Full wwPDB NMR Structure Validation Report (i)

Apr 26, 2016 – 04:46 PM BST

PDB ID	:	1RKJ
Title	:	Solution structure of the complex formed by the two N-terminal RNA-binding domains of nucleolin and a pre-rRNA target
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Deposited on	:	2003-11-21

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We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
http://wwpdb.org/validation/2016/NMRValidationReportHelp
with specific help available everywhere you see the (i) symbol.

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

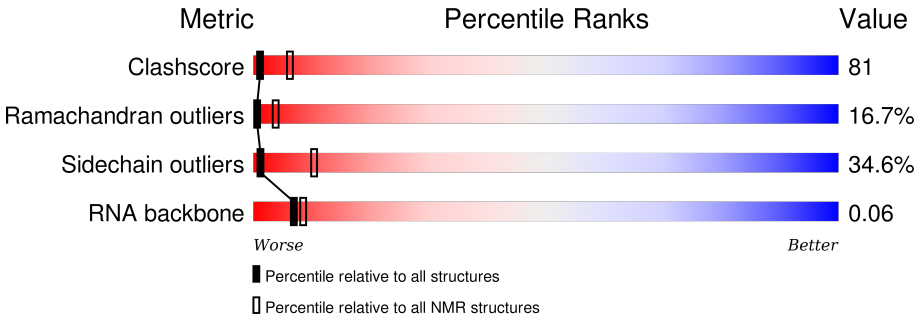
Cyrange	:	Kirchner and Güntert (2011)
NmrClust	:	Kelley et al. (1996)
MolProbity	:	4.02b-467
Mogul	:	unknown
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
ShiftChecker	:	rb-20027457
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20027457

1 Overall quality at a glance (i)

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	114402	11133
Ramachandran outliers	111179	9975
Sidechain outliers	111093	9958
RNA backbone	3027	600

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 <=5%

Mol	Chain	Length	Quality of chain
1	B	21	24% 62% 14%
2	A	175	10% 61% 22% 7%

2 Ensemble composition and analysis

This entry contains 14 models. Model 1 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	A:11-A:172 (162)	1.28	1

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 5 single-model clusters were found.

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

3 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 3403 atoms, of which 1599 are hydrogens and 0 are deuteriums.

- Molecule 1 is a RNA chain called 5'-R(*GP*GP*AP*UP*GP*CP*CP*UP*CP*CP*CP*GP*AP*GP*UP*GP*CP*AP*UP*CP*C)-3'.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	P	
1	B	21	670	198	229	77	146	20	0

- Molecule 2 is a protein called Nucleolin.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
2	A	175	2733	856	1370	229	277	1	0

There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	GLY	-	CLONING ARTIFACT	UNP P08199
A	2	SER	-	CLONING ARTIFACT	UNP P08199
A	3	HIS	-	CLONING ARTIFACT	UNP P08199
A	4	MET	-	CLONING ARTIFACT	UNP P08199
A	37	LEU	PRO	SEE REMARK 999	UNP P08199

4 Residue-property plots (i)

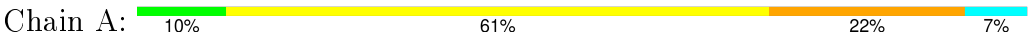
4.1 Average score per residue in the NMR ensemble

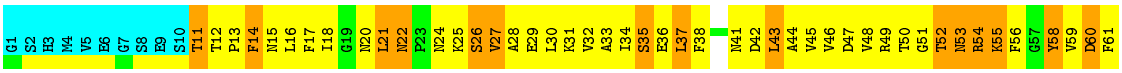
These plots are provided for all protein, RNA and DNA chains in the entry. The first graphic is the same as shown in the summary in section 1 of this report. The second graphic shows the sequence where residues are colour-coded according to the number of geometric quality criteria for which they contain 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.

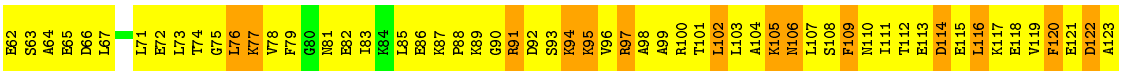
• Molecule 1: 5'-R(*GP*GP*AP*UP*GP*CP*CP*UP*CP*CP*CP*GP*AP*GP*UP*GP*CP*AP*UP*CP*C)-3'

Chain B: 

• Molecule 2: Nucleolin

Chain A: 





4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

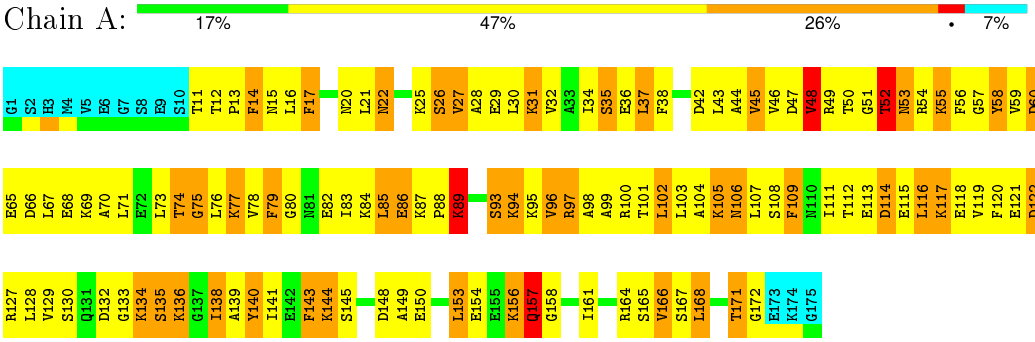
4.2.1 Score per residue for model 1 (medoid)

• Molecule 1: 5'-R(*GP*GP*AP*UP*GP*CP*CP*UP*CP*CP*CP*GP*AP*GP*UP*GP*CP*AP*UP*CP*C)-3'

Chain B: 

• Molecule 2: Nucleolin

Chain A:



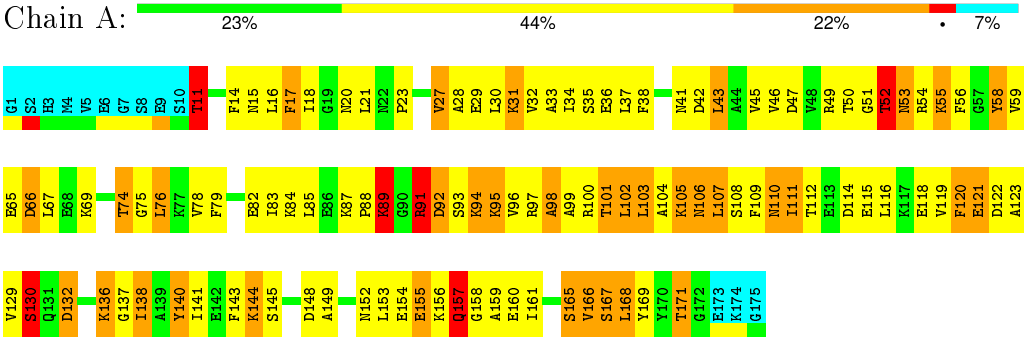
4.2.2 Score per residue for model 2

• Molecule 1: 5'-R(*GP*GP*AP*UP*GP*CP*CP*UP*CP*CP*CP*GP*AP*GP*UP*GP*CP*AP*UP*CP*C)-3'

Chain B:

• Molecule 2: Nucleolin

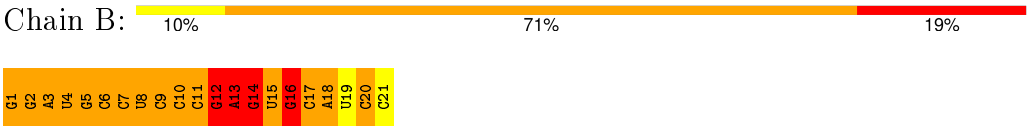
Chain A:



4.2.3 Score per residue for model 3

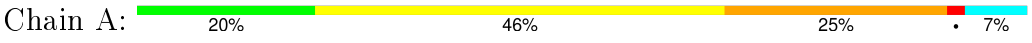
• Molecule 1: 5'-R(*GP*GP*AP*UP*GP*CP*CP*UP*CP*CP*CP*GP*AP*GP*UP*GP*CP*AP*UP*CP*C)-3'

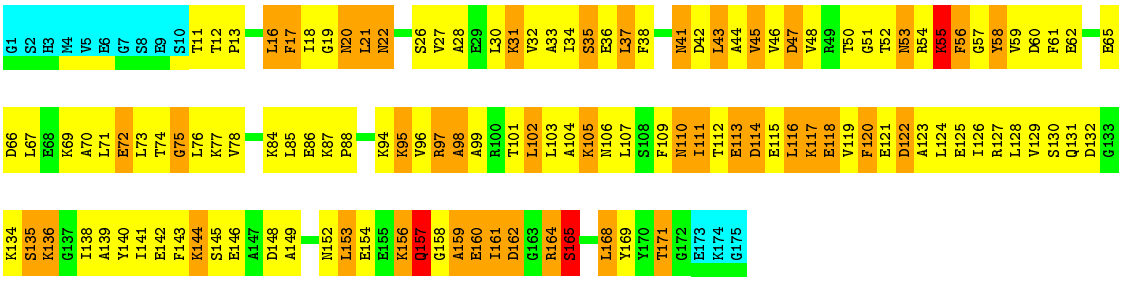
Chain B:



• Molecule 2: Nucleolin

Chain A:





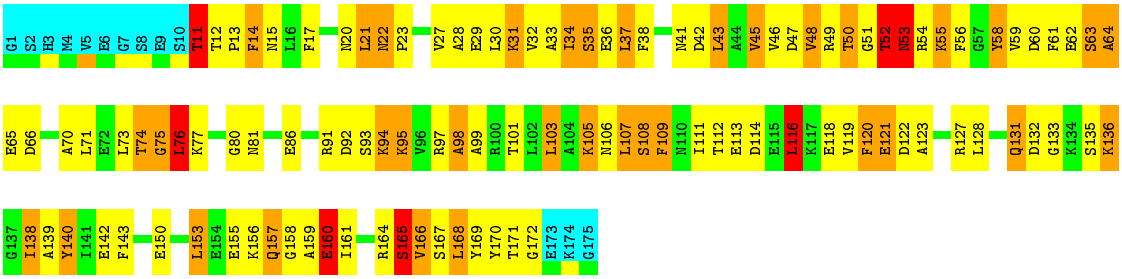
4.2.4 Score per residue for model 4

• Molecule 1: 5'-R(*GP*GP*AP*UP*GP*CP*CP*UP*CP*CP*CP*GP*AP*GP*UP*GP*CP*AP*UP*CP*C)-3'

Chain B: 19% 48% 33%

• Molecule 2: Nucleolin

Chain A: 29% 40% 20% 7%



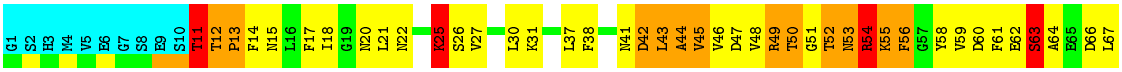
4.2.5 Score per residue for model 5

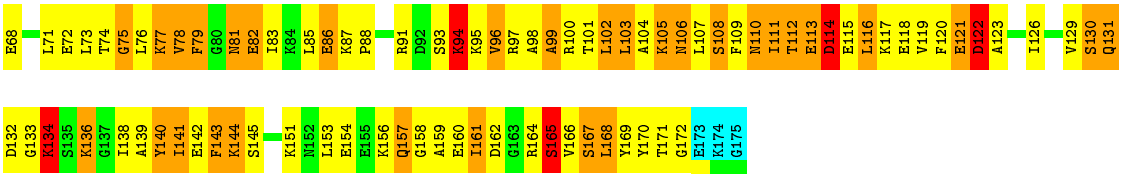
• Molecule 1: 5'-R(*GP*GP*AP*UP*GP*CP*CP*UP*CP*CP*CP*GP*AP*GP*UP*GP*CP*AP*UP*CP*C)-3'

Chain B: 10% 67% 24%

• Molecule 2: Nucleolin

Chain A: 21% 42% 25% 5% 7%





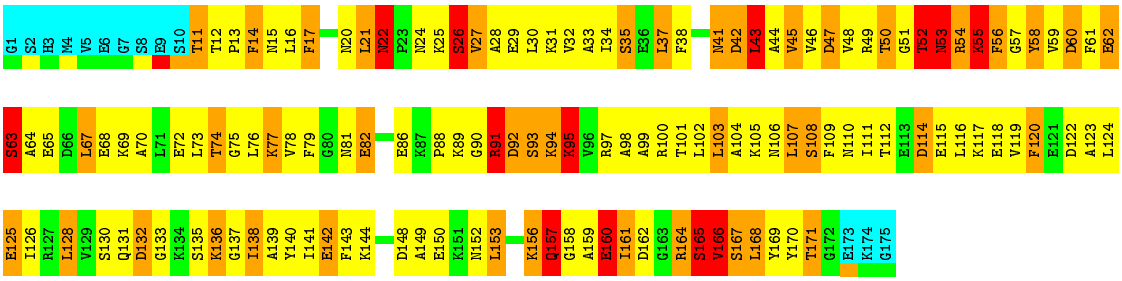
4.2.6 Score per residue for model 6

• Molecule 1: 5'-R(*GP*GP*AP*UP*GP*CP*CP*UP*CP*CP*CP*GP*AP*GP*UP*GP*CP*AP*UP*CP*C)-3'

Chain B: 14% 57% 29%

• Molecule 2: Nucleolin

Chain A: 15% 46% 24% 7% 7%



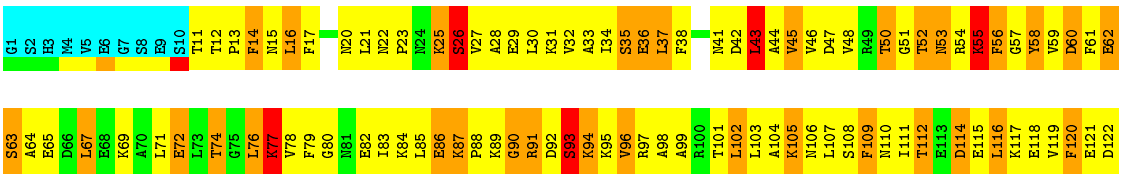
4.2.7 Score per residue for model 7

• Molecule 1: 5'-R(*GP*GP*AP*UP*GP*CP*CP*UP*CP*CP*CP*GP*AP*GP*UP*GP*CP*AP*UP*CP*C)-3'

Chain B: 29% 52% 19%

• Molecule 2: Nucleolin

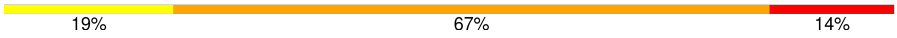
Chain A: 15% 47% 26% 5% 7%



4.2.8 Score per residue for model 8

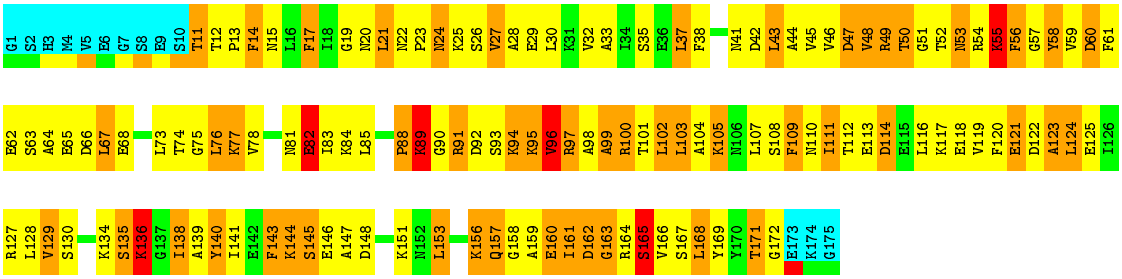
• Molecule 1: 5'-R(*GP*GP*AP*UP*GP*CP*CP*UP*CP*CP*CP*GP*AP*GP*UP*GP*CP*AP*UP*CP*C)-3'

Chain B:



• Molecule 2: Nucleolin

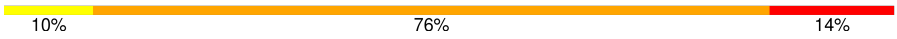
Chain A:



4.2.9 Score per residue for model 9

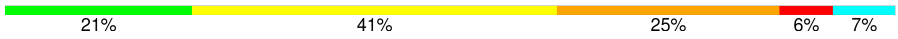
• Molecule 1: 5'-R(*GP*GP*AP*UP*GP*CP*CP*UP*CP*CP*CP*GP*AP*GP*UP*GP*CP*AP*UP*CP*C)-3'

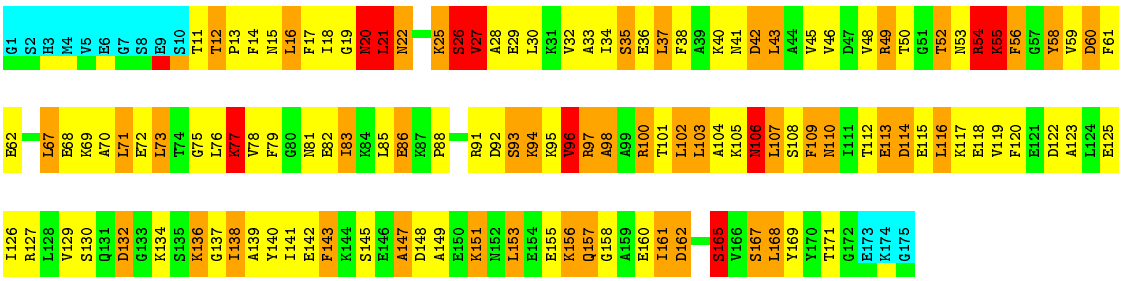
Chain B:



• Molecule 2: Nucleolin

Chain A:





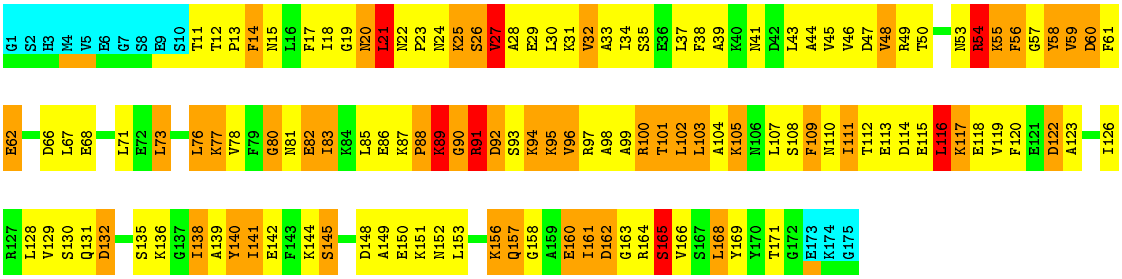
4.2.10 Score per residue for model 10

• Molecule 1: 5'-R(*GP*GP*AP*UP*GP*CP*CP*UP*CP*CP*CP*GP*AP*GP*UP*GP*CP*AP*UP*CP*C)-3'

Chain B: 5% 19% 57% 19%

• Molecule 2: Nucleolin

Chain A: 19% 45% 25% 7%



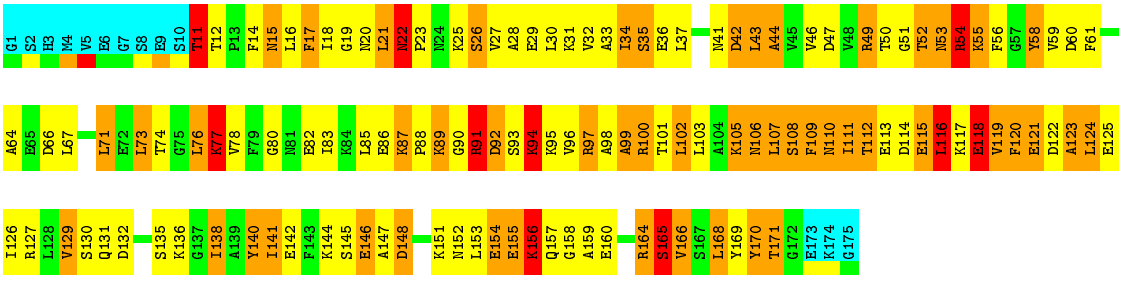
4.2.11 Score per residue for model 11

• Molecule 1: 5'-R(*GP*GP*AP*UP*GP*CP*CP*UP*CP*CP*CP*GP*AP*GP*UP*GP*CP*AP*UP*CP*C)-3'

Chain B: 19% 67% 14%

• Molecule 2: Nucleolin

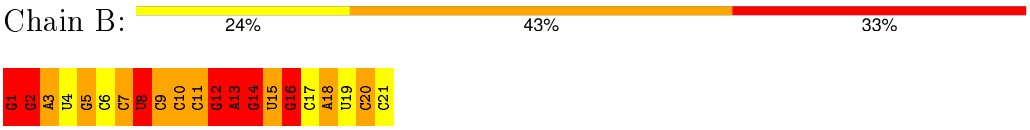
Chain A: 19% 39% 29% 6% 7%



4.2.12 Score per residue for model 12

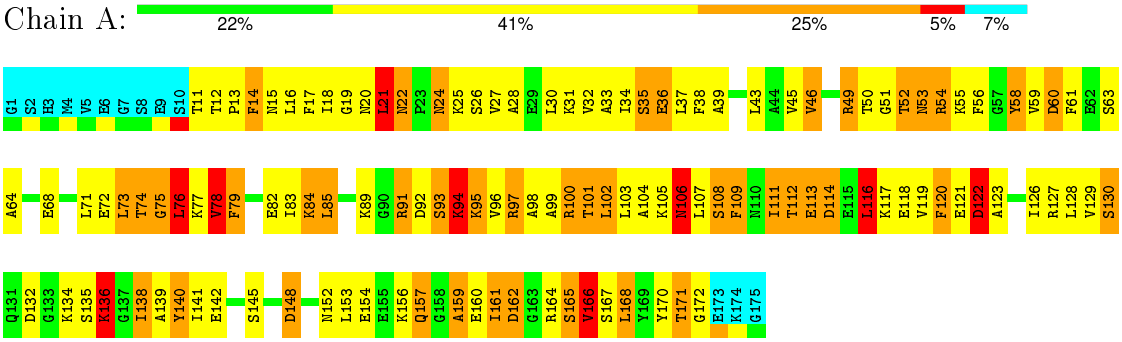
• Molecule 1: 5'-R(*GP*GP*AP*UP*GP*CP*CP*UP*CP*CP*CP*GP*AP*GP*UP*GP*CP*AP*UP*CP*C)-3'

Chain B:



• Molecule 2: Nucleolin

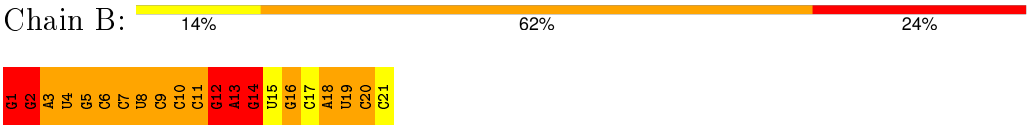
Chain A:



4.2.13 Score per residue for model 13

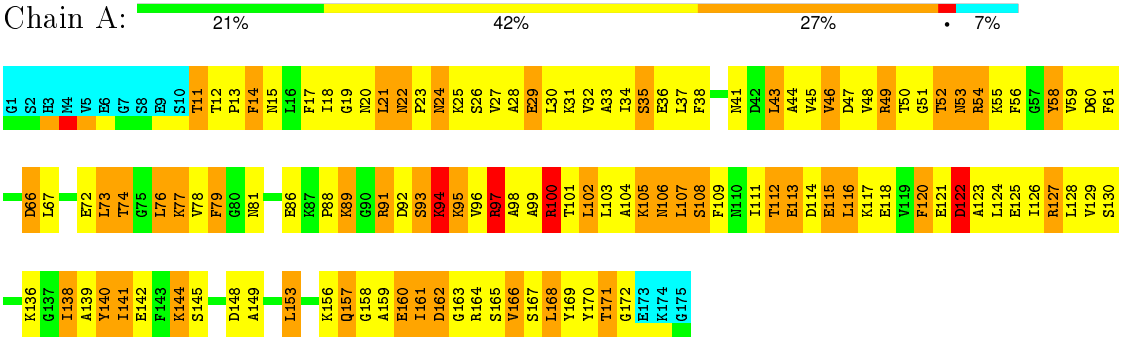
• Molecule 1: 5'-R(*GP*GP*AP*UP*GP*CP*CP*UP*CP*CP*CP*GP*AP*GP*UP*GP*CP*AP*UP*CP*C)-3'

Chain B:



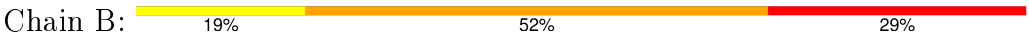
• Molecule 2: Nucleolin

Chain A:

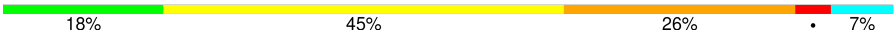


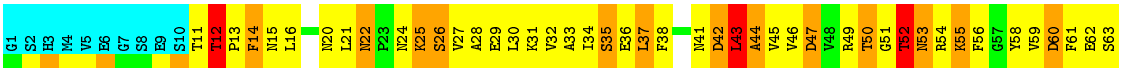
4.2.14 Score per residue for model 14

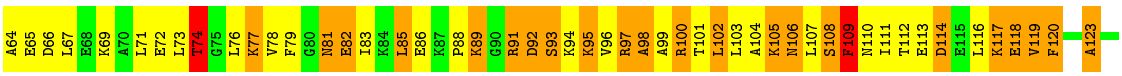
• Molecule 1: 5'-R(*GP*GP*AP*UP*GP*CP*CP*UP*CP*CP*CP*GP*AP*GP*UP*GP*CP*AP*UP*CP*C)-3'

Chain B: 

• Molecule 2: Nucleolin

Chain A: 





5 Refinement protocol and experimental data overview

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

Of the 40 calculated structures, 14 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. No validations of the models with respect to experimental NMR restraints is performed at this time.

6 Model quality

6.1 Standard geometry

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the (average) root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#Z>5	RMSZ	#Z>5
1	B	1.07±0.01	0±0/491 (0.0±0.0%)	1.92±0.01	21±1/763 (2.8±0.1%)
2	A	0.21±0.00	0±0/1287 (0.0±0.0%)	0.34±0.01	0±0/1729 (0.0±0.0%)
All	All	0.59	0/24892 (0.0%)	1.10	300/34888 (0.9%)

There are no bond-length outliers.

All unique angle outliers are listed below. They are sorted according to the Z-score of the worst occurrence in the ensemble.

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
1	B	12	G	N7-C8-N9	9.27	117.74	113.10	2	14
1	B	14	G	N7-C8-N9	9.25	117.72	113.10	7	14
1	B	1	G	N7-C8-N9	9.24	117.72	113.10	6	14
1	B	5	G	N7-C8-N9	9.21	117.71	113.10	13	14
1	B	16	G	N7-C8-N9	9.21	117.71	113.10	13	14
1	B	2	G	N7-C8-N9	9.19	117.70	113.10	10	14
1	B	18	A	N7-C8-N9	7.68	117.64	113.80	11	14
1	B	3	A	N7-C8-N9	7.51	117.55	113.80	1	14
1	B	13	A	N7-C8-N9	7.37	117.48	113.80	7	14
1	B	2	G	C8-N9-C4	-7.36	103.46	106.40	4	14
1	B	14	G	C8-N9-C4	-7.11	103.56	106.40	10	14
1	B	1	G	C8-N9-C4	-7.04	103.58	106.40	11	14
1	B	16	G	C8-N9-C4	-7.03	103.59	106.40	4	14
1	B	5	G	C8-N9-C4	-6.79	103.68	106.40	4	14
1	B	12	G	C8-N9-C4	-6.72	103.71	106.40	2	14
1	B	13	A	C8-N9-C4	-5.96	103.42	105.80	2	14
1	B	18	A	C8-N9-C4	-5.65	103.54	105.80	12	14
1	B	3	A	C8-N9-C4	-5.61	103.56	105.80	1	14
1	B	12	G	C5-N7-C8	-5.37	101.61	104.30	4	12
1	B	8	U	O4'-C1'-N1	5.33	112.47	108.20	12	1
1	B	14	G	C5-N7-C8	-5.23	101.69	104.30	6	10
1	B	5	G	C5-N7-C8	-5.20	101.70	104.30	9	11
1	B	16	G	C5-N7-C8	-5.16	101.72	104.30	14	8

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
1	B	1	G	C5-N7-C8	-5.09	101.76	104.30	5	5
1	B	2	G	C5-N7-C8	-5.00	101.80	104.30	1	1

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	B	441	229	229	92±9
2	A	1271	1287	1287	203±18
All	All	23968	21224	21224	3663

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 81.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:17:C:O2'	1:B:18:A:H5'	1.06	1.50	12	14
2:A:101:THR:HG23	2:A:171:THR:HG23	1.05	1.25	1	5
1:B:2:G:O2'	1:B:3:A:H5'	1.04	1.52	2	14
2:A:11:THR:HG21	2:A:46:VAL:HG11	1.04	1.26	3	4
1:B:8:U:C4	2:A:103:LEU:HD21	1.02	1.88	7	6
2:A:153:LEU:O	2:A:168:LEU:HD12	1.02	1.53	11	1
1:B:1:G:O2'	1:B:2:G:H5'	1.01	1.55	7	8
2:A:123:ALA:HB2	2:A:143:PHE:CZ	1.00	1.91	6	5
1:B:8:U:C6	2:A:103:LEU:HD13	0.97	1.94	5	2
2:A:98:ALA:HB1	2:A:101:THR:CG2	0.95	1.90	10	2
1:B:6:C:O2'	1:B:7:C:H5'	0.95	1.61	7	4
2:A:38:PHE:CD1	2:A:43:LEU:HD11	0.95	1.97	7	2
2:A:123:ALA:HB2	2:A:143:PHE:CE2	0.95	1.97	5	3
1:B:20:C:O2'	1:B:21:C:H5'	0.94	1.62	2	14
1:B:9:C:O4'	2:A:129:VAL:HG13	0.94	1.62	12	5
1:B:12:G:OP2	2:A:52:THR:HG21	0.94	1.62	8	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:13:A:C8	2:A:52:THR:HG23	0.94	1.98	5	4
1:B:8:U:C4	2:A:103:LEU:HD22	0.94	1.97	9	2
1:B:8:U:HO2'	1:B:9:C:H6	0.93	0.94	1	4
1:B:8:U:C4	2:A:103:LEU:HD11	0.93	1.98	14	6
2:A:136:LYS:CD	2:A:138:ILE:HD11	0.93	1.94	11	2
1:B:14:G:OP2	1:B:14:G:H2'	0.93	1.63	10	1
2:A:106:ASN:OD1	2:A:166:VAL:HG23	0.92	1.63	13	1
1:B:9:C:H5'	1:B:10:C:OP2	0.92	1.63	14	1
2:A:124:LEU:HD12	2:A:125:GLU:N	0.92	1.79	7	1
1:B:8:U:C5	2:A:103:LEU:HD22	0.91	1.99	9	2
2:A:37:LEU:HD13	2:A:38:PHE:N	0.91	1.80	6	11
2:A:27:VAL:HG21	2:A:53:ASN:O	0.91	1.65	2	2
2:A:116:LEU:HD11	2:A:139:ALA:HB1	0.91	1.42	13	2
1:B:8:U:O2'	1:B:9:C:H6	0.90	1.49	6	5
2:A:15:ASN:O	2:A:16:LEU:HD22	0.90	1.65	7	1
2:A:102:LEU:HD12	2:A:169:TYR:O	0.90	1.67	6	7
2:A:18:ILE:CG2	2:A:21:LEU:HD21	0.89	1.97	5	2
1:B:7:C:O3'	1:B:8:U:H4'	0.88	1.68	13	1
2:A:136:LYS:CE	2:A:138:ILE:HD11	0.88	1.99	11	2
2:A:101:THR:C	2:A:102:LEU:HD13	0.88	1.88	3	3
1:B:1:G:HO2'	1:B:2:G:H8	0.88	1.02	14	6
2:A:111:ILE:CD1	2:A:161:ILE:HG23	0.88	1.98	12	3
1:B:8:U:C5	2:A:103:LEU:HD13	0.88	2.02	5	2
2:A:104:ALA:HB3	2:A:139:ALA:HB3	0.88	1.44	12	3
2:A:34:ILE:CD1	2:A:76:LEU:HD11	0.87	1.98	9	1
1:B:12:G:N3	1:B:12:G:H3'	0.87	1.84	9	2
2:A:61:PHE:CD2	2:A:67:LEU:HD12	0.87	2.04	11	2
2:A:101:THR:HG23	2:A:171:THR:OG1	0.87	1.70	12	4
2:A:11:THR:HG21	2:A:46:VAL:CG1	0.87	1.98	8	4
1:B:8:U:C6	2:A:103:LEU:HD23	0.86	2.05	10	1
2:A:157:GLN:O	2:A:168:LEU:HD21	0.86	1.70	5	1
2:A:11:THR:CG2	2:A:46:VAL:HG11	0.85	1.99	2	5
1:B:15:U:H4'	1:B:16:G:O5'	0.85	1.72	12	2
2:A:101:THR:HG22	2:A:171:THR:O	0.85	1.71	1	2
2:A:18:ILE:HG21	2:A:21:LEU:HD21	0.85	1.46	5	2
1:B:12:G:O2'	1:B:13:A:H5'	0.84	1.72	12	3
2:A:157:GLN:N	2:A:168:LEU:HD11	0.84	1.86	6	4
2:A:103:LEU:HD12	2:A:140:TYR:CD1	0.84	2.07	9	1
1:B:5:G:O2'	1:B:6:C:H5'	0.84	1.72	9	14
2:A:102:LEU:HD23	2:A:141:ILE:HB	0.84	1.50	3	2
2:A:119:VAL:HG22	2:A:156:LYS:HG3	0.84	1.49	1	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:11:C:H1'	1:B:12:G:OP1	0.83	1.73	5	7
1:B:8:U:O2'	1:B:9:C:C6	0.83	2.32	14	7
1:B:12:G:OP1	1:B:12:G:H3'	0.83	1.72	2	1
2:A:98:ALA:HB1	2:A:101:THR:HG23	0.83	1.51	10	1
2:A:103:LEU:HD12	2:A:104:ALA:N	0.83	1.88	8	5
1:B:7:C:H5"	1:B:8:U:OP2	0.83	1.74	6	2
1:B:13:A:H4'	1:B:14:G:O5'	0.82	1.73	2	5
2:A:157:GLN:NE2	2:A:168:LEU:HD11	0.82	1.89	11	1
1:B:8:U:O4	2:A:103:LEU:HD11	0.82	1.73	2	5
1:B:1:G:O2'	1:B:2:G:H8	0.82	1.56	4	5
2:A:30:LEU:O	2:A:34:ILE:HD12	0.82	1.73	13	4
2:A:156:LYS:HB2	2:A:168:LEU:HD13	0.82	1.50	11	1
2:A:21:LEU:HD22	2:A:34:ILE:HD11	0.82	1.51	3	1
2:A:47:ASP:O	2:A:59:VAL:HG23	0.81	1.75	14	7
2:A:105:LYS:O	2:A:166:VAL:HG22	0.81	1.76	6	5
2:A:103:LEU:HD13	2:A:140:TYR:CD1	0.81	2.11	4	1
1:B:11:C:H4'	1:B:12:G:OP1	0.80	1.75	13	3
2:A:159:ALA:HB3	2:A:166:VAL:HG12	0.80	1.52	11	4
2:A:18:ILE:HG21	2:A:83:ILE:HD12	0.79	1.52	2	3
1:B:8:U:N3	2:A:103:LEU:HD11	0.79	1.91	14	4
2:A:101:THR:HG23	2:A:171:THR:CG2	0.79	2.07	6	5
2:A:102:LEU:HD23	2:A:141:ILE:CD1	0.79	2.08	5	1
2:A:116:LEU:O	2:A:119:VAL:HG12	0.79	1.78	9	6
2:A:102:LEU:HD21	2:A:143:PHE:CD1	0.79	2.13	2	2
2:A:103:LEU:HD22	2:A:140:TYR:CD2	0.78	2.13	10	1
2:A:123:ALA:HB2	2:A:143:PHE:CE1	0.78	2.13	7	3
2:A:20:ASN:OD1	2:A:83:ILE:HG22	0.78	1.77	9	1
1:B:12:G:H5'	1:B:12:G:N3	0.78	1.92	11	4
2:A:101:THR:OG1	2:A:171:THR:HG23	0.78	1.79	4	2
2:A:103:LEU:HD12	2:A:139:ALA:O	0.77	1.78	1	6
2:A:102:LEU:HD11	2:A:143:PHE:HB2	0.77	1.54	1	2
1:B:8:U:C5	2:A:103:LEU:HD21	0.77	2.15	1	8
1:B:12:G:OP2	1:B:12:G:H4'	0.77	1.80	11	1
2:A:136:LYS:CD	2:A:138:ILE:HD12	0.77	2.09	5	1
1:B:8:U:H1'	1:B:9:C:OP1	0.77	1.80	4	3
2:A:98:ALA:HB3	2:A:101:THR:HG21	0.77	1.55	1	4
2:A:129:VAL:HG11	2:A:138:ILE:HD12	0.76	1.57	13	2
2:A:20:ASN:O	2:A:83:ILE:HG22	0.76	1.80	7	2
1:B:9:C:C5	1:B:10:C:C5	0.76	2.72	13	10
2:A:44:ALA:O	2:A:45:VAL:HG12	0.76	1.78	7	2
2:A:12:THR:HG21	2:A:61:PHE:O	0.76	1.80	14	8

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:12:G:H1'	1:B:13:A:O5'	0.76	1.81	3	1
1:B:11:C:OP2	1:B:11:C:H6	0.76	1.63	10	1
2:A:103:LEU:HD13	2:A:140:TYR:CD2	0.76	2.14	1	4
1:B:11:C:H1'	1:B:12:G:O5'	0.76	1.79	13	1
1:B:8:U:O2'	1:B:9:C:C5	0.76	2.39	7	2
1:B:9:C:H5'	1:B:10:C:O5'	0.76	1.81	4	2
2:A:124:LEU:HD11	2:A:142:GLU:OE1	0.76	1.81	6	1
1:B:8:U:O5'	1:B:8:U:H6	0.75	1.63	3	4
2:A:31:LYS:O	2:A:34:ILE:HG22	0.75	1.81	7	5
1:B:9:C:OP2	1:B:10:C:H5	0.75	1.64	8	5
2:A:103:LEU:HD11	2:A:105:LYS:NZ	0.75	1.96	8	1
2:A:84:LYS:C	2:A:85:LEU:HD13	0.75	2.03	12	1
1:B:8:U:H4'	1:B:9:C:OP1	0.74	1.83	7	1
2:A:119:VAL:HG22	2:A:156:LYS:CG	0.74	2.12	5	4
1:B:9:C:H1'	2:A:129:VAL:HG22	0.74	1.59	9	3
2:A:102:LEU:HD11	2:A:168:LEU:HB2	0.74	1.58	13	3
2:A:94:LYS:HE2	2:A:96:VAL:HG13	0.74	1.58	10	1
2:A:102:LEU:HD22	2:A:102:LEU:N	0.74	1.97	3	2
1:B:9:C:O5'	1:B:9:C:H6	0.74	1.66	13	1
2:A:78:VAL:HG13	2:A:83:ILE:CG2	0.74	2.12	5	1
2:A:34:ILE:HD13	2:A:76:LEU:HD11	0.74	1.60	9	1
2:A:11:THR:HG21	2:A:47:ASP:CB	0.73	2.13	5	1
2:A:18:ILE:CG2	2:A:83:ILE:HD12	0.73	2.13	11	3
2:A:102:LEU:HD13	2:A:102:LEU:N	0.73	1.98	2	2
1:B:12:G:O2'	1:B:13:A:P	0.73	2.46	9	6
1:B:9:C:C4	1:B:10:C:C4	0.73	2.77	2	4
2:A:116:LEU:HD21	2:A:139:ALA:HB1	0.73	1.61	3	4
2:A:104:ALA:CB	2:A:139:ALA:HB3	0.73	2.13	13	2
2:A:102:LEU:HD22	2:A:141:ILE:O	0.73	1.83	2	2
1:B:13:A:O2'	1:B:14:G:P	0.73	2.47	7	9
2:A:21:LEU:HD12	2:A:78:VAL:HG11	0.73	1.60	9	1
2:A:76:LEU:CD2	2:A:83:ILE:HD11	0.73	2.14	9	1
1:B:10:C:O2'	1:B:11:C:P	0.72	2.47	11	1
2:A:153:LEU:HG	2:A:168:LEU:HD12	0.72	1.59	3	1
2:A:136:LYS:CE	2:A:138:ILE:HD12	0.72	2.14	14	2
1:B:13:A:H4'	1:B:14:G:OP1	0.72	1.84	12	4
2:A:157:GLN:HA	2:A:168:LEU:HD11	0.72	1.58	10	6
2:A:102:LEU:HD22	2:A:102:LEU:H	0.72	1.45	3	2
2:A:168:LEU:N	2:A:168:LEU:HD12	0.72	1.99	2	1
2:A:16:LEU:HD22	2:A:85:LEU:HD23	0.72	1.61	9	1
2:A:41:ASN:HB3	2:A:43:LEU:HD23	0.72	1.60	8	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:8:U:O2	2:A:129:VAL:HG21	0.72	1.85	2	2
2:A:101:THR:HG22	2:A:142:GLU:HB2	0.72	1.62	5	1
2:A:171:THR:HG23	2:A:171:THR:O	0.71	1.84	5	1
1:B:1:G:C2	1:B:2:G:N7	0.71	2.59	14	6
1:B:7:C:O2'	1:B:8:U:P	0.71	2.47	12	4
1:B:8:U:O2'	1:B:9:C:P	0.71	2.48	12	2
1:B:9:C:N3	2:A:140:TYR:CD2	0.71	2.58	9	3
1:B:8:U:C5	2:A:138:ILE:HG21	0.71	2.20	13	2
2:A:119:VAL:HG22	2:A:158:GLY:O	0.71	1.86	11	1
2:A:157:GLN:CA	2:A:168:LEU:HD11	0.71	2.16	9	6
2:A:119:VAL:HG22	2:A:156:LYS:HG2	0.71	1.62	5	2
1:B:8:U:C5	2:A:103:LEU:HD23	0.71	2.20	10	1
2:A:107:LEU:HD13	2:A:139:ALA:HB2	0.71	1.60	14	2
1:B:9:C:C5	2:A:140:TYR:CE2	0.71	2.78	1	6
2:A:21:LEU:O	2:A:30:LEU:HD13	0.71	1.85	2	3
2:A:78:VAL:HG13	2:A:83:ILE:HG21	0.71	1.63	5	2
1:B:9:C:C4	2:A:140:TYR:CE1	0.71	2.79	2	3
2:A:102:LEU:HD22	2:A:152:ASN:OD1	0.71	1.86	6	1
2:A:128:LEU:HD23	2:A:128:LEU:N	0.71	1.99	6	3
1:B:1:G:N2	1:B:2:G:C5	0.71	2.59	4	6
1:B:9:C:C5	2:A:140:TYR:CD2	0.71	2.79	5	6
2:A:168:LEU:N	2:A:168:LEU:HD23	0.71	2.00	11	1
1:B:9:C:N3	2:A:140:TYR:CE2	0.71	2.59	9	1
1:B:4:U:HO2'	1:B:5:G:C5'	0.70	1.99	14	12
1:B:2:G:HO2'	1:B:3:A:H5'	0.70	1.44	11	10
2:A:160:GLU:O	2:A:161:ILE:HG22	0.70	1.86	10	1
2:A:102:LEU:HD23	2:A:143:PHE:CE1	0.70	2.22	7	2
1:B:8:U:O4	2:A:103:LEU:HD21	0.70	1.86	6	5
1:B:9:C:C4	2:A:140:TYR:CZ	0.70	2.80	6	5
2:A:104:ALA:HB3	2:A:139:ALA:CB	0.70	2.17	13	2
2:A:128:LEU:N	2:A:128:LEU:HD23	0.70	2.01	2	1
1:B:9:C:N4	2:A:140:TYR:CD1	0.70	2.60	8	1
1:B:9:C:N4	1:B:10:C:N3	0.70	2.39	8	1
2:A:102:LEU:N	2:A:102:LEU:HD22	0.70	2.02	1	1
2:A:11:THR:HG21	2:A:47:ASP:HB2	0.69	1.62	5	1
2:A:28:ALA:O	2:A:32:VAL:HG23	0.69	1.87	3	9
1:B:9:C:N3	2:A:140:TYR:CE1	0.69	2.61	3	2
1:B:11:C:N3	2:A:17:PHE:CD2	0.69	2.59	10	2
1:B:12:G:H2'	1:B:12:G:N3	0.69	2.01	2	2
1:B:9:C:C5	1:B:10:C:C4	0.69	2.81	8	6
1:B:9:C:N3	2:A:140:TYR:CG	0.69	2.60	11	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:17:C:HO2'	1:B:18:A:H5'	0.69	1.44	1	8
2:A:11:THR:HG22	2:A:46:VAL:HG11	0.69	1.64	10	1
2:A:104:ALA:O	2:A:138:ILE:HG22	0.69	1.87	9	3
2:A:102:LEU:CD2	2:A:141:ILE:HD13	0.69	2.17	5	2
1:B:9:C:N3	2:A:140:TYR:CD1	0.69	2.61	6	5
2:A:117:LYS:HB2	2:A:126:ILE:HD13	0.69	1.62	14	2
2:A:101:THR:HG23	2:A:171:THR:O	0.69	1.88	8	1
1:B:9:C:N4	2:A:140:TYR:CE1	0.69	2.60	8	4
2:A:157:GLN:O	2:A:168:LEU:HD23	0.69	1.88	14	1
2:A:37:LEU:HD13	2:A:37:LEU:C	0.69	2.09	5	8
2:A:111:ILE:HD11	2:A:161:ILE:HG22	0.69	1.65	1	2
2:A:98:ALA:HB1	2:A:172:GLY:HA2	0.68	1.64	12	1
2:A:16:LEU:HD11	2:A:85:LEU:HB3	0.68	1.63	1	1
2:A:22:ASN:ND2	2:A:30:LEU:HD11	0.68	2.03	14	1
2:A:16:LEU:HD23	2:A:85:LEU:CD2	0.68	2.18	14	1
2:A:103:LEU:HD12	2:A:140:TYR:CD2	0.68	2.24	5	1
1:B:15:U:OP2	1:B:15:U:H4'	0.68	1.89	3	1
1:B:9:C:C1'	2:A:129:VAL:HG22	0.68	2.18	9	4
2:A:103:LEU:HD23	2:A:105:LYS:HD2	0.68	1.66	5	1
1:B:12:G:C3'	1:B:12:G:N3	0.68	2.57	9	2
1:B:9:C:N4	2:A:140:TYR:CZ	0.68	2.62	6	5
2:A:30:LEU:HD12	2:A:55:LYS:HB2	0.68	1.62	8	1
2:A:46:VAL:HG23	2:A:61:PHE:C	0.68	2.10	2	5
2:A:153:LEU:O	2:A:168:LEU:HD21	0.68	1.88	14	1
2:A:85:LEU:N	2:A:85:LEU:HD13	0.67	2.02	12	1
1:B:11:C:H1'	1:B:12:G:N7	0.67	2.04	9	2
2:A:116:LEU:CD1	2:A:139:ALA:HB1	0.67	2.18	13	1
2:A:37:LEU:O	2:A:37:LEU:HD22	0.67	1.89	6	3
2:A:124:LEU:HD12	2:A:144:LYS:HB3	0.67	1.65	3	1
1:B:9:C:H5"	1:B:10:C:OP2	0.67	1.90	1	1
2:A:76:LEU:HD23	2:A:76:LEU:N	0.67	2.02	12	1
2:A:11:THR:O	2:A:12:THR:HG22	0.67	1.87	14	1
2:A:16:LEU:HD23	2:A:85:LEU:HD23	0.67	1.65	14	1
1:B:9:C:C4'	2:A:129:VAL:HG13	0.67	2.18	13	3
2:A:126:ILE:HG12	2:A:141:ILE:HG23	0.67	1.66	11	1
2:A:43:LEU:HD13	2:A:61:PHE:CG	0.67	2.25	11	1
2:A:37:LEU:C	2:A:37:LEU:HD13	0.67	2.09	14	5
1:B:8:U:O2'	2:A:140:TYR:CD2	0.67	2.48	7	1
1:B:12:G:H1'	1:B:13:A:OP2	0.67	1.89	5	1
1:B:8:U:C4	2:A:103:LEU:CD1	0.67	2.78	1	6
1:B:12:G:H4'	1:B:13:A:OP1	0.67	1.90	3	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:A:119:VAL:HG21	2:A:159:ALA:HB2	0.67	1.66	2	1
2:A:157:GLN:C	2:A:168:LEU:HD21	0.67	2.10	5	1
2:A:49:ARG:NH2	2:A:58:TYR:CD2	0.67	2.63	4	2
2:A:120:PHE:CZ	2:A:141:ILE:HD11	0.67	2.25	12	1
2:A:136:LYS:HD2	2:A:138:ILE:HD11	0.67	1.66	11	2
2:A:37:LEU:HD22	2:A:37:LEU:O	0.67	1.90	4	4
1:B:11:C:N3	2:A:17:PHE:CZ	0.67	2.63	12	2
2:A:167:SER:C	2:A:168:LEU:HD23	0.67	2.10	6	1
1:B:8:U:C4	2:A:103:LEU:CD2	0.66	2.78	6	7
2:A:102:LEU:HD23	2:A:141:ILE:HD13	0.66	1.65	5	1
1:B:9:C:C2	2:A:140:TYR:CG	0.66	2.83	6	5
1:B:1:G:O2'	1:B:2:G:C5'	0.66	2.44	8	8
2:A:102:LEU:HD11	2:A:143:PHE:CG	0.66	2.25	2	2
1:B:8:U:C5	2:A:103:LEU:CD2	0.66	2.78	10	8
1:B:8:U:O3'	1:B:9:C:H6	0.66	1.74	7	2
1:B:13:A:C6	2:A:94:LYS:CG	0.66	2.79	1	2
2:A:123:ALA:CB	2:A:143:PHE:CE2	0.66	2.79	8	3
2:A:153:LEU:HA	2:A:168:LEU:HD12	0.66	1.67	13	1
2:A:159:ALA:HB3	2:A:166:VAL:CG1	0.66	2.21	11	3
1:B:9:C:N4	1:B:10:C:C4	0.66	2.64	8	4
2:A:30:LEU:HD22	2:A:78:VAL:CG1	0.66	2.20	13	1
2:A:45:VAL:HG13	2:A:45:VAL:O	0.66	1.91	5	4
2:A:94:LYS:O	2:A:96:VAL:HG22	0.66	1.91	1	2
1:B:13:A:C8	2:A:52:THR:CG2	0.66	2.79	5	3
2:A:112:THR:O	2:A:116:LEU:HD13	0.66	1.90	2	1
2:A:116:LEU:C	2:A:116:LEU:HD13	0.66	2.11	14	1
1:B:8:U:C4	2:A:103:LEU:HD13	0.65	2.26	8	1
1:B:9:C:C4	2:A:140:TYR:CG	0.65	2.84	8	1
1:B:8:U:O3'	1:B:9:C:C6	0.65	2.50	11	2
2:A:129:VAL:CG1	2:A:138:ILE:HD12	0.65	2.22	13	2
1:B:13:A:O2'	1:B:14:G:C4'	0.65	2.45	5	1
2:A:52:THR:O	2:A:52:THR:HG22	0.65	1.91	8	1
1:B:16:G:HO2'	1:B:17:C:H6	0.65	1.35	13	3
1:B:9:C:C6	2:A:140:TYR:CD2	0.65	2.85	1	4
2:A:107:LEU:HD23	2:A:108:SER:O	0.65	1.92	5	1
1:B:12:G:O2'	1:B:13:A:C5'	0.65	2.44	13	5
2:A:101:THR:HG22	2:A:142:GLU:CB	0.65	2.22	5	2
2:A:102:LEU:H	2:A:102:LEU:HD22	0.65	1.49	1	1
2:A:106:ASN:O	2:A:166:VAL:HG23	0.65	1.92	1	3
1:B:2:G:O2'	1:B:3:A:C5'	0.65	2.41	7	14
2:A:16:LEU:CD2	2:A:67:LEU:HD11	0.65	2.22	7	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:A:153:LEU:HD22	2:A:170:TYR:HB3	0.65	1.69	11	1
2:A:140:TYR:OH	2:A:171:THR:HG21	0.65	1.92	10	4
1:B:8:U:C5	2:A:103:LEU:CD1	0.65	2.80	5	2
2:A:136:LYS:HE2	2:A:138:ILE:HD12	0.65	1.67	14	1
2:A:102:LEU:HD13	2:A:153:LEU:HD12	0.65	1.68	6	2
2:A:141:ILE:HG22	2:A:143:PHE:CE1	0.65	2.27	9	2
2:A:141:ILE:HD12	2:A:141:ILE:N	0.65	2.07	11	1
2:A:41:ASN:HB3	2:A:43:LEU:HD12	0.65	1.68	4	2
2:A:125:GLU:O	2:A:141:ILE:HG23	0.65	1.91	6	4
1:B:9:C:C4	2:A:140:TYR:CE2	0.65	2.85	14	5
2:A:140:TYR:CE1	2:A:171:THR:HG21	0.65	2.27	2	4
1:B:4:U:O2'	1:B:5:G:C5'	0.64	2.45	2	14
1:B:5:G:O2'	1:B:6:C:C5'	0.64	2.45	3	14
1:B:11:C:H4'	1:B:12:G:OP2	0.64	1.92	8	3
1:B:12:G:H4'	1:B:13:A:O5'	0.64	1.90	9	1
2:A:107:LEU:HD23	2:A:109:PHE:H	0.64	1.51	13	1
1:B:9:C:C2	2:A:140:TYR:CD1	0.64	2.84	3	5
2:A:17:PHE:CD1	2:A:18:ILE:N	0.64	2.66	10	2
1:B:20:C:O2'	1:B:21:C:C5'	0.64	2.45	6	14
1:B:9:C:N4	2:A:127:ARG:NH2	0.64	2.46	13	2
2:A:45:VAL:HG21	2:A:48:VAL:HG13	0.64	1.69	1	2
1:B:13:A:N6	2:A:94:LYS:CE	0.64	2.60	8	1
2:A:140:TYR:CZ	2:A:171:THR:HG21	0.64	2.27	6	4
2:A:128:LEU:HD23	2:A:128:LEU:H	0.64	1.52	1	1
2:A:153:LEU:HD11	2:A:169:TYR:C	0.64	2.12	6	2
1:B:13:A:O2'	1:B:14:G:C5'	0.64	2.46	5	1
1:B:8:U:C4	2:A:138:ILE:HG21	0.64	2.28	1	6
1:B:11:C:O2'	1:B:12:G:C5'	0.64	2.46	2	2
1:B:8:U:O4	2:A:105:LYS:CE	0.64	2.46	9	2
1:B:4:U:O2'	1:B:5:G:H5'	0.64	1.93	10	13
1:B:18:A:O2'	1:B:19:U:C5'	0.64	2.46	7	11
2:A:102:LEU:HD23	2:A:141:ILE:HG13	0.64	1.70	13	1
2:A:97:ARG:O	2:A:98:ALA:HB3	0.64	1.93	14	7
1:B:12:G:HO2'	1:B:13:A:P	0.64	2.16	10	2
1:B:6:C:N4	1:B:16:G:C6	0.63	2.66	12	2
2:A:101:THR:HG23	2:A:171:THR:HG1	0.63	1.52	13	2
2:A:50:THR:HG23	2:A:51:GLY:N	0.63	2.08	8	1
2:A:22:ASN:OD1	2:A:30:LEU:HD22	0.63	1.93	3	1
1:B:3:A:O2'	1:B:4:U:C5'	0.63	2.46	14	14
1:B:14:G:H4'	1:B:15:U:OP1	0.63	1.92	3	1
1:B:8:U:O2'	1:B:9:C:H5'	0.63	1.93	2	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:A:136:LYS:HD3	2:A:138:ILE:HD12	0.63	1.67	5	1
1:B:8:U:O4	2:A:103:LEU:CD1	0.63	2.46	8	2
2:A:11:THR:CG2	2:A:46:VAL:HG13	0.63	2.23	1	1
2:A:102:LEU:CD2	2:A:141:ILE:HD12	0.63	2.24	13	1
2:A:43:LEU:O	2:A:44:ALA:HB3	0.63	1.94	5	1
2:A:111:ILE:C	2:A:112:THR:HG23	0.63	2.13	11	1
1:B:11:C:O2'	2:A:91:ARG:CB	0.63	2.47	9	3
2:A:45:VAL:CG2	2:A:48:VAL:HG13	0.63	2.22	1	2
1:B:5:G:H8	1:B:5:G:O5'	0.63	1.77	3	3
2:A:161:ILE:O	2:A:161:ILE:HG22	0.63	1.92	13	3
2:A:161:ILE:HG22	2:A:161:ILE:O	0.63	1.92	8	1
2:A:46:VAL:HG23	2:A:62:GLU:N	0.63	2.09	2	2
2:A:17:PHE:CE1	2:A:56:PHE:CD2	0.63	2.86	3	1
2:A:43:LEU:O	2:A:44:ALA:CB	0.63	2.46	14	2
1:B:8:U:C6	2:A:103:LEU:CD1	0.63	2.79	5	2
1:B:18:A:O2'	1:B:19:U:H5'	0.63	1.94	7	6
1:B:12:G:O5'	1:B:12:G:C4	0.63	2.52	10	1
2:A:17:PHE:CD1	2:A:86:GLU:CB	0.63	2.82	13	1
1:B:11:C:O2'	2:A:91:ARG:CG	0.63	2.47	13	1
1:B:13:A:OP1	1:B:13:A:C8	0.62	2.52	14	4
1:B:9:C:H4'	2:A:129:VAL:HG13	0.62	1.71	11	1
1:B:5:G:O5'	1:B:5:G:H8	0.62	1.77	9	11
2:A:120:PHE:CD1	2:A:120:PHE:N	0.62	2.67	14	3
2:A:42:ASP:O	2:A:43:LEU:HD23	0.62	1.95	11	1
2:A:98:ALA:HB2	2:A:140:TYR:OH	0.62	1.95	9	1
2:A:128:LEU:H	2:A:128:LEU:HD23	0.62	1.55	7	2
1:B:13:A:N6	2:A:94:LYS:CD	0.62	2.63	8	1
1:B:16:G:O2'	1:B:17:C:C6	0.62	2.50	12	3
2:A:17:PHE:CB	2:A:58:TYR:CD1	0.62	2.83	11	2
2:A:136:LYS:CG	2:A:138:ILE:HD12	0.62	2.24	3	1
2:A:46:VAL:HG11	2:A:62:GLU:HA	0.62	1.70	14	1
1:B:13:A:OP2	1:B:13:A:N9	0.62	2.33	2	1
1:B:9:C:N3	2:A:140:TYR:CZ	0.62	2.68	14	1
1:B:5:G:H2'	1:B:6:C:O4'	0.62	1.94	7	12
1:B:9:C:OP2	1:B:10:C:C5	0.62	2.53	7	5
2:A:45:VAL:HG21	2:A:48:VAL:CG1	0.62	2.24	4	2
1:B:8:U:O2'	1:B:9:C:O4'	0.62	2.18	14	1
1:B:10:C:OP1	1:B:10:C:H4'	0.61	1.95	6	2
2:A:102:LEU:HA	2:A:171:THR:HG23	0.61	1.70	13	2
2:A:103:LEU:HD12	2:A:140:TYR:CE2	0.61	2.29	5	1
1:B:12:G:N3	1:B:12:G:H2'	0.61	2.10	5	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:A:119:VAL:HG13	2:A:120:PHE:CD2	0.61	2.31	9	4
2:A:16:LEU:HD11	2:A:71:LEU:HD12	0.61	1.71	9	1
2:A:38:PHE:HB3	2:A:43:LEU:HD11	0.61	1.71	10	3
2:A:102:LEU:HD12	2:A:169:TYR:C	0.61	2.15	11	4
2:A:111:ILE:CD1	2:A:161:ILE:HG22	0.61	2.25	1	1
1:B:13:A:OP2	1:B:13:A:C8	0.61	2.53	7	2
1:B:5:G:HO2'	1:B:6:C:H5'	0.61	1.54	8	3
2:A:128:LEU:HD22	2:A:128:LEU:O	0.61	1.95	14	1
2:A:161:ILE:O	2:A:162:ASP:CB	0.61	2.48	10	5
1:B:8:U:O2'	1:B:9:C:OP2	0.61	2.18	8	1
1:B:12:G:O6	2:A:58:TYR:CD1	0.61	2.53	4	1
1:B:12:G:N2	1:B:12:G:OP1	0.61	2.34	4	2
2:A:161:ILE:HD12	2:A:166:VAL:CB	0.61	2.25	2	1
1:B:12:G:P	2:A:93:SER:O	0.61	2.58	13	1
1:B:9:C:O4'	2:A:129:VAL:HG21	0.61	1.96	3	2
1:B:8:U:C3'	1:B:9:C:C6	0.61	2.84	11	1
2:A:161:ILE:HD12	2:A:166:VAL:HB	0.61	1.71	2	2
1:B:1:G:N3	1:B:2:G:C8	0.61	2.69	14	5
1:B:13:A:C4'	1:B:14:G:O5'	0.61	2.49	2	5
2:A:21:LEU:HD22	2:A:34:ILE:CD1	0.61	2.24	3	1
1:B:12:G:C8	1:B:12:G:OP1	0.61	2.53	10	1
1:B:8:U:OP1	1:B:10:C:N4	0.61	2.34	13	1
1:B:9:C:N3	2:A:127:ARG:NE	0.61	2.49	13	1
2:A:55:LYS:O	2:A:56:PHE:CG	0.61	2.54	12	1
2:A:32:VAL:O	2:A:35:SER:N	0.60	2.34	11	13
1:B:11:C:C2	2:A:88:PRO:CG	0.60	2.84	8	1
2:A:106:ASN:C	2:A:107:LEU:HD22	0.60	2.16	11	2
2:A:101:THR:HG22	2:A:142:GLU:HA	0.60	1.72	4	1
1:B:12:G:C4'	1:B:13:A:OP1	0.60	2.49	6	3
2:A:109:PHE:N	2:A:109:PHE:CD1	0.60	2.69	4	4
1:B:11:C:O2	2:A:17:PHE:CE1	0.60	2.55	12	1
1:B:13:A:O2'	1:B:14:G:O5'	0.60	2.20	9	11
2:A:34:ILE:HD12	2:A:76:LEU:HD12	0.60	1.73	12	1
1:B:8:U:C4	2:A:138:ILE:CG2	0.60	2.84	1	4
1:B:12:G:OP2	1:B:12:G:H3'	0.60	1.95	7	2
1:B:6:C:O2'	1:B:7:C:C5'	0.60	2.46	7	4
1:B:8:U:H6	1:B:8:U:O5'	0.60	1.79	2	1
2:A:17:PHE:CZ	2:A:56:PHE:CE2	0.60	2.90	9	1
1:B:11:C:C1'	1:B:12:G:OP1	0.60	2.50	12	7
1:B:11:C:N3	2:A:17:PHE:CE2	0.60	2.70	10	4
2:A:98:ALA:CB	2:A:101:THR:HG21	0.60	2.26	7	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:A:34:ILE:HG23	2:A:76:LEU:CD1	0.60	2.27	12	1
2:A:67:LEU:C	2:A:67:LEU:HD23	0.60	2.18	10	2
1:B:11:C:O2'	1:B:12:G:N2	0.60	2.35	5	1
2:A:98:ALA:HB1	2:A:101:THR:HG21	0.60	1.74	3	2
1:B:11:C:O2	2:A:56:PHE:CG	0.60	2.55	3	1
2:A:170:TYR:CD2	2:A:170:TYR:O	0.60	2.55	5	3
2:A:35:SER:O	2:A:39:ALA:HB2	0.60	1.97	10	1
1:B:11:C:O2	1:B:12:G:N2	0.59	2.35	4	1
2:A:43:LEU:C	2:A:43:LEU:HD12	0.59	2.17	12	1
1:B:13:A:OP1	2:A:56:PHE:CE1	0.59	2.55	3	1
2:A:45:VAL:HG22	2:A:60:ASP:O	0.59	1.97	2	2
1:B:8:U:O4	2:A:103:LEU:HD22	0.59	1.97	9	2
2:A:48:VAL:HG12	2:A:59:VAL:HB	0.59	1.73	9	1
1:B:11:C:O2	2:A:17:PHE:CZ	0.59	2.55	12	1
1:B:12:G:OP1	2:A:56:PHE:CE1	0.59	2.55	12	1
1:B:13:A:OP1	1:B:13:A:N9	0.59	2.36	1	2
1:B:11:C:C4'	1:B:12:G:OP1	0.59	2.50	13	3
1:B:8:U:O2'	1:B:9:C:C5'	0.59	2.51	2	1
1:B:14:G:O2'	1:B:15:U:P	0.59	2.60	14	1
2:A:105:LYS:O	2:A:106:ASN:CB	0.59	2.50	13	5
2:A:30:LEU:HD22	2:A:78:VAL:HG11	0.59	1.74	12	2
1:B:12:G:N2	2:A:91:ARG:NH1	0.59	2.51	13	2
2:A:17:PHE:CB	2:A:58:TYR:CE1	0.59	2.85	2	1
1:B:8:U:O4	2:A:138:ILE:HG22	0.59	1.97	8	1
1:B:19:U:O2'	1:B:20:C:C5'	0.59	2.50	14	14
2:A:43:LEU:HD13	2:A:61:PHE:CD1	0.59	2.33	12	1
2:A:102:LEU:HD22	2:A:152:ASN:ND2	0.59	2.12	7	1
2:A:46:VAL:HG23	2:A:61:PHE:O	0.59	1.98	7	1
2:A:144:LYS:O	2:A:145:SER:CB	0.59	2.51	8	1
1:B:7:C:O5'	1:B:7:C:H6	0.59	1.80	13	1
1:B:6:C:O2'	1:B:7:C:O4'	0.59	2.21	5	2
2:A:99:ALA:O	2:A:172:GLY:CA	0.59	2.50	5	1
1:B:11:C:C4	2:A:17:PHE:CE2	0.59	2.90	13	1
2:A:123:ALA:CA	2:A:143:PHE:CD2	0.59	2.86	5	1
1:B:12:G:O2'	1:B:13:A:OP2	0.58	2.21	8	6
1:B:3:A:O2'	1:B:4:U:O4'	0.58	2.21	6	14
2:A:53:ASN:O	2:A:54:ARG:CB	0.58	2.51	12	6
1:B:7:C:C2'	1:B:8:U:OP1	0.58	2.51	13	6
1:B:12:G:C1'	1:B:13:A:OP1	0.58	2.52	6	3
1:B:8:U:O2'	1:B:9:C:OP1	0.58	2.20	14	4
2:A:111:ILE:CD1	2:A:161:ILE:CG2	0.58	2.81	1	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:A:48:VAL:O	2:A:48:VAL:HG23	0.58	1.98	6	2
2:A:41:ASN:HD21	2:A:73:LEU:HD11	0.58	1.58	13	1
1:B:16:G:O2'	1:B:17:C:O4'	0.58	2.22	12	3
2:A:23:PRO:HA	2:A:30:LEU:HD11	0.58	1.75	2	1
2:A:103:LEU:HD11	2:A:105:LYS:HZ3	0.58	1.58	8	1
2:A:123:ALA:CB	2:A:143:PHE:CZ	0.58	2.86	8	1
2:A:54:ARG:O	2:A:55:LYS:HB3	0.58	1.96	8	1
2:A:88:PRO:O	2:A:89:LYS:CB	0.58	2.52	10	2
2:A:11:THR:CG2	2:A:46:VAL:CG1	0.58	2.81	1	2
2:A:102:LEU:HD23	2:A:143:PHE:CZ	0.58	2.33	7	1
1:B:9:C:N4	2:A:140:TYR:OH	0.58	2.37	14	1
2:A:17:PHE:CE2	2:A:56:PHE:CE2	0.58	2.92	9	1
2:A:159:ALA:O	2:A:161:ILE:HD12	0.58	1.98	5	1
2:A:153:LEU:HD11	2:A:169:TYR:CA	0.58	2.27	6	4
1:B:10:C:N4	2:A:97:ARG:O	0.58	2.36	5	1
2:A:37:LEU:HD22	2:A:37:LEU:C	0.58	2.19	6	4
2:A:170:TYR:CG	2:A:170:TYR:O	0.58	2.57	5	3
2:A:119:VAL:CG1	2:A:120:PHE:CE2	0.58	2.86	5	3
2:A:48:VAL:HG12	2:A:59:VAL:CB	0.58	2.27	9	1
2:A:102:LEU:HD23	2:A:141:ILE:CG1	0.58	2.29	13	1
1:B:9:C:O2	2:A:140:TYR:CD1	0.58	2.57	11	1
1:B:10:C:O2'	1:B:11:C:OP1	0.58	2.21	11	1
1:B:13:A:O2'	1:B:14:G:OP1	0.58	2.22	11	2
1:B:12:G:O2'	1:B:13:A:O5'	0.58	2.21	9	5
2:A:78:VAL:O	2:A:79:PHE:CG	0.58	2.57	2	3
2:A:56:PHE:CE2	2:A:58:TYR:CD1	0.58	2.92	6	1
1:B:12:G:O4'	1:B:13:A:H5"	0.58	1.99	5	1
1:B:8:U:C6	2:A:103:LEU:CD2	0.57	2.84	10	2
1:B:8:U:C1'	1:B:9:C:OP1	0.57	2.52	14	3
2:A:102:LEU:N	2:A:102:LEU:HD13	0.57	2.14	1	1
1:B:11:C:O2'	1:B:12:G:O5'	0.57	2.21	1	2
2:A:168:LEU:O	2:A:169:TYR:CG	0.57	2.57	7	2
1:B:12:G:C4'	1:B:13:A:O5'	0.57	2.52	10	3
2:A:25:LYS:O	2:A:26:SER:CB	0.57	2.52	6	1
1:B:12:G:N7	2:A:50:THR:O	0.57	2.37	5	1
2:A:116:LEU:O	2:A:120:PHE:CE1	0.57	2.57	4	5
1:B:7:C:O2'	1:B:8:U:OP1	0.57	2.21	5	5
2:A:119:VAL:HG13	2:A:120:PHE:CG	0.57	2.34	4	5
2:A:119:VAL:CG1	2:A:120:PHE:CD2	0.57	2.88	9	5
1:B:12:G:C1'	1:B:13:A:O5'	0.57	2.51	3	1
1:B:13:A:HO2'	1:B:14:G:P	0.57	2.22	4	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:A:92:ASP:O	2:A:96:VAL:HG21	0.57	1.99	2	1
2:A:126:ILE:O	2:A:127:ARG:CG	0.57	2.53	9	1
1:B:8:U:C6	1:B:8:U:O5'	0.57	2.51	3	2
1:B:13:A:C8	2:A:52:THR:OG1	0.57	2.55	7	2
2:A:120:PHE:CZ	2:A:157:GLN:OE1	0.57	2.57	14	1
2:A:120:PHE:CE1	2:A:156:LYS:CB	0.57	2.88	8	1
1:B:8:U:O3'	1:B:9:C:O4'	0.57	2.21	11	1
1:B:13:A:N3	2:A:94:LYS:O	0.57	2.37	11	2
1:B:9:C:H3'	1:B:10:C:O4'	0.57	1.99	7	2
1:B:17:C:O2'	1:B:18:A:C5'	0.57	2.46	10	14
1:B:12:G:C5	2:A:49:ARG:NH2	0.57	2.72	4	4
1:B:13:A:O2'	1:B:14:G:O4'	0.57	2.22	1	5
2:A:17:PHE:CD2	2:A:86:GLU:O	0.57	2.57	11	1
2:A:22:ASN:ND2	2:A:30:LEU:CD1	0.57	2.67	14	1
2:A:109:PHE:O	2:A:109:PHE:CG	0.57	2.57	11	1
1:B:13:A:C2'	1:B:14:G:OP2	0.57	2.53	5	2
2:A:61:PHE:HB2	2:A:67:LEU:HD12	0.57	1.77	7	1
2:A:41:ASN:OD1	2:A:73:LEU:HD23	0.57	2.00	14	1
1:B:10:C:C2'	1:B:11:C:OP1	0.57	2.53	9	1
2:A:126:ILE:CG2	2:A:127:ARG:N	0.57	2.68	9	1
1:B:12:G:N7	2:A:49:ARG:NH2	0.57	2.53	5	1
1:B:12:G:C1'	1:B:13:A:OP2	0.57	2.53	5	1
2:A:52:THR:O	2:A:53:ASN:CB	0.57	2.53	13	4
1:B:8:U:O4	2:A:138:ILE:CG2	0.57	2.53	8	3
1:B:15:U:C4'	1:B:16:G:OP1	0.57	2.53	4	1
2:A:22:ASN:CG	2:A:30:LEU:HD11	0.57	2.19	14	1
2:A:111:ILE:CG2	2:A:112:THR:N	0.57	2.68	1	11
2:A:102:LEU:HD11	2:A:143:PHE:CB	0.57	2.30	1	2
2:A:136:LYS:CE	2:A:138:ILE:CD1	0.56	2.83	10	4
2:A:76:LEU:O	2:A:77:LYS:CG	0.56	2.53	9	1
1:B:9:C:O2	2:A:127:ARG:CG	0.56	2.53	13	1
1:B:1:G:N3	1:B:2:G:N7	0.56	2.53	14	5
2:A:127:ARG:O	2:A:128:LEU:HD23	0.56	2.00	12	2
2:A:101:THR:HG21	2:A:140:TYR:CE2	0.56	2.34	9	2
1:B:8:U:O2	2:A:136:LYS:CE	0.56	2.53	9	5
2:A:111:ILE:HD11	2:A:161:ILE:HG23	0.56	1.77	12	2
2:A:151:LYS:O	2:A:155:GLU:CB	0.56	2.53	11	1
2:A:48:VAL:HG13	2:A:59:VAL:HG22	0.56	1.77	3	1
2:A:17:PHE:C	2:A:17:PHE:CD1	0.56	2.78	1	4
2:A:17:PHE:HB2	2:A:58:TYR:CE1	0.56	2.35	2	1
1:B:12:G:O4'	1:B:13:A:C5'	0.56	2.53	5	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:A:50:THR:CG2	2:A:51:GLY:N	0.56	2.69	8	1
2:A:107:LEU:N	2:A:107:LEU:CD2	0.56	2.68	9	3
2:A:111:ILE:HD12	2:A:161:ILE:HG13	0.56	1.78	3	1
2:A:78:VAL:O	2:A:79:PHE:CD1	0.56	2.57	5	4
1:B:13:A:P	2:A:94:LYS:HB2	0.56	2.40	1	2
1:B:1:G:C2	1:B:2:G:C5	0.56	2.94	14	2
2:A:56:PHE:CD1	2:A:57:GLY:N	0.56	2.74	1	2
2:A:56:PHE:CG	2:A:57:GLY:N	0.56	2.73	7	3
2:A:21:LEU:O	2:A:30:LEU:HD22	0.56	2.00	4	1
1:B:12:G:OP2	1:B:12:G:C3'	0.56	2.53	7	1
1:B:14:G:O2'	1:B:15:U:OP1	0.56	2.22	14	1
2:A:18:ILE:N	2:A:18:ILE:HD12	0.56	2.16	9	2
2:A:31:LYS:CG	2:A:32:VAL:N	0.56	2.69	7	4
1:B:9:C:C4	2:A:140:TYR:CD2	0.56	2.93	5	3
2:A:101:THR:HG21	2:A:140:TYR:HE2	0.56	1.61	11	1
1:B:9:C:O2	2:A:127:ARG:CB	0.56	2.54	11	1
2:A:161:ILE:CG2	2:A:162:ASP:N	0.56	2.68	3	1
1:B:11:C:C6	1:B:11:C:OP2	0.56	2.53	10	1
2:A:51:GLY:O	2:A:55:LYS:CB	0.56	2.54	3	9
2:A:27:VAL:HG21	2:A:54:ARG:HG3	0.56	1.77	2	1
2:A:128:LEU:H	2:A:128:LEU:HD13	0.56	1.60	14	1
2:A:78:VAL:HG13	2:A:83:ILE:HD13	0.56	1.77	9	1
2:A:116:LEU:HD11	2:A:139:ALA:CB	0.56	2.24	13	3
2:A:103:LEU:HD22	2:A:140:TYR:CE2	0.56	2.34	10	1
2:A:22:ASN:ND2	2:A:24:ASN:O	0.56	2.39	10	1
2:A:158:GLY:H	2:A:168:LEU:HD21	0.56	1.61	13	1
1:B:8:U:O2	1:B:9:C:C6	0.56	2.59	8	1
1:B:6:C:O2'	1:B:7:C:O5'	0.56	2.22	4	5
2:A:17:PHE:HB3	2:A:58:TYR:CD1	0.56	2.36	11	1
2:A:104:ALA:HB3	2:A:139:ALA:O	0.56	2.00	3	1
1:B:12:G:C6	2:A:92:ASP:OD1	0.56	2.59	7	1
2:A:150:GLU:OE2	2:A:153:LEU:HD23	0.56	2.00	10	1
2:A:103:LEU:HD11	2:A:138:ILE:HG21	0.56	1.76	5	1
1:B:11:C:C2	2:A:17:PHE:CZ	0.55	2.94	12	2
2:A:107:LEU:CD1	2:A:139:ALA:HB2	0.55	2.31	5	2
2:A:168:LEU:HD23	2:A:168:LEU:N	0.55	2.15	13	1
2:A:14:PHE:CD2	2:A:63:SER:N	0.55	2.74	12	1
1:B:11:C:C4'	1:B:12:G:OP2	0.55	2.53	8	2
2:A:136:LYS:CG	2:A:138:ILE:CD1	0.55	2.84	1	1
1:B:13:A:C5	2:A:94:LYS:HG2	0.55	2.37	1	2
2:A:92:ASP:O	2:A:93:SER:CB	0.55	2.54	6	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:A:102:LEU:CG	2:A:169:TYR:O	0.55	2.55	10	5
2:A:153:LEU:HD11	2:A:169:TYR:HA	0.55	1.78	6	2
1:B:8:U:C6	1:B:8:U:OP1	0.55	2.60	6	1
2:A:43:LEU:HD21	2:A:66:ASP:O	0.55	2.01	5	1
2:A:37:LEU:HD12	2:A:38:PHE:CD1	0.55	2.37	13	3
2:A:34:ILE:N	2:A:34:ILE:CD1	0.55	2.70	4	1
2:A:122:ASP:O	2:A:143:PHE:CD2	0.55	2.60	7	1
1:B:12:G:OP1	2:A:93:SER:N	0.55	2.39	2	1
2:A:11:THR:O	2:A:12:THR:CG2	0.55	2.55	14	1
2:A:98:ALA:CB	2:A:101:THR:HG23	0.55	2.30	10	1
2:A:107:LEU:HD11	2:A:116:LEU:HD11	0.55	1.78	11	2
1:B:13:A:C6	2:A:94:LYS:HG3	0.55	2.37	7	3
2:A:120:PHE:O	2:A:123:ALA:HB3	0.55	2.02	10	1
2:A:171:THR:O	2:A:171:THR:CG2	0.55	2.54	5	1
1:B:16:G:O2'	1:B:17:C:O5'	0.55	2.25	13	13
2:A:107:LEU:O	2:A:108:SER:CB	0.55	2.54	14	2
1:B:8:U:C4	2:A:138:ILE:HD13	0.55	2.37	13	2
2:A:52:THR:O	2:A:54:ARG:N	0.55	2.40	1	7
1:B:15:U:H1'	1:B:16:G:OP1	0.55	2.01	4	1
2:A:76:LEU:CD2	2:A:83:ILE:CD1	0.55	2.85	9	1
2:A:161:ILE:HG21	2:A:166:VAL:HB	0.55	1.79	10	1
2:A:108:SER:O	2:A:109:PHE:CG	0.55	2.60	13	1
2:A:165:SER:O	2:A:166:VAL:O	0.55	2.24	12	9
2:A:38:PHE:CD1	2:A:43:LEU:HD21	0.55	2.36	12	1
2:A:41:ASN:O	2:A:42:ASP:CB	0.55	2.54	5	7
2:A:157:GLN:HE22	2:A:168:LEU:HD11	0.55	1.60	11	1
1:B:15:U:C1'	1:B:16:G:OP1	0.55	2.55	4	1
1:B:1:G:N2	1:B:2:G:C4	0.55	2.75	14	1
1:B:4:U:O2'	1:B:5:G:O5'	0.55	2.25	11	14
1:B:9:C:H42	2:A:127:ARG:NH2	0.55	2.00	12	2
1:B:11:C:C2	2:A:88:PRO:HB3	0.55	2.36	8	1
2:A:103:LEU:HD21	2:A:105:LYS:HZ1	0.55	1.62	8	1
1:B:10:C:C4'	1:B:10:C:OP1	0.55	2.55	8	3
2:A:37:LEU:CD1	2:A:38:PHE:N	0.55	2.67	9	9
2:A:147:ALA:O	2:A:151:LYS:CB	0.55	2.55	11	2
2:A:101:THR:HG22	2:A:142:GLU:CA	0.55	2.31	4	1
1:B:8:U:O2'	1:B:9:C:O5'	0.54	2.25	1	2
2:A:91:ARG:O	2:A:92:ASP:CB	0.54	2.53	11	4
2:A:108:SER:C	2:A:109:PHE:CG	0.54	2.81	10	4
2:A:101:THR:OG1	2:A:140:TYR:CE1	0.54	2.60	10	3
2:A:120:PHE:CD2	2:A:156:LYS:HE2	0.54	2.37	10	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:A:51:GLY:O	2:A:52:THR:CB	0.54	2.55	5	2
2:A:56:PHE:C	2:A:56:PHE:CD1	0.54	2.81	6	1
2:A:17:PHE:CD1	2:A:17:PHE:C	0.54	2.81	11	4
2:A:44:ALA:O	2:A:45:VAL:CG1	0.54	2.55	3	2
1:B:11:C:C5	2:A:88:PRO:HG2	0.54	2.36	2	1
1:B:8:U:C5	2:A:138:ILE:HD13	0.54	2.37	13	1
1:B:12:G:OP1	2:A:94:LYS:CD	0.54	2.55	6	1
2:A:42:ASP:O	2:A:43:LEU:CG	0.54	2.56	11	1
2:A:101:THR:CG2	2:A:171:THR:OG1	0.54	2.56	1	5
2:A:156:LYS:O	2:A:158:GLY:N	0.54	2.41	14	7
2:A:17:PHE:CD2	2:A:56:PHE:CD1	0.54	2.96	1	1
2:A:152:ASN:ND2	2:A:153:LEU:N	0.54	2.56	7	1
1:B:8:U:C5	2:A:103:LEU:HG	0.54	2.37	10	1
2:A:43:LEU:HD22	2:A:61:PHE:HE1	0.54	1.62	10	1
1:B:13:A:OP2	2:A:94:LYS:CB	0.54	2.56	12	2
2:A:153:LEU:HD11	2:A:168:LEU:O	0.54	2.02	1	1
2:A:21:LEU:HA	2:A:83:ILE:HG22	0.54	1.78	10	1
2:A:105:LYS:HA	2:A:138:ILE:HG22	0.54	1.78	12	1
2:A:55:LYS:O	2:A:56:PHE:CD1	0.54	2.61	12	1
2:A:122:ASP:C	2:A:143:PHE:CE2	0.54	2.81	3	2
2:A:17:PHE:CD1	2:A:86:GLU:HB3	0.54	2.37	13	1
2:A:160:GLU:CG	2:A:161:ILE:N	0.54	2.70	6	1
2:A:123:ALA:HB1	2:A:141:ILE:HG22	0.54	1.80	5	1
2:A:71:LEU:HD23	2:A:71:LEU:C	0.54	2.23	12	1
2:A:35:SER:OG	2:A:36:GLU:N	0.54	2.41	9	4
2:A:54:ARG:O	2:A:56:PHE:N	0.54	2.41	9	4
2:A:123:ALA:HA	2:A:143:PHE:CD2	0.54	2.37	5	4
2:A:115:GLU:HB3	2:A:161:ILE:HG21	0.54	1.78	5	1
2:A:113:GLU:O	2:A:117:LYS:CG	0.54	2.56	14	3
1:B:13:A:C4	2:A:94:LYS:HB3	0.54	2.38	5	2
2:A:101:THR:HG22	2:A:142:GLU:CG	0.54	2.32	4	1
1:B:9:C:C2	2:A:140:TYR:HB3	0.54	2.37	1	4
2:A:114:ASP:O	2:A:118:GLU:CB	0.54	2.56	5	9
1:B:8:U:H3	2:A:103:LEU:HD11	0.54	1.62	7	1
1:B:13:A:P	1:B:13:A:O4'	0.54	2.66	14	1
1:B:8:U:C4	2:A:138:ILE:HB	0.54	2.37	8	1
2:A:90:GLY:O	2:A:91:ARG:CB	0.54	2.56	10	3
1:B:18:A:O2'	1:B:19:U:O4'	0.54	2.26	7	7
2:A:135:SER:O	2:A:136:LYS:CB	0.54	2.56	7	5
2:A:94:LYS:O	2:A:96:VAL:N	0.54	2.41	10	5
2:A:12:THR:CG2	2:A:61:PHE:O	0.54	2.56	10	11

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:A:102:LEU:CD1	2:A:169:TYR:O	0.54	2.56	8	5
2:A:56:PHE:CD1	2:A:56:PHE:C	0.54	2.81	7	2
2:A:12:THR:HG23	2:A:61:PHE:O	0.54	2.03	11	2
2:A:140:TYR:OH	2:A:171:THR:CB	0.54	2.56	6	3
2:A:20:ASN:OD1	2:A:21:LEU:N	0.54	2.41	9	1
1:B:11:C:C4	2:A:88:PRO:HB3	0.54	2.38	10	1
2:A:116:LEU:O	2:A:120:PHE:CD1	0.53	2.60	4	5
1:B:11:C:O2	2:A:88:PRO:CG	0.53	2.55	8	1
2:A:162:ASP:O	2:A:164:ARG:N	0.53	2.41	7	2
2:A:97:ARG:O	2:A:98:ALA:CB	0.53	2.56	4	6
2:A:28:ALA:O	2:A:31:LYS:CG	0.53	2.56	2	2
2:A:123:ALA:HA	2:A:143:PHE:CE2	0.53	2.38	9	1
2:A:21:LEU:HB3	2:A:30:LEU:HD13	0.53	1.79	12	1
2:A:156:LYS:O	2:A:159:ALA:N	0.53	2.41	8	1
2:A:55:LYS:HD3	2:A:55:LYS:N	0.53	2.18	8	1
1:B:12:G:C6	2:A:49:ARG:NH2	0.53	2.77	9	2
2:A:109:PHE:O	2:A:110:ASN:CB	0.53	2.57	11	1
1:B:1:G:HO2'	1:B:2:G:H5'	0.53	1.63	3	2
2:A:21:LEU:O	2:A:30:LEU:CD1	0.53	2.57	5	2
1:B:13:A:C5	2:A:94:LYS:HG3	0.53	2.37	6	1
2:A:53:ASN:O	2:A:54:ARG:CG	0.53	2.57	5	2
2:A:19:GLY:O	2:A:20:ASN:CB	0.53	2.56	10	5
2:A:62:GLU:O	2:A:63:SER:CB	0.53	2.57	7	5
2:A:112:THR:HA	2:A:128:LEU:HD13	0.53	1.78	2	1
2:A:141:ILE:HG22	2:A:142:GLU:N	0.53	2.17	12	1
1:B:8:U:C4'	1:B:9:C:OP2	0.53	2.56	11	1
2:A:123:ALA:HB1	2:A:142:GLU:O	0.53	2.03	7	2
1:B:10:C:H4'	1:B:11:C:OP1	0.53	2.02	11	1
2:A:34:ILE:CD1	2:A:76:LEU:O	0.53	2.57	7	1
1:B:11:C:C2	2:A:17:PHE:CD2	0.53	2.97	7	1
2:A:160:GLU:O	2:A:162:ASP:N	0.53	2.42	6	2
2:A:34:ILE:HA	2:A:76:LEU:HD11	0.53	1.80	13	1
2:A:111:ILE:HG22	2:A:112:THR:N	0.53	2.18	13	11
1:B:13:A:N7	2:A:52:THR:HA	0.53	2.18	8	1
2:A:143:PHE:CD2	2:A:148:ASP:HB2	0.53	2.38	3	1
2:A:113:GLU:OE2	2:A:128:LEU:HD11	0.53	2.03	10	1
2:A:103:LEU:HD12	2:A:104:ALA:H	0.53	1.63	12	1
2:A:105:LYS:O	2:A:166:VAL:CG2	0.53	2.56	10	5
1:B:13:A:H62	2:A:94:LYS:CE	0.53	2.16	8	1
2:A:103:LEU:HD11	2:A:138:ILE:CG2	0.53	2.34	10	3
2:A:143:PHE:CE2	2:A:148:ASP:HB3	0.53	2.39	3	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:A:45:VAL:CG1	2:A:45:VAL:O	0.53	2.57	5	1
2:A:129:VAL:O	2:A:130:SER:CB	0.53	2.57	12	1
2:A:111:ILE:CG1	2:A:161:ILE:HG23	0.53	2.32	12	2
2:A:101:THR:CG2	2:A:171:THR:O	0.53	2.57	8	1
2:A:63:SER:O	2:A:65:GLU:N	0.53	2.42	8	6
1:B:11:C:N3	2:A:88:PRO:HG3	0.53	2.19	8	1
2:A:94:LYS:O	2:A:95:LYS:CB	0.53	2.57	6	6
1:B:10:C:H4'	1:B:10:C:OP1	0.53	2.03	3	2
2:A:37:LEU:HD11	2:A:41:ASN:ND2	0.53	2.19	2	1
2:A:15:ASN:CB	2:A:59:VAL:O	0.53	2.57	9	2
1:B:13:A:O2'	2:A:95:LYS:HD2	0.53	2.03	14	1
2:A:41:ASN:OD1	2:A:73:LEU:CD2	0.53	2.57	14	1
2:A:102:LEU:HD23	2:A:141:ILE:HD12	0.53	1.79	5	1
2:A:158:GLY:CA	2:A:166:VAL:O	0.53	2.56	8	2
2:A:98:ALA:CB	2:A:101:THR:OG1	0.53	2.57	4	2
2:A:157:GLN:HA	2:A:168:LEU:HD21	0.53	1.80	7	4
2:A:81:ASN:O	2:A:82:GLU:CB	0.53	2.57	10	1
2:A:94:LYS:HG2	2:A:95:LYS:N	0.53	2.19	10	3
2:A:100:ARG:O	2:A:100:ARG:CG	0.53	2.57	8	1
2:A:101:THR:CB	2:A:171:THR:HG23	0.53	2.34	3	1
2:A:140:TYR:CE2	2:A:171:THR:HG21	0.53	2.39	4	1
1:B:9:C:N4	2:A:98:ALA:HB2	0.53	2.19	4	1
2:A:98:ALA:HB1	2:A:101:THR:OG1	0.53	2.03	5	3
2:A:21:LEU:O	2:A:22:ASN:CB	0.53	2.57	4	4
2:A:111:ILE:O	2:A:128:LEU:CD1	0.53	2.57	1	1
2:A:17:PHE:CD1	2:A:86:GLU:HB2	0.53	2.39	7	2
2:A:128:LEU:CD2	2:A:128:LEU:O	0.53	2.57	14	1
1:B:7:C:HO2'	2:A:97:ARG:HG2	0.53	1.64	5	1
2:A:75:GLY:O	2:A:77:LYS:N	0.53	2.42	12	2
2:A:103:LEU:C	2:A:103:LEU:HD12	0.53	2.24	8	2
1:B:9:C:O4'	2:A:129:VAL:CG2	0.53	2.56	3	1
2:A:97:ARG:O	2:A:172:GLY:CA	0.53	2.57	1	1
2:A:89:LYS:O	2:A:90:GLY:C	0.53	2.48	10	3
2:A:103:LEU:CD1	2:A:104:ALA:N	0.53	2.72	10	1
2:A:103:LEU:HD21	2:A:138:ILE:CG2	0.53	2.34	5	1
2:A:153:LEU:O	2:A:157:GLN:CG	0.52	2.57	8	3
2:A:55:LYS:CD	2:A:55:LYS:N	0.52	2.72	8	1
1:B:18:A:O5'	1:B:18:A:H8	0.52	1.88	13	8
2:A:118:GLU:O	2:A:120:PHE:N	0.52	2.43	14	2
2:A:70:ALA:O	2:A:73:LEU:N	0.52	2.42	4	4
2:A:119:VAL:CG1	2:A:120:PHE:N	0.52	2.72	2	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:A:46:VAL:CG2	2:A:61:PHE:O	0.52	2.57	7	1
2:A:61:PHE:CB	2:A:67:LEU:HD12	0.52	2.34	7	1
2:A:149:ALA:O	2:A:153:LEU:CB	0.52	2.57	2	4
1:B:9:C:C6	1:B:10:C:C5	0.52	2.97	13	2
1:B:9:C:N4	2:A:140:TYR:CE2	0.52	2.77	13	2
2:A:140:TYR:OH	2:A:171:THR:CG2	0.52	2.57	5	3
2:A:96:VAL:O	2:A:98:ALA:N	0.52	2.42	3	5
1:B:9:C:C4	1:B:10:C:N3	0.52	2.77	8	1
1:B:9:C:C4	2:A:140:TYR:CD1	0.52	2.98	2	4
2:A:13:PRO:O	2:A:15:ASN:N	0.52	2.42	10	8
2:A:159:ALA:O	2:A:161:ILE:N	0.52	2.43	4	3
1:B:12:G:O4'	1:B:13:A:OP1	0.52	2.26	7	3
2:A:43:LEU:CD2	2:A:66:ASP:O	0.52	2.57	5	1
2:A:121:GLU:O	2:A:122:ASP:CB	0.52	2.58	11	1
2:A:103:LEU:CD1	2:A:139:ALA:O	0.52	2.56	1	2
2:A:131:GLN:O	2:A:132:ASP:CB	0.52	2.58	10	3
2:A:103:LEU:HD12	2:A:140:TYR:CE1	0.52	2.39	9	1
2:A:35:SER:O	2:A:39:ALA:CB	0.52	2.57	10	1
2:A:108:SER:O	2:A:109:PHE:CB	0.52	2.57	13	2
1:B:8:U:N3	2:A:138:ILE:HD13	0.52	2.19	3	2
1:B:13:A:C4	2:A:94:LYS:O	0.52	2.63	9	1
2:A:120:PHE:O	2:A:123:ALA:CB	0.52	2.58	10	1
2:A:22:ASN:O	2:A:24:ASN:N	0.52	2.42	13	2
2:A:71:LEU:HD21	2:A:85:LEU:HD22	0.52	1.80	11	1
2:A:108:SER:O	2:A:110:ASN:N	0.52	2.43	11	5
2:A:102:LEU:CD2	2:A:102:LEU:N	0.52	2.72	1	2
1:B:9:C:N4	1:B:10:C:N4	0.52	2.58	1	2
2:A:11:THR:HG21	2:A:46:VAL:HG13	0.52	1.81	1	1
2:A:92:ASP:O	2:A:96:VAL:CG2	0.52	2.58	2	1
2:A:152:ASN:O	2:A:155:GLU:N	0.52	2.43	2	1
2:A:168:LEU:N	2:A:168:LEU:CD1	0.52	2.68	2	1
2:A:20:ASN:OD1	2:A:83:ILE:CG2	0.52	2.57	9	1
1:B:9:C:C5	1:B:10:C:C6	0.52	2.98	13	1
2:A:14:PHE:CE1	2:A:64:ALA:HB2	0.52	2.39	12	2
2:A:120:PHE:CE1	2:A:156:LYS:HB3	0.52	2.40	8	1
2:A:54:ARG:O	2:A:55:LYS:CB	0.52	2.57	8	1
2:A:98:ALA:O	2:A:100:ARG:N	0.52	2.42	9	4
2:A:101:THR:HB	2:A:142:GLU:CB	0.52	2.35	9	2
2:A:18:ILE:HG22	2:A:21:LEU:HD21	0.52	1.80	3	2
1:B:8:U:C1'	1:B:9:C:P	0.52	2.98	3	3
2:A:63:SER:OG	2:A:64:ALA:N	0.52	2.43	5	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:A:124:LEU:HD12	2:A:124:LEU:C	0.52	2.24	7	1
2:A:95:LYS:O	2:A:97:ARG:N	0.52	2.42	10	2
2:A:43:LEU:HD12	2:A:43:LEU:C	0.52	2.24	10	1
1:B:12:G:C3'	2:A:93:SER:O	0.52	2.57	5	1
1:B:20:C:C2'	1:B:21:C:O5'	0.52	2.58	6	13
2:A:112:THR:O	2:A:114:ASP:N	0.52	2.43	3	5
1:B:13:A:N6	2:A:94:LYS:HD2	0.52	2.20	8	1
2:A:42:ASP:OD1	2:A:43:LEU:N	0.52	2.43	11	1
1:B:12:G:N2	2:A:89:LYS:HB3	0.52	2.20	1	1
2:A:101:THR:OG1	2:A:102:LEU:N	0.52	2.43	2	1
2:A:123:ALA:N	2:A:143:PHE:CE2	0.52	2.77	9	1
1:B:13:A:O2'	1:B:14:G:H5"	0.52	2.04	5	1
2:A:148:ASP:O	2:A:152:ASN:ND2	0.52	2.43	6	2
2:A:119:VAL:O	2:A:156:LYS:CG	0.52	2.57	1	2
2:A:136:LYS:CD	2:A:138:ILE:CD1	0.52	2.88	10	1
2:A:116:LEU:HD23	2:A:126:ILE:CG2	0.52	2.35	13	1
1:B:11:C:C1'	1:B:12:G:O5'	0.52	2.54	13	1
2:A:23:PRO:O	2:A:24:ASN:CB	0.52	2.57	8	1
2:A:58:TYR:O	2:A:59:VAL:CG1	0.52	2.58	7	1
2:A:124:LEU:CD1	2:A:144:LYS:HB2	0.52	2.35	8	2
2:A:37:LEU:HD13	2:A:38:PHE:CA	0.52	2.34	6	7
2:A:119:VAL:HG22	2:A:156:LYS:HB3	0.52	1.82	4	1
2:A:136:LYS:HG2	2:A:138:ILE:HD11	0.52	1.81	6	2
2:A:93:SER:O	2:A:96:VAL:HG22	0.52	2.04	2	1
2:A:153:LEU:O	2:A:168:LEU:CD2	0.52	2.58	14	1
2:A:128:LEU:HD13	2:A:128:LEU:N	0.52	2.20	14	1
1:B:9:C:C6	1:B:10:C:C6	0.52	2.97	13	1
2:A:77:LYS:O	2:A:79:PHE:N	0.52	2.43	5	1
1:B:11:C:OP2	2:A:93:SER:CB	0.51	2.58	12	1
2:A:143:PHE:O	2:A:145:SER:N	0.51	2.43	8	2
2:A:103:LEU:HD11	2:A:138:ILE:HG22	0.51	1.82	10	2
2:A:131:GLN:O	2:A:133:GLY:N	0.51	2.43	6	2
2:A:16:LEU:HD11	2:A:85:LEU:CB	0.51	2.34	1	1
2:A:123:ALA:HA	2:A:143:PHE:CE1	0.51	2.40	2	1
2:A:11:THR:O	2:A:12:THR:CB	0.51	2.57	14	1
2:A:29:GLU:O	2:A:32:VAL:N	0.51	2.43	10	2
2:A:49:ARG:NH1	2:A:60:ASP:OD2	0.51	2.43	13	1
1:B:13:A:OP2	2:A:51:GLY:CA	0.51	2.58	6	1
2:A:49:ARG:NE	2:A:50:THR:O	0.51	2.42	5	1
2:A:54:ARG:O	2:A:55:LYS:C	0.51	2.49	7	4
1:B:13:A:OP1	1:B:13:A:H8	0.51	1.86	14	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:17:C:O5'	1:B:17:C:H6	0.51	1.88	13	2
2:A:168:LEU:O	2:A:169:TYR:CD1	0.51	2.64	3	2
2:A:17:PHE:HB3	2:A:58:TYR:CE1	0.51	2.41	8	1
1:B:11:C:N3	2:A:88:PRO:HB3	0.51	2.20	8	1
2:A:168:LEU:N	2:A:168:LEU:CD2	0.51	2.69	11	1
2:A:111:ILE:O	2:A:112:THR:HG23	0.51	2.05	11	1
2:A:69:LYS:O	2:A:72:GLU:N	0.51	2.43	3	1
2:A:165:SER:OG	2:A:165:SER:O	0.51	2.29	10	4
2:A:122:ASP:HB3	2:A:143:PHE:CE2	0.51	2.40	1	1
2:A:113:GLU:O	2:A:117:LYS:CB	0.51	2.58	14	1
2:A:153:LEU:CD1	2:A:168:LEU:O	0.51	2.57	10	1
1:B:8:U:C5	2:A:103:LEU:CG	0.51	2.93	10	1
2:A:160:GLU:O	2:A:161:ILE:CG2	0.51	2.57	10	1
2:A:102:LEU:CD2	2:A:141:ILE:CD1	0.51	2.88	13	2
2:A:154:GLU:O	2:A:157:GLN:CB	0.51	2.57	12	1
2:A:145:SER:O	2:A:148:ASP:N	0.51	2.42	8	1
2:A:156:LYS:O	2:A:157:GLN:C	0.51	2.49	14	10
2:A:49:ARG:NH1	2:A:60:ASP:OD1	0.51	2.43	8	1
2:A:126:ILE:CG1	2:A:141:ILE:HG23	0.51	2.36	11	1
1:B:11:C:O2	2:A:56:PHE:CD2	0.51	2.63	3	1
2:A:111:ILE:HD12	2:A:161:ILE:CG1	0.51	2.35	3	1
2:A:103:LEU:HB2	2:A:140:TYR:CZ	0.51	2.41	8	3
1:B:11:C:O2'	2:A:89:LYS:HE2	0.51	2.06	1	1
1:B:7:C:O3'	1:B:8:U:O4'	0.51	2.27	5	1
2:A:27:VAL:O	2:A:30:LEU:N	0.51	2.44	12	6
1:B:11:C:O2'	1:B:12:G:OP2	0.51	2.28	11	1
2:A:76:LEU:O	2:A:77:LYS:O	0.51	2.29	9	4
2:A:56:PHE:CZ	2:A:58:TYR:CD1	0.51	2.99	6	4
2:A:47:ASP:N	2:A:60:ASP:OD1	0.51	2.43	3	2
2:A:119:VAL:O	2:A:156:LYS:CD	0.51	2.59	4	2
2:A:102:LEU:HD12	2:A:149:ALA:HB1	0.51	1.83	1	2
1:B:13:A:C6	2:A:94:LYS:HG2	0.51	2.40	1	1
1:B:11:C:O2'	2:A:89:LYS:HG3	0.51	2.05	2	2
2:A:153:LEU:O	2:A:157:GLN:NE2	0.51	2.43	2	1
2:A:20:ASN:O	2:A:22:ASN:N	0.51	2.43	9	2
2:A:126:ILE:HG22	2:A:127:ARG:H	0.51	1.66	13	1
2:A:74:THR:HG23	2:A:75:GLY:N	0.51	2.21	6	1
2:A:119:VAL:CG2	2:A:158:GLY:O	0.51	2.59	11	1
2:A:43:LEU:CD1	2:A:61:PHE:CG	0.51	2.94	11	1
2:A:127:ARG:O	2:A:140:TYR:O	0.51	2.28	13	5
2:A:52:THR:O	2:A:53:ASN:C	0.51	2.49	4	7

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:A:98:ALA:HB3	2:A:101:THR:CG2	0.51	2.32	1	2
1:B:12:G:H1'	1:B:13:A:OP1	0.51	2.06	6	3
2:A:161:ILE:HD12	2:A:166:VAL:CG2	0.51	2.35	2	1
2:A:136:LYS:HE2	2:A:138:ILE:CD1	0.51	2.36	14	2
2:A:25:LYS:O	2:A:25:LYS:CE	0.51	2.59	9	1
2:A:89:LYS:O	2:A:91:ARG:NH1	0.51	2.44	13	1
1:B:9:C:C2'	1:B:10:C:O5'	0.51	2.58	13	1
1:B:11:C:O5'	2:A:93:SER:CB	0.51	2.58	12	1
1:B:11:C:C6	1:B:11:C:OP1	0.51	2.64	8	1
2:A:102:LEU:CD1	2:A:153:LEU:HA	0.51	2.36	11	1
2:A:17:PHE:CE2	2:A:86:GLU:HB2	0.51	2.40	11	1
2:A:17:PHE:CE1	2:A:86:GLU:OE1	0.51	2.64	4	1
2:A:21:LEU:CB	2:A:25:LYS:HB3	0.51	2.35	9	1
2:A:47:ASP:O	2:A:48:VAL:HG23	0.51	2.06	10	1
1:B:11:C:O2'	2:A:91:ARG:HG3	0.51	2.05	13	1
2:A:12:THR:OG1	2:A:13:PRO:CD	0.51	2.58	5	1
2:A:168:LEU:C	2:A:169:TYR:CD1	0.51	2.84	8	2
2:A:88:PRO:O	2:A:89:LYS:HB3	0.51	2.06	8	2
2:A:118:GLU:O	2:A:120:PHE:O	0.51	2.28	11	1
2:A:78:VAL:HG23	2:A:79:PHE:N	0.51	2.21	2	4
1:B:9:C:C2	2:A:140:TYR:CD2	0.51	2.99	9	1
2:A:91:ARG:NE	2:A:91:ARG:N	0.51	2.59	12	1
2:A:153:LEU:O	2:A:157:GLN:CB	0.51	2.58	8	2
1:B:13:A:C5	2:A:94:LYS:HB3	0.51	2.41	5	2
2:A:123:ALA:CB	2:A:143:PHE:CE1	0.51	2.93	4	1
1:B:11:C:C2	2:A:89:LYS:HB2	0.51	2.41	6	1
2:A:21:LEU:O	2:A:22:ASN:C	0.50	2.48	3	3
2:A:158:GLY:O	2:A:160:GLU:N	0.50	2.44	3	1
2:A:76:LEU:CD1	2:A:85:LEU:CD2	0.50	2.89	2	1
2:A:43:LEU:HD22	2:A:61:PHE:CE1	0.50	2.42	10	1
1:B:12:G:C8	2:A:51:GLY:HA2	0.50	2.41	5	1
1:B:12:G:O4'	1:B:13:A:O5'	0.50	2.29	5	1
1:B:8:U:HO2'	1:B:9:C:P	0.50	2.28	12	1
1:B:8:U:O2	1:B:9:C:O4'	0.50	2.28	8	1
2:A:41:ASN:CB	2:A:43:LEU:HD23	0.50	2.37	9	2
2:A:159:ALA:CB	2:A:166:VAL:CG1	0.50	2.89	11	1
2:A:85:LEU:O	2:A:86:GLU:CG	0.50	2.59	11	1
1:B:11:C:C2'	2:A:89:LYS:HE2	0.50	2.37	1	1
2:A:130:SER:OG	2:A:137:GLY:N	0.50	2.44	2	1
2:A:51:GLY:HA3	2:A:56:PHE:CE1	0.50	2.41	14	1
2:A:53:ASN:O	2:A:54:ARG:CD	0.50	2.59	5	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:A:15:ASN:N	2:A:15:ASN:OD1	0.50	2.43	5	1
2:A:52:THR:O	2:A:53:ASN:HB2	0.50	2.07	5	3
2:A:122:ASP:O	2:A:126:ILE:CD1	0.50	2.59	11	1
1:B:12:G:OP2	2:A:89:LYS:CB	0.50	2.60	11	1
2:A:102:LEU:HD12	2:A:149:ALA:CB	0.50	2.36	2	3
1:B:15:U:O4'	1:B:15:U:OP2	0.50	2.30	4	1
2:A:45:VAL:CG2	2:A:48:VAL:CG1	0.50	2.88	4	1
2:A:27:VAL:CG2	2:A:54:ARG:HG3	0.50	2.37	2	1
2:A:22:ASN:OD1	2:A:25:LYS:N	0.50	2.43	14	1
1:B:8:U:O4	2:A:105:LYS:HE3	0.50	2.06	9	2
2:A:21:LEU:CB	2:A:25:LYS:CB	0.50	2.89	9	1
2:A:34:ILE:CG2	2:A:38:PHE:CE2	0.50	2.95	13	2
2:A:41:ASN:CB	2:A:43:LEU:CD2	0.50	2.89	9	1
1:B:15:U:OP2	1:B:15:U:O4'	0.50	2.30	12	1
1:B:13:A:C4'	1:B:14:G:OP1	0.50	2.58	12	3
2:A:30:LEU:CD2	2:A:78:VAL:HG11	0.50	2.37	12	1
2:A:37:LEU:C	2:A:37:LEU:CD1	0.50	2.80	13	6
1:B:11:C:O3'	1:B:13:A:OP2	0.50	2.30	11	1
2:A:35:SER:O	2:A:38:PHE:N	0.50	2.44	3	5
2:A:17:PHE:CB	2:A:86:GLU:O	0.50	2.59	3	1
2:A:27:VAL:CG2	2:A:53:ASN:O	0.50	2.58	4	1
1:B:8:U:O4	2:A:138:ILE:HG21	0.50	2.06	7	1
2:A:76:LEU:CD1	2:A:85:LEU:CD1	0.50	2.89	14	1
2:A:52:THR:HG23	2:A:53:ASN:N	0.50	2.21	9	1
2:A:143:PHE:CD1	2:A:143:PHE:N	0.50	2.78	5	2
2:A:44:ALA:O	2:A:45:VAL:O	0.50	2.29	3	2
2:A:51:GLY:O	2:A:52:THR:O	0.50	2.30	1	4
1:B:13:A:OP1	1:B:13:A:O4'	0.50	2.29	1	1
1:B:8:U:O2'	2:A:129:VAL:HG11	0.50	2.07	9	1
1:B:12:G:O6	2:A:90:GLY:O	0.50	2.30	10	1
1:B:13:A:H3'	1:B:13:A:OP2	0.50	2.07	6	1
2:A:127:ARG:O	2:A:128:LEU:CD2	0.50	2.59	12	1
2:A:27:VAL:HG13	2:A:28:ALA:N	0.50	2.22	13	4
2:A:124:LEU:CD1	2:A:144:LYS:CB	0.50	2.90	8	1
2:A:43:LEU:HD12	2:A:44:ALA:N	0.50	2.21	8	2
2:A:46:VAL:CG2	2:A:47:ASP:N	0.50	2.75	11	1
2:A:31:LYS:HG3	2:A:32:VAL:N	0.50	2.22	7	1
2:A:27:VAL:HG13	2:A:28:ALA:H	0.50	1.66	9	8
2:A:74:THR:O	2:A:75:GLY:C	0.50	2.50	4	7
2:A:17:PHE:CG	2:A:18:ILE:N	0.50	2.80	10	2
1:B:7:C:C5'	1:B:8:U:OP2	0.50	2.53	6	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:A:37:LEU:CD1	2:A:37:LEU:C	0.50	2.80	12	7
2:A:121:GLU:O	2:A:123:ALA:N	0.50	2.45	5	3
1:B:13:A:OP1	2:A:94:LYS:CB	0.50	2.60	1	2
2:A:47:ASP:CB	2:A:60:ASP:HB2	0.50	2.37	14	4
2:A:101:THR:CG2	2:A:171:THR:HG23	0.50	2.19	1	1
2:A:51:GLY:HA3	2:A:56:PHE:CZ	0.50	2.42	2	1
2:A:47:ASP:O	2:A:59:VAL:CG2	0.50	2.57	6	2
1:B:13:A:C6	2:A:94:LYS:HD2	0.50	2.41	14	1
1:B:9:C:H2'	1:B:10:C:O5'	0.50	2.07	13	1
2:A:123:ALA:N	2:A:143:PHE:CD2	0.50	2.80	5	1
2:A:17:PHE:CZ	2:A:18:ILE:O	0.50	2.65	5	1
2:A:99:ALA:O	2:A:101:THR:HG22	0.49	2.07	12	1
2:A:140:TYR:C	2:A:140:TYR:CD1	0.49	2.85	11	1
1:B:13:A:C5	2:A:94:LYS:CG	0.49	2.95	7	2
1:B:11:C:O2'	2:A:89:LYS:HD2	0.49	2.07	2	1
2:A:98:ALA:C	2:A:101:THR:HG22	0.49	2.28	13	1
2:A:105:LYS:CB	2:A:167:SER:O	0.49	2.60	8	1
2:A:123:ALA:O	2:A:124:LEU:CB	0.49	2.60	8	1
1:B:13:A:C8	2:A:94:LYS:CG	0.49	2.94	11	1
2:A:27:VAL:CG2	2:A:54:ARG:CG	0.49	2.89	2	1
2:A:93:SER:O	2:A:96:VAL:CG2	0.49	2.60	2	1
1:B:12:G:O4'	1:B:12:G:OP1	0.49	2.30	10	1
2:A:76:LEU:O	2:A:77:LYS:CB	0.49	2.59	5	1
2:A:165:SER:O	2:A:166:VAL:C	0.49	2.50	13	6
1:B:11:C:C2	2:A:88:PRO:CB	0.49	2.96	8	1
2:A:46:VAL:HG23	2:A:47:ASP:N	0.49	2.21	11	1
2:A:101:THR:CB	2:A:140:TYR:OH	0.49	2.61	3	1
1:B:8:U:O4	2:A:105:LYS:CG	0.49	2.59	3	1
1:B:11:C:O2'	2:A:89:LYS:CG	0.49	2.60	1	2
2:A:119:VAL:CG1	2:A:120:PHE:CZ	0.49	2.96	5	1
1:B:13:A:OP2	2:A:94:LYS:HB3	0.49	2.07	12	1
2:A:122:ASP:O	2:A:123:ALA:C	0.49	2.50	8	5
2:A:153:LEU:HD12	2:A:153:LEU:C	0.49	2.28	11	1
2:A:101:THR:HG23	2:A:171:THR:CB	0.49	2.37	6	2
2:A:103:LEU:CD1	2:A:138:ILE:HG22	0.49	2.38	10	1
2:A:170:TYR:CD1	2:A:170:TYR:O	0.49	2.66	12	1
2:A:97:ARG:O	2:A:98:ALA:HB2	0.49	2.08	3	1
1:B:8:U:O4	2:A:105:LYS:CD	0.49	2.60	3	1
2:A:103:LEU:HB2	2:A:140:TYR:CE2	0.49	2.43	1	4
1:B:8:U:N3	2:A:103:LEU:CD1	0.49	2.72	1	2
2:A:102:LEU:CD1	2:A:153:LEU:HD12	0.49	2.37	14	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:A:107:LEU:CD2	2:A:137:GLY:HA3	0.49	2.37	9	1
2:A:98:ALA:HA	2:A:171:THR:CA	0.49	2.37	8	1
1:B:13:A:OP2	2:A:94:LYS:O	0.49	2.30	8	2
2:A:11:THR:OG1	2:A:46:VAL:HG11	0.49	2.07	9	1
2:A:48:VAL:CA	2:A:58:TYR:O	0.49	2.61	9	1
1:B:9:C:N3	2:A:127:ARG:CZ	0.49	2.75	13	1
2:A:135:SER:O	2:A:136:LYS:CG	0.49	2.60	12	1
2:A:51:GLY:O	2:A:55:LYS:HB2	0.49	2.06	1	5
2:A:47:ASP:CB	2:A:60:ASP:CG	0.49	2.81	8	1
1:B:12:G:N2	2:A:92:ASP:HB2	0.49	2.23	11	1
1:B:8:U:C2	2:A:138:ILE:HD13	0.49	2.42	3	1
2:A:45:VAL:HG23	2:A:59:VAL:CG2	0.49	2.37	4	1
2:A:61:PHE:CE1	2:A:70:ALA:HB2	0.49	2.42	4	1
2:A:89:LYS:O	2:A:90:GLY:O	0.49	2.30	10	2
1:B:13:A:N7	2:A:52:THR:HB	0.49	2.23	9	1
2:A:27:VAL:HG11	2:A:53:ASN:HA	0.49	1.83	5	1
2:A:38:PHE:CD2	2:A:45:VAL:HB	0.49	2.43	5	1
2:A:136:LYS:HE2	2:A:138:ILE:HD11	0.49	1.85	13	2
2:A:136:LYS:HG3	2:A:138:ILE:HD12	0.49	1.84	3	1
2:A:153:LEU:HD11	2:A:169:TYR:N	0.49	2.22	3	2
2:A:103:LEU:HD13	2:A:140:TYR:CE1	0.49	2.43	4	1
1:B:15:U:O2'	1:B:16:G:O5'	0.49	2.22	4	1
2:A:124:LEU:HD11	2:A:142:GLU:HG2	0.49	1.84	7	1
2:A:34:ILE:CG2	2:A:48:VAL:HG11	0.49	2.37	9	1
2:A:32:VAL:HG12	2:A:36:GLU:HG3	0.49	1.83	13	1
1:B:8:U:C5	1:B:8:U:OP1	0.49	2.66	6	1
2:A:33:ALA:HB1	2:A:78:VAL:O	0.49	2.07	6	1
2:A:29:GLU:O	2:A:30:LEU:C	0.49	2.51	10	8
2:A:14:PHE:HD1	2:A:67:LEU:HD13	0.49	1.68	7	2
1:B:11:C:C4	2:A:89:LYS:HE3	0.49	2.43	14	1
1:B:8:U:O4	2:A:105:LYS:HE2	0.49	2.06	9	1
2:A:76:LEU:HD21	2:A:83:ILE:CD1	0.49	2.37	9	1
2:A:17:PHE:CD1	2:A:88:PRO:HG3	0.49	2.43	8	1
1:B:13:A:C4	2:A:94:LYS:HG3	0.49	2.42	11	1
2:A:47:ASP:HB3	2:A:60:ASP:CB	0.49	2.37	11	1
2:A:101:THR:CG2	2:A:171:THR:CG2	0.49	2.89	1	1
1:B:9:C:C2	2:A:140:TYR:CB	0.49	2.96	6	3
2:A:168:LEU:HD12	2:A:168:LEU:N	0.49	2.23	7	1
2:A:98:ALA:O	2:A:172:GLY:CA	0.49	2.61	13	1
2:A:116:LEU:HG	2:A:128:LEU:HD21	0.48	1.85	12	1
2:A:76:LEU:CD2	2:A:76:LEU:N	0.48	2.73	12	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:A:168:LEU:O	2:A:169:TYR:CD2	0.48	2.66	7	2
2:A:58:TYR:CZ	2:A:89:LYS:HE3	0.48	2.43	2	1
2:A:77:LYS:CG	2:A:81:ASN:O	0.48	2.61	14	1
2:A:120:PHE:CD2	2:A:156:LYS:CE	0.48	2.96	10	1
2:A:92:ASP:OD1	2:A:92:ASP:N	0.48	2.46	6	2
2:A:103:LEU:CG	2:A:138:ILE:CG2	0.48	2.91	5	1
1:B:8:U:OP1	2:A:97:ARG:CD	0.48	2.61	5	2
2:A:56:PHE:CZ	2:A:58:TYR:HB2	0.48	2.42	8	2
1:B:9:C:O2	2:A:127:ARG:HB2	0.48	2.08	11	1
2:A:136:LYS:HG2	2:A:138:ILE:CD1	0.48	2.38	1	3
2:A:25:LYS:CE	2:A:25:LYS:C	0.48	2.81	9	1
2:A:67:LEU:HD23	2:A:68:GLU:N	0.48	2.22	10	1
2:A:111:ILE:HD12	2:A:161:ILE:HG23	0.48	1.83	13	1
2:A:42:ASP:O	2:A:43:LEU:CD2	0.48	2.60	11	1
2:A:58:TYR:CE1	2:A:88:PRO:HA	0.48	2.43	11	1
2:A:87:LYS:CB	2:A:88:PRO:HD2	0.48	2.38	11	2
2:A:11:THR:HG23	2:A:12:THR:N	0.48	2.23	9	1
2:A:19:GLY:O	2:A:20:ASN:OD1	0.48	2.31	9	1
2:A:25:LYS:CD	2:A:25:LYS:C	0.48	2.82	9	1
1:B:9:C:O2	2:A:127:ARG:HG2	0.48	2.08	13	1
2:A:107:LEU:HD23	2:A:107:LEU:C	0.48	2.29	5	1
1:B:3:A:O2'	1:B:4:U:O5'	0.48	2.32	9	13
2:A:27:VAL:O	2:A:28:ALA:C	0.48	2.51	10	13
2:A:51:GLY:O	2:A:52:THR:HB	0.48	2.09	11	4
2:A:55:LYS:HB3	2:A:56:PHE:CD1	0.48	2.43	11	1
2:A:131:GLN:OE1	2:A:132:ASP:N	0.48	2.46	11	1
2:A:101:THR:OG1	2:A:171:THR:CG2	0.48	2.61	3	2
2:A:136:LYS:HG3	2:A:138:ILE:HD11	0.48	1.85	1	1
1:B:8:U:O2'	2:A:140:TYR:CE2	0.48	2.67	7	1
1:B:13:A:H8	1:B:13:A:OP2	0.48	1.92	7	1
2:A:103:LEU:HG	2:A:138:ILE:CG2	0.48	2.38	5	1
2:A:53:ASN:O	2:A:54:ARG:HB2	0.48	2.09	12	5
1:B:13:A:OP1	2:A:52:THR:OG1	0.48	2.32	12	1
2:A:47:ASP:CB	2:A:60:ASP:HB3	0.48	2.39	11	1
1:B:14:G:C4'	1:B:15:U:OP1	0.48	2.61	3	1
2:A:65:GLU:OE1	2:A:69:LYS:CD	0.48	2.62	3	1
1:B:9:C:O2'	2:A:127:ARG:HB3	0.48	2.07	14	2
2:A:58:TYR:CE2	2:A:89:LYS:HD3	0.48	2.44	1	1
2:A:20:ASN:ND2	2:A:82:GLU:O	0.48	2.46	14	2
2:A:47:ASP:HB2	2:A:60:ASP:CB	0.48	2.39	14	1
2:A:68:GLU:HG3	2:A:69:LYS:N	0.48	2.23	9	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:12:G:OP2	2:A:92:ASP:O	0.48	2.31	6	1
2:A:117:LYS:O	2:A:120:PHE:O	0.48	2.32	11	1
2:A:153:LEU:O	2:A:168:LEU:CD1	0.48	2.61	3	2
1:B:11:C:C2'	2:A:89:LYS:HD2	0.48	2.38	2	1
2:A:111:ILE:CD1	2:A:115:GLU:CD	0.48	2.82	10	1
2:A:107:LEU:HD11	2:A:139:ALA:HB2	0.48	1.84	6	1
2:A:116:LEU:O	2:A:119:VAL:N	0.48	2.47	10	2
1:B:11:C:C2	2:A:88:PRO:HG3	0.48	2.43	8	1
1:B:13:A:O2'	1:B:14:G:OP2	0.48	2.31	7	5
2:A:103:LEU:HB2	2:A:140:TYR:CD2	0.48	2.44	3	2
2:A:21:LEU:HB3	2:A:25:LYS:CB	0.48	2.39	9	1
1:B:14:G:OP2	2:A:52:THR:O	0.48	2.31	5	1
2:A:99:ALA:O	2:A:100:ARG:C	0.48	2.52	13	2
2:A:162:ASP:O	2:A:163:GLY:C	0.48	2.51	8	1
1:B:12:G:OP1	2:A:90:GLY:O	0.48	2.31	11	1
2:A:17:PHE:CD2	2:A:89:LYS:NZ	0.48	2.78	1	1
2:A:76:LEU:HD21	2:A:83:ILE:HD11	0.48	1.83	9	1
2:A:116:LEU:HD23	2:A:126:ILE:HG22	0.48	1.86	13	1
2:A:106:ASN:ND2	2:A:164:ARG:O	0.48	2.46	5	1
2:A:164:ARG:O	2:A:165:SER:O	0.48	2.31	5	3
2:A:38:PHE:O	2:A:43:LEU:O	0.48	2.32	3	2
1:B:10:C:H2'	1:B:11:C:OP1	0.48	2.07	9	1
1:B:8:U:OP2	2:A:140:TYR:OH	0.48	2.30	10	1
2:A:47:ASP:O	2:A:48:VAL:CG2	0.48	2.62	10	1
2:A:111:ILE:HD11	2:A:161:ILE:O	0.48	2.09	10	1
1:B:12:G:OP1	2:A:94:LYS:HD3	0.48	2.09	6	1
1:B:18:A:H8	1:B:18:A:O5'	0.48	1.91	1	4
2:A:77:LYS:O	2:A:78:VAL:C	0.48	2.52	5	3
1:B:8:U:O4	2:A:139:ALA:O	0.48	2.32	8	1
2:A:73:LEU:O	2:A:76:LEU:HD23	0.48	2.09	11	1
2:A:14:PHE:CD2	2:A:63:SER:HA	0.48	2.44	4	3
2:A:119:VAL:HG13	2:A:120:PHE:N	0.48	2.24	2	1
2:A:78:VAL:C	2:A:79:PHE:CD1	0.48	2.87	2	1
2:A:125:GLU:O	2:A:142:GLU:O	0.48	2.32	9	2
1:B:12:G:C4'	2:A:94:LYS:HB3	0.48	2.39	10	1
2:A:27:VAL:CA	2:A:55:LYS:HB3	0.48	2.39	10	1
2:A:158:GLY:HA2	2:A:166:VAL:O	0.48	2.08	5	1
2:A:120:PHE:CZ	2:A:141:ILE:CD1	0.47	2.95	12	1
2:A:141:ILE:CG2	2:A:142:GLU:N	0.47	2.77	12	1
2:A:161:ILE:O	2:A:162:ASP:OD1	0.47	2.32	12	1
1:B:13:A:OP1	2:A:94:LYS:HB3	0.47	2.09	1	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:A:113:GLU:CB	2:A:117:LYS:HE3	0.47	2.39	11	1
2:A:78:VAL:O	2:A:78:VAL:HG13	0.47	2.09	3	1
2:A:117:LYS:O	2:A:121:GLU:N	0.47	2.46	7	2
2:A:49:ARG:HG2	2:A:50:THR:N	0.47	2.24	4	1
2:A:12:THR:HG22	2:A:46:VAL:HG21	0.47	1.85	7	1
2:A:102:LEU:CD1	2:A:102:LEU:N	0.47	2.69	2	1
2:A:38:PHE:CD2	2:A:45:VAL:HG21	0.47	2.44	9	1
2:A:94:LYS:HD3	2:A:95:LYS:N	0.47	2.24	9	1
2:A:101:THR:O	2:A:171:THR:HG23	0.47	2.09	13	1
2:A:74:THR:O	2:A:75:GLY:O	0.47	2.32	4	2
2:A:124:LEU:CD1	2:A:144:LYS:HB3	0.47	2.39	2	2
1:B:12:G:C1'	1:B:13:A:P	0.47	3.02	7	2
2:A:38:PHE:CG	2:A:45:VAL:HB	0.47	2.44	5	2
2:A:125:GLU:O	2:A:141:ILE:CG2	0.47	2.62	6	1
1:B:13:A:OP2	2:A:51:GLY:HA2	0.47	2.09	6	1
1:B:11:C:OP2	2:A:93:SER:HB3	0.47	2.10	12	1
2:A:136:LYS:HE3	2:A:138:ILE:HD12	0.47	1.85	14	2
2:A:22:ASN:ND2	2:A:30:LEU:HD22	0.47	2.24	3	1
2:A:22:ASN:CG	2:A:30:LEU:HD22	0.47	2.30	3	1
2:A:107:LEU:O	2:A:109:PHE:CE1	0.47	2.68	4	1
2:A:51:GLY:HA3	2:A:56:PHE:CE2	0.47	2.44	2	1
1:B:13:A:N9	2:A:94:LYS:HB3	0.47	2.24	14	1
2:A:64:ALA:O	2:A:68:GLU:CG	0.47	2.62	5	1
2:A:162:ASP:OD1	2:A:164:ARG:N	0.47	2.42	12	1
2:A:164:ARG:O	2:A:165:SER:CB	0.47	2.62	14	2
2:A:26:SER:O	2:A:27:VAL:C	0.47	2.53	10	12
2:A:134:LYS:O	2:A:134:LYS:CG	0.47	2.63	8	1
2:A:130:SER:O	2:A:131:GLN:CB	0.47	2.61	11	1
2:A:38:PHE:CE2	2:A:61:PHE:CZ	0.47	3.02	3	1
1:B:8:U:N3	2:A:138:ILE:HG21	0.47	2.24	3	1
2:A:45:VAL:HG22	2:A:48:VAL:HG13	0.47	1.84	4	1
2:A:88:PRO:HD2	2:A:89:LYS:HZ2	0.47	1.69	1	1
2:A:76:LEU:CD1	2:A:83:ILE:HD11	0.47	2.39	14	1
2:A:30:LEU:HD22	2:A:78:VAL:HB	0.47	1.86	5	1
1:B:12:G:O3'	2:A:56:PHE:CD2	0.47	2.67	12	1
2:A:32:VAL:O	2:A:33:ALA:C	0.47	2.52	8	11
2:A:102:LEU:O	2:A:141:ILE:O	0.47	2.32	8	4
2:A:105:LYS:HG3	2:A:138:ILE:CG2	0.47	2.40	4	7
2:A:103:LEU:HB2	2:A:140:TYR:CE1	0.47	2.45	4	2
1:B:13:A:OP2	2:A:93:SER:O	0.47	2.32	8	1
2:A:93:SER:O	2:A:94:LYS:O	0.47	2.32	5	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:8:U:C6	2:A:103:LEU:HD22	0.47	2.45	11	1
2:A:129:VAL:O	2:A:136:LYS:O	0.47	2.33	11	2
2:A:61:PHE:CD2	2:A:67:LEU:CD1	0.47	2.91	11	1
1:B:10:C:N3	2:A:97:ARG:HG3	0.47	2.24	11	1
1:B:13:A:OP2	2:A:94:LYS:CG	0.47	2.63	3	1
1:B:13:A:H2'	1:B:14:G:OP2	0.47	2.10	1	2
2:A:101:THR:OG1	2:A:141:ILE:O	0.47	2.32	2	2
1:B:1:G:C2	1:B:2:G:C8	0.47	3.02	14	1
2:A:116:LEU:C	2:A:116:LEU:CD1	0.47	2.82	14	1
2:A:141:ILE:HG22	2:A:142:GLU:H	0.47	1.69	14	1
2:A:102:LEU:HB3	2:A:143:PHE:CE1	0.47	2.44	6	1
2:A:116:LEU:HD13	2:A:120:PHE:CE1	0.47	2.45	12	1
2:A:165:SER:O	2:A:165:SER:OG	0.47	2.33	1	7
2:A:101:THR:O	2:A:171:THR:O	0.47	2.32	8	4
1:B:9:C:H41	1:B:10:C:N4	0.47	2.07	1	2
2:A:38:PHE:HD1	2:A:43:LEU:HD11	0.47	1.61	7	1
2:A:120:PHE:HB3	2:A:123:ALA:HB2	0.47	1.84	14	1
2:A:106:ASN:OD1	2:A:106:ASN:O	0.47	2.32	13	1
2:A:102:LEU:CA	2:A:171:THR:HG23	0.47	2.40	13	1
1:B:10:C:H42	2:A:97:ARG:CB	0.47	2.23	12	1
1:B:12:G:OP2	2:A:93:SER:O	0.47	2.31	12	1
2:A:75:GLY:O	2:A:83:ILE:HD11	0.47	2.09	12	1
2:A:60:ASP:OD1	2:A:60:ASP:N	0.47	2.46	8	1
2:A:90:GLY:O	2:A:91:ARG:O	0.47	2.33	8	2
2:A:159:ALA:O	2:A:166:VAL:N	0.47	2.48	2	2
2:A:51:GLY:HA3	2:A:56:PHE:CD2	0.47	2.45	11	1
1:B:12:G:OP2	2:A:89:LYS:CA	0.47	2.63	11	1
2:A:116:LEU:HD22	2:A:128:LEU:HD21	0.47	1.87	4	1
2:A:104:ALA:O	2:A:139:ALA:O	0.47	2.33	6	3
2:A:111:ILE:HD12	2:A:161:ILE:CG2	0.47	2.40	1	1
2:A:12:THR:O	2:A:60:ASP:OD1	0.47	2.33	1	2
1:B:12:G:H3'	1:B:12:G:OP2	0.47	2.09	1	1
2:A:157:GLN:HG2	2:A:168:LEU:HD11	0.47	1.87	7	1
2:A:156:LYS:O	2:A:157:GLN:O	0.47	2.33	5	2
2:A:112:THR:OG1	2:A:114:ASP:OD2	0.47	2.33	2	1
2:A:49:ARG:HG3	2:A:58:TYR:CB	0.47	2.40	9	1
2:A:94:LYS:CE	2:A:96:VAL:HG13	0.47	2.37	10	1
2:A:136:LYS:HD3	2:A:138:ILE:CD1	0.47	2.40	10	1
2:A:17:PHE:HB2	2:A:88:PRO:CG	0.47	2.39	10	1
2:A:45:VAL:O	2:A:45:VAL:HG13	0.47	2.09	13	1
1:B:13:A:OP2	1:B:13:A:O4'	0.47	2.33	12	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:8:U:O2	2:A:136:LYS:HE3	0.47	2.09	9	3
2:A:38:PHE:CE2	2:A:59:VAL:HG11	0.47	2.45	12	2
2:A:13:PRO:O	2:A:14:PHE:C	0.47	2.53	14	9
2:A:166:VAL:HG22	2:A:167:SER:H	0.47	1.69	8	1
2:A:136:LYS:HE3	2:A:138:ILE:CD1	0.47	2.40	14	2
2:A:52:THR:HG23	2:A:94:LYS:HG2	0.47	1.86	8	1
2:A:77:LYS:HA	2:A:83:ILE:HD13	0.47	1.87	11	1
2:A:93:SER:HB3	2:A:94:LYS:CE	0.47	2.39	1	1
2:A:97:ARG:O	2:A:171:THR:OG1	0.47	2.33	1	2
2:A:14:PHE:O	2:A:60:ASP:OD2	0.47	2.33	10	2
1:B:13:A:N6	2:A:94:LYS:HE3	0.47	2.25	5	1
2:A:96:VAL:O	2:A:99:ALA:HB2	0.47	2.10	8	1
2:A:110:ASN:O	2:A:111:ILE:O	0.47	2.33	8	4
2:A:49:ARG:O	2:A:58:TYR:HB2	0.47	2.10	11	1
2:A:98:ALA:O	2:A:101:THR:OG1	0.47	2.33	3	1
2:A:99:ALA:O	2:A:172:GLY:O	0.47	2.33	4	1
2:A:122:ASP:CB	2:A:143:PHE:CE2	0.47	2.98	1	1
2:A:38:PHE:CB	2:A:43:LEU:HD11	0.47	2.39	10	1
2:A:22:ASN:OD1	2:A:24:ASN:O	0.47	2.32	10	1
2:A:129:VAL:O	2:A:138:ILE:O	0.47	2.33	12	3
2:A:46:VAL:HG21	2:A:62:GLU:HA	0.47	1.86	8	1
2:A:123:ALA:CB	2:A:141:ILE:HG22	0.47	2.40	11	2
2:A:17:PHE:CE2	2:A:86:GLU:CB	0.47	2.98	11	1
2:A:98:ALA:N	2:A:172:GLY:N	0.46	2.63	8	1
1:B:11:C:C1'	1:B:12:G:P	0.46	3.03	8	2
2:A:140:TYR:CD1	2:A:140:TYR:O	0.46	2.68	11	1
2:A:49:ARG:O	2:A:58:TYR:O	0.46	2.32	11	1
2:A:46:VAL:CG2	2:A:62:GLU:HA	0.46	2.40	4	2
2:A:14:PHE:O	2:A:60:ASP:OD1	0.46	2.33	7	2
2:A:157:GLN:NE2	2:A:168:LEU:HD13	0.46	2.25	2	1
2:A:12:THR:O	2:A:60:ASP:OD2	0.46	2.33	10	2
1:B:11:C:O4'	1:B:12:G:OP1	0.46	2.33	14	1
1:B:11:C:O2'	2:A:91:ARG:HB3	0.46	2.09	9	1
1:B:10:C:C4	2:A:97:ARG:O	0.46	2.68	5	1
2:A:105:LYS:O	2:A:106:ASN:HB3	0.46	2.11	12	3
2:A:94:LYS:CG	2:A:95:LYS:N	0.46	2.78	12	1
1:B:12:G:N3	1:B:12:G:C5'	0.46	2.74	11	1
2:A:73:LEU:O	2:A:74:THR:O	0.46	2.33	4	2
2:A:28:ALA:O	2:A:31:LYS:HG2	0.46	2.11	1	2
1:B:11:C:C6	2:A:89:LYS:CE	0.46	2.98	1	1
1:B:12:G:O3'	2:A:94:LYS:HB3	0.46	2.11	2	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:A:118:GLU:HG2	2:A:119:VAL:N	0.46	2.26	14	1
1:B:13:A:N7	2:A:94:LYS:HG3	0.46	2.25	8	1
2:A:102:LEU:CD2	2:A:141:ILE:C	0.46	2.84	3	1
1:B:15:U:H4'	1:B:16:G:OP1	0.46	2.11	4	1
2:A:52:THR:CB	2:A:55:LYS:HB2	0.46	2.41	1	1
2:A:15:ASN:OD1	2:A:60:ASP:OD2	0.46	2.33	1	1
1:B:8:U:O5'	1:B:8:U:C6	0.46	2.67	14	1
2:A:37:LEU:C	2:A:37:LEU:HD22	0.46	2.31	14	1
2:A:15:ASN:CA	2:A:59:VAL:O	0.46	2.63	9	1
1:B:12:G:N3	1:B:12:G:C2'	0.46	2.79	9	2
2:A:161:ILE:O	2:A:162:ASP:HB2	0.46	2.10	10	1
2:A:166:VAL:O	2:A:166:VAL:HG13	0.46	2.10	13	1
2:A:51:GLY:O	2:A:52:THR:OG1	0.46	2.33	13	2
2:A:156:LYS:CD	2:A:156:LYS:N	0.46	2.78	5	1
2:A:106:ASN:O	2:A:164:ARG:CG	0.46	2.63	5	1
2:A:112:THR:O	2:A:113:GLU:C	0.46	2.53	13	5
2:A:122:ASP:O	2:A:126:ILE:HD11	0.46	2.11	11	1
2:A:136:LYS:CG	2:A:138:ILE:HD11	0.46	2.41	11	1
2:A:141:ILE:CD1	2:A:141:ILE:N	0.46	2.75	11	1
2:A:17:PHE:HB2	2:A:58:TYR:CD1	0.46	2.46	11	2
2:A:132:ASP:N	2:A:132:ASP:OD1	0.46	2.47	9	1
2:A:12:THR:HG22	2:A:61:PHE:O	0.46	2.10	10	1
2:A:34:ILE:CG2	2:A:35:SER:N	0.46	2.78	10	1
2:A:32:VAL:O	2:A:35:SER:OG	0.46	2.33	13	1
2:A:166:VAL:O	2:A:166:VAL:CG1	0.46	2.64	13	2
2:A:81:ASN:O	2:A:82:GLU:O	0.46	2.34	6	3
1:B:8:U:H4'	1:B:9:C:OP2	0.46	2.09	11	1
2:A:91:ARG:O	2:A:92:ASP:HB2	0.46	2.10	2	2
2:A:74:THR:O	2:A:76:LEU:N	0.46	2.48	3	2
2:A:116:LEU:HD22	2:A:128:LEU:CD2	0.46	2.41	4	1
2:A:23:PRO:HB2	2:A:54:ARG:CD	0.46	2.41	2	1
2:A:53:ASN:CG	2:A:53:ASN:O	0.46	2.54	5	2
2:A:134:LYS:O	2:A:135:SER:O	0.46	2.33	1	3
2:A:122:ASP:O	2:A:123:ALA:O	0.46	2.34	11	1
1:B:12:G:C2'	1:B:13:A:O5'	0.46	2.64	3	1
2:A:47:ASP:O	2:A:60:ASP:OD1	0.46	2.33	13	2
2:A:105:LYS:HB2	2:A:105:LYS:HZ3	0.46	1.70	1	1
2:A:161:ILE:HD12	2:A:166:VAL:HG21	0.46	1.86	1	2
2:A:73:LEU:HB2	2:A:76:LEU:CD1	0.46	2.41	10	1
2:A:17:PHE:O	2:A:86:GLU:O	0.46	2.33	5	1
2:A:96:VAL:O	2:A:97:ARG:C	0.46	2.53	9	4

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:A:43:LEU:HD12	2:A:45:VAL:N	0.46	2.26	12	1
2:A:148:ASP:OD1	2:A:148:ASP:N	0.46	2.49	12	1
2:A:101:THR:OG1	2:A:171:THR:O	0.46	2.34	3	1
2:A:101:THR:CG2	2:A:142:GLU:HA	0.46	2.41	4	1
2:A:63:SER:N	2:A:66:ASP:OD1	0.46	2.49	5	2
2:A:141:ILE:N	2:A:141:ILE:HD12	0.46	2.25	10	1
2:A:25:LYS:O	2:A:26:SER:HB2	0.46	2.10	6	1
2:A:72:GLU:O	2:A:73:LEU:O	0.46	2.33	13	3
2:A:129:VAL:CG1	2:A:136:LYS:HE2	0.46	2.41	8	1
2:A:101:THR:HG21	2:A:172:GLY:O	0.46	2.10	8	1
2:A:12:THR:OG1	2:A:14:PHE:CD2	0.46	2.68	8	1
2:A:52:THR:CG2	2:A:52:THR:O	0.46	2.62	8	1
2:A:153:LEU:HG	2:A:154:GLU:N	0.46	2.26	11	1
2:A:108:SER:C	2:A:109:PHE:CD1	0.46	2.89	1	1
2:A:21:LEU:CB	2:A:30:LEU:HD13	0.46	2.41	7	1
2:A:76:LEU:HD13	2:A:85:LEU:HD21	0.46	1.88	2	1
2:A:120:PHE:CD2	2:A:141:ILE:HG12	0.46	2.45	9	1
2:A:38:PHE:CE2	2:A:59:VAL:HG21	0.46	2.45	9	1
2:A:49:ARG:CG	2:A:58:TYR:HB3	0.46	2.41	9	1
2:A:41:ASN:HB2	2:A:43:LEU:CD2	0.46	2.40	9	1
2:A:127:ARG:O	2:A:139:ALA:HB1	0.46	2.10	8	1
2:A:124:LEU:HD12	2:A:144:LYS:CB	0.46	2.41	8	1
2:A:76:LEU:O	2:A:78:VAL:N	0.46	2.48	8	1
2:A:114:ASP:O	2:A:118:GLU:HB3	0.46	2.11	6	5
2:A:76:LEU:CD1	2:A:85:LEU:HD21	0.46	2.39	3	1
2:A:58:TYR:CE2	2:A:89:LYS:CD	0.46	2.98	1	1
2:A:122:ASP:OD2	2:A:148:ASP:OD1	0.46	2.34	2	1
2:A:58:TYR:CZ	2:A:88:PRO:HA	0.46	2.46	11	1
2:A:144:LYS:O	2:A:144:LYS:CG	0.46	2.64	10	2
2:A:51:GLY:O	2:A:55:LYS:HB3	0.46	2.11	3	3
1:B:13:A:OP1	2:A:95:LYS:CG	0.46	2.64	4	1
2:A:14:PHE:HD2	2:A:67:LEU:HD13	0.46	1.70	1	1
2:A:14:PHE:CD1	2:A:67:LEU:HD13	0.46	2.45	7	2
2:A:106:ASN:O	2:A:107:LEU:HD22	0.46	2.11	2	2
1:B:13:A:O4'	2:A:94:LYS:HG3	0.46	2.11	9	1
2:A:25:LYS:HD2	2:A:55:LYS:CD	0.46	2.41	10	1
1:B:9:C:O4'	2:A:129:VAL:CG1	0.46	2.54	13	1
2:A:159:ALA:O	2:A:160:GLU:C	0.45	2.54	6	3
2:A:120:PHE:CD1	2:A:156:LYS:HG2	0.45	2.47	8	1
1:B:6:C:HO2'	1:B:7:C:C5'	0.45	2.23	3	2
2:A:117:LYS:HB3	2:A:126:ILE:CD1	0.45	2.41	7	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:A:43:LEU:O	2:A:43:LEU:CG	0.45	2.63	7	1
2:A:99:ALA:C	2:A:100:ARG:CG	0.45	2.84	14	1
2:A:18:ILE:O	2:A:56:PHE:CD2	0.45	2.69	9	1
2:A:21:LEU:HG	2:A:30:LEU:CD2	0.45	2.41	9	1
1:B:13:A:O4'	2:A:94:LYS:CG	0.45	2.65	9	1
2:A:107:LEU:CD2	2:A:137:GLY:CA	0.45	2.94	9	1
2:A:120:PHE:CE2	2:A:156:LYS:HB2	0.45	2.46	13	1
1:B:8:U:OP1	2:A:97:ARG:HD2	0.45	2.11	5	1
1:B:13:A:OP1	2:A:56:PHE:CE2	0.45	2.70	12	1
2:A:98:ALA:O	2:A:101:THR:HG22	0.45	2.11	11	1
2:A:161:ILE:HG23	2:A:162:ASP:N	0.45	2.27	3	1
2:A:105:LYS:HB2	2:A:105:LYS:NZ	0.45	2.27	1	1
2:A:132:ASP:O	2:A:133:GLY:C	0.45	2.54	1	1
2:A:61:PHE:CD2	2:A:67:LEU:HA	0.45	2.46	5	3
2:A:115:GLU:HG2	2:A:161:ILE:CG2	0.45	2.41	7	1
2:A:76:LEU:HD13	2:A:83:ILE:HD11	0.45	1.88	14	1
2:A:53:ASN:O	2:A:54:ARG:HB3	0.45	2.11	9	2
2:A:53:ASN:O	2:A:53:ASN:OD1	0.45	2.35	10	1
2:A:140:TYR:OH	2:A:171:THR:OG1	0.45	2.34	6	1
2:A:103:LEU:CD2	2:A:138:ILE:HG23	0.45	2.41	5	1
2:A:143:PHE:O	2:A:144:LYS:C	0.45	2.54	5	1
1:B:13:A:OP1	2:A:56:PHE:CD2	0.45	2.69	12	1
2:A:143:PHE:N	2:A:143:PHE:CD1	0.45	2.84	8	1
1:B:11:C:C2	2:A:17:PHE:CE1	0.45	3.04	3	1
2:A:123:ALA:N	2:A:143:PHE:CZ	0.45	2.84	3	1
2:A:94:LYS:O	2:A:95:LYS:HB3	0.45	2.11	14	3
2:A:116:LEU:HD22	2:A:120:PHE:CE2	0.45	2.47	14	1
2:A:117:LYS:HG2	2:A:118:GLU:N	0.45	2.25	14	1
2:A:157:GLN:HB3	2:A:168:LEU:CD2	0.45	2.42	14	1
2:A:77:LYS:HG2	2:A:81:ASN:O	0.45	2.11	14	1
2:A:161:ILE:O	2:A:161:ILE:CG2	0.45	2.64	13	2
2:A:160:GLU:O	2:A:162:ASP:OD1	0.45	2.35	13	1
2:A:78:VAL:HB	2:A:79:PHE:CD1	0.45	2.46	12	1
2:A:43:LEU:CD1	2:A:61:PHE:CD1	0.45	2.99	11	2
2:A:158:GLY:HA2	2:A:166:VAL:HG12	0.45	1.88	5	2
2:A:111:ILE:C	2:A:112:THR:CG2	0.45	2.83	11	1
2:A:21:LEU:O	2:A:22:ASN:HB3	0.45	2.12	4	3
2:A:25:LYS:HE3	2:A:79:PHE:CD2	0.45	2.46	1	1
2:A:136:LYS:HE3	2:A:138:ILE:HD11	0.45	1.89	10	1
1:B:7:C:HO2'	1:B:8:U:P	0.45	2.34	13	1
1:B:7:C:OP2	1:B:9:C:OP1	0.45	2.34	13	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:A:149:ALA:O	2:A:152:ASN:OD1	0.45	2.34	6	1
2:A:45:VAL:CG2	2:A:59:VAL:CG2	0.45	2.95	12	1
2:A:21:LEU:O	2:A:22:ASN:OD1	0.45	2.33	8	1
2:A:106:ASN:C	2:A:107:LEU:CD2	0.45	2.85	11	1
1:B:13:A:C8	2:A:94:LYS:HG3	0.45	2.47	11	1
1:B:13:A:OP1	2:A:56:PHE:CD1	0.45	2.69	3	1
2:A:130:SER:O	2:A:131:GLN:O	0.45	2.33	7	1
2:A:120:PHE:CE2	2:A:141:ILE:HG12	0.45	2.46	11	1
2:A:42:ASP:O	2:A:43:LEU:CB	0.45	2.64	11	1
1:B:11:C:C5	2:A:88:PRO:CG	0.45	2.99	2	1
2:A:100:ARG:CB	2:A:145:SER:HA	0.45	2.40	9	1
2:A:45:VAL:HG21	2:A:48:VAL:CG2	0.45	2.40	10	1
1:B:9:C:O5'	1:B:9:C:C6	0.45	2.58	13	1
2:A:103:LEU:CD2	2:A:138:ILE:CG2	0.45	2.95	5	1
2:A:36:GLU:O	2:A:39:ALA:HB3	0.45	2.11	12	1
2:A:22:ASN:OD1	2:A:25:LYS:CG	0.45	2.65	12	1
2:A:78:VAL:CG2	2:A:79:PHE:N	0.45	2.79	1	3
2:A:102:LEU:HD22	2:A:152:ASN:HD21	0.45	1.72	7	1
2:A:153:LEU:CD1	2:A:169:TYR:CA	0.45	2.95	7	1
1:B:13:A:N7	2:A:94:LYS:HG2	0.45	2.27	2	2
2:A:66:ASP:OD1	2:A:66:ASP:N	0.45	2.49	2	2
2:A:161:ILE:O	2:A:162:ASP:HB3	0.45	2.10	9	2
2:A:22:ASN:HB2	2:A:23:PRO:HD2	0.45	1.89	10	1
2:A:53:ASN:CG	2:A:54:ARG:N	0.45	2.70	8	1
2:A:42:ASP:O	2:A:43:LEU:C	0.45	2.55	9	3
2:A:98:ALA:CB	2:A:140:TYR:OH	0.45	2.64	9	1
2:A:157:GLN:HA	2:A:168:LEU:CD1	0.45	2.40	6	2
2:A:21:LEU:HD23	2:A:30:LEU:HB3	0.45	1.88	12	1
1:B:19:U:O2'	1:B:20:C:O5'	0.45	2.35	14	7
2:A:61:PHE:CD1	2:A:61:PHE:N	0.45	2.84	11	1
2:A:101:THR:O	2:A:171:THR:OG1	0.45	2.31	9	2
2:A:27:VAL:HB	2:A:55:LYS:CB	0.45	2.42	9	1
1:B:12:G:OP2	2:A:93:SER:HB2	0.45	2.12	9	1
2:A:111:ILE:HG13	2:A:161:ILE:HG23	0.45	1.87	12	2
1:B:11:C:O5'	2:A:93:SER:OG	0.45	2.32	12	1
2:A:116:LEU:O	2:A:120:PHE:CD2	0.45	2.70	11	2
2:A:119:VAL:CG1	2:A:120:PHE:CG	0.45	2.99	4	1
2:A:153:LEU:CD1	2:A:169:TYR:HA	0.45	2.42	4	1
2:A:50:THR:HG22	2:A:56:PHE:O	0.45	2.12	6	2
2:A:87:LYS:CG	2:A:88:PRO:HD2	0.45	2.42	7	1
2:A:150:GLU:HG3	2:A:151:LYS:N	0.45	2.27	7	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:A:111:ILE:HD13	2:A:115:GLU:HG3	0.45	1.87	2	1
2:A:115:GLU:OE2	2:A:118:GLU:OE1	0.45	2.34	2	1
2:A:116:LEU:CD2	2:A:120:PHE:CE2	0.45	3.00	14	1
2:A:158:GLY:HA3	2:A:166:VAL:HG11	0.45	1.89	14	1
2:A:25:LYS:O	2:A:25:LYS:HE2	0.45	2.12	9	1
2:A:48:VAL:HA	2:A:58:TYR:O	0.45	2.12	9	1
2:A:43:LEU:HD11	2:A:45:VAL:HB	0.44	1.87	12	1
2:A:49:ARG:CZ	2:A:60:ASP:OD1	0.44	2.65	8	1
2:A:11:THR:HG21	2:A:46:VAL:HG12	0.44	1.81	8	1
1:B:8:U:O4	2:A:105:LYS:HG3	0.44	2.12	7	2
2:A:153:LEU:HD12	2:A:168:LEU:HB2	0.44	1.90	7	1
2:A:30:LEU:O	2:A:78:VAL:CG1	0.44	2.64	7	1
1:B:11:C:N4	2:A:17:PHE:CE2	0.44	2.85	2	1
2:A:149:ALA:O	2:A:153:LEU:HB3	0.44	2.13	2	1
2:A:15:ASN:HB2	2:A:59:VAL:O	0.44	2.12	9	2
2:A:132:ASP:OD1	2:A:132:ASP:N	0.44	2.49	14	1
2:A:15:ASN:OD1	2:A:58:TYR:CE2	0.44	2.70	13	1
2:A:100:ARG:O	2:A:143:PHE:O	0.44	2.34	6	1
2:A:108:SER:CB	2:A:162:ASP:OD2	0.44	2.65	5	1
2:A:111:ILE:HG13	2:A:161:ILE:CG2	0.44	2.42	6	2
2:A:15:ASN:OD1	2:A:16:LEU:N	0.44	2.49	12	1
2:A:151:LYS:O	2:A:155:GLU:HB2	0.44	2.12	11	1
2:A:20:ASN:O	2:A:21:LEU:C	0.44	2.56	3	3
1:B:13:A:OP2	2:A:94:LYS:C	0.44	2.55	1	1
2:A:123:ALA:CA	2:A:143:PHE:CE1	0.44	3.00	2	1
2:A:165:SER:O	2:A:166:VAL:HG12	0.44	2.12	14	1
1:B:11:C:O2'	2:A:89:LYS:C	0.44	2.56	14	1
2:A:128:LEU:CD2	2:A:128:LEU:N	0.44	2.80	13	1
2:A:123:ALA:O	2:A:124:LEU:HG	0.44	2.12	8	1
2:A:102:LEU:HG	2:A:169:TYR:O	0.44	2.12	9	4
2:A:155:GLU:O	2:A:156:LYS:C	0.44	2.55	11	1
2:A:115:GLU:OE1	2:A:118:GLU:OE1	0.44	2.35	11	1
1:B:11:C:O2'	2:A:89:LYS:HB2	0.44	2.12	11	1
2:A:97:ARG:CB	2:A:172:GLY:HA2	0.44	2.43	1	1
2:A:153:LEU:HA	2:A:157:GLN:CB	0.44	2.42	14	1
2:A:105:LYS:HB2	2:A:167:SER:HB2	0.44	1.89	9	1
2:A:151:LYS:HG2	2:A:155:GLU:OE1	0.44	2.13	9	1
2:A:88:PRO:O	2:A:89:LYS:CG	0.44	2.66	10	1
2:A:153:LEU:HD11	2:A:170:TYR:N	0.44	2.28	6	1
2:A:41:ASN:OD1	2:A:73:LEU:HD22	0.44	2.12	6	1
2:A:158:GLY:HA2	2:A:166:VAL:CG1	0.44	2.42	5	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:A:135:SER:O	2:A:136:LYS:HG2	0.44	2.13	12	1
2:A:85:LEU:O	2:A:86:GLU:HG3	0.44	2.13	11	1
2:A:45:VAL:CG2	2:A:59:VAL:HG23	0.44	2.43	4	1
1:B:14:G:O2'	1:B:16:G:OP2	0.44	2.28	1	1
1:B:12:G:C3'	2:A:94:LYS:HB2	0.44	2.42	2	2
2:A:134:LYS:O	2:A:135:SER:OG	0.44	2.33	14	1
2:A:119:VAL:HG13	2:A:156:LYS:HB3	0.44	1.89	6	1
1:B:12:G:OP1	2:A:56:PHE:CZ	0.44	2.71	12	1
2:A:98:ALA:O	2:A:99:ALA:C	0.44	2.56	5	5
1:B:8:U:O2	2:A:136:LYS:HE2	0.44	2.11	3	3
1:B:8:U:O4	2:A:105:LYS:HD2	0.44	2.12	3	2
2:A:62:GLU:CB	2:A:66:ASP:OD2	0.44	2.65	4	1
2:A:32:VAL:O	2:A:35:SER:CB	0.44	2.65	7	1
2:A:157:GLN:O	2:A:166:VAL:HG11	0.44	2.12	14	1
1:B:13:A:O2'	1:B:14:G:C8	0.44	2.70	9	1
2:A:119:VAL:HG13	2:A:120:PHE:CD1	0.44	2.47	5	1
2:A:118:GLU:O	2:A:119:VAL:C	0.44	2.56	11	2
2:A:136:LYS:O	2:A:138:ILE:HG13	0.44	2.13	11	2
2:A:97:ARG:O	2:A:172:GLY:N	0.44	2.51	1	1
2:A:123:ALA:CA	2:A:143:PHE:CE2	0.44	3.01	9	2
2:A:102:LEU:CD2	2:A:141:ILE:CG1	0.44	2.96	13	1
2:A:27:VAL:HA	2:A:30:LEU:HD12	0.44	1.89	6	1
1:B:12:G:N7	2:A:49:ARG:CZ	0.44	2.81	5	1
2:A:51:GLY:HA3	2:A:56:PHE:HB2	0.44	1.89	12	1
2:A:19:GLY:O	2:A:20:ASN:HB3	0.44	2.13	12	4
1:B:20:C:HO2'	1:B:21:C:H5'	0.44	1.69	8	1
2:A:54:ARG:C	2:A:55:LYS:HD2	0.44	2.32	8	1
2:A:43:LEU:CD2	2:A:70:ALA:HB2	0.44	2.42	3	1
2:A:28:ALA:O	2:A:31:LYS:HG3	0.44	2.13	4	1
2:A:63:SER:O	2:A:64:ALA:C	0.44	2.56	2	3
2:A:131:GLN:O	2:A:132:ASP:HB2	0.44	2.12	10	2
2:A:17:PHE:C	2:A:18:ILE:HD12	0.44	2.33	10	1
2:A:108:SER:O	2:A:109:PHE:CD2	0.44	2.71	10	1
2:A:37:LEU:O	2:A:37:LEU:HD13	0.44	2.12	10	1
2:A:162:ASP:OD1	2:A:163:GLY:N	0.44	2.51	13	1
2:A:51:GLY:HA3	2:A:56:PHE:CB	0.44	2.42	13	1
2:A:14:PHE:HA	2:A:67:LEU:HD12	0.44	1.90	13	1
2:A:111:ILE:CD1	2:A:115:GLU:HG3	0.44	2.43	5	1
2:A:161:ILE:O	2:A:162:ASP:CG	0.44	2.56	9	2
2:A:35:SER:O	2:A:36:GLU:C	0.44	2.56	4	7
2:A:17:PHE:CG	2:A:17:PHE:O	0.44	2.71	8	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:A:164:ARG:O	2:A:165:SER:C	0.44	2.56	11	5
1:B:12:G:OP2	2:A:89:LYS:C	0.44	2.55	11	1
2:A:21:LEU:O	2:A:23:PRO:N	0.44	2.50	11	1
2:A:112:THR:O	2:A:115:GLU:N	0.44	2.51	3	1
2:A:142:GLU:HG3	2:A:143:PHE:N	0.44	2.28	4	1
2:A:101:THR:CG2	2:A:140:TYR:CE2	0.44	3.01	9	1
2:A:21:LEU:HB3	2:A:25:LYS:HB3	0.44	1.88	9	1
2:A:76:LEU:O	2:A:77:LYS:HG3	0.44	2.11	9	1
2:A:24:ASN:C	2:A:25:LYS:CG	0.44	2.86	10	1
2:A:154:GLU:O	2:A:157:GLN:HB2	0.44	2.12	12	1
2:A:117:LYS:HB2	2:A:126:ILE:CD1	0.44	2.43	12	2
2:A:121:GLU:O	2:A:122:ASP:C	0.44	2.56	13	4
2:A:54:ARG:C	2:A:55:LYS:CD	0.44	2.86	8	1
2:A:157:GLN:HG3	2:A:158:GLY:N	0.44	2.28	4	1
1:B:13:A:OP2	2:A:94:LYS:HB2	0.44	2.13	1	3
2:A:161:ILE:CD1	2:A:166:VAL:HG11	0.44	2.42	1	1
2:A:32:VAL:O	2:A:35:SER:HB2	0.44	2.13	7	1
2:A:17:PHE:CE1	2:A:56:PHE:HB2	0.44	2.48	2	1
2:A:76:LEU:CD1	2:A:85:LEU:HD22	0.44	2.43	2	1
2:A:150:GLU:O	2:A:153:LEU:HB3	0.44	2.13	14	1
2:A:62:GLU:N	2:A:66:ASP:OD2	0.44	2.50	14	1
2:A:101:THR:CB	2:A:142:GLU:HB2	0.44	2.43	9	1
2:A:22:ASN:N	2:A:22:ASN:OD1	0.44	2.50	9	1
1:B:12:G:OP1	1:B:12:G:N9	0.44	2.50	10	1
2:A:105:LYS:O	2:A:106:ASN:CG	0.44	2.55	13	1
2:A:27:VAL:HB	2:A:54:ARG:CG	0.44	2.43	13	1
2:A:108:SER:O	2:A:109:PHE:C	0.43	2.56	14	4
2:A:148:ASP:O	2:A:152:ASN:CG	0.43	2.57	11	1
2:A:101:THR:CG2	2:A:142:GLU:OE2	0.43	2.66	3	1
2:A:114:ASP:O	2:A:118:GLU:HB2	0.43	2.13	4	1
2:A:90:GLY:O	2:A:91:ARG:HB2	0.43	2.12	7	1
2:A:76:LEU:O	2:A:77:LYS:HB2	0.43	2.13	5	2
2:A:94:LYS:C	2:A:96:VAL:N	0.43	2.71	10	2
2:A:113:GLU:N	2:A:113:GLU:CD	0.43	2.71	10	1
2:A:43:LEU:CD1	2:A:43:LEU:C	0.43	2.86	12	2
2:A:119:VAL:CG1	2:A:156:LYS:HB3	0.43	2.42	6	2
2:A:43:LEU:CB	2:A:66:ASP:HB3	0.43	2.43	3	2
2:A:18:ILE:CG2	2:A:83:ILE:HB	0.43	2.43	11	1
2:A:18:ILE:HG21	2:A:83:ILE:CD1	0.43	2.41	11	1
2:A:14:PHE:O	2:A:60:ASP:CG	0.43	2.56	14	2
2:A:37:LEU:CD1	2:A:38:PHE:CD1	0.43	3.01	7	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:A:33:ALA:CB	2:A:78:VAL:HB	0.43	2.43	7	2
2:A:117:LYS:HB3	2:A:126:ILE:HD13	0.43	1.88	7	1
2:A:31:LYS:HD3	2:A:50:THR:CG2	0.43	2.43	14	1
2:A:101:THR:OG1	2:A:142:GLU:CA	0.43	2.65	9	1
2:A:101:THR:CB	2:A:142:GLU:HA	0.43	2.43	9	1
2:A:16:LEU:HB2	2:A:59:VAL:CG1	0.43	2.43	9	1
1:B:9:C:C4	2:A:127:ARG:NH2	0.43	2.86	13	1
2:A:122:ASP:N	2:A:122:ASP:OD1	0.43	2.50	5	1
1:B:12:G:N7	2:A:51:GLY:HA2	0.43	2.29	5	1
2:A:15:ASN:CG	2:A:59:VAL:O	0.43	2.57	12	2
2:A:158:GLY:HA3	2:A:166:VAL:O	0.43	2.12	8	1
2:A:58:TYR:C	2:A:59:VAL:CG1	0.43	2.86	7	1
2:A:129:VAL:HB	2:A:138:ILE:CD1	0.43	2.43	9	1
2:A:98:ALA:HB3	2:A:171:THR:OG1	0.43	2.12	10	1
2:A:21:LEU:HB2	2:A:25:LYS:CE	0.43	2.43	10	1
2:A:27:VAL:N	2:A:55:LYS:HB3	0.43	2.28	10	1
2:A:15:ASN:O	2:A:88:PRO:HG2	0.43	2.14	13	1
2:A:15:ASN:C	2:A:15:ASN:OD1	0.43	2.56	12	1
2:A:17:PHE:HA	2:A:57:GLY:O	0.43	2.14	8	1
2:A:47:ASP:OD2	2:A:49:ARG:NE	0.43	2.52	8	1
2:A:52:THR:HG23	2:A:94:LYS:CG	0.43	2.43	8	1
2:A:95:LYS:HA	2:A:95:LYS:CE	0.43	2.42	8	1
1:B:13:A:OP1	2:A:95:LYS:CB	0.43	2.66	4	1
1:B:13:A:OP1	2:A:95:LYS:HB3	0.43	2.12	4	1
2:A:62:GLU:HB2	2:A:66:ASP:OD2	0.43	2.13	4	2
2:A:113:GLU:O	2:A:117:LYS:HG2	0.43	2.14	1	2
1:B:12:G:O3'	2:A:94:LYS:HB2	0.43	2.12	7	1
1:B:13:A:N6	2:A:94:LYS:HE2	0.43	2.28	7	1
2:A:153:LEU:HA	2:A:168:LEU:HD22	0.43	1.89	14	1
2:A:15:ASN:HA	2:A:59:VAL:O	0.43	2.13	9	1
2:A:18:ILE:N	2:A:18:ILE:CD1	0.43	2.80	9	1
2:A:160:GLU:HG2	2:A:163:GLY:N	0.43	2.27	10	1
2:A:113:GLU:HG3	2:A:126:ILE:HG21	0.43	1.90	13	1
2:A:103:LEU:HD13	2:A:140:TYR:CE2	0.43	2.48	12	1
2:A:94:LYS:O	2:A:95:LYS:C	0.43	2.57	10	3
2:A:14:PHE:O	2:A:60:ASP:HA	0.43	2.13	8	4
1:B:10:C:O2'	1:B:11:C:O5'	0.43	2.37	11	1
2:A:58:TYR:CE1	2:A:88:PRO:CA	0.43	3.02	11	1
2:A:100:ARG:CB	2:A:145:SER:CA	0.43	2.97	9	1
2:A:17:PHE:CE1	2:A:18:ILE:C	0.43	2.91	10	1
1:B:8:U:C2	2:A:136:LYS:HE3	0.43	2.48	12	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:A:162:ASP:OD1	2:A:162:ASP:C	0.43	2.57	12	2
1:B:12:G:C2	2:A:91:ARG:NH1	0.43	2.87	12	1
1:B:11:C:P	2:A:93:SER:CB	0.43	3.06	12	1
2:A:101:THR:HG23	2:A:171:THR:C	0.43	2.33	8	1
2:A:55:LYS:CG	2:A:55:LYS:O	0.43	2.66	8	1
2:A:160:GLU:O	2:A:161:ILE:C	0.43	2.57	3	3
2:A:76:LEU:O	2:A:77:LYS:C	0.43	2.57	7	2
2:A:21:LEU:C	2:A:22:ASN:OD1	0.43	2.57	9	2
2:A:144:LYS:CD	2:A:148:ASP:OD2	0.43	2.67	13	1
2:A:43:LEU:HD12	2:A:43:LEU:O	0.43	2.13	3	1
2:A:75:GLY:O	2:A:76:LEU:C	0.43	2.56	3	2
2:A:12:THR:HG22	2:A:46:VAL:HG11	0.43	1.91	4	1
2:A:156:LYS:N	2:A:156:LYS:HD3	0.43	2.27	1	2
2:A:123:ALA:HA	2:A:143:PHE:CD1	0.43	2.49	2	1
2:A:21:LEU:HG	2:A:30:LEU:CD1	0.43	2.43	9	1
2:A:34:ILE:HD12	2:A:76:LEU:HD11	0.43	1.84	9	1
1:B:8:U:OP1	2:A:97:ARG:HG2	0.43	2.13	10	1
2:A:14:PHE:HA	2:A:67:LEU:CD1	0.43	2.43	13	1
2:A:111:ILE:CG2	2:A:115:GLU:HB2	0.43	2.44	11	1
2:A:73:LEU:O	2:A:74:THR:C	0.43	2.56	4	3
2:A:22:ASN:N	2:A:30:LEU:HD13	0.43	2.29	7	1
2:A:150:GLU:O	2:A:151:LYS:C	0.43	2.57	14	1
2:A:48:VAL:HB	2:A:58:TYR:O	0.43	2.14	9	1
2:A:22:ASN:HB2	2:A:23:PRO:CD	0.43	2.44	10	1
2:A:30:LEU:CD1	2:A:55:LYS:HB2	0.43	2.44	10	1
2:A:131:GLN:O	2:A:132:ASP:C	0.43	2.57	6	1
2:A:55:LYS:HG3	2:A:56:PHE:CE2	0.43	2.48	5	1
2:A:98:ALA:O	2:A:172:GLY:HA2	0.43	2.14	12	1
2:A:51:GLY:O	2:A:56:PHE:HB3	0.43	2.14	8	1
2:A:61:PHE:CG	2:A:67:LEU:HD12	0.43	2.49	7	1
1:B:12:G:OP1	2:A:92:ASP:HA	0.43	2.14	2	1
2:A:129:VAL:CG2	2:A:140:TYR:HB2	0.43	2.44	10	1
1:B:7:C:O3'	1:B:8:U:C4'	0.43	2.67	5	2
2:A:48:VAL:HG23	2:A:58:TYR:O	0.43	2.12	13	1
2:A:119:VAL:CG2	2:A:156:LYS:CG	0.43	2.94	5	1
1:B:12:G:N3	1:B:12:G:H5'	0.43	2.29	5	1
2:A:127:ARG:O	2:A:128:LEU:CG	0.43	2.67	12	1
2:A:72:GLU:O	2:A:73:LEU:C	0.43	2.57	12	2
2:A:14:PHE:HB3	2:A:67:LEU:HD12	0.43	1.91	8	1
2:A:16:LEU:HD13	2:A:61:PHE:CE1	0.43	2.48	3	1
2:A:157:GLN:HA	2:A:168:LEU:CG	0.43	2.44	1	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:A:17:PHE:HB3	2:A:86:GLU:O	0.43	2.13	10	2
2:A:152:ASN:O	2:A:153:LEU:C	0.43	2.57	14	3
2:A:27:VAL:HA	2:A:55:LYS:HB3	0.43	1.91	10	1
2:A:18:ILE:HG22	2:A:19:GLY:N	0.43	2.29	13	1
2:A:119:VAL:HG12	2:A:120:PHE:CD2	0.43	2.49	6	1
1:B:12:G:OP1	2:A:94:LYS:HG2	0.43	2.14	6	1
2:A:100:ARG:HD2	2:A:144:LYS:O	0.43	2.14	5	1
1:B:13:A:P	1:B:13:A:C8	0.42	3.12	12	1
2:A:85:LEU:CD1	2:A:85:LEU:N	0.42	2.74	12	1
2:A:152:ASN:O	2:A:156:LYS:CG	0.42	2.67	10	2
2:A:111:ILE:O	2:A:112:THR:OG1	0.42	2.33	11	1
2:A:41:ASN:O	2:A:42:ASP:OD2	0.42	2.36	11	1
1:B:15:U:C4'	1:B:15:U:OP2	0.42	2.64	3	1
2:A:148:ASP:O	2:A:152:ASN:OD1	0.42	2.37	3	1
2:A:56:PHE:CE2	2:A:57:GLY:O	0.42	2.71	7	2
2:A:111:ILE:HD13	2:A:115:GLU:OE1	0.42	2.14	13	1
2:A:120:PHE:HE2	2:A:168:LEU:HD13	0.42	1.74	13	1
1:B:13:A:H2'	2:A:52:THR:HG23	0.42	1.90	6	1
2:A:119:VAL:HG13	2:A:120:PHE:CE1	0.42	2.48	5	1
2:A:43:LEU:HD12	2:A:44:ALA:H	0.42	1.73	8	1
2:A:41:ASN:O	2:A:42:ASP:CG	0.42	2.57	11	1
2:A:157:GLN:HA	2:A:168:LEU:CD2	0.42	2.44	1	1
2:A:152:ASN:C	2:A:152:ASN:ND2	0.42	2.72	7	1
2:A:30:LEU:O	2:A:78:VAL:HG11	0.42	2.14	7	1
2:A:20:ASN:OD1	2:A:83:ILE:HA	0.42	2.14	9	1
1:B:7:C:P	1:B:9:C:OP1	0.42	2.77	13	1
2:A:38:PHE:CZ	2:A:61:PHE:CZ	0.42	3.08	8	1
2:A:152:ASN:O	2:A:156:LYS:HG3	0.42	2.13	11	1
2:A:140:TYR:CD1	2:A:140:TYR:C	0.42	2.92	3	1
2:A:149:ALA:O	2:A:153:LEU:HB2	0.42	2.14	1	3
2:A:17:PHE:CD1	2:A:86:GLU:OE1	0.42	2.72	4	1
2:A:47:ASP:OD1	2:A:48:VAL:N	0.42	2.51	4	1
2:A:42:ASP:O	2:A:44:ALA:N	0.42	2.52	7	1
2:A:99:ALA:HA	2:A:172:GLY:CA	0.42	2.45	7	1
2:A:15:ASN:OD1	2:A:88:PRO:HG3	0.42	2.14	14	1
1:B:13:A:C2	2:A:94:LYS:O	0.42	2.72	9	1
2:A:95:LYS:O	2:A:96:VAL:C	0.42	2.57	9	1
2:A:15:ASN:O	2:A:88:PRO:HD3	0.42	2.13	5	1
2:A:129:VAL:CB	2:A:138:ILE:HD12	0.42	2.44	12	1
2:A:98:ALA:HA	2:A:171:THR:C	0.42	2.34	8	1
2:A:119:VAL:HB	2:A:120:PHE:CE1	0.42	2.49	11	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:A:140:TYR:CE1	2:A:141:ILE:O	0.42	2.71	3	1
2:A:43:LEU:HG	2:A:43:LEU:O	0.42	2.15	7	1
2:A:153:LEU:O	2:A:157:GLN:HG3	0.42	2.14	7	1
2:A:93:SER:O	2:A:94:LYS:C	0.42	2.57	14	1
2:A:13:PRO:O	2:A:15:ASN:CG	0.42	2.58	9	1
2:A:25:LYS:HD2	2:A:26:SER:N	0.42	2.30	9	1
2:A:46:VAL:HG22	2:A:62:GLU:HB2	0.42	1.91	9	1
2:A:159:ALA:O	2:A:160:GLU:HB2	0.42	2.14	13	1
1:B:11:C:O2'	2:A:91:ARG:HB2	0.42	2.14	13	1
2:A:157:GLN:OE1	2:A:168:LEU:CD1	0.42	2.68	12	1
2:A:154:GLU:O	2:A:157:GLN:HB3	0.42	2.15	3	1
2:A:143:PHE:CD2	2:A:148:ASP:CB	0.42	3.02	3	1
2:A:23:PRO:CB	2:A:54:ARG:HG2	0.42	2.44	4	1
2:A:52:THR:OG1	2:A:55:LYS:HB2	0.42	2.15	1	2
2:A:12:THR:HG23	2:A:60:ASP:OD1	0.42	2.14	1	1
2:A:130:SER:CB	2:A:137:GLY:HA2	0.42	2.44	7	1
2:A:106:ASN:O	2:A:107:LEU:CB	0.42	2.67	14	1
2:A:113:GLU:HB3	2:A:117:LYS:CD	0.42	2.44	14	1
2:A:113:GLU:O	2:A:114:ASP:C	0.42	2.58	9	1
2:A:152:ASN:HB2	2:A:156:LYS:HG2	0.42	1.91	6	1
1:B:20:C:H2'	1:B:21:C:O5'	0.42	2.13	6	2
2:A:162:ASP:O	2:A:162:ASP:CG	0.42	2.58	5	1
1:B:7:C:O2'	2:A:97:ARG:HG2	0.42	2.14	5	1
2:A:110:ASN:O	2:A:111:ILE:C	0.42	2.58	5	2
2:A:148:ASP:O	2:A:152:ASN:HB2	0.42	2.14	11	1
2:A:152:ASN:O	2:A:156:LYS:CB	0.42	2.68	11	1
2:A:88:PRO:HD2	2:A:89:LYS:CE	0.42	2.44	2	1
2:A:104:ALA:N	2:A:139:ALA:O	0.42	2.52	9	1
2:A:22:ASN:HB2	2:A:81:ASN:CB	0.42	2.45	10	1
2:A:120:PHE:CD1	2:A:141:ILE:HD13	0.42	2.49	13	1
1:B:9:C:O2	2:A:127:ARG:HB3	0.42	2.14	12	2
2:A:129:VAL:HG23	2:A:139:ALA:HA	0.42	1.91	8	1
2:A:49:ARG:O	2:A:58:TYR:CB	0.42	2.67	11	1
2:A:35:SER:O	2:A:37:LEU:N	0.42	2.52	1	4
1:B:9:C:C1'	2:A:129:VAL:CG2	0.42	2.98	3	1
2:A:58:TYR:C	2:A:59:VAL:HG13	0.42	2.35	7	1
2:A:89:LYS:HD3	2:A:89:LYS:N	0.42	2.29	2	1
2:A:63:SER:O	2:A:66:ASP:OD1	0.42	2.37	14	1
1:B:14:G:OP2	1:B:14:G:C2'	0.42	2.52	10	1
2:A:46:VAL:HG23	2:A:62:GLU:HB3	0.42	1.89	10	1
2:A:73:LEU:O	2:A:74:THR:OG1	0.42	2.32	13	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:A:152:ASN:OD1	2:A:153:LEU:N	0.42	2.51	6	1
2:A:11:THR:HG21	2:A:47:ASP:CG	0.42	2.35	5	1
1:B:8:U:C2	2:A:129:VAL:HG21	0.42	2.50	8	1
2:A:43:LEU:O	2:A:44:ALA:C	0.42	2.57	11	1
2:A:44:ALA:O	2:A:45:VAL:C	0.42	2.57	5	4
2:A:58:TYR:OH	2:A:89:LYS:HD2	0.42	2.15	1	1
2:A:23:PRO:HB3	2:A:54:ARG:NE	0.42	2.29	7	1
2:A:48:VAL:O	2:A:48:VAL:CG2	0.42	2.67	7	1
2:A:92:ASP:CG	2:A:92:ASP:O	0.42	2.57	2	1
1:B:8:U:C2'	1:B:9:C:C6	0.42	3.03	14	1
1:B:13:A:C5	2:A:94:LYS:HD2	0.42	2.49	14	1
2:A:98:ALA:O	2:A:99:ALA:HB3	0.42	2.15	14	1
2:A:101:THR:HB	2:A:142:GLU:CG	0.42	2.45	9	1
2:A:101:THR:CG2	2:A:142:GLU:HB2	0.42	2.44	10	1
2:A:95:LYS:O	2:A:97:ARG:CD	0.42	2.68	10	1
2:A:127:ARG:O	2:A:128:LEU:HG	0.42	2.14	12	1
2:A:129:VAL:HB	2:A:138:ILE:CG1	0.42	2.45	12	1
2:A:53:ASN:O	2:A:54:ARG:HG3	0.42	2.14	12	1
2:A:100:ARG:HG3	2:A:100:ARG:O	0.42	2.15	8	1
2:A:111:ILE:O	2:A:112:THR:CB	0.42	2.66	11	1
2:A:159:ALA:O	2:A:165:SER:HA	0.42	2.15	11	1
1:B:14:G:N7	2:A:52:THR:HA	0.42	2.29	11	1
2:A:102:LEU:N	2:A:102:LEU:CD1	0.42	2.80	1	2
2:A:99:ALA:O	2:A:172:GLY:C	0.42	2.58	4	1
2:A:102:LEU:HD21	2:A:143:PHE:HD1	0.42	1.73	1	1
2:A:156:LYS:C	2:A:158:GLY:N	0.42	2.73	1	2
2:A:58:TYR:O	2:A:59:VAL:HG12	0.42	2.14	7	1
2:A:103:LEU:CD1	2:A:103:LEU:C	0.42	2.88	10	1
2:A:122:ASP:OD1	2:A:122:ASP:N	0.42	2.53	10	1
2:A:95:LYS:C	2:A:97:ARG:N	0.42	2.73	10	1
2:A:12:THR:HG21	2:A:14:PHE:CD2	0.42	2.50	10	1
2:A:45:VAL:O	2:A:45:VAL:CG1	0.42	2.68	13	1
2:A:13:PRO:HB2	2:A:14:PHE:CD1	0.42	2.50	5	1
1:B:13:A:N7	2:A:52:THR:N	0.42	2.68	8	1
2:A:152:ASN:O	2:A:156:LYS:HB2	0.42	2.14	11	1
2:A:168:LEU:HD12	2:A:168:LEU:O	0.42	2.15	4	1
2:A:163:GLY:O	2:A:164:ARG:CB	0.42	2.68	7	1
2:A:46:VAL:HB	2:A:60:ASP:O	0.42	2.15	9	2
2:A:156:LYS:NZ	2:A:156:LYS:HB3	0.42	2.30	10	1
2:A:103:LEU:CD2	2:A:105:LYS:HD2	0.42	2.41	5	1
2:A:111:ILE:HD11	2:A:162:ASP:HB2	0.42	1.91	5	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:A:12:THR:CG2	2:A:46:VAL:HG11	0.42	2.45	5	1
2:A:51:GLY:HA3	2:A:56:PHE:N	0.41	2.30	12	1
2:A:83:ILE:HG13	2:A:85:LEU:HD11	0.41	1.92	12	1
2:A:14:PHE:CE2	2:A:63:SER:HA	0.41	2.50	8	1
2:A:147:ALA:O	2:A:151:LYS:HB3	0.41	2.14	8	1
2:A:48:VAL:HA	2:A:59:VAL:HG12	0.41	1.92	8	1
2:A:21:LEU:CB	2:A:30:LEU:HB3	0.41	2.45	4	1
2:A:124:LEU:CD1	2:A:124:LEU:C	0.41	2.87	7	1
2:A:92:ASP:O	2:A:93:SER:HB2	0.41	2.15	7	1
2:A:153:LEU:CD1	2:A:169:TYR:C	0.41	2.85	6	2
2:A:113:GLU:O	2:A:117:LYS:HB3	0.41	2.14	14	1
2:A:147:ALA:O	2:A:148:ASP:C	0.41	2.58	9	1
2:A:107:LEU:HD21	2:A:137:GLY:CA	0.41	2.44	9	1
2:A:34:ILE:CG1	2:A:76:LEU:HG	0.41	2.44	13	1
1:B:7:C:O2'	1:B:8:U:OP2	0.41	2.38	12	1
2:A:153:LEU:O	2:A:157:GLN:HB2	0.41	2.14	8	3
2:A:47:ASP:HB2	2:A:60:ASP:CG	0.41	2.36	8	1
2:A:56:PHE:CE1	2:A:58:TYR:HB2	0.41	2.50	8	1
2:A:105:LYS:O	2:A:106:ASN:HB2	0.41	2.14	11	2
1:B:8:U:C2'	1:B:9:C:OP1	0.41	2.68	4	3
2:A:84:LYS:HD3	2:A:86:GLU:OE2	0.41	2.15	3	1
2:A:112:THR:C	2:A:114:ASP:N	0.41	2.73	3	1
2:A:122:ASP:CG	2:A:148:ASP:OD2	0.41	2.59	1	1
2:A:62:GLU:OE1	2:A:66:ASP:OD2	0.41	2.38	1	1
2:A:157:GLN:HG2	2:A:168:LEU:CD1	0.41	2.44	7	1
2:A:140:TYR:HH	2:A:171:THR:CB	0.41	2.27	2	1
1:B:13:A:C8	2:A:94:LYS:HB3	0.41	2.50	14	1
1:B:13:A:OP1	2:A:94:LYS:HE3	0.41	2.15	9	1
2:A:18:ILE:HG21	2:A:21:LEU:CD2	0.41	2.33	5	1
2:A:99:ALA:O	2:A:172:GLY:HA2	0.41	2.15	5	1
1:B:12:G:C2'	1:B:13:A:OP2	0.41	2.68	5	1
2:A:128:LEU:CD2	2:A:139:ALA:HB1	0.41	2.44	12	1
2:A:51:GLY:HA3	2:A:56:PHE:CA	0.41	2.45	12	1
2:A:105:LYS:HB3	2:A:167:SER:O	0.41	2.14	8	1
2:A:63:SER:C	2:A:65:GLU:N	0.41	2.74	6	4
1:B:8:U:H3	2:A:138:ILE:HG21	0.41	1.75	3	1
1:B:14:G:H5'	1:B:15:U:OP1	0.41	2.14	4	1
1:B:13:A:H3'	1:B:13:A:OP1	0.41	2.16	2	1
2:A:104:ALA:HA	2:A:167:SER:O	0.41	2.16	9	3
2:A:101:THR:CB	2:A:142:GLU:CB	0.41	2.99	9	1
2:A:126:ILE:O	2:A:127:ARG:HG2	0.41	2.15	9	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:A:103:LEU:CD2	2:A:140:TYR:CE2	0.41	3.03	10	1
2:A:77:LYS:HG3	2:A:80:GLY:CA	0.41	2.46	10	1
2:A:25:LYS:HD2	2:A:30:LEU:HD21	0.41	1.90	5	1
2:A:116:LEU:HD13	2:A:120:PHE:CZ	0.41	2.50	12	1
2:A:46:VAL:N	2:A:60:ASP:O	0.41	2.54	12	1
2:A:71:LEU:HD21	2:A:85:LEU:CD2	0.41	2.45	11	1
2:A:120:PHE:N	2:A:120:PHE:CD1	0.41	2.86	4	2
2:A:103:LEU:HD22	2:A:140:TYR:CE1	0.41	2.51	4	1
2:A:41:ASN:HB3	2:A:43:LEU:CD1	0.41	2.44	4	1
2:A:119:VAL:HG12	2:A:120:PHE:CD1	0.41	2.50	4	1
2:A:118:GLU:O	2:A:121:GLU:OE2	0.41	2.38	4	1
2:A:119:VAL:O	2:A:156:LYS:HG2	0.41	2.16	1	1
2:A:14:PHE:CZ	2:A:64:ALA:N	0.41	2.88	7	1
2:A:82:GLU:OE1	2:A:83:ILE:O	0.41	2.38	14	1
2:A:68:GLU:CG	2:A:69:LYS:N	0.41	2.82	9	1
2:A:22:ASN:CG	2:A:24:ASN:O	0.41	2.59	10	1
2:A:108:SER:HB2	2:A:162:ASP:OD2	0.41	2.15	5	1
2:A:129:VAL:HG12	2:A:136:LYS:HE2	0.41	1.93	8	1
2:A:18:ILE:HD12	2:A:59:VAL:HG21	0.41	1.93	3	1
2:A:105:LYS:HB2	2:A:167:SER:CB	0.41	2.45	4	1
1:B:12:G:OP2	1:B:12:G:O4'	0.41	2.38	4	1
2:A:47:ASP:O	2:A:48:VAL:HG13	0.41	2.15	4	1
2:A:101:THR:OG1	2:A:142:GLU:HB2	0.41	2.15	9	1
2:A:95:LYS:O	2:A:97:ARG:HG3	0.41	2.15	10	1
2:A:160:GLU:HG2	2:A:161:ILE:N	0.41	2.31	13	1
2:A:94:LYS:HE2	2:A:96:VAL:CG1	0.41	2.45	13	1
2:A:120:PHE:CZ	2:A:168:LEU:HD11	0.41	2.51	8	1
2:A:98:ALA:O	2:A:99:ALA:O	0.41	2.37	8	1
2:A:23:PRO:O	2:A:24:ASN:HB3	0.41	2.15	8	1
2:A:32:VAL:O	2:A:35:SER:HB3	0.41	2.16	4	1
1:B:13:A:O4'	2:A:94:LYS:HB2	0.41	2.15	9	1
2:A:34:ILE:HG23	2:A:35:SER:N	0.41	2.30	10	1
2:A:144:LYS:O	2:A:144:LYS:CD	0.41	2.69	10	1
2:A:37:LEU:CD2	2:A:37:LEU:C	0.41	2.87	6	1
2:A:123:ALA:CB	2:A:143:PHE:CD2	0.41	3.03	8	1
2:A:50:THR:HA	2:A:56:PHE:O	0.41	2.15	10	3
2:A:135:SER:O	2:A:136:LYS:HB3	0.41	2.15	11	1
2:A:77:LYS:HG2	2:A:78:VAL:N	0.41	2.31	11	1
1:B:13:A:OP2	2:A:94:LYS:HG3	0.41	2.14	3	1
1:B:12:G:O5'	2:A:92:ASP:HA	0.41	2.16	4	1
2:A:80:GLY:O	2:A:81:ASN:C	0.41	2.59	4	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:A:94:LYS:N	2:A:94:LYS:HD2	0.41	2.30	1	1
2:A:133:GLY:O	2:A:134:LYS:CB	0.41	2.69	1	1
2:A:69:LYS:O	2:A:72:GLU:CB	0.41	2.69	7	1
2:A:111:ILE:HG13	2:A:161:ILE:HG21	0.41	1.93	14	1
2:A:153:LEU:HG	2:A:168:LEU:HD13	0.41	1.91	14	1
2:A:49:ARG:HG3	2:A:58:TYR:HB2	0.41	1.93	9	1
1:B:12:G:OP1	2:A:94:LYS:CG	0.41	2.68	6	1
2:A:25:LYS:HD2	2:A:79:PHE:CD1	0.41	2.50	6	1
2:A:166:VAL:HG22	2:A:167:SER:N	0.41	2.30	8	1
2:A:116:LEU:C	2:A:120:PHE:CE2	0.41	2.94	11	1
2:A:92:ASP:CG	2:A:93:SER:N	0.41	2.73	11	1
1:B:10:C:C2	2:A:97:ARG:HG3	0.41	2.51	11	1
2:A:20:ASN:ND2	2:A:20:ASN:O	0.41	2.53	2	1
2:A:17:PHE:CA	2:A:58:TYR:CD1	0.41	3.04	2	1
2:A:118:GLU:C	2:A:120:PHE:N	0.41	2.74	14	1
1:B:5:G:O5'	1:B:5:G:C8	0.41	2.68	9	1
2:A:93:SER:HA	2:A:96:VAL:CG2	0.41	2.45	9	1
2:A:49:ARG:HG2	2:A:58:TYR:CB	0.41	2.46	12	1
2:A:141:ILE:CG2	2:A:143:PHE:CE1	0.41	3.04	8	1
1:B:13:A:N7	2:A:52:THR:CA	0.41	2.84	8	1
1:B:12:G:OP1	2:A:89:LYS:HB3	0.41	2.16	11	1
2:A:21:LEU:O	2:A:23:PRO:HD3	0.41	2.16	11	1
2:A:41:ASN:HB3	2:A:43:LEU:CD2	0.41	2.45	3	1
2:A:17:PHE:CE1	2:A:56:PHE:CE2	0.41	3.09	3	1
2:A:143:PHE:CE2	2:A:148:ASP:CB	0.41	3.04	3	1
2:A:47:ASP:HB3	2:A:60:ASP:CG	0.41	2.36	4	2
2:A:45:VAL:HG23	2:A:59:VAL:HG23	0.41	1.93	4	1
1:B:11:C:HO2'	1:B:12:G:C5'	0.41	2.26	1	1
2:A:17:PHE:CD1	2:A:86:GLU:O	0.41	2.74	1	1
2:A:103:LEU:HD12	2:A:103:LEU:C	0.41	2.37	2	1
1:B:1:G:N2	1:B:2:G:C8	0.41	2.89	14	1
2:A:130:SER:O	2:A:131:GLN:HB2	0.41	2.14	14	1
2:A:136:LYS:O	2:A:138:ILE:HG12	0.41	2.15	14	1
2:A:158:GLY:HA2	2:A:161:ILE:CD1	0.41	2.46	14	1
2:A:49:ARG:CG	2:A:58:TYR:CB	0.41	2.98	9	1
2:A:143:PHE:CD2	2:A:148:ASP:HB3	0.41	2.51	9	1
2:A:17:PHE:HB3	2:A:86:GLU:CB	0.41	2.46	9	1
2:A:25:LYS:N	2:A:25:LYS:HE2	0.41	2.31	9	1
2:A:126:ILE:HG22	2:A:127:ARG:N	0.41	2.31	9	1
2:A:98:ALA:HB1	2:A:101:THR:CB	0.41	2.42	10	1
1:B:7:C:H2'	1:B:8:U:OP1	0.41	2.16	13	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:9:C:H2'	1:B:10:C:C5'	0.41	2.46	13	1
2:A:49:ARG:HG2	2:A:58:TYR:HB3	0.41	1.93	12	1
2:A:100:ARG:HD3	2:A:146:GLU:N	0.41	2.30	11	1
2:A:15:ASN:HB2	2:A:88:PRO:CG	0.41	2.46	11	1
2:A:103:LEU:HD21	2:A:105:LYS:HD2	0.41	1.93	4	1
2:A:119:VAL:O	2:A:156:LYS:HD2	0.41	2.16	4	1
2:A:152:ASN:O	2:A:154:GLU:N	0.41	2.54	2	1
2:A:157:GLN:NE2	2:A:168:LEU:HD12	0.40	2.31	12	1
2:A:12:THR:OG1	2:A:13:PRO:HD2	0.40	2.17	9	3
2:A:105:LYS:HE2	2:A:169:TYR:CD1	0.40	2.50	3	1
1:B:4:U:H2'	1:B:5:G:C8	0.40	2.51	4	6
2:A:17:PHE:HB3	2:A:86:GLU:C	0.40	2.36	3	1
2:A:111:ILE:CD1	2:A:161:ILE:CG1	0.40	2.98	3	1
1:B:13:A:N7	2:A:52:THR:HG23	0.40	2.30	1	1
2:A:77:LYS:CD	2:A:82:GLU:HA	0.40	2.45	14	1
2:A:48:VAL:CB	2:A:58:TYR:O	0.40	2.68	9	1
2:A:77:LYS:O	2:A:77:LYS:HG2	0.40	2.15	10	1
2:A:133:GLY:O	2:A:134:LYS:O	0.40	2.39	5	1
2:A:106:ASN:OD1	2:A:164:ARG:HD3	0.40	2.15	12	1
2:A:152:ASN:O	2:A:156:LYS:HG2	0.40	2.16	12	1
1:B:10:C:C4'	1:B:11:C:OP1	0.40	2.68	11	1
2:A:87:LYS:CB	2:A:88:PRO:CD	0.40	2.99	11	1
2:A:135:SER:O	2:A:136:LYS:HB2	0.40	2.16	4	1
2:A:136:LYS:HG3	2:A:138:ILE:CD1	0.40	2.46	1	1
2:A:76:LEU:HD13	2:A:85:LEU:CD2	0.40	2.45	2	1
2:A:121:GLU:C	2:A:123:ALA:N	0.40	2.74	5	1
2:A:103:LEU:HD21	2:A:105:LYS:NZ	0.40	2.30	8	1
2:A:148:ASP:O	2:A:152:ASN:CB	0.40	2.69	11	1
2:A:153:LEU:HD22	2:A:170:TYR:CB	0.40	2.45	11	1
2:A:37:LEU:HD22	2:A:41:ASN:OD1	0.40	2.16	11	1
1:B:13:A:O4'	2:A:94:LYS:HB3	0.40	2.16	11	1
1:B:13:A:N6	2:A:94:LYS:CG	0.40	2.83	1	1
2:A:157:GLN:O	2:A:158:GLY:C	0.40	2.60	7	1
2:A:111:ILE:CD1	2:A:115:GLU:HG2	0.40	2.46	7	1
2:A:150:GLU:CG	2:A:151:LYS:N	0.40	2.84	7	1
2:A:65:GLU:HA	2:A:65:GLU:OE1	0.40	2.15	7	1
1:B:13:A:O2'	2:A:95:LYS:CD	0.40	2.69	14	1
2:A:138:ILE:CG2	2:A:139:ALA:N	0.40	2.84	5	1
2:A:47:ASP:O	2:A:59:VAL:HB	0.40	2.16	5	1
2:A:21:LEU:CD2	2:A:30:LEU:HB3	0.40	2.46	12	1
2:A:78:VAL:HG23	2:A:79:PHE:H	0.40	1.77	12	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:18:A:O2'	1:B:19:U:O5'	0.40	2.40	8	1
2:A:152:ASN:HA	2:A:156:LYS:HG2	0.40	1.94	11	1
2:A:92:ASP:OD2	2:A:97:ARG:N	0.40	2.54	11	1
2:A:77:LYS:CD	2:A:77:LYS:N	0.40	2.84	11	1
2:A:119:VAL:O	2:A:156:LYS:CE	0.40	2.70	4	1
2:A:129:VAL:HG11	2:A:136:LYS:NZ	0.40	2.31	1	1
2:A:129:VAL:O	2:A:136:LYS:HB2	0.40	2.16	2	1
1:B:9:C:C5'	1:B:10:C:OP2	0.40	2.53	14	1
2:A:157:GLN:NE2	2:A:157:GLN:O	0.40	2.54	14	1
2:A:30:LEU:CD1	2:A:55:LYS:O	0.40	2.70	9	1
2:A:22:ASN:HB2	2:A:81:ASN:HB2	0.40	1.93	10	1
1:B:12:G:OP2	2:A:94:LYS:HB2	0.40	2.17	6	1
1:B:12:G:C8	2:A:50:THR:O	0.40	2.75	5	1
2:A:115:GLU:CD	2:A:118:GLU:OE1	0.40	2.59	11	1
2:A:98:ALA:O	2:A:101:THR:HG23	0.40	2.16	3	1
2:A:75:GLY:O	2:A:76:LEU:HB2	0.40	2.17	4	1
2:A:74:THR:O	2:A:76:LEU:HG	0.40	2.16	1	1
2:A:61:PHE:O	2:A:62:GLU:C	0.40	2.60	2	1
1:B:19:U:C2'	1:B:20:C:O5'	0.40	2.70	14	1
2:A:131:GLN:HB2	2:A:135:SER:O	0.40	2.17	14	1
2:A:158:GLY:HA2	2:A:165:SER:O	0.40	2.16	13	1
2:A:101:THR:O	2:A:171:THR:CB	0.40	2.70	13	1
1:B:12:G:O2'	1:B:13:A:H5"	0.40	2.15	13	1
2:A:106:ASN:O	2:A:107:LEU:HG	0.40	2.17	6	1
2:A:48:VAL:CG2	2:A:48:VAL:O	0.40	2.69	6	1
2:A:142:GLU:C	2:A:143:PHE:CD1	0.40	2.95	5	1
1:B:12:G:C5'	2:A:94:LYS:HG2	0.40	2.46	5	1
1:B:12:G:O5'	2:A:94:LYS:HG2	0.40	2.16	5	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	A	162/175 (93%)	96±4 (59±2%)	39±4 (24±3%)	27±4 (17±3%)	0 4

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	2268/2450 (93%)	1338 (59%)	551 (24%)	379 (17%)	0 4

All 87 unique Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
2	A	157	GLN	13
2	A	53	ASN	12
2	A	116	LEU	10
2	A	165	SER	10
2	A	166	VAL	9
2	A	52	THR	9
2	A	14	PHE	9
2	A	130	SER	9
2	A	22	ASN	8
2	A	77	LYS	8
2	A	136	LYS	8
2	A	160	GLU	7
2	A	161	ILE	7
2	A	82	GLU	7
2	A	74	THR	7
2	A	97	ARG	7
2	A	111	ILE	7
2	A	106	ASN	7
2	A	54	ARG	6
2	A	45	VAL	6
2	A	75	GLY	6
2	A	64	ALA	6
2	A	99	ALA	5
2	A	91	ARG	5
2	A	98	ALA	5
2	A	55	LYS	5
2	A	21	LEU	5
2	A	109	PHE	5
2	A	27	VAL	5
2	A	63	SER	5
2	A	24	ASN	5
2	A	94	LYS	5
2	A	110	ASN	5
2	A	92	ASP	5
2	A	113	GLU	5
2	A	88	PRO	5

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Mol	Chain	Res	Type	Models (Total)
2	A	95	LYS	4
2	A	135	SER	4
2	A	11	THR	4
2	A	25	LYS	4
2	A	43	LEU	4
2	A	76	LEU	4
2	A	26	SER	4
2	A	96	VAL	4
2	A	80	GLY	4
2	A	79	PHE	4
2	A	35	SER	4
2	A	114	ASP	4
2	A	162	ASP	4
2	A	20	ASN	4
2	A	89	LYS	4
2	A	73	LEU	4
2	A	123	ALA	3
2	A	132	ASP	3
2	A	158	GLY	3
2	A	48	VAL	3
2	A	151	LYS	3
2	A	122	ASP	3
2	A	44	ALA	3
2	A	121	GLU	3
2	A	93	SER	3
2	A	42	ASP	2
2	A	119	VAL	2
2	A	90	GLY	2
2	A	137	GLY	2
2	A	78	VAL	2
2	A	118	GLU	2
2	A	144	LYS	2
2	A	163	GLY	2
2	A	131	GLN	2
2	A	145	SER	2
2	A	159	ALA	2
2	A	153	LEU	2
2	A	46	VAL	2
2	A	108	SER	2
2	A	164	ARG	1
2	A	112	THR	1
2	A	120	PHE	1

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Mol	Chain	Res	Type	Models (Total)
2	A	83	ILE	1
2	A	156	LYS	1
2	A	134	LYS	1
2	A	147	ALA	1
2	A	13	PRO	1
2	A	124	LEU	1
2	A	12	THR	1
2	A	100	ARG	1
2	A	23	PRO	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	A	137/147 (93%)	90±6 (65±4%)	47±6 (35±4%)	1 10
All	All	1918/2058 (93%)	1255 (65%)	663 (35%)	1 10

All 119 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	A	168	LEU	14
2	A	58	TYR	14
2	A	55	LYS	13
2	A	102	LEU	12
2	A	50	THR	12
2	A	43	LEU	12
2	A	138	ILE	12
2	A	105	LYS	11
2	A	94	LYS	11
2	A	171	THR	10
2	A	95	LYS	10
2	A	49	ARG	10
2	A	165	SER	10
2	A	107	LEU	10
2	A	91	ARG	9
2	A	71	LEU	9

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Mol	Chain	Res	Type	Models (Total)
2	A	140	TYR	9
2	A	11	THR	9
2	A	100	ARG	9
2	A	164	ARG	8
2	A	120	PHE	8
2	A	21	LEU	8
2	A	37	LEU	8
2	A	156	LYS	8
2	A	167	SER	8
2	A	122	ASP	8
2	A	60	ASP	8
2	A	77	LYS	8
2	A	56	PHE	8
2	A	114	ASP	8
2	A	89	LYS	8
2	A	87	LYS	7
2	A	132	ASP	7
2	A	153	LEU	7
2	A	76	LEU	7
2	A	145	SER	7
2	A	109	PHE	7
2	A	125	GLU	7
2	A	103	LEU	7
2	A	52	THR	7
2	A	85	LEU	7
2	A	67	LEU	7
2	A	93	SER	7
2	A	31	LYS	6
2	A	25	LYS	6
2	A	117	LYS	6
2	A	17	PHE	6
2	A	144	LYS	6
2	A	26	SER	6
2	A	16	LEU	6
2	A	86	GLU	6
2	A	108	SER	6
2	A	35	SER	6
2	A	72	GLU	5
2	A	42	ASP	5
2	A	141	ILE	5
2	A	47	ASP	5
2	A	84	LYS	5

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Mol	Chain	Res	Type	Models (Total)
2	A	134	LYS	5
2	A	54	ARG	5
2	A	96	VAL	5
2	A	115	GLU	5
2	A	74	THR	5
2	A	136	LYS	5
2	A	112	THR	5
2	A	106	ASN	5
2	A	157	GLN	5
2	A	29	GLU	4
2	A	160	GLU	4
2	A	148	ASP	4
2	A	166	VAL	4
2	A	68	GLU	4
2	A	143	PHE	4
2	A	62	GLU	4
2	A	81	ASN	4
2	A	128	LEU	4
2	A	154	GLU	4
2	A	82	GLU	4
2	A	66	ASP	4
2	A	22	ASN	4
2	A	116	LEU	4
2	A	92	ASP	4
2	A	97	ARG	4
2	A	69	LYS	4
2	A	155	GLU	4
2	A	130	SER	4
2	A	121	GLU	4
2	A	41	ASN	3
2	A	101	THR	3
2	A	83	ILE	3
2	A	48	VAL	3
2	A	27	VAL	3
2	A	63	SER	3
2	A	110	ASN	3
2	A	150	GLU	3
2	A	131	GLN	3
2	A	12	THR	3
2	A	36	GLU	3
2	A	118	GLU	3
2	A	20	ASN	3

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Mol	Chain	Res	Type	Models (Total)
2	A	146	GLU	3
2	A	73	LEU	3
2	A	53	ASN	2
2	A	129	VAL	2
2	A	34	ILE	2
2	A	124	LEU	2
2	A	162	ASP	2
2	A	15	ASN	1
2	A	161	ILE	1
2	A	79	PHE	1
2	A	152	ASN	1
2	A	59	VAL	1
2	A	170	TYR	1
2	A	32	VAL	1
2	A	127	ARG	1
2	A	113	GLU	1
2	A	78	VAL	1
2	A	142	GLU	1
2	A	40	LYS	1

6.3.3 RNA

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers	Suiteness
1	B	21/21 (100%)	13±1 (60±6%)	4±1 (17±7%)	0.06±0.02
All	All	286/294 (97%)	177 (62%)	49 (17%)	0.06

The overall RNA backbone suiteness is 0.06.

All unique RNA backbone outliers are listed below:

Mol	Chain	Res	Type	Models (Total)
1	B	14	G	14
1	B	12	G	14
1	B	20	C	14
1	B	10	C	14
1	B	13	A	14
1	B	11	C	14
1	B	8	U	14
1	B	15	U	13
1	B	6	C	13
1	B	9	C	12
1	B	17	C	10

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Mol	Chain	Res	Type	Models (Total)
1	B	16	G	7
1	B	2	G	6
1	B	4	U	6
1	B	7	C	5
1	B	19	U	5
1	B	18	A	2

All unique RNA pucker outliers are listed below:

Mol	Chain	Res	Type	Models (Total)
1	B	11	C	12
1	B	13	A	10
1	B	12	G	7
1	B	1	G	6
1	B	8	U	6
1	B	7	C	3
1	B	14	G	3
1	B	15	U	1
1	B	10	C	1

6.4 Non-standard residues in protein, DNA, RNA chains

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

6.5 Carbohydrates

There are no carbohydrates in this entry.

6.6 Ligand geometry

There are no ligands in this entry.

6.7 Other polymers

There are no such molecules in this entry.

6.8 Polymer linkage issues

There are no chain breaks in this entry.

7 Chemical shift validation

No chemical shift data were provided