'	2.05	0.57
21:U:14:GLU:O	21:U:17:THR:HB	2.05	0.57
30:0:65:C:O2'	30:0:66:G:H5'	2.03	0.57
28:2:35:ARG:HB2	38:2:2691:HOH:O	2.05	0.57
30:0:119:A:H2'	30:0:120:A:H5''	1.86	0.57
2:B:244:PRO:HB3	30:0:1234:U:N3	2.19	0.57
30:0:2314:G:C2'	30:0:2315:C:H5'	2.34	0.57
30:0:1116:U:O2'	30:0:1118:A:C2	2.50	0.57
9:I:73:LEU:HD12	9:I:107:LYS:HZ2	1.67	0.57
30:0:1333:U:H2'	30:0:1334:C:C6	2.40	0.57
30:0:2282:U:H4'	30:0:2309:C:C5	2.39	0.57
30:0:2507:G:H2'	30:0:2510:C:H42	1.70	0.57
18:R:39:THR:HG23	18:R:107:GLU:O	2.05	0.57
1:A:192:VAL:HG13	1:A:207:GLN:HB3	1.87	0.57
5:E:93:MET:HE1	5:E:165:GLY:N	2.19	0.57
30:0:1515:A:H2'	30:0:1516:U:C6	2.40	0.57
14:N:13:ARG:NH1	30:0:2368:A:C6	2.72	0.57
13:M:30:GLU:O	13:M:34:GLU:HG3	2.04	0.57
30:0:711:G:C2	30:0:718:C:C2	2.92	0.57
8:H:98:LEU:HD11	8:H:127:ALA:HB2	1.86	0.57
30:0:291:C:H2'	30:0:292:G:O4'	2.05	0.57
30:0:1351:G:H1'	38:0:4693:HOH:O	2.04	0.57
30:0:1189:A:O2'	30:0:1208:C:H2'	2.05	0.56
30:0:2831:C:O2'	30:0:2832:C:H5'	2.05	0.56
30:0:2533:C:C6	30:0:2533:C:H5'	2.38	0.56
23:W:13:MET:CE	23:W:18:GLN:HA	2.35	0.56
3:C:174:ILE:CD1	30:0:338:C:H4'	2.35	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
30:0:2897:C:O2'	30:0:2898:G:H5'	2.05	0.56
16:P:59:ARG:O	16:P:63:ARG:HG3	2.05	0.56
30:0:538:C:H5''	30:0:539:G:C8	2.40	0.56
30:0:1504:A:H4'	30:0:1506:U:C5	2.40	0.56
5:E:116:THR:HG22	5:E:151:LEU:HD22	1.87	0.56
30:0:432:G:O2'	30:0:433:C:H5'	2.05	0.56
11:K:118:ALA:HA	11:K:125:ALA:HB2	1.85	0.56
26:Z:81:CYS:SG	26:Z:83:TYR:HB3	2.45	0.56
19:S:11:THR:H	19:S:14:ALA:HB3	1.69	0.56
1:A:105:VAL:CG1	1:A:154:ALA:HB1	2.35	0.56
2:B:294:TYR:HE2	38:B:9116:HOH:O	1.88	0.56
23:W:5:VAL:HG11	23:W:153:MET:CE	2.35	0.56
15:O:14:LEU:HD23	15:O:102:ILE:HD11	1.88	0.56
19:S:57:THR:HG23	38:S:8980:HOH:O	2.05	0.56
30:0:812:A:H2'	30:0:813:C:C6	2.40	0.56
30:0:2781:U:H2'	30:0:2782:G:C5'	2.35	0.56
30:0:1634:G:H2'	30:0:1635:U:C6	2.41	0.56
14:N:139:TRP:HA	14:N:139:TRP:CE3	2.40	0.56
30:0:2297:U:H1'	38:0:5188:HOH:O	2.04	0.56
30:0:851:C:O2	30:0:2022:A:H2	1.87	0.56
30:0:2282:U:H4'	30:0:2309:C:H5	1.71	0.56
30:0:483:C:C4	30:0:484:A:C6	2.94	0.56
30:0:484:A:N1	30:0:506:G:H4'	2.21	0.56
30:0:2300:A:H4'	30:0:2301:A:O5'	2.05	0.56
25:Y:130:ARG:HB2	25:Y:142:SER:O	2.05	0.56
30:0:2472:C:O2'	30:0:2634:G:H4'	2.04	0.56
30:0:1189:A:H1'	30:0:1209:C:O4'	2.05	0.56
8:H:59:GLN:HE21	8:H:129:ARG:NE	1.94	0.56
24:X:72:VAL:HG22	24:X:85:VAL:HG12	1.86	0.56
31:9:35:C:H5''	38:9:9075:HOH:O	2.06	0.56
2:B:7:ARG:HG2	2:B:7:ARG:HH11	1.70	0.56
4:D:56:ARG:NH2	30:0:2332:A:H5'	2.21	0.56
8:H:22:TYR:CZ	30:0:1007:A:H2'	2.41	0.56
13:M:24:GLN:NE2	13:M:27:ARG:HH11	2.04	0.56
4:D:159:PRO:O	4:D:163:VAL:HG23	2.06	0.56
30:0:1130:U:H2'	30:0:1131:G:O4'	2.06	0.56
30:0:559:U:C5	30:0:560:U:C5	2.94	0.56
30:0:2482:G:H5'	38:0:5036:HOH:O	2.05	0.56
1:A:47:HIS:CD2	30:0:1654:U:H2'	2.37	0.56
30:0:282:C:C2'	30:0:282:C:O2	2.54	0.56
2:B:162:MET:HE2	2:B:310:ARG:HD3	1.87	0.56
22:V:42:ASN:HB3	38:V:7247:HOH:O	2.06	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
18:R:29:LYS:HB3	38:R:8936:HOH:O	2.06	0.56
30:0:151:A:C2	30:0:152:A:C2	2.94	0.56
30:0:2831:C:C2'	30:0:2832:C:H5'	2.36	0.56
30:0:1772:C:H5'	30:0:1773:G:C5	2.41	0.56
4:D:103:ASN:ND2	4:D:134:LEU:H	2.04	0.56
10:J:74:ARG:HB3	10:J:74:ARG:HH11	1.70	0.56
15:O:32:ARG:HH21	15:O:35:LYS:NZ	2.04	0.55
38:M:8868:HOH:O	30:0:2244:A:H1'	2.06	0.55
2:B:156:LYS:HD3	38:0:3870:HOH:O	2.05	0.55
31:9:49:G:H2'	31:9:50:G:O4'	2.05	0.55
30:0:1787:C:H4'	30:0:2883:A:O4'	2.06	0.55
14:N:61:ALA:HB3	14:N:88:ALA:HB2	1.88	0.55
3:C:47:GLY:HA2	3:C:92:PRO:HB2	1.87	0.55
30:0:1426:C:H2'	38:0:9598:HOH:O	2.06	0.55
30:0:1545:C:H2'	30:0:1546:G:O4'	2.06	0.55
30:0:553:G:O4'	30:0:1325:G:H5'	2.06	0.55
14:N:37:ARG:HH11	31:9:6:C:C5'	2.15	0.55
30:0:1972:U:C2'	30:0:1973:A:H5''	2.36	0.55
11:K:45:PRO:HB2	38:0:7387:HOH:O	2.06	0.55
12:L:136:ALA:HB3	38:L:8873:HOH:O	2.05	0.55
30:0:2886:C:O2'	30:0:2887:G:H5'	2.07	0.55
14:N:80:SER:HB2	38:N:8833:HOH:O	2.05	0.55
2:B:265:LEU:HD21	2:B:316:ARG:HD3	1.88	0.55
2:B:211:THR:HG23	30:0:2840:A:OP1	2.06	0.55
30:0:1191:A:C2'	30:0:1193:A:H5'	2.37	0.55
30:0:960:G:N3	30:0:960:G:C2'	2.69	0.55
21:U:39:ASN:ND2	21:U:44:ARG:HH11	2.04	0.55
29:3:3:MET:O	29:3:90:PHE:HA	2.06	0.55
30:0:1202:A:H2'	30:0:1203:G:C5'	2.37	0.55
20:T:9:LYS:HD3	38:0:3761:HOH:O	2.06	0.55
2:B:98:THR:HG22	30:0:2820:A:OP1	2.07	0.55
23:W:35:VAL:HG23	23:W:41:TYR:CD2	2.42	0.55
30:0:2599:A:H5''	38:0:3384:HOH:O	2.05	0.55
14:N:37:ARG:HD3	35:N:8807:CL:CL	2.44	0.55
9:I:87:PRO:HG2	30:0:1181:A:H4'	1.87	0.55
6:F:58:GLU:CD	13:M:27:ARG:HH22	2.08	0.55
30:0:669:G:O2'	30:0:670:G:H5'	2.07	0.55
30:0:1120:U:H5'	30:0:1121:G:OP2	2.07	0.55
14:N:12:ARG:HD3	14:N:18:THR:OG1	2.06	0.55
18:R:111:ILE:HG23	18:R:145:LEU:HD11	1.89	0.55
18:R:132:ARG:HG2	18:R:133:ALA:N	2.21	0.55
4:D:173:GLU:HG3	4:D:174:VAL:H	1.71	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
30:0:1790:C:H2'	30:0:1791:U:C6	2.41	0.55
18:R:98:ASN:HD21	30:0:500:G:H21	1.54	0.55
27:1:21:ARG:HD2	27:1:37:CYS:SG	2.47	0.55
15:O:25:VAL:CG1	30:0:710:G:H5'	2.36	0.55
2:B:86:ALA:HA	38:B:9045:HOH:O	2.05	0.55
30:0:1972:U:H2'	30:0:1973:A:C5'	2.37	0.55
3:C:236:THR:HA	38:C:8657:HOH:O	2.07	0.55
10:J:69:TYR:CE1	30:0:2081:A:H4'	2.42	0.55
25:Y:117:LEU:HA	25:Y:174:VAL:HG11	1.88	0.55
18:R:59:PHE:O	18:R:63:ASN:HB3	2.06	0.55
2:B:267:LYS:HE2	38:B:8994:HOH:O	2.06	0.55
31:9:24:U:H3'	31:9:25:G:C5'	2.35	0.55
30:0:2514:U:OP1	30:0:2572:G:H1'	2.06	0.55
30:0:2297:U:H2'	30:0:2298:C:H6	1.71	0.55
4:D:103:ASN:HD22	4:D:134:LEU:H	1.54	0.55
30:0:1544:U:O2'	30:0:1545:C:H5'	2.05	0.55
15:O:96:VAL:HG13	15:O:100:GLN:HB2	1.89	0.55
30:0:794:U:H3	30:0:819:A:H61	1.54	0.55
30:0:512:G:O3'	30:0:513:A:H8	1.89	0.55
30:0:1706:G:C6	30:0:1707:G:C6	2.95	0.55
13:M:46:LEU:HG	38:M:8921:HOH:O	2.06	0.55
13:M:65:VAL:HG21	13:M:105:ALA:HB2	1.89	0.55
23:W:154:ARG:NH1	30:0:588:G:O6	2.40	0.55
30:0:2851:G:C2'	30:0:2852:A:H5'	2.37	0.54
30:0:1504:A:H5'	38:0:4423:HOH:O	2.06	0.54
30:0:88:G:H5'	30:0:88:G:H8	1.72	0.54
30:0:713:U:O5'	30:0:713:U:H6	1.90	0.54
6:F:96:ALA:HA	38:F:3111:HOH:O	2.06	0.54
30:0:1915:U:O2'	30:0:1916:C:H5'	2.06	0.54
30:0:1202:A:H2'	30:0:1203:G:O4'	2.08	0.54
30:0:2790:C:HO2'	30:0:2791:U:H6	1.54	0.54
4:D:131:THR:HG21	30:0:2348:C:H1'	1.89	0.54
30:0:515:C:H5''	38:0:5660:HOH:O	2.06	0.54
30:0:1160:G:H2'	38:0:5647:HOH:O	2.07	0.54
23:W:137:GLN:HE21	23:W:141:HIS:CE1	2.13	0.54
30:0:1202:A:O2'	30:0:1203:G:H5'	2.07	0.54
1:A:190:ARG:NH2	1:A:207:GLN:OE1	2.40	0.54
30:0:1903:U:O2'	30:0:1904:A:N7	2.40	0.54
30:0:644:G:N3	30:0:644:G:H5'	2.22	0.54
23:W:88:THR:HG23	23:W:110:GLN:HE21	1.72	0.54
30:0:1730:G:H5''	30:0:1731:C:H6	1.71	0.54
10:J:127:ILE:CG2	35:J:8801:CL:CL	2.91	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:119:HIS:O	2:B:121:PRO:HD3	2.07	0.54
20:T:38:ARG:NH1	38:T:6217:HOH:O	2.41	0.54
21:U:9:CYS:HA	21:U:52:THR:HG23	1.90	0.54
30:0:2326:C:H4'	30:0:2412:G:H4'	1.89	0.54
30:0:1521:C:H2'	30:0:1522:A:H8	1.72	0.54
27:1:20:ARG:HG2	30:0:111:C:O2'	2.08	0.54
14:N:4:PRO:HG3	31:9:69:U:OP1	2.07	0.54
27:1:25:LYS:CD	28:2:49:GLU:H	2.18	0.54
2:B:162:MET:HE1	2:B:308:LEU:HD21	1.89	0.54
2:B:51:VAL:HG13	2:B:53:LEU:HD13	1.90	0.54
30:0:2314:G:H2'	30:0:2315:C:H5'	1.90	0.54
30:0:553:G:H5'	38:0:3505:HOH:O	2.08	0.54
30:0:1406:A:H5'	30:0:1407:A:C8	2.42	0.54
19:S:17:ASP:HB3	19:S:23:LYS:HB2	1.90	0.54
15:O:37:ARG:HD2	30:0:656:G:OP2	2.08	0.54
30:0:1041:U:H2'	30:0:1042:U:H5'	1.89	0.54
12:L:46:LEU:O	30:0:2430:A:H4'	2.07	0.54
30:0:1559:A:H4'	38:0:5879:HOH:O	2.08	0.54
9:I:118:ASN:HB3	30:0:1185:U:H5''	1.88	0.54
30:0:2421:G:H2'	38:0:4085:HOH:O	2.07	0.54
30:0:920:C:H5''	30:0:921:G:O5'	2.08	0.54
30:0:1573:A:H2'	30:0:1574:C:O4'	2.08	0.54
30:0:2329:C:O2'	30:0:2330:U:H5'	2.08	0.54
4:D:64:ARG:HD3	4:D:67:ASP:HB3	1.90	0.54
19:S:33:SER:O	19:S:37:VAL:HG23	2.08	0.54
30:0:1193:A:C2	30:0:1194:A:N6	2.76	0.54
2:B:212:GLN:HA	30:0:1733:A:H4'	1.89	0.54
23:W:21:LEU:HD22	23:W:26:ILE:HD13	1.89	0.54
30:0:1165:G:O3'	30:0:1174:A:H4'	2.08	0.54
30:0:812:A:H1'	38:0:3964:HOH:O	2.08	0.54
17:Q:25:PRO:HB2	38:9:9079:HOH:O	2.07	0.54
30:0:2460:A:C2	30:0:2461:U:C2	2.95	0.54
1:A:101:GLU:OE2	1:A:131:HIS:HB2	2.08	0.54
30:0:1544:U:H2'	30:0:1545:C:H6	1.72	0.53
30:0:1495:C:H1'	30:0:1573:A:H1'	1.90	0.53
25:Y:151:SER:HB3	25:Y:154:ARG:CB	2.38	0.53
16:P:76:GLY:HA3	30:0:1785:G:OP1	2.08	0.53
2:B:84:LEU:HD23	2:B:142:LEU:HD23	1.91	0.53
30:0:822:C:H2'	30:0:823:U:H6	1.73	0.53
30:0:2134:G:N2	30:0:2242:U:C2	2.76	0.53
24:X:76:ARG:HH11	24:X:76:ARG:HG3	1.71	0.53
22:V:57:LYS:HA	22:V:60:GLN:HE21	1.72	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
30:0:1803:C:H2'	30:0:1804:A:C8	2.43	0.53
31:9:54:A:C2'	31:9:55:U:H5'	2.38	0.53
30:0:2510:C:H5'	30:0:2511:A:OP2	2.08	0.53
8:H:35:LYS:HE3	30:0:968:G:H1'	1.88	0.53
4:D:27:ILE:HB	4:D:69:ILE:O	2.08	0.53
30:0:963:C:H2'	30:0:964:G:C8	2.43	0.53
30:0:2667:G:H1'	30:0:2914:A:N3	2.24	0.53
26:Z:61:HIS:HB2	26:Z:71:VAL:HB	1.90	0.53
30:0:1289:C:O2'	30:0:1290:G:H5'	2.09	0.53
9:I:69:PRO:HA	30:0:1164:U:OP1	2.09	0.53
25:Y:187:VAL:HB	38:Y:8140:HOH:O	2.08	0.53
30:0:2241:C:O2'	30:0:2242:U:H5'	2.09	0.53
30:0:1118:A:N6	30:0:1244:U:H3	1.99	0.53
31:9:29:C:C2'	31:9:30:C:H5'	2.38	0.53
16:P:13:VAL:HG21	16:P:41:ARG:HG2	1.89	0.53
30:0:821:U:O2'	30:0:822:C:H5'	2.08	0.53
30:0:2251:G:H2'	30:0:2252:A:C8	2.43	0.53
30:0:349:U:H2'	30:0:350:G:O4'	2.09	0.53
1:A:51:ARG:NH1	1:A:120:ARG:O	2.39	0.53
30:0:1632:A:C2'	30:0:1633:C:H5'	2.39	0.53
6:F:91:VAL:HG11	30:0:262:A:OP2	2.09	0.53
2:B:53:LEU:HD11	2:B:327:VAL:HG22	1.89	0.53
3:C:184:ARG:NH2	30:0:450:C:OP1	2.29	0.53
10:J:76:ASP:HA	38:J:8865:HOH:O	2.09	0.53
2:B:141:ARG:HD2	2:B:163:GLU:OE2	2.09	0.53
30:0:635:A:H2'	30:0:636:G:H5'	1.90	0.53
30:0:1909:A:N1	30:0:2128:G:H1'	2.24	0.53
14:N:35:VAL:HG12	14:N:37:ARG:HG2	1.91	0.53
30:0:1166:A:C6	30:0:1167:G:C6	2.97	0.53
2:B:312:ARG:HD3	2:B:315:VAL:HG13	1.90	0.53
25:Y:151:SER:HB3	25:Y:154:ARG:HB2	1.90	0.53
5:E:107:PHE:CE1	5:E:152:THR:HB	2.43	0.53
30:0:574:G:O2'	30:0:575:A:H5'	2.09	0.53
30:0:222:A:H2'	30:0:223:G:O4'	2.08	0.53
8:H:26:ILE:HA	8:H:123:ILE:HG21	1.89	0.53
12:L:67:ARG:HB2	12:L:112:GLY:HA3	1.90	0.53
27:1:12:ASN:O	30:0:1415:G:H5'	2.08	0.53
30:0:559:U:C5'	30:0:559:U:H6	2.19	0.53
30:0:2073:G:C6	30:0:2489:G:H4'	2.44	0.53
30:0:2065:C:O2'	30:0:2066:C:H5'	2.09	0.53
14:N:25:ARG:HG2	30:0:2416:G:O2'	2.09	0.53
14:N:132:ASN:O	14:N:135:VAL:HG12	2.09	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
30:0:128:A:O2'	30:0:129:A:H5'	2.09	0.53
10:J:107:ASN:HD22	10:J:109:TYR:H	1.57	0.53
30:0:2111:G:H1'	38:0:9051:HOH:O	2.08	0.53
30:0:2769:C:H2'	30:0:2770:G:O4'	2.09	0.53
5:E:139:GLU:OE2	30:0:2781:U:H1'	2.09	0.53
30:0:441:A:H8	30:0:441:A:O5'	1.92	0.53
30:0:290:C:O2'	30:0:291:C:H5'	2.09	0.53
14:N:139:TRP:HA	14:N:139:TRP:HE3	1.74	0.53
6:F:34:ASN:HA	13:M:4:ALA:HB2	1.91	0.53
30:0:1181:A:H2'	30:0:1182:C:H5'	1.90	0.52
31:9:3:A:H1'	38:9:9037:HOH:O	2.09	0.52
30:0:1594:C:O2'	30:0:1595:G:H5'	2.09	0.52
30:0:24:G:N2	30:0:518:G:H1'	2.24	0.52
30:0:1625:U:H5''	38:0:6037:HOH:O	2.09	0.52
5:E:143:GLN:NE2	30:0:2780:C:H1'	2.13	0.52
30:0:615:G:H2'	30:0:616:U:C6	2.44	0.52
30:0:1733:A:C6	30:0:1734:C:C2	2.98	0.52
30:0:2500:C:O2'	30:0:2501:G:H5'	2.08	0.52
14:N:48:VAL:HG11	14:N:55:ASP:HB3	1.90	0.52
30:0:204:A:H2'	30:0:205:U:H5'	1.90	0.52
4:D:57:THR:HG23	4:D:63:ILE:HA	1.91	0.52
4:D:58:VAL:HB	4:D:62:ASP:HB3	1.89	0.52
30:0:90:A:H2'	30:0:91:G:O4'	2.08	0.52
30:0:1419:U:H2'	30:0:1685:A:C2	2.44	0.52
31:9:59:C:H2'	31:9:60:C:C6	2.43	0.52
30:0:1181:A:H1'	38:0:7132:HOH:O	2.09	0.52
1:A:223:ARG:HB2	30:0:2272:G:H5'	1.90	0.52
28:2:49:GLU:HB2	38:2:719:HOH:O	2.10	0.52
23:W:48:VAL:HG12	23:W:52:VAL:HB	1.90	0.52
35:0:8813:CL:CL	38:0:4697:HOH:O	2.56	0.52
38:L:8841:HOH:O	30:0:2453:G:H5''	2.09	0.52
15:O:47:ARG:HG3	15:O:47:ARG:NH1	2.25	0.52
4:D:28:GLY:HA2	4:D:69:ILE:HG23	1.91	0.52
5:E:91:PHE:CE1	30:0:2694:A:H4'	2.43	0.52
30:0:2598:U:O2	30:0:2600:A:H8	1.92	0.52
30:0:1216:G:O2'	30:0:1217:G:H5'	2.10	0.52
30:0:1461:U:H2'	30:0:1462:C:C6	2.44	0.52
30:0:1161:A:C6	30:0:1162:G:N7	2.77	0.52
30:0:1189:A:H1'	30:0:1209:C:C1'	2.40	0.52
8:H:6:ALA:HB3	30:0:2521:A:OP2	2.09	0.52
30:0:1588:G:C6	30:0:1589:G:N1	2.77	0.52
30:0:1482:A:O2'	30:0:1483:C:H5'	2.10	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
25:Y:99:ALA:HB2	25:Y:233:TYR:CE2	2.44	0.52
2:B:305:ASP:O	2:B:306:LYS:HB2	2.10	0.52
30:0:899:C:H5'	38:0:3209:HOH:O	2.09	0.52
16:P:134:VAL:O	16:P:137:LEU:HB3	2.10	0.52
26:Z:74:GLN:HB2	26:Z:78:ILE:HG22	1.90	0.52
1:A:206:ARG:HD3	38:0:4620:HOH:O	2.08	0.52
30:0:1196:C:H42	30:0:1204:C:H42	1.58	0.52
31:9:91:C:H2'	31:9:92:G:O4'	2.10	0.52
30:0:1202:A:H2'	30:0:1203:G:H5'	1.90	0.52
30:0:1871:U:O4'	30:0:1873:G:C8	2.63	0.52
2:B:17:LYS:O	2:B:260:HIS:HD2	1.91	0.52
30:0:1309:U:O2'	30:0:1310:U:H5'	2.09	0.52
17:Q:19:ARG:HH21	31:9:11:A:P	2.33	0.52
25:Y:169:ARG:HD3	30:0:1328:A:C8	2.44	0.52
16:P:91:LYS:O	16:P:95:GLU:HG3	2.08	0.52
3:C:63:SER:OG	30:0:2101:A:H2'	2.09	0.52
21:U:6:CYS:HB2	21:U:32:CYS:HB3	1.90	0.52
14:N:67:ALA:HA	14:N:71:TRP:HB3	1.92	0.52
11:K:113:ILE:HD12	11:K:128:ALA:HB2	1.92	0.52
30:0:136:C:H2'	30:0:137:U:O4'	2.09	0.52
20:T:38:ARG:HH21	30:0:306:A:P	2.33	0.52
30:0:2866:U:C2	30:0:2891:A:C8	2.98	0.52
30:0:2273:C:H5''	38:0:4515:HOH:O	2.10	0.52
31:9:108:C:H2'	31:9:109:G:C8	2.45	0.52
30:0:1029:U:O2'	30:0:1273:C:OP1	2.25	0.52
23:W:117:ARG:HD3	30:0:1287:A:O4'	2.10	0.52
11:K:10:GLN:H	11:K:10:GLN:NE2	1.96	0.52
30:0:2032:U:O2'	30:0:2033:G:H5''	2.09	0.52
9:I:73:LEU:HD12	9:I:107:LYS:HZ1	1.73	0.52
30:0:1964:U:C2'	30:0:1964:U:O2	2.58	0.52
3:C:217:GLU:HG3	30:0:672:G:O6	2.10	0.52
18:R:33:ARG:NH1	38:R:8947:HOH:O	2.42	0.52
11:K:18:ILE:HG22	11:K:93:ASN:HB2	1.92	0.52
30:0:2112:A:H2'	30:0:2113:G:C8	2.45	0.52
9:I:112:LEU:HD12	30:0:1162:G:H1'	1.92	0.51
30:0:2827:A:H2'	30:0:2828:G:O4'	2.10	0.51
30:0:407:A:H8	38:0:4468:HOH:O	1.93	0.51
30:0:1333:U:H2'	30:0:1334:C:H6	1.75	0.51
30:0:152:A:H2'	30:0:153:C:C6	2.45	0.51
22:V:56:ILE:O	22:V:60:GLN:HG3	2.09	0.51
31:9:59:C:H6	31:9:59:C:O5'	1.92	0.51
30:0:951:A:C2'	30:0:952:G:H5'	2.39	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
8:H:70:LEU:O	8:H:74:ARG:HB2	2.09	0.51
30:0:2636:C:H3'	38:0:9279:HOH:O	2.09	0.51
30:0:876:A:N3	30:0:876:A:H2'	2.23	0.51
30:0:792:G:O2'	30:0:793:A:H5'	2.11	0.51
31:9:58:G:H1'	38:9:9067:HOH:O	2.09	0.51
10:J:54:VAL:HG11	10:J:138:THR:HG21	1.92	0.51
30:0:638:C:H2'	30:0:639:A:C8	2.46	0.51
31:9:42:C:H5'	31:9:43:G:OP2	2.10	0.51
30:0:1163:G:H2'	30:0:1164:U:C5	2.44	0.51
30:0:2896:A:N3	30:0:2896:A:H2'	2.25	0.51
30:0:154:C:H2'	30:0:155:C:H6	1.76	0.51
30:0:821:U:H2'	30:0:822:C:H6	1.75	0.51
24:X:21:PRO:HG2	24:X:24:LYS:HD3	1.91	0.51
30:0:1279:U:O2	30:0:1279:U:H2'	2.09	0.51
22:V:12:THR:HG23	22:V:14:ALA:H	1.74	0.51
30:0:603:A:H4'	30:0:605:C:C6	2.46	0.51
30:0:255:A:H2'	30:0:256:C:H6	1.74	0.51
30:0:1755:A:H2'	30:0:1756:G:O4'	2.11	0.51
2:B:125:GLU:O	2:B:129:ARG:HG3	2.10	0.51
30:0:1137:G:H1'	38:0:3884:HOH:O	2.09	0.51
30:0:2724:U:H2'	30:0:2725:G:O4'	2.10	0.51
2:B:254:GLN:HG2	2:B:255:GLY:N	2.25	0.51
30:0:1525:G:H5'	30:0:1526:A:OP2	2.11	0.51
30:0:2566:A:C2	30:0:2696:G:O4'	2.63	0.51
30:0:2478:U:O2'	30:0:2479:A:H5'	2.10	0.51
30:0:1081:A:H5''	38:0:3158:HOH:O	2.10	0.51
5:E:84:MET:HG2	5:E:168:ILE:HA	1.93	0.51
30:0:877:G:C2	30:0:885:G:O4'	2.63	0.51
30:0:1524:U:H5''	30:0:1524:U:C6	2.46	0.51
23:W:43:GLY:HA3	30:0:945:U:O2'	2.11	0.51
30:0:684:G:H2'	30:0:685:C:C6	2.46	0.51
2:B:248:ARG:O	2:B:251:VAL:HG22	2.11	0.51
30:0:2758:G:H2'	30:0:2759:C:C6	2.46	0.51
31:9:54:A:HO2'	31:9:55:U:H5'	1.75	0.51
23:W:88:THR:HG22	23:W:89:ASP:N	2.18	0.51
31:9:31:C:C2	31:9:50:G:C2	2.99	0.51
30:0:2823:G:H4'	30:0:2827:A:O4'	2.11	0.51
24:X:43:VAL:HG12	24:X:44:ASP:N	2.26	0.51
3:C:111:VAL:HB	38:C:8519:HOH:O	2.11	0.51
6:F:39:SER:HB3	6:F:45:ALA:HB2	1.91	0.51
3:C:43:LYS:HG2	30:0:449:A:N7	2.26	0.51
1:A:33:GLU:CD	1:A:33:GLU:H	2.14	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:69:LEU:HB3	38:A:9039:HOH:O	2.11	0.51
30:0:1185:U:H5'	38:0:7483:HOH:O	2.09	0.51
30:0:2830:U:O2'	30:0:2831:C:H5'	2.11	0.51
25:Y:189:ASN:HA	25:Y:217:ILE:HD11	1.93	0.51
30:0:10:U:C6	30:0:10:U:H3'	2.46	0.51
4:D:99:ASP:HB3	4:D:103:ASN:HB2	1.90	0.51
30:0:821:U:H2'	30:0:822:C:C6	2.46	0.51
30:0:2344:G:N3	30:0:2344:G:H2'	2.26	0.51
30:0:955:A:C2	30:0:1013:A:C4	2.99	0.51
30:0:958:G:O2'	30:0:959:C:H5'	2.10	0.51
12:L:148:GLU:HA	38:L:8872:HOH:O	2.10	0.51
11:K:10:GLN:N	11:K:10:GLN:HE21	1.97	0.51
30:0:2768:A:N3	30:0:2768:A:H3'	2.26	0.51
10:J:45:VAL:HG21	10:J:129:PHE:CD1	2.45	0.51
30:0:1245:C:O5'	30:0:1245:C:H6	1.93	0.51
16:P:40:VAL:O	16:P:44:VAL:HG23	2.11	0.51
30:0:2638:G:H1'	38:0:4596:HOH:O	2.11	0.51
2:B:5:ARG:NH1	30:0:2547:C:OP2	2.44	0.51
30:0:407:A:H5'	38:0:6041:HOH:O	2.11	0.51
1:A:179:MET:HG2	1:A:186:TRP:CB	2.41	0.51
19:S:57:THR:HG22	19:S:58:MET:N	2.26	0.51
25:Y:204:ARG:HH22	30:0:553:G:P	2.33	0.51
30:0:1614:G:H2'	38:0:4642:HOH:O	2.10	0.51
30:0:2102:G:H5'	30:0:2538:A:C2	2.45	0.51
30:0:1118:A:C8	30:0:1119:G:H5''	2.46	0.51
30:0:1667:A:C8	30:0:1667:A:H5'	2.44	0.51
2:B:190:MET:HE2	2:B:194:PHE:CD1	2.46	0.51
30:0:18:C:H2'	30:0:19:U:C6	2.46	0.51
2:B:36:PRO:HA	2:B:168:GLY:HA3	1.93	0.51
26:Z:57:MET:SD	26:Z:73:ARG:HD2	2.51	0.51
30:0:877:G:C5'	30:0:878:G:OP1	2.55	0.50
30:0:1857:A:N6	30:0:2247:C:H1'	2.26	0.50
2:B:140:LEU:HD12	2:B:174:ARG:HG3	1.91	0.50
6:F:38:LYS:HE3	30:0:244:C:OP2	2.11	0.50
14:N:169:PRO:O	14:N:172:PHE:HB3	2.11	0.50
30:0:2858:U:H2'	30:0:2859:C:C6	2.46	0.50
2:B:221:GLN:HE22	11:K:42:ASN:HD22	1.59	0.50
30:0:2347:C:H2'	30:0:2348:C:H6	1.76	0.50
2:B:36:PRO:HG3	2:B:169:GLY:H	1.75	0.50
30:0:2681:A:H8	38:0:5592:HOH:O	1.92	0.50
31:9:52:A:H2'	31:9:53:G:O4'	2.10	0.50
30:0:1829:A:C2'	30:0:1830:C:H5'	2.40	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
30:0:1829:A:H2'	30:0:1830:C:H5'	1.94	0.50
30:0:1284:G:O2'	30:0:1285:U:H5'	2.11	0.50
38:I:5331:HOH:O	30:0:1164:U:H5	1.94	0.50
30:0:1194:A:N1	30:0:1195:G:C6	2.79	0.50
30:0:2505:G:H8	38:0:5653:HOH:O	1.94	0.50
30:0:694:A:C2'	30:0:695:C:H5'	2.41	0.50
2:B:280:VAL:HG13	2:B:334:SER:HA	1.93	0.50
30:0:1163:G:H2'	30:0:1164:U:C6	2.45	0.50
30:0:1166:A:C6	30:0:1181:A:C2	2.99	0.50
4:D:69:ILE:HD12	30:0:2346:C:H5'	1.93	0.50
30:0:2102:G:C2	30:0:2104:C:C4	3.00	0.50
14:N:143:ARG:HH21	14:N:169:PRO:HB2	1.75	0.50
30:0:1921:A:O2'	30:0:1922:A:H5'	2.12	0.50
2:B:62:ARG:HA	2:B:65:MET:CE	2.41	0.50
24:X:78:GLU:HG2	24:X:79:GLU:H	1.75	0.50
1:A:109:GLU:HG2	1:A:116:GLY:H	1.75	0.50
30:0:1190:G:N3	30:0:1190:G:H3'	2.26	0.50
30:0:2718:C:H6	30:0:2718:C:H5'	1.77	0.50
30:0:1118:A:H8	30:0:1119:G:H5''	1.77	0.50
30:0:920:C:H5'	30:0:921:G:C4	2.46	0.50
30:0:255:A:O2'	30:0:256:C:H5'	2.12	0.50
30:0:1762:C:H4'	38:0:4668:HOH:O	2.11	0.50
30:0:2256:G:C2'	30:0:2257:G:H5'	2.42	0.50
17:Q:66:LYS:HB2	17:Q:70:ALA:O	2.11	0.50
30:0:368:C:C2'	30:0:369:G:H5'	2.42	0.50
8:H:59:GLN:HG2	8:H:129:ARG:HG2	1.92	0.50
30:0:12:U:C2'	30:0:13:G:H5'	2.41	0.50
30:0:1819:G:C2'	30:0:1820:G:H5'	2.41	0.50
1:A:191:GLY:HA2	1:A:194:MET:CE	2.41	0.50
10:J:74:ARG:O	10:J:78:ILE:HG12	2.11	0.50
30:0:1521:C:C2	30:0:1522:A:C8	3.00	0.50
10:J:107:ASN:HD21	10:J:109:TYR:HB2	1.76	0.50
10:J:107:ASN:ND2	10:J:109:TYR:H	2.09	0.50
30:0:2553:A:H2'	30:0:2553:A:N3	2.26	0.50
1:A:212:PRO:HB2	38:0:4369:HOH:O	2.12	0.50
30:0:2730:G:O2'	30:0:2731:G:H5'	2.11	0.50
9:I:82:THR:CG2	30:0:1168:C:H5''	2.42	0.50
30:0:1131:G:C6	30:0:1230:A:C4	3.00	0.50
30:0:559:U:C3'	30:0:559:U:C6	2.95	0.50
30:0:1522:A:C2	30:0:1665:G:C6	2.99	0.50
30:0:2729:C:O2'	30:0:2730:G:H5'	2.10	0.50
30:0:1205:U:C2'	30:0:1206:U:C5'	2.84	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
5:E:143:GLN:NE2	30:0:2779:G:H21	2.10	0.50
30:0:1406:A:H4'	30:0:1407:A:H5''	1.93	0.50
30:0:2597:U:H2'	30:0:2598:U:H5'	1.94	0.50
30:0:2445:U:H2'	30:0:2446:G:C8	2.47	0.50
9:I:95:LEU:HD23	9:I:99:GLN:OE1	2.11	0.50
9:I:87:PRO:HD3	38:0:3242:HOH:O	2.12	0.50
30:0:2291:A:N9	30:0:2309:C:H5'	2.26	0.50
30:0:2909:G:H2'	30:0:2910:A:H8	1.76	0.50
30:0:2756:U:H3	30:0:2896:A:H2	1.57	0.50
6:F:58:GLU:HA	6:F:61:MET:HE2	1.94	0.50
30:0:204:A:C2'	30:0:205:U:H5'	2.41	0.50
13:M:28:GLN:O	13:M:32:ARG:HG3	2.12	0.50
4:D:88:LEU:HB2	4:D:89:PRO:HD3	1.94	0.50
30:0:1209:C:C2	30:0:1210:G:C8	3.00	0.49
13:M:171:ARG:NH2	30:0:189:A:OP1	2.45	0.49
31:9:3:A:H2'	38:9:9040:HOH:O	2.11	0.49
30:0:67:A:H5''	30:0:69:A:C8	2.47	0.49
1:A:199:HIS:HE1	30:0:1881:A:OP1	1.95	0.49
2:B:320:GLN:HE21	2:B:321:PRO:CD	2.24	0.49
30:0:73:U:O2'	30:0:74:G:H5'	2.12	0.49
23:W:64:THR:O	23:W:68:THR:HG22	2.11	0.49
30:0:1707:G:H1'	30:0:1711:A:N6	2.26	0.49
14:N:77:ASN:OD1	14:N:79:PRO:HD2	2.12	0.49
30:0:941:G:C5	30:0:942:U:C4	3.00	0.49
26:Z:34:SER:HA	30:0:797:A:H5'	1.94	0.49
30:0:2712:G:H5'	38:0:5233:HOH:O	2.11	0.49
10:J:75:PRO:HG2	10:J:105:LEU:CD2	2.38	0.49
30:0:256:C:H2'	30:0:257:G:O4'	2.12	0.49
2:B:62:ARG:HA	2:B:65:MET:HE2	1.93	0.49
30:0:2831:C:C2	30:0:2910:A:C2	3.00	0.49
30:0:1878:G:O2'	30:0:1879:U:OP2	2.30	0.49
2:B:144:THR:HG22	2:B:145:HIS:N	2.27	0.49
30:0:652:G:H8	38:0:3021:HOH:O	1.95	0.49
6:F:58:GLU:HB3	13:M:8:ILE:HG23	1.93	0.49
3:C:107:ARG:O	3:C:111:VAL:HG23	2.13	0.49
1:A:33:GLU:O	1:A:34:ASP:HB2	2.12	0.49
30:0:946:C:O2'	30:0:947:U:H5'	2.12	0.49
27:1:28:HIS:HE1	30:0:776:A:OP1	1.94	0.49
30:0:333:G:O2'	30:0:334:G:H5'	2.13	0.49
30:0:702:G:C2	30:0:703:G:C8	3.00	0.49
10:J:88:PRO:HA	35:J:8802:CL:CL	2.49	0.49
11:K:34:VAL:HG21	11:K:46:LYS:O	2.12	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
30:0:185:G:H4'	30:0:186:A:H4'	1.93	0.49
30:0:1909:A:H2'	30:0:1910:A:C8	2.48	0.49
4:D:50:VAL:HG13	31:9:41:C:O4'	2.12	0.49
16:P:81:LYS:HG2	38:0:9543:HOH:O	2.12	0.49
30:0:1187:U:O2'	30:0:1189:A:H2	1.95	0.49
30:0:2781:U:O2'	30:0:2782:G:H5'	2.12	0.49
30:0:711:G:N2	30:0:718:C:C2	2.80	0.49
30:0:2004:U:H5''	30:0:2005:G:C8	2.47	0.49
30:0:1377:C:H1'	38:0:9041:HOH:O	2.12	0.49
27:1:16:HIS:HE1	30:0:775:G:OP1	1.95	0.49
30:0:947:U:H2'	30:0:948:G:H8	1.77	0.49
30:0:1768:C:H2'	30:0:1769:C:O4'	2.13	0.49
16:P:7:LYS:HD3	16:P:21:VAL:CG2	2.41	0.49
4:D:51:ARG:HH11	4:D:68:PRO:HB3	1.76	0.49
30:0:95:A:H5''	30:0:97:G:O4'	2.13	0.49
30:0:1607:A:C4	30:0:1608:G:C8	3.00	0.49
20:T:18:GLU:O	20:T:21:LYS:HG2	2.11	0.49
30:0:363:C:H2'	30:0:364:U:H6	1.77	0.49
5:E:47:VAL:HG11	5:E:69:ILE:HD13	1.94	0.49
2:B:162:MET:CE	2:B:308:LEU:HD21	2.42	0.49
30:0:1588:G:C6	30:0:1589:G:C6	3.01	0.49
23:W:5:VAL:HG11	23:W:153:MET:HE3	1.94	0.49
18:R:29:LYS:HE2	30:0:524:A:C5'	2.42	0.49
15:O:25:VAL:HG12	30:0:709:G:O3'	2.13	0.49
30:0:2112:A:H2'	30:0:2113:G:H8	1.77	0.49
30:0:951:A:O2'	30:0:952:G:H5'	2.13	0.49
30:0:1854:C:H2'	30:0:1875:A:H61	1.78	0.49
11:K:130:MET:SD	21:U:25:ASP:O	2.70	0.49
30:0:734:U:O2'	30:0:736:A:N7	2.44	0.49
30:0:1189:A:N7	30:0:1190:G:C8	2.81	0.49
10:J:70:PHE:CD1	30:0:2676:C:H4'	2.46	0.49
30:0:1730:G:C5'	30:0:1731:C:H6	2.25	0.49
30:0:1778:A:H2'	30:0:1779:A:H5'	1.94	0.49
30:0:952:G:N3	30:0:2302:A:H2'	2.28	0.49
29:3:11:CYS:SG	29:3:14:CYS:HB2	2.52	0.49
29:3:30:GLN:NE2	38:3:9043:HOH:O	2.43	0.49
30:0:1568:G:C5	30:0:1569:U:C5	3.01	0.49
31:9:31:C:C2	31:9:50:G:N2	2.81	0.49
30:0:2498:C:C2'	30:0:2499:U:H5'	2.43	0.49
30:0:2481:G:C3'	30:0:2482:G:H5''	2.42	0.49
30:0:1730:G:H5'	30:0:1731:C:H5	1.78	0.49
1:A:53:ALA:HB3	38:A:9068:HOH:O	2.12	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
25:Y:149:GLN:O	25:Y:154:ARG:NH1	2.46	0.49
2:B:142:LEU:HD21	2:B:178:ALA:HB1	1.94	0.49
31:9:73:A:N1	31:9:108:C:O2	2.45	0.49
30:0:1682:A:H5''	38:0:9457:HOH:O	2.13	0.49
30:0:1066:U:H2'	30:0:1067:A:C8	2.47	0.49
30:0:2829:G:O2'	30:0:2830:U:H5'	2.13	0.49
10:J:131:THR:HG22	10:J:133:GLY:H	1.78	0.49
20:T:97:ARG:NH2	30:0:309:C:OP1	2.46	0.49
25:Y:189:ASN:HD22	25:Y:192:ASP:H	1.61	0.49
1:A:81:GLN:HB2	1:A:92:ASN:ND2	2.28	0.49
30:0:2890:A:H8	30:0:2890:A:H5''	1.77	0.49
30:0:1783:A:O2'	30:0:1784:U:H5'	2.12	0.49
30:0:503:G:H2'	30:0:504:G:H8	1.77	0.49
8:H:150:LYS:HA	38:H:230:HOH:O	2.13	0.49
26:Z:55:SER:O	26:Z:59:GLU:HG3	2.12	0.49
30:0:2756:U:N3	30:0:2896:A:C2	2.75	0.49
30:0:2578:G:C8	30:0:2578:G:H5'	2.43	0.49
1:A:48:ASP:HB3	38:A:9068:HOH:O	2.13	0.49
30:0:1398:G:H2'	30:0:1399:A:H8	1.75	0.49
1:A:211:LYS:HD2	38:A:9083:HOH:O	2.13	0.49
30:0:2064:U:H5'	30:0:2652:U:O3'	2.13	0.49
30:0:1007:A:H1'	38:0:3138:HOH:O	2.12	0.49
25:Y:170:SER:OG	25:Y:175:ARG:HG3	2.12	0.49
11:K:82:ARG:NH2	11:K:115:ARG:HG2	2.28	0.49
30:0:2847:G:O2'	30:0:2848:G:H5'	2.12	0.49
30:0:1816:C:H2'	30:0:1817:U:O4'	2.13	0.49
30:0:1180:U:H2'	30:0:1181:A:O4'	2.13	0.48
3:C:76:ARG:HD3	38:C:8570:HOH:O	2.13	0.48
20:T:2:LYS:HG2	30:0:447:A:OP1	2.13	0.48
24:X:23:HIS:HD2	38:0:9959:HOH:O	1.96	0.48
30:0:703:G:O2'	30:0:704:C:H5'	2.13	0.48
30:0:1016:U:O2'	30:0:2303:A:N7	2.38	0.48
23:W:125:HIS:CE1	30:0:1097:A:H5''	2.47	0.48
30:0:1497:G:H4'	30:0:1627:G:O2'	2.13	0.48
31:9:92:G:C6	31:9:93:A:C6	3.01	0.48
15:O:32:ARG:HD3	15:O:32:ARG:O	2.13	0.48
30:0:814:G:H2'	30:0:815:U:C6	2.48	0.48
30:0:69:A:H2'	30:0:70:A:OP2	2.12	0.48
22:V:39:ALA:N	22:V:40:PRO:HD2	2.25	0.48
30:0:613:C:H2'	30:0:614:U:C6	2.44	0.48
12:L:18:HIS:HB2	30:0:903:U:O4	2.13	0.48
30:0:1676:G:H1'	38:0:9434:HOH:O	2.13	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
30:0:499:G:O2'	30:0:500:G:H5'	2.13	0.48
2:B:140:LEU:CD1	2:B:174:ARG:HG3	2.44	0.48
30:0:1323:G:H5'	38:0:4709:HOH:O	2.13	0.48
31:9:61:C:H2'	31:9:62:A:H8	1.77	0.48
30:0:626:U:C4	30:0:627:G:C6	3.01	0.48
30:0:371:U:O2'	30:0:372:A:H5'	2.13	0.48
30:0:2510:C:H42	30:0:2564:G:N2	2.11	0.48
16:P:88:GLN:HE21	30:0:1800:G:H1'	1.76	0.48
30:0:308:U:C4	30:0:342:C:H1'	2.48	0.48
25:Y:187:VAL:HG23	25:Y:192:ASP:HB3	1.93	0.48
30:0:2353:A:H4'	30:0:2354:A:O5'	2.13	0.48
30:0:961:A:H4'	38:0:6790:HOH:O	2.13	0.48
25:Y:154:ARG:HH22	30:0:1071:G:H4'	1.78	0.48
4:D:76:ARG:NE	31:9:44:A:O4'	2.46	0.48
30:0:2433:A:H2'	30:0:2434:A:C8	2.48	0.48
24:X:30:MET:HG2	30:0:1384:C:H5'	1.94	0.48
30:0:2831:C:H6	38:0:7228:HOH:O	1.96	0.48
30:0:581:G:O2'	30:0:582:U:H5'	2.12	0.48
14:N:110:THR:HB	14:N:113:SER:OG	2.13	0.48
30:0:1377:C:H6	30:0:1377:C:C5'	2.25	0.48
5:E:69:ILE:HA	5:E:72:MET:CE	2.44	0.48
31:9:39:U:H1'	31:9:44:A:H61	1.78	0.48
17:Q:7:LEU:HD12	30:0:2424:U:H1'	1.96	0.48
30:0:1087:G:H4'	30:0:1088:A:OP1	2.12	0.48
30:0:466:A:H2'	30:0:467:G:O4'	2.13	0.48
30:0:1190:G:H2'	38:0:4064:HOH:O	2.13	0.48
13:M:99:ARG:HD2	13:M:167:GLY:CA	2.41	0.48
30:0:2908:A:O2'	30:0:2909:G:H5'	2.13	0.48
30:0:2768:A:C2'	30:0:2769:C:O4'	2.61	0.48
1:A:140:LEU:HB3	1:A:141:PRO:HD2	1.94	0.48
27:1:1:THR:HB	38:0:7157:HOH:O	2.13	0.48
15:O:14:LEU:CD2	15:O:102:ILE:HD11	2.43	0.48
30:0:513:A:N3	38:0:3665:HOH:O	2.35	0.48
30:0:2256:G:O2'	30:0:2257:G:H5'	2.14	0.48
2:B:223:ARG:HG3	2:B:232:TRP:O	2.13	0.48
11:K:12:LEU:HB2	11:K:47:ALA:HB3	1.96	0.48
24:X:61:ARG:O	30:0:2744:G:H5''	2.14	0.48
31:9:71:C:H2'	31:9:72:C:H6	1.79	0.48
30:0:790:A:H1'	30:0:1710:A:H2'	1.95	0.48
30:0:802:G:O2'	30:0:803:C:H5'	2.13	0.48
30:0:2754:G:C2'	30:0:2755:G:H5'	2.43	0.48
30:0:1343:C:H2'	30:0:1344:G:O5'	2.14	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
30:0:1520:G:H2'	30:0:1521:C:C6	2.48	0.48
11:K:41:LYS:HA	30:0:2582:G:O3'	2.14	0.48
16:P:7:LYS:HD3	16:P:21:VAL:HG22	1.95	0.48
30:0:305:A:C5	30:0:329:A:C2	3.02	0.48
4:D:23:VAL:HG12	4:D:130:VAL:HG22	1.96	0.48
30:0:1311:G:C2	30:0:1312:G:C8	3.01	0.48
14:N:65:ASP:HB3	38:N:8821:HOH:O	2.13	0.48
8:H:165:ARG:HB3	38:H:235:HOH:O	2.13	0.48
11:K:55:VAL:HG12	11:K:56:SER:N	2.28	0.48
23:W:21:LEU:HD13	23:W:26:ILE:HD11	1.95	0.48
30:0:1422:U:H2'	30:0:1423:C:H6	1.76	0.48
8:H:61:ARG:HG3	8:H:61:ARG:HH11	1.78	0.48
3:C:246:ARG:NE	38:C:8628:HOH:O	2.43	0.48
21:U:17:THR:CG2	21:U:18:GLY:N	2.77	0.48
27:1:28:HIS:HD2	27:1:30:LYS:H	1.59	0.48
30:0:735:C:O5'	30:0:735:C:H6	1.97	0.48
30:0:661:G:C5	30:0:686:A:C2	3.02	0.48
1:A:135:VAL:HG21	1:A:147:ARG:HB3	1.96	0.48
8:H:170:ARG:HD2	38:H:194:HOH:O	2.13	0.48
12:L:117:GLU:HA	38:L:8852:HOH:O	2.13	0.48
30:0:1188:A:C5	30:0:1189:A:C2	3.01	0.48
30:0:1201:C:C2'	30:0:1202:A:H5'	2.42	0.48
30:0:285:A:N6	30:0:367:G:H1'	2.28	0.48
5:E:72:MET:O	5:E:76:VAL:HG22	2.14	0.48
30:0:1789:G:H2'	30:0:1790:C:O5'	2.13	0.48
12:L:143:THR:HG22	12:L:144:ASP:N	2.28	0.48
11:K:9:THR:HA	38:0:3293:HOH:O	2.14	0.48
30:0:1976:G:O2'	30:0:1977:U:H5'	2.14	0.48
30:0:2090:G:H2'	30:0:2091:G:C8	2.49	0.48
30:0:1159:G:H1	30:0:1208:C:H42	1.61	0.48
30:0:2635:A:C2'	30:0:2636:C:H5'	2.44	0.48
30:0:1543:G:N1	30:0:1641:A:OP2	2.34	0.48
30:0:2419:U:H5''	30:0:2420:G:H5'	1.95	0.48
30:0:675:U:H6	30:0:675:U:O5'	1.97	0.48
9:I:97:VAL:HG12	9:I:101:LYS:HE3	1.94	0.48
6:F:53:ASP:OD1	6:F:80:GLN:HB2	2.14	0.48
30:0:2656:G:C2'	30:0:2657:G:H5'	2.44	0.48
30:0:732:C:O2'	30:0:733:U:H5'	2.13	0.48
13:M:171:ARG:CD	30:0:156:C:H5''	2.23	0.48
30:0:506:G:N2	30:0:509:A:H5''	2.20	0.48
30:0:363:C:H2'	30:0:364:U:C6	2.49	0.48
1:A:88:ILE:HD13	1:A:100:PRO:HD3	1.95	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
30:0:1506:U:H6	30:0:1506:U:H5'	1.79	0.48
23:W:41:TYR:OH	30:0:1024:G:H4'	2.14	0.48
30:0:1613:C:H2'	30:0:1614:G:O4'	2.14	0.48
30:0:2858:U:H2'	30:0:2859:C:H6	1.78	0.48
10:J:39:VAL:HG13	10:J:106:GLY:O	2.13	0.48
20:T:77:VAL:HG11	20:T:91:LEU:HD11	1.95	0.48
30:0:2837:U:H2'	38:0:6856:HOH:O	2.14	0.48
30:0:1902:G:N2	30:0:1936:C:C2	2.82	0.48
38:C:8666:HOH:O	30:0:656:G:H1'	2.14	0.47
30:0:2769:C:C2'	30:0:2770:G:C5'	2.78	0.47
31:9:1:U:C4'	31:9:3:A:OP1	2.62	0.47
30:0:250:C:H2'	30:0:251:C:H6	1.79	0.47
30:0:1512:G:O2'	30:0:1513:C:H5'	2.14	0.47
14:N:4:PRO:HB2	30:0:1010:C:H4'	1.94	0.47
30:0:947:U:O2'	30:0:948:G:H5'	2.14	0.47
30:0:2074:A:H1'	38:0:9890:HOH:O	2.14	0.47
13:M:64:ARG:HD2	38:M:8880:HOH:O	2.14	0.47
30:0:814:G:H4'	38:0:3141:HOH:O	2.14	0.47
30:0:2672:C:H2'	30:0:2673:U:H6	1.78	0.47
13:M:34:GLU:HB3	13:M:38:GLU:HG3	1.96	0.47
30:0:128:A:O2'	30:0:129:A:C5'	2.62	0.47
31:9:108:C:H2'	31:9:109:G:H8	1.78	0.47
30:0:1562:C:O2	30:0:1562:C:H2'	2.12	0.47
30:0:2493:C:O2	30:0:2493:C:H2'	2.14	0.47
30:0:843:A:C2	30:0:846:A:C8	3.02	0.47
30:0:2869:G:H5'	38:0:5510:HOH:O	2.14	0.47
30:0:800:G:H2'	30:0:801:U:C6	2.49	0.47
29:3:65:THR:HB	29:3:83:TRP:H	1.79	0.47
30:0:101:C:H2'	30:0:102:A:C8	2.49	0.47
30:0:814:G:H2'	30:0:815:U:H6	1.79	0.47
12:L:41:HIS:CD2	30:0:926:A:O2'	2.65	0.47
9:I:108:HIS:N	9:I:109:PRO:HD2	2.29	0.47
30:0:2134:G:H2'	30:0:2135:A:H8	1.79	0.47
30:0:1321:A:H2'	30:0:1322:G:H8	1.80	0.47
30:0:2253:G:H2'	30:0:2254:G:H8	1.79	0.47
1:A:171:LYS:HB2	30:0:820:G:C6	2.49	0.47
29:3:11:CYS:HB2	29:3:20:HIS:CE1	2.49	0.47
30:0:2795:C:O2'	30:0:2796:U:H5'	2.15	0.47
9:I:120:ALA:O	9:I:124:VAL:HG23	2.14	0.47
26:Z:45:VAL:HG23	30:0:1887:U:OP1	2.14	0.47
1:A:217:ARG:HG2	1:A:229:ALA:HB2	1.96	0.47
31:9:114:G:H2'	31:9:115:C:C6	2.49	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
30:0:1268:C:H2'	30:0:1269:G:H8	1.79	0.47
1:A:65:ARG:O	1:A:66:ARG:HG3	2.15	0.47
30:0:1667:A:H2'	30:0:1668:U:C6	2.49	0.47
5:E:143:GLN:HE21	30:0:2780:C:C1'	2.15	0.47
30:0:1165:G:C4'	30:0:1174:A:O2'	2.60	0.47
3:C:197:SER:HB3	38:C:8577:HOH:O	2.15	0.47
2:B:41:PHE:HB3	2:B:190:MET:HE1	1.96	0.47
1:A:171:LYS:HB2	30:0:820:G:C5	2.50	0.47
30:0:671:A:O2'	30:0:672:G:H2'	2.14	0.47
30:0:2256:G:H2'	30:0:2257:G:C5'	2.45	0.47
30:0:1568:G:O2'	30:0:1569:U:H5'	2.14	0.47
30:0:660:A:H4'	30:0:661:G:O5'	2.14	0.47
3:C:58:ALA:HA	3:C:73:GLN:HE21	1.79	0.47
30:0:834:G:H3'	30:0:835:U:H4'	1.95	0.47
4:D:41:LEU:HA	4:D:44:ILE:HG22	1.96	0.47
26:Z:43:GLY:O	26:Z:47:ARG:HG2	2.14	0.47
30:0:1187:U:H2'	38:0:6916:HOH:O	2.15	0.47
30:0:69:A:H8	30:0:69:A:C5'	2.21	0.47
30:0:2826:G:C6	30:0:2913:A:C6	3.02	0.47
2:B:229:ARG:NH2	30:0:1753:C:O2	2.45	0.47
30:0:1126:C:H6	30:0:1126:C:O5'	1.97	0.47
5:E:108:LEU:HD11	5:E:164:ASP:HB2	1.96	0.47
30:0:2105:C:O2'	30:0:2284:G:N2	2.48	0.47
12:L:92:ASP:HA	12:L:121:ILE:HB	1.96	0.47
8:H:5:PRO:HD2	8:H:8:MET:SD	2.55	0.47
30:0:1166:A:H1'	30:0:1192:A:C2	2.50	0.47
30:0:559:U:H3'	30:0:559:U:C6	2.50	0.47
3:C:114:ALA:HB1	3:C:223:LEU:HB3	1.96	0.47
12:L:134:GLU:HG3	38:L:8856:HOH:O	2.15	0.47
1:A:186:TRP:CD1	1:A:187:PRO:HA	2.49	0.47
30:0:423:A:C5	30:0:424:C:C5	3.02	0.47
14:N:61:ALA:CB	14:N:88:ALA:HB2	2.44	0.47
5:E:91:PHE:HE1	30:0:2694:A:H4'	1.78	0.47
30:0:1014:A:H5''	31:9:101:G:O2'	2.14	0.47
31:9:39:U:C2'	31:9:40:C:OP1	2.63	0.47
30:0:1126:C:HO2'	30:0:1128:U:H6	1.60	0.47
30:0:2411:C:H4'	38:0:4964:HOH:O	2.13	0.47
8:H:64:SER:OG	30:0:2520:G:H5'	2.13	0.47
30:0:2265:U:H2'	30:0:2266:A:C8	2.49	0.47
12:L:35:ARG:O	12:L:40:PHE:HA	2.15	0.47
30:0:1883:U:H5''	30:0:2013:G:OP2	2.14	0.47
3:C:34:ALA:HB3	3:C:220:THR:HG21	1.97	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
13:M:99:ARG:CD	13:M:167:GLY:HA2	2.41	0.47
30:0:2831:C:H2'	30:0:2832:C:C5'	2.45	0.47
30:0:1477:C:C5'	30:0:1868:G:H5''	2.44	0.47
30:0:1730:G:H5'	30:0:1731:C:C6	2.48	0.47
1:A:36:ASP:HA	1:A:83:GLY:HA3	1.97	0.47
4:D:37:ALA:O	4:D:40:ILE:HG12	2.14	0.47
30:0:36:C:C2	30:0:447:A:C2	3.03	0.47
30:0:1948:G:H2'	30:0:1949:G:H8	1.79	0.47
24:X:43:VAL:HG11	24:X:82:GLU:HA	1.95	0.47
30:0:2531:U:O2'	30:0:2532:A:H5'	2.14	0.47
12:L:71:GLU:HG2	30:0:700:A:C2	2.49	0.47
30:0:1391:G:H2'	30:0:1392:A:H5'	1.97	0.47
30:0:304:G:H1'	30:0:347:A:N6	2.29	0.47
18:R:82:GLU:O	18:R:86:LYS:HG3	2.13	0.47
13:M:124:GLY:HA3	30:0:2132:C:H1'	1.96	0.47
25:Y:155:ARG:NH1	38:Y:8128:HOH:O	2.48	0.47
30:0:1471:A:H5'	38:0:3197:HOH:O	2.15	0.47
3:C:154:VAL:O	3:C:158:GLU:HG3	2.15	0.47
6:F:50:VAL:HG13	6:F:60:VAL:HG11	1.96	0.47
30:0:1182:C:C1'	30:0:1192:A:C8	2.97	0.47
30:0:2829:G:C2	30:0:2912:C:C2	3.03	0.47
12:L:133:VAL:HB	38:L:8856:HOH:O	2.15	0.47
30:0:151:A:H2'	30:0:152:A:O4'	2.14	0.47
30:0:2891:A:N3	30:0:2891:A:H2'	2.29	0.47
1:A:27:LEU:HD12	1:A:69:LEU:HD22	1.95	0.47
14:N:11:ARG:HG3	14:N:14:ARG:NH1	2.30	0.47
30:0:2871:G:H2'	30:0:2872:U:C6	2.50	0.47
16:P:54:LYS:HB2	30:0:1717:A:H5''	1.95	0.47
30:0:960:G:H3'	30:0:960:G:C4	2.47	0.47
30:0:560:U:H2'	30:0:561:G:C8	2.44	0.47
12:L:50:GLY:C	30:0:2453:G:H4'	2.35	0.47
27:1:28:HIS:CD2	27:1:31:LYS:HG3	2.50	0.47
30:0:485:A:N3	30:0:487:G:H5''	2.29	0.47
27:1:46:ARG:HA	38:0:3028:HOH:O	2.15	0.47
30:0:2087:C:O2'	30:0:2088:C:H5'	2.15	0.47
2:B:199:TYR:HE2	2:B:268:ARG:HB2	1.79	0.47
30:0:1205:U:H2'	30:0:1206:U:H5'	1.96	0.47
30:0:2831:C:H2'	30:0:2832:C:H5'	1.97	0.47
30:0:1789:G:C2'	30:0:1790:C:O5'	2.63	0.47
30:0:2326:C:H4'	30:0:2412:G:C4'	2.44	0.47
30:0:1788:U:C2	30:0:1805:G:N2	2.83	0.47
14:N:86:LEU:O	14:N:90:LEU:HG	2.14	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
30:0:254:C:C2'	30:0:254:C:O2	2.54	0.46
30:0:2072:G:C6	30:0:2533:C:H1'	2.50	0.46
30:0:1947:G:N2	30:0:1966:U:O2	2.48	0.46
24:X:43:VAL:HG22	24:X:76:ARG:NH1	2.29	0.46
30:0:820:G:O2'	30:0:856:G:H4'	2.14	0.46
30:0:2256:G:H2'	30:0:2257:G:H5'	1.97	0.46
30:0:2833:C:H1'	30:0:2848:G:N2	2.30	0.46
14:N:11:ARG:NH1	31:9:8:G:O6	2.48	0.46
2:B:314:ALA:HB3	2:B:317:PRO:HG3	1.97	0.46
23:W:61:THR:HG23	23:W:151:GLU:HG3	1.97	0.46
30:0:825:U:H5''	30:0:826:U:OP1	2.15	0.46
30:0:2911:C:O2'	30:0:2912:C:H5'	2.15	0.46
14:N:86:LEU:HD12	14:N:125:ALA:HB2	1.97	0.46
30:0:1174:A:C5	30:0:1201:C:H4'	2.50	0.46
30:0:1771:U:O2'	30:0:1773:G:N7	2.46	0.46
1:A:233:THR:HB	30:0:1942:A:H5''	1.98	0.46
14:N:141:ARG:HH21	31:9:48:C:H4'	1.79	0.46
30:0:2825:C:H4'	30:0:2826:G:O5'	2.15	0.46
30:0:920:C:H4'	30:0:921:G:N2	2.30	0.46
30:0:10:U:C6	30:0:10:U:C3'	2.98	0.46
30:0:1706:G:C5	30:0:1707:G:C6	3.03	0.46
24:X:30:MET:HE1	24:X:58:ALA:HB3	1.97	0.46
30:0:2106:C:H1'	30:0:2484:U:C2	2.49	0.46
30:0:2092:G:H2'	30:0:2613:G:OP1	2.15	0.46
28:2:28:LYS:O	30:0:87:C:H2'	2.15	0.46
3:C:200:PRO:HB3	3:C:212:VAL:HG23	1.97	0.46
30:0:789:C:H5'	38:0:6228:HOH:O	2.15	0.46
3:C:35:VAL:HG21	3:C:227:GLY:HA2	1.96	0.46
13:M:43:PRO:HG3	13:M:62:VAL:HG21	1.98	0.46
30:0:2577:A:H8	38:0:9606:HOH:O	1.98	0.46
28:2:22:PRO:HG2	28:2:25:VAL:HG23	1.97	0.46
30:0:544:G:C3'	30:0:545:G:H5''	2.45	0.46
31:9:3:A:H2	31:9:21:G:N3	2.14	0.46
30:0:1596:U:H2'	30:0:1598:A:OP2	2.14	0.46
30:0:1634:G:C4	30:0:1635:U:C5	3.03	0.46
1:A:211:LYS:HD3	38:0:6884:HOH:O	2.15	0.46
30:0:2598:U:O2	30:0:2600:A:C8	2.68	0.46
25:Y:99:ALA:HB2	25:Y:233:TYR:CZ	2.50	0.46
30:0:2871:G:H2'	30:0:2872:U:H6	1.79	0.46
30:0:1400:C:O2'	30:0:1401:G:H5'	2.15	0.46
30:0:277:U:O2'	30:0:278:A:H5'	2.15	0.46
30:0:1557:G:O2'	30:0:1558:C:H5'	2.15	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
31:9:27:C:H2'	31:9:28:U:O4'	2.16	0.46
30:0:1878:G:C4'	38:0:6135:HOH:O	2.64	0.46
30:0:2482:G:H4'	30:0:2483:A:C5'	2.45	0.46
2:B:41:PHE:CZ	2:B:79:MET:HG3	2.50	0.46
15:O:25:VAL:HG12	30:0:709:G:O2'	2.16	0.46
30:0:876:A:N3	30:0:876:A:C2'	2.79	0.46
30:0:2105:C:H2'	30:0:2106:C:C6	2.50	0.46
30:0:2284:G:H1'	38:0:9576:HOH:O	2.15	0.46
30:0:1200:A:H3'	38:0:5769:HOH:O	2.15	0.46
30:0:2802:C:H2'	30:0:2803:C:C6	2.50	0.46
1:A:123:GLY:HA3	1:A:162:GLY:HA2	1.96	0.46
13:M:80:GLY:O	13:M:81:ARG:HD2	2.14	0.46
30:0:354:A:H2'	30:0:355:C:H6	1.80	0.46
30:0:1102:C:H5	38:0:3497:HOH:O	1.98	0.46
3:C:127:ARG:HD3	3:C:129:HIS:CE1	2.48	0.46
2:B:243:ASN:HA	2:B:244:PRO:C	2.35	0.46
30:0:1515:A:H2'	30:0:1516:U:H6	1.80	0.46
30:0:590:A:H2'	30:0:591:A:H5'	1.97	0.46
14:N:11:ARG:HD3	31:9:114:G:O6	2.15	0.46
30:0:1125:U:H3'	30:0:1126:C:C6	2.51	0.46
21:U:49:LEU:HG	38:U:3805:HOH:O	2.15	0.46
16:P:101:GLN:HG3	38:0:3511:HOH:O	2.15	0.46
30:0:228:C:H2'	30:0:229:G:H5'	1.96	0.46
29:3:61:PRO:HG3	30:0:2462:G:O6	2.16	0.46
30:0:343:C:O2'	30:0:344:C:H5'	2.15	0.46
30:0:716:G:C6	30:0:717:C:N4	2.83	0.46
30:0:445:U:H2'	30:0:446:G:H8	1.81	0.46
30:0:1175:G:N7	30:0:1176:C:N3	2.63	0.46
30:0:241:A:C2	30:0:378:A:H4'	2.51	0.46
30:0:2703:A:H2'	30:0:2704:C:C6	2.46	0.46
16:P:59:ARG:HH22	16:P:66:GLN:NE2	2.12	0.46
30:0:1067:A:H5'	38:0:4351:HOH:O	2.15	0.46
30:0:2613:G:O2'	30:0:2614:C:H5'	2.15	0.46
30:0:1420:C:H2'	30:0:1420:C:O2	2.15	0.46
31:9:12:C:H5'	31:9:70:U:O4'	2.15	0.46
14:N:112:GLY:HA2	14:N:137:ALA:HB2	1.96	0.46
2:B:214:PRO:HD2	38:0:9081:HOH:O	2.15	0.46
30:0:1616:A:H5'	30:0:1617:C:OP1	2.16	0.46
30:0:1346:U:H2'	30:0:1347:U:C6	2.51	0.46
17:Q:53:HIS:CD2	30:0:2389:U:H4'	2.50	0.46
5:E:11:VAL:HG12	5:E:12:ASP:N	2.31	0.46
9:I:130:LEU:HA	38:0:7420:HOH:O	2.15	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
14:N:175:LEU:O	14:N:179:LEU:HG	2.15	0.46
3:C:1:MET:CG	3:C:2:GLN:H	2.26	0.46
30:0:138:U:OP2	30:0:139:C:C5	2.69	0.46
2:B:307:ARG:HG3	2:B:307:ARG:NH1	2.30	0.46
30:0:2840:A:H3'	38:0:7661:HOH:O	2.15	0.46
4:D:64:ARG:HB3	4:D:67:ASP:OD2	2.15	0.46
30:0:2346:C:O5'	30:0:2346:C:H6	1.98	0.46
30:0:1617:C:C4	30:0:1643:C:H4'	2.50	0.46
2:B:202:VAL:HG11	2:B:301:VAL:HG13	1.98	0.46
1:A:71:PRO:HD2	1:A:74:VAL:HG21	1.98	0.46
30:0:2061:C:C2'	30:0:2062:A:H5'	2.46	0.46
16:P:64:GLU:HG3	38:P:166:HOH:O	2.15	0.46
30:0:2093:G:H5''	38:0:9483:HOH:O	2.15	0.46
30:0:889:C:H2'	30:0:890:C:C6	2.51	0.46
1:A:127:GLN:HB3	1:A:139:LYS:HB3	1.98	0.46
30:0:2401:A:H2'	30:0:2402:A:C8	2.51	0.46
30:0:370:G:O2'	30:0:371:U:H5'	2.15	0.46
30:0:2908:A:C2'	30:0:2909:G:H5'	2.46	0.46
30:0:1741:U:C4	30:0:2033:G:C8	3.04	0.46
30:0:1202:A:C8	30:0:1203:G:C8	3.04	0.46
31:9:34:A:H2'	31:9:35:C:O4'	2.16	0.46
5:E:3:VAL:HG22	5:E:49:ILE:HB	1.97	0.46
30:0:510:U:O5'	30:0:510:U:H6	1.99	0.46
3:C:103:ASN:HB3	38:0:9117:HOH:O	2.16	0.46
4:D:20:LYS:HA	4:D:75:LEU:O	2.15	0.46
30:0:729:C:C2	30:0:743:G:C2	3.04	0.46
30:0:1463:U:H2'	30:0:1464:C:C6	2.51	0.46
1:A:110:SER:HB2	1:A:117:LYS:HG3	1.98	0.46
30:0:1873:G:H2'	30:0:1874:U:H5'	1.98	0.46
30:0:1845:A:O2'	30:0:1846:U:H5'	2.15	0.46
30:0:162:C:C2'	30:0:163:U:H5'	2.45	0.46
30:0:1453:G:C2	30:0:1675:C:C2	3.04	0.46
4:D:56:ARG:HH22	30:0:2332:A:H5'	1.79	0.46
17:Q:25:PRO:HA	17:Q:26:PRO:HD3	1.81	0.46
1:A:206:ARG:O	1:A:208:HIS:HD2	1.98	0.46
30:0:1309:U:C2'	30:0:1310:U:H5'	2.46	0.46
30:0:1008:C:O2'	30:0:1009:U:H5'	2.16	0.46
30:0:417:G:P	38:0:7436:HOH:O	2.73	0.46
16:P:80:ARG:HG2	16:P:87:ARG:CZ	2.46	0.46
30:0:39:G:N2	30:0:444:C:C2	2.84	0.46
5:E:137:ASP:O	5:E:141:VAL:HG23	2.16	0.46
6:F:13:GLU:OE2	6:F:78:GLU:HG2	2.15	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
30:0:2764:C:O2'	30:0:2765:C:H5'	2.16	0.46
30:0:932:U:H2'	30:0:933:C:C6	2.51	0.46
30:0:1700:C:H5''	30:0:1701:A:OP2	2.15	0.46
31:9:3:A:OP2	31:9:25:G:N2	2.48	0.46
30:0:560:U:C2	30:0:561:G:C8	3.04	0.46
30:0:567:U:C5'	38:0:5300:HOH:O	2.63	0.46
30:0:1838:U:C4	30:0:2644:C:N4	2.84	0.46
23:W:118:LEU:HD12	23:W:153:MET:HE3	1.97	0.46
24:X:56:GLU:HG2	30:0:1400:C:H4'	1.98	0.46
30:0:1156:C:O5'	30:0:1156:C:H6	1.99	0.46
30:0:2103:A:N3	30:0:2103:A:H2'	2.30	0.46
27:1:42:SER:HB2	38:1:8957:HOH:O	2.16	0.46
25:Y:165:GLU:HB3	38:Y:8163:HOH:O	2.16	0.46
2:B:102:THR:HG23	2:B:182:VAL:HG12	1.98	0.46
3:C:156:LEU:O	3:C:160:LEU:HG	2.16	0.46
4:D:91:ALA:HB1	38:D:5198:HOH:O	2.15	0.46
30:0:1535:G:H2'	30:0:1536:C:C6	2.50	0.46
30:0:238:C:H4'	30:0:287:C:OP1	2.16	0.46
30:0:369:G:C2	30:0:370:G:C8	3.04	0.45
30:0:2526:C:H2'	30:0:2527:U:H5'	1.98	0.45
1:A:190:ARG:NH1	30:0:1845:A:OP2	2.47	0.45
30:0:1675:C:O2'	30:0:1676:G:H5'	2.16	0.45
31:9:52:A:O2'	31:9:53:G:H5'	2.16	0.45
28:2:22:PRO:HG2	28:2:25:VAL:CG2	2.46	0.45
30:0:1393:A:H2'	30:0:1394:C:C6	2.51	0.45
21:U:42:LEU:HD22	30:0:1810:C:H1'	1.98	0.45
30:0:630:A:H5'	38:0:9367:HOH:O	2.16	0.45
30:0:1735:C:H2'	30:0:1736:A:C8	2.50	0.45
30:0:1741:U:H3'	38:0:9774:HOH:O	2.16	0.45
30:0:1973:A:H2'	30:0:1974:G:O4'	2.15	0.45
30:0:536:A:N1	30:0:2075:G:O2'	2.44	0.45
30:0:2499:U:H2'	30:0:2500:C:C6	2.51	0.45
31:9:37:C:H2'	31:9:38:A:C8	2.48	0.45
11:K:34:VAL:HB	38:0:7387:HOH:O	2.15	0.45
30:0:137:U:OP1	30:0:259:G:O2'	2.34	0.45
30:0:797:A:H2'	30:0:798:G:O4'	2.16	0.45
30:0:735:C:H2'	30:0:736:A:H5'	1.99	0.45
30:0:340:A:O5'	30:0:340:A:C8	2.69	0.45
30:0:80:A:C2	30:0:94:G:N3	2.85	0.45
30:0:1501:A:H4'	38:0:5614:HOH:O	2.15	0.45
30:0:1636:G:O2'	30:0:1637:A:H5'	2.16	0.45
4:D:15:GLU:HA	4:D:16:PRO:HD3	1.78	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
30:0:2883:A:H2'	30:0:2884:G:O4'	2.17	0.45
30:0:806:A:H2'	30:0:807:A:O4'	2.17	0.45
30:0:2121:G:O2'	30:0:2122:C:H5'	2.16	0.45
30:0:497:A:H2'	30:0:498:A:C5'	2.46	0.45
30:0:2435:U:H1'	38:0:5442:HOH:O	2.16	0.45
38:Y:8136:HOH:O	30:0:1316:G:H5''	2.15	0.45
17:Q:45:PRO:O	30:0:2365:G:H4'	2.16	0.45
2:B:14:GLY:HA2	2:B:15:PRO:C	2.37	0.45
30:0:1160:G:O2'	30:0:1190:G:H1'	2.17	0.45
30:0:2909:G:H2'	30:0:2910:A:C8	2.51	0.45
3:C:127:ARG:CZ	3:C:225:PRO:HG2	2.45	0.45
30:0:364:U:H2'	30:0:365:G:C8	2.51	0.45
30:0:1477:C:C5'	30:0:1868:G:C5'	2.93	0.45
30:0:1730:G:H5''	30:0:1731:C:C6	2.51	0.45
30:0:1041:U:C2'	30:0:1042:U:H5'	2.47	0.45
16:P:105:LEU:HD21	16:P:137:LEU:HD11	1.99	0.45
30:0:883:U:C2'	30:0:883:U:O2	2.64	0.45
10:J:46:ILE:HD11	10:J:53:ILE:HG23	1.97	0.45
5:E:119:HIS:O	5:E:140:ALA:HB1	2.17	0.45
20:T:41:ARG:HH11	20:T:41:ARG:HG2	1.82	0.45
30:0:1163:G:N2	38:0:4740:HOH:O	2.49	0.45
30:0:281:U:H5	38:0:7610:HOH:O	2.00	0.45
30:0:282:C:C2'	30:0:283:U:H5'	2.46	0.45
5:E:143:GLN:NE2	30:0:2780:C:C1'	2.79	0.45
31:9:3:A:C8	31:9:26:C:O2	2.69	0.45
31:9:3:A:H8	31:9:26:C:O2	1.99	0.45
22:V:39:ALA:C	22:V:41:GLU:H	2.20	0.45
30:0:2499:U:H2'	30:0:2500:C:H6	1.81	0.45
5:E:69:ILE:HA	5:E:72:MET:HE2	1.99	0.45
30:0:2064:U:H2'	30:0:2065:C:H6	1.81	0.45
19:S:57:THR:HG22	19:S:59:ASP:H	1.80	0.45
2:B:141:ARG:HG2	2:B:165:ARG:HA	1.98	0.45
1:A:231:LYS:HG3	30:0:1853:C:OP1	2.17	0.45
12:L:33:ALA:HB3	38:L:8892:HOH:O	2.17	0.45
4:D:22:VAL:HG22	4:D:74:THR:HG22	1.97	0.45
4:D:104:PHE:CE2	4:D:132:VAL:HB	2.52	0.45
30:0:2308:U:C5	30:0:2310:G:C8	3.05	0.45
2:B:262:ARG:HD2	30:0:2715:G:O2'	2.17	0.45
30:0:2908:A:H2'	30:0:2909:G:C4'	2.45	0.45
30:0:2421:G:H3'	30:0:2422:U:C5'	2.47	0.45
3:C:236:THR:HG21	38:C:8577:HOH:O	2.17	0.45
30:0:1903:U:O2'	30:0:1904:A:C8	2.69	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
30:0:1120:U:H5''	30:0:1120:U:C6	2.52	0.45
30:0:1521:C:H2'	30:0:1522:A:C8	2.50	0.45
14:N:4:PRO:HD2	38:0:6790:HOH:O	2.17	0.45
31:9:39:U:H3'	31:9:40:C:H5''	1.99	0.45
30:0:1098:A:H2'	30:0:1099:G:O4'	2.17	0.45
12:L:12:THR:HG21	12:L:16:GLY:O	2.17	0.45
30:0:2515:C:H2'	30:0:2516:G:O4'	2.16	0.45
30:0:1149:U:C5	30:0:1215:A:C5	3.04	0.45
30:0:134:U:C2	30:0:145:A:C2	3.05	0.45
30:0:517:U:H1'	38:0:7592:HOH:O	2.16	0.45
30:0:1992:U:H2'	30:0:1994:A:OP2	2.17	0.45
30:0:1815:A:H4'	30:0:2751:C:O4'	2.17	0.45
30:0:1175:G:C1'	30:0:1193:A:C8	2.98	0.45
30:0:1196:C:H42	30:0:1204:C:N4	2.14	0.45
30:0:283:U:H5	30:0:284:C:N3	2.13	0.45
2:B:234:ARG:NH2	30:0:2039:A:OP2	2.50	0.45
30:0:1165:G:N2	30:0:1173:A:H5'	2.32	0.45
30:0:1773:G:N2	30:0:1774:G:C8	2.84	0.45
30:0:581:G:H5'	38:0:7694:HOH:O	2.16	0.45
30:0:2004:U:H6	30:0:2004:U:P	2.40	0.45
31:9:63:C:O2'	31:9:64:C:H5'	2.17	0.45
3:C:54:LEU:HD23	3:C:79:ARG:HG3	1.99	0.45
19:S:57:THR:CG2	19:S:58:MET:N	2.79	0.45
30:0:61:G:C6	30:0:62:C:C4	3.05	0.45
2:B:69:VAL:HA	2:B:70:PRO:HD3	1.82	0.45
22:V:49:LEU:O	22:V:53:ILE:HG13	2.17	0.45
30:0:1249:U:H2'	30:0:1250:C:C6	2.51	0.45
30:0:1996:U:O2'	30:0:1997:A:H5'	2.16	0.45
4:D:10:PHE:HA	38:D:7345:HOH:O	2.15	0.45
30:0:31:C:H4'	38:0:7442:HOH:O	2.17	0.45
30:0:168:C:O2'	30:0:169:A:H5'	2.16	0.45
2:B:81:ALA:HB1	2:B:142:LEU:HD13	1.99	0.45
1:A:206:ARG:HH11	1:A:206:ARG:HG3	1.82	0.45
26:Z:34:SER:HB3	30:0:797:A:H4'	1.99	0.45
4:D:75:LEU:HD22	4:D:79:MET:HB3	1.98	0.45
25:Y:144:ARG:NE	38:Y:8181:HOH:O	2.49	0.45
30:0:844:A:C6	30:0:882:A:C5	3.05	0.45
14:N:171:HIS:CE1	38:N:8861:HOH:O	2.69	0.45
30:0:2583:A:H5'	38:0:9803:HOH:O	2.17	0.45
30:0:559:U:H2'	30:0:560:U:O4'	2.17	0.45
23:W:52:VAL:HG22	23:W:53:ALA:H	1.82	0.45
30:0:2072:G:H3'	30:0:2073:G:C5'	2.47	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
30:0:968:G:H2'	30:0:969:G:H8	1.82	0.45
1:A:35:GLY:O	1:A:36:ASP:HB3	2.16	0.45
13:M:24:GLN:HE22	13:M:27:ARG:HH11	1.64	0.45
30:0:553:G:H3'	38:0:4084:HOH:O	2.15	0.45
2:B:211:THR:HG21	38:0:7472:HOH:O	2.17	0.45
30:0:1711:A:O2'	30:0:1712:A:H5'	2.16	0.45
2:B:5:ARG:NH2	30:0:2548:C:OP2	2.50	0.45
14:N:109:PRO:HB3	30:0:2413:A:N7	2.32	0.45
30:0:240:C:O2	30:0:240:C:H2'	2.17	0.45
30:0:1577:U:O2'	30:0:1578:C:H5'	2.17	0.45
18:R:15:LYS:HE3	38:R:8982:HOH:O	2.16	0.45
3:C:72:LYS:HE3	38:C:8505:HOH:O	2.17	0.45
11:K:64:MET:HA	11:K:67:GLN:HE21	1.81	0.45
6:F:2:VAL:HG22	6:F:57:GLU:OE1	2.17	0.45
23:W:130:HIS:O	23:W:136:GLY:HA3	2.17	0.45
1:A:54:PRO:HG2	1:A:160:ALA:HB3	1.99	0.45
30:0:1825:U:O2'	30:0:1826:C:H5'	2.16	0.45
30:0:960:G:C3'	30:0:960:G:C4	3.00	0.45
2:B:217:ARG:HG3	2:B:257:THR:HB	1.99	0.45
30:0:68:U:O2'	30:0:69:A:H5''	2.17	0.45
30:0:2361:A:C5'	38:0:9009:HOH:O	2.60	0.45
30:0:2828:G:C6	30:0:2913:A:C2	3.05	0.45
30:0:407:A:H3'	38:0:4468:HOH:O	2.16	0.45
27:1:16:HIS:CD2	30:0:470:U:O2'	2.68	0.45
30:0:1626:A:H2'	30:0:1627:G:C5'	2.47	0.45
16:P:20:ARG:NH1	16:P:54:LYS:HD3	2.32	0.45
13:M:81:ARG:HG3	13:M:85:ARG:HB2	1.99	0.45
30:0:2624:A:O2'	30:0:2625:C:H5'	2.17	0.45
18:R:40:ALA:O	18:R:44:VAL:HG23	2.16	0.45
30:0:884:C:H3'	38:0:9406:HOH:O	2.17	0.45
8:H:31:ILE:HG23	38:H:233:HOH:O	2.16	0.45
14:N:37:ARG:NH1	31:9:6:C:OP1	2.50	0.44
30:0:2269:C:H2'	30:0:2270:G:C5'	2.47	0.44
30:0:2653:A:H2'	30:0:2654:C:C6	2.52	0.44
1:A:179:MET:HA	1:A:179:MET:CE	2.47	0.44
3:C:46:TYR:CE1	3:C:92:PRO:HB3	2.51	0.44
23:W:122:ARG:HH12	23:W:154:ARG:N	2.14	0.44
17:Q:26:PRO:O	17:Q:30:VAL:HG23	2.16	0.44
3:C:39:GLN:O	3:C:43:LYS:HD3	2.18	0.44
2:B:214:PRO:C	2:B:220:VAL:HG22	2.37	0.44
30:0:1735:C:H2'	30:0:1736:A:H8	1.82	0.44
4:D:12:GLU:O	4:D:15:GLU:HG2	2.17	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
16:P:1:THR:O	30:0:1396:C:H1'	2.17	0.44
30:0:1718:G:O2'	30:0:1719:G:H5'	2.17	0.44
5:E:75:GLY:HA3	5:E:136:PRO:O	2.18	0.44
30:0:45:A:H5''	30:0:47:G:O4'	2.17	0.44
9:I:121:LYS:HB3	30:0:1184:C:H4'	1.98	0.44
31:9:14:G:H8	31:9:14:G:C5'	2.20	0.44
30:0:2510:C:N4	30:0:2564:G:H22	2.12	0.44
3:C:1:MET:HG2	3:C:2:GLN:N	2.27	0.44
23:W:13:MET:HE2	23:W:17:ILE:HG22	1.98	0.44
5:E:15:GLN:HG3	5:E:20:ILE:HG12	1.99	0.44
25:Y:235:GLU:CD	25:Y:235:GLU:N	2.70	0.44
30:0:1676:G:C2'	30:0:1677:U:H5'	2.47	0.44
28:2:8:LYS:NZ	30:0:1677:U:OP2	2.48	0.44
30:0:255:A:H2'	30:0:256:C:O4'	2.17	0.44
2:B:27:ASN:HD21	30:0:2807:U:P	2.40	0.44
18:R:29:LYS:HE2	30:0:524:A:H5'	1.99	0.44
4:D:52:THR:HG21	30:0:2346:C:O2'	2.17	0.44
14:N:22:GLN:HA	14:N:25:ARG:CZ	2.47	0.44
29:3:60:LYS:HG3	29:3:61:PRO:HD2	1.98	0.44
30:0:1894:C:N4	30:0:1939:U:H2'	2.31	0.44
13:M:159:VAL:HG13	13:M:160:PHE:N	2.32	0.44
2:B:10:SER:O	2:B:16:ARG:NH1	2.49	0.44
11:K:8:VAL:HG13	11:K:80:ILE:HG22	1.98	0.44
30:0:271:C:C2	30:0:273:G:O4'	2.70	0.44
30:0:542:A:H1'	38:0:4691:HOH:O	2.16	0.44
30:0:2526:C:C2'	30:0:2527:U:H5'	2.47	0.44
31:9:3:A:C8	31:9:26:C:N3	2.86	0.44
30:0:2505:G:H2'	30:0:2506:A:H5'	2.00	0.44
23:W:21:LEU:HB3	23:W:26:ILE:HG12	1.99	0.44
30:0:2587:OMU:H2'	30:0:2589:U:H5''	1.99	0.44
13:M:59:GLY:HA3	13:M:141:ILE:CD1	2.47	0.44
4:D:137:PRO:O	31:9:30:C:OP1	2.35	0.44
31:9:65:A:N6	31:9:112:U:C6	2.85	0.44
30:0:74:G:H2'	30:0:75:U:H6	1.82	0.44
12:L:6:ARG:NH1	30:0:1299:G:N7	2.65	0.44
3:C:95:GLU:CD	3:C:95:GLU:H	2.20	0.44
25:Y:126:PRO:HG2	25:Y:128:PHE:CZ	2.52	0.44
25:Y:154:ARG:NH2	30:0:1071:G:H4'	2.31	0.44
16:P:137:LEU:O	16:P:141:ILE:HG13	2.17	0.44
8:H:77:ILE:HG23	8:H:82:GLU:HG2	2.00	0.44
30:0:649:U:O2'	30:0:650:C:H5'	2.16	0.44
13:M:184:ARG:HG3	13:M:185:PRO:HA	2.00	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
30:0:2502:C:O2'	30:0:2503:A:H5'	2.17	0.44
30:0:1116:U:N3	30:0:1246:A:N6	2.59	0.44
11:K:55:VAL:CG1	11:K:56:SER:N	2.80	0.44
2:B:162:MET:CE	2:B:310:ARG:HD3	2.46	0.44
30:0:2064:U:H4'	30:0:2653:A:OP1	2.17	0.44
30:0:1503:U:H2'	30:0:1504:A:O4'	2.17	0.44
4:D:54:ALA:HB2	4:D:69:ILE:CD1	2.48	0.44
30:0:796:A:C2	30:0:797:A:C4	3.05	0.44
30:0:1268:C:O2'	30:0:1269:G:H5'	2.16	0.44
30:0:957:A:H8	30:0:957:A:O5'	2.01	0.44
30:0:1850:U:H2'	30:0:1851:G:H8	1.82	0.44
27:1:8:GLN:HG3	30:0:1688:G:H4'	1.99	0.44
31:9:45:A:C5	31:9:46:C:C5	3.05	0.44
3:C:233:THR:HG22	3:C:234:VAL:N	2.32	0.44
30:0:1925:G:O2'	30:0:1926:G:H5'	2.18	0.44
5:E:95:VAL:HG11	5:E:131:LEU:HD21	1.98	0.44
16:P:19:ASN:OD1	30:0:1720:C:H5	2.00	0.44
30:0:195:C:H2'	30:0:196:G:H5'	1.99	0.44
10:J:70:PHE:HE1	30:0:2676:C:H4'	1.79	0.44
30:0:731:U:O2'	30:0:732:C:H5'	2.18	0.44
30:0:1268:C:H2'	30:0:1269:G:C8	2.53	0.44
1:A:70:ALA:HA	1:A:71:PRO:HD3	1.77	0.44
30:0:397:A:O2'	30:0:417:G:N3	2.36	0.44
1:A:164:ARG:HB2	26:Z:92:SER:OG	2.17	0.44
30:0:1416:G:C2'	30:0:1417:G:H5'	2.47	0.44
30:0:970:U:H2'	38:0:6346:HOH:O	2.18	0.44
30:0:2734:G:O2'	30:0:2735:U:H5'	2.18	0.44
30:0:348:C:H5	38:0:6349:HOH:O	1.99	0.44
30:0:299:U:H5'	38:0:7352:HOH:O	2.16	0.44
30:0:283:U:H5	30:0:284:C:C4	2.36	0.44
30:0:816:G:H5'	30:0:1598:A:H4'	2.00	0.44
30:0:1058:A:H2'	30:0:1060:C:C5'	2.47	0.44
13:M:92:THR:HB	30:0:401:C:O2'	2.17	0.44
30:0:1421:C:H2'	30:0:1422:U:H6	1.82	0.44
27:1:1:THR:O	30:0:1836:A:H1'	2.18	0.44
30:0:535:G:C6	30:0:2064:U:C5	3.06	0.44
30:0:2324:G:H21	30:0:2377:U:H1'	1.83	0.44
30:0:312:U:C2	30:0:320:G:N2	2.86	0.44
27:1:28:HIS:CE1	27:1:31:LYS:HE2	2.53	0.44
30:0:99:A:C8	30:0:100:C:C5	3.06	0.44
30:0:354:A:H2'	30:0:355:C:C6	2.53	0.44
30:0:1020:A:H2'	30:0:1021:G:C8	2.52	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
30:0:2612:A:H4'	38:0:3687:HOH:O	2.16	0.44
18:R:61:GLN:NE2	38:0:4737:HOH:O	2.50	0.44
12:L:79:ASP:HB2	38:L:8858:HOH:O	2.17	0.44
2:B:198:GLU:HA	38:B:9123:HOH:O	2.17	0.44
25:Y:122:ARG:NH2	38:Y:8101:HOH:O	2.51	0.44
31:9:56:A:H2'	31:9:57:A:C5'	2.28	0.44
30:0:545:G:H8	30:0:545:G:C5'	2.14	0.44
30:0:1666:C:C2'	30:0:1667:A:H5'	2.31	0.44
2:B:256:GLN:HG2	38:B:9122:HOH:O	2.17	0.44
30:0:2672:C:H2'	30:0:2673:U:C6	2.52	0.44
11:K:118:ALA:CA	11:K:125:ALA:HB2	2.48	0.44
27:1:21:ARG:HD2	27:1:39:PHE:HB2	1.98	0.44
20:T:19:ARG:HD3	20:T:67:LEU:O	2.18	0.44
5:E:35:TYR:CD2	5:E:36:PRO:HD2	2.53	0.44
30:0:1224:G:H2'	30:0:1225:C:C6	2.52	0.44
30:0:565:A:C6	30:0:566:A:C6	3.05	0.44
24:X:34:ARG:NH1	24:X:48:VAL:O	2.49	0.44
7:G:19:GLU:O	7:G:23:ILE:HG13	2.18	0.44
14:N:160:SER:HB3	31:9:51:A:H5'	1.99	0.44
6:F:107:ASP:O	6:F:111:ILE:HG13	2.18	0.44
30:0:363:C:O2'	30:0:364:U:H5'	2.18	0.44
5:E:81:GLU:HG2	5:E:134:SER:CB	2.45	0.44
1:A:48:ASP:HA	1:A:49:PRO:HD3	1.86	0.44
30:0:1947:G:N2	30:0:1966:U:C2	2.86	0.44
3:C:40:ALA:O	3:C:43:LYS:HB2	2.18	0.44
30:0:777:U:OP2	30:0:777:U:H4'	2.17	0.44
18:R:113:HIS:HE1	18:R:144:GLU:CD	2.21	0.44
13:M:169:ARG:HD2	38:M:8886:HOH:O	2.16	0.44
14:N:154:LEU:C	14:N:156:GLU:H	2.20	0.44
23:W:75:GLY:HA3	38:W:5763:HOH:O	2.17	0.44
4:D:84:LEU:HA	4:D:87:ALA:HB3	1.99	0.44
3:C:153:VAL:O	3:C:157:LEU:HG	2.16	0.44
30:0:1186:C:N4	30:0:1187:U:C4	2.86	0.44
30:0:1206:U:C5'	30:0:1206:U:H6	2.24	0.44
30:0:2456:A:H5'	38:0:5708:HOH:O	2.18	0.44
30:0:1236:A:H2'	30:0:1237:U:O4'	2.17	0.44
30:0:537:G:O4'	30:0:538:C:C5	2.70	0.44
30:0:1520:G:C2	30:0:1521:C:C2	3.06	0.44
30:0:2310:G:C2	30:0:2311:A:C5	3.05	0.44
30:0:970:U:O5'	30:0:970:U:H6	2.01	0.44
3:C:51:TYR:CE2	27:1:53:LYS:HB3	2.53	0.44
30:0:1079:A:OP2	30:0:1080:C:N4	2.46	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
30:0:2717:C:C2'	30:0:2718:C:C5'	2.81	0.43
30:0:1593:C:O2'	30:0:1594:C:H5'	2.18	0.43
30:0:1695:G:C6	30:0:1696:U:C4	3.06	0.43
30:0:2387:U:H2'	30:0:2388:C:C6	2.53	0.43
30:0:758:A:H2'	30:0:759:C:O4'	2.17	0.43
15:O:65:LEU:HD13	30:0:746:A:C6	2.53	0.43
3:C:195:VAL:HA	3:C:213:ALA:O	2.17	0.43
12:L:27:ARG:HH21	12:L:30:ARG:HG2	1.82	0.43
30:0:2842:G:H2'	30:0:2843:A:H5'	2.00	0.43
30:0:2015:A:H2'	30:0:2016:U:O4'	2.18	0.43
13:M:115:LEU:HD13	13:M:116:ASN:HB2	2.00	0.43
30:0:192:A:H5'	38:0:7657:HOH:O	2.17	0.43
30:0:1164:U:H3	30:0:1192:A:H2	1.65	0.43
30:0:2269:C:H2'	30:0:2270:G:H5'	2.00	0.43
17:Q:94:GLN:O	17:Q:95:GLU:HB2	2.18	0.43
30:0:2642:G:H2'	30:0:2643:G:O4'	2.18	0.43
5:E:84:MET:HG2	5:E:168:ILE:HD13	2.00	0.43
30:0:958:G:H2'	30:0:959:C:C6	2.53	0.43
10:J:88:PRO:CA	35:J:8802:CL:CL	3.03	0.43
30:0:1626:A:C2'	30:0:1627:G:H5'	2.48	0.43
30:0:327:A:H4'	30:0:329:A:C8	2.52	0.43
30:0:2649:A:H5'	30:0:2649:A:C8	2.53	0.43
30:0:705:C:H2'	30:0:705:C:O2	2.17	0.43
22:V:4:HIS:O	22:V:8:ILE:HG13	2.18	0.43
30:0:2595:U:O2'	30:0:2596:A:H5'	2.18	0.43
30:0:682:A:H2'	30:0:683:G:O4'	2.18	0.43
5:E:53:GLU:HB3	5:E:55:ASN:ND2	2.33	0.43
30:0:2906:A:H5'	30:0:2907:C:O4'	2.17	0.43
30:0:1069:C:H2'	30:0:1070:A:O4'	2.18	0.43
30:0:2107:U:O2'	30:0:2108:A:H5'	2.19	0.43
18:R:80:TYR:O	30:0:2050:G:H5''	2.18	0.43
30:0:1205:U:H5	38:0:4448:HOH:O	2.00	0.43
9:I:87:PRO:HG3	38:0:7132:HOH:O	2.18	0.43
31:9:23:U:C2'	31:9:24:U:H4'	2.48	0.43
30:0:711:G:C2	30:0:718:C:N3	2.87	0.43
30:0:1889:C:O2	30:0:2010:A:H2	2.02	0.43
27:1:9:GLY:HA3	30:0:1695:G:H1'	2.00	0.43
30:0:1631:A:C6	30:0:1632:A:N1	2.86	0.43
30:0:1298:U:H2'	30:0:1299:G:C8	2.53	0.43
30:0:130:C:H4'	38:0:5803:HOH:O	2.17	0.43
16:P:73:HIS:HE1	30:0:1789:G:O6	2.01	0.43
30:0:100:C:H2'	30:0:101:C:H6	1.84	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
7:G:23:ILE:O	7:G:27:ILE:HG13	2.18	0.43
30:0:745:G:H5''	30:0:746:A:OP1	2.18	0.43
30:0:2801:A:H2'	30:0:2801:A:N3	2.33	0.43
30:0:2349:G:O2'	30:0:2350:G:H5'	2.17	0.43
30:0:622:G:O2'	30:0:623:U:H5'	2.19	0.43
4:D:146:LYS:HE2	14:N:107:ASN:ND2	2.34	0.43
30:0:871:G:H4'	38:0:4418:HOH:O	2.18	0.43
8:H:12:ILE:HG23	8:H:129:ARG:CZ	2.48	0.43
30:0:483:C:N4	30:0:484:A:C6	2.86	0.43
6:F:91:VAL:CG1	6:F:92:GLY:N	2.81	0.43
30:0:367:G:OP2	30:0:367:G:H8	2.01	0.43
30:0:2315:C:H4'	30:0:2425:A:C6	2.53	0.43
30:0:1503:U:H3'	30:0:1503:U:H6	1.82	0.43
30:0:2040:C:H5''	30:0:2759:C:O2'	2.18	0.43
30:0:2649:A:H5'	30:0:2649:A:H8	1.83	0.43
30:0:1368:U:H6	30:0:1368:U:O5'	2.01	0.43
13:M:67:VAL:HB	13:M:97:ILE:HG23	2.01	0.43
10:J:80:LYS:HE3	10:J:101:VAL:O	2.19	0.43
16:P:98:ILE:HD12	16:P:102:ARG:CZ	2.48	0.43
31:9:110:G:C5	31:9:111:U:C5	3.07	0.43
30:0:1074:G:H4'	30:0:1260:G:C6	2.54	0.43
14:N:37:ARG:HH21	14:N:105:GLY:N	2.16	0.43
15:O:32:ARG:HH21	15:O:35:LYS:HZ2	1.67	0.43
14:N:86:LEU:HD23	14:N:179:LEU:HD12	1.98	0.43
30:0:2010:A:C2'	38:0:5975:HOH:O	2.59	0.43
16:P:59:ARG:NH2	16:P:66:GLN:HE22	2.17	0.43
16:P:83:LYS:HG2	30:0:793:A:H5''	1.99	0.43
30:0:1568:G:C6	30:0:1569:U:C4	3.06	0.43
30:0:1626:A:H2'	30:0:1627:G:H5'	1.99	0.43
1:A:64:ASP:OD1	1:A:66:ARG:HD3	2.18	0.43
30:0:1416:G:H2'	30:0:1417:G:H5'	1.99	0.43
30:0:666:A:H2'	30:0:667:C:O4'	2.18	0.43
30:0:113:A:H2'	30:0:115:U:O4	2.19	0.43
30:0:2902:A:H4'	30:0:2903:C:OP1	2.19	0.43
31:9:117:G:H2'	31:9:118:C:H6	1.83	0.43
30:0:2470:A:H5''	38:0:3249:HOH:O	2.18	0.43
15:O:29:VAL:HG11	15:O:98:LEU:HD21	1.99	0.43
30:0:725:C:H2'	30:0:726:C:O5'	2.17	0.43
30:0:1163:G:H1	30:0:1184:C:N4	2.17	0.43
15:O:3:THR:HG22	30:0:656:G:C5'	2.31	0.43
30:0:2829:G:N2	30:0:2912:C:C2	2.86	0.43
23:W:139:GLY:O	23:W:141:HIS:CD2	2.71	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
22:V:59:ILE:O	22:V:63:GLU:HG2	2.17	0.43
3:C:27:ARG:NH1	3:C:29:ASP:OD1	2.50	0.43
3:C:96:LYS:NZ	30:0:1351:G:OP1	2.39	0.43
25:Y:204:ARG:NH2	30:0:1324:G:H21	2.16	0.43
30:0:1023:C:H2'	30:0:1024:G:O4'	2.18	0.43
15:O:25:VAL:HG11	30:0:710:G:H5'	1.99	0.43
30:0:1314:U:H5''	30:0:1316:G:O4'	2.19	0.43
16:P:94:TRP:CH2	16:P:98:ILE:HG13	2.53	0.43
30:0:1585:C:H2'	30:0:1586:G:H8	1.84	0.43
17:Q:47:VAL:HA	17:Q:48:PRO:HD3	1.81	0.43
30:0:1181:A:O2'	30:0:1182:C:H5'	2.18	0.43
30:0:2716:G:O2'	30:0:2717:C:H5'	2.19	0.43
30:0:1474:C:C5'	30:0:1474:C:H6	2.18	0.43
30:0:2421:G:H3'	30:0:2422:U:H5''	2.00	0.43
1:A:94:LEU:N	1:A:94:LEU:HD23	2.33	0.43
1:A:94:LEU:HD12	1:A:98:GLU:HB2	2.00	0.43
3:C:118:THR:HG22	3:C:137:PRO:HB3	1.99	0.43
31:9:64:C:O2'	31:9:65:A:H5'	2.18	0.43
2:B:51:VAL:CG2	2:B:330:VAL:HG22	2.48	0.43
15:O:24:ALA:HB3	30:0:710:G:OP1	2.19	0.43
31:9:59:C:H2'	31:9:60:C:H6	1.83	0.43
30:0:1626:A:H2'	30:0:1627:G:O4'	2.19	0.43
30:0:790:A:H2'	30:0:791:A:O4'	2.18	0.43
30:0:1950:G:O2'	30:0:1951:G:H5'	2.19	0.43
5:E:7:ILE:HG22	5:E:45:ASP:O	2.19	0.43
30:0:912:A:C4	30:0:1294:A:C2	3.06	0.43
30:0:1175:G:O2'	30:0:1193:A:H2'	2.19	0.43
30:0:1132:A:H3'	38:0:4832:HOH:O	2.18	0.43
30:0:1453:G:N2	30:0:1675:C:C2	2.87	0.43
30:0:512:G:O3'	30:0:513:A:C8	2.70	0.43
30:0:1705:C:H2'	30:0:1706:G:O4'	2.19	0.43
12:L:67:ARG:O	12:L:71:GLU:HG3	2.19	0.43
14:N:108:SER:HA	14:N:109:PRO:HD3	1.78	0.43
2:B:242:TRP:CZ2	30:0:2607:U:C4	3.06	0.43
13:M:49:ALA:C	13:M:54:TYR:HB3	2.39	0.43
3:C:25:PRO:HG2	38:C:8520:HOH:O	2.17	0.43
4:D:154:LYS:H	4:D:154:LYS:CD	2.20	0.43
30:0:2589:U:H2'	30:0:2590:U:C6	2.54	0.43
30:0:2362:A:H2'	30:0:2363:G:C8	2.54	0.43
31:9:65:A:C2'	31:9:66:G:OP2	2.66	0.43
30:0:2241:C:H2'	30:0:2242:U:C6	2.54	0.43
30:0:1971:G:H5''	38:0:7084:HOH:O	2.18	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
30:0:64:G:H2'	30:0:65:C:O4'	2.19	0.43
6:F:61:MET:HB3	13:M:19:GLN:OE1	2.19	0.43
30:0:590:A:C2'	30:0:591:A:H5'	2.48	0.43
1:A:217:ARG:NH2	30:0:1853:C:O2'	2.48	0.43
30:0:1463:U:H2'	30:0:1464:C:H6	1.83	0.43
31:9:117:G:H2'	31:9:118:C:C6	2.53	0.43
30:0:1138:G:H4'	38:0:5722:HOH:O	2.18	0.43
23:W:119:HIS:HE1	38:0:9560:HOH:O	2.02	0.43
6:F:59:ILE:CD1	30:0:263:U:C2	3.02	0.43
14:N:44:ARG:HG3	14:N:45:ALA:N	2.34	0.43
30:0:2761:A:H2'	38:0:5654:HOH:O	2.19	0.43
20:T:71:VAL:HG11	20:T:90:PRO:HB3	1.99	0.43
30:0:1158:G:O2'	30:0:1159:G:H5'	2.19	0.43
10:J:75:PRO:HD3	10:J:136:SER:OG	2.18	0.43
30:0:1528:A:H61	30:0:1663:G:H1'	1.84	0.43
23:W:26:ILE:HB	38:W:5420:HOH:O	2.18	0.43
30:0:779:U:H5'	30:0:1836:A:C2	2.54	0.43
3:C:27:ARG:HG3	3:C:27:ARG:HH11	1.83	0.43
30:0:2249:G:C2	30:0:2253:G:C6	3.07	0.43
30:0:2314:G:O2'	30:0:2315:C:H5'	2.19	0.43
18:R:29:LYS:HE2	30:0:524:A:H5''	2.01	0.43
30:0:1559:A:OP2	30:0:1559:A:H8	2.02	0.43
30:0:1483:C:O2'	30:0:1484:G:H5'	2.18	0.43
30:0:1829:A:C8	30:0:1885:A:C8	3.07	0.43
30:0:1015:C:H2'	30:0:1016:U:C6	2.54	0.43
1:A:217:ARG:CG	1:A:217:ARG:HH11	2.32	0.43
5:E:108:LEU:CD1	5:E:164:ASP:HB2	2.49	0.43
7:G:63:ARG:O	7:G:67:LEU:HG	2.18	0.43
31:9:121:C:H6	31:9:121:C:O5'	2.02	0.43
30:0:764:C:H2'	30:0:765:G:O4'	2.19	0.43
4:D:96:SER:O	30:0:2337:G:H5''	2.19	0.43
30:0:1409:G:C2	30:0:1410:G:C8	3.07	0.43
1:A:173:GLY:O	1:A:176:HIS:HB3	2.19	0.43
30:0:69:A:C8	30:0:69:A:C5'	2.98	0.42
30:0:1213:C:C2'	30:0:1214:G:H5'	2.48	0.42
14:N:29:SER:HB3	30:0:2415:A:O2'	2.19	0.42
30:0:2374:G:H2'	30:0:2375:A:H8	1.83	0.42
30:0:1482:A:H1'	38:0:9422:HOH:O	2.19	0.42
24:X:61:ARG:HD2	24:X:65:ASN:O	2.19	0.42
2:B:82:VAL:HG12	2:B:82:VAL:O	2.19	0.42
30:0:1413:A:H2'	30:0:1414:A:O4'	2.19	0.42
30:0:2293:G:C2	30:0:2316:G:C6	3.07	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
30:0:1555:G:H4'	30:0:1630:A:H2	1.84	0.42
28:2:20:ARG:HG2	28:2:21:VAL:N	2.33	0.42
30:0:1116:U:C2	30:0:1246:A:N6	2.87	0.42
23:W:6:GLN:HB2	23:W:26:ILE:HD11	1.98	0.42
30:0:56:G:N3	30:0:70:A:C2	2.87	0.42
20:T:9:LYS:HE3	20:T:13:ARG:NH1	2.33	0.42
18:R:128:ARG:HH22	30:0:2054:A:H2	1.65	0.42
30:0:137:U:H3'	30:0:139:C:H41	1.83	0.42
30:0:808:A:C5	30:0:809:G:H1'	2.54	0.42
30:0:319:A:H4'	30:0:338:C:C4	2.53	0.42
30:0:2347:C:H2'	30:0:2348:C:C6	2.54	0.42
30:0:1406:A:H4'	30:0:1407:A:C5'	2.50	0.42
5:E:91:PHE:HA	5:E:92:PRO:HD3	1.80	0.42
30:0:941:G:C6	30:0:942:U:C4	3.08	0.42
30:0:1769:C:C4	30:0:1770:U:C4	3.08	0.42
30:0:2519:C:H2'	30:0:2520:G:O4'	2.19	0.42
30:0:917:U:H6	30:0:917:U:O5'	2.02	0.42
14:N:73:ALA:HB1	14:N:74:PRO:CD	2.49	0.42
30:0:216:A:O2'	30:0:217:C:H5'	2.19	0.42
17:Q:55:ARG:HD2	38:Q:2875:HOH:O	2.18	0.42
30:0:2726:U:O2	30:0:2749:U:O5'	2.36	0.42
30:0:1185:U:C5'	38:0:7483:HOH:O	2.66	0.42
30:0:2822:C:O2'	30:0:2827:A:H4'	2.19	0.42
1:A:211:LYS:HG2	38:0:7044:HOH:O	2.19	0.42
21:U:52:THR:HG22	21:U:54:THR:N	2.32	0.42
5:E:107:PHE:CZ	5:E:152:THR:HB	2.55	0.42
30:0:2755:G:H1'	38:0:4696:HOH:O	2.19	0.42
4:D:22:VAL:HA	4:D:73:VAL:O	2.19	0.42
2:B:70:PRO:HG3	30:0:2719:A:C2	2.54	0.42
30:0:78:G:C6	30:0:79:G:C6	3.07	0.42
30:0:699:C:C6	30:0:744:G:C4	3.07	0.42
5:E:77:THR:OG1	5:E:78:GLU:N	2.53	0.42
30:0:1167:G:H3'	38:0:7514:HOH:O	2.19	0.42
30:0:1163:G:N2	30:0:1184:C:N3	2.67	0.42
30:0:1189:A:N7	30:0:1190:G:N7	2.67	0.42
30:0:1603:A:H5'	30:0:1605:G:C5'	2.48	0.42
30:0:69:A:C2'	30:0:70:A:OP2	2.67	0.42
30:0:536:A:H8	38:0:5057:HOH:O	2.01	0.42
26:Z:40:ALA:HA	30:0:1773:G:C8	2.54	0.42
30:0:2456:A:H2'	30:0:2457:U:C6	2.55	0.42
30:0:1211:G:H2'	30:0:1212:C:C6	2.48	0.42
30:0:2512:U:O5'	30:0:2512:U:H6	2.02	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
30:0:305:A:C6	30:0:329:A:N3	2.87	0.42
4:D:23:VAL:HG21	4:D:45:THR:CG2	2.49	0.42
16:P:16:VAL:HG22	16:P:20:ARG:CZ	2.50	0.42
30:0:1400:C:C2'	30:0:1401:G:H5'	2.49	0.42
30:0:2061:C:H2'	30:0:2062:A:H5'	2.00	0.42
30:0:1850:U:H2'	30:0:1851:G:C8	2.53	0.42
30:0:2119:C:O2'	30:0:2120:U:H5'	2.19	0.42
30:0:1057:A:H1'	30:0:2492:U:O2'	2.19	0.42
9:I:82:THR:HG22	30:0:1168:C:H5''	2.00	0.42
30:0:2661:U:H3	30:0:2812:A:H62	1.66	0.42
31:9:14:G:C8	31:9:14:G:C5'	2.99	0.42
14:N:55:ASP:OD2	31:9:7:G:H4'	2.20	0.42
30:0:138:U:OP2	30:0:139:C:H5	2.02	0.42
2:B:304:PRO:HD2	2:B:307:ARG:HE	1.84	0.42
30:0:807:A:H2'	30:0:808:A:O4'	2.19	0.42
30:0:2879:A:H2'	30:0:2880:A:O4'	2.19	0.42
30:0:470:U:H2'	30:0:471:G:O4'	2.20	0.42
30:0:952:G:H4'	38:0:4039:HOH:O	2.19	0.42
31:9:39:U:H1'	31:9:44:A:N6	2.35	0.42
4:D:76:ARG:NH1	31:9:42:C:O2	2.53	0.42
30:0:1015:C:H2'	30:0:1016:U:H6	1.85	0.42
30:0:2310:G:N1	30:0:2311:A:C5	2.88	0.42
30:0:939:A:C2	30:0:1027:G:N3	2.88	0.42
30:0:1381:A:N3	30:0:1382:G:H1'	2.35	0.42
2:B:275:GLY:O	2:B:291:ASP:HA	2.19	0.42
30:0:459:A:H4'	38:0:9454:HOH:O	2.20	0.42
9:I:118:ASN:HB3	30:0:1185:U:C5'	2.49	0.42
9:I:130:LEU:HD21	30:0:1167:G:H4'	2.02	0.42
30:0:1603:A:C5'	30:0:1605:G:C5'	2.96	0.42
28:2:48:ASP:O	28:2:49:GLU:HB2	2.19	0.42
30:0:1211:G:O2'	30:0:1212:C:H5'	2.19	0.42
30:0:191:A:C4	30:0:237:G:N7	2.88	0.42
30:0:657:G:H2'	30:0:658:C:C6	2.55	0.42
2:B:310:ARG:HD2	38:B:9114:HOH:O	2.19	0.42
30:0:1966:U:H2'	30:0:1967:U:H2'	2.00	0.42
3:C:206:ASN:HB2	30:0:329:A:OP2	2.19	0.42
30:0:1976:G:O2'	30:0:1977:U:C5'	2.68	0.42
30:0:2388:C:O2'	30:0:2389:U:H5'	2.19	0.42
4:D:101:THR:HG22	4:D:101:THR:O	2.19	0.42
30:0:849:C:H1'	38:0:6632:HOH:O	2.19	0.42
28:2:10:ARG:NH2	30:0:121:U:OP2	2.39	0.42
30:0:2816:A:H5''	30:0:2817:G:H5'	2.01	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
18:R:72:VAL:CG1	18:R:75:TRP:HB3	2.50	0.42
30:0:722:G:H22	30:0:938:G:P	2.42	0.42
30:0:1193:A:H1'	30:0:1194:A:N7	2.35	0.42
30:0:2524:G:H5''	38:0:4744:HOH:O	2.19	0.42
30:0:212:A:O4'	30:0:214:U:C6	2.72	0.42
30:0:307:G:H3'	30:0:342:C:OP2	2.19	0.42
18:R:99:ALA:O	18:R:104:PHE:HB2	2.19	0.42
30:0:137:U:H6	30:0:137:U:O5'	2.02	0.42
30:0:120:A:H2'	30:0:120:A:N3	2.34	0.42
2:B:140:LEU:HD13	2:B:175:LEU:HA	2.01	0.42
38:W:7873:HOH:O	30:0:1287:A:H8	2.03	0.42
30:0:1754:A:H2'	30:0:1755:A:O4'	2.19	0.42
30:0:1097:A:C6	30:0:1098:A:C6	3.08	0.42
3:C:73:GLN:HA	3:C:73:GLN:NE2	2.35	0.42
30:0:485:A:H4'	30:0:486:A:OP1	2.20	0.42
30:0:287:C:O5'	30:0:287:C:H6	2.03	0.42
30:0:85:C:H5''	30:0:86:A:OP2	2.20	0.42
30:0:2355:G:H2'	38:0:5650:HOH:O	2.18	0.42
8:H:6:ALA:CA	8:H:61:ARG:HH12	2.29	0.42
2:B:254:GLN:NE2	38:B:9058:HOH:O	2.52	0.42
20:T:41:ARG:NH1	20:T:42:VAL:O	2.53	0.42
30:0:2333:G:H2'	30:0:2334:C:H6	1.84	0.42
1:A:30:ARG:HG2	1:A:31:LYS:N	2.35	0.42
30:0:2575:C:H2'	30:0:2576:A:O4'	2.19	0.42
30:0:2497:A:C2	30:0:2524:G:C2	3.07	0.42
20:T:9:LYS:HB2	38:0:7442:HOH:O	2.20	0.42
2:B:53:LEU:HD21	2:B:270:ILE:HD12	2.01	0.42
30:0:2324:G:C2	30:0:2377:U:O2	2.73	0.42
30:0:293:A:C4	30:0:360:A:C2	3.08	0.42
2:B:137:LEU:HD21	2:B:140:LEU:HD21	2.02	0.42
4:D:21:VAL:HA	4:D:131:THR:O	2.20	0.42
4:D:19:GLU:O	4:D:76:ARG:HG2	2.19	0.42
4:D:51:ARG:HD3	38:D:7636:HOH:O	2.20	0.42
30:0:834:G:H4'	30:0:835:U:OP2	2.19	0.42
2:B:215:VAL:HA	2:B:220:VAL:HG22	2.01	0.42
1:A:164:ARG:NH2	30:0:1876:C:O3'	2.53	0.42
30:0:295:C:H2'	30:0:296:G:O4'	2.20	0.42
11:K:78:LYS:HA	11:K:79:PRO:HD3	1.94	0.42
30:0:2911:C:H2'	30:0:2912:C:C6	2.54	0.42
30:0:2727:A:C6	30:0:2756:U:C2	3.08	0.42
27:1:25:LYS:HG3	28:2:49:GLU:H	1.85	0.42
23:W:48:VAL:HG12	23:W:48:VAL:O	2.20	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
17:Q:18:PRO:O	17:Q:21:ARG:HB2	2.20	0.42
30:0:130:C:H5'	38:0:5226:HOH:O	2.20	0.42
30:0:2134:G:C6	30:0:2258:A:C8	3.08	0.42
30:0:1544:U:H2'	30:0:1545:C:C6	2.53	0.42
21:U:50:GLU:HB2	30:0:2866:U:C5	2.54	0.42
30:0:844:A:C6	30:0:882:A:C6	3.08	0.42
2:B:75:GLU:C	2:B:77:PRO:HD3	2.39	0.42
30:0:264:G:H1'	30:0:265:U:H5	1.85	0.42
30:0:1175:G:H1'	30:0:1193:A:N9	2.33	0.41
30:0:2269:C:C2'	30:0:2270:G:H5'	2.50	0.41
30:0:583:C:C2	30:0:584:U:C5	3.08	0.41
17:Q:40:HIS:HE1	30:0:949:U:O2'	2.03	0.41
30:0:212:A:N1	30:0:226:A:H5''	2.35	0.41
30:0:2534:C:H2'	30:0:2535:A:C8	2.55	0.41
20:T:48:VAL:HG22	20:T:97:ARG:O	2.19	0.41
11:K:14:LYS:CB	11:K:45:PRO:HG2	2.50	0.41
30:0:2297:U:H2'	30:0:2298:C:C6	2.53	0.41
2:B:84:LEU:O	2:B:99:GLU:HA	2.20	0.41
30:0:803:C:H2'	30:0:804:C:C6	2.55	0.41
30:0:2333:G:H2'	30:0:2334:C:C6	2.55	0.41
7:G:20:VAL:O	7:G:24:VAL:HG23	2.20	0.41
12:L:57:VAL:O	12:L:57:VAL:HG12	2.20	0.41
12:L:57:VAL:HG21	30:0:2443:C:H5'	2.02	0.41
13:M:47:ASP:CG	13:M:48:LYS:N	2.74	0.41
30:0:226:A:H1'	30:0:393:G:C5	2.55	0.41
6:F:99:THR:HG23	6:F:99:THR:O	2.20	0.41
13:M:9:ARG:HD2	30:0:380:A:OP2	2.20	0.41
1:A:179:MET:HG2	1:A:186:TRP:HB2	2.02	0.41
30:0:636:G:H5'	30:0:2059:U:OP2	2.20	0.41
10:J:107:ASN:HD22	10:J:107:ASN:C	2.24	0.41
11:K:41:LYS:O	11:K:42:ASN:HB2	2.20	0.41
26:Z:34:SER:CB	30:0:797:A:H4'	2.50	0.41
2:B:229:ARG:HD2	38:B:8989:HOH:O	2.20	0.41
18:R:79:ARG:HB3	30:0:2050:G:OP1	2.20	0.41
30:0:2350:G:H2'	30:0:2351:C:C6	2.56	0.41
20:T:71:VAL:CG1	20:T:90:PRO:HB3	2.50	0.41
8:H:91:ARG:HG2	8:H:91:ARG:H	1.54	0.41
30:0:830:G:C5	30:0:831:U:C4	3.08	0.41
1:A:97:ALA:HB2	1:A:150:PRO:HB2	2.02	0.41
20:T:28:SER:O	20:T:32:ARG:HG3	2.19	0.41
30:0:1355:A:H4'	38:0:5766:HOH:O	2.19	0.41
5:E:10:ASP:HA	38:E:6017:HOH:O	2.20	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
18:R:96:VAL:HG13	18:R:106:GLY:HA3	2.02	0.41
30:0:1162:G:C6	30:0:1163:G:C6	3.09	0.41
31:9:3:A:C6	31:9:22:G:H1'	2.52	0.41
30:0:1598:A:C2	30:0:1599:U:C2	3.07	0.41
1:A:141:PRO:HG2	30:0:1855:G:O6	2.20	0.41
30:0:567:U:H5''	38:0:5300:HOH:O	2.19	0.41
30:0:1172:G:H1'	38:0:4984:HOH:O	2.20	0.41
30:0:1971:G:C5'	38:0:7084:HOH:O	2.67	0.41
23:W:35:VAL:HA	23:W:36:PRO:HD3	1.83	0.41
18:R:132:ARG:NH2	38:R:8987:HOH:O	2.53	0.41
30:0:349:U:O2'	30:0:350:G:H5'	2.20	0.41
2:B:199:TYR:CE2	2:B:268:ARG:HB2	2.54	0.41
30:0:2766:A:O2'	30:0:2767:C:H5'	2.20	0.41
30:0:1056:U:H2'	30:0:1057:A:O4'	2.20	0.41
2:B:124:ALA:O	2:B:128:ILE:HG13	2.21	0.41
30:0:696:C:O2'	30:0:697:G:H5'	2.19	0.41
30:0:1154:A:H2'	30:0:1155:G:O4'	2.20	0.41
30:0:283:U:C5	30:0:284:C:N3	2.87	0.41
30:0:1421:C:H2'	30:0:1422:U:C6	2.55	0.41
30:0:594:C:C4	30:0:595:U:C4	3.09	0.41
4:D:129:ASP:OD1	30:0:2338:G:H2'	2.20	0.41
30:0:1904:A:C2	30:0:1905:U:H1'	2.54	0.41
30:0:2600:A:H2'	30:0:2601:A:O4'	2.20	0.41
23:W:74:GLU:OE1	30:0:1285:U:H4'	2.21	0.41
30:0:1471:A:H2'	30:0:1472:C:C6	2.55	0.41
30:0:445:U:H2'	30:0:446:G:C8	2.55	0.41
30:0:2310:G:C2	30:0:2311:A:C8	3.08	0.41
30:0:1149:U:H5''	30:0:1151:G:O4'	2.21	0.41
30:0:2699:A:H2'	30:0:2700:G:O4'	2.20	0.41
11:K:22:ASP:HB2	38:K:5264:HOH:O	2.20	0.41
17:Q:34:ASP:O	17:Q:37:GLU:HB2	2.20	0.41
30:0:1946:C:O4'	30:0:1969:A:C2	2.73	0.41
30:0:1139:U:H2'	30:0:1140:C:C6	2.55	0.41
30:0:1795:G:H2'	30:0:1796:A:O4'	2.20	0.41
30:0:177:A:O2'	30:0:892:G:H4'	2.20	0.41
8:H:46:TYR:HA	8:H:47:PRO:HD3	1.88	0.41
30:0:30:U:O2	30:0:460:A:C2	2.74	0.41
30:0:815:U:O2'	30:0:1598:A:H4'	2.20	0.41
29:3:38:ARG:HD2	30:0:396:U:OP2	2.20	0.41
30:0:1060:C:H6	30:0:1060:C:C5'	2.29	0.41
30:0:968:G:H2'	30:0:969:G:C8	2.54	0.41
30:0:625:U:H3'	38:0:3262:HOH:O	2.20	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
24:X:43:VAL:HG12	24:X:44:ASP:H	1.85	0.41
30:0:154:C:O2'	30:0:155:C:H5'	2.20	0.41
30:0:2250:G:N2	30:0:2251:G:H1'	2.36	0.41
3:C:184:ARG:HD2	30:0:1306:U:OP1	2.21	0.41
2:B:248:ARG:NH2	30:0:2549:C:H1'	2.35	0.41
31:9:110:G:C6	31:9:111:U:C5	3.08	0.41
30:0:113:A:OP2	30:0:114:A:H2'	2.20	0.41
5:E:19:ASP:HA	5:E:31:ARG:O	2.21	0.41
30:0:1933:G:O2'	30:0:1934:A:H5'	2.20	0.41
5:E:111:LYS:CE	30:0:2690:U:H4'	2.50	0.41
13:M:72:ALA:HB2	13:M:93:ARG:HG2	2.01	0.41
30:0:1163:G:C2	30:0:1184:C:N3	2.89	0.41
30:0:1184:C:O2'	30:0:1185:U:OP2	2.35	0.41
30:0:1189:A:C8	30:0:1190:G:C8	3.09	0.41
31:9:28:U:O2	31:9:57:A:N6	2.53	0.41
16:P:115:SER:OG	16:P:118:GLN:HG3	2.21	0.41
30:0:563:C:H2'	30:0:564:G:O4'	2.21	0.41
30:0:2003:U:O2'	30:0:2004:U:H5	2.02	0.41
30:0:168:C:O5'	30:0:168:C:H6	2.04	0.41
30:0:1947:G:H2'	30:0:1948:G:C8	2.52	0.41
19:S:57:THR:HG22	19:S:59:ASP:N	2.34	0.41
30:0:1006:A:N3	30:0:2298:C:O2'	2.50	0.41
30:0:2328:U:C4	30:0:2329:C:C5	3.08	0.41
30:0:2891:A:C2	30:0:2892:G:C4	3.09	0.41
30:0:2722:G:C2	30:0:2761:A:C2	3.09	0.41
8:H:91:ARG:HA	30:0:1002:G:O2'	2.20	0.41
30:0:2860:G:H2'	30:0:2861:G:O4'	2.20	0.41
30:0:929:A:O5'	30:0:929:A:H8	2.04	0.41
30:0:571:C:H6	30:0:571:C:O5'	2.03	0.41
13:M:164:THR:CG2	13:M:165:GLY:N	2.82	0.41
30:0:1733:A:H2'	30:0:1734:C:O4'	2.20	0.41
30:0:1615:A:H5'	38:0:4187:HOH:O	2.19	0.41
1:A:36:ASP:CB	1:A:85:SER:H	2.29	0.41
25:Y:234:VAL:HG12	25:Y:235:GLU:N	2.36	0.41
30:0:681:G:H2'	30:0:681:G:N3	2.36	0.41
21:U:56:ARG:NH1	30:0:2890:A:C2	2.89	0.41
12:L:30:ARG:NH1	38:L:8811:HOH:O	2.48	0.41
30:0:940:G:C5	30:0:1027:G:C2	3.09	0.41
25:Y:145:LYS:HD2	38:0:9965:HOH:O	2.20	0.41
30:0:301:C:O2'	30:0:302:A:H5'	2.21	0.41
19:S:6:LYS:HB2	19:S:27:ALA:O	2.20	0.41
30:0:1051:C:H2'	30:0:1052:G:O4'	2.21	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
30:0:1797:A:H2'	30:0:1799:G:O5'	2.21	0.41
31:9:78:G:O2'	31:9:79:U:OP2	2.38	0.41
9:I:87:PRO:HD2	30:0:1180:U:O2'	2.20	0.41
31:9:23:U:H2'	31:9:24:U:H4'	2.03	0.41
30:0:506:G:N1	30:0:509:A:OP2	2.54	0.41
30:0:2712:G:O2'	30:0:2713:G:H5'	2.21	0.41
30:0:2756:U:C2	30:0:2896:A:H2	2.39	0.41
30:0:1597:A:C4	30:0:1598:A:C8	3.09	0.41
30:0:250:C:H2'	30:0:251:C:C6	2.55	0.41
30:0:1730:G:N3	30:0:1730:G:H2'	2.36	0.41
30:0:1819:G:C2'	30:0:1820:G:C5'	2.97	0.41
2:B:307:ARG:HD2	38:B:9119:HOH:O	2.20	0.41
30:0:1517:C:O2	30:0:1670:A:C2	2.74	0.41
2:B:140:LEU:HA	38:B:9045:HOH:O	2.20	0.41
30:0:510:U:H5''	30:0:512:G:OP2	2.21	0.41
25:Y:151:SER:HB3	25:Y:154:ARG:HB3	2.03	0.41
30:0:24:G:H22	30:0:518:G:H1'	1.86	0.41
30:0:2866:U:H4'	30:0:2867:G:H5'	2.01	0.41
23:W:130:HIS:NE2	31:9:88:G:OP1	2.45	0.41
23:W:38:THR:HG22	23:W:39:ASP:N	2.35	0.41
16:P:55:LYS:HA	38:0:5633:HOH:O	2.21	0.41
30:0:519:A:H4'	30:0:1320:C:O3'	2.21	0.41
30:0:1255:A:N3	38:0:7772:HOH:O	2.37	0.41
30:0:271:C:H4'	30:0:272:A:OP1	2.21	0.41
2:B:234:ARG:HD3	30:0:1734:C:OP1	2.21	0.41
23:W:88:THR:HG23	23:W:110:GLN:CB	2.43	0.41
30:0:1840:A:H4'	30:0:1841:C:O5'	2.21	0.41
30:0:2756:U:N3	30:0:2896:A:H2	2.17	0.41
30:0:1597:A:C5	30:0:1598:A:C8	3.08	0.41
23:W:4:LEU:HD22	23:W:52:VAL:CG2	2.49	0.41
30:0:1873:G:C2'	30:0:1874:U:H5'	2.51	0.41
30:0:1942:A:C1'	38:0:9044:HOH:O	2.69	0.41
30:0:1890:U:H4'	30:0:2010:A:C6	2.56	0.41
4:D:173:GLU:HG3	4:D:174:VAL:N	2.36	0.41
30:0:2361:A:H2'	30:0:2362:A:C8	2.55	0.41
31:9:65:A:O2'	31:9:66:G:P	2.79	0.41
30:0:694:A:H2'	30:0:695:C:C5'	2.50	0.41
14:N:7:LYS:HB3	30:0:2353:A:O2'	2.20	0.41
30:0:652:G:H2'	30:0:653:U:O4'	2.20	0.41
25:Y:134:HIS:HE1	30:0:538:C:OP2	2.04	0.41
1:A:105:VAL:HG11	1:A:154:ALA:HB1	2.01	0.41
23:W:5:VAL:HG22	23:W:32:CYS:HB2	2.02	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
4:D:18:ILE:HG12	4:D:134:LEU:HD21	2.03	0.41
30:0:1706:G:C6	30:0:1707:G:N1	2.89	0.41
17:Q:30:VAL:O	17:Q:30:VAL:HG12	2.21	0.41
30:0:822:C:H2'	30:0:823:U:C6	2.54	0.41
30:0:2479:A:H5'	38:0:4665:HOH:O	2.21	0.41
2:B:254:GLN:HG3	38:0:9708:HOH:O	2.21	0.41
23:W:125:HIS:HD2	23:W:127:GLY:H	1.68	0.41
30:0:278:A:H2'	30:0:279:C:O4'	2.19	0.41
29:3:60:LYS:HG3	38:0:7573:HOH:O	2.19	0.41
4:D:49:PRO:HA	4:D:73:VAL:HG22	2.02	0.41
30:0:1718:G:C6	30:0:1719:G:C5	3.08	0.41
2:B:80:ARG:O	2:B:82:VAL:HG23	2.21	0.41
30:0:2689:A:H2'	30:0:2690:U:H5'	2.02	0.41
30:0:106:A:H2'	30:0:107:U:O4'	2.21	0.41
18:R:17:MET:HE3	18:R:19:ARG:NH2	2.36	0.41
30:0:1222:A:H2'	30:0:1223:G:O4'	2.21	0.41
16:P:28:GLN:HE22	30:0:1387:G:C1'	2.33	0.41
23:W:120:PRO:HG2	30:0:1095:U:O2	2.20	0.41
30:0:827:A:H2'	30:0:828:G:O4'	2.21	0.41
13:M:75:ARG:HH21	13:M:78:LYS:HE3	1.85	0.41
30:0:2864:U:C5	30:0:2865:G:C6	3.09	0.41
30:0:1305:C:H5'	38:0:9844:HOH:O	2.20	0.41
30:0:1364:G:H1'	38:0:4812:HOH:O	2.20	0.41
8:H:52:LEU:HD13	8:H:153:PHE:HB3	2.02	0.41
30:0:1175:G:H1'	30:0:1193:A:H2'	2.03	0.41
30:0:2780:C:H2'	30:0:2781:U:C6	2.56	0.41
30:0:364:U:H2'	30:0:365:G:O4'	2.21	0.41
30:0:1819:G:H2'	30:0:1820:G:H5'	1.98	0.41
29:3:48:ASN:ND2	30:0:169:A:H1'	2.36	0.41
30:0:424:C:C2	30:0:425:U:C5	3.09	0.41
3:C:73:GLN:HG2	30:0:475:G:OP1	2.20	0.41
30:0:2722:G:N3	30:0:2761:A:C2	2.89	0.41
30:0:580:A:O4'	30:0:1111:U:H4'	2.21	0.41
30:0:413:G:H2'	30:0:414:C:C6	2.55	0.41
30:0:146:U:O2'	30:0:147:G:H5'	2.21	0.41
30:0:426:G:H2'	30:0:427:C:O4'	2.19	0.41
30:0:2002:C:H2'	30:0:2003:U:H5'	2.03	0.40
4:D:135:VAL:HG22	4:D:136:ARG:N	2.36	0.40
10:J:41:ALA:HB3	38:J:8865:HOH:O	2.19	0.40
30:0:1217:G:C2	30:0:1218:U:C2	3.09	0.40
30:0:334:G:C5	30:0:335:U:C5	3.09	0.40
30:0:1250:C:O2'	30:0:1251:C:H5'	2.21	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
25:Y:144:ARG:CZ	38:Y:8181:HOH:O	2.69	0.40
30:0:772:G:H2'	30:0:773:A:O4'	2.21	0.40
19:S:38:ALA:O	19:S:42:GLU:HG3	2.21	0.40
2:B:24:PRO:HD3	38:B:8991:HOH:O	2.22	0.40
30:0:275:G:C2	30:0:376:C:N3	2.88	0.40
13:M:167:GLY:O	13:M:171:ARG:HG3	2.21	0.40
30:0:371:U:H2'	30:0:372:A:H8	1.86	0.40
3:C:236:THR:CG2	3:C:239:ALA:H	2.34	0.40
30:0:921:G:H4'	30:0:924:G:N1	2.36	0.40
30:0:921:G:H4'	30:0:924:G:C6	2.56	0.40
30:0:1587:U:C4	30:0:1588:G:C5	3.09	0.40
30:0:423:A:C4	30:0:424:C:C6	3.09	0.40
30:0:1295:G:H2'	30:0:1296:A:C8	2.56	0.40
30:0:293:A:C2	30:0:294:C:C6	3.09	0.40
30:0:1669:G:H2'	30:0:1670:A:C8	2.56	0.40
8:H:27:PRO:HD3	8:H:123:ILE:HG22	2.02	0.40
7:G:63:ARG:NH1	30:0:1151:G:OP1	2.54	0.40
3:C:138:VAL:O	3:C:234:VAL:HA	2.21	0.40
30:0:725:C:C2'	30:0:726:C:O5'	2.69	0.40
30:0:1928:C:C2'	30:0:1929:G:H5'	2.51	0.40
23:W:11:VAL:HG11	30:0:1086:A:C6	2.55	0.40
25:Y:152:LYS:HB3	25:Y:160:LYS:HG3	2.03	0.40
30:0:2385:G:H2'	30:0:2386:U:C6	2.56	0.40
30:0:2846:C:H3'	38:0:7101:HOH:O	2.20	0.40
21:U:31:PHE:CG	21:U:37:GLU:HG2	2.56	0.40
30:0:1182:C:H1'	30:0:1192:A:C8	2.41	0.40
30:0:1205:U:O2	30:0:1205:U:H2'	2.21	0.40
30:0:2831:C:H2'	30:0:2832:C:O4'	2.22	0.40
2:B:209:LYS:HB2	2:B:257:THR:O	2.21	0.40
23:W:139:GLY:O	23:W:141:HIS:HD2	2.04	0.40
30:0:1198:U:H1'	30:0:1201:C:H5	1.86	0.40
11:K:81:ARG:HD3	11:K:87:ARG:NH2	2.36	0.40
1:A:38:ILE:HA	1:A:38:ILE:HD13	1.90	0.40
3:C:226:GLY:HA3	30:0:1308:A:O4'	2.21	0.40
30:0:123:U:H2'	30:0:124:C:C6	2.55	0.40
30:0:1947:G:OP1	30:0:1971:G:N7	2.54	0.40
30:0:319:A:H2'	30:0:320:G:C8	2.56	0.40
23:W:5:VAL:HG11	23:W:153:MET:HE1	2.04	0.40
10:J:90:LYS:HB2	35:J:8802:CL:CL	2.58	0.40
24:X:30:MET:HE1	24:X:55:ASN:HA	2.03	0.40
30:0:303:C:N4	30:0:304:G:C6	2.89	0.40
13:M:42:ARG:HA	13:M:43:PRO:HD3	1.93	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
16:P:87:ARG:HG2	38:0:5961:HOH:O	2.22	0.40
30:0:2765:C:H2'	30:0:2766:A:C8	2.56	0.40
25:Y:148:GLY:HA3	30:0:622:G:P	2.61	0.40
17:Q:59:GLN:NE2	30:0:1018:A:H4'	2.36	0.40
30:0:549:A:C6	30:0:550:C:C4	3.10	0.40
30:0:1375:A:C2'	30:0:1376:G:H5'	2.51	0.40
30:0:1167:G:O2'	30:0:1168:C:H5'	2.22	0.40
30:0:272:A:N1	30:0:369:G:H5''	2.35	0.40
30:0:545:G:C8	30:0:545:G:C5'	2.95	0.40
31:9:24:U:H3'	31:9:24:U:H6	1.87	0.40
30:0:2505:G:HO2'	30:0:2506:A:H5'	1.80	0.40
20:T:21:LYS:HA	20:T:24:ARG:HG3	2.04	0.40
28:2:41:HIS:CD2	28:2:44:ARG:H	2.31	0.40
4:D:25:MET:HE1	4:D:37:ALA:O	2.22	0.40
25:Y:187:VAL:HG13	25:Y:205:ILE:HA	2.02	0.40
6:F:56:PRO:HB2	6:F:58:GLU:OE1	2.21	0.40
30:0:2887:G:H2'	30:0:2888:U:O4'	2.22	0.40
30:0:963:C:O2	30:0:1005:A:N1	2.54	0.40
24:X:79:GLU:CD	24:X:80:GLU:H	2.25	0.40
1:A:109:GLU:HG2	1:A:116:GLY:N	2.36	0.40
30:0:803:C:H2'	30:0:804:C:H6	1.87	0.40
30:0:2802:C:H2'	30:0:2803:C:H6	1.85	0.40
12:L:30:ARG:HD3	30:0:164:G:H4'	2.04	0.40
30:0:2118:A:C5	30:0:2470:A:C5	3.09	0.40
30:0:1386:G:O2'	30:0:1387:G:H5'	2.22	0.40
30:0:2437:A:H2'	30:0:2438:G:C8	2.57	0.40
23:W:108:ARG:HG3	23:W:114:PRO:HG3	2.03	0.40
30:0:27:U:H5	38:0:5902:HOH:O	2.04	0.40
30:0:1931:A:H2'	30:0:1932:G:H5'	2.04	0.40
30:0:1189:A:H1'	30:0:1209:C:H1'	2.02	0.40
30:0:1191:A:H2	30:0:1206:U:H3	1.69	0.40
30:0:1207:A:H5'	30:0:1208:C:OP2	2.21	0.40
30:0:2712:G:P	38:0:5233:HOH:O	2.79	0.40
30:0:1342:C:H2'	30:0:1343:C:C5'	2.47	0.40
30:0:365:G:C6	30:0:366:U:C4	3.09	0.40
20:T:49:GLU:OE2	20:T:97:ARG:HD2	2.22	0.40
30:0:1589:G:H4'	38:0:6875:HOH:O	2.20	0.40
30:0:2133:U:H4'	30:0:2134:G:H5'	2.02	0.40
18:R:132:ARG:CZ	38:R:8987:HOH:O	2.70	0.40
30:0:820:G:H5'	30:0:821:U:H5'	2.02	0.40
30:0:2346:C:O5'	30:0:2346:C:C6	2.74	0.40
12:L:113:GLN:C	30:0:700:A:H62	2.24	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
14:N:143:ARG:HG2	14:N:172:PHE:CD2	2.56	0.40
30:O:1102:C:H4'	38:O:9561:HOH:O	2.20	0.40
15:O:44:ASN:OD1	15:O:65:LEU:HB2	2.22	0.40
30:O:2304:G:C6	30:O:2305:A:C5	3.10	0.40
7:G:64:ASN:N	7:G:64:ASN:HD22	2.18	0.40
30:O:2237:G:O2'	30:O:2238:A:C8	2.72	0.40
16:P:104:LYS:HE2	16:P:138:GLU:OE2	2.20	0.40
30:O:2543:G:H2'	30:O:2544:G:O4'	2.21	0.40
25:Y:133:HIS:HD2	38:Y:8150:HOH:O	2.04	0.40
18:R:46:TYR:O	18:R:50:VAL:HG23	2.22	0.40
26:Z:50:VAL:O	26:Z:54:GLU:HG3	2.21	0.40
30:O:461:C:N3	30:O:479:G:H5'	2.36	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%)	211 (90%)	22 (9%)	2 (1%)	25	60
2	B	335/338 (99%)	309 (92%)	21 (6%)	5 (2%)	15	43
3	C	244/246 (99%)	228 (93%)	16 (7%)	0	100	100
4	D	134/177 (76%)	110 (82%)	22 (16%)	2 (2%)	15	43
5	E	170/178 (96%)	160 (94%)	9 (5%)	1 (1%)	33	70
6	F	117/120 (98%)	107 (92%)	8 (7%)	2 (2%)	14	38
7	G	25/348 (7%)	23 (92%)	2 (8%)	0	100	100
8	H	156/177 (88%)	141 (90%)	14 (9%)	1 (1%)	33	70
9	I	68/162 (42%)	53 (78%)	13 (19%)	2 (3%)	7	20
10	J	140/145 (97%)	131 (94%)	8 (6%)	1 (1%)	30	67
11	K	130/132 (98%)	122 (94%)	8 (6%)	0	100	100
12	L	141/165 (86%)	125 (89%)	13 (9%)	3 (2%)	11	30

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
13	M	192/196 (98%)	181 (94%)	10 (5%)	1 (0%)	38	74
14	N	184/187 (98%)	164 (89%)	16 (9%)	4 (2%)	10	29
15	O	113/116 (97%)	110 (97%)	3 (3%)	0	100	100
16	P	141/149 (95%)	137 (97%)	4 (3%)	0	100	100
17	Q	93/96 (97%)	89 (96%)	3 (3%)	1 (1%)	21	53
18	R	148/155 (96%)	141 (95%)	7 (5%)	0	100	100
19	S	79/85 (93%)	74 (94%)	5 (6%)	0	100	100
20	T	117/120 (98%)	108 (92%)	8 (7%)	1 (1%)	25	60
21	U	51/67 (76%)	48 (94%)	3 (6%)	0	100	100
22	V	63/71 (89%)	59 (94%)	3 (5%)	1 (2%)	14	40
23	W	152/154 (99%)	146 (96%)	6 (4%)	0	100	100
24	X	80/92 (87%)	73 (91%)	5 (6%)	2 (2%)	9	25
25	Y	140/241 (58%)	139 (99%)	1 (1%)	0	100	100
26	Z	71/116 (61%)	62 (87%)	9 (13%)	0	100	100
27	1	54/57 (95%)	52 (96%)	2 (4%)	0	100	100
28	2	42/50 (84%)	41 (98%)	1 (2%)	0	100	100
29	3	90/92 (98%)	88 (98%)	2 (2%)	0	100	100
All	All	3705/4472 (83%)	3432 (93%)	244 (7%)	29 (1%)	27	63

All (29) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	37	VAL
8	H	19	ARG
10	J	5	GLU
14	N	154	LEU
14	N	183	ASP
14	N	184	ILE
2	B	184	ASP
9	I	107	LYS
12	L	149	ARG
14	N	162	ASP
1	A	34	ASP
2	B	34	GLY
6	F	101	ALA
12	L	80	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	2	GLN
2	B	245	SER
4	D	56	ARG
12	L	21	ARG
20	T	53	GLY
24	X	87	ALA
4	D	137	PRO
6	F	100	ASP
24	X	70	ILE
22	V	39	ALA
2	B	185	GLY
17	Q	78	GLY
5	E	44	GLY
9	I	83	GLY
13	M	88	VAL

5.3.2 Protein sidechains ⓘ

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	179/182 (98%)	166 (93%)	13 (7%)	20	46
2	B	282/283 (100%)	264 (94%)	18 (6%)	25	55
3	C	193/193 (100%)	179 (93%)	14 (7%)	20	46
4	D	117/148 (79%)	113 (97%)	4 (3%)	49	83
5	E	152/156 (97%)	150 (99%)	2 (1%)	80	96
6	F	93/94 (99%)	92 (99%)	1 (1%)	84	97
7	G	27/282 (10%)	25 (93%)	2 (7%)	20	45
8	H	134/145 (92%)	129 (96%)	5 (4%)	45	80
9	I	58/130 (45%)	58 (100%)	0	100	100
10	J	118/121 (98%)	112 (95%)	6 (5%)	33	67
11	K	106/106 (100%)	105 (99%)	1 (1%)	87	97
12	L	113/127 (89%)	107 (95%)	6 (5%)	32	65
13	M	158/160 (99%)	152 (96%)	6 (4%)	44	79

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
14	N	149/150 (99%)	142 (95%)	7 (5%)	36	71
15	O	93/94 (99%)	93 (100%)	0	100	100
16	P	113/117 (97%)	110 (97%)	3 (3%)	57	88
17	Q	79/80 (99%)	75 (95%)	4 (5%)	33	67
18	R	117/122 (96%)	111 (95%)	6 (5%)	33	67
19	S	71/74 (96%)	70 (99%)	1 (1%)	78	96
20	T	105/106 (99%)	98 (93%)	7 (7%)	23	52
21	U	44/53 (83%)	44 (100%)	0	100	100
22	V	51/57 (90%)	50 (98%)	1 (2%)	68	93
23	W	130/130 (100%)	126 (97%)	4 (3%)	52	85
24	X	66/74 (89%)	62 (94%)	4 (6%)	26	58
25	Y	120/196 (61%)	116 (97%)	4 (3%)	50	83
26	Z	60/94 (64%)	59 (98%)	1 (2%)	73	94
27	1	46/47 (98%)	45 (98%)	1 (2%)	64	92
28	2	42/46 (91%)	41 (98%)	1 (2%)	61	90
29	3	79/79 (100%)	76 (96%)	3 (4%)	44	79
All	All	3095/3646 (85%)	2970 (96%)	125 (4%)	42	77

All (125) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	ARG
1	A	26	ASP
1	A	36	ASP
1	A	38	ILE
1	A	68	ILE
1	A	69	LEU
1	A	94	LEU
1	A	131	HIS
1	A	165	THR
1	A	179	MET
1	A	192	VAL
1	A	206	ARG
1	A	217	ARG
2	B	7	ARG
2	B	11	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	16	ARG
2	B	27	ASN
2	B	51	VAL
2	B	53	LEU
2	B	71	VAL
2	B	88	GLU
2	B	97	LEU
2	B	98	THR
2	B	132	HIS
2	B	149	ASP
2	B	162	MET
2	B	175	LEU
2	B	234	ARG
2	B	254	GLN
2	B	257	THR
2	B	265	LEU
3	C	78	ARG
3	C	91	PRO
3	C	94	THR
3	C	101	ASP
3	C	115	LEU
3	C	132	ASP
3	C	136	VAL
3	C	162	VAL
3	C	187	ARG
3	C	214	THR
3	C	222	ASP
3	C	223	LEU
3	C	234	VAL
3	C	243	VAL
4	D	24	HIS
4	D	29	HIS
4	D	50	VAL
4	D	161	ASP
5	E	102	VAL
5	E	156	ASP
6	F	12	LEU
7	G	72	ASP
7	G	73	ASP
8	H	21	GLU
8	H	62	HIS
8	H	87	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
8	H	91	ARG
8	H	157	TYR
10	J	46	ILE
10	J	52	GLN
10	J	74	ARG
10	J	79	PHE
10	J	93	ARG
10	J	107	ASN
11	K	10	GLN
12	L	35	ARG
12	L	37	LYS
12	L	102	ASP
12	L	104	ASP
12	L	114	VAL
12	L	140	VAL
13	M	46	LEU
13	M	68	ARG
13	M	93	ARG
13	M	99	ARG
13	M	116	ASN
13	M	164	THR
14	N	23	ARG
14	N	26	LEU
14	N	49	THR
14	N	101	VAL
14	N	127	LEU
14	N	139	TRP
14	N	173	ASP
16	P	16	VAL
16	P	91	LYS
16	P	98	ILE
17	Q	11	ARG
17	Q	16	ASN
17	Q	18	PRO
17	Q	57	ASP
18	R	39	THR
18	R	82	GLU
18	R	119	VAL
18	R	132	ARG
18	R	143	VAL
18	R	150	PRO
19	S	44	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
20	T	39	ASN
20	T	48	VAL
20	T	71	VAL
20	T	73	HIS
20	T	89	ARG
20	T	115	GLU
20	T	117	ASP
22	V	12	THR
23	W	26	ILE
23	W	52	VAL
23	W	108	ARG
23	W	146	ILE
24	X	27	ASP
24	X	52	PRO
24	X	72	VAL
24	X	82	GLU
25	Y	95	THR
25	Y	189	ASN
25	Y	191	ASP
25	Y	203	VAL
26	Z	68	GLU
27	1	14	THR
28	2	18	ASN
29	3	14	CYS
29	3	56	PRO
29	3	87	ARG

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	47	HIS
1	A	199	HIS
2	B	2	GLN
2	B	27	ASN
2	B	106	HIS
2	B	145	HIS
2	B	221	GLN
2	B	238	ASN
2	B	256	GLN
2	B	260	HIS
2	B	320	GLN
2	B	332	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	C	73	GLN
3	C	129	HIS
3	C	151	GLN
3	C	163	HIS
4	D	85	GLN
4	D	103	ASN
5	E	143	GLN
7	G	64	ASN
8	H	34	HIS
8	H	59	GLN
8	H	62	HIS
10	J	52	GLN
10	J	107	ASN
10	J	126	ASN
10	J	142	ASN
11	K	10	GLN
11	K	44	HIS
11	K	67	GLN
12	L	18	HIS
12	L	41	HIS
13	M	24	GLN
13	M	58	GLN
13	M	137	ASN
13	M	143	ASN
13	M	170	ASN
14	N	40	ASN
14	N	53	ASN
14	N	107	ASN
14	N	132	ASN
16	P	50	GLN
16	P	66	GLN
16	P	73	HIS
16	P	88	GLN
16	P	118	GLN
17	Q	40	HIS
18	R	22	GLN
18	R	61	GLN
18	R	94	ASN
18	R	98	ASN
18	R	113	HIS
18	R	117	HIS
18	R	122	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
18	R	123	GLN
19	S	44	GLN
19	S	53	ASN
20	T	39	ASN
21	U	39	ASN
22	V	60	GLN
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	189	ASN
27	1	8	GLN
27	1	16	HIS
27	1	28	HIS
28	2	18	ASN
28	2	41	HIS
28	2	45	ASN
29	3	15	ASN
29	3	20	HIS
29	3	48	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
30	0	2745/2923 (93%)	232 (8%)	18 (0%)
31	9	121/122 (99%)	16 (13%)	1 (0%)
All	All	2866/3045 (94%)	248 (8%)	19 (0%)

All (248) 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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
30	0	88	G
30	0	114	A
30	0	115	U
30	0	130	C
30	0	141	C
30	0	151	A
30	0	166	A
30	0	169	A
30	0	186	A
30	0	191	A
30	0	192	A
30	0	198	A
30	0	200	C
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	336	G
30	0	337	A
30	0	358	G
30	0	368	C
30	0	381	G
30	0	397	A
30	0	417	G
30	0	461	C
30	0	487	G
30	0	498	A
30	0	510	U
30	0	511	A
30	0	514	G
30	0	537	G
30	0	538	C
30	0	539	G
30	0	542	A
30	0	545	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
30	0	553	G
30	0	559	U
30	0	588	G
30	0	604	G
30	0	620	A
30	0	632	A
30	0	644	G
30	0	660	A
30	0	688	A
30	0	701	U
30	0	746	A
30	0	759	C
30	0	777	U
30	0	809	G
30	0	821	U
30	0	835	U
30	0	840	U
30	0	857	A
30	0	858	U
30	0	868	G
30	0	869	G
30	0	871	G
30	0	872	U
30	0	875	A
30	0	877	G
30	0	878	G
30	0	884	C
30	0	885	G
30	0	905	C
30	0	920	C
30	0	921	G
30	0	923	A
30	0	953	G
30	0	960	G
30	0	961	A
30	0	1006	A
30	0	1008	C
30	0	1029	U
30	0	1045	G
30	0	1059	G
30	0	1060	C
30	0	1072	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
30	0	1081	A
30	0	1088	A
30	0	1109	U
30	0	1110	G
30	0	1119	G
30	0	1124	A
30	0	1130	U
30	0	1151	G
30	0	1165	G
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	1342	C
30	0	1353	C
30	0	1360	C
30	0	1377	C
30	0	1378	G
30	0	1407	A
30	0	1409	G
30	0	1474	C
30	0	1505	U
30	0	1506	U
30	0	1524	U
30	0	1525	G
30	0	1526	A
30	0	1535	G
30	0	1562	C
30	0	1592	G
30	0	1605	G
30	0	1625	U
30	0	1626	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
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	1710	A
30	0	1722	U
30	0	1723	G
30	0	1725	C
30	0	1731	C
30	0	1732	A
30	0	1742	A
30	0	1752	G
30	0	1778	A
30	0	1798	C
30	0	1820	G
30	0	1829	A
30	0	1856	C
30	0	1879	U
30	0	1919	A
30	0	1942	A
30	0	1968	A
30	0	1971	G
30	0	1973	A
30	0	1979	G
30	0	1980	U
30	0	1996	U
30	0	2006	C
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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
30	0	2101	A
30	0	2102	G
30	0	2110	G
30	0	2238	A
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	2354	A
30	0	2361	A
30	0	2369	A
30	0	2379	G
30	0	2422	U
30	0	2462	G
30	0	2465	A
30	0	2467	A
30	0	2476	C
30	0	2483	A
30	0	2507	G
30	0	2509	A
30	0	2511	A
30	0	2533	C
30	0	2537	G
30	0	2541	U
30	0	2553	A
30	0	2564	G
30	0	2589	U
30	0	2601	A
30	0	2602	G
30	0	2608	C
30	0	2613	G
30	0	2637	A
30	0	2638	G
30	0	2649	A
30	0	2664	A
30	0	2681	A
30	0	2682	C
30	0	2726	U
30	0	2747	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
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	2867	G
30	0	2876	G
30	0	2890	A
30	0	2896	A
30	0	2903	C
30	0	2914	A
31	9	2	U
31	9	7	G
31	9	14	G
31	9	22	G
31	9	23	U
31	9	24	U
31	9	25	G
31	9	40	C
31	9	41	C
31	9	43	G
31	9	52	A
31	9	57	A
31	9	66	G
31	9	77	A
31	9	114	G
31	9	122	C

All (19) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
30	0	129	A
30	0	603	A
30	0	699	C
30	0	834	G
30	0	857	A
30	0	871	G
30	0	877	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
30	0	1237	U
30	0	1352	A
30	0	1377	C
30	0	1506	U
30	0	1685	A
30	0	1979	G
30	0	2467	A
30	0	2649	A
30	0	2718	C
30	0	2726	U
30	0	2761	A
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	0.69	1 (5%)	24,31,34	0.76	0
30	OMG	0	2588	30	24,26,27	0.80	0	32,38,41	4.96	3 (9%)
30	UR3	0	2619	30	20,22,23	0.78	1 (5%)	23,32,35	0.84	0
30	PSU	0	2621	30	19,21,22	1.21	3 (15%)	23,30,33	1.04	1 (4%)
30	1MA	0	628	30	23,25,26	0.83	0	32,37,40	0.90	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

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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	3.13	1.43	1.37
30	0	2621	PSU	C6-N1	2.44	1.34	1.32
30	0	2619	UR3	P-OP1	2.05	1.49	1.46
30	0	2621	PSU	P-OP1	2.03	1.49	1.46
30	0	2587	OMU	P-OP1	2.01	1.49	1.46

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	0	2588	OMG	C6-C5-N7	-27.49	130.44	134.14
30	0	2588	OMG	C6-N1-C2	3.22	125.14	119.51
30	0	628	1MA	C2-N3-C4	-3.15	110.84	116.23
30	0	2588	OMG	C2-N3-C4	-2.30	111.85	115.09
30	0	2621	PSU	C5-C4-N3	-2.15	114.94	118.86

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%)	0.88	31 (13%) 4 4	22, 47, 83, 108	0
2	B	337/338 (99%)	0.56	18 (5%) 25 27	25, 51, 79, 90	0
3	C	246/246 (100%)	-0.05	5 (2%) 62 65	19, 42, 65, 81	0
4	D	140/177 (79%)	2.11	61 (43%) 1 0	58, 101, 124, 135	0
5	E	172/178 (96%)	0.71	14 (8%) 12 12	42, 66, 89, 94	0
6	F	119/120 (99%)	0.99	20 (16%) 2 2	44, 69, 96, 114	0
7	G	29/348 (8%)	1.65	10 (34%) 1 1	71, 91, 100, 102	0
8	H	160/177 (90%)	1.44	43 (26%) 1 1	55, 73, 100, 106	0
9	I	70/162 (43%)	3.59	50 (71%) 0 0	127, 145, 163, 164	0
10	J	142/145 (97%)	0.42	5 (3%) 42 44	34, 51, 71, 94	0
11	K	132/132 (100%)	0.71	9 (6%) 17 17	29, 47, 68, 77	0
12	L	145/165 (87%)	0.50	12 (8%) 11 11	26, 62, 111, 125	0
13	M	194/196 (98%)	0.26	3 (1%) 70 73	24, 38, 55, 62	0
14	N	186/187 (99%)	0.65	17 (9%) 9 9	40, 65, 111, 120	0
15	O	115/116 (99%)	-0.20	0 100 100	34, 49, 67, 76	0
16	P	143/149 (95%)	0.84	14 (9%) 8 7	34, 51, 67, 75	0
17	Q	95/96 (98%)	0.14	0 100 100	34, 45, 61, 74	0
18	R	150/155 (96%)	0.35	2 (1%) 74 77	28, 44, 64, 74	0
19	S	81/85 (95%)	0.50	4 (4%) 28 30	35, 53, 73, 86	0
20	T	119/120 (99%)	0.23	5 (4%) 35 37	34, 52, 80, 109	0
21	U	53/67 (79%)	1.02	7 (13%) 4 4	39, 54, 73, 82	0
22	V	65/71 (91%)	1.11	9 (13%) 4 3	42, 66, 113, 122	0
23	W	154/154 (100%)	0.11	3 (1%) 64 67	36, 49, 67, 83	0
24	X	82/92 (89%)	0.93	7 (8%) 11 10	37, 57, 82, 98	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%)	-0.10	2 (1%) 72 75	23, 44, 65, 87	0
26	Z	73/116 (62%)	1.40	19 (26%) 1 1	47, 66, 82, 97	0
27	1	56/57 (98%)	0.36	0 100 100	21, 28, 35, 45	0
28	2	46/50 (92%)	0.72	5 (10%) 6 6	28, 58, 88, 95	0
29	3	92/92 (100%)	0.28	0 100 100	35, 54, 67, 83	0
30	0	2754/2923 (94%)	0.34	66 (2%) 56 59	19, 43, 89, 167	0
31	9	122/122 (100%)	-0.12	3 (2%) 54 58	37, 67, 86, 146	0
All	All	6651/7517 (88%)	0.51	444 (6%) 17 17	19, 49, 99, 167	0

All (444) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
22	V	1	THR	16.4
4	D	63	ILE	11.8
9	I	100	VAL	11.2
9	I	74	ILE	10.3
9	I	104	ALA	9.8
4	D	66	GLY	9.7
4	D	93	LEU	9.3
9	I	113	SER	8.7
9	I	128	THR	8.5
1	A	237	GLY	7.4
9	I	70	THR	7.1
9	I	111	LEU	7.0
22	V	40	PRO	7.0
9	I	80	PHE	6.7
22	V	43	PRO	6.6
2	B	1	PRO	6.2
14	N	166	ALA	6.2
22	V	39	ALA	6.2
9	I	110	ASP	6.1
4	D	57	THR	6.0
4	D	81	GLU	6.0
9	I	115	ASP	6.0
9	I	117	THR	5.9
9	I	91	PHE	5.9
4	D	27	ILE	5.8
4	D	88	LEU	5.7
4	D	64	ARG	5.7
26	Z	43	GLY	5.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
31	9	1	U	5.7
22	V	38	GLY	5.6
30	0	1172	G	5.5
9	I	78	ALA	5.5
4	D	134	LEU	5.4
20	T	119	ALA	5.4
9	I	95	LEU	5.3
7	G	27	ILE	5.3
19	S	81	ILE	5.2
9	I	103	ILE	5.1
1	A	43	VAL	5.0
5	E	87	PHE	5.0
9	I	116	LEU	4.9
9	I	108	HIS	4.9
26	Z	48	ARG	4.9
9	I	97	VAL	4.9
4	D	69	ILE	4.8
21	U	46	ALA	4.8
30	0	999	C	4.7
4	D	26	GLY	4.5
26	Z	46	SER	4.5
1	A	89	ALA	4.5
4	D	170	TYR	4.4
26	Z	67	GLY	4.4
9	I	132	VAL	4.4
12	L	100	ALA	4.4
4	D	95	THR	4.4
21	U	24	LYS	4.4
14	N	185	GLU	4.4
5	E	100	ASP	4.4
14	N	162	ASP	4.4
24	X	85	VAL	4.3
8	H	81	GLY	4.3
12	L	97	VAL	4.3
8	H	76	LEU	4.2
4	D	85	GLN	4.2
9	I	112	LEU	4.2
6	F	115	VAL	4.2
8	H	97	VAL	4.2
4	D	61	PHE	4.2
4	D	18	ILE	4.2
30	0	1951	G	4.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
30	0	2587	OMU	4.2
30	0	1177	A	4.1
9	I	68	PRO	4.1
4	D	172	VAL	4.1
4	D	165	PHE	4.1
4	D	19	GLU	4.1
22	V	41	GLU	4.1
4	D	75	LEU	4.1
8	H	53	ILE	4.1
30	0	2637	A	4.1
8	H	89	THR	4.1
9	I	118	ASN	4.1
7	G	26	MET	4.1
8	H	133	GLY	4.1
28	2	39	ARG	4.1
30	0	1182	C	4.1
4	D	171	ASP	4.1
9	I	66	GLY	4.0
4	D	128	LEU	4.0
4	D	44	ILE	4.0
8	H	157	TYR	4.0
8	H	48	VAL	4.0
30	0	1171	A	4.0
4	D	62	ASP	3.9
7	G	73	ASP	3.9
4	D	90	LEU	3.9
24	X	14	LEU	3.9
30	0	1196	C	3.9
5	E	159	VAL	3.9
7	G	70	ALA	3.9
6	F	20	LEU	3.9
9	I	93	ALA	3.9
9	I	120	ALA	3.9
26	Z	49	ARG	3.9
16	P	143	ALA	3.9
30	0	1170	U	3.8
9	I	133	THR	3.8
8	H	169	GLU	3.8
8	H	123	ILE	3.8
30	0	1950	G	3.8
9	I	99	GLN	3.8
4	D	166	ILE	3.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
16	P	114	LEU	3.8
22	V	37	GLY	3.8
8	H	77	ILE	3.8
4	D	102	GLY	3.8
2	B	91	PRO	3.7
2	B	119	HIS	3.7
8	H	30	LYS	3.7
4	D	101	THR	3.7
8	H	132	ALA	3.7
11	K	110	LYS	3.7
30	0	2508	C	3.7
1	A	158	VAL	3.7
8	H	161	THR	3.7
9	I	79	GLY	3.7
8	H	152	ALA	3.7
19	S	2	TRP	3.7
8	H	150	LYS	3.6
9	I	114	TYR	3.6
8	H	61	ARG	3.6
9	I	134	ILE	3.6
8	H	16	ALA	3.6
30	0	1195	G	3.6
8	H	54	VAL	3.6
24	X	10	VAL	3.5
9	I	96	SER	3.5
4	D	87	ALA	3.5
14	N	182	GLY	3.5
9	I	87	PRO	3.5
6	F	44	SER	3.4
4	D	129	ASP	3.4
23	W	96	LEU	3.4
1	A	82	VAL	3.4
9	I	75	LYS	3.4
14	N	95	ALA	3.4
6	F	17	LEU	3.4
30	0	1197	G	3.4
30	0	970	U	3.4
4	D	135	VAL	3.4
16	P	112	GLY	3.4
4	D	89	PRO	3.4
4	D	158	ASN	3.4
21	U	51	TRP	3.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
30	0	628	1MA	3.4
26	Z	42	TYR	3.4
2	B	118	ASP	3.4
4	D	104	PHE	3.4
14	N	163	PHE	3.4
24	X	88	GLU	3.4
1	A	91	GLY	3.4
9	I	106	GLN	3.3
12	L	76	LEU	3.3
20	T	116	ASP	3.3
30	0	1181	A	3.3
6	F	105	ASP	3.3
8	H	62	HIS	3.3
10	J	6	PHE	3.3
3	C	62	GLY	3.3
8	H	156	ALA	3.3
16	P	116	SER	3.3
21	U	52	THR	3.2
5	E	45	ASP	3.2
2	B	278	PRO	3.2
12	L	93	VAL	3.2
25	Y	108	ASP	3.2
9	I	88	GLN	3.2
5	E	155	ASN	3.2
4	D	43	GLU	3.1
4	D	23	VAL	3.1
30	0	1203	G	3.1
30	0	1169	U	3.1
30	0	2510	C	3.1
4	D	80	ALA	3.1
6	F	100	ASP	3.1
4	D	10	PHE	3.1
16	P	137	LEU	3.1
5	E	154	ILE	3.1
8	H	85	ASP	3.1
5	E	129	GLU	3.1
1	A	36	ASP	3.1
5	E	168	ILE	3.1
9	I	76	ASP	3.0
7	G	68	GLU	3.0
4	D	74	THR	3.0
12	L	95	ASP	3.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	99	ILE	3.0
26	Z	44	ARG	3.0
11	K	85	GLY	3.0
4	D	173	GLU	3.0
1	A	69	LEU	3.0
9	I	92	VAL	3.0
14	N	147	ILE	3.0
1	A	37	VAL	3.0
30	0	497	A	3.0
9	I	67	VAL	2.9
8	H	174	LEU	2.9
19	S	1	SER	2.9
4	D	103	ASN	2.9
26	Z	58	ASN	2.9
1	A	80	LEU	2.9
8	H	79	GLU	2.9
30	0	282	C	2.9
6	F	99	THR	2.9
11	K	130	MET	2.9
28	2	27	LEU	2.9
26	Z	61	HIS	2.9
30	0	1179	C	2.9
30	0	2100	A	2.9
14	N	159	TYR	2.8
2	B	62	ARG	2.8
9	I	109	PRO	2.8
26	Z	50	VAL	2.8
1	A	145	MET	2.8
6	F	112	ALA	2.8
10	J	41	ALA	2.8
30	0	1000	C	2.8
1	A	124	VAL	2.8
30	0	969	G	2.8
8	H	40	GLN	2.8
9	I	71	ALA	2.8
14	N	164	ASP	2.8
28	2	49	GLU	2.8
1	A	211	LYS	2.8
4	D	94	ALA	2.8
30	0	2507	G	2.8
30	0	1184	C	2.8
4	D	28	GLY	2.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
21	U	43	GLY	2.8
19	S	20	PHE	2.8
14	N	143	ARG	2.8
24	X	80	GLU	2.8
14	N	75	THR	2.8
26	Z	34	SER	2.8
8	H	146	ALA	2.8
30	0	1192	A	2.8
30	0	2506	A	2.8
30	0	2538	A	2.8
1	A	138	VAL	2.7
30	0	1163	G	2.7
30	0	1965	C	2.7
8	H	141	CYS	2.7
30	0	1180	U	2.7
5	E	112	ALA	2.7
2	B	175	LEU	2.7
30	0	1198	U	2.7
1	A	135	VAL	2.7
1	A	40	GLY	2.7
30	0	1173	A	2.7
22	V	24	LYS	2.7
8	H	164	CYS	2.6
1	A	79	GLU	2.6
8	H	29	SER	2.6
9	I	102	GLN	2.6
16	P	113	THR	2.6
9	I	73	LEU	2.6
30	0	1199	A	2.6
21	U	31	PHE	2.6
2	B	138	GLY	2.6
30	0	2237	G	2.6
4	D	60	GLU	2.6
12	L	77	ALA	2.6
8	H	39	LYS	2.6
6	F	49	PHE	2.6
1	A	83	GLY	2.6
4	D	24	HIS	2.6
12	L	74	THR	2.6
1	A	42	VAL	2.6
8	H	125	GLY	2.6
9	I	82	THR	2.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
10	J	94	GLY	2.6
6	F	16	ALA	2.6
30	O	1200	A	2.6
7	G	25	GLU	2.6
9	I	125	GLY	2.5
30	O	1183	C	2.5
1	A	133	ARG	2.5
6	F	91	VAL	2.5
8	H	91	ARG	2.5
8	H	170	ARG	2.5
16	P	98	ILE	2.5
26	Z	106	SER	2.5
8	H	144	GLU	2.5
12	L	44	GLU	2.5
11	K	95	ALA	2.5
24	X	72	VAL	2.5
3	C	65	ARG	2.5
20	T	115	GLU	2.5
1	A	75	GLY	2.5
8	H	127	ALA	2.5
11	K	128	ALA	2.5
30	O	280	C	2.5
2	B	151	VAL	2.5
2	B	161	VAL	2.5
2	B	53	LEU	2.5
30	O	2104	C	2.5
1	A	58	VAL	2.5
4	D	50	VAL	2.5
2	B	106	HIS	2.4
6	F	19	ALA	2.4
26	Z	45	VAL	2.4
3	C	61	PHE	2.4
4	D	106	PHE	2.4
11	K	127	ALA	2.4
14	N	136	LEU	2.4
2	B	18	ARG	2.4
30	O	2289	G	2.4
4	D	39	ASP	2.4
5	E	127	ASP	2.4
6	F	117	GLU	2.4
14	N	175	LEU	2.4
13	M	194	GLY	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
16	P	82	GLY	2.4
4	D	37	ALA	2.4
7	G	23	ILE	2.4
9	I	101	LYS	2.4
30	0	2825	C	2.4
10	J	122	ASP	2.4
30	0	1202	A	2.4
1	A	74	VAL	2.4
22	V	20	LEU	2.4
6	F	119	ARG	2.4
8	H	153	PHE	2.4
9	I	90	ASP	2.4
26	Z	64	PRO	2.3
1	A	151	GLN	2.3
16	P	105	LEU	2.3
30	0	1551	C	2.3
1	A	64	ASP	2.3
8	H	71	SER	2.3
9	I	121	LYS	2.3
4	D	22	VAL	2.3
8	H	6	ALA	2.3
4	D	154	LYS	2.3
30	0	2509	A	2.3
9	I	83	GLY	2.3
1	A	88	ILE	2.3
13	M	1	ALA	2.3
30	0	1178	G	2.3
4	D	92	GLU	2.3
2	B	115	VAL	2.3
6	F	72	VAL	2.3
6	F	62	HIS	2.3
30	0	1701	A	2.3
4	D	133	ASN	2.3
3	C	64	GLY	2.3
23	W	55	GLY	2.3
1	A	55	VAL	2.3
3	C	215	ALA	2.3
23	W	45	VAL	2.3
31	9	2	U	2.3
30	0	1161	A	2.3
2	B	31	SER	2.3
30	0	1819	G	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
4	D	83	PHE	2.3
8	H	9	TYR	2.3
14	N	70	GLY	2.3
12	L	60	GLU	2.2
30	O	1693	A	2.2
12	L	96	VAL	2.2
8	H	37	GLY	2.2
26	Z	85	ASP	2.2
4	D	141	VAL	2.2
11	K	117	VAL	2.2
26	Z	68	GLU	2.2
12	L	145	LEU	2.2
4	D	45	THR	2.2
7	G	21	ASP	2.2
4	D	164	ALA	2.2
26	Z	53	ILE	2.2
2	B	105	PHE	2.2
16	P	68	LYS	2.2
16	P	141	ILE	2.2
30	O	1176	C	2.2
30	O	1175	G	2.2
7	G	22	ALA	2.2
16	P	120	ARG	2.2
24	X	8	ARG	2.2
30	O	2537	G	2.2
8	H	86	TYR	2.2
26	Z	62	ALA	2.2
30	O	10	U	2.2
5	E	107	PHE	2.2
7	G	66	LEU	2.2
1	A	59	GLU	2.2
16	P	55	LYS	2.2
21	U	8	TYR	2.2
8	H	31	ILE	2.2
6	F	116	GLU	2.2
5	E	46	THR	2.1
11	K	58	THR	2.1
13	M	30	GLU	2.1
31	9	24	U	2.1
1	A	29	HIS	2.1
18	R	106	GLY	2.1
6	F	25	ASP	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
12	L	75	LEU	2.1
4	D	136	ARG	2.1
30	0	2725	G	2.1
4	D	168	SER	2.1
30	0	2504	A	2.1
6	F	39	SER	2.1
26	Z	69	ASP	2.1
14	N	178	THR	2.1
10	J	97	ALA	2.1
9	I	69	PRO	2.1
30	0	1626	A	2.1
16	P	108	LEU	2.1
18	R	1	GLY	2.1
6	F	23	ALA	2.1
5	E	22	VAL	2.1
30	0	1537	C	2.1
5	E	91	PHE	2.1
11	K	113	ILE	2.1
4	D	132	VAL	2.0
9	I	98	ASP	2.0
28	2	20	ARG	2.0
30	0	1409	G	2.0
30	0	1730	G	2.0
1	A	90	PRO	2.0
14	N	152	GLU	2.0
20	T	59	GLU	2.0
30	0	735	C	2.0
30	0	2035	C	2.0
14	N	119	GLN	2.0
4	D	56	ARG	2.0
2	B	123	ALA	2.0
2	B	124	ALA	2.0
20	T	60	GLY	2.0
30	0	1525	G	2.0
25	Y	235	GLU	2.0
30	0	2569	A	2.0
8	H	78	LYS	2.0
28	2	21	VAL	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(Å ²)	Q<0.9
30	1MA	0	628	23/24	0.22	1.20	25,27,30,31	0
30	UR3	0	2619	21/22	0.19	0.94	33,35,38,43	0
30	OMU	0	2587	21/22	0.20	0.49	31,33,34,36	0
30	OMG	0	2588	24/25	0.17	-1.35	30,31,35,36	0
30	PSU	0	2621	20/21	0.16	-1.38	30,32,37,37	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(Å ²)	Q<0.9
32	MG	0	8089	1/1	0.51	335.00	53,53,53,53	0
36	SR	0	9006	1/1	0.91	88.18	200,200,200,200	0
34	NA	0	8566	1/1	1.29	75.52	40,40,40,40	0
32	MG	0	8085	1/1	0.80	75.51	82,82,82,82	0
34	NA	0	8502	1/1	1.28	58.09	78,78,78,78	0
36	SR	0	9001	1/1	0.42	51.84	169,169,169,169	0
34	NA	0	8525	1/1	0.63	45.87	91,91,91,91	0
34	NA	0	8514	1/1	0.48	41.96	52,52,52,52	0
36	SR	0	9004	1/1	1.14	39.87	200,200,200,200	0
34	NA	0	8528	1/1	0.83	36.02	51,51,51,51	0
36	SR	0	8982	1/1	0.54	35.45	186,186,186,186	0
34	NA	0	8553	1/1	0.62	29.46	70,70,70,70	0
35	CL	0	8822	1/1	0.34	28.41	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
34	NA	0	8511	1/1	0.59	27.38	54,54,54,54	0
36	SR	0	8997	1/1	0.86	27.27	189,189,189,189	0
34	NA	0	8512	1/1	0.39	27.18	51,51,51,51	0
32	MG	0	8092	1/1	0.32	27.03	40,40,40,40	0
36	SR	0	9000	1/1	0.48	26.39	171,171,171,171	0
34	NA	0	8564	1/1	0.71	25.93	67,67,67,67	0
34	NA	0	8549	1/1	0.66	25.46	42,42,42,42	0
34	NA	0	8559	1/1	0.64	22.84	74,74,74,74	0
32	MG	0	8030	1/1	0.45	22.19	53,53,53,53	0
34	NA	0	8517	1/1	0.61	20.45	38,38,38,38	0
36	SR	0	8994	1/1	0.57	19.88	188,188,188,188	0
34	NA	0	8563	1/1	0.57	19.59	70,70,70,70	0
32	MG	A	8051	1/1	0.60	19.28	64,64,64,64	0
36	SR	0	9007	1/1	0.71	18.96	181,181,181,181	0
34	NA	0	8505	1/1	0.62	18.65	36,36,36,36	0
34	NA	0	8513	1/1	0.49	18.27	44,44,44,44	0
34	NA	0	8548	1/1	0.25	17.42	66,66,66,66	0
32	MG	0	8037	1/1	0.35	17.40	77,77,77,77	0
36	SR	0	8996	1/1	0.38	16.68	200,200,200,200	0
34	NA	0	8509	1/1	0.33	16.52	64,64,64,64	0
36	SR	0	8976	1/1	0.48	16.31	173,173,173,173	0
32	MG	0	8063	1/1	0.70	15.61	98,98,98,98	0
34	NA	0	8575	1/1	0.63	15.35	72,72,72,72	0
32	MG	0	8038	1/1	0.36	15.22	74,74,74,74	0
32	MG	0	8079	1/1	0.32	13.56	67,67,67,67	0
34	NA	0	8522	1/1	0.39	13.35	57,57,57,57	0
34	NA	0	8524	1/1	0.33	13.00	56,56,56,56	0
34	NA	0	8560	1/1	0.38	12.62	58,58,58,58	0
34	NA	0	8569	1/1	0.42	12.50	64,64,64,64	0
34	NA	0	8526	1/1	0.34	12.47	31,31,31,31	0
36	SR	0	8971	1/1	0.17	12.33	172,172,172,172	0
33	K	0	8401	1/1	0.67	12.12	149,149,149,149	0
32	MG	0	8040	1/1	0.45	12.00	69,69,69,69	0
32	MG	0	8069	1/1	0.48	11.71	61,61,61,61	0
34	NA	0	8561	1/1	0.51	11.55	71,71,71,71	0
34	NA	0	8571	1/1	0.35	11.27	72,72,72,72	0
32	MG	0	8082	1/1	0.63	10.78	76,76,76,76	0
32	MG	0	8068	1/1	0.29	10.41	58,58,58,58	0
36	SR	0	8957	1/1	0.61	10.31	200,200,200,200	0
34	NA	0	8558	1/1	0.42	9.56	36,36,36,36	0
34	NA	0	8541	1/1	0.29	9.32	59,59,59,59	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
34	NA	0	8506	1/1	0.33	9.23	74,74,74,74	0
32	MG	0	8073	1/1	0.28	9.11	57,57,57,57	0
34	NA	0	8562	1/1	0.39	8.94	67,67,67,67	0
36	SR	0	8962	1/1	0.39	8.55	157,157,157,157	0
32	MG	0	8062	1/1	0.38	8.20	68,68,68,68	0
32	MG	0	8049	1/1	0.35	8.19	53,53,53,53	0
34	NA	0	8519	1/1	0.33	8.16	35,35,35,35	0
34	NA	0	8530	1/1	0.37	8.05	59,59,59,59	0
34	NA	0	8556	1/1	0.68	7.98	35,35,35,35	0
34	NA	0	8552	1/1	0.36	7.92	47,47,47,47	0
34	NA	0	8518	1/1	0.39	7.77	76,76,76,76	0
32	MG	0	8071	1/1	0.25	7.59	56,56,56,56	0
34	NA	0	8554	1/1	0.37	7.31	50,50,50,50	0
34	NA	0	8567	1/1	0.23	7.12	57,57,57,57	0
32	MG	0	8075	1/1	0.26	7.07	36,36,36,36	0
34	NA	0	8547	1/1	0.32	6.97	36,36,36,36	0
34	NA	0	8551	1/1	0.28	6.79	39,39,39,39	0
36	SR	B	8987	1/1	0.43	6.76	200,200,200,200	0
34	NA	0	8501	1/1	0.19	6.58	30,30,30,30	0
34	NA	0	8507	1/1	0.36	6.34	39,39,39,39	0
32	MG	0	8072	1/1	0.26	6.32	68,68,68,68	0
34	NA	Q	8540	1/1	0.41	6.27	46,46,46,46	0
34	NA	0	8523	1/1	0.33	6.06	62,62,62,62	0
36	SR	0	8979	1/1	0.35	5.99	200,200,200,200	0
36	SR	0	8983	1/1	0.21	5.98	183,183,183,183	0
36	SR	9	8980	1/1	0.17	5.91	154,154,154,154	0
35	CL	R	8806	1/1	0.32	5.81	43,43,43,43	0
34	NA	0	8534	1/1	0.32	5.69	35,35,35,35	0
34	NA	0	8516	1/1	0.22	5.67	31,31,31,31	0
32	MG	0	8008	1/1	0.24	5.45	18,18,18,18	0
36	SR	0	8967	1/1	0.24	5.44	145,145,145,145	0
36	SR	0	8988	1/1	0.21	5.28	144,144,144,144	0
36	SR	0	8991	1/1	0.28	5.20	176,176,176,176	0
35	CL	0	8814	1/1	0.39	5.18	62,62,62,62	0
32	MG	0	8015	1/1	0.24	5.11	36,36,36,36	0
34	NA	0	8573	1/1	0.23	4.80	78,78,78,78	0
34	NA	0	8545	1/1	0.30	4.80	30,30,30,30	0
34	NA	0	8533	1/1	0.33	4.54	65,65,65,65	0
36	SR	0	8972	1/1	0.73	4.52	159,159,159,159	0
32	MG	0	8076	1/1	0.24	4.37	29,29,29,29	0
34	NA	0	8504	1/1	0.27	4.21	39,39,39,39	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	8061	1/1	0.26	4.07	29,29,29,29	0
32	MG	0	8090	1/1	0.24	3.93	45,45,45,45	0
36	SR	0	8947	1/1	0.29	3.60	160,160,160,160	0
34	NA	0	8565	1/1	0.20	3.57	65,65,65,65	0
36	SR	0	8985	1/1	0.19	3.45	137,137,137,137	0
36	SR	0	8914	1/1	0.20	3.32	105,105,105,105	0
34	NA	0	8520	1/1	0.19	3.20	55,55,55,55	0
34	NA	0	8544	1/1	0.18	2.95	59,59,59,59	0
33	K	0	8402	1/1	0.25	2.60	63,63,63,63	0
36	SR	0	8989	1/1	0.22	2.27	182,182,182,182	0
34	NA	0	8574	1/1	0.19	2.24	63,63,63,63	0
34	NA	0	8546	1/1	0.26	2.18	57,57,57,57	0
36	SR	0	8969	1/1	0.27	2.17	143,143,143,143	0
36	SR	0	8938	1/1	0.18	2.06	175,175,175,175	0
35	CL	J	8802	1/1	0.26	2.05	70,70,70,70	0
32	MG	0	8084	1/1	0.17	1.73	30,30,30,30	0
34	NA	0	8521	1/1	0.24	1.71	42,42,42,42	0
36	SR	9	8968	1/1	0.25	1.67	178,178,178,178	0
32	MG	0	8007	1/1	0.22	1.54	28,28,28,28	0
34	NA	0	8555	1/1	0.23	1.39	58,58,58,58	0
36	SR	A	8929	1/1	0.24	1.34	135,135,135,135	0
32	MG	0	8048	1/1	0.23	1.21	20,20,20,20	0
36	SR	0	8993	1/1	0.26	1.15	173,173,173,173	0
32	MG	0	8080	1/1	0.16	1.08	58,58,58,58	0
36	SR	0	8920	1/1	0.17	1.06	106,106,106,106	0
34	NA	0	8508	1/1	0.19	1.05	54,54,54,54	0
36	SR	0	8955	1/1	0.18	1.05	174,174,174,174	0
34	NA	0	8527	1/1	0.20	0.98	43,43,43,43	0
32	MG	0	8056	1/1	0.18	0.86	48,48,48,48	0
34	NA	0	8557	1/1	0.13	0.80	57,57,57,57	0
32	MG	0	8033	1/1	0.19	0.57	46,46,46,46	0
36	SR	0	8986	1/1	0.17	0.44	200,200,200,200	0
36	SR	0	8990	1/1	0.19	0.37	109,109,109,109	0
32	MG	0	8044	1/1	0.21	0.26	40,40,40,40	0
32	MG	0	8078	1/1	0.21	0.26	41,41,41,41	0
32	MG	B	8042	1/1	0.21	0.24	48,48,48,48	0
36	SR	0	8927	1/1	0.17	0.23	167,167,167,167	0
34	NA	0	8570	1/1	0.20	0.23	40,40,40,40	0
32	MG	0	8022	1/1	0.18	0.21	24,24,24,24	0
32	MG	0	8052	1/1	0.19	0.19	40,40,40,40	0
36	SR	0	8926	1/1	0.12	0.19	145,145,145,145	0
36	SR	0	9002	1/1	0.15	0.13	170,170,170,170	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
34	NA	J	8538	1/1	0.20	0.01	58,58,58,58	0
32	MG	0	8077	1/1	0.17	-0.03	24,24,24,24	0
36	SR	0	8917	1/1	0.18	-0.05	114,114,114,114	0
32	MG	0	8047	1/1	0.18	-0.13	45,45,45,45	0
32	MG	0	8039	1/1	0.19	-0.24	55,55,55,55	0
32	MG	0	8058	1/1	0.12	-0.35	18,18,18,18	0
32	MG	Y	8086	1/1	0.17	-0.38	40,40,40,40	0
32	MG	0	8024	1/1	0.20	-0.61	50,50,50,50	0
36	SR	B	8950	1/1	0.13	-0.62	108,108,108,108	0
32	MG	0	8043	1/1	0.16	-0.66	47,47,47,47	0
35	CL	J	8821	1/1	0.17	-0.69	63,63,63,63	0
32	MG	0	8028	1/1	0.17	-0.70	23,23,23,23	0
32	MG	0	8066	1/1	0.18	-0.70	53,53,53,53	0
32	MG	0	8029	1/1	0.14	-0.71	40,40,40,40	0
35	CL	Q	8811	1/1	0.18	-0.74	57,57,57,57	0
35	CL	0	8816	1/1	0.15	-0.74	62,62,62,62	0
35	CL	0	8820	1/1	0.12	-0.75	39,39,39,39	0
36	SR	9	9003	1/1	0.11	-0.77	157,157,157,157	0
32	MG	0	8067	1/1	0.19	-0.78	33,33,33,33	0
35	CL	0	8812	1/1	0.16	-0.87	35,35,35,35	0
32	MG	0	8009	1/1	0.17	-0.96	29,29,29,29	0
36	SR	0	8933	1/1	0.14	-0.98	134,134,134,134	0
32	MG	0	8012	1/1	0.15	-0.99	16,16,16,16	0
34	NA	M	8539	1/1	0.16	-1.00	30,30,30,30	0
32	MG	0	8034	1/1	0.18	-1.02	28,28,28,28	0
36	SR	0	8903	1/1	0.17	-1.04	53,53,53,53	0
32	MG	0	8025	1/1	0.16	-1.05	16,16,16,16	0
35	CL	O	8808	1/1	0.10	-1.06	63,63,63,63	0
34	NA	R	8532	1/1	0.15	-1.07	58,58,58,58	0
36	SR	0	8935	1/1	0.13	-1.19	75,75,75,75	0
32	MG	0	8070	1/1	0.16	-1.26	65,65,65,65	0
36	SR	3	8999	1/1	0.10	-1.30	95,95,95,95	0
34	NA	9	8543	1/1	0.16	-1.31	53,53,53,53	0
36	SR	0	8924	1/1	0.16	-1.33	140,140,140,140	0
36	SR	0	8956	1/1	0.09	-1.38	167,167,167,167	0
32	MG	T	8057	1/1	0.12	-1.43	54,54,54,54	0
35	CL	N	8807	1/1	0.10	-1.51	59,59,59,59	0
32	MG	0	8013	1/1	0.13	-1.53	29,29,29,29	0
37	CD	U	8701	1/1	0.07	-1.58	60,60,60,60	0
32	MG	9	8074	1/1	0.12	-1.58	73,73,73,73	0
32	MG	0	8014	1/1	0.15	-1.59	15,15,15,15	0
35	CL	A	8809	1/1	0.17	-1.65	65,65,65,65	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	K	8054	1/1	0.12	-1.65	29,29,29,29	0
34	NA	0	8537	1/1	0.10	-1.66	39,39,39,39	0
32	MG	0	8026	1/1	0.12	-1.69	35,35,35,35	0
36	SR	0	8928	1/1	0.12	-1.69	167,167,167,167	0
37	CD	Z	8703	1/1	0.08	-1.74	64,64,64,64	0
36	SR	0	8940	1/1	0.12	-1.74	79,79,79,79	0
36	SR	F	9005	1/1	0.10	-1.75	130,130,130,130	0
36	SR	0	8911	1/1	0.10	-1.80	70,70,70,70	0
32	MG	0	8045	1/1	0.11	-1.81	29,29,29,29	0
35	CL	0	8803	1/1	0.15	-1.82	40,40,40,40	0
36	SR	0	8975	1/1	0.07	-1.84	146,146,146,146	0
32	MG	0	8031	1/1	0.11	-1.95	45,45,45,45	0
32	MG	0	8035	1/1	0.16	-1.96	58,58,58,58	0
32	MG	0	8019	1/1	0.17	-1.99	24,24,24,24	0
36	SR	0	8908	1/1	0.13	-2.00	87,87,87,87	0
35	CL	0	8817	1/1	0.09	-2.00	60,60,60,60	0
36	SR	0	8915	1/1	0.09	-2.06	114,114,114,114	0
34	NA	0	8529	1/1	0.08	-2.10	35,35,35,35	0
36	SR	A	8977	1/1	0.09	-2.13	147,147,147,147	0
37	CD	3	8704	1/1	0.10	-2.18	62,62,62,62	0
36	SR	0	8960	1/1	0.11	-2.20	138,138,138,138	0
32	MG	0	8053	1/1	0.11	-2.27	44,44,44,44	0
32	MG	0	8006	1/1	0.11	-2.37	34,34,34,34	0
32	MG	0	8023	1/1	0.12	-2.39	27,27,27,27	0
32	MG	0	8041	1/1	0.13	-2.49	21,21,21,21	0
32	MG	A	8050	1/1	0.17	-2.50	48,48,48,48	0
34	NA	0	8515	1/1	0.11	-2.55	33,33,33,33	0
36	SR	0	8998	1/1	0.15	-2.55	134,134,134,134	0
37	CD	1	8702	1/1	0.08	-2.63	53,53,53,53	0
32	MG	0	8032	1/1	0.10	-2.76	29,29,29,29	0
34	NA	C	8503	1/1	0.12	-2.81	32,32,32,32	0
36	SR	0	8995	1/1	0.14	-2.83	140,140,140,140	0
32	MG	0	8011	1/1	0.14	-2.87	31,31,31,31	0
32	MG	0	8018	1/1	0.11	-2.87	37,37,37,37	0
35	CL	0	8815	1/1	0.12	-2.91	66,66,66,66	0
36	SR	0	8909	1/1	0.09	-2.92	88,88,88,88	0
36	SR	0	8981	1/1	0.10	-3.00	140,140,140,140	0
36	SR	S	8961	1/1	0.09	-3.00	124,124,124,124	0
36	SR	0	8931	1/1	0.11	-3.01	108,108,108,108	0
36	SR	R	8912	1/1	0.08	-3.03	80,80,80,80	0
35	CL	J	8801	1/1	0.06	-3.03	65,65,65,65	0
36	SR	0	8934	1/1	0.14	-3.03	100,100,100,100	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	0	8907	1/1	0.08	-3.06	58,58,58,58	0
32	MG	0	8088	1/1	0.11	-3.06	26,26,26,26	0
36	SR	9	8978	1/1	0.12	-3.07	150,150,150,150	0
32	MG	0	8064	1/1	0.14	-3.10	37,37,37,37	0
32	MG	0	8003	1/1	0.13	-3.11	28,28,28,28	0
36	SR	0	8966	1/1	0.12	-3.12	97,97,97,97	0
36	SR	0	8936	1/1	0.10	-3.13	86,86,86,86	0
36	SR	0	8949	1/1	0.11	-3.14	105,105,105,105	0
32	MG	0	8017	1/1	0.16	-3.19	29,29,29,29	0
35	CL	3	8804	1/1	0.06	-3.29	58,58,58,58	0
36	SR	0	8910	1/1	0.10	-3.37	87,87,87,87	0
36	SR	0	8954	1/1	0.11	-3.37	94,94,94,94	0
36	SR	A	8930	1/1	0.09	-3.41	87,87,87,87	0
34	NA	0	8535	1/1	0.14	-3.50	35,35,35,35	0
36	SR	0	8959	1/1	0.05	-3.52	142,142,142,142	0
32	MG	0	8036	1/1	0.11	-3.57	40,40,40,40	0
36	SR	0	8916	1/1	0.10	-3.59	107,107,107,107	0
34	NA	0	8542	1/1	0.13	-3.62	53,53,53,53	0
32	MG	0	8083	1/1	0.11	-3.63	30,30,30,30	0
35	CL	L	8810	1/1	0.06	-3.69	57,57,57,57	0
36	SR	0	8951	1/1	0.07	-3.69	139,139,139,139	0
36	SR	0	8919	1/1	0.16	-3.77	144,144,144,144	0
32	MG	0	8060	1/1	0.09	-3.78	42,42,42,42	0
36	SR	1	8952	1/1	0.11	-3.95	70,70,70,70	0
36	SR	0	8965	1/1	0.12	-4.00	125,125,125,125	0
32	MG	0	8001	1/1	0.10	-4.11	27,27,27,27	0
34	NA	0	8568	1/1	0.11	-4.13	37,37,37,37	0
36	SR	0	8905	1/1	0.14	-4.15	55,55,55,55	0
36	SR	0	8948	1/1	0.08	-4.20	101,101,101,101	0
35	CL	0	8805	1/1	0.06	-4.24	50,50,50,50	0
36	SR	0	8958	1/1	0.09	-4.24	99,99,99,99	0
36	SR	0	8974	1/1	0.15	-4.29	155,155,155,155	0
36	SR	0	8946	1/1	0.14	-4.30	110,110,110,110	0
36	SR	0	8904	1/1	0.10	-4.34	49,49,49,49	0
32	MG	0	8020	1/1	0.11	-4.40	37,37,37,37	0
32	MG	0	8065	1/1	0.08	-4.43	37,37,37,37	0
36	SR	0	8970	1/1	0.05	-4.44	121,121,121,121	0
36	SR	0	8964	1/1	0.07	-4.45	131,131,131,131	0
36	SR	0	8945	1/1	0.09	-4.56	113,113,113,113	0
36	SR	3	8932	1/1	0.09	-4.59	68,68,68,68	0
35	CL	B	8819	1/1	0.11	-4.63	49,49,49,49	0
36	SR	0	8918	1/1	0.11	-4.65	73,73,73,73	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
35	CL	M	8818	1/1	0.07	-4.65	30,30,30,30	0
36	SR	0	8921	1/1	0.11	-4.71	74,74,74,74	0
32	MG	0	8004	1/1	0.10	-4.73	26,26,26,26	0
32	MG	0	8093	1/1	0.12	-4.86	35,35,35,35	0
32	MG	0	8027	1/1	0.09	-4.93	35,35,35,35	0
32	MG	0	8055	1/1	0.13	-5.11	28,28,28,28	0
36	SR	0	8901	1/1	0.10	-5.13	78,78,78,78	0
32	MG	0	8046	1/1	0.12	-5.16	28,28,28,28	0
36	SR	0	8992	1/1	0.09	-5.19	123,123,123,123	0
32	MG	0	8021	1/1	0.12	-5.27	32,32,32,32	0
34	NA	0	8531	1/1	0.09	-5.39	33,33,33,33	0
36	SR	1	8913	1/1	0.09	-5.41	82,82,82,82	0
32	MG	0	8010	1/1	0.08	-5.46	34,34,34,34	0
36	SR	0	8984	1/1	0.07	-5.50	106,106,106,106	0
32	MG	0	8081	1/1	0.13	-5.50	48,48,48,48	0
34	NA	0	8550	1/1	0.14	-5.54	42,42,42,42	0
32	MG	0	8091	1/1	0.12	-5.57	43,43,43,43	0
36	SR	0	8939	1/1	0.07	-5.57	129,129,129,129	0
32	MG	0	8059	1/1	0.08	-5.71	33,33,33,33	0
32	MG	0	8002	1/1	0.04	-6.43	26,26,26,26	0
37	CD	O	8705	1/1	0.07	-6.52	81,81,81,81	0
36	SR	0	8902	1/1	0.09	-6.78	54,54,54,54	0
35	CL	0	8813	1/1	0.09	-6.86	45,45,45,45	0
32	MG	0	8005	1/1	0.11	-7.48	25,25,25,25	0
36	SR	0	8943	1/1	0.08	-7.49	113,113,113,113	0
36	SR	0	8937	1/1	0.08	-7.63	101,101,101,101	0
36	SR	0	8922	1/1	0.15	-7.67	177,177,177,177	0
32	MG	0	8087	1/1	0.10	-7.69	29,29,29,29	0
36	SR	0	8953	1/1	0.10	-7.83	130,130,130,130	0
34	NA	9	8572	1/1	0.06	-8.12	88,88,88,88	0
32	MG	0	8016	1/1	0.09	-8.88	36,36,36,36	0
36	SR	0	8906	1/1	0.08	-9.03	51,51,51,51	0
36	SR	0	9008	1/1	0.07	-9.44	89,89,89,89	0
36	SR	0	8925	1/1	0.05	-9.71	90,90,90,90	0
36	SR	0	8963	1/1	0.04	-10.18	177,177,177,177	0
36	SR	0	8944	1/1	0.10	-10.60	148,148,148,148	0
34	NA	S	8510	1/1	0.07	-10.83	26,26,26,26	0
36	SR	0	8942	1/1	0.11	-11.64	109,109,109,109	0
36	SR	0	8941	1/1	0.10	-12.62	104,104,104,104	0
36	SR	0	8973	1/1	0.05	-16.40	124,124,124,124	0
36	SR	0	8923	1/1	0.06	-18.52	104,104,104,104	0
34	NA	0	8536	1/1	0.07	-18.93	43,43,43,43	0

6.5 Other polymers ⓘ

There are no such residues in this entry.