



Full wwPDB NMR Structure Validation Report ⓘ

Mar 28, 2026 – 08:28 AM UTC

PDB ID : 1T4L / pdb_00001t4l
Title : Solution structure of double-stranded RNA binding domain of *S. cerevisiae* RNase III (Rnt1p) in complex with the 5' terminal RNA hairpin of snR47 precursor
Authors : Wu, H.; Henras, A.; Chanfreau, G.; Feigon, J.
Deposited on : 2004-04-29

This is a Full wwPDB NMR Structure Validation Report for a publicly released PDB entry.

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity	:	4-5-2 with Phenix2.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
wwPDB-RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
wwPDB-ShiftChecker	:	v1.2
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

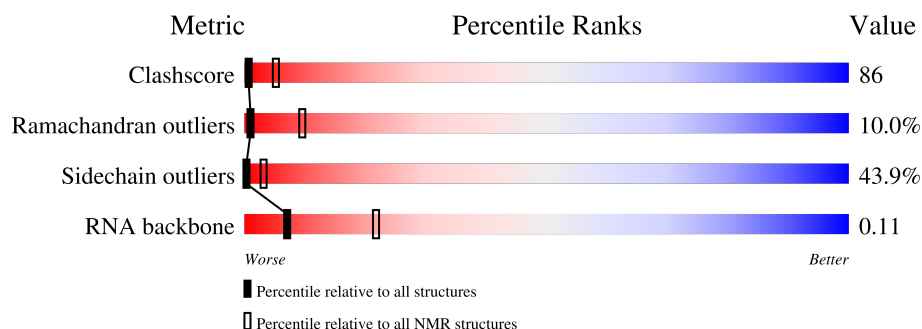
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment was not calculated.

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)	NMR archive (#Entries)
Clashscore	229148	14424
Ramachandran outliers	224038	12848
Sidechain outliers	223484	12823
RNA backbone	8273	777

The table below summarises the geometric issues observed across the polymeric chains and their fit to the experimental data. The red, orange, yellow and green segments indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A cyan segment indicates the fraction of residues that are not part of the well-defined cores, and a grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	A	32	 88% 12%
2	B	90	 9% 49% 29% • 12%

2 Ensemble composition and analysis

This entry contains 15 models. Model 5 is the overall representative, medoid model (most similar to other models).

The following residues are included in the computation of the global validation metrics.

Well-defined (core) protein residues			
Well-defined core	Residue range (total)	Backbone RMSD (Å)	Medoid model
1	B:367-B:445 (79)	0.76	5

Ill-defined regions of proteins are excluded from the global statistics.

Ligands and non-protein polymers are included in the analysis.

The models can be grouped into 3 clusters and 1 single-model cluster was found.

Cluster number	Models
1	1, 3, 5, 6, 12
2	2, 7, 10, 11, 15
3	4, 8, 9, 13
Single-model clusters	14

3 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 2437 atoms, of which 1067 are hydrogens and 0 are deuteriums.

- Molecule 1 is a RNA chain called 5' terminal hairpin of snR47 precursor.

Mol	Chain	Residues	Atoms						Trace
1	A	32	Total	C	H	N	O	P	0
			1028	306	346	124	221	31	

- Molecule 2 is a protein called Ribonuclease III.

Mol	Chain	Residues	Atoms						Trace
2	B	90	Total	C	H	N	O	S	0
			1409	429	721	129	127	3	

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	364	GLY	-	cloning artifact	UNP Q02555
B	365	SER	-	cloning artifact	UNP Q02555

4 Residue-property plots

4.1 Average score per residue in the NMR ensemble

These plots are provided for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic is the same as shown in the summary in section 1 of this report. The second graphic shows the sequence where residues are colour-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. Stretches of 2 or more consecutive residues without any outliers are shown as green connectors. Residues which are classified as ill-defined in the NMR ensemble, are shown in cyan with an underline colour-coded according to the previous scheme. Residues which were present in the experimental sample, but not modelled in the final structure are shown in grey.

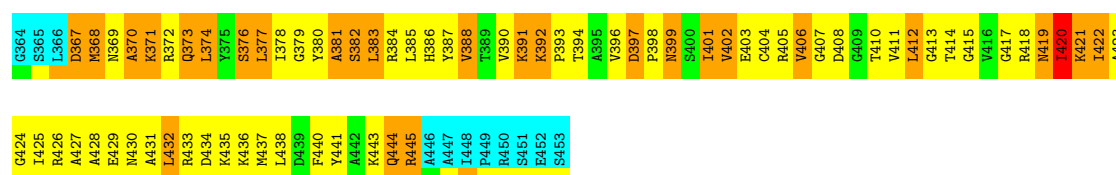
- Molecule 1: 5' terminal hairpin of snR47 precursor

Chain A: 



- Molecule 2: Ribonuclease III

Chain B: 

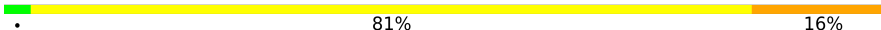


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

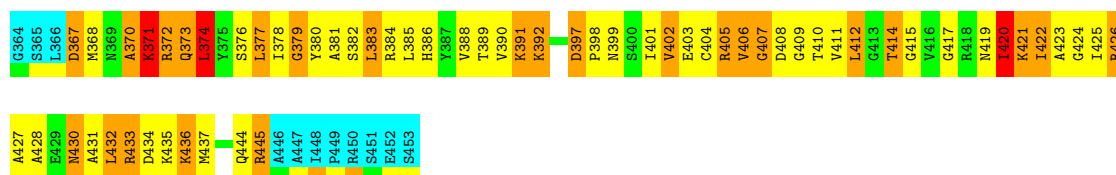
- Molecule 1: 5' terminal hairpin of snR47 precursor

Chain A: 



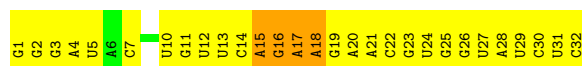
- Molecule 2: Ribonuclease III

Chain B: 

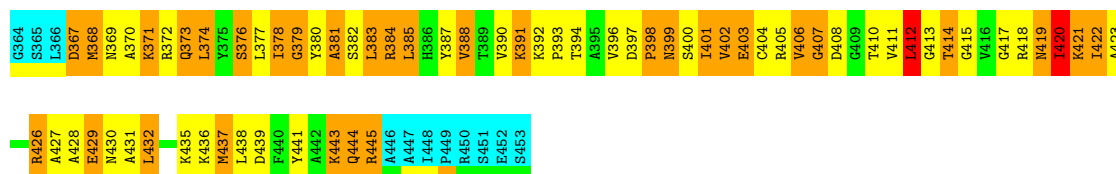


4.2.2 Score per residue for model 2

- Molecule 1: 5' terminal hairpin of snR47 precursor

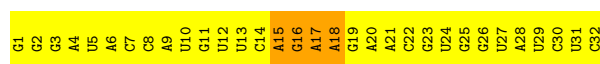
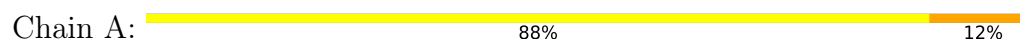


- Molecule 2: Ribonuclease III

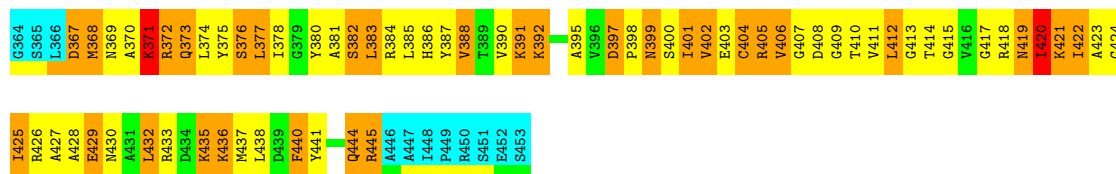
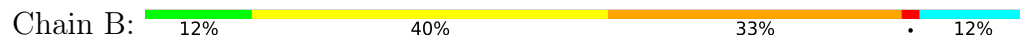


4.2.3 Score per residue for model 3

- Molecule 1: 5' terminal hairpin of snR47 precursor

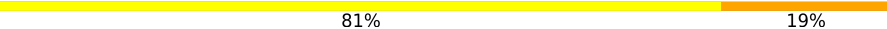


- Molecule 2: Ribonuclease III



4.2.4 Score per residue for model 4

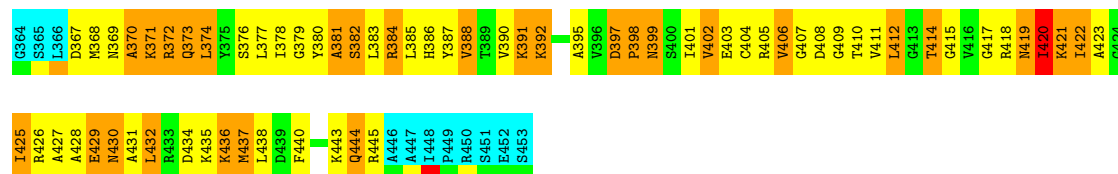
- Molecule 1: 5' terminal hairpin of snR47 precursor

Chain A: 



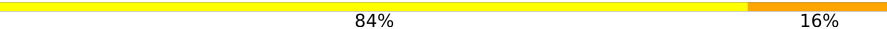
- Molecule 2: Ribonuclease III

Chain B: 



4.2.5 Score per residue for model 5 (medoid)

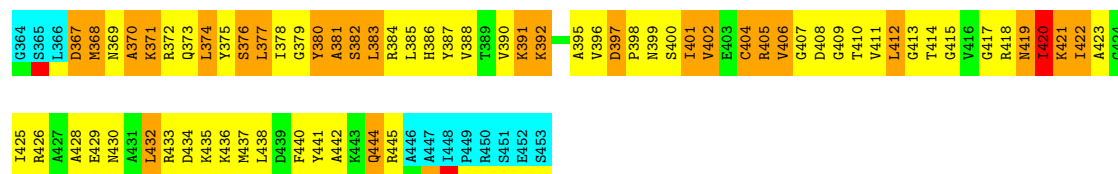
- Molecule 1: 5' terminal hairpin of snR47 precursor

Chain A: 



- Molecule 2: Ribonuclease III

Chain B: 



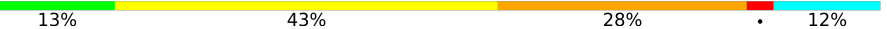
4.2.6 Score per residue for model 6

- Molecule 1: 5' terminal hairpin of snR47 precursor

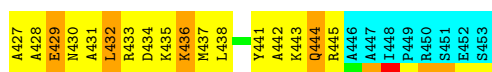
Chain A: 



- Molecule 2: Ribonuclease III

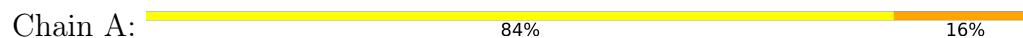
Chain B: 



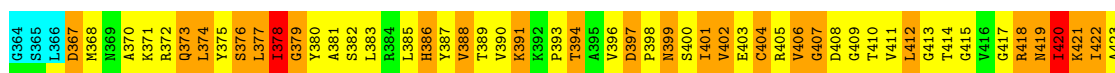


4.2.7 Score per residue for model 7

- Molecule 1: 5' terminal hairpin of snR47 precursor

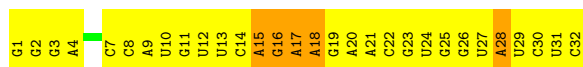


- Molecule 2: Ribonuclease III

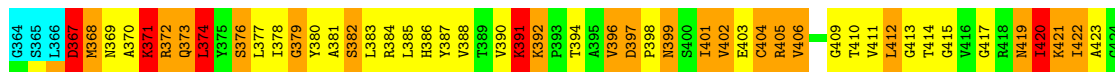


4.2.8 Score per residue for model 8

- Molecule 1: 5' terminal hairpin of snR47 precursor

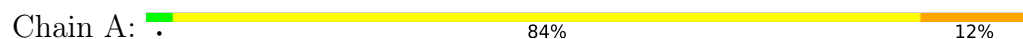


- Molecule 2: Ribonuclease III



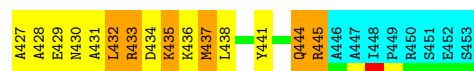
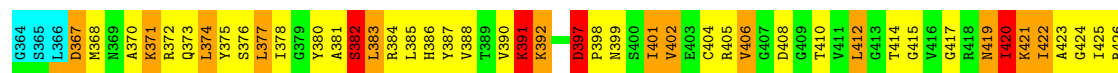
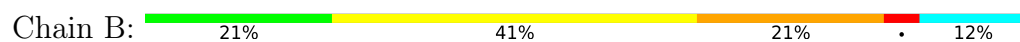
4.2.9 Score per residue for model 9

- Molecule 1: 5' terminal hairpin of snR47 precursor





• Molecule 2: Ribonuclease III

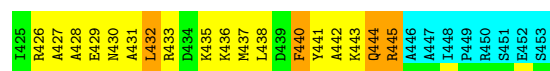
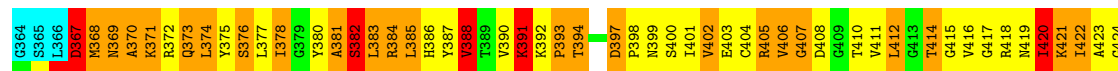


4.2.10 Score per residue for model 10

• Molecule 1: 5' terminal hairpin of snR47 precursor

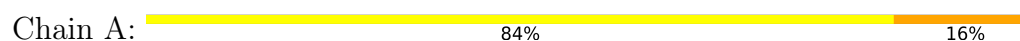


• Molecule 2: Ribonuclease III

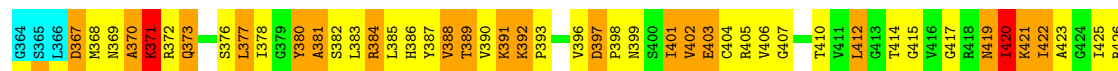
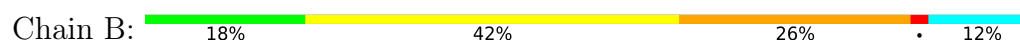


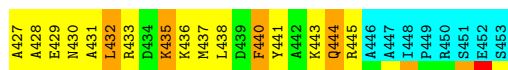
4.2.11 Score per residue for model 11

• Molecule 1: 5' terminal hairpin of snR47 precursor



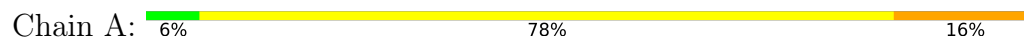
• Molecule 2: Ribonuclease III



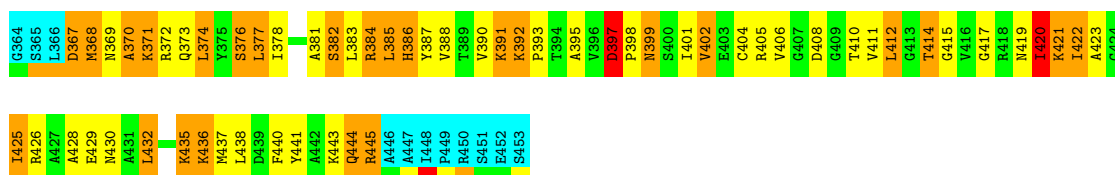
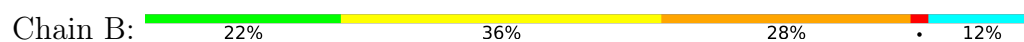


4.2.12 Score per residue for model 12

- Molecule 1: 5' terminal hairpin of snR47 precursor

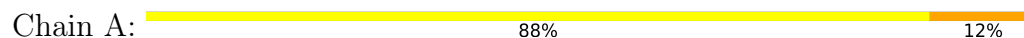


- Molecule 2: Ribonuclease III

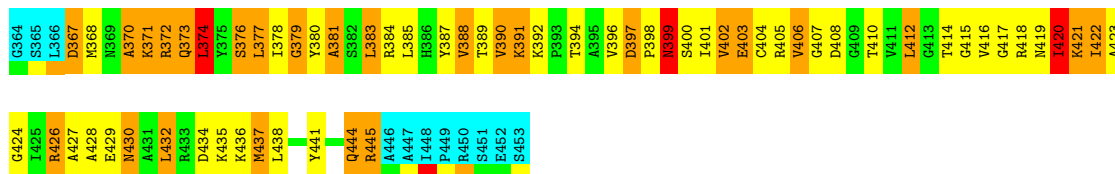


4.2.13 Score per residue for model 13

- Molecule 1: 5' terminal hairpin of snR47 precursor



- Molecule 2: Ribonuclease III



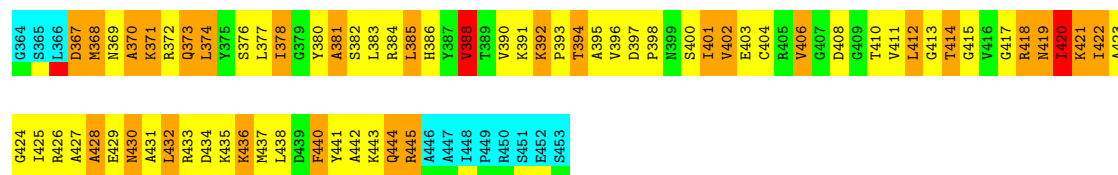
4.2.14 Score per residue for model 14

- Molecule 1: 5' terminal hairpin of snR47 precursor





• Molecule 2: Ribonuclease III

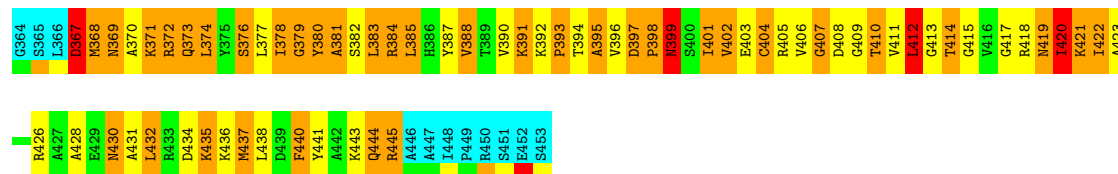


4.2.15 Score per residue for model 15

• Molecule 1: 5' terminal hairpin of snR47 precursor



• Molecule 2: Ribonuclease III



5 Refinement protocol and experimental data overview

The models were refined using the following method: *simulated annealing*.

Of the 100 calculated structures, 15 were deposited, based on the following criterion: *structures with the lowest energy*.

The following table shows the software used for structure solution, optimisation and refinement.

Software name	Classification	Version
X-PLOR	refinement	NIH

No chemical shift data was provided.

6 Model quality ⓘ

6.1 Standard geometry ⓘ

There are no covalent bond-length or bond-angle outliers.

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

There are no planarity outliers.

6.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in each chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes averaged over the ensemble.

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	A	682	346	346	90±10
2	B	612	643	642	111±10
All	All	19410	14835	14820	2932

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 86.

All unique clashes are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:390:VAL:HG23	2:B:401:ILE:HG23	1.04	1.29	6	14
2:B:406:VAL:HG13	2:B:412:LEU:HD21	1.02	1.20	15	3
2:B:380:TYR:CE2	2:B:383:LEU:HD12	1.00	1.91	9	2
1:A:30:C:O2'	1:A:31:U:H5'	0.95	1.61	11	15
2:B:377:LEU:O	2:B:378:ILE:HD13	0.93	1.62	8	12
2:B:370:ALA:HB1	2:B:428:ALA:HB1	0.93	1.40	6	13
1:A:1:G:HO2'	1:A:2:G:H8	0.93	1.07	8	5
1:A:1:G:O2'	1:A:2:G:H5'	0.93	1.62	10	10
2:B:401:ILE:HD12	2:B:415:GLY:O	0.92	1.63	14	5
1:A:4:A:O2'	1:A:5:U:H5'	0.92	1.62	10	1
1:A:9:A:O2'	1:A:10:U:H5'	0.90	1.67	14	5
1:A:27:U:O2'	1:A:28:A:H5'	0.90	1.67	9	13
2:B:406:VAL:CG1	2:B:412:LEU:HD21	0.90	1.97	15	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:29:U:O2'	1:A:30:C:H5'	0.89	1.66	2	13
2:B:368:MET:HE2	2:B:369:ASN:HB3	0.89	1.45	15	1
1:A:15:A:H2'	1:A:16:G:O4'	0.89	1.68	10	13
1:A:6:A:O2'	1:A:7:C:H5'	0.89	1.66	13	3
2:B:412:LEU:HD12	2:B:437:MET:SD	0.88	2.09	5	9
2:B:370:ALA:HB1	2:B:428:ALA:CB	0.86	2.00	9	11
2:B:406:VAL:HG13	2:B:412:LEU:CD2	0.85	1.99	15	1
1:A:12:U:O2'	1:A:13:U:H5'	0.84	1.71	10	15
2:B:419:ASN:O	2:B:420:ILE:HG23	0.83	1.74	15	6
1:A:20:A:H2'	1:A:21:A:O4'	0.83	1.74	13	7
2:B:432:LEU:C	2:B:438:LEU:HD11	0.83	1.98	2	5
1:A:23:G:O2'	1:A:24:U:H5'	0.82	1.73	14	15
2:B:432:LEU:O	2:B:438:LEU:HD11	0.82	1.74	2	2
1:A:1:G:HO5'	1:A:1:G:H8	0.82	1.13	11	5
2:B:432:LEU:HA	2:B:438:LEU:HD11	0.81	1.52	11	9
2:B:402:VAL:O	2:B:414:THR:HG22	0.81	1.74	10	4
2:B:417:GLY:HA3	2:B:422:ILE:HD13	0.81	1.52	12	11
2:B:387:TYR:CE2	2:B:427:ALA:HB1	0.81	2.09	10	2
2:B:373:GLN:OE1	2:B:377:LEU:HD23	0.81	1.75	4	1
2:B:404:CYS:SG	2:B:431:ALA:HB2	0.80	2.16	11	4
2:B:432:LEU:C	2:B:432:LEU:HD23	0.80	2.01	9	1
2:B:390:VAL:HG13	2:B:401:ILE:HG23	0.80	1.51	13	1
2:B:404:CYS:O	2:B:411:VAL:O	0.79	2.00	14	2
1:A:12:U:H6	1:A:12:U:O5'	0.79	1.60	5	5
1:A:2:G:O2'	1:A:3:G:H5'	0.78	1.78	1	6
2:B:419:ASN:O	2:B:421:LYS:N	0.78	2.17	10	9
1:A:20:A:O2'	1:A:21:A:H5'	0.78	1.79	4	12
2:B:432:LEU:CA	2:B:438:LEU:HD11	0.78	2.09	7	10
1:A:22:C:O5'	1:A:22:C:H6	0.77	1.61	10	8
2:B:402:VAL:HG21	2:B:423:ALA:O	0.77	1.80	11	13
2:B:412:LEU:HD12	2:B:437:MET:HE2	0.77	1.55	7	2
1:A:17:A:O2'	1:A:18:A:P	0.77	2.43	1	3
2:B:376:SER:C	2:B:377:LEU:HD22	0.76	2.05	15	2
1:A:30:C:O2'	2:B:396:VAL:HG12	0.76	1.80	14	3
2:B:385:LEU:HA	2:B:406:VAL:HG12	0.76	1.55	1	14
1:A:22:C:O2'	1:A:23:G:H5'	0.75	1.82	9	11
1:A:15:A:O2'	1:A:16:G:H5'	0.75	1.81	6	7
2:B:419:ASN:OD1	2:B:422:ILE:HD11	0.75	1.81	1	1
1:A:16:G:H4'	1:A:17:A:O5'	0.75	1.81	2	1
2:B:417:GLY:CA	2:B:422:ILE:HD13	0.74	2.12	13	14
2:B:390:VAL:HG22	2:B:401:ILE:O	0.74	1.83	15	3

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:26:G:O2'	1:A:27:U:H5'	0.74	1.82	1	9
1:A:1:G:H8	1:A:1:G:O5'	0.74	1.64	11	4
2:B:420:ILE:O	2:B:423:ALA:HB3	0.73	1.82	10	15
1:A:7:C:H6	1:A:7:C:O5'	0.73	1.66	5	6
2:B:383:LEU:HD13	2:B:385:LEU:HB2	0.73	1.58	2	3
2:B:388:VAL:HG23	2:B:403:GLU:O	0.72	1.83	15	4
2:B:401:ILE:HD11	2:B:414:THR:OG1	0.72	1.83	13	3
2:B:432:LEU:HA	2:B:438:LEU:HD21	0.72	1.60	2	4
1:A:22:C:H6	1:A:22:C:O5'	0.72	1.68	4	7
1:A:24:U:H6	1:A:24:U:O5'	0.72	1.68	8	6
2:B:419:ASN:C	2:B:420:ILE:HG23	0.72	2.10	11	6
1:A:8:C:N4	1:A:9:A:N6	0.72	2.37	15	8
1:A:31:U:O2'	1:A:32:C:H5'	0.72	1.84	12	6
2:B:431:ALA:O	2:B:437:MET:HE1	0.72	1.84	14	5
1:A:23:G:C6	1:A:24:U:C4	0.72	2.77	13	6
2:B:428:ALA:O	2:B:432:LEU:HD13	0.72	1.85	3	7
1:A:7:C:N4	1:A:8:C:N4	0.71	2.38	14	7
1:A:15:A:C5	1:A:16:G:N7	0.71	2.59	6	6
1:A:1:G:H8	1:A:1:G:HO5'	0.71	1.26	10	1
2:B:419:ASN:O	2:B:422:ILE:HD12	0.71	1.86	10	1
2:B:412:LEU:HG	2:B:437:MET:HE2	0.71	1.63	14	2
2:B:412:LEU:CG	2:B:437:MET:HE2	0.71	2.16	10	1
1:A:10:U:H6	1:A:10:U:O5'	0.71	1.69	8	3
2:B:420:ILE:HD12	2:B:420:ILE:C	0.70	2.11	5	7
1:A:15:A:C5	1:A:16:G:C8	0.70	2.79	7	13
2:B:425:ILE:HD13	2:B:425:ILE:N	0.70	2.01	4	3
2:B:405:ARG:HB3	2:B:411:VAL:HG22	0.70	1.61	12	5
1:A:18:A:H2'	1:A:19:G:O4'	0.70	1.87	11	12
1:A:16:G:H5''	1:A:17:A:N7	0.70	2.01	14	3
1:A:30:C:C4	1:A:31:U:C4	0.69	2.79	12	10
2:B:374:LEU:HD11	2:B:387:TYR:OH	0.69	1.87	5	2
1:A:1:G:N3	1:A:2:G:C8	0.69	2.60	14	6
2:B:378:ILE:HG23	2:B:441:TYR:CB	0.69	2.17	8	3
2:B:387:TYR:OH	2:B:431:ALA:HB2	0.69	1.87	15	2
1:A:20:A:O5'	1:A:20:A:H8	0.69	1.69	13	8
1:A:28:A:O2'	1:A:29:U:C6	0.69	2.46	13	4
2:B:420:ILE:C	2:B:420:ILE:HD12	0.69	2.11	9	8
1:A:20:A:H8	1:A:20:A:O5'	0.69	1.70	2	5
1:A:1:G:C2	1:A:2:G:C5	0.69	2.81	14	6
1:A:1:G:C2	1:A:2:G:N7	0.69	2.61	14	3
1:A:29:U:H2'	1:A:30:C:O4'	0.69	1.87	3	6

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:374:LEU:HD23	2:B:374:LEU:N	0.69	2.03	14	11
2:B:402:VAL:HG21	2:B:423:ALA:C	0.69	2.13	13	11
1:A:13:U:O2'	1:A:14:C:H5'	0.68	1.88	3	8
1:A:30:C:N4	1:A:31:U:C4	0.68	2.61	12	10
1:A:5:U:H6	1:A:5:U:O5'	0.68	1.70	13	7
1:A:17:A:O2'	1:A:18:A:N9	0.68	2.27	12	3
2:B:432:LEU:HD23	2:B:433:ARG:N	0.68	2.03	9	1
2:B:402:VAL:HG23	2:B:415:GLY:O	0.68	1.88	15	7
2:B:402:VAL:HG23	2:B:423:ALA:HB1	0.68	1.66	14	6
2:B:401:ILE:HD11	2:B:414:THR:CG2	0.68	2.18	6	1
2:B:383:LEU:O	2:B:383:LEU:HD23	0.68	1.89	8	1
1:A:12:U:O2'	1:A:13:U:C5'	0.67	2.42	13	15
1:A:14:C:H2'	1:A:15:A:O4'	0.67	1.89	6	9
1:A:16:G:H4'	1:A:17:A:OP2	0.67	1.87	4	6
2:B:388:VAL:HG23	2:B:403:GLU:CB	0.67	2.19	13	4
1:A:30:C:C4	1:A:31:U:C5	0.67	2.82	12	13
1:A:23:G:O2'	1:A:24:U:C5'	0.67	2.43	5	12
1:A:15:A:C6	1:A:16:G:C8	0.67	2.82	14	9
2:B:401:ILE:HD13	2:B:402:VAL:N	0.67	2.04	9	1
1:A:13:U:O2'	1:A:14:C:C5'	0.67	2.43	2	14
2:B:391:LYS:HB2	2:B:401:ILE:HG22	0.67	1.67	6	5
1:A:22:C:O2'	1:A:23:G:C5'	0.67	2.43	12	11
2:B:401:ILE:HD13	2:B:416:VAL:HB	0.67	1.66	10	1
2:B:401:ILE:HB	2:B:416:VAL:HG22	0.67	1.65	13	1
1:A:11:G:O2'	1:A:12:U:C5'	0.67	2.42	4	14
1:A:21:A:O2'	1:A:22:C:C5'	0.66	2.43	1	4
2:B:419:ASN:H	2:B:422:ILE:HD11	0.66	1.50	12	13
1:A:25:G:C2	1:A:26:G:C5	0.66	2.83	6	2
2:B:379:GLY:HA2	2:B:383:LEU:HD12	0.66	1.66	1	2
1:A:16:G:H1'	1:A:17:A:OP2	0.66	1.90	14	7
2:B:405:ARG:CA	2:B:412:LEU:HD22	0.66	2.21	6	1
1:A:28:A:O2'	1:A:29:U:C5'	0.66	2.43	8	12
2:B:432:LEU:H	2:B:432:LEU:HD13	0.66	1.50	2	2
1:A:29:U:O2'	1:A:30:C:C5'	0.66	2.44	7	10
2:B:402:VAL:HB	2:B:427:ALA:HB2	0.66	1.68	6	8
2:B:412:LEU:HD12	2:B:437:MET:HG3	0.66	1.68	10	2
1:A:20:A:O2'	1:A:21:A:C5'	0.66	2.44	2	13
2:B:383:LEU:CD1	2:B:385:LEU:HD12	0.66	2.19	14	1
2:B:396:VAL:HG23	2:B:397:ASP:OD2	0.65	1.91	11	2
2:B:402:VAL:CG2	2:B:423:ALA:HB1	0.65	2.22	14	9
2:B:405:ARG:HA	2:B:412:LEU:HD22	0.65	1.67	6	2

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:368:MET:HE2	2:B:369:ASN:OD1	0.65	1.91	3	1
1:A:27:U:O2'	1:A:28:A:C5'	0.65	2.44	6	9
1:A:9:A:O2'	1:A:10:U:C5'	0.65	2.44	14	4
2:B:412:LEU:CB	2:B:437:MET:HE2	0.65	2.22	10	1
1:A:14:C:C4	1:A:15:A:C4	0.65	2.83	8	6
2:B:412:LEU:HD13	2:B:412:LEU:N	0.65	2.07	10	3
1:A:7:C:O5'	1:A:7:C:H6	0.65	1.75	8	5
1:A:18:A:H8	1:A:18:A:O5'	0.65	1.75	8	1
1:A:30:C:O2'	1:A:31:U:C5'	0.65	2.45	5	14
1:A:25:G:C6	1:A:26:G:C6	0.65	2.85	11	5
1:A:3:G:O2'	1:A:4:A:C5'	0.64	2.45	6	7
2:B:380:TYR:O	2:B:381:ALA:HB2	0.64	1.93	14	8
2:B:385:LEU:HG	2:B:406:VAL:HG12	0.64	1.68	11	1
2:B:380:TYR:CE1	2:B:445:ARG:CZ	0.64	2.81	5	1
2:B:368:MET:HE2	2:B:369:ASN:CB	0.64	2.22	8	1
1:A:10:U:O2'	1:A:11:G:C5'	0.64	2.45	11	9
2:B:374:LEU:HD21	2:B:432:LEU:HD23	0.64	1.67	15	5
2:B:377:LEU:C	2:B:378:ILE:HD13	0.64	2.18	5	3
1:A:1:G:O2'	1:A:2:G:C5'	0.64	2.45	2	9
1:A:31:U:O2'	1:A:32:C:C5'	0.64	2.46	4	10
2:B:374:LEU:HD22	2:B:431:ALA:HB3	0.64	1.68	15	2
2:B:406:VAL:CG2	2:B:412:LEU:HD22	0.64	2.22	14	1
2:B:385:LEU:HD23	2:B:386:HIS:N	0.63	2.08	4	4
2:B:440:PHE:CE2	2:B:441:TYR:CE1	0.63	2.85	7	2
1:A:28:A:O2'	1:A:29:U:H5'	0.63	1.93	6	9
2:B:378:ILE:CG2	2:B:441:TYR:CG	0.63	2.81	8	1
1:A:18:A:N3	2:B:372:ARG:CG	0.63	2.61	8	4
1:A:15:A:O2'	1:A:18:A:N6	0.63	2.31	15	6
1:A:26:G:O2'	1:A:27:U:C5'	0.63	2.46	6	11
2:B:440:PHE:CE2	2:B:441:TYR:CZ	0.63	2.86	7	2
2:B:380:TYR:CD1	2:B:381:ALA:N	0.63	2.67	14	1
1:A:17:A:O2'	1:A:18:A:C1'	0.62	2.46	12	5
2:B:406:VAL:HG21	2:B:412:LEU:HD22	0.62	1.72	14	1
1:A:17:A:O2'	1:A:18:A:O4'	0.62	2.18	1	11
2:B:420:ILE:HD12	2:B:421:LYS:N	0.62	2.08	5	3
2:B:432:LEU:HD13	2:B:432:LEU:H	0.62	1.55	6	3
1:A:3:G:HO2'	1:A:4:A:C5'	0.62	2.07	13	4
2:B:390:VAL:HG23	2:B:401:ILE:CG2	0.62	2.24	4	7
2:B:422:ILE:O	2:B:426:ARG:CB	0.62	2.48	6	14
2:B:419:ASN:O	2:B:420:ILE:CG2	0.62	2.48	14	6
1:A:14:C:C5	1:A:15:A:C8	0.61	2.87	13	10

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:23:G:C5	1:A:24:U:C5	0.61	2.88	13	6
1:A:3:G:O2'	1:A:4:A:O5'	0.61	2.18	4	12
2:B:381:ALA:O	2:B:382:SER:CB	0.61	2.49	12	6
2:B:432:LEU:HD22	2:B:432:LEU:C	0.61	2.21	11	1
2:B:412:LEU:N	2:B:412:LEU:HD13	0.61	2.08	2	3
2:B:417:GLY:C	2:B:422:ILE:HD13	0.61	2.20	7	11
1:A:16:G:N2	1:A:16:G:OP2	0.61	2.33	6	6
1:A:9:A:C6	1:A:10:U:C4	0.61	2.89	13	1
1:A:28:A:O2'	1:A:29:U:O5'	0.61	2.19	11	14
2:B:383:LEU:H	2:B:383:LEU:HD12	0.61	1.56	2	1
1:A:15:A:N7	1:A:16:G:C8	0.61	2.69	4	2
2:B:380:TYR:CD1	2:B:445:ARG:NE	0.61	2.69	5	1
2:B:378:ILE:HG22	2:B:383:LEU:HD22	0.60	1.71	7	1
1:A:4:A:O2'	1:A:5:U:C5'	0.60	2.44	10	5
1:A:19:G:O2'	1:A:20:A:C5'	0.60	2.49	4	3
1:A:28:A:O2'	1:A:29:U:H6	0.60	1.78	8	4
1:A:18:A:O5'	1:A:18:A:C8	0.60	2.53	8	1
1:A:10:U:O2'	1:A:11:G:O5'	0.60	2.20	4	7
2:B:368:MET:CE	2:B:369:ASN:ND2	0.60	2.65	8	2
1:A:14:C:N4	1:A:15:A:C4	0.60	2.69	13	7
1:A:6:A:O2'	1:A:7:C:C5'	0.60	2.45	13	7
1:A:20:A:OP1	2:B:375:TYR:CE2	0.60	2.55	7	4
2:B:385:LEU:CA	2:B:406:VAL:HG12	0.60	2.26	6	8
1:A:16:G:C5'	1:A:17:A:N7	0.60	2.65	8	2
1:A:24:U:O2'	1:A:25:G:O5'	0.60	2.19	7	4
2:B:387:TYR:CD2	2:B:427:ALA:HB1	0.60	2.31	10	2
1:A:1:G:O2'	1:A:2:G:O5'	0.60	2.20	9	5
2:B:388:VAL:HG23	2:B:403:GLU:HB3	0.60	1.71	13	2
2:B:440:PHE:CD1	2:B:440:PHE:C	0.60	2.80	7	5
2:B:432:LEU:C	2:B:432:LEU:CD2	0.60	2.75	11	7
1:A:30:C:N4	1:A:31:U:O4	0.60	2.35	12	5
2:B:421:LYS:CD	2:B:422:ILE:N	0.60	2.65	2	9
1:A:1:G:C8	1:A:1:G:O5'	0.60	2.54	5	1
1:A:25:G:HO2'	1:A:26:G:C5'	0.59	2.10	6	2
1:A:26:G:HO2'	1:A:27:U:C5'	0.59	2.10	13	7
1:A:17:A:OP2	1:A:17:A:H3'	0.59	1.97	4	1
2:B:373:GLN:NE2	2:B:438:LEU:HD22	0.59	2.12	15	2
1:A:8:C:O2'	1:A:9:A:O5'	0.59	2.20	13	3
1:A:19:G:HO2'	1:A:20:A:C5'	0.59	2.10	4	2
1:A:25:G:O2'	1:A:26:G:O5'	0.59	2.19	1	2
1:A:4:A:HO2'	1:A:5:U:C5'	0.59	2.10	4	3

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:15:A:O2'	1:A:18:A:N1	0.59	2.35	2	3
1:A:16:G:OP2	1:A:16:G:N2	0.59	2.34	5	5
2:B:374:LEU:CD2	2:B:432:LEU:HD12	0.59	2.27	10	3
1:A:3:G:O2'	1:A:4:A:H5'	0.59	1.96	6	6
1:A:11:G:O2'	1:A:12:U:O5'	0.59	2.20	10	15
1:A:16:G:OP1	1:A:17:A:N6	0.59	2.35	4	1
2:B:387:TYR:CE1	2:B:404:CYS:SG	0.59	2.95	12	1
1:A:17:A:O2'	1:A:18:A:O5'	0.59	2.20	1	2
2:B:432:LEU:C	2:B:432:LEU:HD22	0.59	2.23	6	4
1:A:21:A:O2'	1:A:22:C:O5'	0.59	2.21	9	10
1:A:31:U:O2'	1:A:32:C:O4'	0.59	2.21	15	6
1:A:15:A:C6	1:A:16:G:N7	0.59	2.71	6	3
1:A:14:C:N4	1:A:15:A:C5	0.59	2.71	13	5
1:A:10:U:O2'	1:A:11:G:O4'	0.58	2.20	4	4
1:A:1:G:N3	1:A:2:G:N7	0.58	2.51	14	2
1:A:16:G:O4'	1:A:18:A:N6	0.58	2.37	1	1
1:A:1:G:N2	1:A:2:G:C4	0.58	2.71	2	4
2:B:372:ARG:O	2:B:376:SER:CB	0.58	2.51	8	12
1:A:13:U:O2'	1:A:14:C:O4'	0.58	2.20	15	10
2:B:429:GLU:O	2:B:432:LEU:CD2	0.58	2.51	9	3
2:B:386:HIS:CD2	2:B:386:HIS:O	0.58	2.57	14	3
2:B:440:PHE:CZ	2:B:444:GLN:OE1	0.58	2.57	5	1
2:B:391:LYS:CB	2:B:401:ILE:CG2	0.58	2.81	14	2
1:A:17:A:O2'	1:A:18:A:OP1	0.58	2.21	4	3
2:B:435:LYS:CG	2:B:436:LYS:N	0.58	2.67	9	12
2:B:380:TYR:CD1	2:B:445:ARG:CD	0.58	2.86	5	2
2:B:383:LEU:N	2:B:383:LEU:CD1	0.58	2.66	15	1
1:A:24:U:C4	1:A:25:G:N7	0.58	2.72	6	3
1:A:11:G:HO2'	1:A:12:U:C5'	0.58	2.11	15	1
1:A:26:G:O2'	1:A:27:U:O5'	0.58	2.21	4	10
2:B:412:LEU:HD21	2:B:437:MET:HG3	0.58	1.76	14	1
1:A:11:G:O2'	1:A:12:U:O4'	0.58	2.21	4	10
2:B:383:LEU:HD23	2:B:383:LEU:N	0.58	2.14	11	2
2:B:374:LEU:HD13	2:B:387:TYR:OH	0.58	1.99	9	3
2:B:378:ILE:O	2:B:379:GLY:C	0.57	2.46	15	5
1:A:20:A:O5'	1:A:20:A:C8	0.57	2.57	6	8
1:A:4:A:O2'	1:A:5:U:O5'	0.57	2.22	12	6
2:B:391:LYS:CB	2:B:401:ILE:HG22	0.57	2.28	5	5
2:B:386:HIS:C	2:B:386:HIS:CD2	0.57	2.81	7	1
2:B:396:VAL:O	2:B:396:VAL:CG2	0.57	2.51	8	1
2:B:383:LEU:O	2:B:385:LEU:N	0.57	2.38	10	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:18:A:N3	2:B:372:ARG:CD	0.57	2.67	1	2
1:A:29:U:C4	1:A:30:C:C4	0.57	2.92	4	1
1:A:17:A:C2'	1:A:18:A:C8	0.57	2.87	1	1
1:A:20:A:O2'	1:A:21:A:O5'	0.57	2.22	11	4
2:B:398:PRO:O	2:B:399:ASN:C	0.57	2.48	13	12
1:A:8:C:N4	1:A:9:A:H62	0.57	1.98	10	6
2:B:374:LEU:HD11	2:B:428:ALA:HA	0.57	1.74	12	1
1:A:16:G:C4'	1:A:17:A:O5'	0.57	2.53	2	1
1:A:20:A:C2	1:A:21:A:C4	0.57	2.92	6	4
2:B:432:LEU:CD2	2:B:432:LEU:C	0.57	2.78	7	1
2:B:440:PHE:CZ	2:B:441:TYR:CE1	0.57	2.92	7	1
2:B:367:ASP:O	2:B:370:ALA:HB3	0.57	2.00	14	3
2:B:411:VAL:O	2:B:413:GLY:N	0.57	2.37	14	2
2:B:421:LYS:HD3	2:B:422:ILE:N	0.57	2.14	4	9
2:B:383:LEU:N	2:B:383:LEU:HD13	0.57	2.14	15	1
1:A:16:G:C1'	1:A:17:A:OP2	0.57	2.52	5	7
1:A:16:G:C4'	1:A:17:A:OP2	0.57	2.53	9	7
2:B:406:VAL:HG21	2:B:412:LEU:CD2	0.57	2.29	14	1
2:B:420:ILE:O	2:B:423:ALA:N	0.57	2.37	9	15
2:B:378:ILE:HG22	2:B:383:LEU:CD1	0.57	2.30	13	2
2:B:390:VAL:O	2:B:391:LYS:CB	0.57	2.52	1	11
2:B:370:ALA:CB	2:B:428:ALA:CB	0.57	2.83	5	1
2:B:368:MET:HE2	2:B:369:ASN:N	0.57	2.15	8	1
2:B:419:ASN:O	2:B:422:ILE:CD1	0.57	2.53	10	1
2:B:404:CYS:O	2:B:412:LEU:N	0.56	2.38	13	8
2:B:380:TYR:CZ	2:B:383:LEU:HD12	0.56	2.33	9	1
2:B:397:ASP:N	2:B:398:PRO:CD	0.56	2.68	13	7
2:B:393:PRO:C	2:B:394:THR:HG22	0.56	2.25	10	2
1:A:25:G:O2'	1:A:26:G:C5'	0.56	2.54	6	2
2:B:391:LYS:HB3	2:B:401:ILE:HG22	0.56	1.76	14	3
2:B:396:VAL:C	2:B:398:PRO:CD	0.56	2.78	13	1
2:B:374:LEU:N	2:B:374:LEU:CD2	0.56	2.68	5	6
1:A:16:G:OP2	1:A:16:G:N3	0.56	2.38	6	2
1:A:23:G:O2'	1:A:24:U:O5'	0.56	2.24	8	8
2:B:383:LEU:HD22	2:B:383:LEU:C	0.56	2.25	15	1
1:A:15:A:C2'	1:A:16:G:O5'	0.56	2.54	4	1
1:A:25:G:C6	1:A:26:G:C5	0.56	2.94	11	1
2:B:383:LEU:HD11	2:B:385:LEU:HD12	0.56	1.77	14	1
2:B:387:TYR:OH	2:B:431:ALA:CB	0.56	2.54	2	3
1:A:6:A:O2'	1:A:7:C:O5'	0.56	2.24	4	4
2:B:368:MET:CE	2:B:369:ASN:CG	0.56	2.79	14	3

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:25:G:C2	1:A:26:G:N7	0.56	2.74	6	2
1:A:13:U:O2'	1:A:14:C:O5'	0.56	2.24	15	9
1:A:16:G:OP1	2:B:368:MET:HE1	0.56	2.00	2	1
2:B:386:HIS:CB	2:B:405:ARG:O	0.56	2.54	12	1
1:A:18:A:O2'	1:A:19:G:O4'	0.56	2.21	9	5
1:A:8:C:C2	1:A:9:A:N7	0.56	2.74	3	1
2:B:380:TYR:CE1	2:B:445:ARG:NE	0.56	2.74	5	1
2:B:432:LEU:HB2	2:B:438:LEU:HD11	0.56	1.78	6	1
2:B:387:TYR:CE2	2:B:404:CYS:SG	0.56	2.99	7	2
2:B:437:MET:HE3	2:B:441:TYR:CE2	0.56	2.35	9	2
2:B:385:LEU:HD22	2:B:387:TYR:CE1	0.56	2.36	9	1
2:B:385:LEU:CD2	2:B:387:TYR:CE1	0.55	2.89	12	1
1:A:22:C:C2'	1:A:23:G:O5'	0.55	2.55	7	10
2:B:374:LEU:HD21	2:B:432:LEU:HD12	0.55	1.78	10	2
2:B:378:ILE:O	2:B:380:TYR:N	0.55	2.39	8	4
1:A:17:A:O2'	1:A:18:A:C8	0.55	2.59	1	1
2:B:412:LEU:HB3	2:B:437:MET:HE2	0.55	1.76	10	2
1:A:16:G:O2'	1:A:17:A:OP2	0.55	2.22	2	1
1:A:18:A:N3	2:B:372:ARG:HG2	0.55	2.16	8	3
2:B:380:TYR:O	2:B:381:ALA:CB	0.55	2.55	2	6
1:A:21:A:H8	1:A:21:A:O5'	0.55	1.85	1	1
2:B:398:PRO:O	2:B:399:ASN:O	0.55	2.25	15	4
1:A:7:C:C4	1:A:8:C:N4	0.55	2.75	1	3
2:B:367:ASP:O	2:B:370:ALA:N	0.55	2.40	4	8
2:B:373:GLN:HB3	2:B:432:LEU:HD22	0.55	1.79	5	3
1:A:24:U:HO2'	1:A:25:G:C5'	0.55	2.14	4	2
2:B:378:ILE:HG22	2:B:383:LEU:CD2	0.55	2.31	7	1
2:B:412:LEU:HD12	2:B:437:MET:CE	0.55	2.30	7	1
2:B:368:MET:HE2	2:B:369:ASN:CG	0.55	2.25	8	2
2:B:390:VAL:CG2	2:B:401:ILE:O	0.55	2.55	14	2
2:B:380:TYR:CG	2:B:445:ARG:HD3	0.55	2.37	4	6
2:B:401:ILE:HD12	2:B:415:GLY:C	0.55	2.26	2	3
2:B:406:VAL:HG23	2:B:410:THR:HB	0.55	1.78	8	7
2:B:437:MET:HE2	2:B:438:LEU:HD23	0.55	1.78	9	1
2:B:411:VAL:O	2:B:412:LEU:HD22	0.55	2.02	15	1
2:B:367:ASP:OD1	2:B:367:ASP:N	0.55	2.40	13	3
2:B:385:LEU:HD21	2:B:387:TYR:CE1	0.55	2.37	12	2
1:A:16:G:HO2'	1:A:17:A:P	0.55	2.25	14	1
1:A:17:A:C2	2:B:372:ARG:NH1	0.55	2.75	2	2
1:A:18:A:N3	2:B:372:ARG:HG3	0.55	2.17	13	4
2:B:380:TYR:CD1	2:B:445:ARG:CG	0.55	2.90	7	2

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:27:U:H6	1:A:27:U:O5'	0.55	1.84	11	2
2:B:406:VAL:O	2:B:408:ASP:N	0.55	2.40	7	7
2:B:406:VAL:HG22	2:B:410:THR:HB	0.55	1.79	15	2
2:B:378:ILE:HG13	2:B:438:LEU:HD23	0.54	1.79	2	2
1:A:5:U:O2'	1:A:6:A:H5'	0.54	2.02	10	4
1:A:20:A:OP1	2:B:375:TYR:CD2	0.54	2.61	5	3
1:A:21:A:O2'	1:A:22:C:O4'	0.54	2.22	6	1
2:B:419:ASN:O	2:B:420:ILE:CG1	0.54	2.55	14	6
1:A:8:C:C4	1:A:9:A:N7	0.54	2.75	10	8
2:B:380:TYR:OH	2:B:441:TYR:CD1	0.54	2.60	15	1
1:A:12:U:O5'	1:A:12:U:H6	0.54	1.85	15	9
2:B:402:VAL:CG2	2:B:423:ALA:C	0.54	2.81	8	9
2:B:373:GLN:OE1	2:B:438:LEU:HD13	0.54	2.03	3	2
2:B:378:ILE:O	2:B:383:LEU:CD1	0.54	2.55	12	3
2:B:368:MET:HE2	2:B:369:ASN:H	0.54	1.62	8	1
2:B:419:ASN:O	2:B:419:ASN:CG	0.54	2.50	9	2
2:B:374:LEU:O	2:B:379:GLY:N	0.54	2.41	1	4
1:A:20:A:C2'	1:A:21:A:O4'	0.54	2.54	8	5
1:A:15:A:C2'	1:A:18:A:H61	0.54	2.16	6	6
2:B:401:ILE:CD1	2:B:415:GLY:O	0.54	2.55	11	3
1:A:17:A:C2	2:B:372:ARG:NH2	0.54	2.76	9	1
2:B:380:TYR:OH	2:B:444:GLN:CG	0.54	2.56	11	1
1:A:10:U:O5'	1:A:10:U:H6	0.54	1.86	5	3
1:A:25:G:N3	1:A:26:G:C8	0.54	2.76	6	2
2:B:370:ALA:CB	2:B:428:ALA:HB1	0.54	2.32	7	2
2:B:380:TYR:CE2	2:B:383:LEU:CD1	0.54	2.81	9	1
2:B:376:SER:O	2:B:377:LEU:HD22	0.54	2.02	15	1
2:B:420:ILE:O	2:B:423:ALA:CB	0.54	2.54	9	8
2:B:401:ILE:HD11	2:B:414:THR:HG22	0.54	1.79	11	2
2:B:396:VAL:O	2:B:396:VAL:HG22	0.54	2.03	8	1
2:B:419:ASN:C	2:B:420:ILE:CG2	0.54	2.81	7	6
2:B:393:PRO:C	2:B:394:THR:CG2	0.54	2.80	10	3
1:A:5:U:O3'	2:B:393:PRO:CG	0.54	2.56	15	1
2:B:370:ALA:O	2:B:373:GLN:N	0.53	2.41	3	9
2:B:419:ASN:N	2:B:422:ILE:HD11	0.53	2.17	12	9
2:B:370:ALA:O	2:B:371:LYS:C	0.53	2.50	11	14
2:B:399:ASN:O	2:B:399:ASN:ND2	0.53	2.41	12	3
2:B:421:LYS:O	2:B:424:GLY:N	0.53	2.41	1	8
2:B:380:TYR:CE1	2:B:383:LEU:HD13	0.53	2.38	7	1
2:B:394:THR:OG1	2:B:397:ASP:N	0.53	2.41	14	2
1:A:15:A:C2'	1:A:16:G:O4'	0.53	2.54	6	2

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:374:LEU:HD11	2:B:428:ALA:CB	0.53	2.34	9	2
1:A:10:U:O2'	1:A:11:G:H5'	0.53	2.03	11	3
1:A:31:U:H5'	2:B:396:VAL:HG12	0.53	1.80	5	1
2:B:401:ILE:CG1	2:B:415:GLY:O	0.53	2.57	7	3
1:A:17:A:H2'	1:A:18:A:O4'	0.53	2.03	15	1
1:A:19:G:O2'	1:A:20:A:O5'	0.53	2.26	4	2
2:B:412:LEU:N	2:B:412:LEU:CD1	0.53	2.71	15	4
2:B:401:ILE:HG13	2:B:402:VAL:N	0.53	2.19	3	6
2:B:433:ARG:CG	2:B:433:ARG:O	0.53	2.57	11	3
1:A:24:U:O5'	1:A:24:U:H6	0.53	1.86	5	1
1:A:8:C:HO2'	1:A:9:A:C5'	0.53	2.17	14	2
2:B:390:VAL:O	2:B:401:ILE:CG2	0.53	2.56	13	1
1:A:25:G:C4	1:A:26:G:N7	0.53	2.76	6	2
1:A:27:U:C2'	1:A:28:A:O5'	0.53	2.56	4	9
2:B:431:ALA:O	2:B:437:MET:CE	0.53	2.54	14	4
1:A:16:G:H2'	1:A:16:G:N3	0.53	2.18	2	1
2:B:383:LEU:HD22	2:B:383:LEU:O	0.53	2.03	15	1
1:A:9:A:N6	1:A:25:G:O6	0.53	2.42	1	2
1:A:18:A:N3	2:B:372:ARG:HD2	0.53	2.19	9	2
1:A:15:A:O2'	2:B:368:MET:SD	0.53	2.65	9	1
2:B:370:ALA:HB1	2:B:428:ALA:HB3	0.53	1.78	12	2
2:B:385:LEU:HA	2:B:406:VAL:CG1	0.53	2.34	8	12
2:B:441:TYR:O	2:B:444:GLN:N	0.53	2.41	6	4
1:A:7:C:C4	1:A:8:C:C5	0.53	2.96	13	3
2:B:389:THR:CG2	2:B:389:THR:O	0.53	2.56	11	1
2:B:391:LYS:O	2:B:392:LYS:C	0.52	2.52	5	12
2:B:399:ASN:HA	2:B:417:GLY:O	0.52	2.03	1	11
1:A:28:A:HO2'	1:A:29:U:H6	0.52	1.47	14	2
1:A:14:C:N4	1:A:15:A:C2	0.52	2.78	8	3
2:B:401:ILE:CD1	2:B:414:THR:OG1	0.52	2.56	13	2
2:B:414:THR:N	2:B:430:ASN:OD1	0.52	2.42	14	1
1:A:17:A:O2'	2:B:372:ARG:NH1	0.52	2.42	9	1
2:B:380:TYR:CD1	2:B:445:ARG:HG2	0.52	2.39	15	3
2:B:421:LYS:CD	2:B:421:LYS:C	0.52	2.82	12	6
1:A:12:U:O5'	1:A:12:U:C6	0.52	2.53	5	1
2:B:385:LEU:C	2:B:385:LEU:HD23	0.52	2.29	6	1
2:B:427:ALA:O	2:B:430:ASN:CB	0.52	2.57	14	1
2:B:383:LEU:HD13	2:B:383:LEU:H	0.52	1.64	15	1
2:B:428:ALA:O	2:B:431:ALA:N	0.52	2.42	2	5
1:A:22:C:O5'	1:A:22:C:C6	0.52	2.54	10	5
2:B:405:ARG:CG	2:B:406:VAL:N	0.52	2.73	8	3

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:393:PRO:O	2:B:394:THR:HG22	0.52	2.04	10	2
2:B:373:GLN:HG2	2:B:377:LEU:HD22	0.52	1.81	8	1
2:B:406:VAL:O	2:B:409:GLY:N	0.52	2.39	1	5
2:B:412:LEU:HD13	2:B:412:LEU:H	0.52	1.65	11	2
2:B:367:ASP:HA	2:B:425:ILE:HG23	0.52	1.80	5	1
1:A:17:A:H1'	1:A:18:A:OP1	0.52	2.05	12	1
2:B:404:CYS:CB	2:B:413:GLY:O	0.52	2.57	15	1
2:B:388:VAL:O	2:B:390:VAL:N	0.52	2.43	13	1
2:B:402:VAL:CG2	2:B:423:ALA:O	0.52	2.58	14	9
1:A:18:A:C2'	1:A:19:G:O4'	0.52	2.57	11	9
2:B:374:LEU:HD21	2:B:432:LEU:CD1	0.52	2.34	10	1
2:B:425:ILE:N	2:B:425:ILE:CD1	0.52	2.73	3	4
2:B:406:VAL:HG21	2:B:441:TYR:OH	0.52	2.05	8	2
1:A:1:G:C2	1:A:2:G:C8	0.52	2.98	14	2
2:B:430:ASN:O	2:B:433:ARG:CG	0.51	2.57	1	1
1:A:12:U:C2'	1:A:13:U:O5'	0.51	2.59	5	12
1:A:25:G:O6	1:A:26:G:O6	0.51	2.28	11	4
2:B:432:LEU:O	2:B:438:LEU:CD1	0.51	2.56	2	1
2:B:429:GLU:HA	2:B:432:LEU:HD21	0.51	1.82	7	2
2:B:391:LYS:HB3	2:B:401:ILE:CG2	0.51	2.35	14	1
2:B:373:GLN:NE2	2:B:373:GLN:O	0.51	2.44	12	4
2:B:383:LEU:O	2:B:384:ARG:CB	0.51	2.58	1	5
2:B:401:ILE:HD11	2:B:414:THR:HG23	0.51	1.80	6	1
2:B:429:GLU:O	2:B:433:ARG:N	0.51	2.42	6	2
2:B:383:LEU:O	2:B:384:ARG:C	0.51	2.53	14	4
2:B:407:GLY:O	2:B:408:ASP:CG	0.51	2.53	13	1
2:B:394:THR:O	2:B:395:ALA:HB2	0.51	2.05	15	1
2:B:372:ARG:CZ	2:B:376:SER:OG	0.51	2.59	5	1
2:B:426:ARG:HG3	2:B:427:ALA:N	0.51	2.21	13	1
2:B:404:CYS:SG	2:B:413:GLY:N	0.51	2.84	6	1
2:B:419:ASN:OD1	2:B:421:LYS:N	0.51	2.43	14	1
2:B:435:LYS:HG3	2:B:436:LYS:N	0.51	2.20	9	8
2:B:425:ILE:CD1	2:B:425:ILE:N	0.51	2.73	12	1
2:B:414:THR:O	2:B:430:ASN:CG	0.51	2.54	15	8
1:A:24:U:O4	1:A:25:G:O6	0.51	2.29	11	4
1:A:18:A:O2'	2:B:376:SER:OG	0.51	2.23	9	4
1:A:14:C:C5	1:A:15:A:C5	0.51	2.98	10	2
2:B:383:LEU:HD21	2:B:441:TYR:CE1	0.51	2.41	13	2
2:B:387:TYR:CZ	2:B:404:CYS:SG	0.51	2.98	9	5
1:A:31:U:O2'	1:A:32:C:O5'	0.51	2.29	2	4
2:B:383:LEU:HD23	2:B:441:TYR:CD1	0.51	2.40	2	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:397:ASP:N	2:B:398:PRO:HD3	0.51	2.21	10	2
2:B:411:VAL:O	2:B:412:LEU:HB2	0.51	2.04	15	2
1:A:14:C:C5	1:A:15:A:N7	0.51	2.79	1	4
2:B:405:ARG:HA	2:B:410:THR:O	0.51	2.06	11	11
2:B:425:ILE:H	2:B:425:ILE:HD12	0.51	1.66	1	2
2:B:367:ASP:HB3	2:B:425:ILE:HD12	0.51	1.82	5	1
1:A:17:A:C3'	1:A:18:A:C8	0.51	2.94	12	1
2:B:367:ASP:O	2:B:368:MET:C	0.50	2.54	12	12
2:B:419:ASN:O	2:B:420:ILE:HG13	0.50	2.06	11	8
1:A:17:A:HO2'	1:A:18:A:C1'	0.50	2.18	12	1
2:B:422:ILE:O	2:B:426:ARG:HB3	0.50	2.06	7	9
1:A:24:U:O2'	1:A:25:G:C5'	0.50	2.60	2	4
2:B:388:VAL:HG23	2:B:403:GLU:HB2	0.50	1.83	3	2
2:B:403:GLU:CG	2:B:414:THR:OG1	0.50	2.59	6	1
2:B:378:ILE:HG23	2:B:441:TYR:CG	0.50	2.41	8	1
2:B:411:VAL:O	2:B:412:LEU:CB	0.50	2.57	15	1
2:B:412:LEU:CD1	2:B:437:MET:SD	0.50	2.98	13	5
1:A:28:A:HO2'	1:A:29:U:C5'	0.50	2.19	5	1
1:A:29:U:C2'	1:A:30:C:O5'	0.50	2.59	7	4
1:A:5:U:O2'	2:B:393:PRO:HB2	0.50	2.05	14	4
2:B:414:THR:O	2:B:430:ASN:ND2	0.50	2.44	8	2
1:A:21:A:H2'	1:A:22:C:C6	0.50	2.42	8	13
2:B:386:HIS:O	2:B:405:ARG:O	0.50	2.30	11	2
1:A:31:U:O4'	2:B:396:VAL:HG11	0.50	2.07	13	1
2:B:390:VAL:CG2	2:B:401:ILE:HG23	0.50	2.36	12	5
1:A:6:A:HO2'	1:A:7:C:C5'	0.50	2.19	14	1
2:B:385:LEU:HD22	2:B:387:TYR:HE1	0.50	1.66	9	1
2:B:411:VAL:C	2:B:412:LEU:HD13	0.50	2.31	15	1
1:A:15:A:N7	1:A:16:G:N7	0.50	2.60	7	2
1:A:17:A:C4'	1:A:18:A:OP1	0.50	2.60	14	2
2:B:370:ALA:O	2:B:372:ARG:N	0.50	2.45	8	1
1:A:16:G:O2'	1:A:17:A:OP1	0.50	2.29	13	2
2:B:369:ASN:C	2:B:369:ASN:ND2	0.50	2.70	15	1
2:B:434:ASP:HB2	2:B:437:MET:HE3	0.49	1.84	7	2
2:B:390:VAL:O	2:B:401:ILE:HG23	0.49	2.06	13	1
2:B:406:VAL:HG22	2:B:410:THR:CB	0.49	2.37	15	1
2:B:374:LEU:O	2:B:378:ILE:C	0.49	2.55	10	6
2:B:412:LEU:HD22	2:B:412:LEU:H	0.49	1.67	5	1
2:B:384:ARG:O	2:B:386:HIS:ND1	0.49	2.44	8	2
2:B:429:GLU:O	2:B:432:LEU:HD22	0.49	2.07	8	2
2:B:406:VAL:O	2:B:407:GLY:C	0.49	2.56	2	6

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:405:ARG:HD3	2:B:411:VAL:HG22	0.49	1.83	2	1
2:B:380:TYR:CD1	2:B:445:ARG:HD2	0.49	2.42	5	1
2:B:380:TYR:CD1	2:B:380:TYR:N	0.49	2.80	5	1
2:B:380:TYR:CE1	2:B:383:LEU:N	0.49	2.80	6	1
1:A:8:C:O2'	1:A:9:A:C5'	0.49	2.61	13	1
2:B:367:ASP:C	2:B:371:LYS:CD	0.49	2.86	9	1
2:B:380:TYR:N	2:B:380:TYR:CD1	0.49	2.80	11	1
1:A:17:A:H4'	1:A:18:A:OP2	0.49	2.07	12	1
2:B:397:ASP:O	2:B:399:ASN:N	0.49	2.45	6	2
1:A:14:C:N4	1:A:15:A:C6	0.49	2.81	3	3
1:A:29:U:C4	1:A:30:C:C5	0.49	3.00	4	1
2:B:391:LYS:O	2:B:391:LYS:CD	0.49	2.61	11	1
1:A:19:G:O2'	1:A:20:A:O4'	0.49	2.24	15	1
2:B:414:THR:OG1	2:B:415:GLY:N	0.49	2.44	15	1
1:A:1:G:N2	1:A:2:G:C5	0.49	2.81	2	4
1:A:29:U:O2	2:B:395:ALA:CB	0.49	2.61	12	2
2:B:410:THR:CG2	2:B:412:LEU:CD1	0.49	2.91	14	1
2:B:434:ASP:CB	2:B:437:MET:HB3	0.48	2.38	6	6
2:B:438:LEU:O	2:B:441:TYR:N	0.48	2.46	11	2
1:A:1:G:O2'	1:A:2:G:H8	0.48	1.90	3	4
2:B:380:TYR:CD2	2:B:383:LEU:HD12	0.48	2.43	8	1
2:B:410:THR:CG2	2:B:412:LEU:HD13	0.48	2.38	14	1
2:B:412:LEU:O	2:B:430:ASN:O	0.48	2.31	14	1
2:B:421:LYS:O	2:B:422:ILE:C	0.48	2.56	1	10
1:A:30:C:O2'	2:B:395:ALA:O	0.48	2.26	12	3
1:A:20:A:O2'	2:B:371:LYS:HG2	0.48	2.08	5	3
2:B:368:MET:CE	2:B:369:ASN:N	0.48	2.76	14	2
2:B:398:PRO:C	2:B:418:ARG:O	0.48	2.56	14	1
2:B:384:ARG:O	2:B:385:LEU:C	0.48	2.56	9	4
2:B:399:ASN:OD1	2:B:399:ASN:O	0.48	2.32	10	2
2:B:415:GLY:HA2	2:B:426:ARG:CG	0.48	2.38	4	2
2:B:434:ASP:O	2:B:435:LYS:C	0.48	2.57	6	3
2:B:387:TYR:CZ	2:B:404:CYS:HB3	0.48	2.43	7	1
2:B:419:ASN:CG	2:B:422:ILE:HD11	0.48	2.33	6	2
2:B:422:ILE:O	2:B:426:ARG:HB2	0.48	2.08	4	8
2:B:406:VAL:HG23	2:B:408:ASP:OD1	0.48	2.07	3	1
2:B:414:THR:O	2:B:430:ASN:OD1	0.48	2.32	11	3
1:A:19:G:H21	2:B:371:LYS:NZ	0.48	2.07	6	1
2:B:374:LEU:CD2	2:B:432:LEU:HD23	0.48	2.36	15	2
1:A:15:A:H2'	1:A:16:G:O5'	0.48	2.07	4	1
2:B:380:TYR:CD1	2:B:445:ARG:HD3	0.48	2.44	4	2

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:387:TYR:HE2	2:B:427:ALA:HB1	0.48	1.63	10	1
2:B:425:ILE:O	2:B:428:ALA:HB3	0.48	2.08	14	3
2:B:398:PRO:O	2:B:400:SER:N	0.48	2.46	13	1
2:B:404:CYS:CB	2:B:413:GLY:HA3	0.48	2.38	14	1
1:A:20:A:C2'	1:A:21:A:O5'	0.48	2.62	2	2
1:A:29:U:O5'	1:A:29:U:H6	0.48	1.92	3	1
2:B:422:ILE:N	2:B:422:ILE:HD12	0.48	2.23	6	5
2:B:436:LYS:O	2:B:440:PHE:CB	0.48	2.62	12	2
2:B:381:ALA:O	2:B:382:SER:C	0.48	2.56	6	1
2:B:394:THR:OG1	2:B:397:ASP:CG	0.48	2.57	8	1
1:A:17:A:O4'	1:A:17:A:OP1	0.48	2.32	10	1
2:B:406:VAL:CG2	2:B:410:THR:HB	0.48	2.39	15	1
2:B:378:ILE:HG23	2:B:441:TYR:HB2	0.48	1.86	2	1
2:B:390:VAL:O	2:B:401:ILE:O	0.48	2.31	7	3
1:A:18:A:C8	1:A:18:A:OP2	0.48	2.67	15	1
1:A:2:G:C6	1:A:3:G:C5	0.48	3.02	2	3
1:A:5:U:C4'	2:B:398:PRO:HB3	0.48	2.39	4	3
2:B:390:VAL:O	2:B:391:LYS:HB3	0.48	2.08	4	5
2:B:391:LYS:HB2	2:B:401:ILE:CG2	0.48	2.38	6	4
2:B:385:LEU:HD12	2:B:406:VAL:HG12	0.48	1.85	12	1
2:B:373:GLN:HG3	2:B:432:LEU:CB	0.47	2.39	4	8
1:A:30:C:C2'	1:A:31:U:O5'	0.47	2.62	5	11
1:A:10:U:HO2'	1:A:11:G:C5'	0.47	2.21	12	2
2:B:419:ASN:O	2:B:420:ILE:C	0.47	2.57	10	1
1:A:25:G:N3	1:A:26:G:N7	0.47	2.62	6	2
2:B:367:ASP:OD1	2:B:425:ILE:HD12	0.47	2.09	4	1
2:B:380:TYR:CE2	2:B:382:SER:HB2	0.47	2.44	5	1
2:B:429:GLU:O	2:B:433:ARG:CB	0.47	2.62	6	1
1:A:5:U:O2'	1:A:6:A:C5'	0.47	2.61	10	1
1:A:7:C:C4	1:A:8:C:C4	0.47	3.03	3	4
1:A:16:G:C4'	1:A:18:A:N6	0.47	2.78	1	1
2:B:412:LEU:CD1	2:B:437:MET:HE2	0.47	2.35	7	1
2:B:367:ASP:N	2:B:367:ASP:OD1	0.47	2.45	8	2
2:B:380:TYR:CE1	2:B:445:ARG:HG2	0.47	2.44	15	2
2:B:401:ILE:HD13	2:B:401:ILE:C	0.47	2.34	9	1
2:B:368:MET:HG2	2:B:369:ASN:N	0.47	2.24	15	1
2:B:373:GLN:CB	2:B:432:LEU:HD22	0.47	2.39	1	1
2:B:377:LEU:O	2:B:378:ILE:CD1	0.47	2.58	15	2
2:B:380:TYR:O	2:B:381:ALA:HB3	0.47	2.09	6	1
2:B:432:LEU:CB	2:B:438:LEU:HD11	0.47	2.39	6	1
2:B:420:ILE:C	2:B:420:ILE:CD1	0.47	2.84	10	5

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:388:VAL:CG2	2:B:403:GLU:O	0.47	2.62	7	1
2:B:373:GLN:O	2:B:373:GLN:NE2	0.47	2.48	10	1
2:B:419:ASN:C	2:B:421:LYS:N	0.47	2.72	10	1
2:B:408:ASP:OD1	2:B:408:ASP:O	0.47	2.32	13	1
2:B:427:ALA:O	2:B:430:ASN:HB2	0.47	2.09	14	7
2:B:380:TYR:CD2	2:B:445:ARG:HD3	0.47	2.44	6	3
2:B:374:LEU:N	2:B:374:LEU:HD23	0.47	2.25	5	1
2:B:420:ILE:CD1	2:B:421:LYS:N	0.47	2.76	5	1
2:B:372:ARG:CZ	2:B:372:ARG:HB3	0.47	2.39	6	1
1:A:30:C:C5	1:A:31:U:C5	0.47	3.02	7	3
2:B:419:ASN:O	2:B:419:ASN:OD1	0.47	2.32	12	3
2:B:410:THR:HG22	2:B:412:LEU:CD1	0.47	2.39	11	3
2:B:408:ASP:OD1	2:B:408:ASP:C	0.47	2.58	3	1
2:B:426:ARG:O	2:B:427:ALA:C	0.47	2.58	11	3
1:A:19:G:H21	2:B:371:LYS:CE	0.47	2.23	8	1
1:A:1:G:O5'	1:A:1:G:C8	0.47	2.52	10	1
2:B:405:ARG:O	2:B:405:ARG:HG3	0.47	2.09	12	1
1:A:9:A:C2'	1:A:10:U:O5'	0.47	2.63	13	2
2:B:383:LEU:HD23	2:B:406:VAL:HG11	0.47	1.87	15	1
2:B:378:ILE:HG13	2:B:438:LEU:CD2	0.47	2.40	12	4
1:A:24:U:O2'	1:A:25:G:H5'	0.47	2.10	3	2
2:B:396:VAL:O	2:B:397:ASP:OD1	0.47	2.33	11	2
2:B:399:ASN:HB2	2:B:417:GLY:O	0.47	2.10	3	1
2:B:404:CYS:SG	2:B:413:GLY:C	0.47	2.98	8	2
2:B:393:PRO:HA	2:B:398:PRO:HA	0.47	1.86	15	1
1:A:7:C:N4	1:A:8:C:H41	0.46	2.04	13	4
2:B:387:TYR:CE2	2:B:404:CYS:HB3	0.46	2.44	5	3
2:B:416:VAL:O	2:B:426:ARG:NH1	0.46	2.48	13	1
2:B:437:MET:O	2:B:438:LEU:C	0.46	2.59	4	1
2:B:441:TYR:O	2:B:442:ALA:C	0.46	2.59	5	5
2:B:404:CYS:HB3	2:B:413:GLY:N	0.46	2.26	14	1
2:B:373:GLN:O	2:B:377:LEU:HB2	0.46	2.10	14	12
2:B:412:LEU:O	2:B:434:ASP:OD2	0.46	2.33	13	2
2:B:368:MET:HA	2:B:371:LYS:CG	0.46	2.40	8	1
1:A:31:U:C4'	2:B:396:VAL:HG11	0.46	2.40	13	1
2:B:419:ASN:N	2:B:419:ASN:OD1	0.46	2.48	8	2
2:B:373:GLN:O	2:B:377:LEU:CB	0.46	2.63	4	3
2:B:432:LEU:HD13	2:B:432:LEU:N	0.46	2.25	10	1
2:B:405:ARG:CA	2:B:410:THR:O	0.46	2.63	3	3
2:B:372:ARG:O	2:B:376:SER:HB3	0.46	2.11	6	10
2:B:412:LEU:HG	2:B:437:MET:CE	0.46	2.39	3	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:367:ASP:HB3	2:B:425:ILE:CD1	0.46	2.41	5	1
2:B:429:GLU:O	2:B:433:ARG:HB2	0.46	2.10	6	4
2:B:436:LYS:O	2:B:440:PHE:HB3	0.46	2.11	12	1
2:B:368:MET:HE3	2:B:369:ASN:N	0.46	2.25	14	1
2:B:370:ALA:HA	2:B:432:LEU:HD22	0.46	1.86	14	1
2:B:383:LEU:HD22	2:B:406:VAL:HG11	0.46	1.87	5	2
1:A:4:A:H2'	1:A:5:U:C6	0.46	2.46	13	11
1:A:27:U:H2'	1:A:28:A:O5'	0.46	2.10	4	3
1:A:16:G:O2'	1:A:17:A:P	0.46	2.74	14	2
2:B:367:ASP:CG	2:B:425:ILE:HG13	0.46	2.36	3	1
2:B:370:ALA:C	2:B:372:ARG:N	0.46	2.71	8	1
2:B:437:MET:HE3	2:B:441:TYR:HE2	0.46	1.69	9	1
2:B:435:LYS:HG2	2:B:436:LYS:N	0.46	2.26	10	3
2:B:428:ALA:O	2:B:429:GLU:C	0.46	2.58	14	1
2:B:420:ILE:O	2:B:421:LYS:C	0.46	2.59	9	10
2:B:383:LEU:O	2:B:384:ARG:HB3	0.46	2.11	4	2
1:A:23:G:C2'	1:A:24:U:O5'	0.45	2.65	1	10
2:B:421:LYS:HD3	2:B:421:LYS:C	0.45	2.36	4	3
1:A:7:C:O5'	1:A:7:C:C6	0.45	2.58	1	1
1:A:22:C:O3'	2:B:421:LYS:HE3	0.45	2.11	7	2
1:A:21:A:HO2'	1:A:22:C:C5'	0.45	2.24	5	2
1:A:18:A:O2'	2:B:376:SER:CB	0.45	2.64	11	2
2:B:404:CYS:SG	2:B:412:LEU:HD23	0.45	2.51	12	2
2:B:429:GLU:HA	2:B:432:LEU:HD22	0.45	1.87	9	1
2:B:401:ILE:HA	2:B:415:GLY:O	0.45	2.11	2	5
1:A:16:G:OP2	1:A:16:G:C2	0.45	2.69	6	1
2:B:419:ASN:ND2	2:B:422:ILE:HG13	0.45	2.27	12	1
1:A:7:C:O2'	1:A:8:C:H5'	0.45	2.11	14	1
1:A:17:A:O2'	1:A:18:A:C4	0.45	2.68	3	1
2:B:415:GLY:CA	2:B:426:ARG:CG	0.45	2.94	4	1
2:B:426:ARG:HG3	2:B:430:ASN:ND2	0.45	2.26	15	1
1:A:15:A:C2	1:A:19:G:O6	0.45	2.69	13	3
2:B:372:ARG:O	2:B:373:GLN:C	0.45	2.59	1	1
2:B:432:LEU:CA	2:B:438:LEU:HD21	0.45	2.37	2	1
2:B:428:ALA:O	2:B:432:LEU:CD1	0.45	2.61	3	1
2:B:401:ILE:HG13	2:B:415:GLY:O	0.45	2.12	11	3
2:B:397:ASP:CG	2:B:399:ASN:OD1	0.45	2.59	9	1
1:A:20:A:O4'	2:B:371:LYS:CB	0.45	2.65	10	1
2:B:368:MET:HE2	2:B:369:ASN:ND2	0.45	2.27	2	1
2:B:393:PRO:HA	2:B:398:PRO:O	0.45	2.11	2	1
2:B:383:LEU:C	2:B:385:LEU:N	0.45	2.75	10	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:21:A:O2'	1:A:22:C:H5'	0.45	2.09	1	2
1:A:29:U:C2'	1:A:30:C:C5'	0.45	2.94	9	3
2:B:399:ASN:CA	2:B:417:GLY:O	0.45	2.65	3	1
2:B:420:ILE:HG13	2:B:421:LYS:N	0.45	2.27	4	4
2:B:398:PRO:HB2	2:B:418:ARG:O	0.45	2.11	2	1
2:B:419:ASN:O	2:B:420:ILE:CB	0.45	2.65	15	6
2:B:367:ASP:CG	2:B:425:ILE:CG1	0.45	2.90	3	1
2:B:372:ARG:O	2:B:376:SER:HB2	0.45	2.12	12	3
2:B:381:ALA:O	2:B:382:SER:HB2	0.45	2.10	4	1
1:A:2:G:C2'	1:A:3:G:O5'	0.45	2.65	9	1
1:A:9:A:C5	1:A:10:U:C5	0.45	3.05	13	1
2:B:405:ARG:HA	2:B:411:VAL:O	0.45	2.12	15	1
1:A:17:A:H2'	1:A:18:A:C8	0.45	2.47	1	1
2:B:421:LYS:C	2:B:423:ALA:N	0.45	2.71	7	4
1:A:22:C:H2'	1:A:23:G:O5'	0.45	2.12	7	2
2:B:385:LEU:HG	2:B:406:VAL:CG1	0.45	2.41	14	2
2:B:400:SER:O	2:B:416:VAL:HA	0.45	2.12	10	1
1:A:17:A:C4'	1:A:18:A:OP2	0.45	2.65	12	1
2:B:403:GLU:HG2	2:B:404:CYS:N	0.45	2.27	14	1
2:B:393:PRO:HA	2:B:398:PRO:CA	0.45	2.42	15	1
2:B:368:MET:O	2:B:369:ASN:C	0.44	2.59	6	2
2:B:383:LEU:HD12	2:B:385:LEU:HD12	0.44	1.87	14	1
2:B:376:SER:C	2:B:377:LEU:CD2	0.44	2.86	15	1
2:B:381:ALA:O	2:B:382:SER:HB3	0.44	2.13	12	2
2:B:399:ASN:CB	2:B:417:GLY:O	0.44	2.66	3	1
2:B:444:GLN:O	2:B:445:ARG:C	0.44	2.60	3	1
2:B:439:ASP:O	2:B:443:LYS:HG3	0.44	2.12	2	1
2:B:393:PRO:HB3	2:B:398:PRO:O	0.44	2.13	7	2
1:A:20:A:O4'	2:B:371:LYS:HB2	0.44	2.13	11	1
2:B:383:LEU:HD23	2:B:441:TYR:CE1	0.44	2.48	2	1
1:A:5:U:O4'	2:B:398:PRO:HB3	0.44	2.12	3	1
2:B:407:GLY:O	2:B:408:ASP:HB3	0.44	2.12	4	1
1:A:26:G:C2'	1:A:27:U:O5'	0.44	2.65	6	1
2:B:429:GLU:HA	2:B:432:LEU:CD2	0.44	2.42	14	1
2:B:437:MET:HG2	2:B:441:TYR:CE2	0.44	2.47	15	1
2:B:405:ARG:HG3	2:B:406:VAL:N	0.44	2.28	5	1
1:A:29:U:O2'	1:A:30:C:O5'	0.44	2.35	6	1
2:B:377:LEU:CD2	2:B:377:LEU:N	0.44	2.80	15	1
2:B:406:VAL:C	2:B:408:ASP:N	0.44	2.76	7	4
1:A:27:U:O5'	1:A:27:U:H6	0.44	1.95	10	3
2:B:367:ASP:C	2:B:371:LYS:HD2	0.44	2.37	9	2

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:373:GLN:CG	2:B:432:LEU:HB3	0.44	2.42	5	2
2:B:386:HIS:HB3	2:B:405:ARG:O	0.44	2.12	12	1
2:B:401:ILE:CG1	2:B:402:VAL:N	0.44	2.80	12	2
2:B:397:ASP:O	2:B:398:PRO:C	0.44	2.60	2	1
1:A:5:U:C2'	1:A:6:A:O5'	0.44	2.66	10	1
2:B:383:LEU:O	2:B:406:VAL:HG12	0.44	2.12	14	1
1:A:6:A:H2'	1:A:7:C:C6	0.44	2.47	13	8
2:B:415:GLY:CA	2:B:426:ARG:HG2	0.44	2.42	1	1
2:B:383:LEU:HD12	2:B:383:LEU:N	0.44	2.26	2	1
2:B:434:ASP:O	2:B:437:MET:N	0.44	2.50	6	1
2:B:396:VAL:C	2:B:397:ASP:OD1	0.44	2.60	8	1
2:B:401:ILE:HD11	2:B:414:THR:HB	0.44	1.90	10	1
2:B:412:LEU:CG	2:B:437:MET:SD	0.44	3.06	11	2
2:B:378:ILE:HG22	2:B:379:GLY:H	0.44	1.73	4	1
1:A:2:G:O2'	1:A:3:G:C5'	0.44	2.63	9	2
2:B:406:VAL:CG2	2:B:412:LEU:HD11	0.44	2.43	10	1
1:A:30:C:H1'	2:B:395:ALA:HB1	0.44	1.89	12	2
2:B:406:VAL:CG2	2:B:410:THR:CB	0.44	2.96	15	1
2:B:374:LEU:HD21	2:B:432:LEU:CD2	0.43	2.43	1	1
2:B:382:SER:O	2:B:382:SER:OG	0.43	2.33	4	1
1:A:14:C:C4	1:A:15:A:C5	0.43	3.06	3	3
1:A:28:A:H2'	1:A:29:U:C6	0.43	2.48	3	2
2:B:405:ARG:CB	2:B:411:VAL:HA	0.43	2.43	3	4
2:B:369:ASN:O	2:B:372:ARG:CB	0.43	2.66	5	1
1:A:17:A:C1'	1:A:18:A:OP1	0.43	2.66	12	1
2:B:394:THR:OG1	2:B:397:ASP:C	0.43	2.62	2	1
2:B:425:ILE:N	2:B:425:ILE:HD12	0.43	2.29	3	1
2:B:441:TYR:HA	2:B:444:GLN:HG2	0.43	1.91	7	5
1:A:11:G:O2'	1:A:12:U:H5'	0.43	2.13	4	1
2:B:385:LEU:HD23	2:B:385:LEU:C	0.43	2.37	4	2
2:B:380:TYR:HB3	2:B:445:ARG:NE	0.43	2.28	7	2
2:B:419:ASN:OD1	2:B:419:ASN:N	0.43	2.51	1	1
2:B:367:ASP:CG	2:B:425:ILE:HD12	0.43	2.38	4	1
1:A:11:G:H2'	1:A:12:U:C6	0.43	2.49	5	1
2:B:380:TYR:CZ	2:B:383:LEU:HG	0.43	2.48	6	1
2:B:399:ASN:N	2:B:418:ARG:O	0.43	2.52	6	2
2:B:391:LYS:CD	2:B:391:LYS:C	0.43	2.91	7	1
1:A:5:U:OP1	2:B:419:ASN:CA	0.43	2.67	9	1
2:B:417:GLY:HA3	2:B:422:ILE:CD1	0.43	2.37	13	2
1:A:19:G:HO2'	1:A:20:A:H8	0.43	1.50	2	1
1:A:15:A:H2'	1:A:16:G:C5'	0.43	2.43	4	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:387:TYR:OH	2:B:404:CYS:SG	0.43	2.77	9	2
1:A:25:G:C5	1:A:26:G:N7	0.43	2.87	11	1
2:B:372:ARG:HD2	2:B:376:SER:CB	0.43	2.44	6	1
2:B:396:VAL:O	2:B:397:ASP:HB3	0.43	2.14	7	1
2:B:404:CYS:O	2:B:411:VAL:HG13	0.43	2.13	7	1
2:B:402:VAL:O	2:B:414:THR:HG23	0.43	2.14	11	1
1:A:11:G:HO2'	1:A:12:U:C4'	0.43	2.27	3	2
2:B:422:ILE:HD12	2:B:422:ILE:H	0.43	1.74	12	3
2:B:411:VAL:HG12	2:B:413:GLY:O	0.43	2.13	6	2
2:B:368:MET:HA	2:B:371:LYS:HD2	0.43	1.91	7	1
2:B:383:LEU:N	2:B:383:LEU:CD2	0.43	2.81	11	1
2:B:428:ALA:C	2:B:430:ASN:N	0.43	2.77	2	4
2:B:432:LEU:HA	2:B:438:LEU:CD2	0.43	2.43	10	2
1:A:5:U:OP1	2:B:419:ASN:CB	0.43	2.67	9	1
2:B:441:TYR:O	2:B:444:GLN:HG3	0.43	2.14	10	1
2:B:391:LYS:C	2:B:391:LYS:CD	0.43	2.92	13	1
1:A:19:G:H2'	1:A:20:A:C8	0.43	2.49	7	4
1:A:23:G:H2'	1:A:24:U:C6	0.43	2.49	15	4
2:B:379:GLY:HA2	2:B:383:LEU:HD13	0.43	1.90	8	1
2:B:410:THR:HG22	2:B:412:LEU:HD13	0.43	1.90	10	1
2:B:404:CYS:HB2	2:B:413:GLY:O	0.43	2.13	15	1
2:B:415:GLY:HA3	2:B:426:ARG:CG	0.42	2.44	9	2
2:B:368:MET:C	2:B:368:MET:SD	0.42	3.01	7	1
2:B:391:LYS:HD3	2:B:392:LYS:N	0.42	2.29	13	1
2:B:411:VAL:C	2:B:413:GLY:N	0.42	2.76	2	3
2:B:387:TYR:HA	2:B:403:GLU:O	0.42	2.14	3	2
2:B:401:ILE:CD1	2:B:402:VAL:N	0.42	2.79	9	1
2:B:396:VAL:C	2:B:398:PRO:HD2	0.42	2.38	13	1
2:B:402:VAL:CG2	2:B:423:ALA:CB	0.42	2.97	3	3
1:A:19:G:HO2'	1:A:20:A:C4'	0.42	2.27	4	1
2:B:422:ILE:HD12	2:B:422:ILE:N	0.42	2.29	7	1
2:B:394:THR:HG23	2:B:397:ASP:HB3	0.42	1.91	10	1
2:B:419:ASN:C	2:B:419:ASN:OD1	0.42	2.62	7	1
1:A:25:G:O6	1:A:26:G:C6	0.42	2.72	11	1
1:A:9:A:C5	1:A:10:U:C4	0.42	3.07	13	1
2:B:401:ILE:CG1	2:B:414:THR:OG1	0.42	2.67	13	1
2:B:394:THR:OG1	2:B:397:ASP:HB2	0.42	2.15	14	1
2:B:368:MET:HE1	2:B:369:ASN:ND2	0.42	2.30	5	1
1:A:12:U:H2'	1:A:13:U:O5'	0.42	2.15	10	1
2:B:396:VAL:C	2:B:397:ASP:CG	0.42	2.87	11	1
1:A:17:A:H3'	1:A:18:A:C8	0.42	2.48	12	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:416:VAL:CG1	2:B:417:GLY:N	0.42	2.81	13	1
1:A:26:G:H2'	1:A:27:U:C6	0.42	2.49	4	3
2:B:405:ARG:HB2	2:B:410:THR:O	0.42	2.14	3	1
2:B:368:MET:CE	2:B:369:ASN:OD1	0.42	2.68	4	1
2:B:391:LYS:HD2	2:B:391:LYS:C	0.42	2.40	5	1
1:A:1:G:C2'	1:A:2:G:O5'	0.42	2.68	10	2
2:B:401:ILE:HG23	2:B:401:ILE:O	0.42	2.15	10	1
1:A:20:A:N3	2:B:371:LYS:HE2	0.42	2.29	11	1
2:B:388:VAL:N	2:B:403:GLU:O	0.42	2.52	14	1
1:A:17:A:N3	2:B:372:ARG:NH2	0.42	2.68	8	1
2:B:405:ARG:CZ	2:B:405:ARG:CB	0.42	2.98	10	1
2:B:396:VAL:C	2:B:398:PRO:HD3	0.42	2.39	13	1
2:B:411:VAL:CG1	2:B:413:GLY:O	0.42	2.68	7	1
2:B:426:ARG:HD2	2:B:430:ASN:ND2	0.42	2.29	10	1
2:B:380:TYR:OH	2:B:444:GLN:HG3	0.42	2.15	11	1
1:A:17:A:C2'	1:A:18:A:O4'	0.42	2.67	15	1
2:B:415:GLY:HA2	2:B:426:ARG:HG2	0.42	1.92	4	1
2:B:386:HIS:O	2:B:386:HIS:CD2	0.42	2.73	5	1
2:B:397:ASP:O	2:B:397:ASP:OD1	0.42	2.37	7	1
2:B:380:TYR:HB3	2:B:445:ARG:CZ	0.42	2.45	11	1
1:A:15:A:HO2'	1:A:18:A:N6	0.42	2.12	13	1
1:A:23:G:C5	1:A:24:U:C4	0.42	3.08	2	1
2:B:441:TYR:O	2:B:444:GLN:HB2	0.42	2.15	5	1
1:A:17:A:C6	2:B:372:ARG:NH1	0.42	2.87	6	1
2:B:368:MET:HA	2:B:371:LYS:CD	0.42	2.45	7	1
1:A:11:G:C2	1:A:23:G:C4	0.42	3.07	8	1
1:A:9:A:H2'	1:A:10:U:C6	0.42	2.50	9	1
2:B:412:LEU:CD1	2:B:412:LEU:N	0.42	2.83	14	1
2:B:386:HIS:CD2	2:B:386:HIS:C	0.41	2.97	1	1
1:A:5:U:OP1	2:B:419:ASN:HB3	0.41	2.15	2	1
1:A:8:C:O2'	1:A:9:A:H8	0.41	1.97	3	1
2:B:369:ASN:O	2:B:372:ARG:HB2	0.41	2.15	8	1
1:A:21:A:O5'	1:A:21:A:H8	0.41	1.97	11	1
2:B:385:LEU:HD21	2:B:387:TYR:HE1	0.41	1.73	13	1
2:B:413:GLY:O	2:B:414:THR:HB	0.41	2.14	3	1
1:A:30:C:C2'	1:A:31:U:C5'	0.41	2.99	6	1
2:B:373:GLN:NE2	2:B:432:LEU:HB3	0.41	2.30	11	1
2:B:373:GLN:NE2	2:B:373:GLN:C	0.41	2.78	5	2
2:B:404:CYS:O	2:B:411:VAL:HA	0.41	2.16	10	2
2:B:433:ARG:O	2:B:433:ARG:HD3	0.41	2.14	6	1
2:B:380:TYR:HE1	2:B:383:LEU:HD13	0.41	1.73	7	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:419:ASN:ND2	2:B:422:ILE:HD11	0.41	2.29	11	1
1:A:29:U:H2'	1:A:30:C:O5'	0.41	2.16	15	1
2:B:374:LEU:CD1	2:B:387:TYR:OH	0.41	2.65	5	1
1:A:20:A:O2'	1:A:21:A:O4'	0.41	2.35	7	1
2:B:384:ARG:O	2:B:407:GLY:N	0.41	2.50	11	1
2:B:380:TYR:OH	2:B:441:TYR:HB3	0.41	2.15	15	1
2:B:397:ASP:H	2:B:398:PRO:CD	0.41	2.29	3	1
2:B:381:ALA:O	2:B:383:LEU:N	0.41	2.54	6	1
2:B:434:ASP:HB3	2:B:437:MET:HB3	0.41	1.92	9	1
2:B:437:MET:SD	2:B:441:TYR:CE1	0.41	3.14	12	1
1:A:12:U:O2'	1:A:13:U:O5'	0.41	2.38	9	2
2:B:440:PHE:CE2	2:B:441:TYR:CE2	0.41	3.08	3	1
2:B:383:LEU:HD23	2:B:383:LEU:H	0.41	1.75	4	1
2:B:418:ARG:HG3	2:B:419:ASN:OD1	0.41	2.15	5	1
2:B:368:MET:N	2:B:371:LYS:HE3	0.41	2.31	6	1
2:B:391:LYS:O	2:B:391:LYS:HD2	0.41	2.16	6	1
2:B:433:ARG:O	2:B:433:ARG:HG2	0.41	2.15	6	1
2:B:406:VAL:HG22	2:B:410:THR:O	0.41	2.16	15	1
1:A:20:A:O2'	1:A:21:A:C4'	0.41	2.69	3	1
2:B:368:MET:CG	2:B:369:ASN:N	0.41	2.84	15	1
2:B:373:GLN:HG3	2:B:432:LEU:HB2	0.41	1.92	7	3
2:B:397:ASP:C	2:B:399:ASN:N	0.41	2.79	4	1
2:B:403:GLU:OE1	2:B:411:VAL:CG1	0.41	2.69	8	1
2:B:419:ASN:OD1	2:B:421:LYS:HB2	0.41	2.16	14	1
2:B:412:LEU:HG	2:B:437:MET:SD	0.41	2.55	15	1
1:A:21:A:C2'	1:A:22:C:O5'	0.41	2.69	1	1
2:B:433:ARG:O	2:B:433:ARG:NE	0.41	2.53	1	1
1:A:2:G:C5	1:A:3:G:N7	0.41	2.89	2	1
2:B:399:ASN:C	2:B:399:ASN:OD1	0.41	2.64	3	1
2:B:402:VAL:O	2:B:414:THR:OG1	0.41	2.32	3	1
2:B:369:ASN:O	2:B:372:ARG:HB3	0.41	2.15	5	1
2:B:373:GLN:HG3	2:B:432:LEU:HB3	0.41	1.91	5	1
2:B:433:ARG:O	2:B:433:ARG:CD	0.41	2.69	6	1
1:A:29:U:H2'	1:A:30:C:C5'	0.41	2.46	9	1
1:A:5:U:O3'	2:B:393:PRO:HG2	0.41	2.16	12	1
2:B:372:ARG:HG2	2:B:376:SER:CB	0.41	2.46	14	1
2:B:412:LEU:CD2	2:B:437:MET:HG3	0.41	2.45	14	1
2:B:437:MET:O	2:B:440:PHE:HB3	0.41	2.15	14	1
2:B:368:MET:O	2:B:372:ARG:HB2	0.41	2.16	2	1
2:B:420:ILE:CG1	2:B:421:LYS:N	0.41	2.84	5	1
1:A:6:A:OP1	2:B:393:PRO:HG2	0.41	2.15	7	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:11:G:N2	1:A:23:G:C4	0.41	2.89	8	1
2:B:390:VAL:O	2:B:391:LYS:HB2	0.41	2.16	9	1
2:B:405:ARG:O	2:B:405:ARG:CG	0.41	2.70	12	1
1:A:17:A:H2'	1:A:18:A:C4	0.40	2.51	1	1
2:B:380:TYR:CD1	2:B:380:TYR:C	0.40	2.99	3	1
1:A:20:A:C5'	2:B:375:TYR:CD2	0.40	3.05	9	1
2:B:377:LEU:C	2:B:378:ILE:HG12	0.40	2.40	15	1
1:A:15:A:C4	1:A:16:G:C8	0.40	3.09	6	1
2:B:380:TYR:CE2	2:B:382:SER:CB	0.40	3.04	10	1
1:A:12:U:O2'	1:A:13:U:C4'	0.40	2.69	12	1
2:B:373:GLN:OE1	2:B:377:LEU:HD22	0.40	2.16	12	1
1:A:9:A:N6	1:A:10:U:O4	0.40	2.54	13	1
1:A:24:U:O2'	1:A:25:G:C8	0.40	2.74	13	1
1:A:22:C:H2'	1:A:23:G:O4'	0.40	2.16	15	1
2:B:377:LEU:HD22	2:B:377:LEU:N	0.40	2.31	15	1
2:B:374:LEU:HD22	2:B:431:ALA:CB	0.40	2.45	10	1
2:B:429:GLU:HA	2:B:432:LEU:HG	0.40	1.91	14	1
2:B:440:PHE:CD1	2:B:440:PHE:O	0.40	2.75	15	1
2:B:368:MET:HE3	2:B:368:MET:HB2	0.40	1.83	3	1
1:A:20:A:O4'	2:B:371:LYS:HB3	0.40	2.17	7	1
2:B:416:VAL:HG22	2:B:417:GLY:N	0.40	2.32	10	1
2:B:380:TYR:CE2	2:B:383:LEU:HD22	0.40	2.52	11	1
2:B:374:LEU:HD11	2:B:428:ALA:CA	0.40	2.45	12	1
2:B:378:ILE:CG2	2:B:441:TYR:CD2	0.40	3.04	14	1
2:B:411:VAL:C	2:B:413:GLY:H	0.40	2.21	14	1
1:A:29:U:HO2'	1:A:30:C:H5'	0.40	1.70	15	1
1:A:15:A:O3'	2:B:368:MET:SD	0.40	2.80	2	1
2:B:373:GLN:OE1	2:B:438:LEU:HD22	0.40	2.17	3	1
2:B:405:ARG:N	2:B:412:LEU:HD22	0.40	2.31	6	1
1:A:20:A:N3	2:B:371:LYS:HE3	0.40	2.31	8	1
2:B:412:LEU:HB3	2:B:437:MET:CE	0.40	2.45	10	1
2:B:429:GLU:HA	2:B:432:LEU:CG	0.40	2.46	13	1
1:A:30:C:O2'	2:B:396:VAL:CG1	0.40	2.63	14	1
2:B:427:ALA:C	2:B:430:ASN:HB2	0.40	2.41	14	1

6.3 Torsion angles ⓘ

6.3.1 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 PDB entries followed by that with respect to all NMR

entries. 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	
2	B	79/90 (88%)	56±3 (70±3%)	16±2 (20±3%)	8±2 (10±3%)	1	9
All	All	1185/1350 (88%)	834 (70%)	233 (20%)	118 (10%)	1	9

All 23 unique Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
2	B	420	ILE	15
2	B	391	LYS	11
2	B	397	ASP	10
2	B	381	ALA	10
2	B	370	ALA	9
2	B	382	SER	9
2	B	407	GLY	8
2	B	399	ASN	7
2	B	379	GLY	6
2	B	371	LYS	4
2	B	398	PRO	4
2	B	367	ASP	4
2	B	374	LEU	3
2	B	378	ILE	3
2	B	393	PRO	3
2	B	412	LEU	2
2	B	384	ARG	2
2	B	409	GLY	2
2	B	388	VAL	2
2	B	392	LYS	1
2	B	389	THR	1
2	B	428	ALA	1
2	B	395	ALA	1

6.3.2 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 PDB entries followed by that with respect to all NMR entries. 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	
2	B	64/72 (89%)	36±3 (56±5%)	28±3 (44±5%)	0	3
All	All	960/1080 (89%)	539 (56%)	421 (44%)	0	3

All 54 unique residues with a non-rotameric sidechain are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
2	B	388	VAL	15
2	B	402	VAL	15
2	B	412	LEU	15
2	B	420	ILE	15
2	B	421	LYS	15
2	B	422	ILE	15
2	B	432	LEU	15
2	B	371	LYS	14
2	B	367	ASP	13
2	B	374	LEU	13
2	B	444	GLN	13
2	B	373	GLN	12
2	B	406	VAL	12
2	B	445	ARG	11
2	B	419	ASN	11
2	B	401	ILE	10
2	B	383	LEU	9
2	B	392	LYS	9
2	B	368	MET	9
2	B	376	SER	9
2	B	443	LYS	9
2	B	377	LEU	8
2	B	397	ASP	8
2	B	418	ARG	8
2	B	372	ARG	7
2	B	414	THR	7
2	B	430	ASN	7
2	B	436	LYS	7
2	B	440	PHE	7
2	B	391	LYS	7
2	B	405	ARG	6
2	B	382	SER	6
2	B	384	ARG	6
2	B	404	CYS	6
2	B	429	GLU	6
2	B	437	MET	6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Models (Total)
2	B	425	ILE	6
2	B	435	LYS	6
2	B	385	LEU	5
2	B	400	SER	5
2	B	403	GLU	4
2	B	426	ARG	4
2	B	394	THR	4
2	B	389	THR	3
2	B	433	ARG	3
2	B	380	TYR	3
2	B	378	ILE	3
2	B	386	HIS	3
2	B	399	ASN	3
2	B	396	VAL	2
2	B	369	ASN	2
2	B	408	ASP	2
2	B	390	VAL	1
2	B	410	THR	1

6.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers	Suiteness
1	A	31/32 (97%)	4±0 (13±0%)	2±1 (6±3%)	0.13±0.00
All	All	466/480 (97%)	60 (13%)	30 (6%)	0.13

The overall RNA backbone suiteness is 0.11.

All unique RNA backbone outliers are listed below:

Mol	Chain	Res	Type	Models (Total)
1	A	15	A	15
1	A	16	G	15
1	A	17	A	15
1	A	18	A	15

All unique RNA pucker outliers are listed below:

Mol	Chain	Res	Type	Models (Total)
1	A	16	G	11
1	A	17	A	8
1	A	28	A	3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Models (Total)
1	A	25	G	2
1	A	3	G	2
1	A	20	A	2
1	A	1	G	1
1	A	18	A	1

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

There are no non-standard protein/DNA/RNA residues in this entry.

6.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.6 Ligand geometry [i](#)

There are no ligands in this entry.

6.7 Other polymers [i](#)

There are no such molecules in this entry.

6.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

7 Chemical shift validation

No chemical shift data were provided