



# Full wwPDB NMR Structure Validation Report ⓘ

Feb 21, 2020 – 05:00 PM EST

PDB ID : 2KM8  
Title : Interdomain RRM packing contributes to RNA recognition in the rna15, hrp1, anchor RNA 3' processing ternary complex  
Authors : Leeper, T.C.; Varani, G.  
Deposited on : 2009-07-24

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

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

Cyrange : Kirchner and Güntert (2011)  
NmrClust : Kelley et al. (1996)  
MolProbity : 4.02b-467  
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)  
RCI : v\_1n\_11\_5\_13\_A (Berjanski et al., 2005)  
PANAV : Wang et al. (2010)  
ShiftChecker : 2.8  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.8

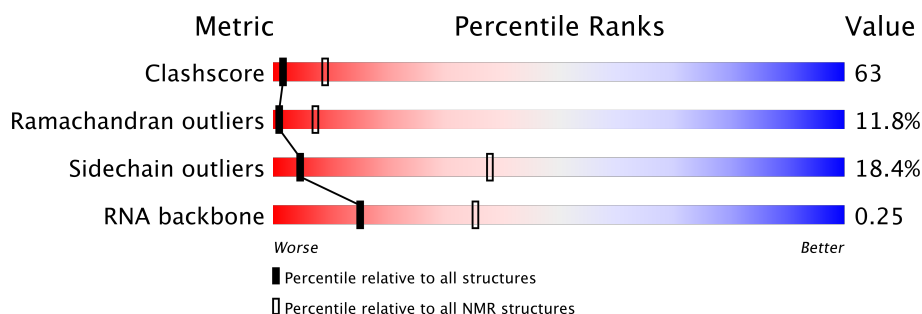
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*SOLUTION NMR*

The overall completeness of chemical shifts assignment is 25%.

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	136327	12091
Ramachandran outliers	132723	10835
Sidechain outliers	132532	10811
RNA backbone	3747	647

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. A cyan segment indicates the fraction of residues that are not part of the well-defined cores, and a grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	A	13	<div> <div style="width: 77%; background-color: orange;"></div> <div style="width: 23%; background-color: red;"></div> </div> <div>77% 23%</div>
2	B	84	<div> <div style="width: 14%; background-color: green;"></div> <div style="width: 65%; background-color: yellow;"></div> <div style="width: 17%; background-color: orange;"></div> <div style="width: 2%; background-color: red;"></div> <div style="width: 2%; background-color: cyan;"></div> </div> <div>14% 65% 17% ..</div>
3	C	167	<div> <div style="width: 23%; background-color: green;"></div> <div style="width: 62%; background-color: yellow;"></div> <div style="width: 12%; background-color: orange;"></div> <div style="width: 3%; background-color: cyan;"></div> </div> <div>23% 62% 12% .</div>

## 2 Ensemble composition and analysis

This entry contains 10 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	B:22-B:103, C:158-C:319 (244)	1.31	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 4 clusters. No single-model clusters were found.

Cluster number	Models
1	1, 3, 4, 6
2	7, 8
3	2, 5
4	9, 10

### 3 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 4375 atoms, of which 2102 are hydrogens and 0 are deuteriums.

- Molecule 1 is a RNA chain called 5'-R(P\*UP\*AP\*UP\*AP\*UP\*AP\*UP\*AP\*AP\*UP\*AP\*AP\*U)-3'.

Mol	Chain	Residues	Atoms						Trace
1	A	13	Total	C	H	N	O	P	0
			414	124	139	47	91	13	

- Molecule 2 is a protein called mRNA 3'-end-processing protein RNA15.

Mol	Chain	Residues	Atoms						Trace
2	B	84	Total	C	H	N	O	S	0
			1296	411	640	112	129	4	

- Molecule 3 is a protein called Nuclear polyadenylated RNA-binding protein 4.


Mol	Chain	Residues	Atoms						Trace
3	C	167	Total	C	H	N	O	S	0
			2665	849	1323	232	256	5	

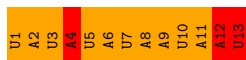
## 4 Residue-property plots [i](#)

### 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.

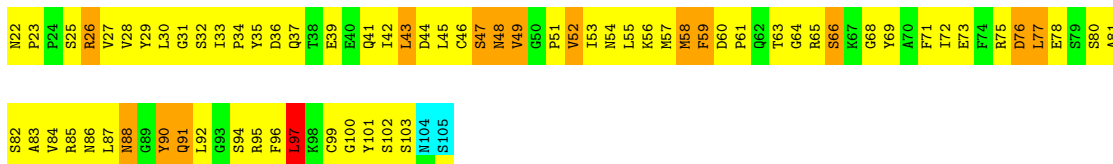
- Molecule 1: 5'-R(P\*UP\*AP\*UP\*AP\*UP\*AP\*UP\*AP\*AP\*UP\*AP\*AP\*U)-3'

Chain A: 




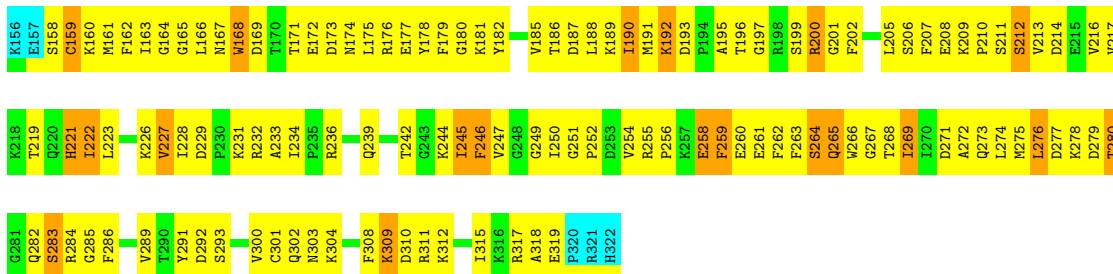
- Molecule 2: mRNA 3'-end-processing protein RNA15

Chain B: 



- Molecule 3: Nuclear polyadenylated RNA-binding protein 4

Chain C: 



### 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)

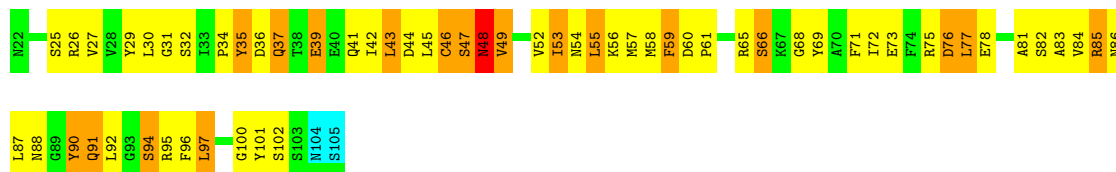
- Molecule 1: 5'-R(P\*UP\*AP\*UP\*AP\*UP\*AP\*UP\*AP\*AP\*UP\*AP\*AP\*U)-3'

Chain A:



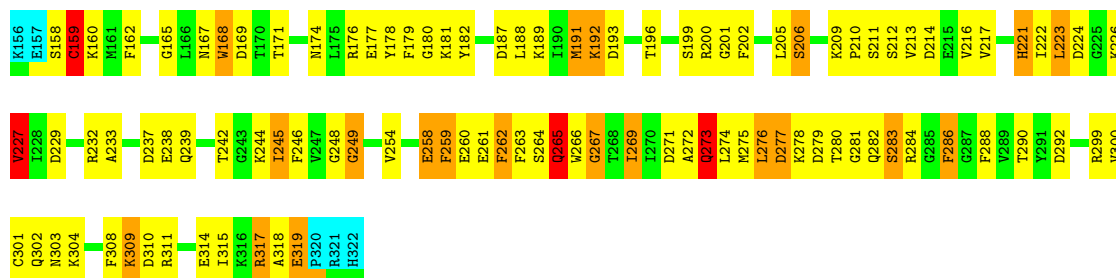
- Molecule 2: mRNA 3'-end-processing protein RNA15

Chain B:



- Molecule 3: Nuclear polyadenylated RNA-binding protein 4

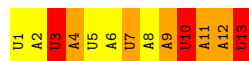
Chain C:



### 4.2.2 Score per residue for model 2

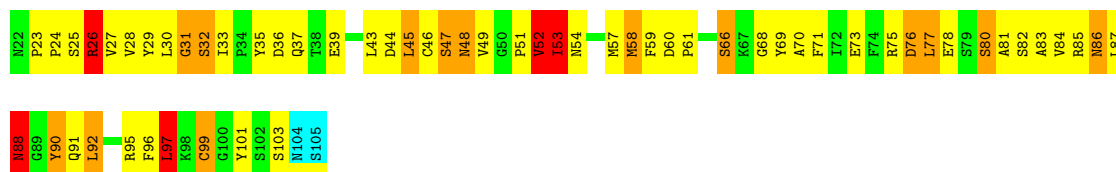
- Molecule 1: 5'-R(P\*UP\*AP\*UP\*AP\*UP\*AP\*UP\*AP\*AP\*UP\*AP\*AP\*U)-3'

Chain A:

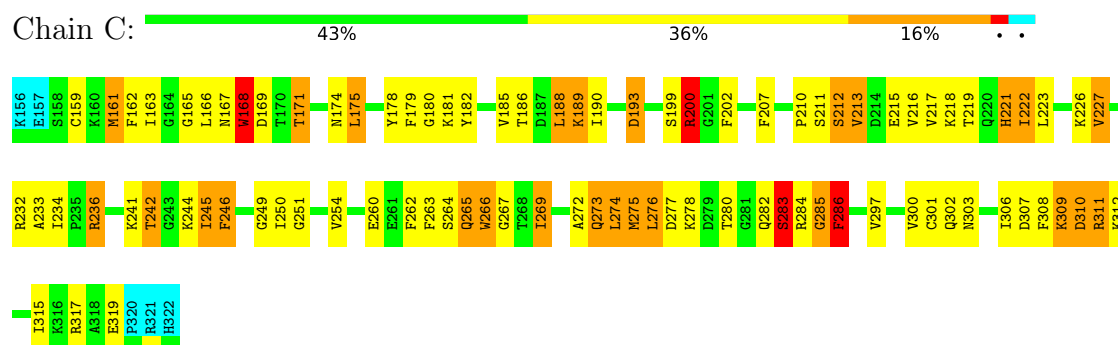


- Molecule 2: mRNA 3'-end-processing protein RNA15

Chain B:

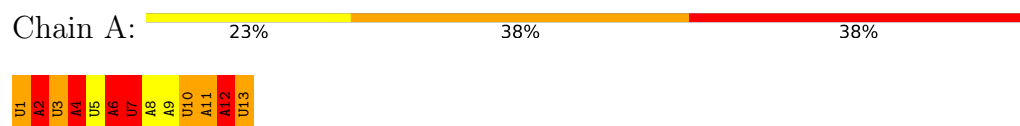


- Molecule 3: Nuclear polyadenylated RNA-binding protein 4

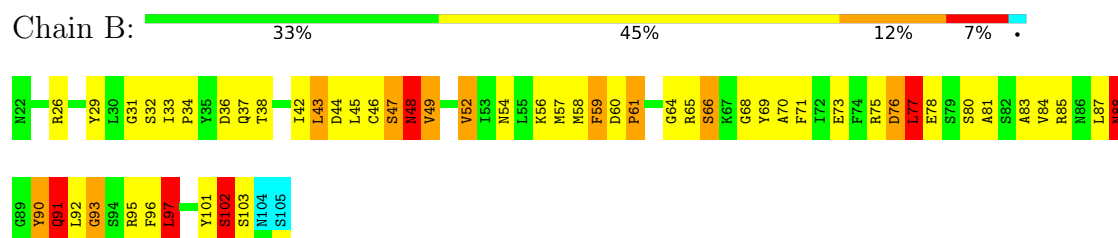


#### 4.2.3 Score per residue for model 3

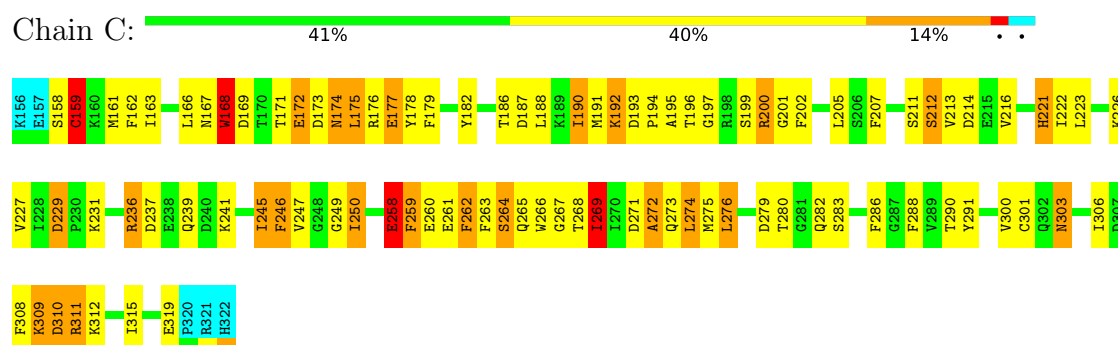
- Molecule 1: 5'-R(P\*UP\*AP\*UP\*AP\*UP\*AP\*UP\*AP\*AP\*UP\*AP\*AP\*U)-3'



- Molecule 2: mRNA 3'-end-processing protein RNA15



- Molecule 3: Nuclear polyadenylated RNA-binding protein 4



#### 4.2.4 Score per residue for model 4

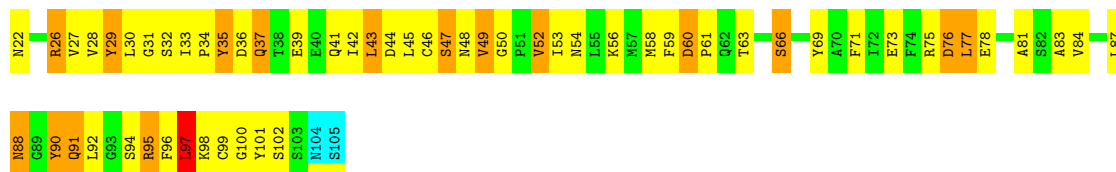
- Molecule 1: 5'-R(P\*UP\*AP\*UP\*AP\*UP\*AP\*UP\*AP\*AP\*UP\*AP\*AP\*U)-3'

Chain A: 23% 38% 38%



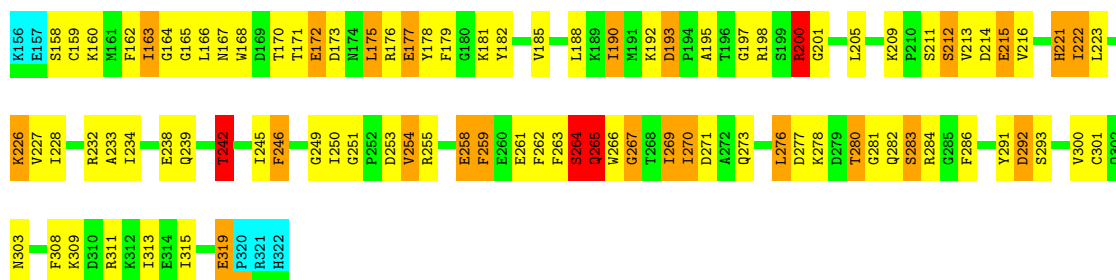
- Molecule 2: mRNA 3'-end-processing protein RNA15

Chain B: 29% 49% 19% ..



- Molecule 3: Nuclear polyadenylated RNA-binding protein 4

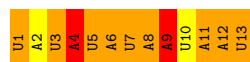
Chain C: 41% 40% 14% ..



#### 4.2.5 Score per residue for model 5

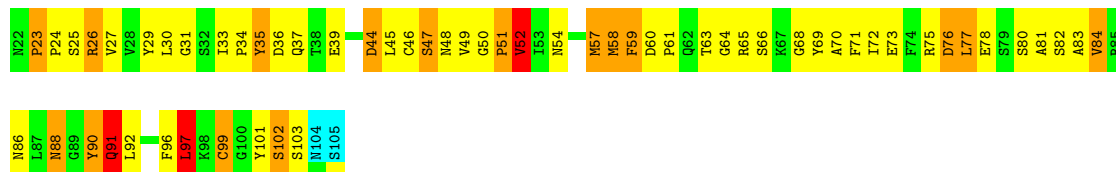
- Molecule 1: 5'-R(P\*UP\*AP\*UP\*AP\*UP\*AP\*UP\*AP\*AP\*UP\*AP\*AP\*U)-3'

Chain A: 15% 69% 15%



- Molecule 2: mRNA 3'-end-processing protein RNA15

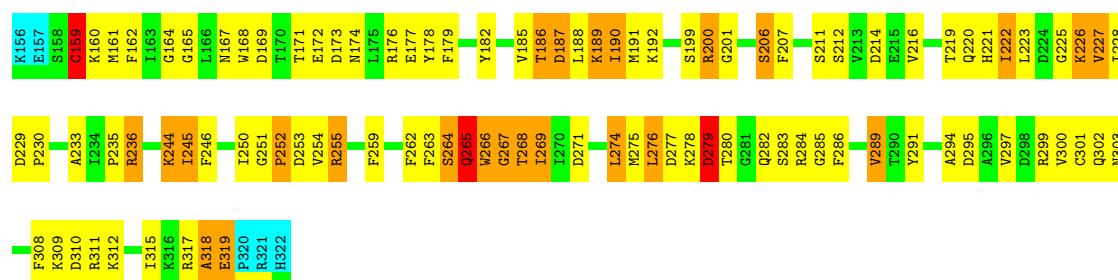
Chain B: 27% 48% 19% ..



- Molecule 3: Nuclear polyadenylated RNA-binding protein 4

Chain C: 38% 43% 14% ..





#### 4.2.6 Score per residue for model 6

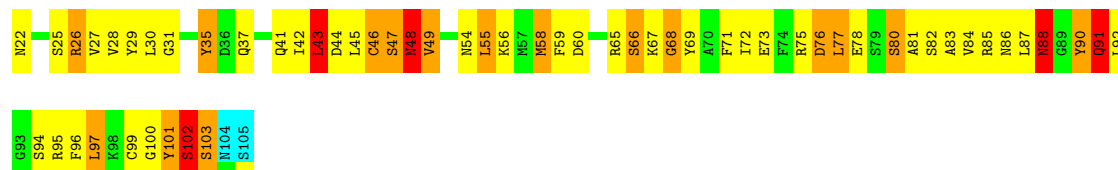
- Molecule 1: 5'-R(P\*UP\*AP\*UP\*AP\*UP\*AP\*UP\*AP\*AP\*UP\*AP\*AP\*U)-3'

Chain A: 62% 38%



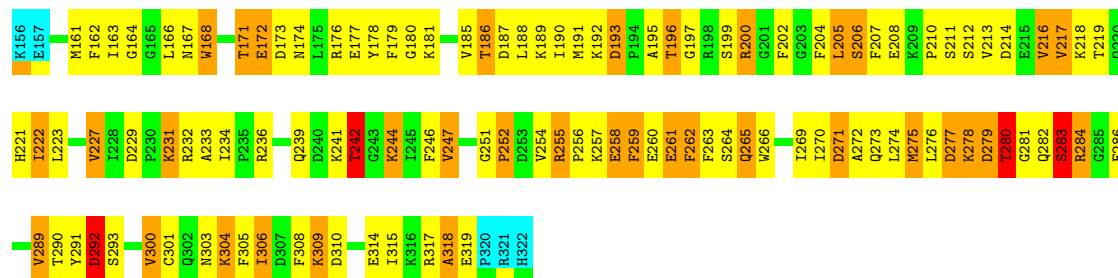
- Molecule 2: mRNA 3'-end-processing protein RNA15

Chain B: 29% 44% 19% 6%



- Molecule 3: Nuclear polyadenylated RNA-binding protein 4

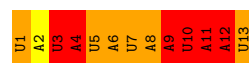
Chain C: 29% 44% 21% 6%



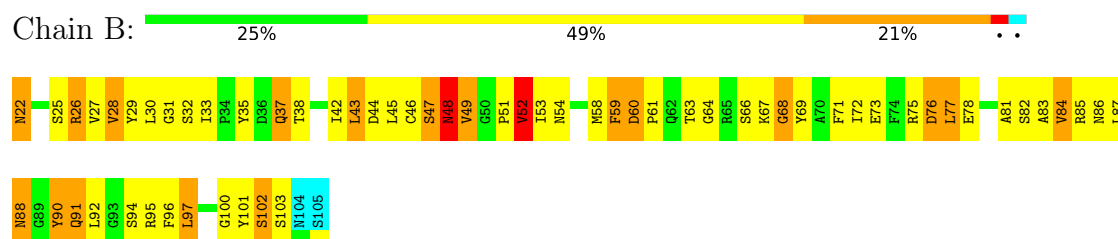
#### 4.2.7 Score per residue for model 7

- Molecule 1: 5'-R(P\*UP\*AP\*UP\*AP\*UP\*AP\*UP\*AP\*AP\*UP\*AP\*AP\*U)-3'

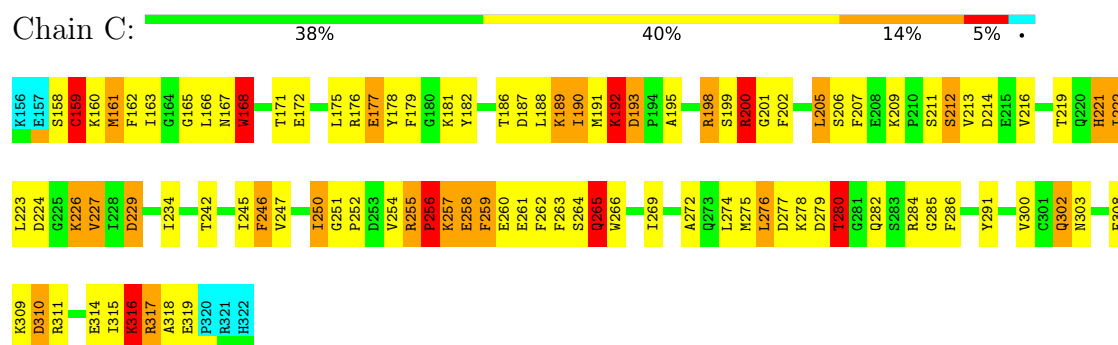
Chain A: 8% 46% 46%



- Molecule 2: mRNA 3'-end-processing protein RNA15



- Molecule 3: Nuclear polyadenylated RNA-binding protein 4

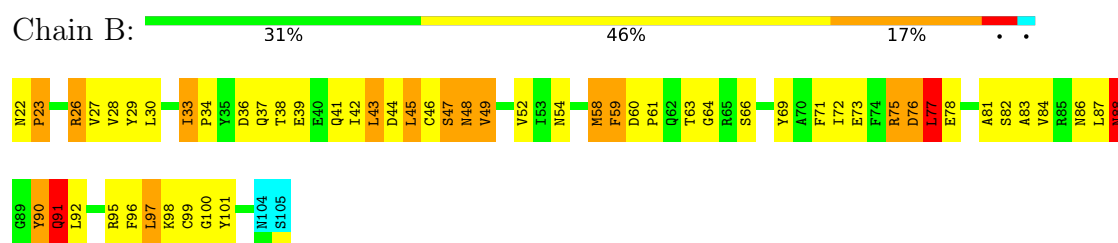


#### 4.2.8 Score per residue for model 8

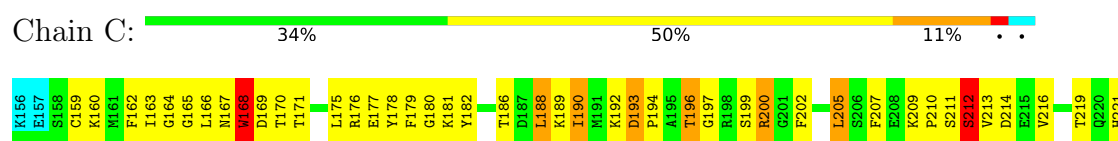
- Molecule 1: 5'-R(P\*UP\*AP\*UP\*AP\*UP\*AP\*UP\*AP\*AP\*UP\*AP\*AP\*U)-3'

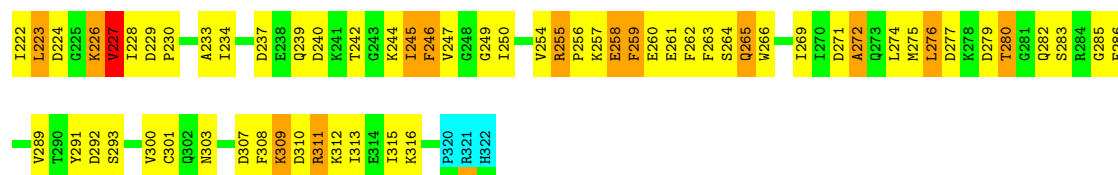


- Molecule 2: mRNA 3'-end-processing protein RNA15



- Molecule 3: Nuclear polyadenylated RNA-binding protein 4



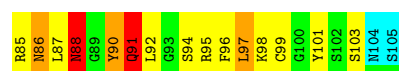
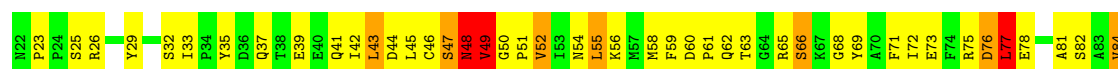


#### 4.2.9 Score per residue for model 9

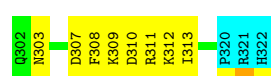
- Molecule 1: 5'-R(P\*UP\*AP\*UP\*AP\*UP\*AP\*UP\*AP\*AP\*UP\*AP\*AP\*U)-3'



- Molecule 2: mRNA 3'-end-processing protein RNA15



- Molecule 3: Nuclear polyadenylated RNA-binding protein 4

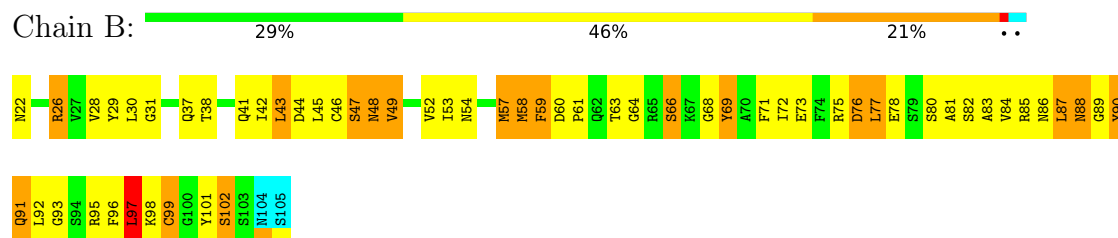


#### 4.2.10 Score per residue for model 10

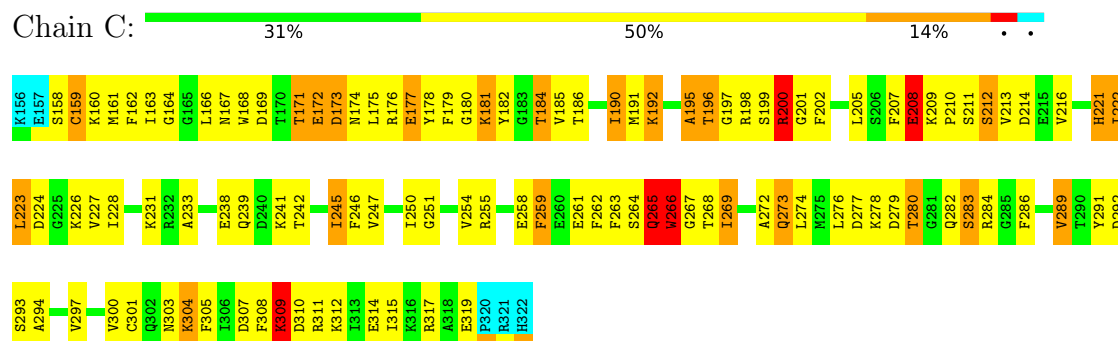
- Molecule 1: 5'-R(P\*UP\*AP\*UP\*AP\*UP\*AP\*UP\*AP\*AP\*UP\*AP\*AP\*U)-3'



- Molecule 2: mRNA 3'-end-processing protein RNA15



• Molecule 3: Nuclear polyadenylated RNA-binding protein 4



## 5 Refinement protocol and experimental data overview

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

Of the 100 calculated structures, 10 were deposited, based on the following criterion: *structures with the lowest energy*.

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

Software name	Classification	Version
X-PLOR NIH	refinement	
CYANA	structure solution	

The following table shows chemical shift validation statistics as aggregates over all chemical shift files. Detailed validation can be found in section 6 of this report.

Chemical shift file(s)	2km8_cs.cif
Number of chemical shift lists	1
Total number of shifts	922
Number of shifts mapped to atoms	922
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	25%

No validations of the models with respect to experimental NMR restraints is performed at this time.

COVALENT-GEOMETRY INFOmissingINFO

### 5.1 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	A	275	139	138	98±23
2	B	641	629	626	99±25
3	C	1295	1274	1273	134±14
All	All	22110	20420	20370	2660

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 63.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:11:A:H3'	2:B:69:TYR:N	1.31	1.37	7	1
1:A:6:A:H4'	1:A:7:U:H5'	1.13	1.17	9	7
1:A:12:A:H5'	2:B:67:LYS:O	1.09	1.47	7	1
1:A:12:A:C5'	2:B:67:LYS:O	1.07	2.00	7	1
1:A:10:U:H5'	2:B:71:PHE:CE1	1.03	1.86	5	4
1:A:12:A:P	2:B:58:MET:O	1.03	2.17	7	1
1:A:12:A:O5'	2:B:68:GLY:HA2	1.02	1.54	7	1
2:B:49:VAL:HG11	2:B:83:ALA:HB2	0.98	1.29	5	4
1:A:11:A:H4'	2:B:58:MET:C	0.97	1.79	7	1
1:A:3:U:O2'	1:A:4:A:H5'	0.96	1.60	2	1
2:B:90:TYR:CE1	2:B:97:LEU:HD11	0.95	1.96	5	2
1:A:12:A:HO2'	1:A:13:U:H6	0.95	0.98	3	4
3:C:188:LEU:HD12	3:C:189:LYS:N	0.94	1.76	8	2
1:A:12:A:P	2:B:68:GLY:HA2	0.94	2.03	7	1
1:A:6:A:O4'	1:A:7:U:H5''	0.94	1.62	3	2
1:A:6:A:H4'	1:A:7:U:C5'	0.93	1.94	5	8
1:A:6:A:C4'	1:A:7:U:H5'	0.92	1.94	4	7
2:B:47:SER:O	2:B:49:VAL:N	0.92	2.02	9	7
1:A:11:A:H4'	2:B:58:MET:O	0.92	1.63	7	1
1:A:11:A:H5'	2:B:69:TYR:O	0.91	1.64	7	1
1:A:9:A:H5''	2:B:69:TYR:OH	0.90	1.65	6	3
3:C:179:PHE:O	3:C:181:LYS:N	0.89	2.05	9	5
1:A:11:A:O2'	2:B:68:GLY:N	0.89	2.05	7	1
1:A:11:A:H3'	2:B:69:TYR:H	0.88	1.28	7	1
3:C:269:ILE:HG23	3:C:291:TYR:CE1	0.88	2.03	3	2
1:A:2:A:HO2'	1:A:3:U:H6	0.88	0.97	2	3
1:A:11:A:C3'	2:B:69:TYR:N	0.87	2.32	7	1
1:A:9:A:HO2'	1:A:10:U:H6	0.87	1.07	2	1
1:A:11:A:HO2'	1:A:12:A:H8	0.87	0.92	10	4
3:C:276:LEU:H	3:C:276:LEU:HD22	0.87	1.30	7	1
2:B:80:SER:O	2:B:84:VAL:HG22	0.86	1.70	10	1
1:A:6:A:C4'	1:A:7:U:H5''	0.86	2.01	8	2
2:B:97:LEU:N	2:B:97:LEU:HD12	0.85	1.86	5	1
2:B:72:ILE:N	2:B:72:ILE:HD12	0.85	1.86	5	3
1:A:9:A:H2'	1:A:10:U:C6	0.85	2.05	3	1
3:C:274:LEU:O	3:C:274:LEU:HD23	0.85	1.70	5	1
1:A:12:A:C8	2:B:68:GLY:N	0.85	2.44	7	1
1:A:1:U:HO2'	1:A:2:A:H8	0.85	0.90	8	5
1:A:9:A:H5''	2:B:69:TYR:CZ	0.85	2.06	2	2
3:C:245:ILE:HD13	3:C:245:ILE:O	0.84	1.71	9	1
1:A:10:U:H5''	2:B:69:TYR:CZ	0.84	2.07	10	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:8:A:H4'	2:B:95:ARG:NH2	0.84	1.88	10	2
1:A:4:A:C6	3:C:168:TRP:CD1	0.84	2.65	6	1
1:A:9:A:H4'	2:B:69:TYR:CE1	0.83	2.08	8	4
3:C:274:LEU:HD23	3:C:274:LEU:O	0.83	1.73	3	2
2:B:72:ILE:HD12	2:B:72:ILE:N	0.83	1.88	9	3
1:A:2:A:H4'	3:C:286:PHE:CD1	0.83	2.08	10	2
3:C:226:LYS:O	3:C:227:VAL:HG13	0.83	1.74	8	2
1:A:10:U:H5'	2:B:71:PHE:CZ	0.83	2.07	7	6
1:A:7:U:H4'	3:C:202:PHE:CZ	0.82	2.09	8	3
1:A:11:A:C4'	2:B:58:MET:O	0.82	2.28	7	1
2:B:97:LEU:HD12	2:B:97:LEU:N	0.81	1.90	2	3
1:A:12:A:H5''	2:B:35:TYR:OH	0.81	1.75	7	1
3:C:226:LYS:O	3:C:227:VAL:HG23	0.81	1.76	5	1
1:A:9:A:H1'	2:B:71:PHE:CZ	0.81	2.11	9	2
1:A:9:A:N3	2:B:71:PHE:CZ	0.80	2.50	8	8
1:A:10:U:H5'	2:B:71:PHE:CE2	0.80	2.11	7	1
3:C:276:LEU:HD12	3:C:276:LEU:H	0.80	1.34	3	1
1:A:10:U:H4'	2:B:71:PHE:CE2	0.80	2.12	5	3
1:A:9:A:H5''	2:B:69:TYR:CE2	0.80	2.10	9	1
3:C:210:PRO:O	3:C:213:VAL:HG22	0.80	1.75	6	2
2:B:90:TYR:CD1	2:B:97:LEU:HD11	0.79	2.12	5	2
3:C:221:HIS:C	3:C:222:ILE:HD13	0.79	1.98	4	3
3:C:276:LEU:HD12	3:C:276:LEU:N	0.79	1.92	3	1
3:C:226:LYS:NZ	3:C:280:THR:HG23	0.79	1.91	5	1
1:A:6:A:H5'	1:A:8:A:OP2	0.79	1.76	3	2
3:C:212:SER:O	3:C:216:VAL:HG23	0.79	1.78	3	8
1:A:11:A:O2'	1:A:12:A:H8	0.78	1.62	4	6
2:B:77:LEU:O	2:B:81:ALA:HB2	0.78	1.78	9	10
1:A:5:U:H1'	3:C:201:GLY:O	0.78	1.77	7	1
3:C:222:ILE:N	3:C:222:ILE:HD13	0.78	1.94	4	1
3:C:309:LYS:O	3:C:311:ARG:N	0.78	2.16	3	2
1:A:9:A:H4'	2:B:69:TYR:CE2	0.78	2.14	1	2
1:A:9:A:H2'	1:A:10:U:C5	0.78	2.14	3	2
1:A:6:A:H1'	1:A:7:U:OP2	0.78	1.79	3	3
1:A:2:A:H4'	3:C:286:PHE:CE1	0.77	2.14	5	2
1:A:10:U:H2'	1:A:11:A:H8	0.77	1.39	10	4
1:A:10:U:OP2	2:B:69:TYR:CG	0.77	2.37	5	2
1:A:1:U:O2'	1:A:2:A:H8	0.77	1.63	8	5
3:C:303:ASN:O	3:C:303:ASN:ND2	0.77	2.18	3	1
1:A:10:U:H6	1:A:10:U:O5'	0.77	1.62	6	2
1:A:9:A:N3	2:B:71:PHE:CE1	0.76	2.53	5	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:7:U:N3	3:C:202:PHE:CG	0.76	2.54	6	1
3:C:221:HIS:CD2	3:C:221:HIS:H	0.76	1.96	10	1
2:B:45:LEU:O	2:B:45:LEU:HD12	0.76	1.81	8	1
1:A:5:U:C2	3:C:162:PHE:CE2	0.75	2.74	6	4
3:C:163:ILE:HD11	3:C:205:LEU:HD12	0.75	1.58	10	1
3:C:276:LEU:N	3:C:276:LEU:HD13	0.75	1.97	7	1
1:A:12:A:H8	2:B:68:GLY:N	0.75	1.79	7	1
3:C:275:MET:C	3:C:276:LEU:HD13	0.75	2.02	7	1
3:C:308:PHE:O	3:C:309:LYS:O	0.74	2.04	2	2
3:C:258:GLU:O	3:C:261:GLU:N	0.74	2.20	8	8
3:C:163:ILE:HG22	3:C:166:LEU:HD21	0.74	1.58	2	1
1:A:6:A:C5	3:C:162:PHE:CE2	0.74	2.75	6	7
1:A:10:U:HO2'	1:A:11:A:H8	0.74	1.19	8	2
1:A:10:U:H4'	2:B:71:PHE:CZ	0.74	2.17	6	3
1:A:9:A:C2	2:B:29:TYR:CZ	0.74	2.76	5	9
1:A:10:U:H2'	1:A:11:A:C8	0.74	2.17	10	7
1:A:9:A:C4	2:B:29:TYR:CE2	0.73	2.76	4	1
1:A:9:A:H4'	2:B:69:TYR:CD1	0.73	2.17	2	1
1:A:4:A:C4	3:C:168:TRP:CZ2	0.73	2.77	1	3
1:A:9:A:C2	2:B:71:PHE:CE2	0.73	2.76	4	4
1:A:9:A:C2	2:B:29:TYR:CE1	0.72	2.77	6	8
3:C:276:LEU:N	3:C:276:LEU:HD22	0.72	1.98	7	1
1:A:10:U:O2'	1:A:11:A:H8	0.72	1.68	8	2
1:A:9:A:N1	2:B:29:TYR:CZ	0.72	2.58	10	5
3:C:188:LEU:HD12	3:C:188:LEU:O	0.72	1.84	4	1
1:A:12:A:C8	2:B:67:LYS:N	0.72	2.57	7	1
1:A:4:A:C6	3:C:168:TRP:CZ3	0.72	2.77	4	9
1:A:3:U:H5'	3:C:286:PHE:CZ	0.72	2.20	9	6
1:A:6:A:C6	3:C:162:PHE:CD2	0.72	2.78	8	7
1:A:2:A:C4	3:C:246:PHE:CE2	0.72	2.77	4	3
1:A:11:A:O3'	2:B:59:PHE:HA	0.72	1.85	7	1
2:B:43:LEU:HD13	2:B:43:LEU:O	0.72	1.85	9	1
1:A:11:A:H1'	2:B:66:SER:O	0.71	1.85	7	1
1:A:10:U:H5''	2:B:60:ASP:CG	0.71	2.06	4	1
1:A:6:A:C6	3:C:162:PHE:CG	0.71	2.79	7	5
1:A:10:U:O5'	1:A:10:U:H6	0.71	1.69	2	2
2:B:69:TYR:OH	2:B:71:PHE:CZ	0.71	2.43	10	1
1:A:10:U:H1'	2:B:58:MET:CE	0.71	2.15	4	1
2:B:87:LEU:O	2:B:97:LEU:HD11	0.71	1.85	9	1
1:A:10:U:C5'	2:B:71:PHE:CZ	0.71	2.73	7	4
1:A:12:A:O5'	2:B:67:LYS:O	0.71	2.09	7	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:6:A:H5''	1:A:8:A:C8	0.71	2.21	3	1
1:A:10:U:H5''	2:B:69:TYR:OH	0.71	1.84	10	1
3:C:221:HIS:CD2	3:C:221:HIS:N	0.70	2.59	1	2
1:A:5:U:N3	3:C:162:PHE:CD2	0.70	2.59	6	2
1:A:5:U:C2	3:C:162:PHE:CD2	0.70	2.79	2	2
1:A:12:A:O2'	1:A:13:U:H6	0.70	1.68	3	4
1:A:5:U:H5'	3:C:200:ARG:CD	0.70	2.16	3	1
1:A:4:A:N1	3:C:168:TRP:NE1	0.70	2.38	6	1
1:A:12:A:P	2:B:67:LYS:O	0.70	2.49	7	1
1:A:2:A:H4'	3:C:286:PHE:CG	0.70	2.21	10	1
1:A:6:A:N7	3:C:162:PHE:CZ	0.70	2.60	7	2
1:A:10:U:C5	2:B:71:PHE:CZ	0.70	2.80	1	1
3:C:188:LEU:HD23	3:C:188:LEU:N	0.70	2.02	6	2
1:A:12:A:OP2	2:B:69:TYR:N	0.70	2.25	7	1
1:A:12:A:OP1	2:B:59:PHE:CD2	0.70	2.45	7	1
1:A:7:U:C2	3:C:202:PHE:CE2	0.70	2.80	6	1
3:C:181:LYS:NZ	3:C:182:TYR:CZ	0.70	2.60	7	1
3:C:216:VAL:O	3:C:221:HIS:NE2	0.70	2.25	8	2
2:B:46:CYS:O	2:B:48:ASN:N	0.69	2.24	7	10
3:C:221:HIS:N	3:C:221:HIS:CD2	0.69	2.61	3	6
2:B:38:THR:O	2:B:42:ILE:HD13	0.69	1.88	10	1
3:C:221:HIS:O	3:C:222:ILE:HD13	0.69	1.87	2	2
1:A:9:A:C2	2:B:29:TYR:CE2	0.69	2.80	9	4
3:C:161:MET:SD	3:C:162:PHE:N	0.69	2.65	7	1
1:A:6:A:C8	3:C:162:PHE:CZ	0.69	2.81	1	5
3:C:205:LEU:HD22	3:C:207:PHE:CE1	0.69	2.22	6	1
1:A:11:A:H3'	2:B:68:GLY:C	0.69	2.08	7	1
2:B:83:ALA:O	2:B:87:LEU:N	0.69	2.26	4	7
1:A:2:A:C6	3:C:246:PHE:CD2	0.69	2.81	2	1
1:A:5:U:H5'	3:C:200:ARG:NE	0.69	2.01	3	1
1:A:5:U:N3	3:C:201:GLY:O	0.69	2.25	5	2
3:C:254:VAL:O	3:C:255:ARG:O	0.69	2.11	8	1
1:A:6:A:C4	3:C:162:PHE:CZ	0.69	2.80	2	4
3:C:226:LYS:NZ	3:C:278:LYS:NZ	0.69	2.40	2	1
1:A:5:U:O4	3:C:165:GLY:N	0.69	2.26	5	5
3:C:226:LYS:HZ1	3:C:279:ASP:N	0.69	1.85	5	2
1:A:12:A:H5''	2:B:35:TYR:CE1	0.69	2.22	7	1
3:C:161:MET:SD	3:C:163:ILE:N	0.69	2.65	7	1
1:A:10:U:H5''	2:B:69:TYR:CE2	0.69	2.22	10	1
3:C:172:GLU:OE1	3:C:190:ILE:HG23	0.69	1.87	3	1
2:B:59:PHE:CD1	2:B:59:PHE:N	0.68	2.61	5	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:C:267:GLY:O	3:C:269:ILE:N	0.68	2.24	5	1
2:B:59:PHE:N	2:B:59:PHE:CD1	0.68	2.60	7	2
1:A:6:A:N7	3:C:239:GLN:NE2	0.68	2.40	3	3
3:C:226:LYS:NZ	3:C:280:THR:N	0.68	2.42	5	1
1:A:10:U:C5'	2:B:71:PHE:CE1	0.68	2.76	7	4
3:C:266:TRP:O	3:C:266:TRP:CD1	0.68	2.47	10	1
1:A:5:U:O2'	1:A:6:A:H5'	0.68	1.88	7	7
1:A:10:U:C4'	2:B:71:PHE:CZ	0.68	2.77	8	3
1:A:7:U:C2	3:C:202:PHE:CD2	0.68	2.82	6	1
1:A:7:U:C4	3:C:202:PHE:CD1	0.68	2.81	6	1
1:A:2:A:O2'	1:A:3:U:H6	0.68	1.71	2	6
1:A:10:U:P	2:B:69:TYR:CD1	0.67	2.88	7	1
2:B:45:LEU:HD13	2:B:45:LEU:O	0.67	1.90	3	6
1:A:6:A:C2	3:C:162:PHE:CD1	0.67	2.83	9	3
3:C:275:MET:N	3:C:275:MET:SD	0.67	2.67	6	1
1:A:4:A:OP2	3:C:280:THR:HG21	0.67	1.88	10	1
3:C:259:PHE:CE1	3:C:274:LEU:HD23	0.67	2.24	8	1
1:A:4:A:C2	3:C:168:TRP:CH2	0.67	2.82	9	6
1:A:6:A:C4	3:C:162:PHE:CE1	0.67	2.82	2	4
1:A:9:A:C2	2:B:29:TYR:CD1	0.67	2.83	4	2
3:C:227:VAL:HG11	3:C:279:ASP:O	0.67	1.90	8	1
1:A:12:A:H5''	2:B:35:TYR:CZ	0.67	2.24	7	1
1:A:2:A:C2	3:C:246:PHE:CD2	0.67	2.82	9	5
1:A:7:U:C2	3:C:191:MET:SD	0.67	2.88	3	1
3:C:275:MET:O	3:C:276:LEU:HD12	0.67	1.89	8	1
1:A:10:U:C6	1:A:10:U:O5'	0.67	2.48	10	3
3:C:275:MET:O	3:C:276:LEU:HD22	0.67	1.91	1	2
1:A:6:A:P	3:C:236:ARG:NH2	0.67	2.68	5	1
1:A:1:U:H4'	3:C:284:ARG:NH1	0.67	2.05	5	1
2:B:76:ASP:O	2:B:78:GLU:N	0.66	2.27	6	10
3:C:195:ALA:O	3:C:196:THR:HG23	0.66	1.90	6	1
1:A:12:A:C5'	2:B:35:TYR:OH	0.66	2.43	7	1
3:C:188:LEU:HD23	3:C:188:LEU:C	0.66	2.10	9	1
1:A:4:A:C2	3:C:168:TRP:NE1	0.66	2.64	6	1
1:A:1:U:H3	3:C:249:GLY:H	0.66	1.31	4	1
3:C:251:GLY:N	3:C:252:PRO:CD	0.66	2.59	7	4
3:C:226:LYS:NZ	3:C:279:ASP:N	0.66	2.43	7	1
1:A:2:A:N1	3:C:246:PHE:CG	0.66	2.64	9	2
3:C:274:LEU:HD13	3:C:275:MET:N	0.66	2.05	8	1
1:A:2:A:C5	3:C:246:PHE:CE2	0.66	2.83	2	3
2:B:69:TYR:CE2	2:B:71:PHE:CE1	0.66	2.84	10	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:6:A:C8	3:C:239:GLN:NE2	0.66	2.63	1	2
1:A:9:A:N3	2:B:29:TYR:CD2	0.66	2.64	5	2
1:A:4:A:C2	3:C:168:TRP:CE2	0.66	2.84	6	1
3:C:219:THR:CG2	3:C:221:HIS:CE1	0.66	2.79	7	1
3:C:258:GLU:O	3:C:259:PHE:C	0.66	2.34	9	8
2:B:90:TYR:CZ	2:B:97:LEU:HD21	0.66	2.25	5	1
1:A:8:A:H4'	2:B:95:ARG:HH21	0.66	1.49	10	1
2:B:28:VAL:HG23	2:B:98:LYS:O	0.65	1.92	4	1
2:B:35:TYR:CD1	2:B:35:TYR:N	0.65	2.59	6	2
2:B:90:TYR:OH	2:B:97:LEU:HD21	0.65	1.91	5	1
1:A:6:A:C2	3:C:162:PHE:CG	0.65	2.84	10	4
2:B:72:ILE:N	2:B:72:ILE:CD1	0.65	2.60	5	3
3:C:269:ILE:O	3:C:269:ILE:HG22	0.65	1.90	2	4
2:B:45:LEU:C	2:B:45:LEU:HD13	0.65	2.12	7	3
3:C:254:VAL:O	3:C:254:VAL:HG12	0.65	1.91	8	1
3:C:311:ARG:O	3:C:313:ILE:N	0.65	2.30	9	1
3:C:207:PHE:O	3:C:208:GLU:O	0.65	2.13	10	1
1:A:3:U:H5'	3:C:286:PHE:CE2	0.65	2.25	10	4
3:C:226:LYS:NZ	3:C:280:THR:H	0.65	1.90	5	1
1:A:10:U:C5	2:B:65:ARG:NH2	0.65	2.65	6	1
1:A:7:U:C4'	3:C:202:PHE:CZ	0.65	2.80	8	2
3:C:245:ILE:HD13	3:C:245:ILE:C	0.65	2.12	9	1
1:A:2:A:N3	1:A:3:U:C6	0.65	2.64	9	3
2:B:97:LEU:H	2:B:97:LEU:HD12	0.65	1.52	2	2
1:A:6:A:N7	3:C:162:PHE:CE2	0.65	2.65	5	6
1:A:9:A:C4'	2:B:69:TYR:CE1	0.65	2.79	6	3
3:C:188:LEU:HD23	3:C:188:LEU:H	0.65	1.51	6	1
3:C:179:PHE:C	3:C:181:LYS:H	0.65	1.95	8	5
1:A:2:A:C6	3:C:246:PHE:CD1	0.65	2.84	9	1
1:A:2:A:C4	1:A:3:U:C5	0.64	2.84	10	2
1:A:10:U:H5'	2:B:71:PHE:CD2	0.64	2.27	7	1
3:C:305:PHE:CE1	3:C:314:GLU:CG	0.64	2.80	10	1
1:A:8:A:N3	2:B:29:TYR:CD2	0.64	2.65	9	1
2:B:90:TYR:O	2:B:92:LEU:N	0.64	2.29	5	10
3:C:308:PHE:CG	3:C:309:LYS:N	0.64	2.64	5	8
3:C:250:ILE:CG2	3:C:254:VAL:HG11	0.64	2.23	2	1
3:C:161:MET:SD	3:C:216:VAL:HG11	0.64	2.32	3	2
1:A:11:A:H5'	2:B:69:TYR:C	0.64	2.12	7	1
1:A:3:U:O2'	1:A:4:A:H5''	0.64	1.93	1	2
1:A:8:A:C2	2:B:29:TYR:CE2	0.64	2.85	3	7
3:C:276:LEU:CD1	3:C:276:LEU:N	0.64	2.58	3	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:11:A:C3'	2:B:58:MET:O	0.64	2.46	7	1
2:B:84:VAL:O	2:B:88:ASN:N	0.64	2.30	9	4
3:C:226:LYS:O	3:C:227:VAL:CG2	0.64	2.46	5	1
3:C:245:ILE:HD12	3:C:315:ILE:CG2	0.64	2.23	7	6
1:A:10:U:O5'	1:A:10:U:C6	0.64	2.51	2	3
3:C:263:PHE:O	3:C:265:GLN:N	0.64	2.31	4	5
3:C:286:PHE:N	3:C:286:PHE:CD1	0.64	2.66	2	2
1:A:2:A:N1	3:C:246:PHE:CD2	0.64	2.66	2	1
1:A:2:A:N3	3:C:246:PHE:CD2	0.64	2.66	5	4
1:A:5:U:H3	3:C:165:GLY:H	0.64	1.36	7	2
1:A:11:A:C4	2:B:66:SER:OG	0.63	2.51	7	1
2:B:45:LEU:HD13	2:B:45:LEU:C	0.63	2.14	10	4
1:A:10:U:O2	1:A:11:A:C5	0.63	2.51	4	1
3:C:255:ARG:N	3:C:255:ARG:CD	0.63	2.60	5	2
3:C:251:GLY:O	3:C:254:VAL:HG12	0.63	1.94	2	2
3:C:226:LYS:HZ1	3:C:279:ASP:H	0.63	1.36	5	1
3:C:205:LEU:HD13	3:C:207:PHE:CZ	0.63	2.27	7	1
3:C:158:SER:O	3:C:160:LYS:N	0.63	2.32	9	2
2:B:27:VAL:O	2:B:100:GLY:N	0.63	2.31	1	4
1:A:4:A:C4	3:C:168:TRP:CH2	0.63	2.85	10	4
1:A:11:A:N7	2:B:58:MET:CE	0.63	2.62	9	3
1:A:3:U:O2'	1:A:4:A:H4'	0.63	1.94	6	1
1:A:12:A:P	2:B:68:GLY:CA	0.63	2.86	7	1
1:A:11:A:C8	2:B:58:MET:SD	0.63	2.91	3	1
3:C:274:LEU:C	3:C:274:LEU:HD23	0.63	2.14	5	2
1:A:4:A:N1	3:C:199:SER:O	0.63	2.32	6	1
3:C:188:LEU:HD23	3:C:189:LYS:N	0.63	2.09	7	1
1:A:6:A:C6	3:C:234:ILE:O	0.63	2.52	8	2
2:B:35:TYR:N	2:B:35:TYR:CD1	0.63	2.62	1	1
1:A:11:A:O3'	2:B:67:LYS:O	0.63	2.16	7	1
2:B:42:ILE:O	2:B:44:ASP:N	0.63	2.32	7	8
3:C:226:LYS:HZ3	3:C:280:THR:HG23	0.63	1.52	5	1
1:A:10:U:C6	1:A:11:A:N7	0.63	2.66	7	1
3:C:308:PHE:O	3:C:310:ASP:N	0.63	2.32	8	3
2:B:44:ASP:O	2:B:48:ASN:ND2	0.62	2.32	8	7
2:B:32:SER:OG	2:B:95:ARG:N	0.62	2.27	7	3
1:A:5:U:O2'	1:A:7:U:N3	0.62	2.32	6	1
1:A:7:U:H5	3:C:204:PHE:CE2	0.62	2.10	6	1
3:C:308:PHE:O	3:C:309:LYS:C	0.62	2.37	3	8
2:B:57:MET:SD	2:B:70:ALA:HB2	0.62	2.34	2	2
3:C:199:SER:O	3:C:201:GLY:N	0.62	2.33	3	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:12:A:H8	2:B:67:LYS:N	0.62	1.89	7	1
1:A:10:U:P	1:A:10:U:C6	0.62	2.92	10	1
3:C:178:TYR:CD2	3:C:223:LEU:HD12	0.62	2.29	1	3
3:C:188:LEU:C	3:C:188:LEU:HD12	0.62	2.14	8	2
1:A:4:A:H8	3:C:166:LEU:O	0.62	1.77	9	3
2:B:84:VAL:HG13	2:B:99:CYS:CB	0.62	2.25	4	1
2:B:97:LEU:N	2:B:97:LEU:CD1	0.62	2.58	5	1
3:C:168:TRP:CZ2	3:C:198:ARG:CZ	0.62	2.83	10	1
1:A:2:A:N3	1:A:3:U:C5	0.62	2.68	3	4
1:A:9:A:C5'	2:B:69:TYR:CE1	0.62	2.82	2	2
1:A:2:A:C5	3:C:246:PHE:CZ	0.62	2.87	9	2
3:C:226:LYS:C	3:C:227:VAL:HG22	0.62	2.15	8	2
1:A:4:A:C5	3:C:168:TRP:CZ3	0.62	2.87	10	7
3:C:301:CYS:SG	3:C:317:ARG:NH2	0.62	2.73	6	1
3:C:182:TYR:OH	3:C:221:HIS:ND1	0.62	2.32	2	5
3:C:264:SER:O	3:C:266:TRP:N	0.62	2.33	8	2
2:B:46:CYS:O	2:B:49:VAL:N	0.62	2.33	5	2
1:A:3:U:C5'	3:C:286:PHE:CZ	0.62	2.83	3	3
1:A:11:A:C8	2:B:58:MET:CE	0.62	2.83	5	2
3:C:188:LEU:O	3:C:188:LEU:HD23	0.62	1.94	5	2
2:B:30:LEU:HD13	2:B:72:ILE:CD1	0.62	2.25	6	1
3:C:316:LYS:O	3:C:317:ARG:O	0.62	2.18	7	1
1:A:5:U:H3'	1:A:5:U:O2	0.61	1.95	3	1
1:A:5:U:C5'	3:C:200:ARG:NE	0.61	2.63	3	1
1:A:12:A:N6	2:B:58:MET:SD	0.61	2.72	8	1
2:B:101:TYR:O	2:B:103:SER:N	0.61	2.33	3	3
3:C:236:ARG:N	3:C:236:ARG:HE	0.61	1.92	3	1
1:A:7:U:O4	3:C:162:PHE:CE1	0.61	2.53	6	1
1:A:12:A:OP1	2:B:59:PHE:CG	0.61	2.53	7	1
2:B:52:VAL:HG12	2:B:53:ILE:H	0.61	1.56	1	1
1:A:7:U:H4'	1:A:8:A:OP2	0.61	1.93	4	3
3:C:166:LEU:N	3:C:166:LEU:HD12	0.61	2.10	3	1
3:C:259:PHE:CZ	3:C:289:VAL:HG13	0.61	2.31	10	1
3:C:238:GLU:O	3:C:242:THR:HG23	0.61	1.95	9	4
1:A:6:A:C5	3:C:162:PHE:CZ	0.61	2.88	6	3
3:C:263:PHE:CD2	3:C:266:TRP:CH2	0.61	2.88	3	9
3:C:276:LEU:O	3:C:282:GLN:N	0.61	2.34	8	1
3:C:301:CYS:SG	3:C:317:ARG:CZ	0.61	2.89	6	1
1:A:4:A:N7	3:C:167:ASN:O	0.61	2.33	2	5
2:B:90:TYR:CE1	2:B:97:LEU:HD21	0.61	2.31	5	1
2:B:85:ARG:O	2:B:88:ASN:ND2	0.61	2.33	7	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:12:A:N3	1:A:13:U:C6	0.61	2.68	7	1
3:C:276:LEU:N	3:C:280:THR:OG1	0.61	2.33	8	3
1:A:6:A:N6	3:C:162:PHE:CD2	0.61	2.68	8	2
3:C:282:GLN:O	3:C:284:ARG:N	0.61	2.31	1	7
2:B:35:TYR:OH	2:B:59:PHE:CG	0.61	2.54	2	2
3:C:262:PHE:O	3:C:265:GLN:NE2	0.61	2.34	5	2
2:B:32:SER:OG	2:B:94:SER:N	0.61	2.34	7	1
1:A:1:U:O2'	1:A:2:A:H2'	0.61	1.95	9	1
1:A:8:A:H4'	2:B:95:ARG:NH1	0.60	2.11	6	1
1:A:6:A:H4'	1:A:7:U:H3'	0.60	1.73	3	2
2:B:88:ASN:N	2:B:88:ASN:OD1	0.60	2.34	9	3
3:C:317:ARG:CD	3:C:317:ARG:H	0.60	2.08	1	1
2:B:84:VAL:O	2:B:88:ASN:CB	0.60	2.49	9	7
3:C:266:TRP:CD1	3:C:266:TRP:O	0.60	2.55	8	1
2:B:82:SER:O	2:B:86:ASN:ND2	0.60	2.34	5	7
3:C:216:VAL:HG12	3:C:216:VAL:O	0.60	1.96	6	1
1:A:6:A:C4	3:C:162:PHE:CD1	0.60	2.90	7	3
3:C:269:ILE:CG2	3:C:269:ILE:O	0.60	2.49	5	3
2:B:48:ASN:O	2:B:49:VAL:HG23	0.60	1.95	9	2
1:A:6:A:C5	3:C:162:PHE:CD2	0.60	2.90	5	6
3:C:176:ARG:O	3:C:178:TYR:N	0.60	2.35	10	8
3:C:227:VAL:HG12	3:C:227:VAL:O	0.60	1.94	5	1
1:A:11:A:O3'	2:B:67:LYS:C	0.60	2.40	7	1
2:B:58:MET:SD	2:B:59:PHE:O	0.60	2.59	2	3
2:B:22:ASN:OD1	2:B:22:ASN:N	0.60	2.34	7	1
1:A:10:U:O2'	1:A:11:A:H5'	0.60	1.97	5	6
2:B:90:TYR:CE1	2:B:91:GLN:O	0.60	2.55	3	8
2:B:53:ILE:HG22	2:B:54:ASN:OD1	0.60	1.97	10	2
3:C:266:TRP:CD1	3:C:267:GLY:N	0.60	2.69	3	1
3:C:277:ASP:O	3:C:280:THR:N	0.60	2.32	4	1
1:A:10:U:OP1	2:B:70:ALA:N	0.60	2.35	5	1
3:C:219:THR:O	3:C:221:HIS:CD2	0.60	2.55	6	3
2:B:68:GLY:O	2:B:69:TYR:CD2	0.60	2.54	7	1
1:A:7:U:C5	3:C:204:PHE:CE2	0.60	2.89	6	1
1:A:9:A:N1	2:B:29:TYR:CE2	0.60	2.70	10	1
3:C:283:SER:O	3:C:285:GLY:N	0.59	2.31	2	1
3:C:246:PHE:CD1	3:C:246:PHE:O	0.59	2.55	9	3
3:C:219:THR:O	3:C:221:HIS:NE2	0.59	2.35	6	4
3:C:250:ILE:O	3:C:286:PHE:N	0.59	2.35	9	3
1:A:11:A:C8	2:B:58:MET:HE1	0.59	2.32	8	1
1:A:5:U:O2'	1:A:6:A:C5'	0.59	2.50	1	7

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:54:ASN:ND2	2:B:73:GLU:OE1	0.59	2.35	2	9
1:A:3:U:O2'	1:A:4:A:C5'	0.59	2.51	6	4
1:A:6:A:C5'	1:A:7:U:H5'	0.59	2.27	2	1
2:B:30:LEU:HD11	2:B:97:LEU:HD23	0.59	1.74	2	1
2:B:60:ASP:OD2	2:B:66:SER:N	0.59	2.36	8	4
3:C:159:CYS:SG	3:C:207:PHE:O	0.59	2.61	3	2
3:C:221:HIS:HB3	3:C:228:ILE:HD11	0.59	1.74	5	2
1:A:1:U:N3	3:C:314:GLU:OE1	0.59	2.35	10	2
3:C:238:GLU:OE1	3:C:238:GLU:N	0.59	2.36	10	1
3:C:167:ASN:O	3:C:168:TRP:CG	0.59	2.56	7	3
1:A:8:A:H2	2:B:29:TYR:CD2	0.59	2.16	3	1
2:B:29:TYR:CD1	2:B:29:TYR:N	0.59	2.70	4	2
2:B:88:ASN:O	2:B:97:LEU:HD13	0.59	1.95	5	1
2:B:22:ASN:ND2	2:B:102:SER:O	0.59	2.36	6	1
3:C:300:VAL:O	3:C:303:ASN:N	0.59	2.36	9	9
2:B:33:ILE:HD12	2:B:33:ILE:N	0.59	2.13	8	3
1:A:9:A:C4'	2:B:69:TYR:CE2	0.59	2.85	3	1
2:B:22:ASN:OD1	2:B:101:TYR:CE2	0.59	2.56	4	1
2:B:58:MET:CG	2:B:59:PHE:N	0.59	2.66	7	1
3:C:261:GLU:OE1	3:C:261:GLU:N	0.59	2.35	7	1
2:B:22:ASN:N	2:B:23:PRO:CD	0.59	2.65	8	1
1:A:10:U:C5	1:A:10:U:P	0.59	2.95	10	1
3:C:237:ASP:OD1	3:C:238:GLU:N	0.59	2.36	1	2
2:B:82:SER:O	2:B:86:ASN:OD1	0.59	2.20	2	1
1:A:6:A:N9	3:C:162:PHE:CZ	0.59	2.71	2	1
2:B:35:TYR:OH	2:B:59:PHE:CD1	0.59	2.55	9	2
3:C:187:ASP:OD2	3:C:189:LYS:NZ	0.59	2.35	5	1
1:A:6:A:N6	3:C:234:ILE:H	0.59	1.96	6	1
1:A:5:U:H4'	3:C:200:ARG:CB	0.59	2.28	10	1
3:C:199:SER:O	3:C:200:ARG:C	0.59	2.41	6	8
1:A:9:A:C6	2:B:29:TYR:OH	0.59	2.56	2	2
2:B:101:TYR:N	2:B:101:TYR:CD1	0.59	2.67	6	2
3:C:181:LYS:NZ	3:C:182:TYR:OH	0.59	2.36	7	1
1:A:1:U:C4	1:A:3:U:O4	0.59	2.56	9	1
3:C:211:SER:O	3:C:213:VAL:N	0.59	2.36	4	8
1:A:5:U:C5'	3:C:200:ARG:HE	0.59	2.10	3	1
3:C:176:ARG:O	3:C:179:PHE:N	0.59	2.35	4	7
2:B:45:LEU:C	2:B:45:LEU:HD12	0.59	2.19	8	1
3:C:167:ASN:O	3:C:169:ASP:N	0.58	2.35	1	2
3:C:160:LYS:NZ	3:C:189:LYS:NZ	0.58	2.51	1	1
3:C:282:GLN:O	3:C:286:PHE:CZ	0.58	2.56	1	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:C:210:PRO:O	3:C:213:VAL:HG12	0.58	1.97	2	1
3:C:269:ILE:HG21	3:C:272:ALA:HB2	0.58	1.75	7	1
3:C:279:ASP:OD1	3:C:280:THR:N	0.58	2.35	7	1
3:C:302:GLN:NE2	3:C:303:ASN:OD1	0.58	2.36	7	1
1:A:1:U:O2	1:A:2:A:N7	0.58	2.36	9	1
1:A:6:A:C4	3:C:162:PHE:CE2	0.58	2.91	10	2
2:B:69:TYR:OH	2:B:71:PHE:CE2	0.58	2.51	10	1
1:A:4:A:P	3:C:280:THR:HG21	0.58	2.38	10	1
2:B:84:VAL:O	2:B:88:ASN:ND2	0.58	2.36	2	3
2:B:52:VAL:CG1	2:B:53:ILE:N	0.58	2.66	4	1
2:B:90:TYR:C	2:B:90:TYR:CD1	0.58	2.76	6	3
1:A:5:U:O4	3:C:231:LYS:NZ	0.58	2.37	9	1
2:B:60:ASP:O	2:B:64:GLY:N	0.58	2.36	10	1
3:C:220:GLN:O	3:C:221:HIS:CG	0.58	2.55	5	1
3:C:277:ASP:OD1	3:C:278:LYS:N	0.58	2.36	10	3
1:A:11:A:C2	2:B:63:THR:OG1	0.58	2.54	7	1
1:A:2:A:N6	3:C:319:GLU:O	0.58	2.36	7	1
3:C:170:THR:OG1	3:C:192:LYS:NZ	0.58	2.36	9	1
1:A:10:U:H3'	2:B:69:TYR:OH	0.58	1.97	10	1
1:A:9:A:C5'	2:B:69:TYR:CZ	0.58	2.84	2	1
3:C:249:GLY:O	3:C:311:ARG:NH1	0.58	2.36	2	1
2:B:84:VAL:O	2:B:88:ASN:CA	0.58	2.51	5	6
1:A:10:U:OP1	2:B:69:TYR:CG	0.58	2.56	8	2
1:A:12:A:H2'	2:B:68:GLY:HA3	0.58	1.75	7	1
1:A:10:U:C2'	1:A:11:A:H8	0.58	2.11	8	4
2:B:87:LEU:O	2:B:88:ASN:C	0.58	2.40	9	2
2:B:27:VAL:HG12	2:B:102:SER:N	0.58	2.13	6	1
1:A:2:A:C6	3:C:246:PHE:CE2	0.58	2.92	2	1
3:C:171:THR:OG1	3:C:174:ASN:ND2	0.58	2.36	2	2
1:A:2:A:O4'	3:C:286:PHE:CE1	0.58	2.57	2	1
1:A:7:U:O4	3:C:162:PHE:CZ	0.58	2.57	6	1
3:C:279:ASP:C	3:C:280:THR:HG22	0.58	2.18	7	1
3:C:193:ASP:OD2	3:C:197:GLY:N	0.58	2.37	8	1
2:B:97:LEU:CD1	2:B:97:LEU:H	0.58	2.10	2	1
1:A:2:A:O2'	1:A:3:U:C6	0.58	2.56	10	5
2:B:45:LEU:O	2:B:48:ASN:ND2	0.58	2.36	4	2
1:A:12:A:O5'	2:B:68:GLY:CA	0.58	2.45	7	1
3:C:250:ILE:N	3:C:285:GLY:O	0.58	2.37	8	1
2:B:27:VAL:O	2:B:100:GLY:CA	0.58	2.52	6	2
2:B:99:CYS:O	2:B:99:CYS:SG	0.58	2.61	10	2
3:C:269:ILE:HD11	3:C:289:VAL:HB	0.58	1.75	5	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:C:174:ASN:OD1	3:C:175:LEU:N	0.58	2.35	10	1
2:B:50:GLY:O	2:B:52:VAL:N	0.58	2.37	5	1
3:C:249:GLY:O	3:C:313:ILE:HG22	0.58	1.98	8	1
2:B:87:LEU:HD12	2:B:87:LEU:O	0.58	1.99	1	1
3:C:200:ARG:NE	3:C:200:ARG:C	0.58	2.57	2	1
3:C:277:ASP:N	3:C:283:SER:OG	0.58	2.36	6	1
1:A:10:U:C5	1:A:11:A:N7	0.58	2.72	7	1
2:B:26:ARG:NE	2:B:76:ASP:OD1	0.58	2.37	8	1
2:B:90:TYR:CD1	2:B:90:TYR:C	0.57	2.77	4	5
3:C:263:PHE:O	3:C:264:SER:C	0.57	2.43	9	10
3:C:297:VAL:O	3:C:301:CYS:SG	0.57	2.62	10	2
2:B:26:ARG:NH2	2:B:76:ASP:OD2	0.57	2.37	8	1
3:C:167:ASN:ND2	3:C:224:ASP:OD2	0.57	2.36	1	2
1:A:2:A:C2	1:A:3:U:C5	0.57	2.92	2	4
3:C:193:ASP:N	3:C:197:GLY:O	0.57	2.36	6	1
3:C:164:GLY:O	3:C:166:LEU:N	0.57	2.37	10	1
1:A:9:A:O2'	1:A:10:U:C5'	0.57	2.53	2	4
3:C:199:SER:O	3:C:200:ARG:O	0.57	2.23	2	3
1:A:10:U:H1'	2:B:58:MET:HE3	0.57	1.75	4	1
2:B:99:CYS:SG	2:B:99:CYS:O	0.57	2.62	5	3
3:C:303:ASN:OD1	3:C:303:ASN:O	0.57	2.22	6	1
2:B:23:PRO:O	2:B:101:TYR:CG	0.57	2.57	2	1
3:C:280:THR:OG1	3:C:281:GLY:N	0.57	2.35	4	1
3:C:178:TYR:OH	3:C:222:ILE:N	0.57	2.37	6	3
3:C:180:GLY:O	3:C:182:TYR:N	0.57	2.36	10	1
3:C:244:LYS:O	3:C:318:ALA:HB2	0.57	2.00	1	1
1:A:4:A:C8	3:C:167:ASN:O	0.57	2.57	7	4
3:C:258:GLU:H	3:C:258:GLU:CD	0.57	2.03	3	1
3:C:166:LEU:HA	3:C:228:ILE:HG22	0.57	1.76	4	2
1:A:8:A:O2'	1:A:9:A:O5'	0.57	2.23	5	5
3:C:211:SER:O	3:C:214:ASP:N	0.57	2.37	4	9
1:A:9:A:H2'	1:A:10:U:H6	0.57	1.54	3	1
1:A:9:A:C4	2:B:29:TYR:CD2	0.57	2.92	4	1
2:B:48:ASN:OD1	2:B:49:VAL:N	0.57	2.32	4	1
3:C:190:ILE:HG23	3:C:190:ILE:O	0.57	1.99	7	1
1:A:4:A:C8	3:C:166:LEU:O	0.57	2.58	7	7
2:B:33:ILE:N	2:B:33:ILE:HD12	0.57	2.15	4	1
2:B:26:ARG:N	2:B:80:SER:OG	0.57	2.38	10	2
3:C:292:ASP:OD1	3:C:293:SER:N	0.57	2.36	10	3
2:B:45:LEU:O	2:B:45:LEU:HD13	0.57	2.00	10	1
1:A:11:A:O2'	1:A:12:A:O5'	0.57	2.23	4	6

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:30:LEU:CD1	2:B:97:LEU:HD23	0.57	2.30	2	1
3:C:303:ASN:ND2	3:C:306:ILE:CG1	0.57	2.67	3	1
3:C:172:GLU:H	3:C:172:GLU:CD	0.57	2.03	10	2
3:C:294:ALA:O	3:C:297:VAL:N	0.57	2.38	5	1
3:C:173:ASP:O	3:C:176:ARG:N	0.57	2.38	10	2
1:A:8:A:C6	2:B:101:TYR:OH	0.57	2.55	6	1
1:A:11:A:O2'	2:B:67:LYS:C	0.57	2.43	7	1
2:B:77:LEU:O	2:B:81:ALA:CB	0.56	2.53	2	10
1:A:4:A:O2'	1:A:5:U:C4	0.56	2.56	4	1
1:A:3:U:H3'	3:C:277:ASP:OD2	0.56	2.00	4	1
1:A:2:A:C2	3:C:246:PHE:CG	0.56	2.94	9	2
1:A:5:U:O2	3:C:163:ILE:O	0.56	2.23	9	3
3:C:263:PHE:CD2	3:C:266:TRP:CZ2	0.56	2.94	9	3
3:C:274:LEU:CD1	3:C:286:PHE:O	0.56	2.54	7	3
2:B:30:LEU:N	2:B:30:LEU:CD2	0.56	2.68	2	1
1:A:4:A:N1	3:C:168:TRP:CZ3	0.56	2.73	4	2
1:A:6:A:P	3:C:236:ARG:HH22	0.56	2.24	5	1
3:C:190:ILE:O	3:C:191:MET:SD	0.56	2.64	5	1
3:C:271:ASP:O	3:C:272:ALA:C	0.56	2.44	8	2
2:B:97:LEU:H	2:B:97:LEU:CD1	0.56	2.11	5	1
2:B:67:LYS:O	2:B:69:TYR:N	0.56	2.38	6	1
3:C:276:LEU:O	3:C:278:LYS:N	0.56	2.33	6	1
1:A:10:U:OP1	2:B:69:TYR:CD2	0.56	2.59	8	3
1:A:1:U:O2	1:A:2:A:N6	0.56	2.38	9	1
1:A:9:A:O2'	1:A:10:U:C6	0.56	2.56	2	2
1:A:6:A:O2'	3:C:236:ARG:NH1	0.56	2.38	9	2
3:C:268:THR:O	3:C:269:ILE:C	0.56	2.43	3	4
1:A:7:U:N3	3:C:202:PHE:CD2	0.56	2.74	6	1
2:B:60:ASP:OD2	2:B:65:ARG:N	0.56	2.37	1	2
3:C:167:ASN:OD1	3:C:168:TRP:N	0.56	2.36	2	3
3:C:282:GLN:O	3:C:283:SER:C	0.56	2.44	2	1
1:A:7:U:OP2	3:C:236:ARG:NH1	0.56	2.39	3	1
3:C:266:TRP:CG	3:C:267:GLY:N	0.56	2.73	3	1
1:A:7:U:O2	3:C:191:MET:SD	0.56	2.63	7	2
2:B:58:MET:C	2:B:58:MET:SD	0.56	2.84	5	1
3:C:261:GLU:CD	3:C:261:GLU:N	0.56	2.58	6	1
1:A:8:A:C4'	2:B:95:ARG:NH2	0.56	2.65	10	1
1:A:5:U:OP2	1:A:5:U:C5	0.56	2.59	1	5
3:C:200:ARG:O	3:C:200:ARG:NE	0.56	2.38	2	1
3:C:166:LEU:C	3:C:166:LEU:HD12	0.56	2.21	4	1
3:C:220:GLN:C	3:C:221:HIS:CG	0.56	2.79	5	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:11:A:O2'	1:A:12:A:N7	0.56	2.37	6	1
1:A:6:A:H4'	1:A:7:U:O5'	0.56	1.99	6	1
2:B:42:ILE:O	2:B:46:CYS:SG	0.56	2.64	6	2
1:A:8:A:N1	2:B:99:CYS:O	0.56	2.38	6	1
1:A:6:A:C1'	1:A:7:U:OP2	0.56	2.54	3	2
1:A:6:A:C5	3:C:162:PHE:CE1	0.56	2.94	7	1
3:C:275:MET:SD	3:C:279:ASP:OD2	0.56	2.63	1	1
2:B:51:PRO:O	2:B:52:VAL:O	0.56	2.24	2	2
3:C:246:PHE:C	3:C:246:PHE:CD1	0.56	2.78	3	2
1:A:12:A:C2	1:A:13:U:C6	0.56	2.94	7	1
3:C:163:ILE:HD12	3:C:175:LEU:HD21	0.56	1.76	7	1
1:A:7:U:O4'	3:C:202:PHE:CZ	0.56	2.59	9	2
3:C:254:VAL:HG13	3:C:309:LYS:HG3	0.56	1.76	8	1
1:A:5:U:O2	3:C:201:GLY:O	0.56	2.24	1	2
1:A:2:A:N1	3:C:318:ALA:O	0.56	2.39	1	1
1:A:2:A:O2'	1:A:3:U:C5	0.56	2.59	4	2
1:A:5:U:C4	1:A:5:U:OP2	0.56	2.59	7	1
3:C:191:MET:O	3:C:202:PHE:CZ	0.56	2.59	7	1
2:B:43:LEU:C	2:B:43:LEU:HD13	0.56	2.22	9	1
1:A:12:A:O2'	1:A:13:U:C5'	0.55	2.54	5	9
1:A:4:A:N6	3:C:279:ASP:OD2	0.55	2.39	5	1
1:A:10:U:H5'	2:B:71:PHE:CD1	0.55	2.36	7	1
1:A:5:U:C6	1:A:5:U:O5'	0.55	2.58	4	2
2:B:45:LEU:HD21	2:B:90:TYR:CE2	0.55	2.36	5	1
1:A:10:U:O5'	2:B:71:PHE:CE1	0.55	2.60	7	1
3:C:191:MET:O	3:C:192:LYS:C	0.55	2.45	10	3
2:B:101:TYR:O	2:B:102:SER:C	0.55	2.43	6	5
3:C:246:PHE:CD1	3:C:246:PHE:C	0.55	2.80	7	6
1:A:10:U:OP1	2:B:58:MET:SD	0.55	2.63	2	1
1:A:9:A:C8	1:A:10:U:H5	0.55	2.19	3	1
3:C:166:LEU:HD12	3:C:167:ASN:O	0.55	2.00	10	2
1:A:11:A:O2'	1:A:12:A:C5'	0.55	2.55	2	6
3:C:226:LYS:NZ	3:C:278:LYS:HZ2	0.55	1.99	2	1
1:A:9:A:N3	2:B:29:TYR:CE2	0.55	2.75	5	1
3:C:316:LYS:O	3:C:317:ARG:C	0.55	2.45	7	1
1:A:6:A:C1'	1:A:7:U:H5''	0.55	2.31	8	2
3:C:200:ARG:NE	3:C:200:ARG:N	0.55	2.55	4	1
2:B:90:TYR:CE1	2:B:97:LEU:CD1	0.55	2.84	5	1
1:A:11:A:O3'	2:B:58:MET:O	0.55	2.24	7	1
1:A:9:A:N1	2:B:29:TYR:OH	0.55	2.35	2	5
3:C:222:ILE:N	3:C:222:ILE:CD1	0.55	2.61	4	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:10:U:C5	1:A:10:U:OP1	0.55	2.60	10	1
2:B:27:VAL:HG13	2:B:73:GLU:HA	0.55	1.78	1	1
1:A:10:U:H5''	2:B:60:ASP:OD1	0.55	2.01	4	1
3:C:215:GLU:CD	3:C:215:GLU:H	0.55	2.04	4	1
1:A:11:A:OP2	2:B:58:MET:SD	0.55	2.65	6	3
1:A:11:A:H2'	2:B:69:TYR:HB2	0.55	1.79	7	1
1:A:7:U:H4'	3:C:202:PHE:CE2	0.55	2.37	8	2
1:A:10:U:O4	2:B:65:ARG:CZ	0.55	2.54	9	1
3:C:182:TYR:OH	3:C:219:THR:HG21	0.55	2.02	9	1
1:A:6:A:C8	3:C:162:PHE:CE2	0.55	2.95	1	1
1:A:10:U:O2'	1:A:11:A:C5'	0.55	2.55	5	5
3:C:163:ILE:HG22	3:C:166:LEU:HD11	0.55	1.78	3	1
3:C:246:PHE:CD1	3:C:247:VAL:N	0.55	2.75	3	2
1:A:10:U:O2	1:A:11:A:N7	0.55	2.39	4	1
1:A:2:A:O2'	1:A:3:U:H5	0.55	1.84	4	2
3:C:198:ARG:C	3:C:198:ARG:NE	0.55	2.60	7	1
1:A:11:A:O2'	1:A:12:A:C8	0.55	2.59	2	3
3:C:175:LEU:HD12	3:C:190:ILE:CD1	0.55	2.32	2	1
1:A:8:A:H2	2:B:29:TYR:CE2	0.55	2.18	3	1
2:B:38:THR:O	2:B:42:ILE:CG1	0.55	2.54	7	2
1:A:10:U:OP2	2:B:69:TYR:CD2	0.55	2.59	5	1
1:A:12:A:N6	2:B:57:MET:O	0.55	2.40	10	2
1:A:12:A:O2'	1:A:13:U:O5'	0.54	2.25	8	9
1:A:6:A:N7	3:C:239:GLN:CD	0.54	2.60	4	2
1:A:6:A:N6	3:C:234:ILE:O	0.54	2.40	7	1
3:C:181:LYS:NZ	3:C:181:LYS:CB	0.54	2.70	8	1
1:A:9:A:C2	2:B:29:TYR:CD2	0.54	2.95	10	1
3:C:173:ASP:O	3:C:174:ASN:C	0.54	2.43	3	3
3:C:292:ASP:CG	3:C:293:SER:N	0.54	2.60	4	2
2:B:24:PRO:O	2:B:99:CYS:SG	0.54	2.63	5	1
3:C:226:LYS:HZ2	3:C:280:THR:N	0.54	1.99	5	1
3:C:307:ASP:OD1	3:C:312:LYS:NZ	0.54	2.37	10	1
1:A:5:U:O5'	1:A:5:U:C6	0.54	2.61	8	3
3:C:226:LYS:O	3:C:227:VAL:CB	0.54	2.56	5	2
1:A:5:U:O2	1:A:5:U:C3'	0.54	2.55	3	1
2:B:45:LEU:O	2:B:48:ASN:OD1	0.54	2.25	4	1
3:C:300:VAL:O	3:C:303:ASN:OD1	0.54	2.24	6	1
1:A:11:A:C5'	2:B:69:TYR:CB	0.54	2.86	7	1
1:A:4:A:C5	3:C:168:TRP:CH2	0.54	2.94	10	3
2:B:27:VAL:HG21	2:B:102:SER:O	0.54	2.01	1	2
2:B:49:VAL:HG11	2:B:83:ALA:CB	0.54	2.19	5	6

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:88:ASN:O	2:B:97:LEU:CB	0.54	2.55	6	2
3:C:188:LEU:CD2	3:C:188:LEU:N	0.54	2.70	6	2
1:A:11:A:C5'	2:B:69:TYR:O	0.54	2.50	7	1
1:A:4:A:O5'	1:A:4:A:N3	0.54	2.40	3	1
2:B:26:ARG:NH1	2:B:76:ASP:OD1	0.54	2.40	6	1
3:C:168:TRP:HE1	3:C:198:ARG:HH21	0.54	1.43	7	1
1:A:10:U:O4	2:B:65:ARG:NH1	0.54	2.41	9	1
2:B:96:PHE:N	2:B:96:PHE:CD1	0.54	2.71	9	1
3:C:277:ASP:O	3:C:279:ASP:N	0.54	2.41	9	1
3:C:245:ILE:HD11	3:C:315:ILE:CG2	0.54	2.32	10	2
3:C:188:LEU:C	3:C:188:LEU:HD23	0.54	2.23	5	1
3:C:317:ARG:O	3:C:319:GLU:N	0.54	2.41	5	2
3:C:164:GLY:C	3:C:166:LEU:N	0.54	2.60	10	1
2:B:87:LEU:HD12	2:B:87:LEU:C	0.54	2.23	1	1
2:B:75:ARG:O	2:B:76:ASP:CB	0.54	2.55	4	9
2:B:31:GLY:O	2:B:68:GLY:O	0.54	2.26	10	4
1:A:9:A:N3	2:B:71:PHE:CE2	0.54	2.76	8	4
3:C:309:LYS:O	3:C:310:ASP:C	0.54	2.46	3	2
3:C:186:THR:OG1	3:C:208:GLU:N	0.54	2.40	6	1
1:A:10:U:H5''	1:A:11:A:OP2	0.54	2.03	7	1
3:C:162:PHE:CD2	3:C:162:PHE:O	0.54	2.61	7	1
3:C:171:THR:O	3:C:174:ASN:OD1	0.54	2.26	10	1
3:C:317:ARG:CD	3:C:317:ARG:N	0.54	2.70	1	1
1:A:8:A:C2	2:B:29:TYR:CD2	0.54	2.95	10	5
2:B:88:ASN:OD1	2:B:99:CYS:SG	0.54	2.66	2	1
3:C:241:LYS:O	3:C:242:THR:C	0.54	2.46	6	3
1:A:5:U:O2	3:C:162:PHE:CD2	0.54	2.61	2	1
3:C:250:ILE:HG23	3:C:254:VAL:HG11	0.54	1.79	2	1
3:C:258:GLU:CD	3:C:258:GLU:N	0.54	2.62	3	1
3:C:166:LEU:HD12	3:C:167:ASN:N	0.54	2.17	4	1
1:A:2:A:C6	3:C:246:PHE:CE1	0.54	2.96	9	2
1:A:9:A:OP2	3:C:200:ARG:NE	0.54	2.40	6	1
1:A:13:U:N3	2:B:94:SER:OG	0.54	2.41	7	1
3:C:182:TYR:OH	3:C:219:THR:CG2	0.54	2.56	9	1
3:C:265:GLN:CG	3:C:266:TRP:H	0.54	2.16	5	2
3:C:178:TYR:O	3:C:181:LYS:NZ	0.54	2.41	8	1
2:B:66:SER:CB	2:B:69:TYR:CD1	0.53	2.91	3	1
2:B:37:GLN:HE22	2:B:92:LEU:HD11	0.53	1.63	4	1
3:C:254:VAL:HG22	3:C:255:ARG:N	0.53	2.18	4	1
1:A:4:A:C2	1:A:4:A:OP1	0.53	2.61	7	3
1:A:11:A:N3	2:B:66:SER:O	0.53	2.41	7	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:25:SER:O	2:B:77:LEU:CD2	0.53	2.56	1	1
1:A:10:U:C2	2:B:58:MET:CE	0.53	2.91	1	1
3:C:176:ARG:O	3:C:177:GLU:C	0.53	2.44	4	9
1:A:11:A:C2'	1:A:12:A:C8	0.53	2.91	2	1
1:A:9:A:N1	2:B:102:SER:CB	0.53	2.71	7	1
2:B:47:SER:OG	2:B:52:VAL:HG21	0.53	2.03	10	1
3:C:266:TRP:CG	3:C:266:TRP:O	0.53	2.59	10	1
3:C:226:LYS:O	3:C:227:VAL:CG1	0.53	2.53	8	2
3:C:216:VAL:CG1	3:C:217:VAL:N	0.53	2.71	2	1
2:B:84:VAL:HG12	2:B:88:ASN:ND2	0.53	2.18	8	2
3:C:276:LEU:CA	3:C:283:SER:OG	0.53	2.56	3	1
3:C:262:PHE:O	3:C:265:GLN:HG2	0.53	2.03	4	1
1:A:4:A:OP2	3:C:282:GLN:NE2	0.53	2.41	7	1
3:C:158:SER:C	3:C:160:LYS:N	0.53	2.61	7	1
2:B:92:LEU:O	2:B:95:ARG:O	0.53	2.26	10	6
3:C:258:GLU:O	3:C:260:GLU:N	0.53	2.42	8	6
3:C:242:THR:O	3:C:291:TYR:O	0.53	2.27	7	2
1:A:9:A:O2'	1:A:10:U:O4'	0.53	2.26	5	2
3:C:254:VAL:CG1	3:C:310:ASP:OD2	0.53	2.56	6	1
3:C:278:LYS:CD	3:C:278:LYS:N	0.53	2.70	9	1
3:C:269:ILE:O	3:C:269:ILE:CG2	0.53	2.57	1	1
3:C:158:SER:C	3:C:159:CYS:SG	0.53	2.87	10	3
2:B:23:PRO:O	2:B:101:TYR:CB	0.53	2.57	2	2
3:C:200:ARG:NH2	3:C:202:PHE:CE2	0.53	2.77	2	1
1:A:6:A:O2'	1:A:7:U:OP2	0.53	2.26	8	2
1:A:1:U:O4	3:C:249:GLY:N	0.53	2.42	4	1
3:C:226:LYS:HZ2	3:C:280:THR:HG23	0.53	1.62	5	1
1:A:3:U:HO2'	1:A:4:A:C5'	0.53	2.16	6	1
1:A:12:A:O2'	1:A:13:U:P	0.53	2.66	7	1
2:B:53:ILE:N	2:B:73:GLU:O	0.53	2.42	7	1
3:C:254:VAL:O	3:C:274:LEU:CD2	0.53	2.56	7	1
1:A:12:A:H61	2:B:57:MET:N	0.53	2.02	10	1
2:B:88:ASN:O	2:B:97:LEU:O	0.53	2.27	9	9
1:A:4:A:N3	1:A:4:A:O5'	0.53	2.41	9	3
3:C:205:LEU:HD23	3:C:207:PHE:CE2	0.53	2.39	8	1
1:A:11:A:N7	2:B:58:MET:HE3	0.53	2.18	9	1
1:A:7:U:H4'	3:C:202:PHE:CE1	0.53	2.38	9	1
1:A:10:U:O4	2:B:71:PHE:CD2	0.53	2.61	1	1
1:A:4:A:N3	3:C:168:TRP:CH2	0.53	2.77	1	2
1:A:6:A:C2'	3:C:236:ARG:HH22	0.53	2.16	2	1
3:C:226:LYS:HZ3	3:C:278:LYS:NZ	0.53	2.00	2	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:46:CYS:O	2:B:87:LEU:CD1	0.53	2.56	7	3
2:B:90:TYR:CE1	2:B:92:LEU:HD13	0.53	2.38	5	1
1:A:8:A:O2'	1:A:9:A:P	0.53	2.67	6	3
3:C:166:LEU:CD1	3:C:192:LYS:HZ1	0.53	2.16	8	1
3:C:212:SER:O	3:C:216:VAL:CG2	0.53	2.55	1	3
3:C:239:GLN:O	3:C:242:THR:OG1	0.53	2.27	6	5
3:C:200:ARG:NH1	3:C:201:GLY:O	0.53	2.42	3	1
1:A:6:A:N1	3:C:162:PHE:CG	0.53	2.76	9	3
1:A:9:A:N3	2:B:29:TYR:CG	0.53	2.77	4	1
1:A:10:U:H5'	2:B:69:TYR:CG	0.53	2.39	4	1
2:B:34:PRO:O	2:B:36:ASP:N	0.53	2.42	5	3
1:A:7:U:C4	3:C:202:PHE:CG	0.53	2.96	6	1
2:B:86:ASN:HD22	2:B:86:ASN:N	0.53	2.02	9	1
1:A:11:A:O2'	2:B:66:SER:C	0.53	2.47	7	1
1:A:6:A:N1	3:C:234:ILE:N	0.53	2.48	7	1
2:B:29:TYR:OH	2:B:101:TYR:N	0.53	2.42	10	1
1:A:1:U:O2'	1:A:2:A:O5'	0.53	2.27	6	6
1:A:2:A:C6	3:C:246:PHE:CG	0.53	2.97	9	2
1:A:4:A:C6	3:C:168:TRP:CE3	0.53	2.97	4	1
2:B:27:VAL:HG12	2:B:102:SER:H	0.53	1.62	6	1
2:B:87:LEU:N	2:B:87:LEU:HD22	0.53	2.18	6	1
1:A:12:A:OP2	2:B:58:MET:O	0.53	2.26	7	1
2:B:32:SER:C	2:B:33:ILE:HD12	0.53	2.24	7	1
3:C:254:VAL:HG11	3:C:308:PHE:CE2	0.53	2.38	7	2
1:A:9:A:H1'	2:B:71:PHE:CE1	0.53	2.38	9	2
3:C:159:CYS:SG	3:C:213:VAL:HG21	0.53	2.44	9	1
3:C:208:GLU:CG	3:C:209:LYS:H	0.53	2.15	10	1
1:A:12:A:H8	2:B:67:LYS:CA	0.52	2.17	7	1
1:A:9:A:O2'	1:A:10:U:O5'	0.52	2.27	10	6
3:C:229:ASP:OD2	3:C:231:LYS:NZ	0.52	2.42	3	1
3:C:262:PHE:O	3:C:263:PHE:C	0.52	2.48	9	5
3:C:172:GLU:CD	3:C:172:GLU:H	0.52	2.07	6	1
2:B:87:LEU:O	2:B:97:LEU:CD1	0.52	2.56	9	1
2:B:46:CYS:C	2:B:48:ASN:N	0.52	2.63	10	9
2:B:90:TYR:O	2:B:91:GLN:C	0.52	2.48	3	9
3:C:226:LYS:HZ2	3:C:226:LYS:HB2	0.52	1.64	4	1
3:C:193:ASP:CB	3:C:197:GLY:O	0.52	2.57	6	1
1:A:11:A:C5'	2:B:69:TYR:HB2	0.52	2.35	7	1
1:A:2:A:O2'	1:A:3:U:P	0.52	2.68	5	5
3:C:227:VAL:O	3:C:227:VAL:HG22	0.52	2.03	7	2
1:A:11:A:C2'	1:A:12:A:H8	0.52	2.17	2	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:6:A:N1	3:C:162:PHE:CB	0.52	2.73	3	1
1:A:1:U:O2	1:A:2:A:C5	0.52	2.62	9	1
3:C:276:LEU:O	3:C:277:ASP:O	0.52	2.27	9	1
2:B:97:LEU:CD1	2:B:97:LEU:N	0.52	2.60	2	1
3:C:276:LEU:N	3:C:280:THR:O	0.52	2.33	2	1
1:A:2:A:C4'	3:C:286:PHE:CE1	0.52	2.93	2	1
3:C:269:ILE:HG23	3:C:291:TYR:CZ	0.52	2.39	3	1
3:C:274:LEU:HD23	3:C:274:LEU:C	0.52	2.25	3	1
3:C:182:TYR:OH	3:C:221:HIS:CE1	0.52	2.63	4	3
3:C:270:ILE:HD13	3:C:291:TYR:O	0.52	2.03	6	1
3:C:247:VAL:HG21	3:C:263:PHE:CZ	0.52	2.40	10	1
3:C:164:GLY:O	3:C:229:ASP:N	0.52	2.34	8	1
3:C:207:PHE:O	3:C:208:GLU:C	0.52	2.48	10	1
3:C:229:ASP:N	3:C:229:ASP:OD1	0.52	2.43	7	1
2:B:36:ASP:CB	2:B:37:GLN:NE2	0.52	2.72	2	1
3:C:307:ASP:O	3:C:307:ASP:OD1	0.52	2.28	8	2
3:C:166:LEU:N	3:C:166:LEU:CD1	0.52	2.73	3	1
1:A:10:U:H1'	2:B:58:MET:HE2	0.52	1.82	4	1
1:A:12:A:H8	2:B:67:LYS:C	0.52	2.08	7	1
2:B:96:PHE:O	2:B:97:LEU:C	0.52	2.48	4	9
3:C:165:GLY:O	3:C:227:VAL:O	0.52	2.28	4	2
3:C:227:VAL:HG12	3:C:273:GLN:OE1	0.52	2.05	6	1
1:A:10:U:H4'	2:B:66:SER:CB	0.51	2.34	1	1
3:C:172:GLU:O	3:C:175:LEU:N	0.51	2.43	4	1
1:A:2:A:C4	3:C:246:PHE:CD2	0.51	2.99	9	3
3:C:269:ILE:HB	3:C:272:ALA:HB2	0.51	1.81	3	1
2:B:60:ASP:OD1	2:B:63:THR:CG2	0.51	2.58	4	1
3:C:313:ILE:O	3:C:313:ILE:CG1	0.51	2.57	4	1
3:C:264:SER:N	3:C:269:ILE:HD11	0.51	2.19	9	1
2:B:34:PRO:C	2:B:36:ASP:H	0.51	2.08	5	5
2:B:23:PRO:CB	2:B:24:PRO:CD	0.51	2.89	5	2
1:A:10:U:P	2:B:30:LEU:O	0.51	2.68	5	1
3:C:266:TRP:HE1	3:C:300:VAL:CG1	0.51	2.17	6	1
1:A:10:U:H5'	2:B:71:PHE:CG	0.51	2.40	7	1
3:C:167:ASN:N	3:C:167:ASN:OD1	0.51	2.43	7	2
3:C:254:VAL:O	3:C:255:ARG:C	0.51	2.48	8	1
1:A:10:U:O2	2:B:58:MET:SD	0.51	2.68	1	1
3:C:179:PHE:C	3:C:181:LYS:N	0.51	2.60	6	4
3:C:172:GLU:CD	3:C:172:GLU:N	0.51	2.64	3	1
2:B:60:ASP:CG	2:B:60:ASP:O	0.51	2.48	7	3
3:C:308:PHE:CD2	3:C:309:LYS:N	0.51	2.78	4	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:47:SER:O	2:B:50:GLY:N	0.51	2.38	9	1
3:C:168:TRP:CZ2	3:C:198:ARG:NH2	0.51	2.79	10	1
3:C:226:LYS:NZ	3:C:278:LYS:O	0.51	2.36	1	1
1:A:10:U:H5''	2:B:60:ASP:OD2	0.51	2.05	4	1
3:C:236:ARG:CG	3:C:236:ARG:HH11	0.51	2.18	5	1
1:A:4:A:H2'	1:A:4:A:N3	0.51	2.21	10	1
3:C:175:LEU:CD2	3:C:205:LEU:HD11	0.51	2.35	10	1
2:B:55:LEU:HD23	2:B:56:LYS:N	0.51	2.21	1	3
2:B:36:ASP:CB	2:B:37:GLN:HE22	0.51	2.19	2	1
1:A:5:U:H3	3:C:201:GLY:C	0.51	2.06	4	2
2:B:53:ILE:O	2:B:54:ASN:OD1	0.51	2.29	7	2
1:A:12:A:O4'	2:B:67:LYS:CB	0.51	2.59	7	1
3:C:185:VAL:HG12	3:C:207:PHE:CE1	0.51	2.41	9	1
3:C:276:LEU:N	3:C:283:SER:OG	0.51	2.43	3	1
3:C:221:HIS:CD2	3:C:230:PRO:CG	0.51	2.94	5	1
1:A:3:U:O2'	1:A:4:A:C4'	0.51	2.59	6	1
1:A:12:A:OP1	2:B:58:MET:O	0.51	2.28	7	1
1:A:12:A:OP1	2:B:59:PHE:CB	0.51	2.58	7	1
1:A:11:A:H5'	2:B:69:TYR:CB	0.51	2.36	7	1
2:B:72:ILE:CD1	2:B:72:ILE:N	0.51	2.72	10	1
1:A:5:U:C2	3:C:201:GLY:O	0.51	2.64	7	2
2:B:60:ASP:CG	2:B:66:SER:H	0.51	2.09	2	1
1:A:10:U:OP1	2:B:69:TYR:CB	0.51	2.59	8	3
3:C:161:MET:SD	3:C:216:VAL:CG1	0.51	2.99	3	1
3:C:250:ILE:HD11	3:C:286:PHE:O	0.51	2.06	3	1
1:A:6:A:C8	3:C:162:PHE:CE1	0.51	2.99	7	1
3:C:186:THR:O	3:C:187:ASP:OD1	0.51	2.29	7	2
3:C:245:ILE:HD12	3:C:315:ILE:HG23	0.51	1.81	7	1
1:A:5:U:H4'	3:C:200:ARG:HB2	0.51	1.82	10	1
1:A:6:A:H5''	1:A:8:A:H8	0.51	1.64	3	1
3:C:166:LEU:HD12	3:C:202:PHE:CA	0.51	2.36	6	1
1:A:6:A:C5	3:C:162:PHE:CD1	0.51	2.99	7	1
3:C:163:ILE:HD11	3:C:205:LEU:HD13	0.51	1.83	8	1
3:C:178:TYR:CD1	3:C:178:TYR:C	0.51	2.84	4	3
3:C:193:ASP:O	3:C:195:ALA:N	0.51	2.44	3	1
1:A:8:A:C2	2:B:29:TYR:CZ	0.51	2.98	4	1
1:A:9:A:C2	2:B:71:PHE:CZ	0.51	2.99	5	1
3:C:311:ARG:CG	3:C:312:LYS:N	0.51	2.74	5	1
3:C:161:MET:SD	3:C:217:VAL:CG2	0.51	2.99	6	1
3:C:175:LEU:HD22	3:C:190:ILE:CD1	0.51	2.36	7	1
3:C:308:PHE:C	3:C:310:ASP:N	0.51	2.64	10	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:C:178:TYR:C	3:C:178:TYR:CD1	0.50	2.85	3	5
1:A:11:A:N7	2:B:58:MET:HE2	0.50	2.21	2	1
1:A:6:A:C8	3:C:236:ARG:NH2	0.50	2.79	2	1
2:B:80:SER:O	2:B:84:VAL:HG23	0.50	2.06	2	1
2:B:27:VAL:CG2	2:B:28:VAL:N	0.50	2.75	6	2
2:B:81:ALA:O	2:B:85:ARG:CG	0.50	2.59	10	3
3:C:241:LYS:O	3:C:242:THR:O	0.50	2.29	6	1
3:C:262:PHE:O	3:C:264:SER:N	0.50	2.45	6	1
1:A:11:A:H3'	2:B:69:TYR:CA	0.50	2.32	7	1
3:C:300:VAL:HG23	3:C:303:ASN:OD1	0.50	2.05	3	1
1:A:6:A:H4'	1:A:7:U:H5''	0.50	1.78	8	2
2:B:60:ASP:CG	2:B:63:THR:HG1	0.50	2.09	4	1
2:B:87:LEU:N	2:B:87:LEU:CD2	0.50	2.74	6	1
3:C:229:ASP:OD1	3:C:271:ASP:OD2	0.50	2.29	6	1
3:C:188:LEU:CD2	3:C:188:LEU:C	0.50	2.78	9	1
2:B:46:CYS:O	2:B:47:SER:C	0.50	2.50	5	10
3:C:272:ALA:O	3:C:273:GLN:CB	0.50	2.55	10	3
2:B:31:GLY:N	2:B:33:ILE:CD1	0.50	2.74	2	1
2:B:60:ASP:CB	2:B:66:SER:O	0.50	2.59	7	3
2:B:27:VAL:HG11	2:B:102:SER:O	0.50	2.06	5	1
2:B:77:LEU:CD2	2:B:77:LEU:N	0.50	2.74	5	2
3:C:207:PHE:CZ	3:C:216:VAL:HG21	0.50	2.41	6	1
3:C:262:PHE:CD1	3:C:262:PHE:C	0.50	2.82	6	1
3:C:259:PHE:CD1	3:C:274:LEU:HD23	0.50	2.41	8	1
2:B:32:SER:H	2:B:95:ARG:NH1	0.50	2.04	9	1
3:C:180:GLY:C	3:C:182:TYR:H	0.50	2.09	10	1
3:C:213:VAL:O	3:C:217:VAL:HG12	0.50	2.07	1	1
3:C:200:ARG:CZ	3:C:202:PHE:CE2	0.50	2.94	2	1
3:C:215:GLU:OE2	3:C:219:THR:OG1	0.50	2.30	2	1
3:C:237:ASP:O	3:C:241:LYS:N	0.50	2.43	3	1
2:B:77:LEU:N	2:B:77:LEU:CD2	0.50	2.74	2	2
2:B:84:VAL:HG13	2:B:99:CYS:SG	0.50	2.47	4	1
3:C:166:LEU:HD12	3:C:167:ASN:C	0.50	2.27	4	1
3:C:301:CYS:SG	3:C:317:ARG:NH1	0.50	2.85	1	1
3:C:193:ASP:O	3:C:193:ASP:OD1	0.50	2.30	4	1
2:B:77:LEU:CD2	2:B:77:LEU:H	0.50	2.20	5	1
3:C:257:LYS:O	3:C:261:GLU:OE1	0.50	2.29	7	1
1:A:8:A:C2	2:B:29:TYR:CG	0.50	2.99	9	1
2:B:97:LEU:HD23	2:B:97:LEU:H	0.50	1.66	9	1
2:B:76:ASP:C	2:B:78:GLU:N	0.50	2.64	9	10
3:C:163:ILE:CG2	3:C:166:LEU:HD21	0.50	2.34	2	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:C:216:VAL:HG13	3:C:217:VAL:N	0.50	2.22	2	1
1:A:2:A:H1'	3:C:286:PHE:CE2	0.50	2.41	2	1
3:C:182:TYR:N	3:C:182:TYR:CD1	0.50	2.79	5	1
3:C:190:ILE:O	3:C:190:ILE:CG2	0.50	2.59	7	1
3:C:166:LEU:CB	3:C:192:LYS:HZ1	0.50	2.20	8	1
1:A:11:A:O2'	1:A:12:A:H5'	0.50	2.07	2	1
3:C:300:VAL:O	3:C:301:CYS:C	0.50	2.50	3	8
2:B:96:PHE:O	2:B:97:LEU:O	0.50	2.30	6	1
2:B:27:VAL:O	2:B:100:GLY:O	0.50	2.29	8	1
3:C:221:HIS:CB	3:C:228:ILE:HD11	0.50	2.36	8	2
2:B:30:LEU:HD12	2:B:72:ILE:HD11	0.50	1.84	10	1
3:C:276:LEU:O	3:C:280:THR:O	0.49	2.30	2	1
1:A:12:A:OP1	2:B:58:MET:C	0.49	2.49	7	1
2:B:68:GLY:O	2:B:69:TYR:CG	0.49	2.65	7	1
3:C:188:LEU:HD12	3:C:189:LYS:H	0.49	1.63	2	1
1:A:11:A:O4'	2:B:58:MET:SD	0.49	2.70	3	1
1:A:10:U:C2	1:A:11:A:N7	0.49	2.80	4	1
1:A:3:U:O2'	1:A:4:A:O5'	0.49	2.30	4	2
2:B:60:ASP:OD1	2:B:63:THR:OG1	0.49	2.30	4	1
1:A:9:A:C6	2:B:29:TYR:CE2	0.49	3.00	10	1
3:C:192:LYS:O	3:C:199:SER:OG	0.49	2.29	10	1
3:C:168:TRP:O	3:C:169:ASP:OD1	0.49	2.30	1	1
3:C:260:GLU:O	3:C:264:SER:CB	0.49	2.61	2	1
3:C:282:GLN:O	3:C:285:GLY:N	0.49	2.46	2	1
2:B:92:LEU:O	2:B:93:GLY:O	0.49	2.30	3	1
3:C:166:LEU:CD2	3:C:201:GLY:O	0.49	2.61	4	1
1:A:4:A:C6	3:C:168:TRP:NE1	0.49	2.79	6	1
2:B:90:TYR:CD1	2:B:91:GLN:N	0.49	2.80	7	3
3:C:162:PHE:O	3:C:162:PHE:CG	0.49	2.65	7	1
3:C:176:ARG:C	3:C:178:TYR:N	0.49	2.64	10	7
1:A:10:U:OP1	2:B:70:ALA:O	0.49	2.31	5	1
3:C:214:ASP:OD1	3:C:218:LYS:NZ	0.49	2.45	6	1
3:C:259:PHE:CD1	3:C:259:PHE:C	0.49	2.86	6	1
1:A:4:A:OP2	1:A:4:A:C2	0.49	2.65	1	1
2:B:76:ASP:O	2:B:77:LEU:C	0.49	2.51	6	10
2:B:77:LEU:H	2:B:77:LEU:CD2	0.49	2.20	7	3
2:B:84:VAL:O	2:B:88:ASN:CG	0.49	2.51	4	4
2:B:60:ASP:OD2	2:B:66:SER:O	0.49	2.29	5	2
3:C:226:LYS:HZ1	3:C:278:LYS:C	0.49	2.09	7	1
3:C:221:HIS:HB2	3:C:228:ILE:HD11	0.49	1.83	9	2
2:B:60:ASP:OD2	2:B:66:SER:OG	0.49	2.31	10	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:C:236:ARG:CG	3:C:236:ARG:NH1	0.49	2.72	5	1
3:C:208:GLU:CG	3:C:209:LYS:N	0.49	2.75	10	1
3:C:232:ARG:O	3:C:233:ALA:C	0.49	2.50	6	4
3:C:275:MET:SD	3:C:280:THR:O	0.49	2.70	5	1
3:C:231:LYS:HG2	3:C:234:ILE:HD11	0.49	1.85	6	1
2:B:60:ASP:CG	2:B:66:SER:O	0.49	2.51	5	6
3:C:211:SER:O	3:C:212:SER:C	0.49	2.51	9	10
1:A:6:A:H2'	3:C:236:ARG:HH22	0.49	1.67	2	1
3:C:260:GLU:O	3:C:264:SER:OG	0.49	2.29	2	1
2:B:102:SER:OG	2:B:102:SER:O	0.49	2.29	3	2
2:B:77:LEU:N	2:B:77:LEU:HD22	0.49	2.23	4	2
1:A:10:U:OP2	1:A:10:U:C6	0.49	2.65	7	1
3:C:262:PHE:CD2	3:C:308:PHE:CE1	0.49	3.00	9	1
2:B:60:ASP:N	2:B:60:ASP:OD1	0.49	2.42	1	1
3:C:158:SER:C	3:C:160:LYS:H	0.49	2.10	7	2
3:C:251:GLY:O	3:C:252:PRO:O	0.49	2.30	9	3
3:C:274:LEU:C	3:C:275:MET:SD	0.49	2.92	6	1
1:A:10:U:O5'	2:B:71:PHE:CZ	0.49	2.66	7	1
2:B:88:ASN:O	2:B:97:LEU:HG	0.49	2.08	9	1
3:C:164:GLY:C	3:C:166:LEU:H	0.49	2.11	10	1
1:A:3:U:O4	3:C:319:GLU:OE1	0.48	2.31	1	1
3:C:178:TYR:CG	3:C:223:LEU:HD12	0.48	2.43	1	2
3:C:172:GLU:O	3:C:173:ASP:C	0.48	2.50	3	6
2:B:30:LEU:HD13	2:B:72:ILE:HD13	0.48	1.85	6	1
2:B:48:ASN:O	2:B:49:VAL:CB	0.48	2.61	9	2
1:A:6:A:C5	3:C:162:PHE:CG	0.48	3.01	1	3
1:A:4:A:OP1	1:A:4:A:H3'	0.48	2.08	9	1
1:A:11:A:N7	2:B:58:MET:SD	0.48	2.86	9	1
3:C:182:TYR:CD1	3:C:182:TYR:N	0.48	2.82	8	2
3:C:166:LEU:CD1	3:C:167:ASN:O	0.48	2.61	4	1
2:B:88:ASN:O	2:B:97:LEU:C	0.48	2.52	6	2
3:C:255:ARG:HH11	3:C:255:ARG:CG	0.48	2.21	6	1
3:C:317:ARG:C	3:C:319:GLU:H	0.48	2.12	7	2
2:B:69:TYR:CD1	2:B:69:TYR:C	0.48	2.86	10	1
3:C:305:PHE:CZ	3:C:314:GLU:OE2	0.48	2.65	10	1
3:C:305:PHE:CE1	3:C:314:GLU:OE2	0.48	2.67	10	1
2:B:34:PRO:C	2:B:36:ASP:N	0.48	2.67	5	5
2:B:26:ARG:C	2:B:80:SER:HG	0.48	2.12	2	1
3:C:262:PHE:O	3:C:265:GLN:CD	0.48	2.51	7	2
3:C:256:PRO:O	3:C:257:LYS:C	0.48	2.50	7	3
3:C:168:TRP:NE1	3:C:198:ARG:NH2	0.48	2.60	7	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:C:175:LEU:HD13	3:C:190:ILE:CD1	0.48	2.38	9	1
3:C:262:PHE:CG	3:C:263:PHE:N	0.48	2.80	6	1
3:C:191:MET:O	3:C:202:PHE:CE1	0.48	2.66	7	1
3:C:277:ASP:C	3:C:279:ASP:N	0.48	2.66	9	1
3:C:242:THR:HG22	3:C:292:ASP:HA	0.48	1.86	1	1
3:C:200:ARG:O	3:C:202:PHE:CD1	0.48	2.66	9	1
3:C:307:ASP:OD1	3:C:307:ASP:O	0.48	2.31	9	1
3:C:195:ALA:O	3:C:196:THR:C	0.48	2.52	10	1
2:B:45:LEU:C	2:B:45:LEU:CD1	0.48	2.82	8	6
2:B:43:LEU:O	2:B:47:SER:OG	0.48	2.30	2	1
3:C:276:LEU:N	3:C:276:LEU:CD1	0.48	2.67	7	1
1:A:10:U:OP1	2:B:69:TYR:CE2	0.48	2.67	10	1
3:C:227:VAL:O	3:C:227:VAL:HG12	0.48	2.09	3	1
1:A:4:A:N6	3:C:279:ASP:OD1	0.48	2.46	3	1
2:B:52:VAL:HG13	2:B:53:ILE:H	0.48	1.69	4	1
3:C:167:ASN:O	3:C:167:ASN:OD1	0.48	2.31	5	1
3:C:163:ILE:HG21	3:C:166:LEU:HD21	0.48	1.84	8	1
2:B:88:ASN:O	2:B:97:LEU:CG	0.48	2.61	1	2
1:A:6:A:C4'	1:A:7:U:C5'	0.48	2.87	3	6
1:A:2:A:N6	3:C:246:PHE:CE1	0.48	2.82	2	2
1:A:10:U:OP2	2:B:69:TYR:CD1	0.48	2.67	5	2
1:A:8:A:N6	2:B:101:TYR:CZ	0.48	2.81	8	1
3:C:170:THR:H	3:C:192:LYS:CD	0.48	2.21	8	1
3:C:262:PHE:O	3:C:265:GLN:OE1	0.48	2.32	2	1
3:C:178:TYR:CE2	3:C:223:LEU:HD23	0.48	2.44	5	1
1:A:12:A:OP1	2:B:59:PHE:CA	0.48	2.62	7	1
3:C:248:GLY:O	3:C:249:GLY:O	0.47	2.32	1	1
2:B:26:ARG:CA	2:B:80:SER:OG	0.47	2.61	2	1
1:A:10:U:C5	2:B:71:PHE:CE1	0.47	3.02	1	1
2:B:75:ARG:O	2:B:76:ASP:HB2	0.47	2.09	2	1
3:C:211:SER:C	3:C:213:VAL:N	0.47	2.67	10	7
1:A:12:A:O2'	1:A:13:U:C6	0.47	2.57	3	4
1:A:5:U:C4	3:C:165:GLY:N	0.47	2.82	4	1
2:B:28:VAL:HG23	2:B:98:LYS:C	0.47	2.28	4	1
2:B:31:GLY:C	2:B:33:ILE:HD12	0.47	2.30	7	3
3:C:255:ARG:NH1	3:C:255:ARG:CG	0.47	2.76	6	1
3:C:161:MET:HE1	3:C:217:VAL:HG22	0.47	1.85	9	1
2:B:87:LEU:O	2:B:87:LEU:CD1	0.47	2.63	1	1
3:C:209:LYS:O	3:C:211:SER:N	0.47	2.48	1	2
3:C:266:TRP:O	3:C:267:GLY:O	0.47	2.32	4	2
1:A:2:A:O4'	3:C:286:PHE:CD1	0.47	2.67	2	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:C:193:ASP:CA	3:C:197:GLY:O	0.47	2.62	6	1
3:C:306:ILE:HG21	3:C:315:ILE:HD11	0.47	1.86	6	1
3:C:193:ASP:OD1	3:C:199:SER:OG	0.47	2.32	7	1
3:C:184:THR:OG1	3:C:208:GLU:OE2	0.47	2.31	10	1
3:C:160:LYS:NZ	3:C:189:LYS:HZ2	0.47	2.08	1	1
2:B:60:ASP:OD1	2:B:60:ASP:O	0.47	2.32	3	2
3:C:196:THR:HG23	3:C:197:GLY:N	0.47	2.24	3	1
2:B:30:LEU:CD1	2:B:72:ILE:HD11	0.47	2.39	10	1
2:B:72:ILE:H	2:B:72:ILE:HD12	0.47	1.68	10	1
1:A:4:A:C8	3:C:168:TRP:CE2	0.47	3.02	1	1
2:B:97:LEU:H	2:B:97:LEU:HD23	0.47	1.70	10	2
1:A:5:U:O2'	1:A:6:A:O5'	0.47	2.31	5	3
1:A:4:A:OP1	3:C:275:MET:CE	0.47	2.62	3	1
2:B:30:LEU:HB3	2:B:33:ILE:HD11	0.47	1.85	4	2
2:B:60:ASP:CG	2:B:63:THR:OG1	0.47	2.52	4	1
3:C:277:ASP:O	3:C:278:LYS:C	0.47	2.53	4	1
1:A:4:A:OP2	3:C:280:THR:O	0.47	2.32	5	1
1:A:10:U:OP1	2:B:30:LEU:O	0.47	2.32	5	1
3:C:277:ASP:OD1	3:C:281:GLY:N	0.47	2.37	6	1
2:B:38:THR:HG23	2:B:39:GLU:N	0.47	2.24	8	1
3:C:193:ASP:OD1	3:C:196:THR:OG1	0.47	2.31	8	1
1:A:1:U:C4	3:C:314:GLU:OE1	0.47	2.67	10	1
3:C:211:SER:O	3:C:215:GLU:OE2	0.47	2.32	4	1
3:C:269:ILE:CG2	3:C:272:ALA:HB2	0.47	2.39	6	2
3:C:167:ASN:C	3:C:169:ASP:H	0.47	2.13	1	2
3:C:282:GLN:C	3:C:284:ARG:H	0.47	2.11	5	4
3:C:221:HIS:H	3:C:221:HIS:CD2	0.47	2.27	4	3
3:C:246:PHE:CG	3:C:247:VAL:N	0.47	2.82	7	4
3:C:274:LEU:CD2	3:C:274:LEU:C	0.47	2.80	5	2
2:B:60:ASP:OD2	2:B:69:TYR:CE2	0.47	2.67	4	1
3:C:160:LYS:O	3:C:233:ALA:HB2	0.47	2.08	5	2
3:C:176:ARG:CD	3:C:185:VAL:HG11	0.47	2.39	6	1
3:C:166:LEU:HD12	3:C:202:PHE:HA	0.47	1.87	6	1
3:C:195:ALA:O	3:C:196:THR:CG2	0.47	2.61	6	1
1:A:11:A:H5'	2:B:69:TYR:CA	0.47	2.40	7	1
1:A:5:U:H3	3:C:165:GLY:N	0.47	2.07	7	1
2:B:45:LEU:CD1	2:B:45:LEU:C	0.47	2.82	7	2
3:C:249:GLY:O	3:C:313:ILE:CG2	0.47	2.62	8	1
3:C:274:LEU:C	3:C:274:LEU:HD13	0.47	2.30	8	1
3:C:267:GLY:CA	3:C:291:TYR:CE1	0.47	2.97	10	1
3:C:283:SER:O	3:C:283:SER:OG	0.47	2.31	1	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:75:ARG:O	2:B:76:ASP:CG	0.47	2.53	5	9
2:B:37:GLN:OE1	2:B:92:LEU:HD11	0.47	2.09	7	2
1:A:5:U:O4'	3:C:200:ARG:CZ	0.47	2.63	3	1
3:C:300:VAL:CG2	3:C:303:ASN:HD21	0.47	2.23	3	1
3:C:172:GLU:OE2	3:C:192:LYS:NZ	0.47	2.46	5	1
3:C:270:ILE:N	3:C:290:THR:O	0.47	2.47	6	1
2:B:85:ARG:O	2:B:88:ASN:CG	0.47	2.54	7	2
2:B:28:VAL:HG22	2:B:72:ILE:HD13	0.47	1.87	7	1
3:C:200:ARG:O	3:C:202:PHE:CD2	0.47	2.68	10	3
2:B:52:VAL:HG13	2:B:53:ILE:N	0.47	2.25	4	1
2:B:88:ASN:O	2:B:97:LEU:HB2	0.47	2.09	6	1
2:B:60:ASP:OD1	2:B:64:GLY:N	0.47	2.37	7	1
3:C:222:ILE:HD13	3:C:222:ILE:N	0.47	2.23	7	1
3:C:271:ASP:OD1	3:C:271:ASP:O	0.47	2.33	8	1
3:C:273:GLN:CG	3:C:274:LEU:N	0.47	2.78	10	1
2:B:42:ILE:C	2:B:44:ASP:N	0.47	2.68	3	6
3:C:161:MET:SD	3:C:216:VAL:HG21	0.47	2.49	2	1
2:B:60:ASP:OD2	2:B:64:GLY:C	0.47	2.54	5	3
1:A:9:A:O2'	1:A:10:U:H5'	0.46	2.10	10	2
1:A:5:U:O2	3:C:200:ARG:C	0.46	2.54	4	2
2:B:46:CYS:O	2:B:48:ASN:OD1	0.46	2.33	4	1
3:C:310:ASP:CG	3:C:311:ARG:H	0.46	2.14	10	3
2:B:52:VAL:HG11	2:B:72:ILE:CG2	0.46	2.40	7	2
3:C:167:ASN:OD1	3:C:170:THR:OG1	0.46	2.32	9	1
3:C:305:PHE:CE1	3:C:314:GLU:HG2	0.46	2.45	10	1
3:C:253:ASP:O	3:C:254:VAL:O	0.46	2.33	4	1
3:C:278:LYS:O	3:C:279:ASP:CG	0.46	2.53	6	1
1:A:13:U:OP2	2:B:33:ILE:O	0.46	2.33	7	1
1:A:8:A:OP1	3:C:199:SER:OG	0.46	2.33	9	1
3:C:283:SER:C	3:C:285:GLY:H	0.46	2.11	2	1
2:B:39:GLU:O	2:B:43:LEU:CB	0.46	2.63	8	3
1:A:10:U:OP1	2:B:66:SER:OG	0.46	2.33	3	1
3:C:167:ASN:O	3:C:168:TRP:C	0.46	2.53	10	2
2:B:51:PRO:O	2:B:52:VAL:C	0.46	2.53	5	2
3:C:178:TYR:CD2	3:C:223:LEU:HD13	0.46	2.46	6	1
2:B:48:ASN:O	2:B:49:VAL:CG2	0.46	2.62	9	1
1:A:10:U:C3'	2:B:69:TYR:OH	0.46	2.63	10	1
1:A:7:U:H1'	3:C:202:PHE:CZ	0.46	2.46	3	1
2:B:60:ASP:OD2	2:B:65:ARG:C	0.46	2.54	5	1
3:C:259:PHE:CE1	3:C:263:PHE:CE1	0.46	3.03	5	2
2:B:26:ARG:HE	2:B:103:SER:CB	0.46	2.24	7	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:37:GLN:HE21	2:B:37:GLN:N	0.46	2.09	7	1
1:A:9:A:HO2'	1:A:10:U:P	0.46	2.33	10	1
2:B:69:TYR:CZ	2:B:71:PHE:CE1	0.46	3.04	10	1
3:C:175:LEU:HD23	3:C:175:LEU:O	0.46	2.11	10	1
3:C:265:GLN:C	3:C:267:GLY:H	0.46	2.14	10	1
3:C:175:LEU:HD12	3:C:190:ILE:HD13	0.46	1.86	2	2
3:C:283:SER:C	3:C:285:GLY:N	0.46	2.68	2	1
3:C:289:VAL:CG2	3:C:291:TYR:CE2	0.46	2.98	5	1
3:C:308:PHE:O	3:C:310:ASP:O	0.46	2.33	9	2
3:C:182:TYR:HH	3:C:221:HIS:CE1	0.46	2.26	1	2
1:A:3:U:OP1	3:C:282:GLN:OE1	0.46	2.34	3	1
3:C:277:ASP:C	3:C:279:ASP:H	0.46	2.14	9	1
3:C:169:ASP:OD1	3:C:192:LYS:CD	0.46	2.64	3	1
3:C:206:SER:O	3:C:206:SER:OG	0.46	2.33	5	1
3:C:291:TYR:O	3:C:292:ASP:CB	0.46	2.64	6	1
2:B:30:LEU:C	2:B:33:ILE:HD11	0.46	2.31	8	1
3:C:275:MET:SD	3:C:275:MET:N	0.46	2.88	9	1
1:A:7:U:C2	3:C:191:MET:HE1	0.46	2.45	1	1
2:B:82:SER:O	2:B:86:ASN:CG	0.46	2.54	9	3
1:A:6:A:O2'	3:C:236:ARG:CZ	0.46	2.64	2	1
1:A:4:A:C5	3:C:168:TRP:CD1	0.46	3.02	6	1
3:C:223:LEU:N	3:C:223:LEU:HD12	0.46	2.26	9	1
3:C:263:PHE:C	3:C:265:GLN:N	0.46	2.66	9	1
3:C:275:MET:HB2	3:C:286:PHE:CE1	0.46	2.46	1	1
3:C:226:LYS:C	3:C:227:VAL:CG2	0.46	2.85	8	2
3:C:163:ILE:HG22	3:C:166:LEU:CD2	0.46	2.36	2	1
2:B:32:SER:OG	2:B:95:ARG:CG	0.46	2.63	3	1
3:C:226:LYS:HZ1	3:C:280:THR:H	0.46	1.54	5	1
2:B:27:VAL:HG22	2:B:28:VAL:N	0.46	2.25	6	1
2:B:77:LEU:HD22	2:B:77:LEU:N	0.46	2.25	7	1
1:A:3:U:O4'	3:C:288:PHE:CZ	0.46	2.69	1	1
1:A:9:A:N6	2:B:102:SER:OG	0.46	2.40	1	1
1:A:10:U:O4'	2:B:69:TYR:CB	0.46	2.64	1	1
3:C:187:ASP:O	3:C:206:SER:CB	0.46	2.64	1	2
2:B:76:ASP:OD2	2:B:77:LEU:N	0.46	2.49	2	1
3:C:309:LYS:C	3:C:311:ARG:H	0.46	2.12	2	1
3:C:280:THR:OG1	3:C:280:THR:O	0.46	2.31	6	2
1:A:10:U:O2'	1:A:11:A:C8	0.46	2.59	8	1
3:C:292:ASP:OD1	3:C:292:ASP:C	0.45	2.54	1	2
1:A:4:A:C6	3:C:168:TRP:CH2	0.45	3.04	2	2
2:B:76:ASP:CG	2:B:77:LEU:H	0.45	2.14	2	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:C:277:ASP:C	3:C:277:ASP:OD1	0.45	2.55	5	2
2:B:91:GLN:NE2	2:B:96:PHE:CZ	0.45	2.85	9	1
3:C:169:ASP:C	3:C:169:ASP:OD1	0.45	2.55	8	1
2:B:22:ASN:ND2	2:B:101:TYR:CD2	0.45	2.84	10	1
2:B:46:CYS:C	2:B:48:ASN:H	0.45	2.14	7	4
3:C:178:TYR:O	3:C:178:TYR:CD1	0.45	2.70	8	1
1:A:1:U:C2	1:A:2:A:C6	0.45	3.05	9	1
3:C:250:ILE:O	3:C:285:GLY:C	0.45	2.55	9	1
1:A:2:A:C2	1:A:3:U:C6	0.45	3.04	1	1
2:B:81:ALA:C	2:B:85:ARG:HE	0.45	2.14	2	1
2:B:35:TYR:OH	2:B:59:PHE:CB	0.45	2.65	5	1
3:C:223:LEU:CD2	3:C:223:LEU:N	0.45	2.78	6	1
1:A:1:U:C2	1:A:2:A:C5	0.45	3.04	9	1
2:B:43:LEU:HD13	2:B:44:ASP:OD1	0.45	2.11	9	1
3:C:226:LYS:HZ1	3:C:278:LYS:NZ	0.45	2.06	2	1
1:A:11:A:C4	2:B:56:LYS:NZ	0.45	2.74	3	1
1:A:10:U:O2'	1:A:11:A:OP2	0.45	2.33	3	1
1:A:6:A:H61	3:C:234:ILE:H	0.45	1.53	6	1
3:C:303:ASN:O	3:C:304:LYS:C	0.45	2.55	6	2
1:A:12:A:O4'	2:B:67:LYS:C	0.45	2.55	7	1
3:C:276:LEU:N	3:C:276:LEU:CD2	0.45	2.68	7	1
3:C:161:MET:CE	3:C:217:VAL:HG22	0.45	2.42	9	1
1:A:4:A:OP2	3:C:277:ASP:OD1	0.45	2.34	4	1
3:C:167:ASN:OD1	3:C:167:ASN:C	0.45	2.54	6	1
3:C:250:ILE:O	3:C:286:PHE:CA	0.45	2.65	9	1
3:C:161:MET:HE2	3:C:163:ILE:HD13	0.45	1.88	10	1
3:C:307:ASP:C	3:C:307:ASP:OD1	0.45	2.55	2	1
3:C:310:ASP:C	3:C:310:ASP:OD1	0.45	2.55	2	1
3:C:169:ASP:OD1	3:C:192:LYS:NZ	0.45	2.36	3	1
3:C:286:PHE:CD1	3:C:286:PHE:C	0.45	2.89	8	2
2:B:72:ILE:HD12	2:B:72:ILE:H	0.45	1.66	5	1
3:C:191:MET:CB	3:C:202:PHE:CZ	0.45	2.99	6	1
1:A:7:U:O2	3:C:202:PHE:CE2	0.45	2.69	6	1
1:A:1:U:O2	1:A:2:A:C6	0.45	2.70	9	1
1:A:8:A:C2	2:B:29:TYR:CD1	0.45	3.05	9	1
3:C:208:GLU:CD	3:C:209:LYS:H	0.45	2.14	10	1
1:A:5:U:O2	3:C:201:GLY:C	0.45	2.55	1	1
3:C:185:VAL:HG22	3:C:207:PHE:CE1	0.45	2.46	10	2
2:B:58:MET:O	2:B:69:TYR:O	0.45	2.35	4	1
3:C:200:ARG:HE	3:C:200:ARG:N	0.45	2.10	4	1
3:C:244:LYS:N	3:C:317:ARG:HH12	0.45	2.09	5	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:C:262:PHE:C	3:C:264:SER:N	0.45	2.66	6	1
3:C:276:LEU:C	3:C:282:GLN:O	0.45	2.55	8	1
3:C:165:GLY:O	3:C:228:ILE:HG22	0.45	2.12	9	1
3:C:171:THR:O	3:C:172:GLU:C	0.45	2.55	4	1
1:A:10:U:OP2	2:B:65:ARG:NH2	0.45	2.49	6	1
3:C:178:TYR:CD2	3:C:223:LEU:CD2	0.45	3.00	8	2
3:C:174:ASN:C	3:C:174:ASN:OD1	0.44	2.55	1	1
1:A:11:A:H2'	1:A:12:A:C8	0.44	2.47	2	1
1:A:2:A:N6	3:C:246:PHE:CD1	0.44	2.85	2	2
3:C:265:GLN:CG	3:C:266:TRP:N	0.44	2.80	5	2
2:B:56:LYS:CG	2:B:58:MET:SD	0.44	3.05	4	1
3:C:167:ASN:ND2	3:C:169:ASP:O	0.44	2.50	5	1
3:C:173:ASP:OD1	3:C:176:ARG:NH2	0.44	2.50	5	1
3:C:255:ARG:H	3:C:255:ARG:NE	0.44	2.10	6	1
3:C:262:PHE:CD2	3:C:263:PHE:CD1	0.44	3.05	6	1
1:A:11:A:C3'	2:B:69:TYR:H	0.44	2.09	7	1
3:C:167:ASN:CG	3:C:168:TRP:H	0.44	2.15	7	2
3:C:245:ILE:C	3:C:245:ILE:CD1	0.44	2.78	9	1
3:C:291:TYR:C	3:C:293:SER:H	0.44	2.15	9	1
3:C:274:LEU:CD1	3:C:275:MET:O	0.44	2.64	2	1
3:C:178:TYR:CD1	3:C:178:TYR:O	0.44	2.71	4	1
2:B:59:PHE:O	2:B:61:PRO:CD	0.44	2.65	1	5
3:C:303:ASN:HD21	3:C:306:ILE:HD11	0.44	1.72	3	1
1:A:12:A:O2'	1:A:13:U:H5'	0.44	2.12	5	2
2:B:37:GLN:CD	2:B:41:GLN:HE21	0.44	2.15	4	1
3:C:294:ALA:O	3:C:295:ASP:C	0.44	2.56	5	1
3:C:264:SER:C	3:C:266:TRP:N	0.44	2.69	6	2
1:A:11:A:C3'	2:B:68:GLY:C	0.44	2.80	7	1
3:C:224:ASP:OD1	3:C:224:ASP:O	0.44	2.36	7	1
1:A:9:A:H5''	2:B:69:TYR:CD2	0.44	2.44	9	1
2:B:71:PHE:C	2:B:72:ILE:HD12	0.44	2.32	9	1
2:B:31:GLY:C	2:B:33:ILE:H	0.44	2.15	2	1
2:B:49:VAL:HG12	2:B:50:GLY:N	0.44	2.27	4	1
3:C:251:GLY:N	3:C:252:PRO:HD2	0.44	2.26	9	3
2:B:60:ASP:C	2:B:60:ASP:OD1	0.44	2.55	7	1
3:C:170:THR:CB	3:C:192:LYS:NZ	0.44	2.81	9	1
3:C:317:ARG:CB	3:C:317:ARG:NH1	0.44	2.80	10	1
3:C:275:MET:C	3:C:283:SER:OG	0.44	2.56	3	1
3:C:300:VAL:HG23	3:C:303:ASN:HD21	0.44	1.71	3	1
1:A:5:U:C5	3:C:164:GLY:HA2	0.44	2.48	4	1
1:A:5:U:N3	3:C:162:PHE:CE2	0.44	2.84	6	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:C:261:GLU:O	3:C:264:SER:OG	0.44	2.33	9	1
3:C:158:SER:OG	3:C:232:ARG:NE	0.44	2.46	1	1
3:C:224:ASP:O	3:C:224:ASP:OD1	0.44	2.35	1	2
3:C:292:ASP:C	3:C:292:ASP:OD1	0.44	2.54	9	2
1:A:2:A:O2'	1:A:3:U:OP2	0.44	2.35	5	1
1:A:9:A:H5''	2:B:69:TYR:CE1	0.44	2.48	7	1
1:A:8:A:H2	2:B:29:TYR:CD1	0.44	2.31	9	1
2:B:23:PRO:O	2:B:101:TYR:CD2	0.44	2.71	9	1
1:A:10:U:O2	2:B:58:MET:CE	0.44	2.66	1	1
1:A:9:A:H4'	2:B:69:TYR:CZ	0.44	2.47	1	1
3:C:193:ASP:CG	3:C:196:THR:OG1	0.44	2.55	1	2
1:A:2:A:N1	3:C:319:GLU:O	0.44	2.50	7	1
3:C:289:VAL:HG11	3:C:291:TYR:CZ	0.44	2.47	8	1
2:B:29:TYR:N	2:B:29:TYR:CD1	0.44	2.80	10	1
2:B:43:LEU:HD23	2:B:44:ASP:OD1	0.44	2.13	10	1
3:C:277:ASP:O	3:C:281:GLY:N	0.44	2.50	1	1
3:C:301:CYS:C	3:C:303:ASN:N	0.44	2.71	5	2
2:B:32:SER:CB	2:B:94:SER:H	0.44	2.25	7	1
3:C:279:ASP:C	3:C:280:THR:CG2	0.44	2.86	7	1
3:C:254:VAL:HG21	3:C:308:PHE:CE2	0.44	2.48	1	1
1:A:6:A:O2'	3:C:236:ARG:NH2	0.44	2.50	2	1
1:A:5:U:O4	3:C:164:GLY:C	0.44	2.56	5	1
2:B:45:LEU:CD2	2:B:90:TYR:OH	0.44	2.65	5	1
3:C:164:GLY:O	3:C:165:GLY:C	0.44	2.56	5	1
1:A:11:A:C2	2:B:63:THR:CB	0.44	3.00	7	1
3:C:269:ILE:HG23	3:C:291:TYR:CE2	0.44	2.48	9	1
2:B:30:LEU:CD2	2:B:30:LEU:N	0.43	2.80	1	1
3:C:277:ASP:OD1	3:C:277:ASP:C	0.43	2.56	1	1
3:C:176:ARG:CG	3:C:177:GLU:N	0.43	2.81	3	1
3:C:246:PHE:CE1	3:C:247:VAL:C	0.43	2.92	3	1
3:C:318:ALA:O	3:C:319:GLU:C	0.43	2.56	5	1
1:A:11:A:C2'	2:B:69:TYR:HB2	0.43	2.43	7	1
1:A:5:U:C1'	3:C:201:GLY:O	0.43	2.59	7	1
2:B:29:TYR:OH	2:B:101:TYR:O	0.43	2.35	10	1
3:C:253:ASP:O	3:C:254:VAL:C	0.43	2.56	4	1
3:C:277:ASP:O	3:C:281:GLY:O	0.43	2.36	4	1
2:B:31:GLY:CA	2:B:69:TYR:CE1	0.43	3.01	5	1
3:C:270:ILE:CG1	3:C:291:TYR:O	0.43	2.65	6	1
3:C:249:GLY:O	3:C:310:ASP:OD2	0.43	2.36	8	1
1:A:4:A:C5	3:C:168:TRP:CE3	0.43	3.06	1	1
2:B:27:VAL:HG13	2:B:73:GLU:CA	0.43	2.42	1	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:1:U:O2'	1:A:2:A:C8	0.43	2.57	6	1
1:A:11:A:C3'	2:B:69:TYR:HB2	0.43	2.44	7	1
1:A:2:A:H5''	3:C:284:ARG:HD2	0.43	1.88	9	1
3:C:208:GLU:OE1	3:C:208:GLU:C	0.43	2.56	9	1
1:A:6:A:N3	3:C:162:PHE:CE1	0.43	2.86	2	1
3:C:232:ARG:O	3:C:234:ILE:N	0.43	2.51	4	1
1:A:11:A:H4'	2:B:58:MET:HG2	0.43	1.90	7	1
2:B:102:SER:O	2:B:102:SER:OG	0.43	2.31	10	1
2:B:38:THR:O	2:B:42:ILE:CD1	0.43	2.64	10	1
2:B:26:ARG:C	2:B:80:SER:OG	0.43	2.56	2	2
2:B:43:LEU:O	2:B:47:SER:CB	0.43	2.66	2	1
1:A:11:A:OP1	2:B:61:PRO:CG	0.43	2.67	3	1
3:C:250:ILE:O	3:C:251:GLY:C	0.43	2.56	4	1
3:C:187:ASP:H	3:C:206:SER:CB	0.43	2.26	5	1
3:C:227:VAL:CG1	3:C:227:VAL:O	0.43	2.65	5	1
3:C:227:VAL:CG1	3:C:273:GLN:OE1	0.43	2.66	6	1
1:A:10:U:OP2	1:A:10:U:C5	0.43	2.71	7	1
2:B:31:GLY:HA2	2:B:69:TYR:CD1	0.43	2.48	7	1
3:C:193:ASP:N	3:C:194:PRO:CD	0.43	2.81	8	1
1:A:4:A:OP1	1:A:4:A:H2	0.43	1.97	10	1
2:B:39:GLU:CD	2:B:39:GLU:C	0.43	2.77	1	1
1:A:9:A:C5	2:B:29:TYR:CE2	0.43	3.07	4	1
2:B:39:GLU:N	2:B:57:MET:SD	0.43	2.92	5	1
3:C:254:VAL:O	3:C:254:VAL:HG23	0.43	2.13	6	1
1:A:12:A:P	2:B:69:TYR:H	0.43	2.35	7	1
2:B:60:ASP:HB3	2:B:66:SER:H	0.43	1.72	8	1
3:C:271:ASP:O	3:C:272:ALA:O	0.43	2.37	8	1
3:C:310:ASP:OD1	3:C:311:ARG:N	0.43	2.52	1	1
2:B:90:TYR:N	2:B:90:TYR:CD1	0.43	2.85	5	1
2:B:48:ASN:O	2:B:87:LEU:HD11	0.43	2.14	10	1
2:B:81:ALA:O	2:B:85:ARG:CB	0.43	2.67	1	2
2:B:83:ALA:HA	2:B:86:ASN:OD1	0.43	2.14	2	1
1:A:9:A:OP1	2:B:69:TYR:OH	0.43	2.34	7	1
3:C:254:VAL:O	3:C:254:VAL:CG1	0.43	2.62	8	1
1:A:10:U:OP1	1:A:10:U:C6	0.43	2.72	10	1
3:C:299:ARG:O	3:C:302:GLN:CG	0.43	2.67	1	1
1:A:7:U:C4'	1:A:8:A:OP2	0.43	2.64	4	2
3:C:217:VAL:HG13	3:C:218:LYS:N	0.43	2.28	2	1
3:C:174:ASN:OD1	3:C:174:ASN:C	0.43	2.58	3	1
3:C:276:LEU:HD12	3:C:278:LYS:N	0.43	2.29	6	1
1:A:6:A:H5''	1:A:7:U:C5'	0.43	2.43	2	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:30:LEU:N	2:B:30:LEU:HD22	0.43	2.29	2	1
3:C:197:GLY:O	3:C:198:ARG:C	0.43	2.55	4	1
3:C:207:PHE:CG	3:C:212:SER:OG	0.43	2.68	10	1
3:C:202:PHE:CD1	3:C:202:PHE:C	0.42	2.92	1	1
2:B:49:VAL:HG21	2:B:87:LEU:HD11	0.42	1.90	2	1
2:B:48:ASN:OD1	2:B:48:ASN:N	0.42	2.52	4	1
3:C:185:VAL:HG11	3:C:188:LEU:HD23	0.42	1.91	4	1
1:A:5:U:C2	3:C:164:GLY:CA	0.42	3.02	6	1
3:C:186:THR:OG1	3:C:208:GLU:CA	0.42	2.67	6	1
3:C:308:PHE:CE2	3:C:309:LYS:CG	0.42	3.02	6	1
1:A:9:A:C2	2:B:29:TYR:CG	0.42	3.07	10	1
1:A:11:A:H5''	2:B:61:PRO:HD2	0.42	1.90	1	1
3:C:158:SER:CB	3:C:232:ARG:HE	0.42	2.27	1	1
2:B:76:ASP:CG	2:B:77:LEU:N	0.42	2.72	2	1
3:C:200:ARG:CD	3:C:200:ARG:N	0.42	2.82	4	1
3:C:254:VAL:CG2	3:C:255:ARG:N	0.42	2.82	4	1
3:C:190:ILE:C	3:C:191:MET:SD	0.42	2.98	5	1
3:C:283:SER:O	3:C:284:ARG:C	0.42	2.57	6	1
1:A:4:A:H2	1:A:4:A:OP1	0.42	1.96	7	1
3:C:163:ILE:CD1	3:C:175:LEU:HD21	0.42	2.45	7	1
1:A:12:A:C6	2:B:58:MET:SD	0.42	3.12	8	1
3:C:275:MET:CB	3:C:286:PHE:CE1	0.42	3.03	1	1
2:B:42:ILE:O	2:B:43:LEU:C	0.42	2.58	3	5
2:B:71:PHE:N	2:B:71:PHE:CD1	0.42	2.86	3	1
1:A:10:U:H5'	2:B:69:TYR:CD2	0.42	2.49	4	1
3:C:215:GLU:CD	3:C:215:GLU:N	0.42	2.73	4	1
3:C:262:PHE:CD2	3:C:308:PHE:CD1	0.42	3.07	9	1
2:B:88:ASN:CG	2:B:89:GLY:N	0.42	2.73	10	1
3:C:250:ILE:HG21	3:C:274:LEU:HD22	0.42	1.91	10	1
1:A:10:U:H5'	2:B:71:PHE:HZ	0.42	1.74	2	1
2:B:48:ASN:O	2:B:49:VAL:C	0.42	2.56	2	2
1:A:5:U:O5'	1:A:5:U:O2	0.42	2.37	3	1
3:C:168:TRP:O	3:C:197:GLY:O	0.42	2.37	3	1
2:B:45:LEU:HD21	2:B:92:LEU:HD22	0.42	1.90	8	1
2:B:90:TYR:CZ	2:B:92:LEU:HD13	0.42	2.49	2	1
3:C:211:SER:C	3:C:215:GLU:OE2	0.42	2.57	4	1
2:B:44:ASP:OD1	2:B:44:ASP:O	0.42	2.38	7	2
1:A:7:U:H5	3:C:204:PHE:CZ	0.42	2.32	6	1
2:B:84:VAL:CG1	2:B:99:CYS:CB	0.42	2.98	6	1
1:A:2:A:C6	3:C:319:GLU:O	0.42	2.72	7	1
3:C:317:ARG:C	3:C:319:GLU:N	0.42	2.72	7	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:10:U:C2'	1:A:11:A:C8	0.42	2.95	8	1
3:C:222:ILE:CG2	3:C:226:LYS:O	0.42	2.68	10	1
1:A:10:U:O4	2:B:71:PHE:CE2	0.42	2.73	1	1
3:C:264:SER:O	3:C:265:GLN:O	0.42	2.37	4	2
1:A:8:A:H4'	2:B:95:ARG:HH22	0.42	1.75	4	1
2:B:47:SER:C	2:B:49:VAL:H	0.42	2.17	5	1
2:B:60:ASP:HB3	2:B:66:SER:N	0.42	2.30	5	1
3:C:252:PRO:C	3:C:254:VAL:H	0.42	2.18	5	1
3:C:269:ILE:HG23	3:C:269:ILE:O	0.42	2.13	5	1
2:B:33:ILE:CD1	2:B:33:ILE:N	0.42	2.81	8	1
3:C:284:ARG:O	3:C:285:GLY:C	0.42	2.57	2	1
2:B:83:ALA:O	2:B:84:VAL:C	0.42	2.56	6	1
3:C:205:LEU:HD13	3:C:207:PHE:CE2	0.42	2.49	7	1
1:A:10:U:C5	2:B:63:THR:HG21	0.42	2.50	8	1
1:A:5:U:O4'	3:C:201:GLY:O	0.42	2.37	9	1
1:A:2:A:HO2'	1:A:3:U:P	0.42	2.37	1	1
2:B:85:ARG:CD	2:B:85:ARG:C	0.42	2.87	1	1
2:B:32:SER:OG	2:B:94:SER:CB	0.42	2.68	1	1
2:B:35:TYR:OH	2:B:59:PHE:CD2	0.42	2.71	2	1
3:C:222:ILE:CD1	3:C:222:ILE:N	0.42	2.83	7	1
3:C:168:TRP:CE2	3:C:198:ARG:CZ	0.42	3.03	10	1
3:C:213:VAL:CG2	3:C:214:ASP:N	0.42	2.82	10	1
3:C:262:PHE:O	3:C:265:GLN:CG	0.42	2.67	1	2
3:C:193:ASP:OD2	3:C:199:SER:OG	0.42	2.29	2	1
1:A:5:U:O2	3:C:162:PHE:CE2	0.42	2.72	9	1
2:B:38:THR:C	2:B:57:MET:SD	0.42	2.98	10	1
3:C:186:THR:CG2	3:C:187:ASP:N	0.42	2.83	3	1
3:C:300:VAL:HG23	3:C:303:ASN:ND2	0.42	2.30	3	1
3:C:221:HIS:CD2	3:C:230:PRO:HG3	0.42	2.49	5	2
3:C:180:GLY:C	3:C:182:TYR:N	0.42	2.72	10	1
2:B:80:SER:O	2:B:84:VAL:CG2	0.41	2.67	2	1
3:C:162:PHE:O	3:C:163:ILE:C	0.41	2.58	8	2
3:C:226:LYS:NZ	3:C:279:ASP:CA	0.41	2.83	7	1
1:A:10:U:C2	2:B:58:MET:HE2	0.41	2.50	1	1
3:C:282:GLN:C	3:C:284:ARG:N	0.41	2.74	5	2
3:C:244:LYS:O	3:C:318:ALA:CB	0.41	2.68	6	3
2:B:57:MET:SD	2:B:70:ALA:CB	0.41	3.07	2	1
1:A:3:U:O4'	3:C:288:PHE:CE1	0.41	2.73	3	1
2:B:27:VAL:CG1	2:B:102:SER:N	0.41	2.83	6	1
3:C:255:ARG:O	3:C:256:PRO:C	0.41	2.58	7	1
2:B:32:SER:OG	2:B:32:SER:O	0.41	2.37	9	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:C:271:ASP:O	3:C:290:THR:OG1	0.41	2.30	1	1
3:C:232:ARG:O	3:C:234:ILE:CD1	0.41	2.68	2	1
1:A:11:A:H3'	1:A:12:A:C8	0.41	2.51	5	1
3:C:186:THR:N	3:C:206:SER:O	0.41	2.50	5	1
1:A:11:A:O5'	2:B:58:MET:HB3	0.41	2.14	7	1
1:A:11:A:C1'	2:B:66:SER:O	0.41	2.64	7	1
1:A:12:A:C8	2:B:67:LYS:C	0.41	2.91	7	1
1:A:8:A:C5'	2:B:95:ARG:NH2	0.41	2.84	10	1
1:A:10:U:C5'	2:B:69:TYR:OH	0.41	2.62	10	1
3:C:175:LEU:HD23	3:C:175:LEU:C	0.41	2.35	10	1
1:A:2:A:C4'	3:C:286:PHE:CG	0.41	3.01	10	1
2:B:88:ASN:O	2:B:97:LEU:HD12	0.41	2.15	1	1
3:C:158:SER:O	3:C:159:CYS:CB	0.41	2.68	1	2
3:C:301:CYS:O	3:C:302:GLN:C	0.41	2.58	5	2
3:C:186:THR:HG23	3:C:187:ASP:N	0.41	2.30	3	1
2:B:54:ASN:HD22	2:B:73:GLU:CD	0.41	2.17	5	1
2:B:27:VAL:HG22	2:B:73:GLU:HG3	0.41	1.91	7	1
1:A:8:A:O2'	1:A:9:A:H5'	0.41	2.15	8	1
1:A:8:A:N3	2:B:29:TYR:CG	0.41	2.89	9	1
2:B:62:GLN:O	2:B:63:THR:C	0.41	2.58	9	1
1:A:4:A:C2	3:C:168:TRP:CZ3	0.41	3.09	9	1
1:A:4:A:N1	3:C:279:ASP:O	0.41	2.52	10	1
3:C:161:MET:CE	3:C:163:ILE:HD13	0.41	2.46	10	1
2:B:59:PHE:O	2:B:61:PRO:HD3	0.41	2.15	5	1
2:B:29:TYR:C	2:B:30:LEU:HD12	0.41	2.35	6	1
2:B:65:ARG:NH1	3:C:200:ARG:NH2	0.41	2.68	6	1
1:A:8:A:OP1	3:C:192:LYS:O	0.41	2.39	7	1
2:B:31:GLY:HA2	2:B:69:TYR:CE1	0.41	2.50	7	1
3:C:175:LEU:HD22	3:C:190:ILE:HD11	0.41	1.92	8	1
2:B:87:LEU:O	2:B:87:LEU:CG	0.41	2.67	1	1
3:C:271:ASP:O	3:C:290:THR:CB	0.41	2.69	1	1
3:C:159:CYS:SG	3:C:213:VAL:CG2	0.41	3.08	2	1
1:A:9:A:C2'	1:A:10:U:H6	0.41	2.26	3	1
3:C:282:GLN:O	3:C:286:PHE:CE2	0.41	2.74	3	1
1:A:5:U:C6	1:A:5:U:P	0.41	3.14	4	1
3:C:270:ILE:HG22	3:C:271:ASP:N	0.41	2.29	4	1
3:C:186:THR:OG1	3:C:206:SER:O	0.41	2.34	5	1
3:C:301:CYS:O	3:C:303:ASN:N	0.41	2.53	5	1
3:C:289:VAL:CG2	3:C:291:TYR:CE1	0.41	3.03	6	1
3:C:167:ASN:O	3:C:168:TRP:CD2	0.41	2.74	7	1
3:C:186:THR:HG22	3:C:206:SER:O	0.41	2.16	7	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:6:A:C5'	1:A:8:A:OP2	0.41	2.66	8	1
3:C:273:GLN:HG3	3:C:274:LEU:N	0.41	2.30	10	1
1:A:9:A:H4'	2:B:69:TYR:CD2	0.41	2.51	3	1
3:C:200:ARG:O	3:C:202:PHE:CE2	0.41	2.72	3	1
3:C:159:CYS:CB	3:C:209:LYS:O	0.41	2.69	4	1
3:C:166:LEU:C	3:C:166:LEU:CD1	0.41	2.89	4	1
3:C:226:LYS:CB	3:C:226:LYS:NZ	0.41	2.83	4	1
1:A:8:A:N6	2:B:101:TYR:OH	0.41	2.54	6	1
3:C:264:SER:O	3:C:265:GLN:C	0.41	2.59	6	1
3:C:305:PHE:CE2	3:C:314:GLU:CG	0.41	3.04	6	1
2:B:28:VAL:HG13	2:B:98:LYS:O	0.41	2.14	8	1
3:C:174:ASN:CG	3:C:175:LEU:N	0.41	2.73	10	1
3:C:178:TYR:CG	3:C:223:LEU:CD1	0.41	3.04	1	1
2:B:52:VAL:O	2:B:53:ILE:HG12	0.41	2.16	2	1
1:A:9:A:C6	2:B:29:TYR:CZ	0.41	3.08	4	2
1:A:11:A:O2'	2:B:67:LYS:N	0.41	2.54	7	1
1:A:2:A:O2'	1:A:3:U:O5'	0.41	2.38	1	1
3:C:309:LYS:C	3:C:311:ARG:N	0.41	2.74	2	1
2:B:35:TYR:CE1	2:B:59:PHE:CD1	0.41	3.09	2	1
3:C:306:ILE:HD12	3:C:315:ILE:HD11	0.41	1.91	2	1
3:C:193:ASP:C	3:C:195:ALA:H	0.41	2.19	3	1
3:C:251:GLY:O	3:C:254:VAL:CG1	0.41	2.69	4	1
2:B:31:GLY:N	2:B:33:ILE:HD11	0.41	2.31	4	1
3:C:281:GLY:C	3:C:283:SER:N	0.41	2.71	6	1
1:A:6:A:C8	3:C:239:GLN:OE1	0.41	2.74	6	1
1:A:11:A:N3	2:B:60:ASP:HB2	0.41	2.31	7	1
1:A:12:A:C8	2:B:67:LYS:CA	0.41	3.00	7	1
1:A:6:A:N9	3:C:162:PHE:CE1	0.41	2.89	7	1
3:C:174:ASN:ND2	3:C:175:LEU:N	0.41	2.69	9	1
3:C:289:VAL:CG1	3:C:291:TYR:CE1	0.41	3.02	9	1
1:A:6:A:OP1	3:C:200:ARG:NH2	0.41	2.54	10	1
1:A:7:U:OP1	1:A:8:A:N7	0.41	2.53	10	1
3:C:294:ALA:O	3:C:297:VAL:CG1	0.41	2.69	10	1
2:B:27:VAL:CG2	2:B:102:SER:O	0.41	2.69	1	1
1:A:3:U:H5'	3:C:286:PHE:CE1	0.41	2.51	3	1
3:C:266:TRP:C	3:C:266:TRP:CD1	0.41	2.94	3	1
3:C:170:THR:O	3:C:190:ILE:CD1	0.41	2.69	4	1
1:A:8:A:C2	2:B:99:CYS:O	0.41	2.73	6	1
3:C:270:ILE:CD1	3:C:291:TYR:O	0.41	2.69	6	1
1:A:3:U:HO2'	1:A:4:A:P	0.41	2.39	7	1
2:B:32:SER:O	2:B:32:SER:OG	0.41	2.35	7	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:C:161:MET:SD	3:C:162:PHE:C	0.41	2.99	7	1
1:A:2:A:C2	1:A:3:U:C4	0.40	3.09	1	1
2:B:30:LEU:CD2	2:B:42:ILE:HD12	0.40	2.47	6	1
3:C:216:VAL:CG1	3:C:216:VAL:O	0.40	2.67	6	1
3:C:255:ARG:N	3:C:255:ARG:NE	0.40	2.69	6	1
3:C:188:LEU:CD1	3:C:188:LEU:C	0.40	2.80	8	1
1:A:10:U:OP2	2:B:30:LEU:O	0.40	2.39	5	1
3:C:289:VAL:HG21	3:C:291:TYR:CZ	0.40	2.52	5	1
2:B:38:THR:O	2:B:42:ILE:HG12	0.40	2.16	7	1
3:C:170:THR:H	3:C:192:LYS:HD2	0.40	1.77	8	1
2:B:69:TYR:CZ	2:B:71:PHE:CZ	0.40	3.09	10	1
1:A:5:U:H6	1:A:5:U:H2'	0.40	1.53	1	1
3:C:272:ALA:C	3:C:273:GLN:CG	0.40	2.90	2	2
3:C:273:GLN:O	3:C:288:PHE:O	0.40	2.39	3	1
3:C:263:PHE:HB3	3:C:269:ILE:HD12	0.40	1.93	5	1
3:C:240:ASP:OD1	3:C:244:LYS:NZ	0.40	2.53	8	1
2:B:35:TYR:CZ	2:B:59:PHE:CD1	0.40	3.09	9	1
3:C:167:ASN:C	3:C:169:ASP:N	0.40	2.74	1	1
3:C:200:ARG:NE	3:C:202:PHE:CE2	0.40	2.89	2	1
3:C:264:SER:HA	3:C:269:ILE:HD13	0.40	1.92	2	1
1:A:11:A:N3	2:B:56:LYS:NZ	0.40	2.60	3	1
2:B:84:VAL:CG1	2:B:99:CYS:SG	0.40	3.09	4	1
3:C:291:TYR:N	3:C:291:TYR:CD1	0.40	2.90	7	1
2:B:39:GLU:C	2:B:39:GLU:CD	0.40	2.80	9	1
3:C:275:MET:CG	3:C:286:PHE:CE2	0.40	3.05	9	1
3:C:251:GLY:O	3:C:254:VAL:N	0.40	2.49	10	1
2:B:31:GLY:O	2:B:33:ILE:N	0.40	2.55	2	1
2:B:51:PRO:C	2:B:52:VAL:O	0.40	2.60	2	1
3:C:297:VAL:C	3:C:299:ARG:N	0.40	2.75	5	1
2:B:60:ASP:CG	2:B:66:SER:C	0.40	2.79	8	1
3:C:233:ALA:O	3:C:234:ILE:CG1	0.40	2.70	8	1
3:C:250:ILE:CD1	3:C:259:PHE:CD1	0.40	3.04	9	1

## 5.2 Torsion angles [i](#)

### 5.2.1 Protein backbone [i](#)

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	81/84 (96%)	56±2 (69±3%)	13±2 (16±3%)	12±2 (15±2%)	1	5
3	C	162/167 (97%)	119±3 (74±2%)	26±3 (16±2%)	17±2 (10±1%)	1	9
All	All	2430/2510 (97%)	1752 (72%)	392 (16%)	286 (12%)	1	7

All 83 unique Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
2	B	77	LEU	10
2	B	26	ARG	10
2	B	91	GLN	10
2	B	76	ASP	10
2	B	47	SER	10
3	C	200	ARG	8
2	B	43	LEU	8
3	C	283	SER	8
3	C	259	PHE	8
3	C	265	GLN	8
3	C	212	SER	7
3	C	258	GLU	7
2	B	49	VAL	7
2	B	48	ASN	7
3	C	168	TRP	6
2	B	97	LEU	6
2	B	88	ASN	6
2	B	102	SER	5
3	C	180	GLY	5
2	B	52	VAL	5
3	C	159	CYS	5
3	C	309	LYS	5
3	C	227	VAL	5
3	C	192	LYS	4
3	C	269	ILE	4
2	B	68	GLY	4
2	B	61	PRO	4
3	C	177	GLU	4
3	C	277	ASP	4
3	C	267	GLY	4
3	C	242	THR	3
3	C	264	SER	3
3	C	252	PRO	3
3	C	280	THR	3
3	C	318	ALA	3

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Mol	Chain	Res	Type	Models (Total)
3	C	310	ASP	3
3	C	311	ARG	3
3	C	273	GLN	3
3	C	285	GLY	3
3	C	304	LYS	3
3	C	195	ALA	3
3	C	262	PHE	3
2	B	35	TYR	2
2	B	53	ILE	2
2	B	103	SER	2
3	C	197	GLY	2
2	B	23	PRO	2
2	B	93	GLY	2
3	C	312	LYS	2
2	B	51	PRO	2
3	C	279	ASP	2
3	C	196	THR	2
3	C	210	PRO	2
3	C	272	ALA	2
3	C	190	ILE	2
2	B	44	ASP	2
3	C	249	GLY	2
3	C	225	GLY	1
3	C	268	THR	1
3	C	276	LEU	1
3	C	317	ARG	1
2	B	31	GLY	1
2	B	32	SER	1
3	C	278	LYS	1
3	C	173	ASP	1
3	C	286	PHE	1
3	C	222	ILE	1
3	C	257	LYS	1
3	C	254	VAL	1
3	C	216	VAL	1
3	C	194	PRO	1
3	C	316	LYS	1
3	C	217	VAL	1
3	C	181	LYS	1
3	C	266	TRP	1
3	C	255	ARG	1
3	C	208	GLU	1

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Mol	Chain	Res	Type	Models (Total)
3	C	253	ASP	1
3	C	256	PRO	1
3	C	292	ASP	1
3	C	235	PRO	1
3	C	233	ALA	1
3	C	319	GLU	1

### 5.2.2 Protein sidechains ⓘ

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	B	72/74 (97%)	58±2 (80±3%)	14±2 (20±3%)	4	34
3	C	140/145 (97%)	115±3 (82±2%)	25±3 (18±2%)	5	40
All	All	2120/2190 (97%)	1730 (82%)	390 (18%)	5	38

All 129 unique residues with a non-rotameric sidechain are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
2	B	90	TYR	10
3	C	276	LEU	9
3	C	171	THR	9
2	B	37	GLN	9
3	C	222	ILE	9
2	B	97	LEU	9
2	B	88	ASN	8
3	C	280	THR	7
2	B	66	SER	7
3	C	245	ILE	7
3	C	205	LEU	6
3	C	159	CYS	6
2	B	52	VAL	6
3	C	246	PHE	6
3	C	193	ASP	6
2	B	48	ASN	6
3	C	190	ILE	6
3	C	186	THR	6

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Mol	Chain	Res	Type	Models (Total)
2	B	59	PHE	6
3	C	221	HIS	6
3	C	189	LYS	5
3	C	168	TRP	5
3	C	265	GLN	5
2	B	58	MET	5
3	C	226	LYS	5
3	C	269	ILE	5
2	B	41	GLN	5
2	B	91	GLN	5
2	B	25	SER	5
3	C	172	GLU	5
3	C	192	LYS	4
3	C	229	ASP	4
3	C	274	LEU	4
2	B	94	SER	4
3	C	223	LEU	4
3	C	283	SER	4
3	C	227	VAL	4
3	C	289	VAL	4
3	C	236	ARG	4
3	C	200	ARG	4
3	C	188	LEU	4
3	C	255	ARG	4
3	C	275	MET	3
2	B	80	SER	3
2	B	84	VAL	3
2	B	33	ILE	3
2	B	77	LEU	3
3	C	244	LYS	3
2	B	99	CYS	3
2	B	55	LEU	3
3	C	311	ARG	3
2	B	102	SER	3
2	B	57	MET	3
3	C	319	GLU	3
3	C	175	LEU	3
3	C	206	SER	3
3	C	250	ILE	3
3	C	266	TRP	3
2	B	63	THR	2
3	C	286	PHE	2

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Mol	Chain	Res	Type	Models (Total)
3	C	196	THR	2
3	C	309	LYS	2
2	B	86	ASN	2
2	B	35	TYR	2
2	B	28	VAL	2
2	B	26	ARG	2
3	C	161	MET	2
3	C	209	LYS	2
3	C	231	LYS	2
2	B	60	ASP	2
3	C	316	LYS	2
3	C	278	LYS	2
3	C	242	THR	2
3	C	213	VAL	2
3	C	312	LYS	2
2	B	45	LEU	2
3	C	271	ASP	2
2	B	46	CYS	2
3	C	284	ARG	2
3	C	181	LYS	2
2	B	49	VAL	2
2	B	103	SER	2
3	C	264	SER	2
3	C	174	ASN	2
2	B	98	LYS	2
3	C	273	GLN	2
3	C	292	ASP	2
3	C	163	ILE	1
3	C	277	ASP	1
3	C	314	GLU	1
2	B	32	SER	1
3	C	215	GLU	1
3	C	191	MET	1
2	B	69	TYR	1
3	C	185	VAL	1
2	B	101	TYR	1
3	C	208	GLU	1
3	C	167	ASN	1
3	C	279	ASP	1
2	B	43	LEU	1
3	C	247	VAL	1
2	B	22	ASN	1

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Mol	Chain	Res	Type	Models (Total)
3	C	300	VAL	1
2	B	85	ARG	1
3	C	169	ASP	1
3	C	262	PHE	1
3	C	212	SER	1
3	C	258	GLU	1
3	C	170	THR	1
3	C	184	THR	1
3	C	303	ASN	1
3	C	187	ASP	1
2	B	29	TYR	1
2	B	87	LEU	1
2	B	75	ARG	1
3	C	317	ARG	1
2	B	39	GLU	1
3	C	290	THR	1
2	B	53	ILE	1
2	B	92	LEU	1
3	C	302	GLN	1
3	C	261	GLU	1
3	C	160	LYS	1
3	C	306	ILE	1
3	C	270	ILE	1
2	B	95	ARG	1
3	C	198	ARG	1
3	C	256	PRO	1
3	C	301	CYS	1

### 5.2.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers	Suiteness
1	A	12/13 (92%)	6±1 (46±11%)	1±1 (8±8%)	0.25±0.07
All	All	120/130 (92%)	55 (46%)	9 (8%)	0.25

The overall RNA backbone suiteness is 0.25.

All unique RNA backbone outliers are listed below:

Mol	Chain	Res	Type	Models (Total)
1	A	3	U	8
1	A	13	U	7
1	A	4	A	6

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Mol	Chain	Res	Type	Models (Total)
1	A	10	U	6
1	A	12	A	6
1	A	9	A	5
1	A	6	A	5
1	A	2	A	5
1	A	11	A	3
1	A	7	U	3
1	A	5	U	1

All unique RNA pucker outliers are listed below:

Mol	Chain	Res	Type	Models (Total)
1	A	5	U	3
1	A	6	A	3
1	A	10	U	3

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

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

### 5.4 Carbohydrates [i](#)

There are no carbohydrates in this entry.

### 5.5 Ligand geometry [i](#)

There are no ligands in this entry.

### 5.6 Other polymers [i](#)

There are no such molecules in this entry.

### 5.7 Polymer linkage issues [i](#)

There are no chain breaks in this entry.



## 6 Chemical shift validation [i](#)

The completeness of assignment taking into account all chemical shift lists is 25% for the well-defined parts and 25% for the entire structure.

### 6.1 Chemical shift list 1

File name: 2km8\_cs.cif

Chemical shift list name: *assigned\_chem\_shift\_list\_1*

#### 6.1.1 Bookkeeping [i](#)

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

Total number of shifts	922
Number of shifts mapped to atoms	922
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	1

#### 6.1.2 Chemical shift referencing [i](#)

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction $\pm$ precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	80	$-0.14 \pm 0.15$	None needed ( $< 0.5$ ppm)
$^{13}\text{C}_\beta$	65	$0.11 \pm 0.13$	None needed ( $< 0.5$ ppm)
$^{13}\text{C}'$	77	$-0.38 \pm 0.19$	None needed ( $< 0.5$ ppm)
$^{15}\text{N}$	78	$0.61 \pm 0.72$	None needed (imprecise)

#### 6.1.3 Completeness of resonance assignments [i](#)

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 25%, i.e. 812 atoms were assigned a chemical shift out of a possible 3265. 9 out of 30 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	$^1\text{H}$	$^{13}\text{C}$	$^{15}\text{N}$
Backbone	387/1198 (32%)	158/477 (33%)	153/488 (31%)	76/233 (33%)
Sidechain	392/1583 (25%)	264/933 (28%)	119/568 (21%)	9/82 (11%)

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	Total	<sup>1</sup> H	<sup>13</sup> C	<sup>15</sup> N
Aromatic	33/249 (13%)	33/133 (25%)	0/112 (0%)	0/4 (0%)
Overall	812/3265 (25%)	455/1674 (27%)	272/1259 (22%)	85/332 (26%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 25%, i.e. 831 atoms were assigned a chemical shift out of a possible 3366. 9 out of 30 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	<sup>1</sup> H	<sup>13</sup> C	<sup>15</sup> N
Backbone	397/1231 (32%)	162/490 (33%)	157/502 (31%)	78/239 (33%)
Sidechain	401/1643 (24%)	270/970 (28%)	121/586 (21%)	10/87 (11%)
Aromatic	33/257 (13%)	33/137 (24%)	0/114 (0%)	0/6 (0%)
Overall	831/3366 (25%)	465/1728 (27%)	278/1293 (22%)	88/345 (26%)

#### 6.1.4 Statistically unusual chemical shifts ⓘ

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

Mol	Chain	Res	Type	Atom	Shift, ppm	Expected range, ppm	Z-score
2	B	23	PRO	HA	1.69	6.05 – 2.75	-8.2

#### 6.1.5 Random Coil Index (RCI) plots ⓘ

The image below reports *random coil index* values for the protein chains in the structure. The height of each bar gives a probability of a given residue to be disordered, as predicted from the available chemical shifts and the amino acid sequence. A value above 0.2 is an indication of significant predicted disorder. The colour of the bar shows whether the residue is in the well-defined core (black) or in the ill-defined residue ranges (cyan), as described in section 2 on ensemble composition.

Random coil index (RCI) for chain B:

