



Full wwPDB NMR Structure Validation Report ⓘ

Mar 8, 2026 – 05:00 PM UTC

PDB ID : 2LBS / pdb_00002lbs
BMRB ID : 17574
Title : Solution structure of double-stranded RNA binding domain of *S. cerevisiae* RNase III (Rnt1p) in complex with AAGU tetraloop hairpin
Authors : Wang, Z.; Hartman, E.; Roy, K.; Chanfreau, G.; Feigon, J.
Deposited on : 2011-04-06

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

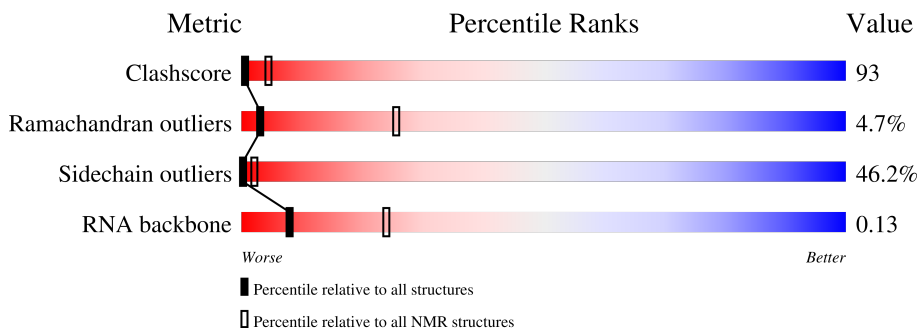
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 51%.

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	 75% 25%
2	B	90	 7% 58% 29% 7%

2 Ensemble composition and analysis

This entry contains 16 models. Model 8 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *lowest energy*.

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:365-B:448 (84)	1.01	8

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 2 clusters and 1 single-model cluster was found.

Cluster number	Models
1	1, 4, 5, 6, 7, 8, 9, 10, 11, 12, 13, 15, 16
2	3, 14
Single-model clusters	2

3 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 2434 atoms, of which 1066 are hydrogens and 0 are deuteriums.

- Molecule 1 is a RNA chain called RNA (32-MER).

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	P	
1	A	32	1025	305	345	121	223	31	0

- Molecule 2 is a protein called Ribonuclease 3.

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

There are 2 discrepancies between the modelled and reference sequences:

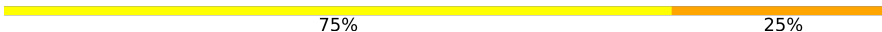
Chain	Residue	Modelled	Actual	Comment	Reference
B	364	GLY	-	expression tag	UNP Q02555
B	365	SER	-	expression tag	UNP Q02555

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.

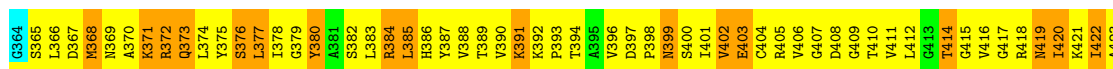
- Molecule 1: RNA (32-MER)

Chain A:  75% 25%



- Molecule 2: Ribonuclease 3

Chain B:  7% 58% 29% 7%

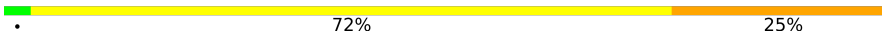


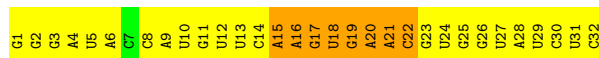
4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

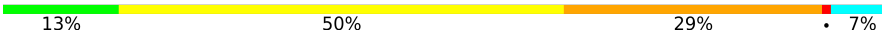
4.2.1 Score per residue for model 1

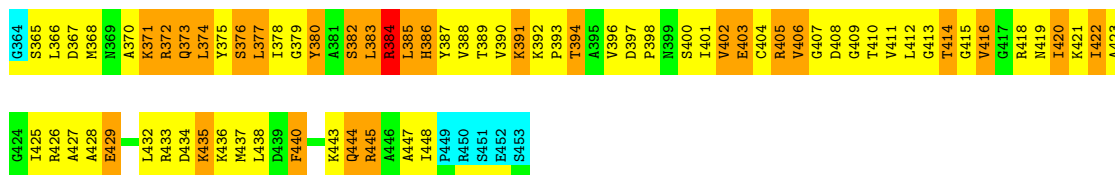
- Molecule 1: RNA (32-MER)

Chain A:  72% 25%



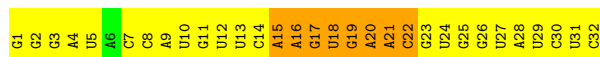
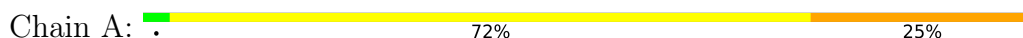
- Molecule 2: Ribonuclease 3

Chain B:  13% 50% 29% 7%

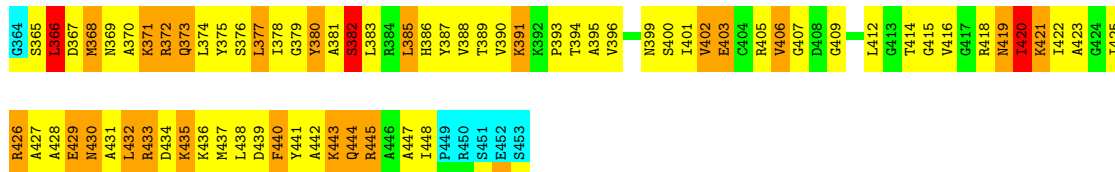
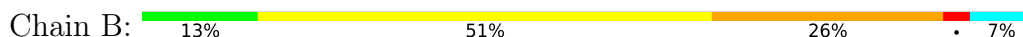


4.2.2 Score per residue for model 2

- Molecule 1: RNA (32-MER)



- Molecule 2: Ribonuclease 3

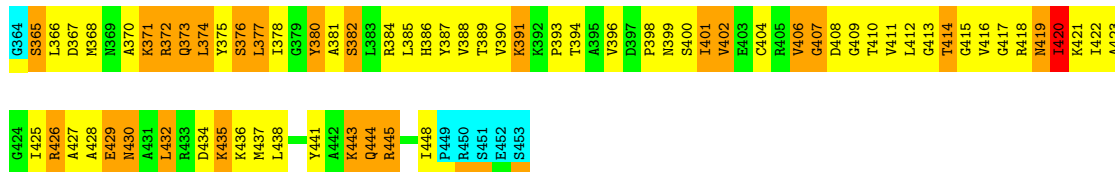
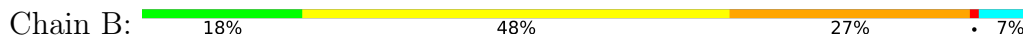


4.2.3 Score per residue for model 3

- Molecule 1: RNA (32-MER)



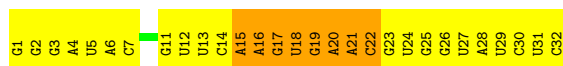
- Molecule 2: Ribonuclease 3



4.2.4 Score per residue for model 4

- Molecule 1: RNA (32-MER)

Chain A: 9% 66% 25%



- Molecule 2: Ribonuclease 3

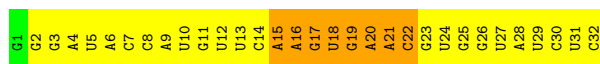
Chain B: 10% 52% 30% 7%



4.2.5 Score per residue for model 5

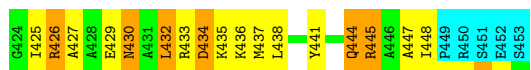
- Molecule 1: RNA (32-MER)

Chain A: 72% 25%



- Molecule 2: Ribonuclease 3

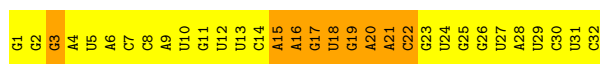
Chain B: 13% 57% 23% 7%



4.2.6 Score per residue for model 6

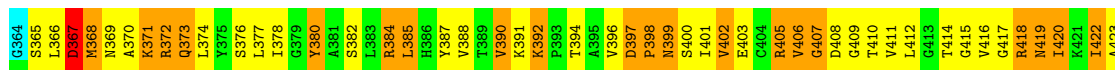
- Molecule 1: RNA (32-MER)

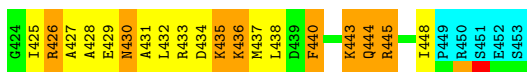
Chain A: 72% 28%



- Molecule 2: Ribonuclease 3

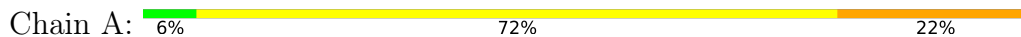
Chain B: 19% 42% 31% 7%





4.2.7 Score per residue for model 7

- Molecule 1: RNA (32-MER)

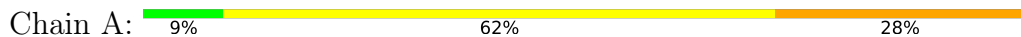


- Molecule 2: Ribonuclease 3

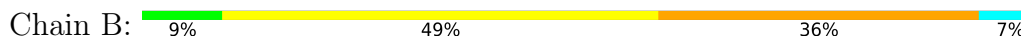


4.2.8 Score per residue for model 8 (medoid)

- Molecule 1: RNA (32-MER)

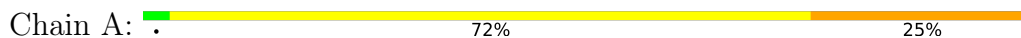


- Molecule 2: Ribonuclease 3



4.2.9 Score per residue for model 9

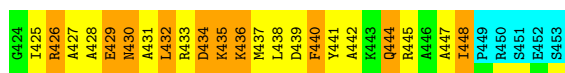
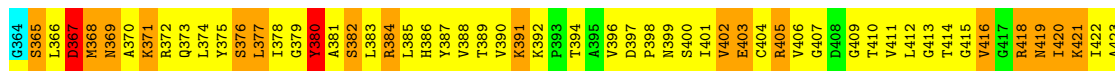
- Molecule 1: RNA (32-MER)





- Molecule 2: Ribonuclease 3

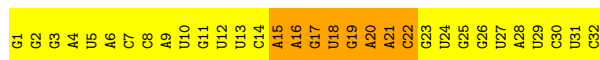
Chain B: 8% 53% 30% 7%



4.2.10 Score per residue for model 10

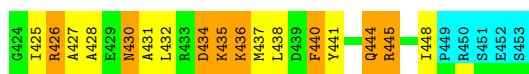
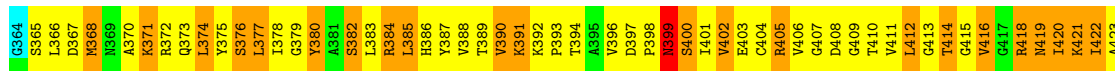
- Molecule 1: RNA (32-MER)

Chain A: 75% 25%



- Molecule 2: Ribonuclease 3

Chain B: 13% 46% 33% 7%



4.2.11 Score per residue for model 11

- Molecule 1: RNA (32-MER)

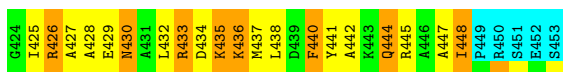
Chain A: 9% 62% 28%



- Molecule 2: Ribonuclease 3

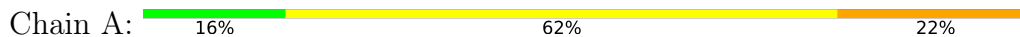
Chain B: 11% 47% 34% 7%



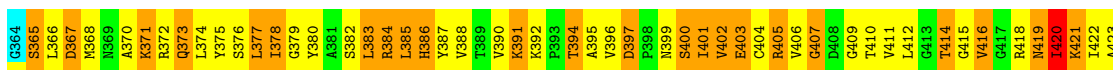


4.2.12 Score per residue for model 12

- Molecule 1: RNA (32-MER)

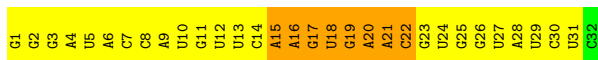
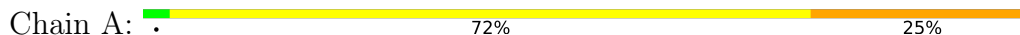


- Molecule 2: Ribonuclease 3

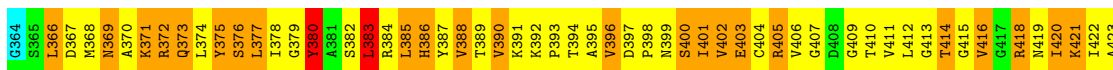
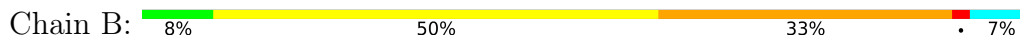


4.2.13 Score per residue for model 13

- Molecule 1: RNA (32-MER)

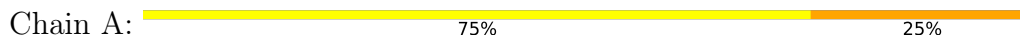


- Molecule 2: Ribonuclease 3



4.2.14 Score per residue for model 14

- Molecule 1: RNA (32-MER)



G1 G2 G3 G4 G5 G6 G7 G8 G9 G10 G11 G12 G13 G14 A15 A16 A17 A18 A19 A20 A21 A22 G23 G24 G25 G26 G27 G28 G29 G30 G31 G32

- Molecule 2: Ribonuclease 3

Chain B: 13% 46% 32% 7%

G364 S365 L366 D367 N368 N369 A370 K371 R372 Q373 L374 Y375 S376 L377 I378 G379 G380 Y381 A381 S382 L383 R384 R385 H386 Y387 V388 T389 K391 P393 T394 A395 V396 D397 P398 N399 S400 S401 V402 E403 C404 R405 V406 G407 D408 G409 T410 V411 L412 G413 T414 G415 V416 G417 R418 N419 I420 K421 I422 A423

G424 I425 R426 A427 N428 N429 M430 A431 R432 D433 K434 K435 M437 D438 F440 A441 K442 Q443 R444 R445 I448 P449 R450 S451 E452 S453

4.2.15 Score per residue for model 15

- Molecule 1: RNA (32-MER)

Chain A: 6% 69% 25%

G1 G2 G3 G4 G5 G6 G7 G8 G9 G10 G11 G12 G13 G14 A15 A16 A17 A18 A19 A20 A21 A22 G23 G24 G25 G26 U27 C30 C32

- Molecule 2: Ribonuclease 3

Chain B: 16% 44% 32% 7%

G364 S365 L366 N369 A370 K371 R372 Q373 L374 Y375 S376 L377 I378 G379 G380 Y381 A381 S382 L383 R384 R385 H386 Y387 V388 T389 K391 P393 T394 A395 V396 D397 P398 N399 S400 S401 V402 E403 C404 R405 V406 G407 D408 G409 T410 V411 L412 G413 T414 G415 V416 G417 R418 N419 I420 K421 I422 A423

R426 A427 E428 N429 M430 A431 R432 D433 K434 K435 M437 D438 F440 A441 K442 Q443 R444 R445 I448 P449 R450 S451 E452 S453

4.2.16 Score per residue for model 16

- Molecule 1: RNA (32-MER)

Chain A: 72% 25%

G1 G2 G3 G4 G5 G6 G7 G8 G9 G10 G11 G12 G13 G14 A15 A16 A17 A18 A19 A20 A21 A22 G23 G24 G25 G26 A28 U29 C30 U31 G32

- Molecule 2: Ribonuclease 3

Chain B: 14% 47% 30% 7%

G364 S365 L366 D367 N369 A370 K371 R372 Q373 L374 Y375 S376 L377 I378 G379 G380 Y381 A381 S382 L383 R384 R385 H386 Y387 V388 T389 K391 P393 T394 A395 V396 D397 P398 N399 S400 S401 V402 E403 C404 R405 V406 G407 D408 G409 T410 V411 L412 G413 T414 G415 V416 G417 R418 N419 I420 K421 I422 A423

E427
I425
R426
A427
A428
E429
M430
A431
L432
R433
D434
K435
K436
M437
L438
D439
F440
Y441
A442
K443
Q444
R445
A446
A447
I448
F449
R450
S451
E452
S453

5 Refinement protocol and experimental data overview

The models were refined using the following method: *torsion angle dynamics*.

Of the 100 calculated structures, 16 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 NIH	structure solution	2.24
X-PLOR NIH	refinement	2.24

The following table shows chemical shift validation statistics as aggregates over all chemical shift files. Detailed validation can be found in section 7 of this report.

Chemical shift file(s)	working_cs.cif
Number of chemical shift lists	1
Total number of shifts	952
Number of shifts mapped to atoms	952
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	51%

6 Model quality i

6.1 Standard geometry i

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 i

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	680	345	345	86±11
2	B	644	680	679	136±15
All	All	21184	16400	16384	3479

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 93.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:412:LEU:HD22	2:B:437:MET:HE2	1.11	1.22	16	12
2:B:404:CYS:C	2:B:411:VAL:HG23	1.02	1.80	8	1
1:A:15:A:N3	1:A:16:A:H2'	1.00	1.69	16	1
2:B:370:ALA:HB1	2:B:428:ALA:HB1	0.99	1.28	13	8
2:B:390:VAL:O	2:B:401:ILE:HG22	0.97	1.57	9	13
2:B:390:VAL:HG23	2:B:401:ILE:CG2	0.96	1.89	16	9
2:B:373:GLN:CD	2:B:438:LEU:HD13	0.95	1.87	5	7
2:B:425:ILE:HG22	2:B:429:GLU:OE1	0.95	1.60	11	2
1:A:30:C:O2'	1:A:31:U:H5'	0.94	1.61	11	16
1:A:1:G:O2'	1:A:2:G:H5'	0.94	1.61	13	7
2:B:388:VAL:HG22	2:B:403:GLU:O	0.93	1.62	2	4
2:B:374:LEU:HD12	2:B:387:TYR:OH	0.93	1.64	6	9
1:A:12:U:O2'	1:A:13:U:H5'	0.92	1.64	5	13

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:389:THR:HG22	2:B:402:VAL:HG13	0.90	1.41	16	3
2:B:432:LEU:HD12	2:B:432:LEU:O	0.90	1.66	8	1
1:A:29:U:H2'	1:A:30:C:O4'	0.89	1.67	5	11
2:B:377:LEU:O	2:B:378:ILE:HD13	0.89	1.68	9	4
1:A:15:A:C2	1:A:16:A:C4	0.89	2.60	16	1
1:A:29:U:O2'	1:A:30:C:H5'	0.89	1.68	6	10
2:B:368:MET:HE3	2:B:369:ASN:HA	0.89	1.45	2	1
2:B:403:GLU:CD	2:B:411:VAL:HG21	0.88	1.92	12	1
2:B:373:GLN:OE1	2:B:374:LEU:HD23	0.88	1.69	9	1
1:A:16:A:H1'	1:A:18:U:O4	0.88	1.69	15	7
2:B:388:VAL:HG22	2:B:403:GLU:CB	0.87	1.98	4	9
2:B:373:GLN:NE2	2:B:438:LEU:HD13	0.87	1.84	1	15
2:B:419:ASN:ND2	2:B:422:ILE:HD11	0.87	1.84	6	2
2:B:373:GLN:OE1	2:B:377:LEU:HD13	0.86	1.70	15	4
2:B:373:GLN:NE2	2:B:438:LEU:HD22	0.86	1.84	10	3
2:B:366:LEU:HD22	2:B:368:MET:HG3	0.85	1.46	4	2
1:A:23:G:O2'	1:A:24:U:H5'	0.85	1.70	10	14
2:B:373:GLN:OE1	2:B:377:LEU:HD23	0.85	1.72	7	6
1:A:2:G:O2'	1:A:3:G:H5'	0.85	1.72	14	12
2:B:401:ILE:HD12	2:B:416:VAL:CG2	0.85	2.01	5	4
2:B:420:ILE:C	2:B:420:ILE:HD13	0.84	1.97	13	6
2:B:370:ALA:CB	2:B:428:ALA:HB1	0.84	2.01	14	8
2:B:412:LEU:HD22	2:B:437:MET:SD	0.83	2.13	8	3
2:B:432:LEU:O	2:B:432:LEU:HD22	0.83	1.74	15	2
1:A:22:C:O2'	1:A:23:G:H5'	0.83	1.73	7	15
2:B:370:ALA:HB2	2:B:429:GLU:OE1	0.83	1.74	6	8
2:B:435:LYS:HA	2:B:438:LEU:HD12	0.82	1.51	1	4
2:B:425:ILE:HG22	2:B:429:GLU:OE2	0.82	1.75	14	1
2:B:401:ILE:CB	2:B:416:VAL:HG13	0.81	2.05	9	2
2:B:444:GLN:O	2:B:448:ILE:HG23	0.81	1.75	3	11
2:B:378:ILE:HD11	2:B:438:LEU:O	0.81	1.76	2	10
2:B:402:VAL:HG23	2:B:415:GLY:O	0.81	1.75	14	14
1:A:15:A:O2'	2:B:368:MET:HE2	0.81	1.75	13	1
2:B:432:LEU:HD23	2:B:432:LEU:O	0.81	1.76	1	3
2:B:367:ASP:HB2	2:B:425:ILE:HG23	0.80	1.53	11	2
2:B:401:ILE:HG13	2:B:416:VAL:HG22	0.80	1.52	4	7
1:A:13:U:O2'	1:A:14:C:H5'	0.80	1.77	7	15
1:A:16:A:O4'	1:A:17:G:H8	0.80	1.60	16	1
2:B:366:LEU:HD22	2:B:368:MET:CG	0.80	2.07	4	2
1:A:9:A:O2'	1:A:10:U:H5'	0.80	1.75	10	9
2:B:420:ILE:HD13	2:B:420:ILE:O	0.79	1.78	8	5

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:412:LEU:HD22	2:B:437:MET:CE	0.79	2.07	11	6
1:A:15:A:N1	1:A:19:G:C2	0.79	2.50	16	1
2:B:420:ILE:O	2:B:423:ALA:HB3	0.78	1.79	14	10
1:A:28:A:O2'	1:A:29:U:H5'	0.78	1.79	6	7
2:B:388:VAL:HG22	2:B:403:GLU:HB3	0.77	1.56	1	6
1:A:22:C:O5'	1:A:22:C:H6	0.77	1.63	1	14
1:A:18:U:H4'	1:A:19:G:OP1	0.77	1.80	5	1
2:B:373:GLN:HE21	2:B:438:LEU:HD13	0.77	1.40	12	7
1:A:20:A:HO2'	1:A:21:A:H8	0.76	1.21	10	4
2:B:437:MET:HE3	2:B:441:TYR:CE2	0.76	2.15	15	1
2:B:389:THR:HG22	2:B:402:VAL:CG1	0.76	2.11	16	1
2:B:366:LEU:HD23	2:B:367:ASP:N	0.75	1.96	8	10
2:B:420:ILE:HD13	2:B:420:ILE:C	0.75	2.07	8	1
1:A:5:U:O2'	1:A:6:A:H5'	0.75	1.81	7	3
2:B:390:VAL:HG23	2:B:401:ILE:HG23	0.75	1.57	11	4
1:A:22:C:H6	1:A:22:C:O5'	0.74	1.64	6	2
1:A:15:A:C4	1:A:16:A:C8	0.74	2.76	16	1
1:A:21:A:O5'	1:A:21:A:H8	0.74	1.64	13	11
1:A:31:U:O2'	1:A:32:C:H5'	0.74	1.82	15	5
2:B:434:ASP:HB2	2:B:437:MET:HE3	0.74	1.60	12	2
2:B:403:GLU:CD	2:B:411:VAL:HG11	0.74	2.07	15	2
2:B:390:VAL:O	2:B:401:ILE:HG23	0.74	1.83	2	3
2:B:412:LEU:CD2	2:B:437:MET:HE2	0.74	2.08	11	4
2:B:419:ASN:OD1	2:B:422:ILE:HD11	0.73	1.82	1	4
2:B:378:ILE:HD13	2:B:441:TYR:HB3	0.73	1.57	15	1
2:B:419:ASN:C	2:B:420:ILE:HG23	0.73	2.09	16	6
2:B:405:ARG:HB3	2:B:411:VAL:HG22	0.73	1.60	6	9
2:B:370:ALA:HB3	2:B:428:ALA:HB1	0.73	1.59	14	3
1:A:26:G:O2'	1:A:27:U:H5'	0.73	1.82	16	11
2:B:385:LEU:CB	2:B:406:VAL:HG12	0.73	2.13	6	3
2:B:367:ASP:CB	2:B:425:ILE:HG23	0.73	2.13	11	2
1:A:15:A:N3	1:A:16:A:C2'	0.73	2.50	16	1
1:A:16:A:O4'	1:A:17:G:C8	0.72	2.43	16	1
1:A:26:G:HO2'	1:A:27:U:C5'	0.72	1.98	3	4
2:B:432:LEU:C	2:B:432:LEU:HD23	0.72	2.10	16	4
2:B:383:LEU:HD12	2:B:384:ARG:N	0.72	1.99	9	2
1:A:15:A:N1	1:A:19:G:C6	0.72	2.58	10	6
2:B:429:GLU:HA	2:B:432:LEU:HD23	0.72	1.59	8	1
1:A:7:C:O2'	1:A:8:C:H5'	0.72	1.84	9	3
2:B:419:ASN:O	2:B:420:ILE:HG22	0.71	1.86	12	4
2:B:410:THR:HG21	2:B:441:TYR:OH	0.71	1.83	5	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:1:G:N3	1:A:2:G:C8	0.71	2.58	4	3
1:A:27:U:O2'	1:A:28:A:H5'	0.71	1.85	1	5
2:B:388:VAL:HG23	2:B:403:GLU:HB2	0.71	1.61	6	5
2:B:378:ILE:HG23	2:B:380:TYR:CZ	0.71	2.20	16	1
1:A:1:G:C2	1:A:2:G:N7	0.71	2.58	4	2
1:A:29:U:H6	1:A:29:U:O5'	0.71	1.68	5	6
2:B:366:LEU:HD23	2:B:367:ASP:H	0.71	1.45	8	4
2:B:406:VAL:HG22	2:B:410:THR:HB	0.71	1.62	16	13
2:B:403:GLU:HG2	2:B:411:VAL:HG11	0.71	1.63	12	2
1:A:14:C:N4	1:A:15:A:C6	0.71	2.59	12	8
1:A:14:C:C4	1:A:15:A:N7	0.71	2.59	14	13
1:A:7:C:N4	1:A:8:C:N4	0.71	2.39	3	4
1:A:18:U:H6	1:A:18:U:O5'	0.71	1.68	13	2
2:B:373:GLN:OE1	2:B:377:LEU:HD22	0.70	1.86	10	2
2:B:380:TYR:CE1	2:B:383:LEU:HD13	0.70	2.20	14	1
2:B:374:LEU:HD13	2:B:387:TYR:OH	0.70	1.85	13	2
1:A:15:A:N6	1:A:16:A:C6	0.70	2.59	14	14
2:B:370:ALA:HB1	2:B:428:ALA:CB	0.70	2.11	13	3
2:B:386:HIS:NE2	2:B:388:VAL:HG12	0.70	2.02	4	1
2:B:373:GLN:HE21	2:B:374:LEU:HD23	0.70	1.46	14	3
1:A:23:G:C5	1:A:24:U:C5	0.70	2.79	14	12
1:A:23:G:C6	1:A:24:U:C4	0.70	2.79	7	12
2:B:401:ILE:CG1	2:B:416:VAL:HG13	0.69	2.17	9	3
1:A:21:A:H8	1:A:21:A:O5'	0.69	1.69	11	3
2:B:440:PHE:CZ	2:B:441:TYR:CE1	0.69	2.80	9	3
1:A:12:U:H6	1:A:12:U:O5'	0.69	1.71	14	7
2:B:374:LEU:O	2:B:379:GLY:N	0.69	2.25	15	1
2:B:403:GLU:CG	2:B:411:VAL:HG11	0.69	2.16	12	2
2:B:440:PHE:CE2	2:B:441:TYR:CE2	0.69	2.81	14	6
2:B:388:VAL:HG23	2:B:403:GLU:HG3	0.69	1.65	2	3
2:B:440:PHE:CE2	2:B:441:TYR:CE1	0.69	2.81	13	3
2:B:385:LEU:N	2:B:385:LEU:HD23	0.69	2.03	12	1
2:B:378:ILE:HD12	2:B:378:ILE:C	0.69	2.12	15	1
2:B:401:ILE:HG12	2:B:416:VAL:HG13	0.69	1.64	12	2
1:A:1:G:C2	1:A:2:G:C5	0.69	2.81	4	5
2:B:388:VAL:HG22	2:B:403:GLU:HB2	0.69	1.63	16	3
2:B:389:THR:OG1	2:B:402:VAL:HG13	0.68	1.88	5	1
1:A:4:A:O2'	1:A:5:U:H5'	0.68	1.89	2	3
2:B:401:ILE:CG1	2:B:416:VAL:HG22	0.68	2.19	10	8
2:B:384:ARG:C	2:B:385:LEU:HD23	0.68	2.14	12	1
1:A:15:A:N7	1:A:16:A:N7	0.68	2.41	1	11

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:377:LEU:HD12	2:B:442:ALA:HB2	0.68	1.66	7	1
2:B:406:VAL:HG21	2:B:441:TYR:OH	0.67	1.88	2	1
2:B:373:GLN:HG3	2:B:432:LEU:HD23	0.67	1.66	15	2
1:A:18:U:O2'	1:A:19:G:C8	0.67	2.47	1	6
1:A:6:A:O2'	1:A:7:C:H5'	0.67	1.89	14	4
1:A:8:C:N4	1:A:9:A:N6	0.67	2.41	8	2
2:B:378:ILE:HD11	2:B:383:LEU:CD2	0.67	2.20	15	1
1:A:13:U:O2'	1:A:14:C:C5'	0.67	2.43	16	15
1:A:22:C:O2'	1:A:23:G:C5'	0.67	2.43	7	14
1:A:14:C:N4	1:A:15:A:N6	0.67	2.43	3	7
2:B:432:LEU:C	2:B:432:LEU:HD13	0.67	2.14	12	2
1:A:24:U:O2'	1:A:25:G:C5'	0.67	2.43	12	8
2:B:401:ILE:CD1	2:B:416:VAL:HG22	0.67	2.19	12	4
1:A:24:U:C2	1:A:25:G:N7	0.67	2.63	8	3
2:B:388:VAL:HG23	2:B:403:GLU:CB	0.67	2.20	11	4
1:A:21:A:O2'	1:A:22:C:C5'	0.67	2.43	4	16
2:B:432:LEU:HA	2:B:438:LEU:HD11	0.67	1.66	7	5
2:B:366:LEU:HD22	2:B:368:MET:HG2	0.67	1.66	8	1
2:B:370:ALA:HB2	2:B:429:GLU:CD	0.66	2.15	7	4
1:A:21:A:O2'	1:A:22:C:H5'	0.66	1.90	4	10
2:B:403:GLU:OE1	2:B:411:VAL:HG21	0.66	1.90	12	2
1:A:28:A:O2'	1:A:29:U:C5'	0.66	2.44	9	10
1:A:30:C:C4	1:A:31:U:C5	0.66	2.82	10	5
2:B:386:HIS:CD2	2:B:387:TYR:N	0.66	2.64	4	2
1:A:16:A:N1	2:B:372:ARG:CG	0.66	2.59	16	1
1:A:19:G:O2'	1:A:20:A:C5'	0.66	2.43	13	8
1:A:30:C:O2'	1:A:31:U:C5'	0.66	2.43	6	13
2:B:425:ILE:HG23	2:B:429:GLU:OE2	0.66	1.91	12	1
1:A:15:A:C2	1:A:19:G:C6	0.66	2.82	16	13
2:B:378:ILE:HG22	2:B:383:LEU:CD2	0.66	2.20	2	1
1:A:23:G:O2'	1:A:24:U:C5'	0.66	2.43	15	6
1:A:17:G:H5'	1:A:18:U:OP2	0.66	1.90	6	2
1:A:29:U:O2'	1:A:30:C:C5'	0.66	2.43	11	5
2:B:401:ILE:CB	2:B:416:VAL:HG22	0.66	2.21	6	3
1:A:16:A:C2	2:B:372:ARG:CG	0.66	2.79	16	1
1:A:24:U:HO2'	1:A:25:G:C5'	0.65	2.03	8	6
1:A:31:U:O2'	1:A:32:C:C5'	0.65	2.44	15	8
1:A:14:C:N4	1:A:15:A:C5	0.65	2.64	7	7
2:B:402:VAL:CG2	2:B:423:ALA:HB1	0.65	2.22	15	5
2:B:380:TYR:CD2	2:B:445:ARG:CB	0.65	2.80	15	3
1:A:15:A:C6	1:A:19:G:C2	0.65	2.84	16	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:440:PHE:CD1	2:B:440:PHE:C	0.65	2.75	9	14
1:A:18:U:O5'	1:A:18:U:C6	0.65	2.49	13	2
2:B:389:THR:HG23	2:B:389:THR:O	0.65	1.90	4	5
2:B:380:TYR:CE2	2:B:382:SER:CB	0.65	2.80	10	3
2:B:385:LEU:HD23	2:B:385:LEU:O	0.65	1.91	13	3
1:A:15:A:O2'	1:A:16:A:O5'	0.65	2.14	16	1
2:B:402:VAL:HG21	2:B:423:ALA:O	0.65	1.91	5	10
2:B:378:ILE:HD13	2:B:441:TYR:CD1	0.65	2.27	12	1
1:A:3:G:O2'	1:A:4:A:C5'	0.65	2.45	11	5
1:A:11:G:O2'	1:A:12:U:C5'	0.65	2.45	4	15
1:A:12:U:O2'	1:A:13:U:C5'	0.65	2.45	15	12
2:B:401:ILE:HG12	2:B:416:VAL:HG22	0.65	1.68	12	2
2:B:380:TYR:CE2	2:B:445:ARG:CB	0.65	2.81	15	6
1:A:1:G:C8	1:A:1:G:O5'	0.65	2.50	14	2
2:B:378:ILE:HD12	2:B:379:GLY:H	0.65	1.52	12	1
2:B:373:GLN:NE2	2:B:374:LEU:HD23	0.65	2.06	14	1
2:B:390:VAL:HG23	2:B:401:ILE:HG22	0.64	1.67	3	5
1:A:26:G:O2'	1:A:27:U:C5'	0.64	2.45	14	8
2:B:422:ILE:O	2:B:426:ARG:CB	0.64	2.46	1	15
2:B:374:LEU:HD11	2:B:387:TYR:OH	0.64	1.93	14	1
1:A:25:G:O2'	1:A:26:G:C5'	0.64	2.45	15	1
1:A:17:G:C8	2:B:372:ARG:CD	0.64	2.80	2	4
2:B:378:ILE:HD11	2:B:383:LEU:HD23	0.64	1.70	15	1
2:B:401:ILE:HG12	2:B:414:THR:HG22	0.64	1.67	15	2
1:A:30:C:H1'	2:B:395:ALA:HB1	0.64	1.70	2	5
2:B:383:LEU:C	2:B:383:LEU:HD12	0.64	2.17	16	1
1:A:1:G:O2'	1:A:2:G:C5'	0.64	2.46	1	6
1:A:16:A:C8	1:A:17:G:C8	0.64	2.85	16	1
2:B:380:TYR:CZ	2:B:445:ARG:CB	0.64	2.81	5	2
1:A:24:U:O2'	1:A:25:G:O5'	0.63	2.16	8	12
2:B:380:TYR:CD1	2:B:445:ARG:CZ	0.63	2.81	4	1
2:B:380:TYR:CD1	2:B:445:ARG:NE	0.63	2.67	4	2
2:B:373:GLN:CG	2:B:438:LEU:HD13	0.63	2.23	10	4
2:B:405:ARG:CB	2:B:411:VAL:HG22	0.63	2.23	14	5
2:B:432:LEU:O	2:B:432:LEU:HD13	0.63	1.93	12	2
1:A:5:U:H6	1:A:5:U:O5'	0.63	1.76	7	8
2:B:422:ILE:O	2:B:426:ARG:HB3	0.63	1.94	7	16
1:A:1:G:HO2'	1:A:2:G:C5'	0.63	2.07	4	4
1:A:24:U:O2'	1:A:25:G:H5'	0.63	1.92	5	4
1:A:20:A:O2'	1:A:21:A:C5'	0.63	2.46	8	3
1:A:15:A:C6	1:A:16:A:C5	0.63	2.87	16	11

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:380:TYR:HH	2:B:441:TYR:C	0.63	2.01	16	1
2:B:421:LYS:O	2:B:425:ILE:HD12	0.63	1.93	8	6
1:A:4:A:O2'	1:A:5:U:C5'	0.63	2.46	2	4
1:A:15:A:C5	1:A:16:A:N7	0.62	2.67	14	13
2:B:388:VAL:HG23	2:B:403:GLU:CG	0.62	2.24	8	3
2:B:368:MET:HE2	2:B:369:ASN:ND2	0.62	2.10	4	2
2:B:378:ILE:O	2:B:380:TYR:CD2	0.62	2.52	15	1
2:B:386:HIS:NE2	2:B:388:VAL:CG1	0.62	2.61	12	8
1:A:9:A:N1	1:A:25:G:C6	0.62	2.67	8	3
2:B:419:ASN:O	2:B:420:ILE:CG2	0.62	2.47	5	4
2:B:370:ALA:HB3	2:B:429:GLU:OE2	0.62	1.95	16	1
1:A:15:A:N1	1:A:19:G:O6	0.62	2.33	1	13
1:A:18:U:C5	1:A:18:U:OP2	0.62	2.53	5	1
1:A:12:U:H2'	1:A:13:U:O4'	0.61	1.94	6	10
2:B:372:ARG:O	2:B:376:SER:CB	0.61	2.47	3	16
2:B:419:ASN:C	2:B:420:ILE:HG22	0.61	2.19	2	3
2:B:432:LEU:O	2:B:432:LEU:HD23	0.61	1.94	6	2
1:A:18:U:C6	1:A:18:U:O5'	0.61	2.53	6	3
2:B:406:VAL:HG23	2:B:407:GLY:N	0.61	2.09	2	1
1:A:15:A:C6	1:A:19:G:O6	0.61	2.53	2	10
2:B:401:ILE:HB	2:B:416:VAL:HG13	0.61	1.72	9	4
1:A:7:C:C4	1:A:8:C:C5	0.61	2.89	13	4
2:B:380:TYR:CD2	2:B:445:ARG:HB2	0.61	2.29	15	4
1:A:23:G:N7	1:A:24:U:C5	0.61	2.68	16	2
1:A:2:G:C6	1:A:3:G:C5	0.61	2.88	2	6
1:A:18:U:O2	1:A:19:G:N7	0.61	2.33	13	8
2:B:373:GLN:O	2:B:377:LEU:CB	0.61	2.49	8	15
2:B:403:GLU:CB	2:B:411:VAL:HG21	0.61	2.25	8	1
2:B:380:TYR:CG	2:B:445:ARG:HG3	0.61	2.31	12	1
1:A:8:C:O2'	1:A:9:A:O5'	0.61	2.18	13	9
2:B:385:LEU:HB2	2:B:406:VAL:HG12	0.61	1.72	6	2
2:B:388:VAL:HG23	2:B:388:VAL:O	0.61	1.94	10	6
2:B:366:LEU:HD21	2:B:369:ASN:CG	0.61	2.21	9	2
1:A:18:U:O2'	1:A:19:G:O4'	0.61	2.19	7	15
2:B:419:ASN:O	2:B:420:ILE:HG23	0.61	1.95	9	7
1:A:15:A:O2'	1:A:16:A:H3'	0.61	1.95	16	1
1:A:10:U:O2'	1:A:11:G:O5'	0.60	2.19	7	13
1:A:20:A:O2'	1:A:21:A:O5'	0.60	2.19	11	15
2:B:380:TYR:CD1	2:B:380:TYR:N	0.60	2.68	11	7
2:B:386:HIS:CD2	2:B:386:HIS:O	0.60	2.54	12	1
2:B:379:GLY:C	2:B:383:LEU:HD21	0.60	2.21	13	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:402:VAL:HG21	2:B:423:ALA:C	0.60	2.21	12	8
2:B:415:GLY:HA3	2:B:427:ALA:HB2	0.60	1.73	14	9
1:A:18:U:O2'	1:A:19:G:O5'	0.60	2.19	5	1
2:B:385:LEU:N	2:B:385:LEU:CD2	0.60	2.64	12	1
2:B:370:ALA:CB	2:B:428:ALA:CB	0.60	2.80	14	4
2:B:386:HIS:NE2	2:B:388:VAL:HG13	0.60	2.11	1	11
1:A:19:G:O2'	1:A:20:A:H5'	0.60	1.97	13	4
1:A:18:U:C4'	1:A:19:G:OP1	0.60	2.50	5	1
2:B:419:ASN:O	2:B:421:LYS:N	0.60	2.35	13	2
2:B:402:VAL:O	2:B:414:THR:HG22	0.60	1.96	8	1
1:A:20:A:OP1	2:B:375:TYR:CD2	0.60	2.54	11	7
2:B:368:MET:HE3	2:B:369:ASN:CA	0.60	2.25	2	1
2:B:386:HIS:CE1	2:B:388:VAL:CG1	0.60	2.85	1	9
1:A:9:A:O2'	1:A:10:U:C5'	0.59	2.50	13	9
1:A:6:A:O2'	1:A:7:C:C5'	0.59	2.50	14	3
2:B:378:ILE:HD12	2:B:441:TYR:HB3	0.59	1.74	9	2
1:A:1:G:N3	1:A:2:G:N7	0.59	2.49	4	2
1:A:17:G:C8	2:B:372:ARG:NE	0.59	2.71	2	2
2:B:388:VAL:CG2	2:B:403:GLU:CB	0.59	2.80	5	9
2:B:386:HIS:CD2	2:B:386:HIS:C	0.59	2.80	4	1
2:B:377:LEU:HD12	2:B:442:ALA:CB	0.59	2.27	7	1
1:A:16:A:N6	2:B:368:MET:O	0.59	2.35	16	1
2:B:386:HIS:C	2:B:386:HIS:CD2	0.59	2.80	1	9
2:B:380:TYR:N	2:B:380:TYR:CD1	0.59	2.70	3	1
2:B:384:ARG:O	2:B:407:GLY:N	0.59	2.35	9	10
2:B:402:VAL:HG22	2:B:423:ALA:HB1	0.59	1.74	16	6
1:A:16:A:C2	2:B:372:ARG:HG3	0.59	2.33	16	1
1:A:16:A:N3	1:A:18:U:O4	0.59	2.35	5	5
2:B:378:ILE:HD12	2:B:378:ILE:O	0.59	1.97	15	1
1:A:3:G:O2'	1:A:4:A:O5'	0.59	2.21	2	8
1:A:10:U:O2'	1:A:11:G:O4'	0.59	2.21	14	8
1:A:17:G:C6	2:B:372:ARG:NH1	0.59	2.71	8	1
1:A:8:C:N4	1:A:9:A:H62	0.59	1.95	9	1
2:B:380:TYR:CD2	2:B:445:ARG:CG	0.59	2.86	15	3
1:A:25:G:O2'	1:A:26:G:O5'	0.59	2.19	15	2
1:A:11:G:O2'	1:A:12:U:O5'	0.59	2.21	15	14
1:A:28:A:O2'	1:A:29:U:O5'	0.58	2.21	1	6
2:B:401:ILE:HG13	2:B:416:VAL:HG13	0.58	1.74	9	2
1:A:15:A:C2	1:A:18:U:C4	0.58	2.90	3	2
1:A:17:G:O6	2:B:368:MET:HE1	0.58	1.98	3	1
1:A:20:A:OP1	2:B:375:TYR:CE2	0.58	2.56	12	7

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:378:ILE:HG22	2:B:378:ILE:O	0.58	1.98	2	2
2:B:440:PHE:CE2	2:B:441:TYR:CD2	0.58	2.91	7	7
1:A:19:G:O2'	1:A:20:A:O4'	0.58	2.21	16	11
1:A:8:C:C4	1:A:9:A:N7	0.58	2.71	8	2
2:B:380:TYR:CE1	2:B:383:LEU:HB2	0.58	2.33	8	1
1:A:29:U:HO2'	1:A:30:C:H5'	0.58	1.57	6	1
2:B:378:ILE:HD12	2:B:379:GLY:N	0.58	2.13	12	1
2:B:420:ILE:C	2:B:420:ILE:CD1	0.58	2.70	13	6
2:B:388:VAL:CG2	2:B:403:GLU:CG	0.58	2.81	10	2
1:A:19:G:O2'	1:A:20:A:O5'	0.58	2.22	16	4
2:B:379:GLY:O	2:B:380:TYR:CD2	0.58	2.57	4	1
1:A:31:U:O2'	1:A:32:C:O4'	0.58	2.21	3	8
1:A:30:C:C4	1:A:31:U:C4	0.58	2.92	10	4
2:B:379:GLY:C	2:B:380:TYR:CG	0.58	2.81	5	4
2:B:401:ILE:HD12	2:B:416:VAL:HG21	0.58	1.72	5	2
2:B:404:CYS:O	2:B:411:VAL:HG23	0.58	1.98	8	1
2:B:412:LEU:N	2:B:412:LEU:HD12	0.58	2.14	8	1
1:A:25:G:O2'	1:A:26:G:H5'	0.58	1.99	15	1
1:A:6:A:N6	1:A:28:A:N6	0.58	2.52	14	4
1:A:13:U:O2'	1:A:14:C:O4'	0.58	2.20	1	4
2:B:435:LYS:CG	2:B:436:LYS:N	0.58	2.67	6	16
1:A:15:A:N3	1:A:16:A:C8	0.58	2.72	16	1
1:A:21:A:O5'	1:A:21:A:C8	0.58	2.53	13	9
1:A:16:A:C1'	1:A:18:U:O4	0.58	2.52	6	1
2:B:390:VAL:CG2	2:B:401:ILE:CG2	0.58	2.80	9	5
1:A:7:C:N4	1:A:8:C:H41	0.58	1.97	5	3
1:A:15:A:C6	1:A:16:A:C6	0.58	2.92	16	3
2:B:366:LEU:C	2:B:366:LEU:HD12	0.58	2.24	11	1
1:A:7:C:O5'	1:A:7:C:H6	0.57	1.82	14	6
2:B:390:VAL:O	2:B:401:ILE:CG2	0.57	2.51	10	9
2:B:405:ARG:HB2	2:B:411:VAL:HG22	0.57	1.75	15	2
1:A:21:A:O2'	1:A:22:C:O5'	0.57	2.22	8	16
2:B:380:TYR:CE2	2:B:445:ARG:O	0.57	2.57	12	1
2:B:415:GLY:CA	2:B:426:ARG:CD	0.57	2.82	16	1
1:A:30:C:N4	1:A:31:U:C4	0.57	2.73	10	5
2:B:399:ASN:CA	2:B:418:ARG:O	0.57	2.52	4	4
2:B:379:GLY:O	2:B:380:TYR:CD1	0.57	2.57	7	1
1:A:15:A:N6	1:A:19:G:N2	0.57	2.52	16	1
2:B:378:ILE:O	2:B:378:ILE:HG22	0.57	1.99	13	4
2:B:440:PHE:CE2	2:B:441:TYR:CD1	0.57	2.93	16	3
1:A:4:A:HO2'	1:A:5:U:C5'	0.57	2.13	13	5

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:18:U:OP1	1:A:18:U:C4'	0.57	2.52	4	3
1:A:1:G:C2	1:A:2:G:C8	0.57	2.92	1	3
1:A:3:G:O2'	1:A:4:A:H5'	0.57	2.00	11	2
1:A:11:G:C2	1:A:23:G:C2	0.57	2.92	8	6
1:A:15:A:C5	1:A:16:A:C5	0.57	2.92	15	10
1:A:23:G:C5	1:A:24:U:C4	0.57	2.92	16	3
2:B:400:SER:O	2:B:423:ALA:HB2	0.57	1.99	8	4
2:B:402:VAL:CG2	2:B:415:GLY:O	0.57	2.53	4	3
2:B:380:TYR:CE2	2:B:382:SER:HB3	0.57	2.34	10	1
2:B:415:GLY:N	2:B:427:ALA:HB2	0.57	2.14	12	2
1:A:15:A:C4'	1:A:16:A:OP1	0.57	2.52	16	1
1:A:30:C:N4	1:A:31:U:O4	0.57	2.38	10	2
1:A:15:A:O2'	1:A:17:G:N7	0.57	2.37	6	1
2:B:367:ASP:CA	2:B:425:ILE:HG23	0.57	2.30	11	4
2:B:383:LEU:O	2:B:384:ARG:CB	0.57	2.53	7	3
2:B:445:ARG:O	2:B:448:ILE:CD1	0.57	2.53	5	12
2:B:419:ASN:O	2:B:420:ILE:CB	0.56	2.52	12	2
2:B:373:GLN:OE1	2:B:438:LEU:HD13	0.56	1.98	14	1
1:A:14:C:C4	1:A:15:A:C5	0.56	2.94	12	8
1:A:26:G:O2'	1:A:27:U:O5'	0.56	2.22	14	7
1:A:1:G:O2'	1:A:2:G:O5'	0.56	2.21	4	7
1:A:11:G:O2'	1:A:12:U:O4'	0.56	2.22	7	8
2:B:381:ALA:O	2:B:382:SER:CB	0.56	2.52	3	5
2:B:379:GLY:O	2:B:380:TYR:CB	0.56	2.53	9	3
1:A:17:G:C5	2:B:372:ARG:NH1	0.56	2.74	8	2
2:B:412:LEU:C	2:B:412:LEU:CD2	0.56	2.79	14	1
1:A:3:G:HO2'	1:A:4:A:C5'	0.56	2.13	1	3
2:B:444:GLN:HG3	2:B:445:ARG:N	0.56	2.15	14	14
1:A:25:G:C6	1:A:26:G:C6	0.56	2.92	1	5
2:B:366:LEU:N	2:B:366:LEU:HD23	0.56	2.15	15	2
2:B:401:ILE:HD11	2:B:416:VAL:HG22	0.56	1.77	12	1
1:A:1:G:N2	1:A:2:G:C4	0.56	2.73	3	5
2:B:422:ILE:O	2:B:426:ARG:CG	0.56	2.54	5	12
2:B:387:TYR:CZ	2:B:404:CYS:SG	0.56	2.97	13	3
2:B:437:MET:SD	2:B:441:TYR:CD1	0.56	2.99	5	2
1:A:15:A:C2'	1:A:16:A:O5'	0.56	2.54	10	2
2:B:374:LEU:O	2:B:378:ILE:HG23	0.56	2.00	12	1
2:B:403:GLU:OE2	2:B:411:VAL:HG21	0.56	2.01	12	1
1:A:15:A:C6	1:A:19:G:C6	0.56	2.94	2	1
2:B:380:TYR:HD2	2:B:383:LEU:HD13	0.56	1.60	2	1
2:B:402:VAL:HG23	2:B:427:ALA:HB2	0.56	1.76	2	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:373:GLN:NE2	2:B:373:GLN:C	0.56	2.64	15	4
1:A:17:G:C4	2:B:372:ARG:NH1	0.56	2.74	6	1
2:B:437:MET:O	2:B:440:PHE:CD2	0.56	2.59	15	5
1:A:6:A:O2'	1:A:7:C:O5'	0.56	2.24	8	4
2:B:385:LEU:HD23	2:B:385:LEU:H	0.56	1.61	10	7
2:B:388:VAL:CG2	2:B:403:GLU:HB2	0.56	2.31	12	13
1:A:12:U:O5'	1:A:12:U:H6	0.56	1.84	11	8
2:B:401:ILE:HB	2:B:416:VAL:HG22	0.56	1.77	6	1
1:A:20:A:O2'	1:A:21:A:H5'	0.56	2.01	8	1
1:A:2:G:O2'	1:A:3:G:O5'	0.56	2.24	9	1
2:B:380:TYR:CD1	2:B:445:ARG:HG2	0.56	2.36	14	2
2:B:405:ARG:CG	2:B:411:VAL:HG22	0.56	2.31	5	1
2:B:380:TYR:OH	2:B:446:ALA:HB2	0.56	2.01	12	1
1:A:4:A:O2'	1:A:5:U:O5'	0.55	2.23	14	7
1:A:8:C:N4	1:A:9:A:C6	0.55	2.74	8	1
2:B:366:LEU:HD12	2:B:366:LEU:O	0.55	2.01	2	1
2:B:367:ASP:O	2:B:371:LYS:CG	0.55	2.55	2	1
2:B:445:ARG:O	2:B:448:ILE:CG1	0.55	2.53	11	3
2:B:445:ARG:O	2:B:448:ILE:HG12	0.55	2.02	15	12
2:B:380:TYR:CE1	2:B:445:ARG:HG2	0.55	2.37	5	3
2:B:380:TYR:CE1	2:B:383:LEU:CB	0.55	2.88	8	1
2:B:382:SER:O	2:B:383:LEU:C	0.55	2.49	12	2
2:B:386:HIS:CD2	2:B:405:ARG:HG3	0.55	2.36	10	3
2:B:419:ASN:C	2:B:420:ILE:CG2	0.55	2.79	16	9
1:A:2:G:O2'	1:A:3:G:C5'	0.55	2.55	9	3
2:B:405:ARG:CG	2:B:411:VAL:CG2	0.55	2.84	5	1
2:B:380:TYR:N	2:B:383:LEU:HD21	0.55	2.15	13	1
2:B:374:LEU:HD11	2:B:431:ALA:HB3	0.55	1.78	2	2
2:B:380:TYR:CE2	2:B:445:ARG:CG	0.55	2.90	4	3
2:B:432:LEU:HD12	2:B:432:LEU:C	0.55	2.24	8	1
2:B:380:TYR:CE2	2:B:445:ARG:HG2	0.55	2.36	4	5
2:B:366:LEU:HD12	2:B:367:ASP:N	0.55	2.17	11	1
2:B:378:ILE:HG23	2:B:380:TYR:OH	0.55	2.02	16	1
1:A:8:C:HO2'	1:A:9:A:C5'	0.55	2.14	13	4
2:B:420:ILE:HG23	2:B:421:LYS:HD2	0.55	1.77	10	3
1:A:7:C:O2'	1:A:8:C:O5'	0.55	2.24	6	2
2:B:419:ASN:OD1	2:B:422:ILE:CD1	0.55	2.55	1	2
1:A:2:G:C5	1:A:3:G:N7	0.55	2.75	2	2
2:B:370:ALA:CB	2:B:429:GLU:OE1	0.55	2.55	2	2
2:B:406:VAL:O	2:B:408:ASP:N	0.55	2.39	6	6
2:B:399:ASN:N	2:B:418:ARG:O	0.55	2.40	4	5

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:375:TYR:O	2:B:379:GLY:CA	0.55	2.55	7	4
1:A:5:U:O2'	1:A:6:A:C5'	0.55	2.55	15	2
2:B:383:LEU:HD22	2:B:441:TYR:CD2	0.55	2.36	16	1
1:A:27:U:C4	1:A:28:A:N7	0.54	2.75	1	1
2:B:380:TYR:CE2	2:B:382:SER:HB2	0.54	2.37	10	2
2:B:419:ASN:CG	2:B:422:ILE:CD1	0.54	2.80	4	1
1:A:17:G:O2'	2:B:372:ARG:NH1	0.54	2.40	10	3
1:A:17:G:H8	1:A:18:U:O2	0.54	1.85	4	2
2:B:378:ILE:CD1	2:B:438:LEU:O	0.54	2.56	6	10
2:B:381:ALA:O	2:B:445:ARG:CZ	0.54	2.56	7	1
2:B:380:TYR:N	2:B:383:LEU:CD2	0.54	2.70	13	1
2:B:380:TYR:HE1	2:B:383:LEU:HD13	0.54	1.62	14	1
2:B:406:VAL:O	2:B:409:GLY:N	0.54	2.40	3	15
2:B:419:ASN:H	2:B:422:ILE:HD13	0.54	1.62	4	1
2:B:410:THR:CG2	2:B:441:TYR:OH	0.54	2.56	5	1
2:B:402:VAL:O	2:B:414:THR:CG2	0.54	2.55	8	1
1:A:23:G:O2'	1:A:24:U:O5'	0.54	2.25	9	2
2:B:374:LEU:O	2:B:378:ILE:O	0.54	2.25	12	7
1:A:10:U:O2'	1:A:11:G:C5'	0.54	2.55	6	4
2:B:380:TYR:CE2	2:B:383:LEU:HD22	0.54	2.38	2	1
1:A:9:A:C6	1:A:10:U:C4	0.54	2.95	2	3
2:B:434:ASP:O	2:B:437:MET:N	0.54	2.39	4	13
1:A:23:G:C6	1:A:24:U:N3	0.54	2.75	16	2
1:A:11:G:HO2'	1:A:12:U:C5'	0.54	2.16	16	7
2:B:373:GLN:HE22	2:B:438:LEU:HD22	0.54	1.63	10	1
1:A:16:A:C2	2:B:372:ARG:HG2	0.54	2.37	16	1
1:A:13:U:O2'	1:A:14:C:O5'	0.54	2.26	10	6
2:B:391:LYS:O	2:B:393:PRO:CD	0.54	2.56	7	9
2:B:380:TYR:CE2	2:B:445:ARG:HB3	0.54	2.37	5	5
2:B:401:ILE:CD1	2:B:416:VAL:CG2	0.54	2.83	5	2
1:A:1:G:O5'	1:A:1:G:H8	0.54	1.86	14	1
2:B:401:ILE:HG13	2:B:416:VAL:HG12	0.54	1.79	16	1
2:B:373:GLN:CD	2:B:377:LEU:CD1	0.54	2.81	1	1
2:B:374:LEU:CD1	2:B:387:TYR:OH	0.54	2.55	7	5
2:B:379:GLY:O	2:B:380:TYR:CG	0.54	2.61	9	2
1:A:1:G:O2'	1:A:2:G:H8	0.54	1.86	12	3
2:B:378:ILE:HG22	2:B:379:GLY:N	0.54	2.18	11	4
2:B:380:TYR:CD2	2:B:383:LEU:HD13	0.54	2.38	2	1
2:B:406:VAL:CG2	2:B:441:TYR:OH	0.54	2.56	2	1
2:B:384:ARG:C	2:B:385:LEU:CD2	0.54	2.81	12	1
2:B:374:LEU:HD23	2:B:374:LEU:N	0.53	2.17	4	6

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:380:TYR:CD2	2:B:445:ARG:HD3	0.53	2.39	4	2
2:B:402:VAL:CG2	2:B:423:ALA:O	0.53	2.56	10	9
2:B:370:ALA:CB	2:B:429:GLU:OE2	0.53	2.56	15	3
2:B:383:LEU:HD11	2:B:406:VAL:CG1	0.53	2.33	16	1
1:A:22:C:C2'	1:A:23:G:O5'	0.53	2.56	15	11
2:B:380:TYR:CD2	2:B:445:ARG:HG2	0.53	2.39	16	4
2:B:400:SER:O	2:B:423:ALA:CB	0.53	2.56	8	4
1:A:30:C:H2'	1:A:31:U:O4'	0.53	2.02	9	1
1:A:15:A:N1	1:A:16:A:C5	0.53	2.77	16	1
2:B:385:LEU:HB2	2:B:405:ARG:O	0.53	2.02	9	9
2:B:445:ARG:CD	2:B:445:ARG:C	0.53	2.81	3	2
2:B:388:VAL:CG2	2:B:388:VAL:O	0.53	2.56	4	2
2:B:380:TYR:CZ	2:B:445:ARG:HB3	0.53	2.38	5	2
2:B:368:MET:CG	2:B:369:ASN:N	0.53	2.70	16	2
2:B:440:PHE:CZ	2:B:441:TYR:CE2	0.53	2.96	4	3
2:B:380:TYR:CD1	2:B:445:ARG:CD	0.53	2.92	9	1
1:A:30:C:HO2'	1:A:31:U:H5'	0.53	1.58	13	1
2:B:389:THR:O	2:B:389:THR:CG2	0.53	2.56	4	2
2:B:366:LEU:CD1	2:B:367:ASP:N	0.53	2.72	11	1
1:A:3:G:C2	1:A:4:A:C5	0.53	2.96	7	1
2:B:366:LEU:O	2:B:369:ASN:ND2	0.53	2.41	11	2
2:B:380:TYR:CD1	2:B:445:ARG:HB2	0.53	2.39	1	4
1:A:18:U:OP2	1:A:18:U:C6	0.53	2.61	5	1
2:B:444:GLN:OE1	2:B:445:ARG:NH2	0.53	2.42	7	1
2:B:448:ILE:N	2:B:448:ILE:HD12	0.53	2.18	7	1
2:B:378:ILE:HD12	2:B:380:TYR:OH	0.53	2.04	16	1
2:B:419:ASN:ND2	2:B:422:ILE:CD1	0.53	2.72	4	1
1:A:15:A:H2'	1:A:16:A:O4'	0.53	2.03	5	1
2:B:418:ARG:N	2:B:418:ARG:CD	0.53	2.72	9	3
1:A:15:A:C5	1:A:16:A:C8	0.53	2.97	14	7
2:B:429:GLU:O	2:B:433:ARG:CG	0.53	2.57	5	5
2:B:444:GLN:O	2:B:448:ILE:CG2	0.53	2.56	14	1
2:B:406:VAL:HG11	2:B:441:TYR:CE1	0.53	2.39	4	1
2:B:373:GLN:HG3	2:B:438:LEU:HD13	0.53	1.81	10	3
2:B:425:ILE:CG2	2:B:429:GLU:OE2	0.53	2.57	12	2
1:A:5:U:O5'	1:A:5:U:H6	0.52	1.86	14	3
2:B:367:ASP:O	2:B:370:ALA:N	0.52	2.41	11	5
2:B:388:VAL:O	2:B:388:VAL:CG2	0.52	2.57	10	2
2:B:386:HIS:CE1	2:B:388:VAL:HG12	0.52	2.39	12	1
1:A:17:G:C8	1:A:18:U:O2	0.52	2.62	3	3
2:B:367:ASP:N	2:B:425:ILE:HG23	0.52	2.19	6	4

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:372:ARG:NH1	2:B:376:SER:CB	0.52	2.72	5	1
1:A:15:A:C2	1:A:16:A:N9	0.52	2.77	16	1
2:B:420:ILE:O	2:B:423:ALA:CB	0.52	2.56	14	7
2:B:421:LYS:O	2:B:425:ILE:N	0.52	2.39	12	3
2:B:405:ARG:CA	2:B:410:THR:O	0.52	2.57	16	5
2:B:404:CYS:O	2:B:412:LEU:N	0.52	2.40	7	1
1:A:19:G:HO2'	1:A:20:A:C4'	0.52	2.16	10	1
2:B:420:ILE:HD12	2:B:420:ILE:C	0.52	2.28	6	1
1:A:19:G:O2'	1:A:20:A:C8	0.52	2.61	14	2
2:B:389:THR:CG2	2:B:389:THR:O	0.52	2.57	2	1
1:A:19:G:N3	2:B:371:LYS:HE2	0.52	2.20	8	7
2:B:388:VAL:CG2	2:B:403:GLU:HB3	0.52	2.35	7	6
1:A:2:G:C6	1:A:3:G:N7	0.52	2.78	2	1
1:A:20:A:O2'	1:A:21:A:C8	0.52	2.59	10	2
2:B:415:GLY:HA3	2:B:426:ARG:CD	0.52	2.34	16	1
2:B:389:THR:O	2:B:389:THR:HG23	0.52	2.04	2	3
2:B:419:ASN:OD1	2:B:419:ASN:N	0.52	2.43	6	3
2:B:383:LEU:CD1	2:B:408:ASP:OD1	0.52	2.57	7	1
2:B:404:CYS:CB	2:B:413:GLY:O	0.52	2.58	9	1
1:A:1:G:N2	1:A:2:G:C5	0.52	2.78	4	4
2:B:373:GLN:NE2	2:B:373:GLN:O	0.52	2.42	6	5
2:B:414:THR:O	2:B:430:ASN:CG	0.52	2.53	14	5
2:B:445:ARG:O	2:B:448:ILE:HD11	0.52	2.03	7	1
1:A:29:U:O2'	1:A:30:C:O5'	0.52	2.28	11	1
1:A:5:U:C4	1:A:6:A:N7	0.52	2.77	14	2
1:A:20:A:O5'	1:A:20:A:H8	0.52	1.88	14	1
1:A:18:U:O2'	1:A:19:G:P	0.52	2.68	5	1
2:B:383:LEU:HD12	2:B:383:LEU:C	0.52	2.30	10	1
2:B:391:LYS:CB	2:B:400:SER:CB	0.52	2.88	11	1
1:A:6:A:HO2'	1:A:7:C:C5'	0.52	2.18	13	1
2:B:420:ILE:HD13	2:B:421:LYS:N	0.52	2.18	13	1
2:B:378:ILE:O	2:B:379:GLY:C	0.52	2.52	15	1
1:A:15:A:C2	1:A:16:A:C5	0.52	2.98	16	1
2:B:379:GLY:O	2:B:380:TYR:C	0.51	2.53	16	3
1:A:15:A:C8	1:A:16:A:N7	0.51	2.78	3	2
2:B:386:HIS:C	2:B:387:TYR:CD1	0.51	2.88	4	2
1:A:11:G:N3	1:A:23:G:C2	0.51	2.78	6	3
2:B:405:ARG:HA	2:B:410:THR:O	0.51	2.06	16	13
2:B:444:GLN:C	2:B:444:GLN:CD	0.51	2.78	2	12
2:B:417:GLY:HA3	2:B:422:ILE:CG2	0.51	2.35	4	2
2:B:389:THR:OG1	2:B:402:VAL:CG1	0.51	2.58	5	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:17:G:O4'	1:A:17:G:OP1	0.51	2.28	6	1
1:A:15:A:H2'	1:A:16:A:O5'	0.51	2.06	10	1
2:B:378:ILE:O	2:B:380:TYR:CG	0.51	2.63	15	1
2:B:367:ASP:O	2:B:368:MET:C	0.51	2.53	6	14
1:A:11:G:N3	1:A:23:G:N2	0.51	2.58	6	2
1:A:29:U:C4	1:A:30:C:C5	0.51	2.98	7	1
2:B:414:THR:O	2:B:430:ASN:CB	0.51	2.59	10	4
1:A:27:U:O5'	1:A:27:U:H6	0.51	1.88	14	1
1:A:18:U:OP1	1:A:18:U:O4'	0.51	2.29	14	3
2:B:391:LYS:O	2:B:393:PRO:HD3	0.51	2.06	3	11
1:A:2:G:O5'	1:A:2:G:H8	0.51	1.88	5	1
2:B:366:LEU:CD1	2:B:368:MET:N	0.51	2.74	11	1
1:A:18:U:C2'	1:A:19:G:C8	0.51	2.94	5	2
2:B:402:VAL:CG2	2:B:423:ALA:C	0.51	2.83	6	4
2:B:420:ILE:HG13	2:B:421:LYS:N	0.51	2.21	3	6
2:B:406:VAL:HG23	2:B:410:THR:O	0.51	2.06	5	2
2:B:434:ASP:N	2:B:434:ASP:OD1	0.51	2.43	5	3
2:B:373:GLN:NE2	2:B:438:LEU:CD2	0.51	2.68	10	1
2:B:406:VAL:CG1	2:B:412:LEU:HD12	0.51	2.36	2	1
2:B:373:GLN:OE1	2:B:377:LEU:CD2	0.51	2.59	11	4
2:B:383:LEU:HD13	2:B:406:VAL:CG1	0.51	2.36	10	1
1:A:4:A:O5'	1:A:4:A:H8	0.51	1.89	11	1
1:A:19:G:O2'	2:B:371:LYS:HG3	0.51	2.05	11	1
2:B:402:VAL:O	2:B:414:THR:CB	0.51	2.58	11	1
2:B:373:GLN:OE1	2:B:377:LEU:CD1	0.51	2.58	5	4
1:A:17:G:O6	2:B:368:MET:HE2	0.51	2.06	16	2
2:B:444:GLN:O	2:B:448:ILE:N	0.51	2.44	14	1
2:B:401:ILE:CG1	2:B:416:VAL:HG12	0.51	2.36	16	1
2:B:380:TYR:CD2	2:B:445:ARG:HG3	0.51	2.41	12	1
2:B:379:GLY:O	2:B:380:TYR:O	0.50	2.29	2	3
2:B:401:ILE:HD12	2:B:416:VAL:HG22	0.50	1.82	11	2
2:B:394:THR:CB	2:B:397:ASP:OD2	0.50	2.58	8	1
2:B:380:TYR:CE1	2:B:445:ARG:HB2	0.50	2.41	8	5
2:B:406:VAL:HG11	2:B:441:TYR:OH	0.50	2.07	13	2
1:A:15:A:C2	1:A:16:A:C2'	0.50	2.94	16	1
2:B:385:LEU:CB	2:B:406:VAL:HA	0.50	2.36	6	6
2:B:397:ASP:OD2	2:B:399:ASN:ND2	0.50	2.45	6	1
1:A:17:G:O2'	2:B:372:ARG:NH2	0.50	2.45	15	1
1:A:27:U:H6	1:A:27:U:O5'	0.50	1.89	5	1
2:B:432:LEU:O	2:B:432:LEU:CD2	0.50	2.59	6	4
1:A:24:U:O5'	1:A:24:U:H6	0.50	1.89	9	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:373:GLN:CD	2:B:373:GLN:C	0.50	2.79	14	2
1:A:18:U:OP1	1:A:18:U:H4'	0.50	2.07	4	1
2:B:417:GLY:HA3	2:B:422:ILE:HG22	0.50	1.83	4	1
1:A:25:G:HO2'	1:A:26:G:C5'	0.50	2.19	6	1
2:B:366:LEU:HD11	2:B:368:MET:HB3	0.50	1.81	11	1
2:B:387:TYR:CE2	2:B:404:CYS:SG	0.50	3.05	4	1
1:A:16:A:C2	1:A:18:U:O4	0.50	2.65	11	2
2:B:383:LEU:CD1	2:B:384:ARG:N	0.50	2.73	10	1
2:B:380:TYR:CD1	2:B:445:ARG:CG	0.50	2.94	14	1
1:A:17:G:O2'	1:A:18:U:OP1	0.50	2.26	16	1
2:B:373:GLN:O	2:B:377:LEU:HB2	0.50	2.06	15	12
1:A:30:C:C1'	2:B:395:ALA:HB1	0.50	2.37	2	1
2:B:419:ASN:O	2:B:420:ILE:HG13	0.50	2.07	11	6
2:B:385:LEU:O	2:B:385:LEU:HG	0.50	2.06	6	1
1:A:15:A:N6	1:A:16:A:C5	0.50	2.80	14	1
2:B:372:ARG:O	2:B:376:SER:HB2	0.50	2.07	5	14
1:A:8:C:C4	1:A:9:A:C5	0.50	3.00	8	1
1:A:17:G:N7	2:B:372:ARG:HD3	0.50	2.22	8	2
2:B:437:MET:HE3	2:B:441:TYR:HE2	0.50	1.64	15	1
2:B:432:LEU:C	2:B:432:LEU:CD2	0.50	2.81	2	2
2:B:425:ILE:HD12	2:B:425:ILE:H	0.50	1.67	5	2
2:B:444:GLN:OE1	2:B:448:ILE:CG2	0.50	2.60	15	2
2:B:378:ILE:C	2:B:378:ILE:CD1	0.50	2.81	15	1
1:A:16:A:O4'	1:A:17:G:O4'	0.50	2.30	16	1
2:B:366:LEU:HD11	2:B:432:LEU:HD13	0.49	1.84	2	1
2:B:443:LYS:O	2:B:447:ALA:HB2	0.49	2.07	2	2
2:B:380:TYR:CD1	2:B:445:ARG:HD3	0.49	2.42	9	2
1:A:6:A:N6	1:A:7:C:N4	0.49	2.60	15	1
1:A:7:C:HO2'	1:A:8:C:C5'	0.49	2.20	15	1
1:A:15:A:O2'	1:A:16:A:C3'	0.49	2.59	16	1
2:B:415:GLY:CA	2:B:426:ARG:HD2	0.49	2.37	16	1
2:B:380:TYR:CG	2:B:445:ARG:HD3	0.49	2.42	10	5
2:B:390:VAL:HG23	2:B:401:ILE:HG21	0.49	1.81	9	3
2:B:378:ILE:HG23	2:B:441:TYR:HB3	0.49	1.84	3	2
2:B:371:LYS:HD2	2:B:372:ARG:N	0.49	2.23	8	5
1:A:15:A:O2'	2:B:368:MET:CE	0.49	2.60	5	1
1:A:24:U:O4	1:A:25:G:O6	0.49	2.29	9	2
2:B:391:LYS:CG	2:B:400:SER:HA	0.49	2.37	15	6
2:B:399:ASN:HA	2:B:418:ARG:O	0.49	2.07	7	4
2:B:397:ASP:CG	2:B:397:ASP:O	0.49	2.55	9	3
2:B:415:GLY:N	2:B:427:ALA:CB	0.49	2.76	11	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:366:LEU:C	2:B:429:GLU:CD	0.49	2.80	14	2
1:A:15:A:O4'	1:A:16:A:OP1	0.49	2.30	16	1
1:A:28:A:HO2'	1:A:29:U:C5'	0.49	2.20	1	6
2:B:405:ARG:CB	2:B:410:THR:O	0.49	2.59	16	2
2:B:412:LEU:HD12	2:B:412:LEU:H	0.49	1.67	8	1
2:B:391:LYS:HG2	2:B:400:SER:N	0.49	2.22	9	2
2:B:410:THR:HG22	2:B:412:LEU:HD13	0.49	1.83	14	1
2:B:398:PRO:O	2:B:399:ASN:C	0.49	2.55	15	11
2:B:380:TYR:HD2	2:B:383:LEU:HD11	0.49	1.68	5	1
2:B:380:TYR:CZ	2:B:383:LEU:HB2	0.49	2.42	11	2
2:B:378:ILE:HG22	2:B:379:GLY:H	0.49	1.67	10	1
1:A:17:G:OP2	1:A:18:U:O4	0.49	2.29	16	1
2:B:373:GLN:CD	2:B:377:LEU:HD13	0.49	2.32	1	1
2:B:381:ALA:O	2:B:445:ARG:NE	0.49	2.45	7	1
2:B:401:ILE:CA	2:B:416:VAL:HG13	0.49	2.37	9	1
2:B:435:LYS:CG	2:B:436:LYS:HD2	0.49	2.37	11	2
2:B:435:LYS:HG2	2:B:436:LYS:CD	0.49	2.37	13	5
2:B:443:LYS:O	2:B:447:ALA:CB	0.49	2.61	2	1
2:B:382:SER:O	2:B:383:LEU:O	0.49	2.31	13	2
2:B:447:ALA:O	2:B:448:ILE:C	0.49	2.56	7	10
1:A:20:A:H2'	1:A:21:A:C8	0.49	2.43	13	12
2:B:445:ARG:C	2:B:445:ARG:CD	0.49	2.85	8	3
2:B:368:MET:HG3	2:B:369:ASN:N	0.49	2.21	16	2
2:B:369:ASN:ND2	2:B:370:ALA:N	0.49	2.61	11	2
2:B:383:LEU:O	2:B:384:ARG:CD	0.49	2.61	1	1
1:A:21:A:C2'	1:A:22:C:O5'	0.49	2.61	4	9
2:B:391:LYS:CB	2:B:400:SER:HA	0.49	2.38	3	9
2:B:381:ALA:CB	2:B:445:ARG:HA	0.49	2.38	9	1
2:B:380:TYR:CE1	2:B:383:LEU:HG	0.49	2.41	10	1
2:B:423:ALA:O	2:B:427:ALA:HB2	0.49	2.08	14	1
2:B:406:VAL:O	2:B:407:GLY:C	0.48	2.56	16	13
2:B:366:LEU:O	2:B:429:GLU:CD	0.48	2.56	15	3
2:B:380:TYR:CD2	2:B:445:ARG:CD	0.48	2.96	4	1
1:A:5:U:C2'	1:A:6:A:O5'	0.48	2.62	15	3
2:B:385:LEU:HA	2:B:406:VAL:HA	0.48	1.85	7	1
2:B:432:LEU:C	2:B:432:LEU:CD1	0.48	2.85	12	2
2:B:440:PHE:CZ	2:B:441:TYR:CD1	0.48	3.01	9	1
2:B:406:VAL:HG11	2:B:412:LEU:HD12	0.48	1.83	2	1
2:B:432:LEU:CD2	2:B:432:LEU:O	0.48	2.61	5	1
1:A:18:U:H2'	1:A:19:G:C8	0.48	2.43	5	7
2:B:368:MET:SD	2:B:368:MET:C	0.48	2.97	2	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:380:TYR:CE1	2:B:445:ARG:CG	0.48	2.97	5	2
2:B:385:LEU:HA	2:B:405:ARG:O	0.48	2.08	15	7
2:B:420:ILE:O	2:B:420:ILE:CD1	0.48	2.58	8	1
2:B:425:ILE:C	2:B:429:GLU:OE1	0.48	2.56	11	2
1:A:15:A:C2	1:A:18:U:N3	0.48	2.81	6	2
2:B:380:TYR:CD1	2:B:445:ARG:HG3	0.48	2.44	7	1
2:B:386:HIS:CD2	2:B:405:ARG:CG	0.48	2.96	10	1
2:B:371:LYS:HG2	2:B:372:ARG:N	0.48	2.22	12	2
2:B:401:ILE:HG12	2:B:416:VAL:CG2	0.48	2.38	12	2
2:B:387:TYR:N	2:B:387:TYR:CD1	0.48	2.81	4	1
2:B:373:GLN:OE1	2:B:377:LEU:CB	0.48	2.62	5	2
1:A:24:U:O2'	1:A:25:G:H8	0.48	1.92	8	2
2:B:397:ASP:O	2:B:397:ASP:OD1	0.48	2.31	8	1
2:B:379:GLY:C	2:B:380:TYR:CD1	0.48	2.92	9	1
2:B:391:LYS:CG	2:B:399:ASN:C	0.48	2.86	9	1
1:A:17:G:C8	2:B:372:ARG:HD3	0.48	2.43	13	2
2:B:445:ARG:HD2	2:B:448:ILE:HD11	0.48	1.85	15	1
1:A:22:C:H2'	1:A:23:G:O5'	0.48	2.08	7	4
2:B:372:ARG:O	2:B:376:SER:OG	0.48	2.32	6	5
2:B:388:VAL:HG23	2:B:403:GLU:HG2	0.48	1.85	8	1
2:B:419:ASN:O	2:B:421:LYS:HD3	0.48	2.09	13	1
2:B:427:ALA:O	2:B:430:ASN:HB2	0.48	2.09	11	11
2:B:385:LEU:O	2:B:385:LEU:CG	0.48	2.62	6	1
1:A:5:U:O4	1:A:6:A:N6	0.48	2.46	14	1
1:A:30:C:C2'	1:A:31:U:O5'	0.48	2.62	4	8
2:B:366:LEU:O	2:B:429:GLU:OE1	0.48	2.31	2	5
2:B:421:LYS:C	2:B:425:ILE:HD12	0.48	2.34	12	2
2:B:416:VAL:O	2:B:426:ARG:NH2	0.48	2.46	6	1
1:A:29:U:C4	1:A:30:C:C4	0.48	3.01	7	1
2:B:383:LEU:HG	2:B:384:ARG:N	0.48	2.23	16	3
2:B:365:SER:O	2:B:429:GLU:HG2	0.48	2.09	11	1
2:B:374:LEU:HA	2:B:378:ILE:HG23	0.48	1.83	12	1
2:B:387:TYR:CE1	2:B:404:CYS:SG	0.48	3.04	13	2
2:B:387:TYR:CE2	2:B:404:CYS:HB2	0.48	2.43	13	2
2:B:378:ILE:CG2	2:B:383:LEU:CD2	0.48	2.92	2	1
2:B:383:LEU:C	2:B:384:ARG:CG	0.48	2.86	4	1
2:B:380:TYR:CE2	2:B:445:ARG:HB2	0.48	2.44	5	1
2:B:403:GLU:OE1	2:B:405:ARG:NH2	0.48	2.47	12	1
2:B:439:ASP:O	2:B:442:ALA:N	0.47	2.46	13	6
2:B:372:ARG:HD2	2:B:376:SER:CB	0.47	2.39	7	4
2:B:375:TYR:O	2:B:378:ILE:O	0.47	2.31	10	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:419:ASN:OD1	2:B:422:ILE:CG1	0.47	2.62	7	2
1:A:11:G:O2'	1:A:12:U:H5'	0.47	2.08	4	3
2:B:368:MET:C	2:B:368:MET:SD	0.47	2.98	7	2
2:B:425:ILE:O	2:B:429:GLU:CD	0.47	2.57	11	2
2:B:421:LYS:CA	2:B:425:ILE:HD12	0.47	2.39	12	1
1:A:22:C:OP1	2:B:421:LYS:CD	0.47	2.61	1	1
1:A:31:U:O2'	1:A:32:C:O5'	0.47	2.32	3	4
2:B:415:GLY:CA	2:B:426:ARG:HG3	0.47	2.39	1	3
2:B:370:ALA:HB3	2:B:428:ALA:CB	0.47	2.37	3	2
1:A:7:C:O2'	1:A:8:C:C5'	0.47	2.58	9	3
2:B:421:LYS:HD2	2:B:421:LYS:N	0.47	2.23	7	2
2:B:391:LYS:HG2	2:B:399:ASN:C	0.47	2.35	9	2
2:B:388:VAL:CG2	2:B:403:GLU:HG3	0.47	2.39	16	2
1:A:5:U:OP1	2:B:419:ASN:O	0.47	2.32	15	1
2:B:418:ARG:N	2:B:418:ARG:HD2	0.47	2.23	9	1
2:B:402:VAL:CG2	2:B:427:ALA:HB2	0.47	2.39	10	2
2:B:412:LEU:CD2	2:B:437:MET:SD	0.47	2.98	8	3
2:B:419:ASN:O	2:B:420:ILE:CG1	0.47	2.62	14	4
2:B:401:ILE:HB	2:B:416:VAL:CG2	0.47	2.39	6	1
2:B:433:ARG:CZ	2:B:433:ARG:CB	0.47	2.92	11	1
2:B:401:ILE:HG12	2:B:416:VAL:CG1	0.47	2.36	12	2
1:A:15:A:C2	1:A:19:G:N1	0.47	2.82	16	1
1:A:25:G:O6	1:A:26:G:O6	0.47	2.33	11	3
2:B:387:TYR:CD1	2:B:387:TYR:N	0.47	2.83	10	3
2:B:374:LEU:HD11	2:B:428:ALA:HA	0.47	1.87	4	1
2:B:391:LYS:CD	2:B:400:SER:OG	0.47	2.63	11	3
2:B:399:ASN:HB2	2:B:417:GLY:O	0.47	2.09	5	4
2:B:391:LYS:CG	2:B:400:SER:OG	0.47	2.63	5	1
1:A:23:G:C2'	1:A:24:U:O5'	0.47	2.62	8	4
2:B:425:ILE:O	2:B:429:GLU:OE1	0.47	2.33	13	3
1:A:8:C:O2'	1:A:9:A:C5'	0.47	2.62	13	2
1:A:15:A:C4	1:A:16:A:N7	0.47	2.82	16	1
1:A:16:A:N1	2:B:372:ARG:HG3	0.47	2.24	16	1
1:A:19:G:O2'	1:A:20:A:P	0.47	2.73	16	1
2:B:434:ASP:O	2:B:435:LYS:C	0.47	2.58	8	12
1:A:15:A:C2	1:A:18:U:O2	0.47	2.68	2	1
2:B:375:TYR:O	2:B:379:GLY:HA3	0.47	2.10	14	4
2:B:434:ASP:CG	2:B:437:MET:CB	0.47	2.88	2	1
2:B:445:ARG:C	2:B:445:ARG:HD2	0.47	2.35	3	4
2:B:398:PRO:O	2:B:399:ASN:O	0.47	2.33	14	4
2:B:425:ILE:O	2:B:429:GLU:OE2	0.47	2.33	4	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:410:THR:OG1	2:B:441:TYR:OH	0.47	2.32	5	2
2:B:419:ASN:ND2	2:B:421:LYS:HB2	0.47	2.25	7	1
2:B:386:HIS:NE2	2:B:405:ARG:HG2	0.47	2.24	10	1
1:A:14:C:C5	1:A:15:A:N7	0.47	2.82	12	1
2:B:444:GLN:NE2	2:B:448:ILE:HG22	0.47	2.24	14	1
2:B:444:GLN:CD	2:B:448:ILE:HG22	0.47	2.35	14	1
1:A:10:U:O2'	1:A:11:G:C8	0.47	2.68	16	1
1:A:15:A:C6	1:A:19:G:N2	0.47	2.82	16	1
1:A:18:U:O3'	2:B:376:SER:OG	0.47	2.33	16	1
2:B:383:LEU:CD1	2:B:406:VAL:HB	0.47	2.39	16	1
2:B:403:GLU:HA	2:B:414:THR:HG23	0.47	1.85	16	1
2:B:398:PRO:C	2:B:418:ARG:O	0.47	2.58	1	1
2:B:415:GLY:HA3	2:B:427:ALA:CA	0.47	2.39	11	9
2:B:373:GLN:O	2:B:377:LEU:HB3	0.47	2.10	12	3
2:B:405:ARG:CB	2:B:411:VAL:HB	0.47	2.40	8	1
2:B:391:LYS:CB	2:B:400:SER:HB2	0.47	2.40	11	1
2:B:383:LEU:HD22	2:B:445:ARG:CZ	0.47	2.40	12	1
2:B:391:LYS:CD	2:B:399:ASN:HB3	0.47	2.38	12	1
2:B:422:ILE:O	2:B:426:ARG:HG2	0.47	2.10	12	8
2:B:386:HIS:CE1	2:B:388:VAL:HG13	0.47	2.45	13	3
1:A:15:A:O2'	1:A:16:A:H5'	0.47	2.09	7	2
2:B:370:ALA:HB2	2:B:429:GLU:OE2	0.47	2.10	15	2
2:B:394:THR:OG1	2:B:397:ASP:OD2	0.47	2.33	8	2
2:B:374:LEU:CD2	2:B:438:LEU:HD21	0.47	2.40	16	1
2:B:380:TYR:OH	2:B:441:TYR:C	0.47	2.56	16	1
2:B:414:THR:C	2:B:430:ASN:OD1	0.47	2.58	16	1
2:B:367:ASP:OD1	2:B:367:ASP:C	0.47	2.57	2	1
2:B:406:VAL:HG11	2:B:441:TYR:CZ	0.47	2.44	4	1
2:B:380:TYR:O	2:B:445:ARG:HD2	0.47	2.10	7	1
2:B:366:LEU:HD22	2:B:368:MET:HB3	0.47	1.87	14	1
1:A:19:G:HO2'	1:A:20:A:C5'	0.47	2.23	15	1
1:A:17:G:N7	2:B:368:MET:CE	0.47	2.78	16	1
2:B:406:VAL:CG2	2:B:407:GLY:N	0.46	2.78	2	1
2:B:420:ILE:O	2:B:423:ALA:N	0.46	2.48	11	4
2:B:399:ASN:CB	2:B:417:GLY:O	0.46	2.63	7	2
2:B:373:GLN:NE2	2:B:377:LEU:HB3	0.46	2.25	9	1
2:B:420:ILE:C	2:B:420:ILE:HD12	0.46	2.34	9	1
1:A:11:G:HO2'	1:A:12:U:H6	0.46	1.51	1	2
1:A:20:A:HO2'	1:A:21:A:C5'	0.46	2.23	7	3
2:B:405:ARG:CD	2:B:406:VAL:N	0.46	2.78	1	1
2:B:404:CYS:CB	2:B:413:GLY:HA3	0.46	2.40	8	4

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:10:U:O2'	1:A:11:G:H8	0.46	1.92	16	2
2:B:391:LYS:HG3	2:B:392:LYS:N	0.46	2.25	6	1
2:B:374:LEU:O	2:B:378:ILE:C	0.46	2.58	14	2
2:B:380:TYR:O	2:B:383:LEU:O	0.46	2.33	10	1
2:B:431:ALA:O	2:B:434:ASP:OD1	0.46	2.33	10	1
2:B:391:LYS:CG	2:B:400:SER:HB2	0.46	2.41	11	1
2:B:418:ARG:O	2:B:419:ASN:OD1	0.46	2.32	13	1
2:B:429:GLU:O	2:B:433:ARG:HG3	0.46	2.09	5	9
2:B:380:TYR:CG	2:B:445:ARG:HG2	0.46	2.45	2	2
2:B:445:ARG:NH1	2:B:448:ILE:HG21	0.46	2.25	7	1
1:A:18:U:O2	1:A:18:U:H2'	0.46	2.10	10	1
2:B:434:ASP:OD1	2:B:434:ASP:N	0.46	2.48	10	1
2:B:380:TYR:CE2	2:B:383:LEU:HB2	0.46	2.45	11	1
2:B:397:ASP:OD1	2:B:397:ASP:C	0.46	2.58	13	1
1:A:7:C:C2	1:A:8:C:C5	0.46	3.04	7	1
2:B:397:ASP:O	2:B:397:ASP:CG	0.46	2.57	8	2
1:A:27:U:O2'	1:A:28:A:C5'	0.46	2.63	11	3
2:B:373:GLN:OE1	2:B:374:LEU:CD2	0.46	2.56	9	1
1:A:12:U:C2'	1:A:13:U:O5'	0.46	2.62	15	1
2:B:405:ARG:HB2	2:B:410:THR:O	0.46	2.11	6	4
2:B:391:LYS:HG3	2:B:400:SER:CB	0.46	2.41	5	1
1:A:27:U:C2'	1:A:28:A:O5'	0.46	2.63	11	3
2:B:383:LEU:HD11	2:B:406:VAL:HG12	0.46	1.88	16	1
2:B:370:ALA:O	2:B:373:GLN:N	0.46	2.48	14	3
2:B:403:GLU:HG2	2:B:414:THR:HG23	0.46	1.86	12	1
1:A:31:U:HO2'	1:A:32:C:C5'	0.46	2.24	14	1
2:B:410:THR:HG22	2:B:412:LEU:CD1	0.46	2.41	14	1
1:A:16:A:N3	1:A:18:U:HI'	0.46	2.26	16	1
1:A:12:U:C2'	1:A:13:U:O4'	0.46	2.63	7	2
2:B:402:VAL:HG23	2:B:415:GLY:C	0.46	2.36	14	1
1:A:16:A:C4	1:A:18:U:O4	0.46	2.68	6	2
2:B:403:GLU:OE1	2:B:414:THR:HG23	0.46	2.11	8	1
2:B:414:THR:O	2:B:430:ASN:OD1	0.46	2.34	16	1
1:A:9:A:C2	1:A:25:G:C2	0.46	3.04	2	1
1:A:11:G:H2'	1:A:12:U:C6	0.46	2.46	2	6
2:B:372:ARG:CZ	2:B:372:ARG:HB3	0.46	2.41	8	2
2:B:388:VAL:CG2	2:B:403:GLU:O	0.46	2.61	6	3
2:B:419:ASN:CG	2:B:422:ILE:HD11	0.46	2.35	6	2
2:B:373:GLN:NE2	2:B:438:LEU:HB3	0.46	2.26	9	1
2:B:428:ALA:HB3	2:B:429:GLU:OE2	0.46	2.11	2	1
1:A:5:U:OP1	2:B:420:ILE:HG22	0.46	2.11	7	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:404:CYS:N	2:B:411:VAL:HG23	0.46	2.26	8	1
2:B:366:LEU:O	2:B:429:GLU:OE2	0.46	2.34	16	2
2:B:404:CYS:HB2	2:B:413:GLY:O	0.46	2.10	9	1
2:B:401:ILE:CG1	2:B:414:THR:HG22	0.46	2.41	15	1
2:B:444:GLN:CG	2:B:445:ARG:N	0.45	2.78	12	9
2:B:377:LEU:O	2:B:380:TYR:OH	0.45	2.30	4	2
2:B:383:LEU:HD13	2:B:441:TYR:CE2	0.45	2.47	16	1
2:B:401:ILE:HG13	2:B:416:VAL:CG2	0.45	2.40	15	3
2:B:368:MET:O	2:B:371:LYS:HG3	0.45	2.10	13	5
1:A:19:G:OP1	2:B:376:SER:CB	0.45	2.64	5	1
2:B:373:GLN:OE1	2:B:377:LEU:HB3	0.45	2.12	5	1
2:B:389:THR:CB	2:B:402:VAL:HG13	0.45	2.42	7	1
1:A:6:A:OP1	2:B:420:ILE:HG21	0.45	2.11	14	1
2:B:382:SER:CB	2:B:448:ILE:HD13	0.45	2.41	15	1
2:B:437:MET:SD	2:B:441:TYR:CD2	0.45	3.10	4	2
2:B:385:LEU:CD2	2:B:385:LEU:N	0.45	2.79	10	3
2:B:444:GLN:OE1	2:B:448:ILE:HG23	0.45	2.10	7	1
2:B:445:ARG:C	2:B:448:ILE:HG13	0.45	2.37	7	1
2:B:398:PRO:O	2:B:418:ARG:O	0.45	2.34	9	1
2:B:405:ARG:HD2	2:B:405:ARG:C	0.45	2.37	9	1
1:A:15:A:C6	1:A:16:A:C4	0.45	3.04	15	1
2:B:434:ASP:O	2:B:437:MET:HB3	0.45	2.11	8	13
1:A:4:A:H2'	1:A:5:U:C6	0.45	2.47	5	11
2:B:400:SER:HB3	2:B:423:ALA:HB2	0.45	1.87	1	1
2:B:377:LEU:C	2:B:378:ILE:HD13	0.45	2.37	4	3
2:B:380:TYR:CE1	2:B:445:ARG:NE	0.45	2.85	4	1
2:B:383:LEU:HD11	2:B:408:ASP:OD1	0.45	2.12	7	1
2:B:419:ASN:O	2:B:421:LYS:HG2	0.45	2.12	13	1
2:B:426:ARG:HG3	2:B:427:ALA:N	0.45	2.27	13	6
2:B:422:ILE:HD12	2:B:422:ILE:H	0.45	1.72	4	1
2:B:381:ALA:O	2:B:445:ARG:HD2	0.45	2.10	7	1
2:B:448:ILE:O	2:B:448:ILE:CD1	0.45	2.64	7	1
2:B:404:CYS:N	2:B:411:VAL:CG2	0.45	2.80	8	1
2:B:382:SER:OG	2:B:448:ILE:CD1	0.45	2.65	15	1
2:B:367:ASP:HB3	2:B:425:ILE:HG23	0.45	1.87	16	1
2:B:391:LYS:HG3	2:B:400:SER:N	0.45	2.26	12	2
2:B:429:GLU:N	2:B:429:GLU:CD	0.45	2.74	2	1
2:B:415:GLY:CA	2:B:427:ALA:HB2	0.45	2.41	11	3
1:A:9:A:C2'	1:A:10:U:O5'	0.45	2.64	13	3
1:A:6:A:C6	1:A:7:C:C4	0.45	3.04	15	1
2:B:367:ASP:HB3	2:B:425:ILE:CG2	0.45	2.42	16	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:21:A:H2'	1:A:22:C:C6	0.45	2.47	8	15
1:A:7:C:C4	1:A:8:C:C4	0.45	3.05	3	2
1:A:15:A:C8	1:A:16:A:C8	0.45	3.05	5	1
2:B:384:ARG:O	2:B:385:LEU:C	0.45	2.60	6	1
2:B:436:LYS:N	2:B:436:LYS:HD2	0.45	2.26	11	1
1:A:15:A:N3	1:A:16:A:N9	0.45	2.65	16	1
2:B:405:ARG:CD	2:B:405:ARG:C	0.45	2.90	1	1
2:B:445:ARG:O	2:B:445:ARG:HD2	0.45	2.13	6	6
2:B:397:ASP:OD2	2:B:399:ASN:OD1	0.45	2.35	10	1
2:B:434:ASP:CG	2:B:437:MET:HB2	0.44	2.37	2	3
1:A:28:A:H2'	1:A:29:U:C6	0.44	2.47	7	7
2:B:391:LYS:HG3	2:B:400:SER:HA	0.44	1.89	3	3
2:B:405:ARG:HD3	2:B:406:VAL:O	0.44	2.12	5	1
2:B:445:ARG:NE	2:B:445:ARG:HA	0.44	2.27	7	1
2:B:422:ILE:HD13	2:B:422:ILE:N	0.44	2.27	14	2
2:B:391:LYS:HD3	2:B:400:SER:OG	0.44	2.12	11	1
2:B:378:ILE:O	2:B:379:GLY:O	0.44	2.34	8	1
1:A:20:A:C2'	1:A:21:A:C8	0.44	3.00	10	2
2:B:368:MET:HE1	2:B:372:ARG:HD3	0.44	1.89	13	1
2:B:366:LEU:CA	2:B:429:GLU:OE2	0.44	2.65	14	1
1:A:23:G:O6	1:A:24:U:C4	0.44	2.71	16	1
2:B:439:ASP:O	2:B:440:PHE:C	0.44	2.61	12	3
2:B:414:THR:O	2:B:427:ALA:HA	0.44	2.13	7	2
1:A:3:G:C2	1:A:31:U:O2	0.44	2.70	5	2
2:B:384:ARG:O	2:B:407:GLY:CA	0.44	2.65	8	1
2:B:447:ALA:O	2:B:448:ILE:O	0.44	2.36	9	1
2:B:403:GLU:OE2	2:B:411:VAL:HG11	0.44	2.11	15	1
2:B:366:LEU:CD1	2:B:432:LEU:HD13	0.44	2.42	2	1
2:B:379:GLY:O	2:B:380:TYR:HB2	0.44	2.12	4	1
2:B:421:LYS:HB3	2:B:425:ILE:CD1	0.44	2.42	4	1
2:B:435:LYS:HG3	2:B:436:LYS:N	0.44	2.27	10	1
2:B:374:LEU:CD2	2:B:438:LEU:CD2	0.44	2.95	16	1
1:A:20:A:C5'	2:B:375:TYR:CD2	0.44	3.01	1	1
2:B:370:ALA:HA	2:B:432:LEU:HD12	0.44	1.90	2	1
2:B:419:ASN:O	2:B:420:ILE:HB	0.44	2.13	12	2
2:B:399:ASN:HA	2:B:417:GLY:O	0.44	2.13	15	7
1:A:8:C:O2'	1:A:9:A:C8	0.44	2.71	5	1
2:B:380:TYR:CD2	2:B:383:LEU:HD11	0.44	2.47	5	1
2:B:391:LYS:HG2	2:B:400:SER:CA	0.44	2.43	9	1
1:A:20:A:C4'	2:B:371:LYS:HG3	0.44	2.43	11	1
2:B:400:SER:OG	2:B:401:ILE:N	0.44	2.48	11	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:26:G:C6	1:A:27:U:C4	0.44	3.05	15	1
1:A:15:A:N1	1:A:16:A:C4	0.44	2.85	16	1
1:A:22:C:OP1	2:B:421:LYS:HG3	0.44	2.13	1	2
2:B:421:LYS:O	2:B:422:ILE:C	0.44	2.61	1	3
2:B:437:MET:SD	2:B:441:TYR:CE2	0.44	3.11	4	1
2:B:394:THR:N	2:B:397:ASP:O	0.44	2.51	12	2
2:B:373:GLN:OE1	2:B:377:LEU:HG	0.44	2.13	6	1
2:B:448:ILE:HD12	2:B:448:ILE:O	0.44	2.13	7	1
2:B:390:VAL:HG23	2:B:390:VAL:O	0.44	2.12	11	1
2:B:396:VAL:O	2:B:398:PRO:HD3	0.44	2.13	13	2
2:B:402:VAL:O	2:B:414:THR:HA	0.44	2.13	14	6
2:B:380:TYR:CZ	2:B:445:ARG:HG2	0.44	2.48	13	2
2:B:381:ALA:HB2	2:B:445:ARG:HA	0.44	1.88	9	1
2:B:420:ILE:HG23	2:B:421:LYS:CD	0.44	2.43	10	1
2:B:366:LEU:HD12	2:B:368:MET:N	0.44	2.28	11	1
2:B:368:MET:O	2:B:371:LYS:NZ	0.44	2.49	11	2
1:A:19:G:O2'	1:A:20:A:C4'	0.44	2.66	13	1
1:A:25:G:C6	1:A:26:G:C5	0.43	3.06	1	1
2:B:394:THR:OG1	2:B:397:ASP:O	0.43	2.35	1	1
2:B:419:ASN:OD1	2:B:422:ILE:HD12	0.43	2.12	8	1
1:A:4:A:C6	1:A:5:U:C4	0.43	3.05	11	1
2:B:448:ILE:O	2:B:448:ILE:HG13	0.43	2.13	13	1
2:B:385:LEU:CD1	2:B:406:VAL:HG12	0.43	2.43	6	1
1:A:14:C:C4	1:A:15:A:C8	0.43	3.06	7	1
1:A:15:A:O2'	2:B:368:MET:SD	0.43	2.74	9	1
2:B:380:TYR:OH	2:B:444:GLN:OE1	0.43	2.32	11	1
2:B:380:TYR:HB3	2:B:445:ARG:NE	0.43	2.28	11	3
2:B:406:VAL:CG2	2:B:410:THR:HB	0.43	2.43	10	2
2:B:440:PHE:CD1	2:B:441:TYR:N	0.43	2.87	10	2
2:B:380:TYR:CE1	2:B:383:LEU:CD2	0.43	3.02	10	1
2:B:401:ILE:HB	2:B:416:VAL:CG1	0.43	2.42	10	1
2:B:365:SER:O	2:B:429:GLU:CG	0.43	2.66	11	1
2:B:369:ASN:ND2	2:B:369:ASN:C	0.43	2.76	11	1
2:B:372:ARG:HD2	2:B:376:SER:OG	0.43	2.13	12	1
2:B:366:LEU:N	2:B:429:GLU:OE2	0.43	2.51	13	1
2:B:430:ASN:O	2:B:433:ARG:HB2	0.43	2.13	14	1
2:B:404:CYS:HB3	2:B:413:GLY:CA	0.43	2.43	13	3
2:B:408:ASP:O	2:B:408:ASP:CG	0.43	2.61	1	1
2:B:388:VAL:HG21	2:B:403:GLU:OE1	0.43	2.13	2	1
1:A:13:U:C2'	1:A:14:C:O5'	0.43	2.67	3	2
2:B:431:ALA:O	2:B:434:ASP:OD2	0.43	2.35	9	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:415:GLY:HA3	2:B:427:ALA:N	0.43	2.27	11	1
1:A:17:G:O6	2:B:369:ASN:ND2	0.43	2.51	13	1
2:B:415:GLY:HA3	2:B:426:ARG:HD3	0.43	1.90	16	1
2:B:433:ARG:CZ	2:B:433:ARG:HB3	0.43	2.43	2	1
2:B:385:LEU:CA	2:B:406:VAL:HA	0.43	2.44	6	1
2:B:401:ILE:HG13	2:B:402:VAL:N	0.43	2.27	11	1
2:B:401:ILE:HD13	2:B:402:VAL:N	0.43	2.29	13	1
1:A:24:U:O2'	1:A:25:G:C8	0.43	2.71	3	1
1:A:18:U:HO2'	1:A:19:G:C1'	0.43	2.26	4	1
1:A:14:C:N4	1:A:15:A:N7	0.43	2.67	7	1
1:A:30:C:O2'	2:B:395:ALA:CB	0.43	2.67	7	1
2:B:367:ASP:HB2	2:B:425:ILE:CG1	0.43	2.44	8	2
2:B:415:GLY:HA3	2:B:427:ALA:CB	0.43	2.41	14	2
2:B:430:ASN:O	2:B:434:ASP:OD1	0.43	2.35	12	1
2:B:387:TYR:CD2	2:B:404:CYS:HB2	0.43	2.49	13	1
2:B:399:ASN:OD1	2:B:418:ARG:HD2	0.43	2.14	16	2
1:A:22:C:O5'	1:A:22:C:C6	0.43	2.60	4	6
2:B:406:VAL:C	2:B:408:ASP:N	0.43	2.76	6	1
1:A:9:A:O2'	1:A:10:U:O5'	0.43	2.36	9	1
2:B:367:ASP:HB3	2:B:425:ILE:CG1	0.43	2.43	9	2
2:B:399:ASN:ND2	2:B:418:ARG:HA	0.43	2.29	10	1
2:B:435:LYS:CG	2:B:436:LYS:CD	0.43	2.97	11	2
2:B:380:TYR:CG	2:B:445:ARG:CG	0.43	3.02	12	1
1:A:16:A:H4'	1:A:17:G:O5'	0.43	2.12	16	1
1:A:9:A:C5	1:A:10:U:C4	0.43	3.06	2	1
2:B:368:MET:O	2:B:371:LYS:HD2	0.43	2.14	3	2
2:B:397:ASP:OD1	2:B:399:ASN:ND2	0.43	2.52	7	1
2:B:398:PRO:O	2:B:418:ARG:HA	0.43	2.14	9	2
1:A:15:A:N6	1:A:19:G:C2	0.43	2.86	16	1
2:B:383:LEU:O	2:B:384:ARG:HD3	0.43	2.12	1	1
2:B:388:VAL:O	2:B:388:VAL:HG23	0.43	2.14	15	2
2:B:420:ILE:HD12	2:B:420:ILE:O	0.43	2.14	2	2
2:B:367:ASP:N	2:B:425:ILE:CG2	0.43	2.81	11	1
2:B:384:ARG:HD2	2:B:384:ARG:N	0.43	2.29	14	1
1:A:16:A:N7	2:B:368:MET:HE3	0.43	2.29	16	1
1:A:2:G:C2'	1:A:3:G:O5'	0.42	2.67	3	2
2:B:417:GLY:CA	2:B:422:ILE:HB	0.42	2.44	3	1
1:A:15:A:C2	1:A:19:G:O6	0.42	2.72	4	1
2:B:383:LEU:C	2:B:384:ARG:HG3	0.42	2.38	4	1
2:B:404:CYS:HB3	2:B:413:GLY:HA3	0.42	1.91	7	1
1:A:18:U:OP2	1:A:18:U:H6	0.42	1.97	10	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:15:A:C2	1:A:18:U:C2	0.42	3.07	11	1
1:A:20:A:O4'	2:B:371:LYS:HB2	0.42	2.13	14	1
1:A:17:G:OP1	1:A:17:G:O4'	0.42	2.36	1	1
2:B:394:THR:HB	2:B:397:ASP:OD2	0.42	2.12	8	1
2:B:394:THR:OG1	2:B:396:VAL:HG13	0.42	2.13	11	1
2:B:437:MET:SD	2:B:441:TYR:CE1	0.42	3.12	13	1
2:B:418:ARG:H	2:B:422:ILE:HD12	0.42	1.74	1	1
2:B:390:VAL:O	2:B:401:ILE:O	0.42	2.37	11	2
2:B:368:MET:HA	2:B:371:LYS:CE	0.42	2.44	3	1
2:B:391:LYS:HB3	2:B:400:SER:OG	0.42	2.14	4	3
2:B:439:ASP:O	2:B:442:ALA:HB3	0.42	2.14	8	2
2:B:405:ARG:C	2:B:405:ARG:CD	0.42	2.92	9	1
2:B:429:GLU:CD	2:B:429:GLU:N	0.42	2.77	12	1
2:B:434:ASP:CB	2:B:437:MET:HE3	0.42	2.40	12	1
2:B:438:LEU:O	2:B:441:TYR:HB2	0.42	2.14	15	2
2:B:444:GLN:NE2	2:B:448:ILE:HA	0.42	2.30	14	1
2:B:398:PRO:HB2	2:B:418:ARG:O	0.42	2.14	1	1
2:B:404:CYS:N	2:B:413:GLY:O	0.42	2.52	5	2
2:B:410:THR:HG22	2:B:412:LEU:HD11	0.42	1.89	10	1
2:B:382:SER:CB	2:B:448:ILE:CD1	0.42	2.98	15	1
2:B:426:ARG:HB2	2:B:426:ARG:CZ	0.42	2.43	16	1
2:B:415:GLY:HA2	2:B:426:ARG:CG	0.42	2.43	2	1
2:B:420:ILE:HG23	2:B:421:LYS:HD3	0.42	1.91	2	1
1:A:19:G:O2'	2:B:371:LYS:HG2	0.42	2.15	3	1
2:B:405:ARG:HB3	2:B:411:VAL:HA	0.42	1.91	16	1
2:B:399:ASN:C	2:B:399:ASN:OD1	0.42	2.62	4	2
2:B:381:ALA:O	2:B:445:ARG:CD	0.42	2.67	7	1
2:B:378:ILE:CD1	2:B:442:ALA:N	0.42	2.83	11	1
2:B:394:THR:HG1	2:B:397:ASP:C	0.42	2.21	13	1
2:B:444:GLN:OE1	2:B:448:ILE:HG21	0.42	2.14	15	1
1:A:17:G:O6	2:B:369:ASN:OD1	0.42	2.37	5	1
2:B:391:LYS:HB2	2:B:400:SER:CB	0.42	2.44	11	1
2:B:412:LEU:C	2:B:412:LEU:HD23	0.42	2.39	14	1
2:B:415:GLY:HA2	2:B:426:ARG:HG3	0.42	1.90	2	1
2:B:414:THR:O	2:B:430:ASN:HB2	0.42	2.15	8	2
2:B:440:PHE:O	2:B:443:LYS:HG2	0.42	2.15	13	1
1:A:18:U:O2	1:A:19:G:C5	0.42	2.73	5	1
1:A:19:G:OP1	2:B:376:SER:HB3	0.42	2.14	5	1
2:B:399:ASN:ND2	2:B:399:ASN:H	0.42	2.12	10	1
2:B:383:LEU:O	2:B:384:ARG:HB3	0.42	2.13	1	1
1:A:5:U:O2'	2:B:393:PRO:HB2	0.42	2.15	2	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:366:LEU:HB3	2:B:369:ASN:OD1	0.42	2.14	4	1
2:B:385:LEU:HD23	2:B:385:LEU:N	0.42	2.29	7	1
2:B:378:ILE:HD12	2:B:441:TYR:CB	0.42	2.45	13	2
2:B:380:TYR:CE1	2:B:445:ARG:CD	0.42	3.03	9	1
2:B:385:LEU:HB3	2:B:406:VAL:HG22	0.42	1.92	10	1
1:A:20:A:O4'	2:B:371:LYS:NZ	0.42	2.53	16	1
2:B:391:LYS:CG	2:B:393:PRO:HG3	0.41	2.44	2	1
2:B:375:TYR:O	2:B:379:GLY:N	0.41	2.53	5	1
2:B:378:ILE:CG2	2:B:379:GLY:N	0.41	2.83	11	1
1:A:1:G:HO5'	1:A:1:G:H8	0.41	1.55	13	1
2:B:378:ILE:CG2	2:B:383:LEU:HD23	0.41	2.45	16	1
2:B:379:GLY:C	2:B:380:TYR:CD2	0.41	2.98	4	1
2:B:379:GLY:O	2:B:380:TYR:HB3	0.41	2.14	9	1
2:B:403:GLU:HA	2:B:413:GLY:O	0.41	2.14	10	1
1:A:5:U:OP1	2:B:419:ASN:CB	0.41	2.68	11	1
2:B:400:SER:O	2:B:416:VAL:HG13	0.41	2.15	11	1
2:B:396:VAL:C	2:B:398:PRO:HD3	0.41	2.40	13	1
2:B:398:PRO:HG2	2:B:418:ARG:O	0.41	2.15	16	2
2:B:385:LEU:HB3	2:B:406:VAL:HG12	0.41	1.90	6	1
2:B:391:LYS:HG2	2:B:399:ASN:O	0.41	2.15	6	2
1:A:17:G:N7	2:B:368:MET:HE1	0.41	2.30	16	2
2:B:366:LEU:O	2:B:366:LEU:CG	0.41	2.67	2	1
2:B:415:GLY:HA3	2:B:427:ALA:HA	0.41	1.91	5	1
1:A:7:C:O2'	1:A:8:C:O4'	0.41	2.39	6	1
2:B:368:MET:O	2:B:372:ARG:HB2	0.41	2.15	9	1
2:B:371:LYS:NZ	2:B:372:ARG:HB2	0.41	2.30	12	1
2:B:405:ARG:HB2	2:B:410:THR:C	0.41	2.41	12	1
1:A:12:U:O5'	1:A:12:U:C6	0.41	2.63	14	1
1:A:18:U:O5'	1:A:18:U:H6	0.41	1.97	15	1
1:A:30:C:C5	1:A:31:U:C5	0.41	3.08	15	1
2:B:400:SER:HB3	2:B:419:ASN:O	0.41	2.16	1	1
2:B:401:ILE:HA	2:B:415:GLY:O	0.41	2.15	2	1
2:B:372:ARG:HA	2:B:376:SER:OG	0.41	2.15	4	1
2:B:391:LYS:CG	2:B:392:LYS:N	0.41	2.84	6	1
2:B:405:ARG:HA	2:B:411:VAL:HA	0.41	1.92	8	1
2:B:405:ARG:CG	2:B:411:VAL:HB	0.41	2.44	8	1
2:B:444:GLN:CD	2:B:444:GLN:C	0.41	2.88	11	1
2:B:378:ILE:O	2:B:380:TYR:N	0.41	2.53	15	1
2:B:380:TYR:CE2	2:B:383:LEU:CD2	0.41	3.03	2	1
2:B:437:MET:HE2	2:B:438:LEU:HD23	0.41	1.90	8	1
2:B:433:ARG:NH1	2:B:433:ARG:HB3	0.41	2.31	1	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:380:TYR:HB3	2:B:445:ARG:CZ	0.41	2.46	3	1
2:B:443:LYS:HG2	2:B:444:GLN:N	0.41	2.30	3	1
2:B:385:LEU:H	2:B:385:LEU:CD2	0.41	2.29	5	1
2:B:434:ASP:HB3	2:B:437:MET:HB3	0.41	1.92	6	1
1:A:23:G:C6	1:A:24:U:C5	0.41	3.09	10	1
1:A:30:C:C2'	1:A:31:U:C5'	0.41	2.99	11	1
2:B:366:LEU:C	2:B:366:LEU:CD1	0.41	2.94	11	1
2:B:435:LYS:HG2	2:B:436:LYS:HD3	0.41	1.93	12	2
2:B:388:VAL:O	2:B:402:VAL:HA	0.41	2.16	4	1
1:A:2:G:O5'	1:A:2:G:C8	0.41	2.72	5	1
1:A:3:G:N1	1:A:31:U:C2	0.41	2.89	5	1
2:B:412:LEU:HD12	2:B:412:LEU:N	0.41	2.31	10	1
2:B:435:LYS:CG	2:B:436:LYS:HD3	0.41	2.45	10	1
1:A:6:A:H2'	1:A:7:C:C6	0.41	2.51	11	2
2:B:419:ASN:O	2:B:421:LYS:CD	0.41	2.69	13	1
2:B:394:THR:CB	2:B:397:ASP:O	0.41	2.69	1	1
2:B:400:SER:OG	2:B:423:ALA:CB	0.41	2.69	1	1
2:B:374:LEU:O	2:B:378:ILE:HB	0.41	2.16	7	3
2:B:383:LEU:O	2:B:384:ARG:CG	0.41	2.68	4	1
2:B:440:PHE:O	2:B:443:LYS:HG3	0.41	2.16	4	1
2:B:373:GLN:OE1	2:B:377:LEU:CG	0.41	2.69	5	1
2:B:378:ILE:HA	2:B:380:TYR:CZ	0.41	2.51	5	1
2:B:408:ASP:OD1	2:B:408:ASP:N	0.41	2.54	7	2
2:B:403:GLU:HB2	2:B:411:VAL:HG21	0.41	1.90	8	1
2:B:421:LYS:CD	2:B:421:LYS:H	0.41	2.29	10	1
2:B:380:TYR:CB	2:B:445:ARG:HD3	0.41	2.46	11	1
2:B:371:LYS:HG3	2:B:372:ARG:N	0.41	2.30	13	1
2:B:383:LEU:HD22	2:B:441:TYR:CE2	0.41	2.51	16	1
2:B:401:ILE:HG12	2:B:414:THR:CG2	0.41	2.46	16	1
1:A:8:C:O2'	1:A:9:A:H8	0.41	1.99	5	1
2:B:403:GLU:CD	2:B:411:VAL:CG2	0.41	2.81	12	1
2:B:380:TYR:CG	2:B:445:ARG:NE	0.40	2.89	4	1
2:B:410:THR:CB	2:B:441:TYR:OH	0.40	2.69	5	1
2:B:387:TYR:HA	2:B:403:GLU:O	0.40	2.17	10	1
2:B:401:ILE:CG1	2:B:416:VAL:CG2	0.40	2.97	15	1
1:A:7:C:H6	1:A:7:C:O5'	0.40	1.99	3	1
2:B:417:GLY:O	2:B:418:ARG:C	0.40	2.64	4	1
2:B:391:LYS:HZ2	2:B:393:PRO:HB3	0.40	1.76	5	1
2:B:405:ARG:HG3	2:B:411:VAL:CG2	0.40	2.46	5	1
2:B:374:LEU:CD1	2:B:404:CYS:SG	0.40	3.10	8	1
2:B:434:ASP:CB	2:B:437:MET:HB3	0.40	2.46	8	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:27:U:H2'	1:A:28:A:O5'	0.40	2.17	11	1
1:A:1:G:HO2'	1:A:2:G:H8	0.40	1.57	12	1
2:B:391:LYS:O	2:B:391:LYS:HD2	0.40	2.16	2	1
1:A:19:G:O2'	2:B:371:LYS:CG	0.40	2.70	3	1
2:B:417:GLY:HA3	2:B:422:ILE:CB	0.40	2.46	4	1
2:B:389:THR:HB	2:B:402:VAL:HG13	0.40	1.94	7	1
1:A:24:U:O2	1:A:25:G:C8	0.40	2.74	12	1
2:B:440:PHE:O	2:B:444:GLN:HB3	0.40	2.16	12	1
1:A:22:C:OP1	2:B:421:LYS:HD2	0.40	2.17	1	1
2:B:378:ILE:HD12	2:B:438:LEU:O	0.40	2.17	3	1
2:B:443:LYS:HD2	2:B:443:LYS:C	0.40	2.41	6	1
2:B:380:TYR:CD1	2:B:383:LEU:HB3	0.40	2.52	8	1
2:B:371:LYS:HD3	2:B:372:ARG:N	0.40	2.31	9	1
2:B:385:LEU:CA	2:B:405:ARG:O	0.40	2.70	15	1
1:A:13:U:O2'	1:A:14:C:C4'	0.40	2.70	1	1
1:A:14:C:C2'	1:A:15:A:O5'	0.40	2.70	9	1
2:B:418:ARG:H	2:B:422:ILE:HD13	0.40	1.76	11	1
2:B:383:LEU:CG	2:B:384:ARG:N	0.40	2.82	16	1

6.3 Torsion angles [i](#)

6.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all 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	84/90 (93%)	66±2 (79±3%)	14±2 (16±3%)	4±1 (5±2%)	3	25
All	All	1344/1440 (93%)	1062 (79%)	219 (16%)	63 (5%)	3	25

All 14 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	365	SER	8
2	B	399	ASN	8
2	B	407	GLY	7
2	B	420	ILE	6

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Mol	Chain	Res	Type	Models (Total)
2	B	398	PRO	6
2	B	380	TYR	5
2	B	383	LEU	4
2	B	384	ARG	4
2	B	382	SER	4
2	B	379	GLY	3
2	B	367	ASP	3
2	B	448	ILE	3
2	B	366	LEU	1
2	B	409	GLY	1

6.3.2 Protein sidechains [i](#)

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	67/72 (93%)	36±3 (54±4%)	31±3 (46±4%)	0 2
All	All	1072/1152 (93%)	577 (54%)	495 (46%)	0 2

All 61 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	371	LYS	16
2	B	396	VAL	16
2	B	402	VAL	16
2	B	420	ILE	16
2	B	444	GLN	16
2	B	377	LEU	15
2	B	414	THR	15
2	B	394	THR	14
2	B	440	PHE	14
2	B	426	ARG	14
2	B	430	ASN	14
2	B	391	LYS	13
2	B	435	LYS	13
2	B	432	LEU	13
2	B	376	SER	12

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Mol	Chain	Res	Type	Models (Total)
2	B	384	ARG	12
2	B	392	LYS	12
2	B	419	ASN	12
2	B	373	GLN	11
2	B	403	GLU	10
2	B	443	LYS	10
2	B	445	ARG	10
2	B	368	MET	10
2	B	418	ARG	10
2	B	372	ARG	9
2	B	380	TYR	9
2	B	385	LEU	9
2	B	429	GLU	9
2	B	436	LYS	9
2	B	382	SER	8
2	B	416	VAL	8
2	B	422	ILE	8
2	B	434	ASP	8
2	B	405	ARG	7
2	B	406	VAL	7
2	B	421	LYS	7
2	B	390	VAL	7
2	B	365	SER	6
2	B	374	LEU	5
2	B	401	ILE	5
2	B	397	ASP	5
2	B	369	ASN	5
2	B	399	ASN	4
2	B	412	LEU	4
2	B	367	ASP	4
2	B	408	ASP	4
2	B	386	HIS	3
2	B	366	LEU	3
2	B	433	ARG	3
2	B	388	VAL	3
2	B	383	LEU	3
2	B	378	ILE	3
2	B	400	SER	3
2	B	389	THR	2
2	B	411	VAL	2
2	B	404	CYS	2
2	B	448	ILE	2

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Mol	Chain	Res	Type	Models (Total)
2	B	437	MET	2
2	B	439	ASP	1
2	B	410	THR	1
2	B	375	TYR	1

6.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers	Suiteness
1	A	31/32 (97%)	8±0 (26±0%)	2±1 (7±2%)	0.18±0.00
All	All	496/512 (97%)	128 (26%)	35 (7%)	0.18

The overall RNA backbone suiteness is 0.13.

All unique RNA backbone outliers are listed below:

Mol	Chain	Res	Type	Models (Total)
1	A	15	A	16
1	A	16	A	16
1	A	17	G	16
1	A	18	U	16
1	A	19	G	16
1	A	20	A	16
1	A	21	A	16
1	A	22	C	16

All unique RNA pucker outliers are listed below:

Mol	Chain	Res	Type	Models (Total)
1	A	18	U	16
1	A	17	G	7
1	A	21	A	4
1	A	24	U	2
1	A	16	A	2
1	A	3	G	1
1	A	28	A	1
1	A	20	A	1
1	A	15	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 i

The completeness of assignment taking into account all chemical shift lists is 51% for the well-defined parts and 52% for the entire structure.

7.1 Chemical shift list 1

File name: working_cs.cif

Chemical shift list name: *assigned_chem_shift_list_1*

7.1.1 Bookkeeping i

The following table shows the results of parsing the chemical shift list and reports the number of nuclei with statistically unusual chemical shifts.

Total number of shifts	952
Number of shifts mapped to atoms	952
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	2

7.1.2 Chemical shift referencing i

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction \pm precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	88	-0.34 ± 0.11	None needed (< 0.5 ppm)
$^{13}\text{C}_\beta$	81	0.20 ± 0.14	None needed (< 0.5 ppm)
$^{13}\text{C}'$	79	-0.23 ± 0.25	None needed (< 0.5 ppm)
^{15}N	82	-0.15 ± 0.35	None needed (< 0.5 ppm)

7.1.3 Completeness of resonance assignments i

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 51%, i.e. 896 atoms were assigned a chemical shift out of a possible 1762. 0 out of 15 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	403/423 (95%)	167/173 (97%)	158/168 (94%)	78/82 (95%)
Sidechain	476/686 (69%)	322/448 (72%)	149/204 (73%)	5/34 (15%)

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	Total	¹ H	¹³ C	¹⁵ N
Aromatic	17/54 (31%)	17/25 (68%)	0/27 (0%)	0/2 (0%)
Sugar	0/352 (0%)	0/192 (0%)	0/160 (0%)	0/0 (—%)
Base	0/247 (0%)	0/151 (0%)	0/55 (0%)	0/41 (0%)
Overall	896/1762 (51%)	506/989 (51%)	307/614 (50%)	83/159 (52%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 52%, i.e. 948 atoms were assigned a chemical shift out of a possible 1831. 0 out of 15 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹ H	¹³ C	¹⁵ N
Backbone	425/452 (94%)	176/185 (95%)	167/180 (93%)	82/87 (94%)
Sidechain	506/726 (70%)	342/473 (72%)	159/216 (74%)	5/37 (14%)
Aromatic	17/54 (31%)	17/25 (68%)	0/27 (0%)	0/2 (0%)
Sugar	0/352 (0%)	0/192 (0%)	0/160 (0%)	0/0 (—%)
Base	0/247 (0%)	0/151 (0%)	0/55 (0%)	0/41 (0%)
Overall	948/1831 (52%)	535/1026 (52%)	326/638 (51%)	87/167 (52%)

7.1.4 Statistically unusual chemical shifts [i](#)

The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

List Id	Chain	Res	Type	Atom	Shift, ppm	Expected range, ppm	Z-score
1	B	448	ILE	CG1	16.40	19.24 – 36.26	-6.7
1	B	420	ILE	CG1	18.29	19.24 – 36.26	-5.6

7.1.5 Random Coil Index (RCI) plots [i](#)

The image below reports *random coil index* values for the protein chains in the structure. The height of each bar gives a probability of a given residue to be disordered, as predicted from the available chemical shifts and the amino acid sequence. A value above 0.2 is an indication of significant predicted disorder. The colour of the bar shows whether the residue is in the well-defined core (black) or in the ill-defined residue ranges (cyan), as described in section 2 on ensemble composition. If well-defined core and ill-defined regions are not identified then it is shown as gray bars.

Random coil index (RCI) for chain B:

