



# Full wwPDB NMR Structure Validation Report ⓘ

Feb 12, 2017 – 10:01 pm GMT

PDB ID : 2H3C  
Title : Structural basis for nucleic acid and toxin recognition of the bacterial antitoxin CcdA  
Authors : Madl, T.; Van Melderren, L.; Respondek, M.; Oberer, M.; Keller, W.; Zangger, K.  
Deposited on : 2006-05-22

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

<http://wwpdb.org/validation/2016/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 : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
RCI : v\_1n\_11\_5\_13\_A (Berjanski et al., 2005)  
PANAV : Wang et al. (2010)  
ShiftChecker : trunk28760  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : recalc28949

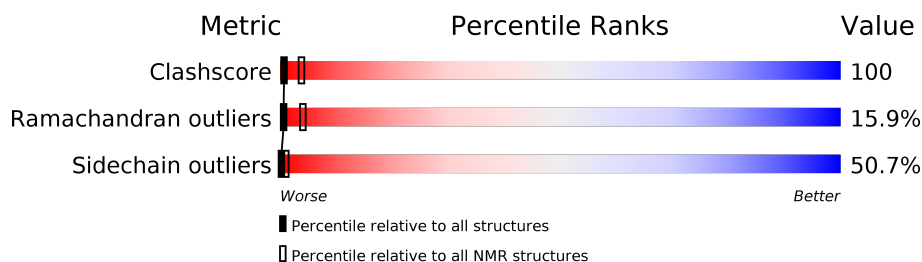
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*SOLUTION NMR*

The overall completeness of chemical shifts assignment was not calculated.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	NMR archive (#Entries)
Clashscore	125131	11601
Ramachandran outliers	121729	10391
Sidechain outliers	121581	10367

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	C	13	<div> <div style="width: 8%; background-color: green;"></div> <div style="width: 92%; background-color: yellow;"></div> </div> <div>8% 92%</div>
2	D	13	<div> <div style="width: 23%; background-color: green;"></div> <div style="width: 77%; background-color: yellow;"></div> </div> <div>23% 77%</div>
3	A	72	<div> <div style="width: 26%; background-color: green;"></div> <div style="width: 21%; background-color: orange;"></div> <div style="width: 49%; background-color: cyan;"></div> </div> <div>• 26% 21% • 49%</div>
3	B	72	<div> <div style="width: 24%; background-color: green;"></div> <div style="width: 24%; background-color: orange;"></div> <div style="width: 49%; background-color: cyan;"></div> </div> <div>• 24% 24% • 49%</div>

## 2 Ensemble composition and analysis

This entry contains 20 models. Model 16 is the overall representative, medoid model (most similar to other models).

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

Well-defined (core) protein residues			
Well-defined core	Residue range (total)	Backbone RMSD (Å)	Medoid model
1	A:2-A:38, B:102-B:138 (74)	0.41	16

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 and 5 single-model clusters were found.

Cluster number	Models
1	3, 4, 5, 8, 10, 12, 15, 16
2	7, 9, 18
3	1, 17
4	2, 6
Single-model clusters	11; 13; 14; 19; 20

### 3 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 3159 atoms, of which 1448 are hydrogens and 0 are deuteriums.

- Molecule 1 is a DNA chain called 5'-D(P\*AP\*TP\*AP\*TP\*GP\*TP\*AP\*TP\*AP\*CP\*CP\*CP\*G)-3'.

Mol	Chain	Residues	Atoms						Trace
1	C	13	Total	C	H	N	O	P	0
			415	127	149	47	79	13	

- Molecule 2 is a DNA chain called 5'-D(P\*TP\*CP\*GP\*GP\*GP\*TP\*AP\*TP\*AP\*CP\*AP\*TP\*A)-3'.

Mol	Chain	Residues	Atoms						Trace
2	D	13	Total	C	H	N	O	P	0
			418	128	149	49	79	13	

- Molecule 3 is a protein called CcdA.

Mol	Chain	Residues	Atoms						Trace
3	A	72	Total	C	H	N	O	S	0
			1163	362	575	105	117	4	
3	B	72	Total	C	H	N	O	S	0
			1163	362	575	105	117	4	

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	70	LYS	ARG	ENGINEERED	UNP Q9S0Z5
B	170	LYS	ARG	ENGINEERED	UNP Q9S0Z5

## 4 Residue-property plots

### 4.1 Average score per residue in the NMR ensemble

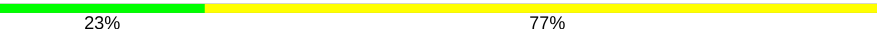
These plots are provided for all protein, RNA and DNA chains in the entry. The first graphic is the same as shown in the summary in section 1 of this report. The second graphic shows the sequence where residues are colour-coded according to the number of geometric quality criteria for which they contain 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'-D(P\*AP\*TP\*AP\*TP\*GP\*TP\*AP\*TP\*AP\*CP\*CP\*CP\*G)-3'

Chain C: 

A173  
T174  
A175  
T176  
G177  
T178  
A179  
T180  
A181  
C182  
C183  
C184  
G185

- Molecule 2: 5'-D(P\*TP\*CP\*GP\*GP\*GP\*TP\*AP\*TP\*AP\*CP\*AP\*TP\*A)-3'

Chain D: 

T186  
C187  
G188  
G189  
G190  
T191  
A192  
T193  
A194  
C195  
A196  
T197  
A198


- Molecule 3: CcdA

Chain A: 

M1  
K2  
Q3  
R4  
I5  
T6  
V7  
T8  
V9  
D10  
S11  
D12  
S13  
Y14  
Q15  
L16  
L17  
K18  
A19  
Y20  
D21  
V22  
N23  
I24  
S25  
G26  
L27  
V28  
S29  
T30  
T31  
M32  
Q33  
N34  
E35  
A36  
R37  
R38  
L39  
R40  
A41  
E42  
R43  
W44  
K45  
V46  
E47  
N48  
Q49  
E50  
G51  
M52  
V53  
E54  
V55  
A56  
R57  
F58  
I59  
E60

M61  
M62  
G63  
S64  
F65  
A66  
D67  
E68  
M69  
K70  
D71  
W72

- Molecule 3: CcdA

Chain B: 

M101  
K102  
Q103  
R104  
T105  
T106  
V107  
T108  
V109  
D110  
S111  
D112  
S113  
Y114  
Q115  
L116  
L117  
K118  
A119  
Y120  
D121  
V122  
N123  
I124  
S125  
G126  
L127  
V128  
S129  
T130  
T131  
M132  
Q133  
N134  
E135  
A136  
R137  
R138  
L139  
R140  
A141  
E142  
R143  
W144  
K145  
V146  
E147  
N148  
Q149  
E150  
G151  
M152  
V153  
E154  
V155  
A156  
R157  
F158  
I159  
E160

M161  
M162  
G163  
S164  
F165  
A166  
D167  
E168  
M169  
K170  
D171  
W172

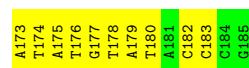
## 4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

### 4.2.1 Score per residue for model 1

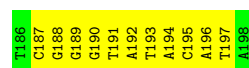
- Molecule 1: 5'-D(P\*AP\*TP\*AP\*TP\*GP\*TP\*AP\*TP\*AP\*CP\*CP\*CP\*G)-3'

Chain C: 



- Molecule 2: 5'-D(P\*TP\*CP\*GP\*GP\*GP\*TP\*AP\*TP\*AP\*CP\*AP\*TP\*A)-3'

Chain D: 



- Molecule 3: CcdA

Chain A: 



- Molecule 3: CcdA

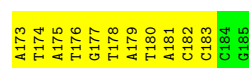
Chain B: 



### 4.2.2 Score per residue for model 2

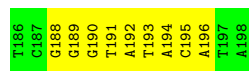
- Molecule 1: 5'-D(P\*AP\*TP\*AP\*TP\*GP\*TP\*AP\*TP\*AP\*CP\*CP\*CP\*G)-3'

Chain C: 



- Molecule 2: 5'-D(P\*TP\*CP\*GP\*GP\*GP\*TP\*AP\*TP\*AP\*CP\*AP\*TP\*A)-3'

Chain D:  31% 69%




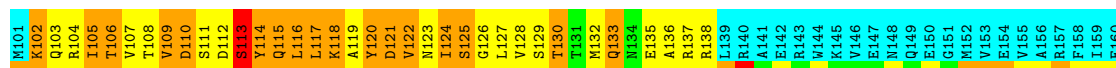
- Molecule 3: CcdA

Chain A:  25% 17% 6% 49%



- Molecule 3: CcdA

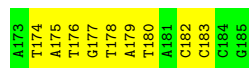
Chain B:  24% 24% 49%



#### 4.2.3 Score per residue for model 3

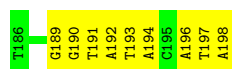
- Molecule 1: 5'-D(P\*AP\*TP\*AP\*TP\*GP\*TP\*AP\*TP\*AP\*CP\*CP\*CP\*G)-3'

Chain C:  31% 69%



- Molecule 2: 5'-D(P\*TP\*CP\*GP\*GP\*GP\*TP\*AP\*TP\*AP\*CP\*AP\*TP\*A)-3'

Chain D:  31% 69%



- Molecule 3: CcdA

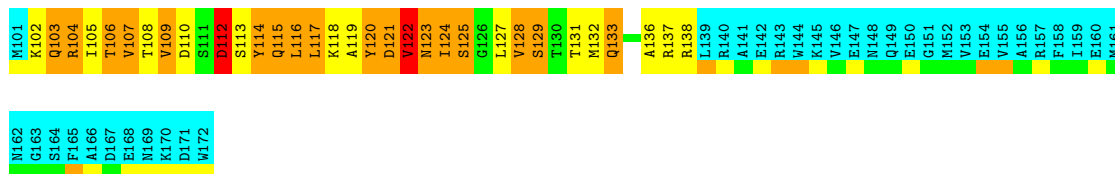
Chain A:  17% 28% 49%





• Molecule 3: CcdA

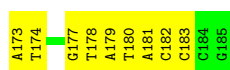
Chain B: 7% 18% 24% • 49%



#### 4.2.4 Score per residue for model 4

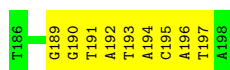
• Molecule 1: 5'-D(P\*AP\*TP\*AP\*TP\*GP\*TP\*AP\*TP\*AP\*CP\*CP\*CP\*G)-3'

Chain C: 31% 69%



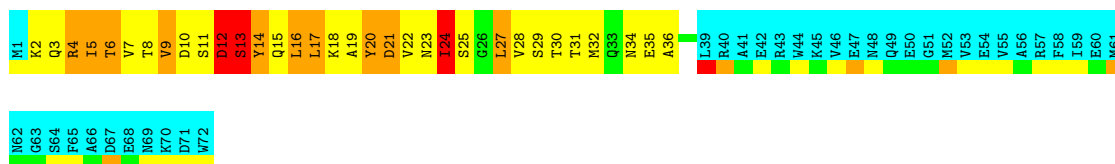
• Molecule 2: 5'-D(P\*TP\*CP\*GP\*GP\*GP\*TP\*AP\*TP\*AP\*CP\*AP\*TP\*A)-3'

Chain D: 31% 69%



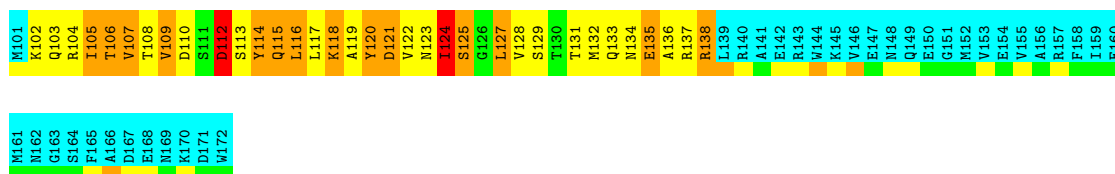
• Molecule 3: CcdA

Chain A: 6% 28% 14% • 49%



• Molecule 3: CcdA

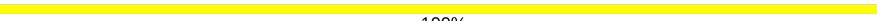
Chain B: • 25% 19% • 49%





### 4.2.5 Score per residue for model 5

- Molecule 1: 5'-D(P\*AP\*TP\*AP\*TP\*GP\*TP\*AP\*TP\*AP\*CP\*CP\*CP\*G)-3'

Chain C:  100%

A173  
T174  
A175  
T176  
G177  
T178  
A179  
T180  
A181  
C182  
C183  
C184  
G185

- Molecule 2: 5'-D(P\*TP\*CP\*GP\*GP\*GP\*TP\*AP\*TP\*AP\*CP\*AP\*TP\*A)-3'

Chain D:  38% 62%

T186  
C187  
G188  
G189  
T190  
T191  
A192  
T193  
A194  
C195  
A198

- Molecule 3: CcdA

Chain A:  18% 28% 49%

M1  
K2  
Q3  
R4  
T5  
T6  
V7  
T8  
V9  
D10  
S11  
D12  
S13  
Y14  
Q15  
L16  
L17  
K18  
A19  
Y20  
D21  
V22  
N23  
I24  
S25  
G26  
L27  
V28  
S29  
T30  
T31  
K32  
Q33  
N34  
E35  
A36  
R37  
P38  
L39  
R40  
A41  
E42  
R43  
V44  
K45  
V46  
E47  
N48  
Q49  
S50  
S51  
M52  
V53  
E54  
V55  
A56  
S57  
F58  
I59  
E60

M61  
G62  
G63  
S64  
F65  
A66  
D67  
E68  
N69  
K70  
D71  
W72

- Molecule 3: CcdA

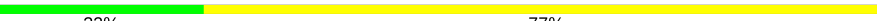
Chain B:  8% 18% 24% 49%

M101  
K102  
Q103  
R104  
I105  
T106  
V107  
T108  
V109  
D110  
S111  
D112  
S113  
Y114  
Q115  
L116  
L117  
K118  
A119  
Y120  
D121  
V122  
N123  
I124  
S125  
G126  
L127  
V128  
S129  
T130  
T131  
M132  
Q133  
A136  
R137  
R138  
L139  
R140  
A141  
E142  
R143  
M144  
K145  
V146  
E147  
N148  
Q149  
E150  
G151  
M152  
V153  
E154  
V155  
A156  
R157  
F158  
I159  
E160  
M161

M162  
G163  
S164  
F165  
A166  
D167  
S168  
M169  
M170  
D171  
M172

### 4.2.6 Score per residue for model 6

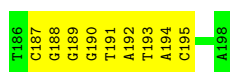
- Molecule 1: 5'-D(P\*AP\*TP\*AP\*TP\*GP\*TP\*AP\*TP\*AP\*CP\*CP\*CP\*G)-3'

Chain C:  23% 77%

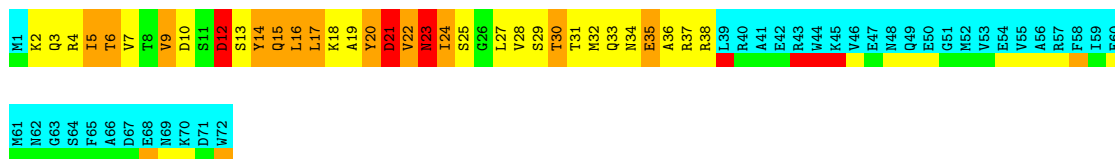
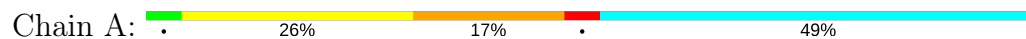
A173  
T174  
A175  
T176  
G177  
T178  
A179  
T180  
A181  
C182  
C183  
C184  
G185

- Molecule 2: 5'-D(P\*TP\*CP\*GP\*GP\*GP\*TP\*AP\*TP\*AP\*CP\*AP\*TP\*A)-3'

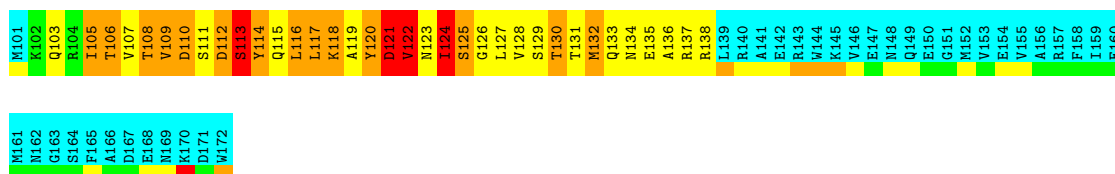
Chain D:  31% 69%



• Molecule 3: CcdA

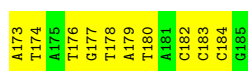
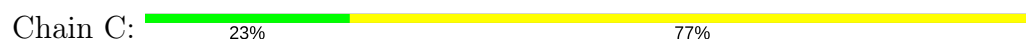


• Molecule 3: CcdA



#### 4.2.7 Score per residue for model 7

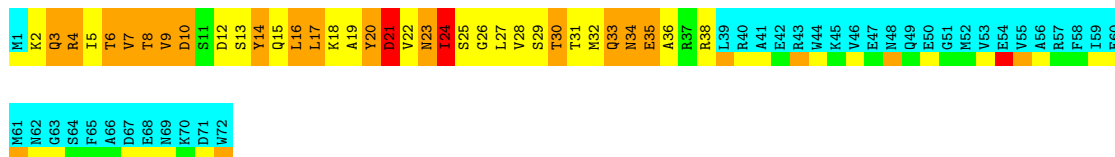
• Molecule 1: 5'-D(P\*AP\*TP\*AP\*TP\*GP\*TP\*AP\*TP\*AP\*CP\*CP\*CP\*G)-3'




• Molecule 2: 5'-D(P\*TP\*CP\*GP\*GP\*GP\*TP\*AP\*TP\*AP\*CP\*AP\*TP\*A)-3'

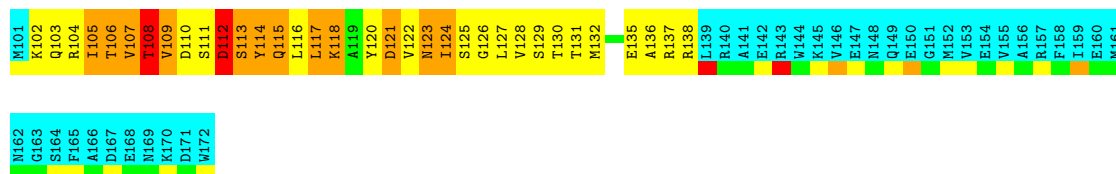


• Molecule 3: CcdA



• Molecule 3: CcdA

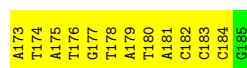
Chain B: 



#### 4.2.8 Score per residue for model 8

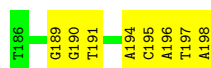
- Molecule 1: 5'-D(P\*AP\*TP\*AP\*TP\*GP\*TP\*AP\*TP\*AP\*CP\*CP\*CP\*G)-3'

Chain C: 



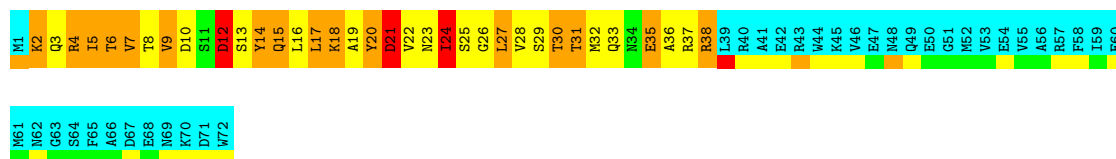
- Molecule 2: 5'-D(P\*TP\*CP\*GP\*GP\*GP\*TP\*AP\*TP\*AP\*CP\*AP\*TP\*A)-3'

Chain D: 



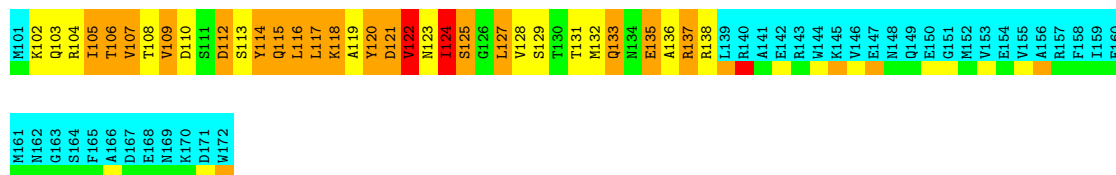
- Molecule 3: CcdA

Chain A: 



- Molecule 3: CcdA

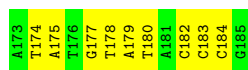
Chain B: 



#### 4.2.9 Score per residue for model 9

- Molecule 1: 5'-D(P\*AP\*TP\*AP\*TP\*GP\*TP\*AP\*TP\*AP\*CP\*CP\*CP\*G)-3'

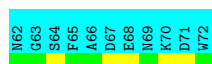
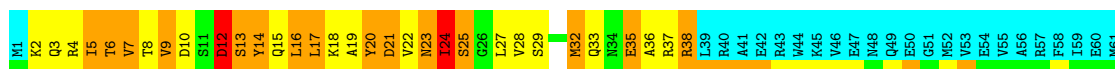
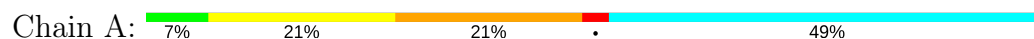
Chain C: 



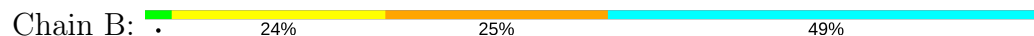
- Molecule 2: 5'-D(P\*TP\*CP\*GP\*GP\*GP\*TP\*AP\*TP\*AP\*CP\*AP\*TP\*A)-3'



- Molecule 3: CcdA

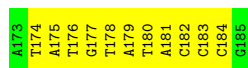


- Molecule 3: CcdA

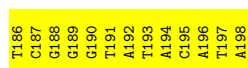


#### 4.2.10 Score per residue for model 10

- Molecule 1: 5'-D(P\*AP\*TP\*AP\*TP\*GP\*TP\*AP\*TP\*AP\*CP\*CP\*CP\*G)-3'

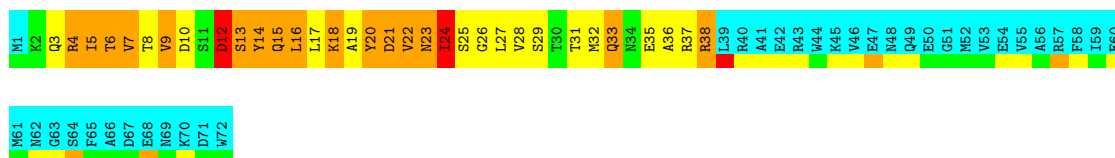


- Molecule 2: 5'-D(P\*TP\*CP\*GP\*GP\*GP\*TP\*AP\*TP\*AP\*CP\*AP\*TP\*A)-3'



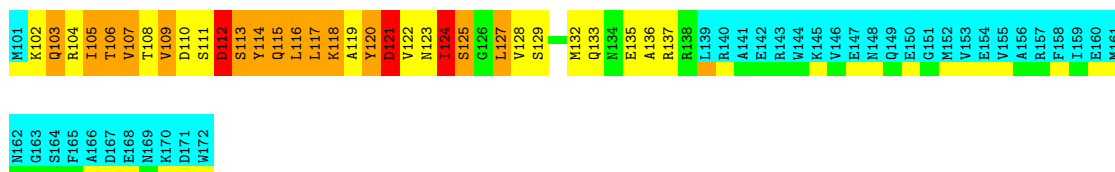
- Molecule 3: CcdA





• Molecule 3: CcdA

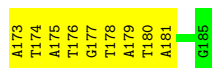
Chain B: 7% 21% 19% 49%



#### 4.2.11 Score per residue for model 11

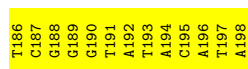
• Molecule 1: 5'-D(P\*AP\*TP\*AP\*TP\*GP\*TP\*AP\*TP\*AP\*CP\*CP\*CP\*G)-3'

Chain C: 31% 69%



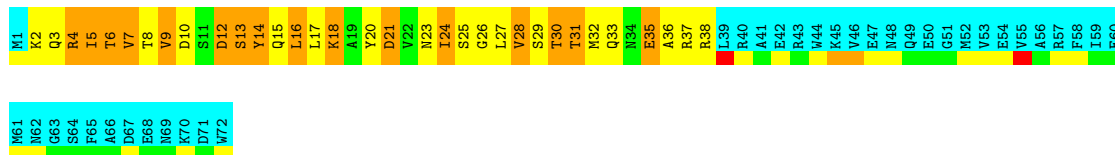
• Molecule 2: 5'-D(P\*TP\*CP\*GP\*GP\*GP\*TP\*AP\*TP\*AP\*CP\*AP\*TP\*A)-3'

Chain D: 100%



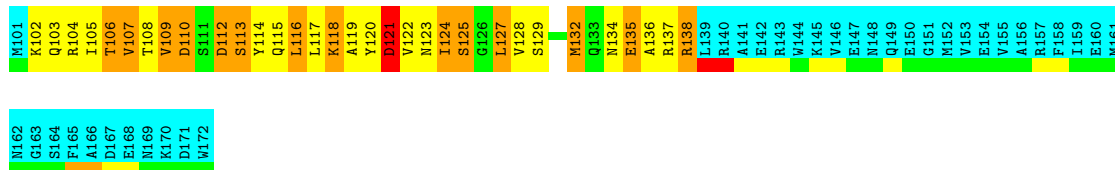
• Molecule 3: CcdA

Chain A: 6% 24% 22% 49%



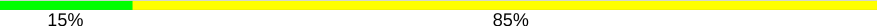
• Molecule 3: CcdA

Chain B: 7% 24% 19% 49%



#### 4.2.12 Score per residue for model 12

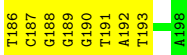
- Molecule 1: 5'-D(P\*AP\*TP\*AP\*TP\*GP\*TP\*AP\*TP\*AP\*CP\*CP\*CP\*G)-3'

Chain C: 


  
A173 T174 A175 T176 G177 T178 A179 T180 A181 C182 C183 C184 G185

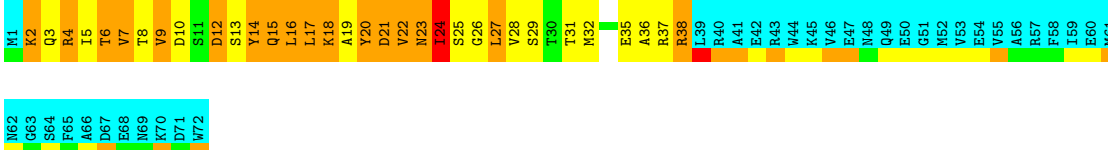
- Molecule 2: 5'-D(P\*TP\*CP\*GP\*GP\*GP\*TP\*AP\*TP\*AP\*CP\*AP\*TP\*A)-3'

Chain D: 

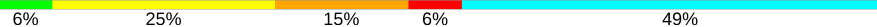
  
T186 C187 G188 G189 G190 T191 A192 T193 A198

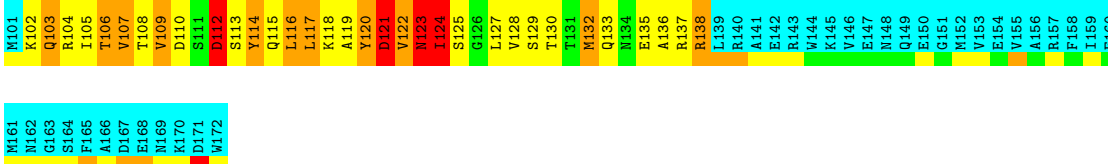
- Molecule 3: CcdA

Chain A: 

  
M1 K2 Q3 R4 T5 T6 V7 T8 V9 S11 D12 S13 Y14 Q15 L16 L17 K18 A19 Y20 D21 V22 N23 I24 S25 G26 L27 V28 S29 T30 T31 M32 E35 A36 R37 R38 L39 R40 A41 E42 R43 W44 K45 V46 E47 N48 Q49 E50 G51 M52 V53 E54 V55 A56 R57 F58 I59 E60 M61 M62 G63 S64 F65 A66 D67 E68 M69 D71 W72


- Molecule 3: CcdA

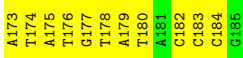
Chain B: 

  
M101 K102 Q103 R104 T105 T106 V107 T108 V109 D110 S111 D112 S113 Y114 Q115 L116 L117 K118 A119 Y120 D121 V122 N123 I124 S125 G126 L127 V128 S129 T130 T131 M132 Q133 M134 E135 A136 R137 R138 L139 R140 A141 E142 R143 K144 V145 V146 E147 N148 Q149 E150 G151 M152 V153 E154 V155 A156 R157 F158 I159 E160 M161 M162 G163 S164 F165 A166 D167 E168 M169 D170 K171 W172

#### 4.2.13 Score per residue for model 13

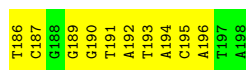
- Molecule 1: 5'-D(P\*AP\*TP\*AP\*TP\*GP\*TP\*AP\*TP\*AP\*CP\*CP\*CP\*G)-3'

Chain C: 

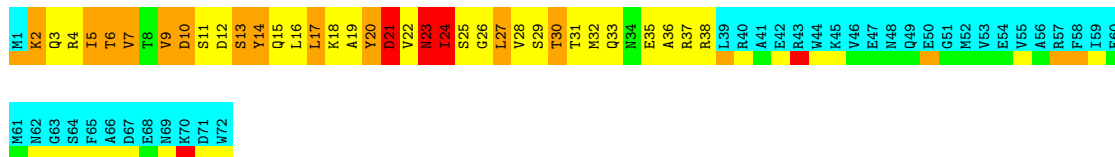
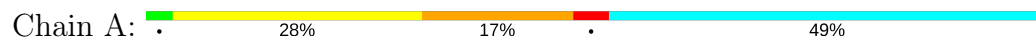
  
A173 T174 A175 T176 G177 T178 A179 T180 A181 C182 C183 C184 G185

- Molecule 2: 5'-D(P\*TP\*CP\*GP\*GP\*GP\*TP\*AP\*TP\*AP\*CP\*AP\*TP\*A)-3'

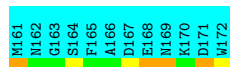
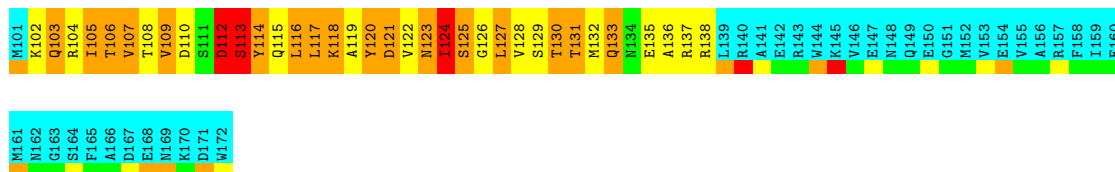
Chain D: 



• Molecule 3: CcdA

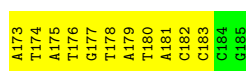
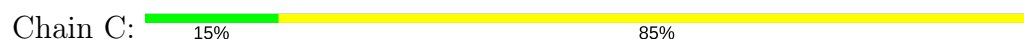


• Molecule 3: CcdA

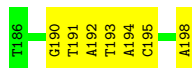


#### 4.2.14 Score per residue for model 14

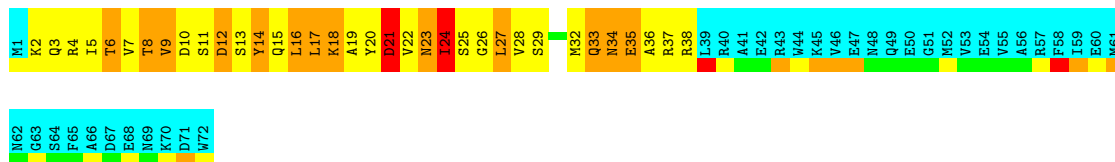
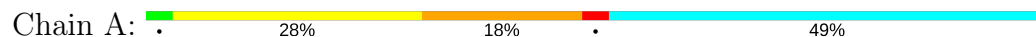
• Molecule 1: 5'-D(P\*AP\*TP\*AP\*TP\*GP\*TP\*AP\*TP\*AP\*CP\*CP\*CP\*G)-3'



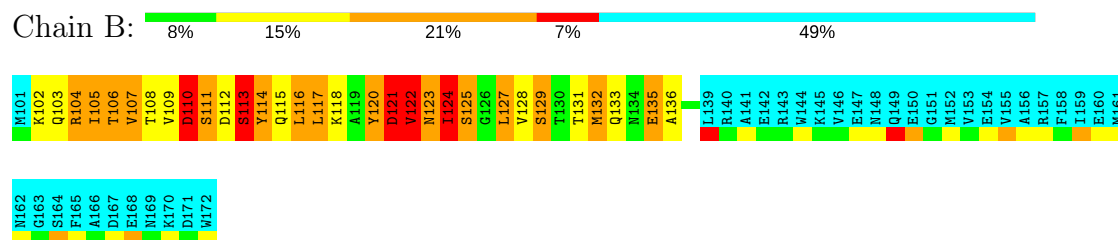
• Molecule 2: 5'-D(P\*TP\*CP\*GP\*GP\*GP\*TP\*AP\*TP\*AP\*CP\*AP\*TP\*A)-3'



• Molecule 3: CcdA



• Molecule 3: CcdA



#### 4.2.15 Score per residue for model 15

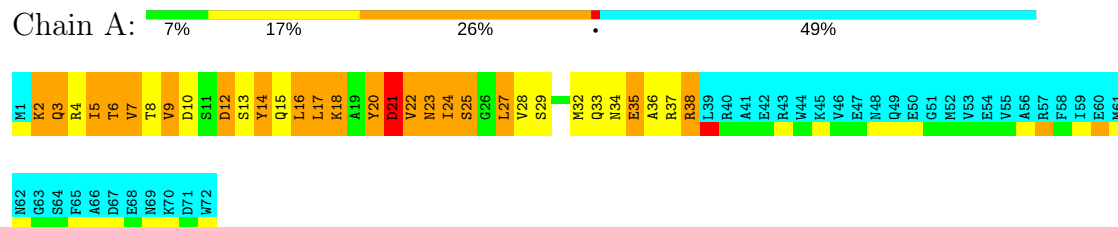
- Molecule 1: 5'-D(P\*AP\*TP\*AP\*TP\*GP\*TP\*AP\*TP\*AP\*CP\*CP\*CP\*G)-3'



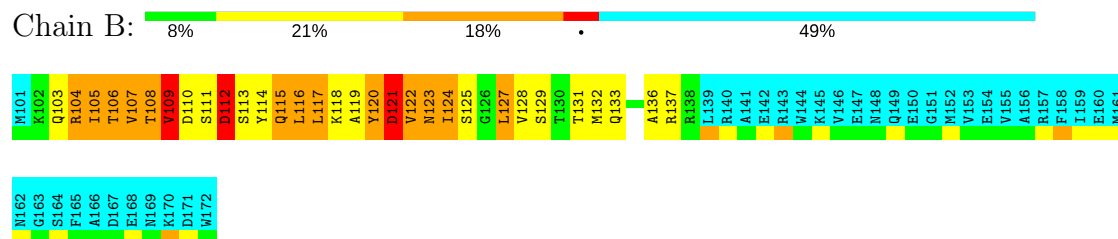
- Molecule 2: 5'-D(P\*TP\*CP\*GP\*GP\*GP\*TP\*AP\*TP\*AP\*CP\*AP\*TP\*A)-3'



- Molecule 3: CcdA



- Molecule 3: CcdA



#### 4.2.16 Score per residue for model 16 (medoid)

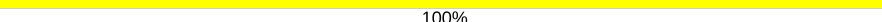
- Molecule 1: 5'-D(P\*AP\*TP\*AP\*TP\*GP\*TP\*AP\*TP\*AP\*CP\*CP\*CP\*G)-3'



Chain C:  23% 77%

A173  
T174  
A175  
T176  
G177  
T178  
A179  
T180  
A181  
C182  
C183  
G184  
G185

- Molecule 2: 5'-D(P\*TP\*CP\*GP\*GP\*GP\*TP\*AP\*TP\*AP\*CP\*AP\*TP\*A)-3'

Chain D:  100%

T186  
C187  
G188  
G189  
G190  
T191  
A192  
T193  
A194  
C195  
A196  
T197  
A198


- Molecule 3: CcdA

Chain A:  21% 26% 49%

M1  
K2  
Q3  
R4  
I5  
T6  
V7  
T8  
V9  
D10  
S11  
D12  
S13  
Y14  
Q15  
L16  
L17  
K18  
A19  
Y20  
D21  
V22  
N23  
I24  
S25  
G26  
L27  
V28  
S29  
T30  
T31  
K32  
Q33  
N34  
E35  
A36  
R37  
R38  
L39  
R40  
A41  
E42  
R43  
R44  
K45  
V46  
E47  
N48  
Q49  
E50  
G51  
M52  
V53  
E54  
V55  
A56  
R57  
F58  
I59  
E60

M61  
M62  
G63  
S64  
F65  
A66  
D67  
S68  
M69  
K70  
D71  
W72

- Molecule 3: CcdA

Chain B:  28% 17% 49%

M101  
K102  
Q103  
R104  
I105  
T106  
V107  
T108  
V109  
D110  
S111  
D112  
S113  
Y114  
Q115  
L116  
L117  
K118  
A119  
Y120  
D121  
V122  
N123  
I124  
S125  
G126  
L127  
V128  
S129  
T130  
T131  
M132  
Q133  
N134  
E135  
A136  
R137  
R138  
L139  
R140  
A141  
E142  
R143  
R144  
K145  
V146  
E147  
N148  
Q149  
E150  
G151  
M152  
V153  
E154  
V155  
A156  
R157  
F158  
I159  
E160

M161  
M162  
G163  
S164  
F165  
A166  
D167  
E168  
M169  
K170  
D171  
W172

#### 4.2.17 Score per residue for model 17

- Molecule 1: 5'-D(P\*AP\*TP\*AP\*TP\*GP\*TP\*AP\*TP\*AP\*CP\*CP\*CP\*G)-3'

Chain C:  15% 85%

A173  
T174  
A175  
T176  
G177  
T178  
A179  
T180  
A181  
C182  
C183  
G184  
G185

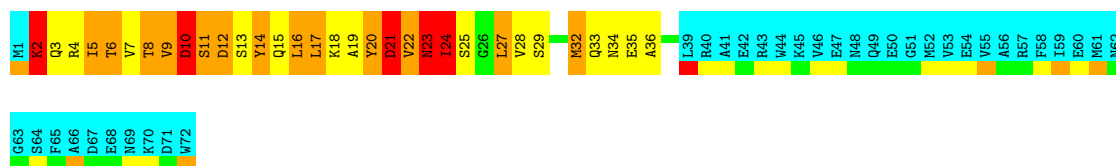
- Molecule 2: 5'-D(P\*TP\*CP\*GP\*GP\*GP\*TP\*AP\*TP\*AP\*CP\*AP\*TP\*A)-3'

Chain D:  31% 69%

T186  
C187  
G188  
G189  
G190  
T191  
A194  
C195  
A196  
T197  
A198

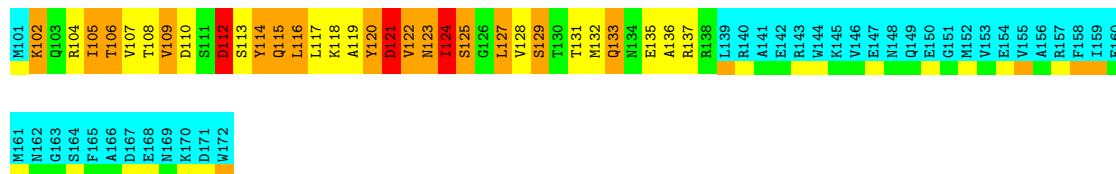
- Molecule 3: CcdA

Chain A: 



• Molecule 3: CcdA

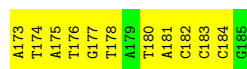
Chain B: 



#### 4.2.18 Score per residue for model 18

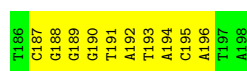
• Molecule 1: 5'-D(P\*AP\*TP\*AP\*TP\*GP\*TP\*AP\*TP\*AP\*CP\*CP\*CP\*G)-3'

Chain C: 

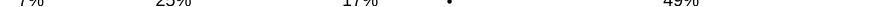


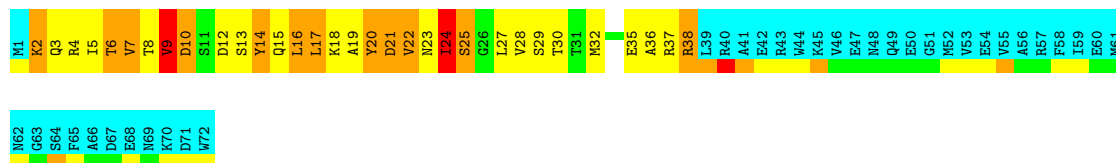
• Molecule 2: 5'-D(P\*TP\*CP\*GP\*GP\*GP\*TP\*AP\*TP\*AP\*CP\*AP\*TP\*A)-3'

Chain D: 




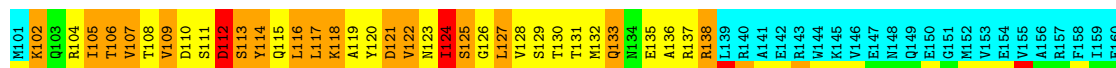
• Molecule 3: CcdA

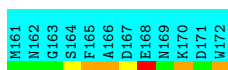
Chain A: 



• Molecule 3: CcdA

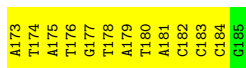
Chain B: 



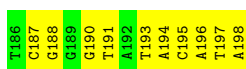


#### 4.2.19 Score per residue for model 19

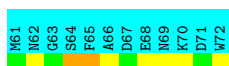
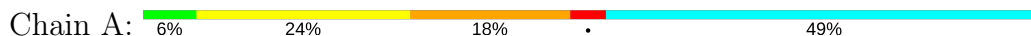
- Molecule 1: 5'-D(P\*AP\*TP\*AP\*TP\*GP\*TP\*AP\*TP\*AP\*CP\*CP\*CP\*G)-3'



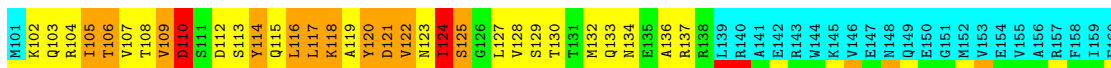
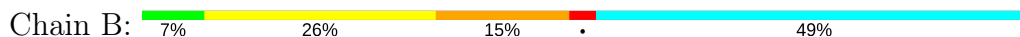
- Molecule 2: 5'-D(P\*TP\*CP\*GP\*GP\*GP\*TP\*AP\*TP\*AP\*CP\*AP\*TP\*A)-3'



- Molecule 3: CcdA

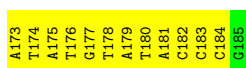


- Molecule 3: CcdA



#### 4.2.20 Score per residue for model 20

- Molecule 1: 5'-D(P\*AP\*TP\*AP\*TP\*GP\*TP\*AP\*TP\*AP\*CP\*CP\*CP\*G)-3'



- Molecule 2: 5'-D(P\*TP\*CP\*GP\*GP\*GP\*TP\*AP\*TP\*AP\*CP\*AP\*TP\*A)-3'

Chain D:  15% 85%

T186  
C187  
G188  
G189  
G190  
T191  
A192  
T193  
A194  
C195  
A196  
T197  
A198

• Molecule 3: CcdA

Chain A:  7% 22% 17% 6% 49%

M1  
K2  
Q3  
R4  
I5  
T6  
V7  
T8  
V9  
D10  
S11  
D12  
S13  
Y14  
Q15  
L16  
L17  
K18  
A19  
Y20  
D21  
V22  
N23  
I24  
S25  
G26  
L27  
V28  
S29  
T30  
T31  
K32  
Q33  
N34  
E35  
A36  
R37  
R38  
L39  
R40  
A41  
E42  
R43  
M44  
K45  
V46  
E47  
N48  
D49  
P50  
G51  
M52  
V53  
E54  
V55  
A56  
R57  
F58  
I59  
E60

M61  
M62  
G63  
S64  
F65  
A66  
D67  
E68  
M69  
K70  
D71  
W72

• Molecule 3: CcdA

Chain B:  6% 21% 21% 49%

M101  
K102  
Q103  
R104  
I105  
T106  
V107  
T108  
V109  
D110  
S111  
D112  
S113  
Y114  
Q115  
L116  
L117  
K118  
A119  
Y120  
D121  
V122  
N123  
I124  
L127  
V128  
S129  
T130  
T131  
M132  
Q133  
N134  
E135  
A136  
R137  
R138  
L139  
R140  
A141  
E142  
R143  
M144  
K145  
V146  
E147  
N148  
Q149  
E150  
G151  
M152  
V153  
E154  
V155  
A156  
R157  
F158  
I159  
E160  
M161

N162  
G163  
S164  
F165  
A166  
D167  
E168  
M169  
K170  
D171  
M172

## 5 Refinement protocol and experimental data overview ⓘ

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

Of the 100 calculated structures, 20 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
CNS	structure solution	1.1
CNS	refinement	1.1

No chemical shift data was provided. No validations of the models with respect to experimental NMR restraints is performed at this time.

## 6 Model quality [i](#)

### 6.1 Standard geometry [i](#)

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

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 6.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	C	266	149	148	16±5
2	D	269	149	148	13±4
3	A	293	298	298	132±7
3	B	293	298	298	132±9
All	All	22420	17880	17840	4044

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 100.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:B:109:VAL:HG21	3:B:114:TYR:CD1	1.22	1.69	13	1
3:B:128:VAL:HG13	3:B:132:MET:SD	1.08	1.88	1	3
3:A:9:VAL:HG21	3:A:14:TYR:CD1	1.07	1.82	11	2
3:A:5:ILE:HD11	3:B:107:VAL:HG13	1.06	1.23	15	6
3:A:32:MET:HA	3:B:117:LEU:HD12	1.06	1.15	4	6
3:B:124:ILE:CG2	3:B:128:VAL:HG23	1.03	1.83	2	17
3:A:17:LEU:HD12	3:B:132:MET:HA	1.01	1.29	8	5
3:A:9:VAL:HG21	3:A:14:TYR:CD2	1.01	1.90	3	4
3:A:7:VAL:HG12	3:B:124:ILE:HD13	1.00	1.28	10	3
3:B:123:ASN:O	3:B:124:ILE:HD12	1.00	1.56	13	10
3:B:109:VAL:HG21	3:B:114:TYR:CB	1.00	1.85	17	13

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:A:14:TYR:CD1	3:B:105:ILE:HD13	1.00	1.91	12	11
3:B:124:ILE:HG22	3:B:128:VAL:HG23	0.99	1.30	13	3
3:B:117:LEU:HD22	3:B:122:VAL:HG11	0.99	1.31	4	3
3:A:17:LEU:HD23	3:A:20:TYR:CE2	0.98	1.93	3	4
3:A:24:ILE:CG2	3:A:28:VAL:HG23	0.97	1.89	13	20
3:A:28:VAL:HG22	3:B:128:VAL:CG2	0.97	1.89	18	10
3:A:23:ASN:C	3:A:24:ILE:HD12	0.97	1.79	19	11
3:A:24:ILE:HD11	3:B:105:ILE:HD12	0.97	1.33	15	5
3:A:28:VAL:HG22	3:B:128:VAL:HG22	0.97	1.34	7	8
3:B:117:LEU:HD23	3:B:120:TYR:CE2	0.96	1.95	4	4
3:A:23:ASN:O	3:A:24:ILE:HD12	0.95	1.60	19	11
3:A:7:VAL:HG21	3:B:128:VAL:HB	0.95	1.37	7	3
3:A:32:MET:CE	3:B:124:ILE:HG21	0.94	1.92	3	3
3:B:109:VAL:HG11	3:B:114:TYR:CB	0.93	1.92	18	8
3:A:9:VAL:HG21	3:A:14:TYR:CB	0.93	1.93	6	11
3:B:109:VAL:HG21	3:B:114:TYR:HB3	0.93	1.38	4	11
3:A:5:ILE:CD1	3:B:107:VAL:HG13	0.90	1.96	15	6
3:A:9:VAL:HG21	3:A:14:TYR:HB3	0.90	1.43	16	12
3:A:5:ILE:HG21	3:B:114:TYR:CZ	0.89	2.02	15	8
3:A:17:LEU:CD1	3:A:27:LEU:HD12	0.89	1.98	14	3
3:A:28:VAL:HG22	3:B:124:ILE:HG21	0.89	1.43	15	9
3:A:28:VAL:HG13	3:A:32:MET:SD	0.89	2.08	3	1
3:A:5:ILE:HD13	3:B:114:TYR:CD1	0.88	2.03	18	10
3:A:16:LEU:HB3	3:B:136:ALA:HB1	0.88	1.45	15	13
3:A:32:MET:HE1	3:B:124:ILE:HG23	0.88	1.45	15	3
3:A:28:VAL:HG21	3:B:128:VAL:HG22	0.88	1.43	14	1
3:A:17:LEU:CD1	3:A:27:LEU:HD22	0.87	1.98	11	3
3:A:9:VAL:HG11	3:A:14:TYR:CB	0.87	1.98	4	11
3:A:17:LEU:HD13	3:A:22:VAL:HG13	0.87	1.42	12	1
3:A:5:ILE:HD13	3:B:107:VAL:HG13	0.87	1.47	10	1
3:A:17:LEU:HB2	3:B:132:MET:SD	0.86	2.09	19	15
3:A:4:ARG:HG3	3:B:108:THR:HG22	0.86	1.46	1	19
3:A:17:LEU:HD13	3:A:22:VAL:CG1	0.86	1.98	12	2
3:A:8:THR:HG23	3:B:104:ARG:CZ	0.86	2.00	1	1
3:A:7:VAL:HG22	3:B:125:SER:HA	0.86	1.46	9	6
3:B:117:LEU:CD1	3:B:127:LEU:HD12	0.86	2.01	20	3
3:A:35:GLU:HG2	3:B:127:LEU:HD11	0.86	1.47	7	1
3:A:9:VAL:HG11	3:A:14:TYR:CG	0.86	2.05	9	5
3:A:24:ILE:HG21	3:B:128:VAL:HG22	0.85	1.45	15	9
3:A:32:MET:SD	3:B:117:LEU:HB2	0.84	2.12	17	15
1:C:174:DT:H2"	1:C:175:DA:N7	0.84	1.87	6	6

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:D:187:DC:H2''	2:D:188:DG:N7	0.84	1.87	18	6
3:B:109:VAL:HG11	3:B:114:TYR:HB3	0.84	1.50	13	13
3:A:9:VAL:HG11	3:A:14:TYR:HB3	0.84	1.48	6	13
3:A:14:TYR:CE1	3:B:105:ILE:HD11	0.84	2.07	15	4
3:A:17:LEU:HD11	3:A:27:LEU:HD12	0.84	1.49	14	2
3:A:9:VAL:HG21	3:A:14:TYR:CE2	0.83	2.08	9	1
3:A:24:ILE:CG2	3:A:27:LEU:HD23	0.83	2.03	1	5
3:A:32:MET:HE3	3:B:124:ILE:HG21	0.82	1.50	3	2
3:A:14:TYR:CE1	3:B:105:ILE:HD13	0.82	2.09	20	1
1:C:180:DT:H2''	1:C:181:DA:N7	0.82	1.88	10	8
2:D:188:DG:H2''	2:D:189:DG:N7	0.82	1.90	10	2
3:A:9:VAL:HG21	3:A:14:TYR:CG	0.81	2.10	12	10
3:B:124:ILE:HG21	3:B:128:VAL:HG23	0.81	1.50	2	12
3:A:8:THR:HG23	3:B:104:ARG:NE	0.81	1.89	1	1
2:D:189:DG:H2'	2:D:190:DG:O4'	0.81	1.75	17	4
3:A:32:MET:SD	3:B:117:LEU:CB	0.81	2.68	10	15
3:A:32:MET:SD	3:B:114:TYR:HA	0.81	2.14	17	5
3:A:14:TYR:CD1	3:B:105:ILE:HG13	0.81	2.11	14	4
3:A:7:VAL:HG22	3:A:9:VAL:HG13	0.81	1.50	3	4
3:B:124:ILE:HB	3:B:128:VAL:HG23	0.81	1.49	14	12
3:A:24:ILE:HD13	3:B:107:VAL:HG23	0.81	1.51	17	2
3:A:14:TYR:HA	3:B:132:MET:SD	0.81	2.16	10	7
3:A:5:ILE:HG21	3:B:114:TYR:CE2	0.81	2.10	15	9
3:B:109:VAL:HG11	3:B:114:TYR:CG	0.81	2.12	10	4
3:A:24:ILE:N	3:A:24:ILE:HD12	0.81	1.91	13	3
3:A:24:ILE:HG21	3:A:28:VAL:HG23	0.80	1.51	3	14
3:A:29:SER:CB	3:B:112:ASP:HB3	0.80	2.07	16	19
3:A:17:LEU:HD21	3:B:135:GLU:HB3	0.80	1.54	16	5
3:A:17:LEU:CB	3:B:132:MET:SD	0.79	2.71	9	15
3:A:7:VAL:HG22	3:A:9:VAL:HG22	0.79	1.53	18	3
3:A:28:VAL:HG13	3:A:32:MET:CE	0.79	2.07	3	6
3:B:117:LEU:HD12	3:B:127:LEU:HD12	0.79	1.52	20	1
3:A:17:LEU:HD12	3:B:132:MET:HG2	0.79	1.55	2	2
3:A:4:ARG:HG3	3:B:108:THR:CG2	0.79	2.08	7	20
3:B:124:ILE:HD12	3:B:124:ILE:N	0.79	1.93	20	6
3:A:35:GLU:HB3	3:B:117:LEU:HD11	0.79	1.52	1	6
3:A:12:ASP:HB2	3:B:129:SER:CB	0.79	2.08	12	6
3:A:24:ILE:HB	3:A:28:VAL:HG23	0.79	1.53	10	12
3:A:28:VAL:CG2	3:B:128:VAL:HG22	0.79	2.08	7	11
3:A:32:MET:HE2	3:B:124:ILE:HG23	0.78	1.53	20	9
2:D:188:DG:H2'	2:D:189:DG:O4'	0.78	1.78	16	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:A:17:LEU:HG	3:B:132:MET:SD	0.78	2.19	5	8
3:A:5:ILE:HG21	3:B:114:TYR:CD2	0.78	2.14	3	15
3:A:20:TYR:CZ	3:A:22:VAL:HG11	0.78	2.13	12	1
3:B:109:VAL:HG21	3:B:114:TYR:HB2	0.78	1.53	11	7
3:A:6:THR:HB	3:B:106:THR:CB	0.78	2.07	1	12
3:A:14:TYR:CE1	3:B:105:ILE:HG13	0.78	2.13	13	3
3:A:8:THR:HG23	3:B:104:ARG:HH11	0.78	1.38	7	1
3:A:24:ILE:HG22	3:A:28:VAL:HG23	0.78	1.55	19	6
3:A:4:ARG:NH2	3:A:6:THR:HG21	0.78	1.94	14	2
3:A:24:ILE:HG23	3:B:132:MET:HE2	0.78	1.56	13	10
3:A:7:VAL:HG12	3:B:105:ILE:HG22	0.78	1.53	14	2
1:C:173:DA:H2''	1:C:174:DT:O5'	0.77	1.77	19	5
3:A:14:TYR:CE1	3:B:105:ILE:CG1	0.77	2.67	9	4
3:A:9:VAL:HG22	3:B:103:GLN:O	0.77	1.78	9	1
3:A:14:TYR:CD2	3:B:105:ILE:HD13	0.77	2.14	11	1
3:A:17:LEU:HD13	3:A:20:TYR:CE2	0.76	2.15	1	9
3:A:9:VAL:HG13	3:A:14:TYR:HB3	0.76	1.56	20	1
3:A:4:ARG:HG3	3:B:108:THR:HG23	0.76	1.58	15	6
3:A:16:LEU:HB3	3:B:136:ALA:CB	0.76	2.10	12	13
3:A:24:ILE:HD13	3:B:105:ILE:HD13	0.76	1.56	19	1
3:A:24:ILE:HD12	3:A:24:ILE:N	0.76	1.95	2	6
3:B:109:VAL:HG21	3:B:114:TYR:CG	0.76	2.15	8	5
3:A:12:ASP:HB3	3:B:129:SER:HB3	0.76	1.56	5	3
3:A:14:TYR:CE1	3:B:105:ILE:CD1	0.76	2.69	15	5
3:A:24:ILE:HG22	3:A:27:LEU:HB3	0.75	1.58	2	12
3:B:123:ASN:C	3:B:124:ILE:HD12	0.75	2.01	6	8
3:A:24:ILE:CB	3:A:28:VAL:HG23	0.75	2.11	10	15
3:A:6:THR:HB	3:B:106:THR:HB	0.75	1.57	1	14
3:A:12:ASP:HB3	3:B:129:SER:CB	0.75	2.12	5	12
3:B:124:ILE:N	3:B:124:ILE:HD12	0.74	1.96	1	4
3:B:117:LEU:HD22	3:B:122:VAL:CG1	0.74	2.12	11	4
3:A:17:LEU:O	3:A:22:VAL:HG12	0.74	1.83	12	1
2:D:189:DG:H2'	3:B:108:THR:OG1	0.74	1.82	6	4
3:A:9:VAL:HG11	3:A:14:TYR:CD2	0.74	2.16	9	1
3:B:104:ARG:NH2	3:B:106:THR:HG21	0.74	1.96	13	2
3:B:107:VAL:HG22	3:B:109:VAL:HG22	0.74	1.59	15	10
3:A:3:GLN:CB	3:B:110:ASP:HB2	0.74	2.13	20	4
3:B:117:LEU:HD22	3:B:122:VAL:HB	0.74	1.59	13	1
3:A:7:VAL:CG2	3:A:9:VAL:HG13	0.74	2.12	3	1
3:A:32:MET:HA	3:B:117:LEU:CD1	0.73	2.13	1	8
3:A:12:ASP:CB	3:B:129:SER:CB	0.73	2.66	4	12

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:A:27:LEU:HD12	3:B:132:MET:SD	0.73	2.23	8	4
1:C:177:DG:C8	1:C:178:DT:H72	0.73	2.19	14	10
3:A:28:VAL:HG22	3:B:128:VAL:HG21	0.73	1.61	18	1
3:A:32:MET:CE	3:B:124:ILE:HG12	0.73	2.14	9	4
3:A:35:GLU:HB3	3:B:117:LEU:HD21	0.73	1.60	6	8
3:A:36:ALA:HB1	3:B:116:LEU:HB3	0.73	1.59	3	13
3:A:9:VAL:HG13	3:A:10:ASP:H	0.73	1.41	20	1
3:A:9:VAL:HG11	3:A:14:TYR:HB2	0.73	1.61	12	6
3:B:124:ILE:HG22	3:B:127:LEU:HD22	0.72	1.59	7	1
3:A:5:ILE:HG21	3:B:114:TYR:CE1	0.72	2.19	10	7
3:B:128:VAL:CG1	3:B:132:MET:SD	0.72	2.77	2	3
3:B:117:LEU:HD13	3:B:120:TYR:CE2	0.72	2.18	6	5
3:A:6:THR:HA	3:B:105:ILE:O	0.72	1.84	9	20
3:A:24:ILE:HG21	3:B:128:VAL:HG13	0.72	1.61	7	3
3:A:12:ASP:CB	3:B:129:SER:HB2	0.72	2.15	20	11
1:C:179:DA:H2'	1:C:180:DT:H71	0.72	1.60	5	9
3:A:24:ILE:HG23	3:A:27:LEU:HD23	0.72	1.62	1	2
3:B:109:VAL:CG2	3:B:114:TYR:HB3	0.72	2.15	17	11
3:A:5:ILE:HG21	3:B:114:TYR:CG	0.72	2.20	6	15
3:A:9:VAL:CG2	3:A:14:TYR:CD2	0.72	2.73	9	4
3:A:17:LEU:HD22	3:A:20:TYR:CE2	0.72	2.20	12	2
3:A:5:ILE:CD1	3:B:114:TYR:CD1	0.71	2.74	1	12
3:A:29:SER:CB	3:B:112:ASP:CB	0.71	2.69	10	10
3:A:5:ILE:CG1	3:B:124:ILE:HD11	0.71	2.15	8	3
3:B:109:VAL:HG13	3:B:112:ASP:HB2	0.71	1.62	17	8
3:A:5:ILE:HG21	3:B:114:TYR:CD1	0.71	2.21	9	15
3:B:124:ILE:HG22	3:B:127:LEU:HB3	0.71	1.63	14	13
3:A:12:ASP:HB2	3:B:129:SER:HB3	0.71	1.63	15	7
3:B:107:VAL:CG2	3:B:109:VAL:HG22	0.71	2.15	6	4
3:A:14:TYR:CE2	3:A:15:GLN:HG2	0.71	2.19	19	1
3:B:128:VAL:HG13	3:B:132:MET:HE1	0.71	1.60	14	2
2:D:186:DT:O5'	2:D:187:DC:H5''	0.71	1.86	20	1
3:A:5:ILE:HD12	3:B:109:VAL:CG2	0.71	2.15	15	1
3:A:29:SER:HB3	3:B:112:ASP:HB3	0.71	1.62	5	8
1:C:174:DT:H2'	1:C:175:DA:C8	0.71	2.20	1	3
3:A:5:ILE:HD11	3:B:107:VAL:CG1	0.71	2.12	15	3
3:A:17:LEU:HB3	3:B:132:MET:SD	0.71	2.26	4	3
3:A:7:VAL:HG23	3:B:124:ILE:HD13	0.70	1.62	20	4
3:A:24:ILE:CD1	3:B:105:ILE:HD13	0.70	2.15	19	1
3:A:3:GLN:HB3	3:B:110:ASP:CB	0.70	2.15	14	2
3:B:109:VAL:HB	3:B:112:ASP:HB2	0.70	1.62	20	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:A:36:ALA:CB	3:B:116:LEU:HB3	0.70	2.16	13	13
1:C:174:DT:H2''	1:C:175:DA:C8	0.70	2.21	6	13
3:A:27:LEU:CD2	3:B:132:MET:SD	0.70	2.80	5	2
3:A:17:LEU:HD13	3:A:27:LEU:HD11	0.70	1.64	4	2
3:A:18:LYS:HA	3:A:22:VAL:O	0.70	1.87	8	1
3:B:124:ILE:HD12	3:B:124:ILE:H	0.69	1.47	15	6
3:A:17:LEU:CD1	3:B:132:MET:HA	0.69	2.17	4	4
3:B:124:ILE:H	3:B:124:ILE:HD12	0.69	1.46	2	4
3:A:32:MET:SD	3:B:127:LEU:CD1	0.69	2.80	20	2
3:B:122:VAL:HG13	3:B:122:VAL:O	0.69	1.86	17	4
1:C:181:DA:H3'	2:D:186:DT:OP3	0.69	1.88	12	1
3:A:9:VAL:CG2	3:A:14:TYR:HB3	0.69	2.18	14	9
3:A:5:ILE:HD12	3:B:124:ILE:HG12	0.69	1.65	13	4
3:A:28:VAL:HG13	3:A:32:MET:HE1	0.69	1.63	18	1
3:A:29:SER:HB3	3:B:112:ASP:HB2	0.69	1.64	10	4
3:B:117:LEU:HD12	3:B:122:VAL:CG1	0.69	2.17	18	3
3:B:117:LEU:HG	3:B:120:TYR:CE2	0.69	2.22	2	3
3:A:14:TYR:CZ	3:B:105:ILE:HB	0.69	2.23	20	1
3:A:6:THR:HG23	3:B:104:ARG:NH2	0.69	2.02	7	1
3:A:32:MET:HG3	3:B:114:TYR:HA	0.69	1.65	9	9
3:A:7:VAL:HG13	3:B:105:ILE:CG1	0.69	2.18	11	7
3:A:5:ILE:O	3:B:106:THR:HA	0.69	1.88	14	17
2:D:191:DT:H73	3:B:106:THR:HG23	0.69	1.64	8	3
2:D:190:DG:OP1	3:B:107:VAL:HG22	0.69	1.88	17	2
1:C:174:DT:H2''	1:C:175:DA:O5'	0.68	1.85	1	3
3:A:6:THR:OG1	3:B:104:ARG:CG	0.68	2.42	7	12
3:B:114:TYR:CZ	3:B:118:LYS:HD3	0.68	2.24	19	14
3:A:17:LEU:HD22	3:A:22:VAL:HB	0.68	1.63	3	1
1:C:176:DT:H2'	3:A:8:THR:OG1	0.68	1.87	14	6
3:A:17:LEU:HD11	3:A:27:LEU:HG	0.68	1.63	10	3
3:B:129:SER:HA	3:B:132:MET:HG2	0.68	1.64	3	1
3:A:28:VAL:HG13	3:A:32:MET:HE2	0.68	1.64	17	3
3:A:24:ILE:HD11	3:B:105:ILE:CD1	0.68	2.18	9	3
1:C:175:DA:C2'	1:C:176:DT:C6	0.68	2.77	16	3
3:A:24:ILE:HD13	3:B:107:VAL:HG12	0.68	1.64	6	2
3:A:12:ASP:HB3	3:B:129:SER:HB2	0.68	1.63	2	11
1:C:178:DT:H73	3:A:6:THR:HG23	0.68	1.65	14	6
3:A:7:VAL:CG1	3:B:124:ILE:HD13	0.68	2.14	10	1
2:D:186:DT:OP3	2:D:187:DC:H3'	0.68	1.89	13	1
3:A:14:TYR:CD1	3:B:105:ILE:CD1	0.68	2.76	12	11
3:A:35:GLU:CB	3:B:117:LEU:HD21	0.68	2.19	6	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:A:29:SER:HB2	3:B:112:ASP:HB3	0.67	1.66	8	12
3:A:25:SER:HA	3:B:107:VAL:HG22	0.67	1.64	2	3
3:A:17:LEU:HD11	3:B:135:GLU:CB	0.67	2.19	8	2
3:A:28:VAL:HG13	3:A:32:MET:HE3	0.67	1.63	8	1
3:B:128:VAL:O	3:B:132:MET:HG2	0.67	1.90	13	12
3:A:7:VAL:HG12	3:A:9:VAL:HG12	0.67	1.67	20	4
1:C:178:DT:H71	3:B:104:ARG:HD3	0.67	1.64	1	1
3:A:3:GLN:HB3	3:B:110:ASP:HB3	0.67	1.67	14	1
3:A:5:ILE:HD11	3:A:28:VAL:HG11	0.67	1.66	19	10
3:A:5:ILE:HG12	3:B:107:VAL:HG13	0.67	1.66	1	9
3:A:24:ILE:HG23	3:B:132:MET:HE3	0.67	1.67	2	2
1:C:173:DA:H1'	1:C:174:DT:O4'	0.67	1.90	7	2
3:A:3:GLN:HB3	3:B:110:ASP:HB2	0.67	1.64	20	6
3:A:3:GLN:CB	3:B:110:ASP:HB3	0.67	2.20	14	1
3:A:5:ILE:CG1	3:B:107:VAL:HG13	0.66	2.20	1	11
3:A:7:VAL:HG22	3:B:125:SER:CA	0.66	2.21	9	3
3:A:24:ILE:HG23	3:B:132:MET:CE	0.66	2.19	19	12
3:A:24:ILE:HD12	3:A:24:ILE:H	0.66	1.50	15	5
3:B:117:LEU:HD23	3:B:122:VAL:CG1	0.66	2.20	14	1
3:A:29:SER:HB3	3:B:112:ASP:CB	0.66	2.20	15	10
3:A:32:MET:HE1	3:B:124:ILE:HG12	0.66	1.66	9	4
3:B:117:LEU:HD23	3:B:120:TYR:CZ	0.66	2.25	4	2
3:A:17:LEU:HD21	3:B:135:GLU:CB	0.66	2.21	17	4
3:A:36:ALA:HB1	3:B:116:LEU:HD22	0.65	1.66	7	12
3:A:35:GLU:CB	3:B:117:LEU:HD11	0.65	2.20	4	4
1:C:182:DC:H2''	1:C:183:DC:O5'	0.65	1.91	2	18
3:A:10:ASP:HB2	3:B:103:GLN:HB3	0.65	1.66	7	5
3:A:24:ILE:HG12	3:B:132:MET:HE1	0.65	1.67	14	3
3:B:107:VAL:HG22	3:B:107:VAL:O	0.65	1.90	7	4
3:A:14:TYR:CE1	3:B:105:ILE:HB	0.65	2.27	20	7
3:B:124:ILE:CG2	3:B:127:LEU:HD12	0.65	2.21	6	4
3:A:12:ASP:HB2	3:B:129:SER:HB2	0.65	1.68	14	5
3:B:120:TYR:O	3:B:121:ASP:HB2	0.65	1.92	16	19
3:A:17:LEU:HG	3:B:132:MET:HA	0.65	1.69	12	3
3:A:32:MET:SD	3:B:127:LEU:HD12	0.65	2.32	10	5
3:B:109:VAL:CG1	3:B:114:TYR:HB3	0.65	2.22	18	12
3:A:32:MET:SD	3:B:117:LEU:HD13	0.65	2.32	15	4
1:C:173:DA:C2'	1:C:174:DT:H5''	0.65	2.22	20	3
3:A:24:ILE:CG2	3:B:132:MET:HE2	0.64	2.22	17	9
3:A:14:TYR:CZ	3:B:105:ILE:HG21	0.64	2.26	12	5
3:A:28:VAL:CG2	3:B:128:VAL:CG2	0.64	2.75	12	8

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:B:124:ILE:CB	3:B:128:VAL:HG23	0.64	2.22	14	15
3:B:105:ILE:HD11	3:B:128:VAL:HG11	0.64	1.70	6	9
3:B:117:LEU:HD21	3:B:127:LEU:HD13	0.64	1.69	2	1
3:A:14:TYR:CD2	3:B:105:ILE:HG21	0.64	2.27	7	11
3:A:7:VAL:CG1	3:A:9:VAL:HG22	0.64	2.23	6	2
3:A:5:ILE:CG2	3:B:114:TYR:CZ	0.64	2.79	15	11
3:A:18:LYS:HB3	3:A:23:ASN:HA	0.64	1.70	13	6
3:B:120:TYR:O	3:B:121:ASP:HB3	0.64	1.92	4	1
3:A:7:VAL:CG1	3:B:105:ILE:HG22	0.64	2.23	14	2
3:A:14:TYR:CG	3:B:105:ILE:HG21	0.64	2.27	7	13
3:A:24:ILE:CG2	3:A:27:LEU:HD12	0.64	2.23	10	3
3:A:31:THR:HG21	3:B:131:THR:HG21	0.64	1.69	3	2
3:A:14:TYR:CD1	3:B:105:ILE:CG1	0.64	2.81	9	2
3:B:109:VAL:HG11	3:B:114:TYR:H	0.63	1.53	9	9
3:A:17:LEU:HD11	3:A:27:LEU:CD1	0.63	2.23	3	2
3:A:10:ASP:HB2	3:B:103:GLN:CB	0.63	2.23	4	6
2:D:191:DT:H72	3:B:106:THR:CG2	0.63	2.23	1	7
3:A:7:VAL:CG1	3:B:105:ILE:CG2	0.63	2.76	14	2
3:A:9:VAL:CG1	3:A:14:TYR:HB3	0.63	2.20	6	14
3:A:6:THR:HB	3:B:106:THR:CA	0.63	2.22	7	5
3:A:17:LEU:HD21	3:B:135:GLU:HB2	0.63	1.71	9	3
3:B:117:LEU:HD13	3:B:127:LEU:HG	0.63	1.70	13	2
3:A:32:MET:SD	3:B:124:ILE:HG23	0.63	2.33	14	3
3:A:32:MET:O	3:A:36:ALA:N	0.63	2.31	3	17
1:C:178:DT:H72	3:A:6:THR:OG1	0.63	1.93	16	3
3:A:17:LEU:HG	3:B:132:MET:HG3	0.63	1.70	1	1
3:A:32:MET:SD	3:B:117:LEU:HG	0.63	2.33	6	6
1:C:179:DA:C2	2:D:194:DA:C2	0.63	2.87	9	2
3:A:14:TYR:HA	3:B:132:MET:HG3	0.63	1.71	7	6
3:A:9:VAL:HG21	3:A:14:TYR:HB2	0.63	1.68	6	2
3:A:17:LEU:HG	3:A:27:LEU:CD2	0.63	2.24	1	1
3:A:20:TYR:O	3:A:21:ASP:HB2	0.62	1.94	10	18
3:A:7:VAL:HG13	3:B:105:ILE:HG12	0.62	1.71	2	6
3:A:14:TYR:CE1	3:B:105:ILE:HG21	0.62	2.29	12	5
3:B:128:VAL:HG13	3:B:132:MET:CE	0.62	2.23	1	7
3:A:5:ILE:HG13	3:B:124:ILE:HD11	0.62	1.71	8	2
3:A:9:VAL:O	3:A:10:ASP:CB	0.62	2.46	13	13
3:A:12:ASP:CB	3:B:129:SER:HB3	0.62	2.24	8	7
2:D:190:DG:H2'	3:B:106:THR:O	0.62	1.92	4	1
2:D:191:DT:H3'	3:B:104:ARG:O	0.62	1.94	12	2
3:A:24:ILE:HG23	3:A:27:LEU:HD12	0.62	1.71	19	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:D:188:DG:H8	2:D:188:DG:O5'	0.62	1.76	12	2
3:B:132:MET:O	3:B:136:ALA:N	0.62	2.33	6	20
3:A:24:ILE:HG21	3:B:132:MET:CE	0.62	2.24	1	1
1:C:174:DT:C2'	1:C:175:DA:C8	0.62	2.81	1	3
3:A:14:TYR:CE2	3:B:105:ILE:HG21	0.62	2.30	11	5
3:A:32:MET:HA	3:B:117:LEU:HD23	0.62	1.71	7	2
3:B:109:VAL:O	3:B:111:SER:N	0.62	2.33	14	2
3:A:16:LEU:CB	3:B:136:ALA:HB1	0.62	2.22	15	3
3:A:6:THR:OG1	3:B:104:ARG:NH1	0.62	2.32	1	1
3:A:9:VAL:CG1	3:A:14:TYR:CB	0.62	2.77	20	5
3:A:17:LEU:HG	3:A:27:LEU:CD1	0.62	2.24	16	2
3:B:120:TYR:O	3:B:121:ASP:CB	0.62	2.48	16	16
3:B:126:GLY:O	3:B:130:THR:HB	0.62	1.94	9	4
3:A:9:VAL:HG22	3:A:10:ASP:H	0.62	1.54	4	6
3:A:4:ARG:NH1	3:B:106:THR:HG21	0.62	2.10	14	1
3:B:109:VAL:CG2	3:B:112:ASP:HB2	0.62	2.24	2	2
3:A:32:MET:SD	3:B:124:ILE:HG21	0.62	2.34	3	3
3:B:117:LEU:HD13	3:B:120:TYR:CZ	0.62	2.30	8	5
1:C:178:DT:H2''	1:C:179:DA:O5'	0.61	1.95	7	11
3:A:24:ILE:HG13	3:B:132:MET:HE1	0.61	1.72	4	7
3:A:27:LEU:HD13	3:B:132:MET:SD	0.61	2.35	16	1
3:A:28:VAL:O	3:A:32:MET:HG2	0.61	1.96	19	15
3:B:118:LYS:HB3	3:B:123:ASN:HA	0.61	1.70	20	9
3:A:9:VAL:HG13	3:A:12:ASP:HB2	0.61	1.71	10	4
3:A:17:LEU:HD12	3:B:132:MET:SD	0.61	2.35	14	3
3:A:5:ILE:CD1	3:A:28:VAL:HG11	0.61	2.24	19	4
3:A:9:VAL:O	3:A:10:ASP:HB3	0.61	1.96	12	10
3:A:17:LEU:HD13	3:A:20:TYR:CZ	0.61	2.29	1	5
3:A:24:ILE:HG21	3:B:132:MET:HE1	0.61	1.71	1	2
3:A:17:LEU:HD12	3:B:132:MET:CA	0.61	2.17	8	2
3:B:128:VAL:O	3:B:132:MET:CG	0.61	2.48	20	10
3:A:15:GLN:O	3:A:19:ALA:HB2	0.61	1.93	7	10
3:B:122:VAL:O	3:B:122:VAL:CG1	0.61	2.48	6	4
3:B:117:LEU:HD22	3:B:127:LEU:HD22	0.61	1.71	2	1
3:B:109:VAL:HG21	3:B:114:TYR:CE1	0.61	2.25	13	1
3:B:117:LEU:HG	3:B:127:LEU:HD22	0.61	1.70	19	1
3:A:14:TYR:CZ	3:A:18:LYS:HD3	0.61	2.31	4	13
3:A:24:ILE:H	3:A:24:ILE:HD12	0.61	1.54	6	3
3:A:10:ASP:HB2	3:B:103:GLN:N	0.61	2.11	13	7
3:B:117:LEU:HD13	3:B:127:LEU:CD1	0.61	2.25	4	3
3:A:6:THR:HG22	3:B:106:THR:HB	0.61	1.72	8	4

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:A:17:LEU:HD22	3:A:22:VAL:HG11	0.61	1.73	12	1
3:A:7:VAL:HG23	3:A:9:VAL:HB	0.61	1.73	17	1
3:A:14:TYR:O	3:B:132:MET:SD	0.61	2.59	19	3
3:B:105:ILE:O	3:B:105:ILE:HG13	0.61	1.95	7	8
3:A:7:VAL:HG23	3:A:9:VAL:HG13	0.61	1.71	1	1
3:B:103:GLN:OE1	3:B:105:ILE:HG22	0.61	1.96	10	2
3:A:32:MET:HA	3:B:117:LEU:HG	0.61	1.73	20	2
3:B:109:VAL:O	3:B:110:ASP:HB3	0.60	1.95	9	9
3:A:9:VAL:HG12	3:A:12:ASP:OD1	0.60	1.96	19	1
3:A:17:LEU:CG	3:B:132:MET:SD	0.60	2.88	5	8
3:B:105:ILE:CD1	3:B:128:VAL:HG11	0.60	2.26	16	4
3:A:24:ILE:HG21	3:B:128:VAL:CG2	0.60	2.25	11	2
3:A:32:MET:HE2	3:B:124:ILE:CG1	0.60	2.27	10	1
3:B:107:VAL:HG12	3:B:109:VAL:HG12	0.60	1.72	2	2
1:C:173:DA:H2''	1:C:174:DT:C5'	0.60	2.25	15	2
3:B:115:GLN:O	3:B:118:LYS:HG3	0.60	1.96	5	16
1:C:173:DA:N3	1:C:173:DA:H5''	0.60	2.11	1	1
3:A:5:ILE:HB	3:B:114:TYR:CE1	0.60	2.31	6	9
3:A:32:MET:SD	3:B:117:LEU:HB3	0.60	2.37	13	4
3:A:6:THR:HG21	3:B:104:ARG:CZ	0.60	2.26	10	1
3:A:31:THR:HG21	3:B:131:THR:CG2	0.60	2.25	3	1
3:B:109:VAL:HG23	3:B:110:ASP:N	0.60	2.11	13	1
3:A:17:LEU:HD21	3:B:135:GLU:HG3	0.60	1.73	12	1
3:A:14:TYR:CZ	3:B:105:ILE:CG2	0.60	2.85	7	11
3:A:7:VAL:HG12	3:A:9:VAL:CG1	0.60	2.27	9	3
2:D:191:DT:H72	3:B:106:THR:OG1	0.60	1.96	14	5
3:A:22:VAL:CG1	3:A:22:VAL:O	0.60	2.50	1	1
3:A:29:SER:CB	3:B:112:ASP:HB2	0.60	2.27	10	4
3:A:24:ILE:HG23	3:B:132:MET:SD	0.60	2.37	20	3
3:A:9:VAL:HG12	3:A:12:ASP:CB	0.60	2.27	19	1
3:A:13:SER:O	3:B:132:MET:HB3	0.59	1.97	19	1
3:B:109:VAL:HG22	3:B:110:ASP:H	0.59	1.57	7	5
3:A:22:VAL:O	3:A:24:ILE:N	0.59	2.33	19	4
3:B:107:VAL:HG12	3:B:109:VAL:CG1	0.59	2.28	19	2
2:D:190:DG:OP2	3:B:107:VAL:HA	0.59	1.97	11	3
3:A:18:LYS:CB	3:A:23:ASN:HA	0.59	2.27	19	1
3:B:107:VAL:O	3:B:107:VAL:HG12	0.59	1.96	17	3
3:A:6:THR:CB	3:B:106:THR:HB	0.59	2.27	1	10
3:A:3:GLN:N	3:B:109:VAL:O	0.59	2.33	19	1
3:A:5:ILE:HG13	3:B:114:TYR:CE2	0.59	2.31	10	1
3:B:107:VAL:O	3:B:107:VAL:HG22	0.59	1.97	20	5

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:C:175:DA:H2'	1:C:176:DT:C6	0.59	2.31	16	1
3:A:17:LEU:HD11	3:B:135:GLU:HB3	0.59	1.74	4	2
3:B:117:LEU:CD1	3:B:127:LEU:CD1	0.59	2.81	17	4
3:A:7:VAL:HG12	3:A:9:VAL:CG2	0.59	2.28	6	2
3:B:124:ILE:HG22	3:B:128:VAL:CG2	0.59	2.18	13	1
2:D:193:DT:O4	3:B:104:ARG:HD3	0.59	1.98	10	2
3:A:32:MET:CE	3:B:124:ILE:CG2	0.59	2.80	9	4
3:B:110:ASP:HA	3:B:114:TYR:CD2	0.59	2.33	14	1
3:A:17:LEU:CD1	3:A:27:LEU:HG	0.59	2.27	2	3
3:A:28:VAL:HB	3:B:107:VAL:HG11	0.59	1.72	5	1
3:A:14:TYR:CE1	3:B:105:ILE:HG12	0.59	2.32	9	1
3:A:24:ILE:CG2	3:B:132:MET:CE	0.59	2.81	19	8
1:C:178:DT:H72	3:A:6:THR:CG2	0.59	2.27	11	5
3:B:114:TYR:CE2	3:B:118:LYS:HD3	0.59	2.32	11	4
2:D:190:DG:C5	2:D:191:DT:H72	0.58	2.32	4	1
3:A:17:LEU:HD12	3:A:22:VAL:O	0.58	1.98	16	2
3:A:32:MET:HE2	3:B:124:ILE:CG2	0.58	2.28	20	7
3:A:32:MET:CE	3:B:124:ILE:HG13	0.58	2.27	11	11
1:C:175:DA:H2''	1:C:176:DT:O5'	0.58	1.98	16	2
3:B:104:ARG:HH21	3:B:106:THR:HG21	0.58	1.57	13	1
3:A:20:TYR:CD1	3:A:21:ASP:N	0.58	2.71	4	15
3:A:20:TYR:CE1	3:A:22:VAL:HB	0.58	2.33	12	4
3:A:32:MET:CG	3:B:117:LEU:HD12	0.58	2.27	16	2
3:A:29:SER:HA	3:B:112:ASP:O	0.58	1.98	2	5
3:A:14:TYR:CE1	3:A:18:LYS:HD3	0.58	2.34	11	2
3:A:5:ILE:O	3:A:5:ILE:CG1	0.58	2.50	4	7
3:A:9:VAL:HG13	3:A:14:TYR:CD2	0.58	2.32	13	2
3:B:122:VAL:CG1	3:B:127:LEU:HB2	0.58	2.29	13	1
3:A:23:ASN:C	3:A:24:ILE:CD1	0.58	2.65	19	6
3:A:17:LEU:HD13	3:A:27:LEU:HG	0.58	1.74	19	1
1:C:183:DC:H2''	1:C:184:DC:C6	0.58	2.33	10	11
3:A:4:ARG:CG	3:B:108:THR:HG22	0.58	2.28	5	6
3:A:7:VAL:CG1	3:A:9:VAL:HG12	0.58	2.29	20	2
3:B:109:VAL:HG21	3:B:114:TYR:HD1	0.58	1.43	13	1
3:A:14:TYR:CD1	3:B:105:ILE:HG21	0.58	2.33	18	10
3:A:6:THR:OG1	3:B:104:ARG:HG2	0.58	1.99	1	12
2:D:194:DA:H1'	2:D:195:DC:O4'	0.58	1.97	9	5
3:A:24:ILE:HB	3:A:28:VAL:CG2	0.58	2.29	10	5
3:B:124:ILE:HG22	3:B:127:LEU:CG	0.58	2.28	9	1
3:A:2:LYS:HA	3:B:109:VAL:O	0.58	1.99	12	4
1:C:173:DA:H3'	1:C:174:DT:H72	0.58	1.74	11	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:B:124:ILE:HG22	3:B:127:LEU:CB	0.58	2.28	9	1
3:A:5:ILE:CD1	3:B:124:ILE:HD11	0.58	2.29	3	1
3:B:114:TYR:CG	3:B:115:GLN:N	0.58	2.71	6	4
3:A:9:VAL:HG11	3:A:14:TYR:H	0.57	1.59	6	5
3:B:129:SER:CA	3:B:132:MET:HG2	0.57	2.29	3	1
3:A:9:VAL:HG23	3:B:103:GLN:HB3	0.57	1.76	3	3
3:A:13:SER:CB	3:B:133:GLN:CB	0.57	2.82	9	1
2:D:190:DG:OP1	3:B:107:VAL:HG23	0.57	1.99	4	1
3:A:9:VAL:HG13	3:A:14:TYR:CB	0.57	2.29	20	1
2:D:186:DT:H2''	2:D:187:DC:O5'	0.57	1.99	11	1
3:A:24:ILE:CG2	3:A:27:LEU:HB3	0.57	2.29	2	4
3:A:24:ILE:CG1	3:B:132:MET:CE	0.57	2.83	3	7
3:A:20:TYR:CZ	3:A:22:VAL:CG1	0.57	2.88	12	1
3:A:17:LEU:HD11	3:B:135:GLU:HB2	0.57	1.75	8	1
3:A:20:TYR:O	3:A:21:ASP:CB	0.57	2.53	11	17
3:A:9:VAL:CG1	3:A:14:TYR:CD2	0.57	2.87	13	2
3:B:117:LEU:HD23	3:B:122:VAL:HG11	0.57	1.74	14	1
1:C:179:DA:C5	1:C:180:DT:C4	0.57	2.93	9	5
3:B:107:VAL:O	3:B:107:VAL:CG2	0.57	2.53	14	1
3:B:109:VAL:HB	3:B:112:ASP:CB	0.57	2.30	20	2
3:B:127:LEU:C	3:B:127:LEU:HD23	0.57	2.20	20	1
2:D:190:DG:H2''	2:D:191:DT:O5'	0.57	2.00	17	5
3:A:17:LEU:CD2	3:A:20:TYR:CE2	0.57	2.88	10	5
3:A:32:MET:CE	3:B:124:ILE:HG23	0.57	2.30	13	8
3:B:117:LEU:CD2	3:B:122:VAL:HG11	0.57	2.29	14	2
3:A:7:VAL:HG23	3:B:125:SER:HA	0.57	1.75	14	1
3:A:5:ILE:CG2	3:B:114:TYR:CE1	0.57	2.88	19	6
3:B:117:LEU:HD13	3:B:122:VAL:O	0.57	1.99	20	1
3:B:118:LYS:CB	3:B:123:ASN:HA	0.57	2.30	13	1
3:A:17:LEU:HD13	3:A:27:LEU:CD1	0.57	2.30	4	3
3:A:3:GLN:O	3:B:108:THR:HA	0.57	2.00	20	7
3:A:6:THR:CG2	3:B:106:THR:HB	0.57	2.30	8	4
3:A:23:ASN:O	3:B:132:MET:HE1	0.56	2.00	16	3
3:A:5:ILE:O	3:A:5:ILE:HG13	0.56	1.98	18	8
3:A:24:ILE:HG13	3:B:132:MET:CE	0.56	2.30	11	11
3:A:9:VAL:CG2	3:A:12:ASP:CB	0.56	2.84	17	1
3:A:9:VAL:HG12	3:A:12:ASP:HB2	0.56	1.76	19	1
3:B:120:TYR:CD1	3:B:121:ASP:N	0.56	2.73	17	11
3:B:109:VAL:CB	3:B:114:TYR:HB3	0.56	2.30	16	6
3:B:123:ASN:O	3:B:125:SER:N	0.56	2.37	6	9
3:A:10:ASP:CB	3:B:102:LYS:HA	0.56	2.31	9	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:A:9:VAL:HG23	3:A:12:ASP:HB2	0.56	1.76	4	2
3:A:17:LEU:HD23	3:A:22:VAL:HB	0.56	1.77	4	1
3:A:7:VAL:CG2	3:B:125:SER:HA	0.56	2.31	16	3
3:B:127:LEU:CD2	3:B:127:LEU:C	0.56	2.74	20	1
3:A:14:TYR:CE2	3:B:103:GLN:HG2	0.56	2.35	5	2
3:A:32:MET:HG3	3:B:117:LEU:HG	0.56	1.76	3	1
3:A:4:ARG:NH1	3:B:108:THR:CG2	0.56	2.69	9	2
3:B:117:LEU:CD2	3:B:120:TYR:CE2	0.56	2.81	4	4
3:A:9:VAL:HG22	3:A:10:ASP:N	0.56	2.15	7	4
2:D:190:DG:OP1	3:A:25:SER:HA	0.56	2.01	17	4
3:A:9:VAL:O	3:A:11:SER:N	0.56	2.37	20	1
3:A:23:ASN:O	3:A:25:SER:N	0.56	2.39	19	11
3:A:32:MET:SD	3:B:117:LEU:CG	0.56	2.93	20	4
2:D:190:DG:P	3:A:25:SER:HB2	0.56	2.41	3	2
3:B:129:SER:HA	3:B:132:MET:CG	0.56	2.30	3	1
3:A:32:MET:HB2	3:B:113:SER:HB2	0.56	1.78	2	2
3:A:3:GLN:HB3	3:B:109:VAL:HG23	0.56	1.78	13	1
3:B:105:ILE:O	3:B:105:ILE:HG22	0.56	2.01	13	1
3:A:32:MET:HE3	3:B:124:ILE:HG12	0.56	1.78	7	1
3:A:4:ARG:HG2	3:B:106:THR:OG1	0.56	2.01	17	9
3:A:32:MET:CG	3:B:117:LEU:HG	0.56	2.31	3	1
3:A:7:VAL:O	3:A:7:VAL:HG12	0.56	2.01	13	2
3:A:29:SER:HB2	3:B:112:ASP:CB	0.56	2.30	8	6
1:C:177:DG:H2'	1:C:178:DT:H72	0.56	1.78	1	7
3:A:7:VAL:HG22	3:A:9:VAL:CG2	0.56	2.31	8	4
3:A:7:VAL:CG2	3:A:9:VAL:HG22	0.56	2.30	1	5
3:B:124:ILE:CG2	3:B:127:LEU:HB3	0.56	2.29	14	6
3:B:105:ILE:O	3:B:105:ILE:CG1	0.56	2.54	16	9
1:C:173:DA:H2''	1:C:174:DT:H5'	0.56	1.77	15	1
3:A:2:LYS:HA	3:B:110:ASP:HB3	0.55	1.77	1	3
3:B:114:TYR:CZ	3:B:118:LYS:HG2	0.55	2.35	10	3
2:D:196:DA:H2'	2:D:197:DT:H71	0.55	1.78	10	1
3:A:7:VAL:CG1	3:A:9:VAL:CG1	0.55	2.83	20	1
3:A:9:VAL:CG2	3:A:12:ASP:HB2	0.55	2.30	17	2
3:A:32:MET:SD	3:B:127:LEU:CD2	0.55	2.94	19	2
3:A:5:ILE:HG22	3:B:114:TYR:CZ	0.55	2.36	14	5
3:A:5:ILE:CG2	3:B:114:TYR:CE2	0.55	2.89	3	10
3:A:24:ILE:HG12	3:B:132:MET:CE	0.55	2.31	14	4
3:B:117:LEU:HD13	3:B:122:VAL:CG1	0.55	2.31	9	1
3:A:17:LEU:HD12	3:B:132:MET:CE	0.55	2.31	12	1
3:A:32:MET:HE1	3:B:124:ILE:HG13	0.55	1.78	5	5

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:A:22:VAL:HG13	3:A:22:VAL:O	0.55	2.01	1	1
3:B:128:VAL:O	3:B:132:MET:HG3	0.55	2.02	15	1
2:D:192:DA:H62	3:B:104:ARG:NH2	0.55	1.99	12	2
3:A:20:TYR:C	3:A:20:TYR:CD1	0.55	2.79	8	6
3:B:107:VAL:HG22	3:B:109:VAL:CG2	0.55	2.32	1	5
3:A:5:ILE:HD12	3:B:114:TYR:CD1	0.55	2.36	16	3
3:A:24:ILE:CG2	3:B:132:MET:SD	0.55	2.95	3	1
3:A:15:GLN:O	3:A:18:LYS:HG3	0.55	2.02	16	13
3:A:5:ILE:HG13	3:A:5:ILE:O	0.55	2.02	3	2
1:C:174:DT:H72	1:C:174:DT:OP1	0.55	2.01	12	2
3:A:12:ASP:O	3:B:129:SER:HB2	0.55	2.01	18	3
1:C:178:DT:H72	3:A:6:THR:HG23	0.55	1.77	18	1
3:A:18:LYS:HB3	3:A:23:ASN:HB3	0.55	1.78	6	1
3:B:124:ILE:CD1	3:B:124:ILE:N	0.55	2.67	8	2
3:A:13:SER:HB3	3:B:133:GLN:HB2	0.55	1.79	2	2
1:C:178:DT:H72	3:A:6:THR:HG21	0.55	1.77	8	3
3:A:14:TYR:CD1	3:B:105:ILE:HD12	0.55	2.37	17	2
3:B:127:LEU:HD22	3:B:127:LEU:C	0.55	2.22	13	1
3:A:16:LEU:HD13	3:B:136:ALA:HB1	0.55	1.79	7	1
1:C:175:DA:O5'	1:C:175:DA:C8	0.55	2.60	19	2
2:D:193:DT:H2''	2:D:194:DA:C8	0.55	2.37	7	9
3:B:117:LEU:HD13	3:B:123:ASN:O	0.55	2.02	11	1
3:B:117:LEU:CD1	3:B:122:VAL:HG13	0.55	2.32	9	1
1:C:178:DT:C7	3:A:6:THR:HG23	0.54	2.32	10	3
3:A:17:LEU:HB2	3:B:132:MET:HB3	0.54	1.78	9	2
3:B:107:VAL:O	3:B:107:VAL:CG1	0.54	2.55	2	3
3:A:9:VAL:HG21	3:B:129:SER:HB3	0.54	1.77	7	2
3:B:109:VAL:CG2	3:B:112:ASP:CB	0.54	2.85	19	1
3:A:17:LEU:CG	3:B:132:MET:HG3	0.54	2.33	1	1
3:A:13:SER:CB	3:B:133:GLN:HB2	0.54	2.33	2	3
3:B:109:VAL:HG21	3:B:112:ASP:HB2	0.54	1.77	2	1
3:A:7:VAL:HG22	3:A:9:VAL:CG1	0.54	2.32	11	3
1:C:179:DA:H62	3:B:104:ARG:NH1	0.54	2.01	12	2
3:A:9:VAL:O	3:A:10:ASP:HB2	0.54	2.03	13	4
3:A:24:ILE:HG22	3:A:27:LEU:HD23	0.54	1.77	1	1
3:A:32:MET:HE3	3:B:124:ILE:CG2	0.54	2.27	3	2
3:B:105:ILE:HG22	3:B:105:ILE:O	0.54	2.01	15	2
3:A:17:LEU:CD1	3:A:22:VAL:HG13	0.54	2.25	12	1
3:A:32:MET:HG2	3:B:117:LEU:HG	0.54	1.79	8	1
3:B:132:MET:O	3:B:136:ALA:CB	0.54	2.55	12	9
3:B:114:TYR:OH	3:B:118:LYS:HD3	0.54	2.02	4	9

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:B:109:VAL:O	3:B:110:ASP:CB	0.54	2.56	15	16
3:A:3:GLN:N	3:B:110:ASP:HB2	0.54	2.18	10	9
2:D:191:DT:H2''	2:D:192:DA:O5'	0.54	2.01	18	2
3:A:4:ARG:NH1	3:A:4:ARG:HB3	0.54	2.18	6	1
3:A:35:GLU:OE1	3:B:117:LEU:HD11	0.54	2.02	13	1
2:D:190:DG:OP1	3:A:25:SER:HB2	0.54	2.02	5	1
3:A:32:MET:SD	3:B:117:LEU:HD12	0.54	2.43	16	3
3:A:8:THR:HG23	3:B:104:ARG:NH1	0.54	2.13	7	1
3:B:107:VAL:HG12	3:B:107:VAL:O	0.54	2.02	8	1
3:A:7:VAL:HG12	3:A:7:VAL:O	0.54	2.03	20	5
3:A:17:LEU:HG	3:A:20:TYR:CE2	0.54	2.37	4	1
3:B:107:VAL:CG2	3:B:107:VAL:O	0.54	2.56	20	4
1:C:178:DT:H73	3:A:6:THR:CG2	0.54	2.32	14	1
3:B:128:VAL:HG13	3:B:132:MET:HE3	0.54	1.80	15	1
3:A:11:SER:HA	3:A:15:GLN:HG2	0.54	1.78	1	2
3:A:17:LEU:HD11	3:A:27:LEU:HD22	0.54	1.79	1	1
3:A:24:ILE:HG12	3:B:132:MET:HE2	0.54	1.77	3	4
3:A:28:VAL:HG12	3:A:29:SER:N	0.54	2.17	3	3
3:A:5:ILE:CG1	3:A:5:ILE:O	0.54	2.55	1	5
2:D:194:DA:C2	2:D:195:DC:C2	0.54	2.96	9	2
3:B:114:TYR:CE2	3:B:118:LYS:HG2	0.54	2.38	7	1
3:A:17:LEU:HD12	3:A:27:LEU:HD22	0.54	1.79	11	1
3:B:128:VAL:O	3:B:131:THR:HG22	0.53	2.03	4	2
2:D:191:DT:C7	3:B:106:THR:OG1	0.53	2.57	7	2
3:A:24:ILE:HG23	3:B:132:MET:HE1	0.53	1.81	3	2
3:B:117:LEU:CD2	3:B:120:TYR:CZ	0.53	2.91	4	1
2:D:197:DT:C4	2:D:198:DA:C6	0.53	2.96	16	2
2:D:192:DA:H8	2:D:192:DA:O5'	0.53	1.87	12	1
3:B:124:ILE:HB	3:B:128:VAL:CG2	0.53	2.34	18	3
3:B:107:VAL:HG12	3:B:109:VAL:CG2	0.53	2.33	8	2
3:B:117:LEU:HD12	3:B:122:VAL:HG11	0.53	1.80	8	1
3:A:28:VAL:O	3:A:32:MET:CG	0.53	2.57	16	7
3:A:27:LEU:HD22	3:B:132:MET:SD	0.53	2.44	5	1
1:C:179:DA:H2''	1:C:180:DT:O5'	0.53	2.02	5	5
3:A:32:MET:O	3:A:36:ALA:CB	0.53	2.56	14	7
3:A:7:VAL:HG11	3:B:128:VAL:HG11	0.53	1.80	3	2
3:A:9:VAL:CG2	3:A:14:TYR:CD1	0.53	2.76	11	2
3:A:32:MET:HE1	3:B:124:ILE:CG2	0.53	2.33	5	3
3:A:17:LEU:HD23	3:B:132:MET:O	0.53	2.03	9	5
3:A:17:LEU:CD1	3:B:132:MET:HG2	0.53	2.31	2	1
1:C:179:DA:H62	3:A:4:ARG:NH2	0.53	2.02	14	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:B:124:ILE:HG22	3:B:127:LEU:CD2	0.53	2.32	7	1
3:A:17:LEU:CD1	3:A:27:LEU:CD2	0.53	2.81	11	1
3:B:117:LEU:HD13	3:B:122:VAL:HG13	0.53	1.81	9	1
3:A:24:ILE:N	3:A:24:ILE:CD1	0.53	2.63	13	3
3:A:24:ILE:HG13	3:B:132:MET:HE2	0.53	1.80	13	3
3:A:32:MET:SD	3:B:114:TYR:CA	0.53	2.96	8	3
3:A:9:VAL:HG12	3:A:12:ASP:CG	0.53	2.24	19	1
3:A:6:THR:CA	3:B:105:ILE:O	0.53	2.56	9	8
3:B:115:GLN:O	3:B:119:ALA:N	0.53	2.41	18	8
3:A:15:GLN:HA	3:A:18:LYS:HE2	0.53	1.81	13	3
3:A:9:VAL:CG2	3:B:103:GLN:HB3	0.53	2.34	9	1
2:D:193:DT:O4	3:B:104:ARG:NE	0.53	2.41	2	2
1:C:175:DA:O5'	1:C:175:DA:H8	0.53	1.87	6	1
3:B:115:GLN:HA	3:B:118:LYS:CG	0.52	2.34	7	5
3:A:32:MET:CA	3:B:117:LEU:HD12	0.52	2.23	13	2
3:A:14:TYR:CE2	3:B:105:ILE:CG2	0.52	2.93	7	7
2:D:190:DG:OP1	3:A:25:SER:HB3	0.52	2.04	20	5
3:B:109:VAL:CG2	3:B:114:TYR:CD1	0.52	2.65	13	1
3:A:32:MET:HE2	3:B:124:ILE:HG13	0.52	1.82	19	2
3:B:127:LEU:HD13	3:B:127:LEU:C	0.52	2.24	9	1
3:A:16:LEU:HD22	3:B:136:ALA:HB1	0.52	1.80	2	7
3:A:6:THR:HB	3:B:106:THR:HG22	0.52	1.81	13	4
3:B:114:TYR:CE1	3:B:118:LYS:HG2	0.52	2.38	15	2
3:A:18:LYS:HG3	3:A:19:ALA:N	0.52	2.18	8	2
3:B:109:VAL:CG1	3:B:114:TYR:CB	0.52	2.81	7	3
3:A:3:GLN:N	3:B:110:ASP:HB3	0.52	2.19	14	1
1:C:183:DC:H2''	1:C:184:DC:C5	0.52	2.40	19	1
1:C:180:DT:H2''	1:C:181:DA:C8	0.52	2.39	10	5
3:A:28:VAL:O	3:A:32:MET:HG3	0.52	2.04	8	2
3:B:107:VAL:CG1	3:B:109:VAL:HG22	0.52	2.35	8	2
1:C:173:DA:C2'	1:C:174:DT:O5'	0.52	2.58	7	3
3:A:14:TYR:OH	3:A:18:LYS:HD3	0.52	2.04	14	10
3:A:32:MET:HG2	3:B:117:LEU:HB2	0.52	1.81	3	1
3:A:4:ARG:HA	3:B:108:THR:HA	0.52	1.82	6	4
3:A:17:LEU:HD12	3:A:27:LEU:HD12	0.52	1.76	14	1
3:A:29:SER:HB2	3:B:112:ASP:O	0.52	2.05	11	3
3:A:24:ILE:CG2	3:B:132:MET:HE1	0.52	2.35	14	2
1:C:175:DA:C2	2:D:198:DA:C2	0.52	2.97	17	5
2:D:190:DG:H2'	2:D:191:DT:H71	0.52	1.81	11	2
3:A:24:ILE:HA	3:A:27:LEU:HB3	0.52	1.81	19	6
2:D:193:DT:O4	3:B:104:ARG:HD2	0.52	2.05	5	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:B:110:ASP:O	3:B:115:GLN:HG2	0.52	2.05	20	4
3:A:9:VAL:N	3:B:103:GLN:O	0.52	2.42	9	10
1:C:173:DA:H2''	1:C:174:DT:C6	0.52	2.40	14	3
3:B:124:ILE:HG22	3:B:127:LEU:HD12	0.52	1.80	3	2
3:A:3:GLN:CB	3:B:110:ASP:CB	0.52	2.84	14	1
3:B:107:VAL:HG12	3:B:109:VAL:HG22	0.52	1.81	8	1
3:B:128:VAL:HG12	3:B:129:SER:N	0.52	2.20	1	3
3:A:32:MET:CE	3:B:124:ILE:CG1	0.52	2.88	17	5
3:A:17:LEU:CD1	3:A:27:LEU:CD1	0.52	2.87	3	2
1:C:178:DT:C7	3:A:6:THR:OG1	0.52	2.57	14	2
2:D:188:DG:O5'	2:D:188:DG:H8	0.52	1.88	18	2
1:C:173:DA:H2''	1:C:174:DT:H5''	0.52	1.82	20	3
3:A:5:ILE:HG23	3:B:109:VAL:HG12	0.52	1.81	10	2
3:A:7:VAL:O	3:A:7:VAL:CG1	0.52	2.58	20	4
3:B:109:VAL:HG23	3:B:114:TYR:HB3	0.52	1.82	14	2
3:B:107:VAL:HG23	3:B:109:VAL:HG13	0.52	1.82	20	3
3:B:117:LEU:HD22	3:B:122:VAL:CB	0.52	2.33	13	1
3:A:8:THR:CG2	3:B:104:ARG:NE	0.52	2.69	1	1
3:B:124:ILE:N	3:B:124:ILE:CD1	0.52	2.72	11	6
3:A:17:LEU:CD2	3:B:132:MET:HA	0.51	2.35	15	3
3:B:124:ILE:HA	3:B:127:LEU:CB	0.51	2.35	4	2
3:A:14:TYR:HE1	3:B:105:ILE:HD11	0.51	1.58	15	3
3:B:124:ILE:HA	3:B:127:LEU:HB3	0.51	1.83	4	6
3:B:117:LEU:HD12	3:B:122:VAL:HG13	0.51	1.82	18	1
3:A:7:VAL:N	3:B:105:ILE:O	0.51	2.43	14	7
3:A:17:LEU:HD23	3:A:20:TYR:HE2	0.51	1.61	19	1
3:A:35:GLU:HG3	3:B:127:LEU:HD11	0.51	1.81	19	1
3:A:9:VAL:CB	3:A:14:TYR:HB3	0.51	2.36	2	6
2:D:190:DG:C8	2:D:191:DT:C7	0.51	2.94	14	4
2:D:191:DT:H72	3:B:106:THR:HG21	0.51	1.82	10	2
3:B:122:VAL:O	3:B:122:VAL:HG13	0.51	2.04	3	1
3:B:107:VAL:HG13	3:B:109:VAL:HB	0.51	1.82	2	1
3:B:110:ASP:CG	3:B:111:SER:N	0.51	2.63	14	1
3:A:17:LEU:HB2	3:B:132:MET:HG2	0.51	1.81	18	1
3:A:7:VAL:CG2	3:A:9:VAL:HB	0.51	2.36	17	1
3:A:9:VAL:CG1	3:A:12:ASP:HB2	0.51	2.35	19	1
3:A:24:ILE:CG1	3:B:132:MET:HE2	0.51	2.36	3	3
3:A:7:VAL:HG13	3:A:9:VAL:HB	0.51	1.82	20	1
3:B:105:ILE:HD12	3:B:106:THR:N	0.51	2.21	19	1
3:B:109:VAL:O	3:B:110:ASP:HB2	0.51	2.05	19	2
3:A:35:GLU:HB3	3:B:117:LEU:CD1	0.51	2.30	1	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:A:17:LEU:CD1	3:A:22:VAL:HB	0.51	2.36	20	1
3:A:3:GLN:O	3:B:109:VAL:HG22	0.51	2.06	13	1
3:A:28:VAL:O	3:A:32:MET:N	0.51	2.40	16	3
3:A:14:TYR:CG	3:A:15:GLN:N	0.51	2.77	1	3
3:B:117:LEU:HD11	3:B:127:LEU:CD1	0.51	2.36	11	2
3:A:32:MET:SD	3:B:127:LEU:HD13	0.51	2.45	20	1
3:A:24:ILE:HA	3:A:27:LEU:CB	0.51	2.36	15	3
2:D:189:DG:H4'	3:A:25:SER:OG	0.51	2.06	8	1
3:A:13:SER:O	3:B:132:MET:HB2	0.51	2.06	3	3
3:B:127:LEU:O	3:B:131:THR:HB	0.51	2.05	13	3
3:A:14:TYR:CD2	3:B:105:ILE:CD1	0.51	2.91	11	2
3:B:115:GLN:HA	3:B:118:LYS:HE2	0.51	1.83	12	3
3:A:10:ASP:HA	3:B:103:GLN:HB3	0.50	1.82	1	1
2:D:191:DT:C2	2:D:192:DA:C6	0.50	2.99	2	1
2:D:190:DG:C4	2:D:191:DT:H72	0.50	2.42	4	1
3:A:6:THR:HA	3:B:106:THR:HA	0.50	1.83	20	3
3:A:7:VAL:CG1	3:A:9:VAL:CG2	0.50	2.89	6	2
3:B:128:VAL:O	3:B:132:MET:N	0.50	2.39	19	3
3:A:24:ILE:CG1	3:B:132:MET:HE1	0.50	2.37	19	5
3:B:109:VAL:HG22	3:B:110:ASP:N	0.50	2.20	18	5
3:B:117:LEU:HD13	3:B:127:LEU:HD11	0.50	1.82	15	3
3:A:9:VAL:HG13	3:A:10:ASP:N	0.50	2.20	17	3
1:C:177:DG:OP1	3:B:125:SER:HB2	0.50	2.06	6	1
3:A:5:ILE:HG12	3:B:124:ILE:HD11	0.50	1.81	8	1
2:D:190:DG:OP1	3:A:25:SER:CB	0.50	2.59	19	1
1:C:176:DT:H72	3:A:8:THR:HG21	0.50	1.83	8	2
3:A:10:ASP:HB2	3:B:103:GLN:HB2	0.50	1.83	3	2
3:A:31:THR:HG23	3:B:127:LEU:HD21	0.50	1.84	2	1
3:A:9:VAL:CG1	3:A:14:TYR:HB2	0.50	2.36	20	1
3:B:117:LEU:HD22	3:B:120:TYR:CE2	0.50	2.41	20	1
3:B:117:LEU:CD1	3:B:122:VAL:CG1	0.50	2.89	18	2
1:C:175:DA:H2'	1:C:176:DT:C5	0.50	2.41	16	1
3:A:17:LEU:HD12	3:B:132:MET:HE1	0.50	1.83	12	1
3:A:7:VAL:HG21	3:B:128:VAL:CB	0.50	2.25	7	1
3:B:109:VAL:HG23	3:B:112:ASP:HB2	0.50	1.82	7	1
3:A:32:MET:HE1	3:B:124:ILE:HG21	0.50	1.78	9	1
3:A:7:VAL:CG1	3:A:9:VAL:HB	0.50	2.36	13	2
3:A:36:ALA:HB1	3:B:116:LEU:HD13	0.50	1.84	8	3
3:A:26:GLY:O	3:A:30:THR:HB	0.50	2.06	13	5
1:C:176:DT:H2'	3:A:8:THR:HG1	0.50	1.67	14	1
3:B:120:TYR:CD1	3:B:120:TYR:N	0.50	2.78	18	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:A:6:THR:OG1	3:B:104:ARG:HG3	0.50	2.06	7	2
1:C:177:DG:P	3:B:125:SER:HB3	0.50	2.47	15	1
3:A:7:VAL:HG12	3:B:124:ILE:CD1	0.50	2.19	10	1
3:B:118:LYS:HG3	3:B:119:ALA:N	0.50	2.22	4	3
3:A:32:MET:HG2	3:B:117:LEU:HD12	0.50	1.84	17	2
3:A:33:GLN:CB	3:B:113:SER:HB3	0.50	2.37	5	2
3:A:15:GLN:O	3:A:19:ALA:N	0.50	2.42	13	9
1:C:175:DA:C5	1:C:176:DT:C4	0.50	2.99	8	6
3:B:127:LEU:C	3:B:127:LEU:HD13	0.50	2.27	3	1
3:A:9:VAL:CG1	3:A:14:TYR:CD1	0.50	2.95	4	1
2:D:189:DG:O3'	3:A:25:SER:HB3	0.50	2.07	17	2
3:B:114:TYR:CE1	3:B:118:LYS:HD3	0.50	2.42	8	2
3:A:15:GLN:O	3:A:19:ALA:CB	0.49	2.59	7	10
1:C:174:DT:C2'	1:C:175:DA:N7	0.49	2.69	6	3
3:A:3:GLN:O	3:B:109:VAL:N	0.49	2.45	1	7
2:D:197:DT:H2''	2:D:198:DA:C8	0.49	2.41	10	1
3:A:9:VAL:CB	3:A:14:TYR:CD2	0.49	2.94	9	1
3:A:27:LEU:O	3:A:31:THR:HB	0.49	2.07	5	3
1:C:178:DT:C2	1:C:179:DA:N7	0.49	2.80	6	4
3:B:114:TYR:CD1	3:B:115:GLN:N	0.49	2.81	13	3
3:B:122:VAL:O	3:B:124:ILE:N	0.49	2.44	6	4
3:A:32:MET:HE3	3:B:114:TYR:HA	0.49	1.83	6	2
3:B:117:LEU:HD13	3:B:122:VAL:HG12	0.49	1.83	20	1
3:A:24:ILE:CD1	3:B:105:ILE:HD12	0.49	2.22	15	1
3:A:17:LEU:HD13	3:A:23:ASN:O	0.49	2.07	11	1
3:A:33:GLN:HB2	3:B:113:SER:HB3	0.49	1.83	10	2
3:B:109:VAL:HG11	3:B:114:TYR:CD1	0.49	2.42	10	1
2:D:192:DA:H2''	2:D:193:DT:C6	0.49	2.43	16	9
1:C:180:DT:O4	3:A:4:ARG:HD2	0.49	2.07	9	1
2:D:196:DA:C5	2:D:197:DT:C4	0.49	3.00	3	5
1:C:177:DG:N2	2:D:196:DA:C4	0.49	2.79	2	3
3:B:117:LEU:O	3:B:122:VAL:HG12	0.49	2.07	4	1
3:A:27:LEU:CD1	3:B:132:MET:SD	0.49	3.00	4	3
1:C:181:DA:C2	1:C:182:DC:C2	0.49	3.01	5	5
3:B:114:TYR:CD2	3:B:115:GLN:N	0.49	2.81	14	6
3:A:14:TYR:CZ	3:B:105:ILE:HG12	0.49	2.42	9	1
3:B:116:LEU:O	3:B:119:ALA:HB3	0.49	2.08	2	1
3:A:33:GLN:CA	3:B:113:SER:HB3	0.49	2.37	14	1
3:A:12:ASP:O	3:A:13:SER:HB2	0.49	2.08	18	2
3:A:14:TYR:CA	3:B:132:MET:SD	0.49	2.99	19	5
2:D:195:DC:C2	2:D:196:DA:N7	0.49	2.81	9	5

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:A:9:VAL:HG23	3:A:10:ASP:N	0.49	2.22	2	4
3:A:24:ILE:HG21	3:B:132:MET:HE2	0.49	1.82	20	1
3:A:7:VAL:HG22	3:A:9:VAL:HB	0.49	1.84	15	1
3:A:32:MET:SD	3:B:114:TYR:O	0.49	2.71	8	1
3:A:12:ASP:O	3:B:129:SER:HA	0.49	2.07	19	2
3:A:28:VAL:CG1	3:A:32:MET:HE3	0.49	2.37	8	2
3:B:105:ILE:CG1	3:B:105:ILE:O	0.49	2.60	5	1
3:B:118:LYS:HB3	3:B:123:ASN:CA	0.49	2.38	20	1
3:A:7:VAL:HG13	3:B:105:ILE:CG2	0.49	2.38	15	1
3:A:7:VAL:HG13	3:B:105:ILE:HB	0.49	1.84	15	1
1:C:173:DA:H2'	1:C:174:DT:H72	0.49	1.84	17	1
3:B:120:TYR:CD1	3:B:120:TYR:C	0.49	2.87	17	6
3:A:7:VAL:HG23	3:B:124:ILE:CD1	0.49	2.38	6	1
3:A:6:THR:HG23	3:B:104:ARG:CZ	0.49	2.38	7	1
3:A:3:GLN:HG2	3:B:114:TYR:CE2	0.48	2.43	19	1
1:C:184:DC:N4	2:D:187:DC:C4	0.48	2.81	19	1
2:D:191:DT:H2'	2:D:192:DA:C8	0.48	2.43	10	3
3:A:15:GLN:HA	3:A:18:LYS:CG	0.48	2.38	12	3
3:A:14:TYR:CZ	3:B:105:ILE:CG1	0.48	2.95	13	1
2:D:191:DT:H73	3:A:4:ARG:HH11	0.48	1.69	1	1
1:C:174:DT:H2'	1:C:175:DA:N7	0.48	2.23	1	2
3:A:7:VAL:HG22	3:A:7:VAL:O	0.48	2.07	10	4
3:A:10:ASP:CB	3:B:103:GLN:HB3	0.48	2.38	20	2
1:C:173:DA:C4'	1:C:174:DT:OP1	0.48	2.61	11	1
3:A:9:VAL:CG2	3:B:105:ILE:CG2	0.48	2.91	19	1
3:A:24:ILE:CD1	3:A:24:ILE:N	0.48	2.66	2	4
3:A:14:TYR:CE2	3:A:18:LYS:HD3	0.48	2.43	12	3
3:A:3:GLN:HB3	3:B:110:ASP:HA	0.48	1.84	6	2
2:D:190:DG:O5'	3:B:107:VAL:HA	0.48	2.08	4	1
2:D:189:DG:O3'	3:A:25:SER:HB2	0.48	2.08	8	3
3:A:5:ILE:HG23	3:B:107:VAL:O	0.48	2.08	17	2
3:B:117:LEU:HD23	3:B:122:VAL:O	0.48	2.08	15	2
2:D:192:DA:N6	3:B:104:ARG:NH2	0.48	2.62	13	1
3:B:127:LEU:HD22	3:B:131:THR:HB	0.48	1.83	13	1
2:D:196:DA:C8	2:D:197:DT:H72	0.48	2.42	19	1
3:A:28:VAL:CB	3:B:107:VAL:HG11	0.48	2.37	5	1
3:B:115:GLN:O	3:B:119:ALA:HB2	0.48	2.08	4	9
3:A:21:ASP:O	3:A:22:VAL:HG23	0.48	2.07	10	2
3:A:14:TYR:CE1	3:B:105:ILE:CG2	0.48	2.97	18	4
3:A:17:LEU:CD2	3:A:22:VAL:HB	0.48	2.37	3	1
1:C:177:DG:C2	2:D:196:DA:C2	0.48	3.01	3	6

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:A:7:VAL:CG2	3:B:124:ILE:O	0.48	2.62	7	2
2:D:186:DT:H5'	2:D:187:DC:C5	0.48	2.44	10	1
1:C:180:DT:O4	3:A:4:ARG:CD	0.48	2.61	9	1
3:A:27:LEU:CD2	3:B:135:GLU:HG2	0.48	2.39	14	1
3:A:5:ILE:HG23	3:B:109:VAL:HG23	0.48	1.85	15	1
3:A:12:ASP:CG	3:B:129:SER:HB3	0.48	2.29	12	1
2:D:194:DA:C4	2:D:195:DC:C6	0.48	3.02	11	10
3:A:32:MET:CE	3:B:123:ASN:O	0.48	2.62	20	6
1:C:177:DG:C4	1:C:178:DT:C5	0.48	3.01	9	3
3:A:27:LEU:HD21	3:B:135:GLU:HG2	0.48	1.85	14	1
3:A:14:TYR:CD2	3:B:105:ILE:CG2	0.48	2.97	20	1
3:B:127:LEU:O	3:B:127:LEU:HD22	0.48	2.08	13	1
3:B:120:TYR:CE1	3:B:122:VAL:HB	0.48	2.43	16	3
3:A:13:SER:CB	3:B:133:GLN:HB3	0.48	2.39	9	1
3:A:32:MET:HA	3:B:117:LEU:CD2	0.48	2.39	6	2
3:B:105:ILE:HD12	3:B:105:ILE:C	0.48	2.29	20	2
3:A:14:TYR:CZ	3:A:18:LYS:HG2	0.48	2.44	14	3
2:D:190:DG:C8	2:D:191:DT:H72	0.48	2.44	20	2
3:A:31:THR:HG21	3:B:131:THR:OG1	0.48	2.08	7	1
2:D:190:DG:O3'	3:A:23:ASN:HB3	0.48	2.09	8	1
3:A:13:SER:OG	3:B:133:GLN:HB2	0.47	2.09	18	3
2:D:189:DG:O5'	2:D:189:DG:C8	0.47	2.67	18	2
2:D:188:DG:H2''	2:D:189:DG:C8	0.47	2.43	6	3
1:C:177:DG:N7	3:B:104:ARG:NH2	0.47	2.62	18	2
3:A:14:TYR:CD2	3:A:15:GLN:N	0.47	2.82	15	4
1:C:181:DA:O5'	1:C:181:DA:H8	0.47	1.92	8	1
3:B:115:GLN:HA	3:B:118:LYS:HE3	0.47	1.85	5	1
3:A:6:THR:HB	3:B:106:THR:CG2	0.47	2.38	10	3
3:A:7:VAL:O	3:A:9:VAL:N	0.47	2.47	14	6
3:A:32:MET:CA	3:B:117:LEU:HD23	0.47	2.37	7	3
3:B:123:ASN:C	3:B:124:ILE:CD1	0.47	2.82	13	2
2:D:196:DA:O5'	2:D:196:DA:H8	0.47	1.91	16	1
3:A:15:GLN:HA	3:A:18:LYS:HE3	0.47	1.85	7	1
1:C:174:DT:H6	1:C:174:DT:O5'	0.47	1.91	10	2
1:C:176:DT:C2	1:C:177:DG:C8	0.47	3.02	2	4
3:A:14:TYR:CE2	3:B:105:ILE:CB	0.47	2.97	4	1
3:A:24:ILE:HD13	3:B:105:ILE:CD1	0.47	2.34	19	1
1:C:175:DA:H2'	1:C:176:DT:H71	0.47	1.85	19	2
3:A:13:SER:HB3	3:B:133:GLN:CB	0.47	2.40	9	2
3:A:9:VAL:HG11	3:A:14:TYR:CD1	0.47	2.44	4	1
3:B:107:VAL:HG23	3:B:109:VAL:CG1	0.47	2.39	14	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:D:191:DT:H2''	2:D:192:DA:N7	0.47	2.24	14	1
3:A:17:LEU:HD12	3:A:22:VAL:CG1	0.47	2.40	20	1
3:A:2:LYS:HD2	3:B:109:VAL:O	0.47	2.09	12	1
1:C:174:DT:C7	1:C:174:DT:OP1	0.47	2.62	12	1
2:D:190:DG:C2	2:D:191:DT:C2	0.47	3.03	1	1
3:B:122:VAL:HG13	3:B:124:ILE:H	0.47	1.70	4	1
2:D:192:DA:C8	2:D:192:DA:O5'	0.47	2.68	12	1
1:C:178:DT:C4	1:C:179:DA:N6	0.47	2.83	1	1
3:B:117:LEU:HD11	3:B:127:LEU:HD12	0.47	1.83	20	1
3:B:107:VAL:HG22	3:B:109:VAL:CG1	0.47	2.40	13	1
3:B:109:VAL:HB	3:B:114:TYR:HB3	0.47	1.86	15	1
2:D:186:DT:H71	2:D:187:DC:C2'	0.47	2.40	16	1
1:C:179:DA:C2	1:C:180:DT:C2	0.47	3.02	20	3
3:A:32:MET:HA	3:B:117:LEU:HD13	0.47	1.87	15	3
3:A:32:MET:O	3:A:36:ALA:HB2	0.47	2.09	14	1
3:B:117:LEU:HB3	3:B:122:VAL:O	0.47	2.09	20	1
2:D:191:DT:OP2	3:B:105:ILE:HA	0.47	2.09	11	2
3:A:8:THR:HA	3:B:104:ARG:HA	0.47	1.87	7	1
3:B:124:ILE:C	3:B:124:ILE:HD12	0.47	2.30	7	1
3:A:5:ILE:CD1	3:B:107:VAL:HB	0.47	2.40	8	1
3:B:121:ASP:O	3:B:122:VAL:HG23	0.47	2.09	19	3
3:A:33:GLN:O	3:A:37:ARG:HB2	0.47	2.10	5	2
1:C:179:DA:H62	3:B:104:ARG:CZ	0.47	2.23	10	1
3:A:32:MET:HE3	3:B:114:TYR:CA	0.47	2.39	14	1
3:B:123:ASN:HB2	3:B:124:ILE:HD12	0.47	1.87	20	1
3:B:124:ILE:CG2	3:B:127:LEU:HD13	0.47	2.39	18	1
3:A:14:TYR:CZ	3:B:105:ILE:HG22	0.47	2.43	16	1
3:B:107:VAL:O	3:B:109:VAL:HG23	0.47	2.10	11	1
3:A:14:TYR:CE2	3:B:105:ILE:HG22	0.47	2.44	8	2
3:B:117:LEU:CD2	3:B:122:VAL:O	0.47	2.63	1	2
3:A:5:ILE:HG22	3:B:114:TYR:CE2	0.47	2.45	6	3
2:D:191:DT:OP2	3:B:105:ILE:HB	0.47	2.09	4	1
1:C:176:DT:C7	3:B:102:LYS:HG3	0.47	2.40	18	1
3:A:24:ILE:HG12	3:B:105:ILE:HD12	0.47	1.86	18	2
3:A:35:GLU:HG3	3:B:127:LEU:HD21	0.47	1.86	11	2
3:A:28:VAL:CG1	3:A:32:MET:HE2	0.47	2.40	7	1
3:A:14:TYR:CE1	3:B:105:ILE:CB	0.47	2.98	7	1
1:C:175:DA:H2''	1:C:176:DT:C6	0.47	2.45	19	3
1:C:177:DG:H2'	1:C:178:DT:H71	0.47	1.86	18	3
3:B:105:ILE:CG2	3:B:105:ILE:O	0.47	2.63	13	1
3:A:32:MET:HB3	3:B:113:SER:O	0.47	2.10	11	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:A:20:TYR:CD1	3:A:21:ASP:HB2	0.47	2.45	8	1
3:A:17:LEU:CG	3:A:27:LEU:HD22	0.46	2.40	1	1
1:C:179:DA:N6	2:D:192:DA:N6	0.46	2.63	1	3
3:B:122:VAL:O	3:B:122:VAL:HG12	0.46	2.08	10	1
2:D:191:DT:H2'	2:D:192:DA:N7	0.46	2.24	12	3
3:A:22:VAL:O	3:A:22:VAL:HG12	0.46	2.09	7	3
3:A:10:ASP:HB3	3:B:102:LYS:HA	0.46	1.87	9	2
3:A:31:THR:HG21	3:B:131:THR:HB	0.46	1.87	4	1
3:A:6:THR:HG21	3:B:104:ARG:NH1	0.46	2.25	13	1
3:A:32:MET:HE1	3:B:123:ASN:O	0.46	2.10	12	4
3:A:4:ARG:HA	3:B:108:THR:HG22	0.46	1.87	14	1
3:B:117:LEU:CD2	3:B:122:VAL:CG1	0.46	2.92	14	1
3:A:36:ALA:HB1	3:B:116:LEU:CB	0.46	2.40	13	1
3:A:5:ILE:CB	3:B:114:TYR:CE1	0.46	2.97	17	1
1:C:178:DT:H73	3:B:104:ARG:HD3	0.46	1.87	8	1
3:B:109:VAL:HG13	3:B:110:ASP:N	0.46	2.25	19	2
3:A:24:ILE:O	3:A:25:SER:C	0.46	2.54	2	17
3:B:111:SER:HA	3:B:115:GLN:HG2	0.46	1.87	2	1
3:B:128:VAL:HG12	3:B:132:MET:SD	0.46	2.51	18	1
3:B:124:ILE:CG2	3:B:127:LEU:HD22	0.46	2.37	7	1
3:A:7:VAL:O	3:A:7:VAL:CG2	0.46	2.62	17	1
3:B:107:VAL:O	3:B:109:VAL:N	0.46	2.46	19	3
1:C:173:DA:O4'	1:C:174:DT:H5'	0.46	2.10	19	1
2:D:191:DT:C4	2:D:192:DA:N6	0.46	2.84	10	1
2:D:190:DG:OP2	3:A:25:SER:HB3	0.46	2.10	6	1
3:A:9:VAL:HG12	3:A:10:ASP:N	0.46	2.25	8	2
3:A:17:LEU:HD11	3:A:27:LEU:HD11	0.46	1.86	3	1
3:A:28:VAL:HG21	3:B:107:VAL:HG11	0.46	1.86	7	2
3:B:130:THR:CG2	3:B:131:THR:N	0.46	2.79	20	1
3:A:4:ARG:CZ	3:B:108:THR:HG21	0.46	2.41	11	3
3:A:20:TYR:CD1	3:A:20:TYR:C	0.46	2.88	9	4
3:B:117:LEU:CD2	3:B:120:TYR:OH	0.46	2.64	4	1
3:A:9:VAL:HG21	3:A:12:ASP:HB2	0.46	1.88	20	1
3:A:18:LYS:NZ	3:B:103:GLN:OE1	0.46	2.48	13	1
3:A:4:ARG:NE	3:B:108:THR:HG23	0.46	2.26	15	1
3:A:15:GLN:OE1	3:A:18:LYS:NZ	0.46	2.43	7	3
3:A:21:ASP:O	3:A:22:VAL:CG2	0.46	2.63	10	3
3:A:14:TYR:CE2	3:B:105:ILE:HG13	0.46	2.46	4	1
3:A:7:VAL:HB	3:B:105:ILE:CD1	0.46	2.41	4	1
3:B:117:LEU:CD1	3:B:127:LEU:HG	0.46	2.40	6	3
3:B:107:VAL:HG22	3:B:109:VAL:HB	0.46	1.88	18	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:D:190:DG:C5	2:D:191:DT:C4	0.46	3.04	12	2
3:B:104:ARG:CZ	3:B:106:THR:HG21	0.46	2.41	13	1
3:B:124:ILE:O	3:B:125:SER:C	0.46	2.54	6	15
3:A:22:VAL:HG12	3:A:23:ASN:N	0.46	2.26	8	1
1:C:177:DG:C2	1:C:178:DT:C2	0.46	3.04	9	2
2:D:190:DG:P	3:A:25:SER:HB3	0.46	2.51	12	3
3:B:112:ASP:O	3:B:114:TYR:N	0.46	2.49	14	3
3:A:17:LEU:HG	3:B:132:MET:HG2	0.46	1.88	15	2
2:D:187:DC:O5'	2:D:187:DC:C6	0.46	2.68	6	2
1:C:183:DC:C2	1:C:184:DC:C5	0.46	3.03	7	1
3:A:5:ILE:HD13	3:A:5:ILE:O	0.45	2.11	5	2
2:D:189:DG:C8	2:D:190:DG:N7	0.45	2.84	10	1
3:A:14:TYR:CE1	3:A:18:LYS:HG2	0.45	2.46	9	1
3:B:124:ILE:CG2	3:B:127:LEU:HD23	0.45	2.41	2	1
3:A:5:ILE:O	3:A:5:ILE:HG12	0.45	2.10	13	2
3:B:109:VAL:HG21	3:B:112:ASP:HB3	0.45	1.87	19	1
2:D:191:DT:H2''	2:D:192:DA:C8	0.45	2.46	1	1
3:B:128:VAL:CG1	3:B:132:MET:HE3	0.45	2.41	15	2
3:B:115:GLN:OE1	3:B:118:LYS:NZ	0.45	2.41	13	1
3:A:5:ILE:O	3:B:107:VAL:N	0.45	2.49	19	4
3:B:118:LYS:HB3	3:B:123:ASN:CG	0.45	2.32	19	1
1:C:175:DA:N6	2:D:196:DA:N6	0.45	2.64	9	1
3:A:20:TYR:CE1	3:A:22:VAL:HG23	0.45	2.47	19	1
3:B:120:TYR:CE1	3:B:122:VAL:HG23	0.45	2.46	19	2
2:D:187:DC:H2''	2:D:188:DG:C8	0.45	2.46	17	6
3:A:14:TYR:CE2	3:A:18:LYS:HG2	0.45	2.47	20	2
3:B:120:TYR:CE1	3:B:122:VAL:CG2	0.45	3.00	19	1
1:C:173:DA:C1'	1:C:174:DT:H5'	0.45	2.42	19	1
3:A:8:THR:HA	3:B:103:GLN:O	0.45	2.12	16	2
3:B:107:VAL:CG1	3:B:109:VAL:CG1	0.45	2.94	2	1
3:A:9:VAL:HG23	3:A:12:ASP:CB	0.45	2.42	4	1
1:C:174:DT:OP1	1:C:174:DT:H72	0.45	2.11	20	1
3:B:109:VAL:CG2	3:B:114:TYR:CB	0.45	2.90	16	4
3:A:17:LEU:HD13	3:A:20:TYR:OH	0.45	2.12	15	1
3:A:3:GLN:NE2	3:B:114:TYR:CD1	0.45	2.85	15	1
2:D:189:DG:C6	2:D:190:DG:C6	0.45	3.05	7	1
2:D:189:DG:O3'	3:A:25:SER:CB	0.45	2.65	8	1
3:B:117:LEU:CD1	3:B:122:VAL:HG11	0.45	2.42	8	1
3:A:5:ILE:HB	3:B:114:TYR:CZ	0.45	2.46	3	1
3:A:32:MET:HB2	3:B:113:SER:O	0.45	2.12	13	2
3:A:14:TYR:CD2	3:B:132:MET:HE3	0.45	2.46	4	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:D:191:DT:H71	3:B:106:THR:OG1	0.45	2.12	17	1
2:D:190:DG:OP1	3:B:107:VAL:HG13	0.45	2.11	8	1
1:C:179:DA:H2'	1:C:180:DT:H72	0.45	1.88	14	2
3:A:29:SER:CB	3:B:112:ASP:O	0.45	2.65	11	2
3:A:31:THR:OG1	3:B:131:THR:HG21	0.45	2.12	7	2
3:A:31:THR:HB	3:B:127:LEU:HD21	0.45	1.88	13	1
3:A:5:ILE:O	3:A:5:ILE:HD13	0.45	2.11	15	1
3:A:32:MET:HG2	3:B:117:LEU:CB	0.45	2.42	3	1
1:C:179:DA:N7	3:A:4:ARG:NH2	0.45	2.65	2	1
1:C:174:DT:O5'	1:C:174:DT:H6	0.45	1.95	6	1
3:A:17:LEU:HD11	3:A:27:LEU:HD13	0.45	1.89	7	2
3:A:28:VAL:HG12	3:A:32:MET:HG3	0.45	1.87	17	1
3:A:22:VAL:HG12	3:A:23:ASN:H	0.45	1.70	8	1
2:D:194:DA:C8	2:D:195:DC:C5	0.44	3.05	10	2
3:A:4:ARG:CZ	3:B:108:THR:CG2	0.44	2.96	15	3
1:C:178:DT:H71	3:A:6:THR:OG1	0.44	2.13	14	1
3:B:107:VAL:CG2	3:B:109:VAL:CG2	0.44	2.93	6	2
3:B:116:LEU:HD22	3:B:120:TYR:OH	0.44	2.12	7	1
3:A:32:MET:CG	3:B:117:LEU:CG	0.44	2.94	3	1
3:B:117:LEU:CD2	3:B:127:LEU:HD13	0.44	2.42	2	1
3:A:32:MET:HE1	3:B:124:ILE:CG1	0.44	2.42	18	2
3:B:127:LEU:O	3:B:127:LEU:HD23	0.44	2.12	20	1
3:B:126:GLY:O	3:B:130:THR:CB	0.44	2.65	7	2
3:B:107:VAL:HG22	3:B:109:VAL:HG13	0.44	1.90	13	1
3:B:120:TYR:C	3:B:120:TYR:CD1	0.44	2.90	5	5
1:C:177:DG:OP1	3:B:125:SER:HB3	0.44	2.11	9	1
3:B:121:ASP:O	3:B:122:VAL:CG2	0.44	2.65	20	2
1:C:178:DT:OP2	3:A:5:ILE:HA	0.44	2.11	16	1
3:A:17:LEU:HD23	3:A:20:TYR:CZ	0.44	2.43	3	1
3:B:127:LEU:HD13	3:B:128:VAL:N	0.44	2.28	3	1
1:C:178:DT:O4	3:B:104:ARG:NE	0.44	2.45	3	1
3:B:123:ASN:N	3:B:123:ASN:OD1	0.44	2.48	9	1
3:A:14:TYR:CZ	3:A:18:LYS:CG	0.44	3.01	14	1
3:B:128:VAL:C	3:B:132:MET:HG2	0.44	2.32	12	1
1:C:185:DG:C2	2:D:188:DG:C6	0.44	3.05	5	1
3:B:110:ASP:HA	3:B:114:TYR:CE2	0.44	2.47	14	1
3:A:28:VAL:HG13	3:A:32:MET:HG3	0.44	1.88	6	1
3:A:3:GLN:OE1	3:B:114:TYR:CE1	0.44	2.70	15	1
1:C:178:DT:C2	1:C:179:DA:C8	0.44	3.06	6	5
3:A:32:MET:SD	3:B:127:LEU:HD22	0.44	2.53	2	2
3:B:124:ILE:HG22	3:B:127:LEU:CD1	0.44	2.42	9	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:A:24:ILE:HD13	3:B:107:VAL:CG1	0.44	2.43	20	1
3:A:4:ARG:NH1	3:B:108:THR:HG21	0.44	2.27	20	1
3:A:27:LEU:HD23	3:A:27:LEU:C	0.44	2.32	16	1
3:A:32:MET:CB	3:B:113:SER:O	0.44	2.66	9	1
2:D:190:DG:OP1	3:A:25:SER:CA	0.44	2.66	13	1
3:A:6:THR:CB	3:B:106:THR:HG22	0.44	2.42	10	1
3:A:24:ILE:HG22	3:A:27:LEU:HD22	0.44	1.90	16	1
3:A:24:ILE:HG12	3:B:105:ILE:CD1	0.44	2.43	7	1
3:A:7:VAL:O	3:A:7:VAL:HG22	0.44	2.12	5	2
3:A:23:ASN:O	3:B:132:MET:CE	0.44	2.66	15	2
3:B:109:VAL:CG1	3:B:114:TYR:CD1	0.44	3.01	10	1
3:A:22:VAL:CG1	3:A:27:LEU:HB2	0.44	2.43	9	1
3:B:109:VAL:HG23	3:B:112:ASP:OD2	0.44	2.13	2	1
3:A:8:THR:CG2	3:B:104:ARG:NH1	0.44	2.81	4	2
3:A:28:VAL:HA	3:A:31:THR:OG1	0.44	2.12	13	1
3:A:4:ARG:NE	3:B:108:THR:CG2	0.44	2.81	15	1
1:C:176:DT:H2''	1:C:177:DG:O5'	0.44	2.12	15	1
3:B:105:ILE:HG13	3:B:105:ILE:O	0.44	2.13	11	1
3:A:33:GLN:HB2	3:B:113:SER:CB	0.43	2.43	10	2
3:B:115:GLN:O	3:B:119:ALA:CB	0.43	2.66	6	5
3:A:14:TYR:HA	3:B:132:MET:HG2	0.43	1.88	1	1
3:A:9:VAL:HG12	3:A:10:ASP:H	0.43	1.73	10	1
3:A:5:ILE:HD13	3:B:124:ILE:HD11	0.43	1.89	3	1
3:A:17:LEU:CD1	3:B:132:MET:SD	0.43	3.05	3	2
3:A:22:VAL:HG12	3:A:22:VAL:O	0.43	2.12	18	2
3:A:25:SER:HA	3:B:107:VAL:CG2	0.43	2.40	2	1
1:C:173:DA:C4	1:C:174:DT:C2	0.43	3.06	18	1
3:A:14:TYR:HA	3:B:132:MET:CG	0.43	2.43	13	1
3:A:20:TYR:CE1	3:A:22:VAL:CG1	0.43	3.01	12	1
3:A:5:ILE:O	3:B:106:THR:CA	0.43	2.66	11	1
3:A:8:THR:CG2	3:B:104:ARG:CZ	0.43	2.88	1	2
3:A:14:TYR:CD1	3:A:15:GLN:N	0.43	2.86	11	2
3:B:117:LEU:CD1	3:B:127:LEU:HD11	0.43	2.43	4	1
3:B:109:VAL:O	3:B:110:ASP:C	0.43	2.55	14	1
3:B:132:MET:O	3:B:136:ALA:HB2	0.43	2.13	13	2
3:A:17:LEU:CB	3:B:132:MET:HG2	0.43	2.43	18	1
2:D:195:DC:H2''	2:D:196:DA:O5'	0.43	2.13	18	1
2:D:186:DT:H2''	2:D:187:DC:O4'	0.43	2.13	11	1
3:B:117:LEU:HG	3:B:127:LEU:CD2	0.43	2.42	19	1
1:C:179:DA:C2'	1:C:180:DT:C6	0.43	3.01	1	2
1:C:179:DA:N6	3:B:104:ARG:CZ	0.43	2.82	10	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:A:17:LEU:HD13	3:A:22:VAL:HB	0.43	1.89	14	1
3:B:109:VAL:HG11	3:B:114:TYR:N	0.43	2.28	16	2
3:A:33:GLN:HG3	3:A:34:ASN:N	0.43	2.27	7	2
2:D:189:DG:C5	2:D:190:DG:N7	0.43	2.86	20	1
1:C:181:DA:N1	2:D:192:DA:C2	0.43	2.87	18	1
2:D:197:DT:N3	2:D:198:DA:C6	0.43	2.87	19	1
3:A:12:ASP:HB2	3:B:129:SER:OG	0.43	2.12	3	1
3:A:32:MET:CG	3:B:114:TYR:HA	0.43	2.44	20	3
2:D:187:DC:C6	2:D:187:DC:O5'	0.43	2.71	15	1
3:B:128:VAL:HG13	3:B:132:MET:CG	0.43	2.44	16	1
2:D:193:DT:O4	3:B:104:ARG:CD	0.43	2.66	16	1
3:B:117:LEU:HG	3:B:124:ILE:CG2	0.43	2.43	7	1
3:A:7:VAL:CG2	3:A:7:VAL:O	0.43	2.66	1	2
2:D:189:DG:C4	2:D:190:DG:C8	0.43	3.07	2	1
3:B:117:LEU:HD13	3:B:127:LEU:CG	0.43	2.43	4	1
3:A:16:LEU:CD2	3:A:20:TYR:OH	0.43	2.66	20	1
3:A:2:LYS:HE3	3:B:109:VAL:HA	0.43	1.91	20	1
3:B:109:VAL:CG2	3:B:110:ASP:N	0.43	2.78	13	1
2:D:196:DA:C4	2:D:197:DT:C5	0.43	3.07	20	2
1:C:176:DT:C4	1:C:177:DG:C6	0.43	3.07	6	1
1:C:183:DC:N4	2:D:188:DG:C6	0.43	2.87	6	1
3:A:17:LEU:HD21	3:B:135:GLU:CG	0.43	2.44	12	1
3:A:9:VAL:HG23	3:A:14:TYR:CD2	0.43	2.48	19	1
1:C:174:DT:C2'	1:C:175:DA:O5'	0.43	2.65	1	1
3:A:8:THR:O	3:B:102:LYS:HD3	0.43	2.12	3	1
3:A:33:GLN:HB2	3:B:113:SER:OG	0.43	2.14	2	1
3:A:7:VAL:HG13	3:B:105:ILE:CD1	0.43	2.44	18	2
3:B:128:VAL:CG1	3:B:132:MET:HE1	0.43	2.44	18	1
3:A:30:THR:CG2	3:A:31:THR:N	0.43	2.82	5	4
1:C:177:DG:H2'	1:C:178:DT:C7	0.43	2.44	1	2
3:B:125:SER:OG	3:B:126:GLY:N	0.43	2.52	7	2
3:A:14:TYR:OH	3:A:18:LYS:NZ	0.43	2.39	13	1
2:D:190:DG:H2'	2:D:191:DT:H73	0.43	1.91	13	1
1:C:174:DT:C4	1:C:175:DA:N6	0.42	2.87	5	1
3:A:12:ASP:C	3:A:14:TYR:H	0.42	2.16	1	1
3:A:8:THR:OG1	3:B:104:ARG:NH2	0.42	2.52	1	1
3:A:5:ILE:CG2	3:B:114:TYR:CD2	0.42	3.02	6	2
2:D:188:DG:H2'	2:D:189:DG:C8	0.42	2.49	2	1
3:B:124:ILE:HG23	3:B:127:LEU:HD12	0.42	1.90	13	2
3:B:102:LYS:HG2	3:B:102:LYS:O	0.42	2.13	18	1
3:A:35:GLU:HG2	3:B:117:LEU:HD11	0.42	1.90	18	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:A:3:GLN:HG2	3:B:114:TYR:CE1	0.42	2.48	13	1
3:A:29:SER:O	3:B:113:SER:HB2	0.42	2.14	19	1
1:C:173:DA:C4'	1:C:174:DT:H5'	0.42	2.44	19	1
1:C:175:DA:H2'	1:C:176:DT:C7	0.42	2.44	19	1
2:D:193:DT:H2''	2:D:194:DA:O5'	0.42	2.14	10	1
3:A:25:SER:OG	3:A:26:GLY:N	0.42	2.52	12	3
3:B:109:VAL:HG11	3:B:114:TYR:HB2	0.42	1.89	2	2
2:D:194:DA:H2''	2:D:195:DC:O5'	0.42	2.14	7	1
3:A:16:LEU:HD13	3:B:136:ALA:CB	0.42	2.44	10	1
3:A:28:VAL:CG1	3:A:29:SER:N	0.42	2.83	3	1
1:C:177:DG:C8	1:C:178:DT:C7	0.42	3.03	9	2
3:A:33:GLN:HG2	3:A:34:ASN:N	0.42	2.29	20	1
2:D:189:DG:C5	2:D:190:DG:C5	0.42	3.07	18	1
1:C:173:DA:C3'	1:C:174:DT:H73	0.42	2.44	15	1
3:B:109:VAL:HG12	3:B:110:ASP:N	0.42	2.29	1	4
3:A:5:ILE:HG13	3:B:114:TYR:CD2	0.42	2.49	10	1
3:A:31:THR:HG21	3:B:127:LEU:HD21	0.42	1.91	20	1
2:D:187:DC:C2'	2:D:188:DG:N7	0.42	2.80	12	2
3:A:13:SER:HB3	3:B:133:GLN:N	0.42	2.29	17	2
3:A:27:LEU:HD21	3:B:131:THR:CG2	0.42	2.44	16	1
3:A:6:THR:HG23	3:B:104:ARG:HH21	0.42	1.69	7	1
2:D:186:DT:H5''	2:D:187:DC:C5	0.42	2.50	7	1
3:A:6:THR:HB	3:B:106:THR:HA	0.42	1.92	17	2
2:D:194:DA:C5	2:D:195:DC:C4	0.42	3.08	10	2
3:A:9:VAL:O	3:B:102:LYS:HA	0.42	2.14	2	2
3:B:110:ASP:CG	3:B:111:SER:H	0.42	2.17	14	1
3:A:13:SER:HB2	3:B:129:SER:O	0.42	2.13	20	2
1:C:173:DA:H2''	1:C:174:DT:OP1	0.42	2.14	20	1
1:C:174:DT:N3	1:C:175:DA:N6	0.42	2.68	16	1
2:D:189:DG:C5	2:D:190:DG:C6	0.42	3.07	12	1
3:A:28:VAL:CG1	3:A:32:MET:CE	0.42	2.98	19	1
3:A:28:VAL:CG2	3:B:124:ILE:HG21	0.42	2.31	15	2
3:B:109:VAL:HG23	3:B:110:ASP:H	0.42	1.74	6	1
2:D:191:DT:C2'	2:D:192:DA:C8	0.42	3.02	15	1
3:A:17:LEU:CG	3:A:27:LEU:CD1	0.42	2.96	16	1
1:C:178:DT:H73	3:B:104:ARG:NE	0.42	2.30	11	2
3:A:17:LEU:HD13	3:B:132:MET:HA	0.42	1.89	4	1
3:A:18:LYS:HB3	3:A:23:ASN:CA	0.42	2.44	13	1
1:C:175:DA:H3'	3:B:102:LYS:HE2	0.42	1.91	12	1
3:A:5:ILE:HG13	3:B:114:TYR:CE1	0.42	2.50	5	1
2:D:190:DG:C4	2:D:191:DT:C5	0.42	3.08	1	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:A:12:ASP:O	3:A:13:SER:CB	0.42	2.67	18	1
3:A:9:VAL:CG2	3:B:103:GLN:HG2	0.42	2.45	12	1
3:A:24:ILE:O	3:A:28:VAL:N	0.42	2.49	7	1
1:C:175:DA:C8	1:C:176:DT:C7	0.42	3.02	5	1
3:A:12:ASP:O	3:A:14:TYR:N	0.42	2.52	17	2
3:A:31:THR:HG21	3:B:131:THR:CB	0.42	2.45	4	1
3:A:14:TYR:HD1	3:B:132:MET:HE2	0.42	1.74	18	1
3:A:17:LEU:CG	3:B:132:MET:HG2	0.42	2.45	18	1
2:D:191:DT:C7	3:A:4:ARG:HD2	0.42	2.44	6	1
3:A:17:LEU:CD1	3:A:27:LEU:HD13	0.42	2.45	7	2
3:B:138:ARG:HA	3:B:138:ARG:NE	0.42	2.28	13	1
3:A:9:VAL:O	3:B:102:LYS:NZ	0.42	2.41	8	1
1:C:177:DG:C8	3:B:104:ARG:NH2	0.42	2.88	1	1
3:B:114:TYR:CZ	3:B:118:LYS:CG	0.42	3.03	10	1
3:A:29:SER:HB3	3:B:109:VAL:HG21	0.42	1.91	14	1
3:B:118:LYS:HB2	3:B:123:ASN:HA	0.42	1.91	13	1
3:A:24:ILE:CG2	3:A:27:LEU:HD22	0.42	2.45	16	1
3:B:109:VAL:HG13	3:B:112:ASP:CB	0.42	2.39	17	1
1:C:175:DA:N1	2:D:198:DA:C2	0.41	2.88	16	2
3:A:15:GLN:CA	3:A:18:LYS:HE2	0.41	2.44	15	1
2:D:188:DG:C4	2:D:189:DG:N7	0.41	2.88	17	1
3:A:29:SER:OG	3:B:112:ASP:HB2	0.41	2.16	3	1
3:A:14:TYR:CE2	3:B:105:ILE:HB	0.41	2.51	4	1
3:A:31:THR:HG23	3:B:127:LEU:HD11	0.41	1.92	11	1
1:C:174:DT:OP1	1:C:174:DT:C7	0.41	2.68	1	1
3:A:9:VAL:HG12	3:B:105:ILE:CG2	0.41	2.45	4	1
3:B:105:ILE:HG12	3:B:105:ILE:O	0.41	2.15	4	1
3:A:34:ASN:O	3:A:38:ARG:HG2	0.41	2.15	14	1
3:B:128:VAL:CG1	3:B:132:MET:CE	0.41	2.98	14	1
3:A:32:MET:SD	3:B:117:LEU:CD1	0.41	3.09	20	2
3:A:32:MET:HE2	3:B:124:ILE:HG21	0.41	1.90	6	1
3:A:3:GLN:HB3	3:B:109:VAL:CG2	0.41	2.43	13	1
1:C:174:DT:H2''	1:C:175:DA:C5'	0.41	2.45	12	1
2:D:190:DG:H2'	2:D:191:DT:H72	0.41	1.91	19	2
3:A:5:ILE:CG1	3:B:114:TYR:CE2	0.41	3.03	10	1
3:B:115:GLN:HA	3:B:118:LYS:CE	0.41	2.46	2	1
3:B:109:VAL:O	3:B:112:ASP:N	0.41	2.40	14	1
3:B:118:LYS:HB2	3:B:123:ASN:OD1	0.41	2.15	2	1
3:A:32:MET:HA	3:B:117:LEU:CG	0.41	2.45	13	1
3:B:117:LEU:HD22	3:B:122:VAL:HG12	0.41	1.92	16	1
3:A:17:LEU:CD1	3:A:22:VAL:CG1	0.41	2.87	12	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:A:22:VAL:O	3:A:22:VAL:HG13	0.41	2.14	12	1
2:D:188:DG:C8	2:D:188:DG:O5'	0.41	2.66	12	1
3:A:17:LEU:HD12	3:B:132:MET:CG	0.41	2.45	19	1
3:A:17:LEU:HD13	3:A:27:LEU:CG	0.41	2.42	19	1
3:A:4:ARG:CG	3:B:106:THR:OG1	0.41	2.68	5	2
3:B:117:LEU:HD22	3:B:122:VAL:O	0.41	2.16	5	1
3:B:128:VAL:O	3:B:132:MET:SD	0.41	2.79	1	1
2:D:192:DA:C5	2:D:193:DT:C4	0.41	3.08	10	1
3:B:109:VAL:HG13	3:B:110:ASP:H	0.41	1.76	2	1
3:B:120:TYR:OH	3:B:122:VAL:HG11	0.41	2.14	16	1
1:C:178:DT:C7	3:B:104:ARG:HE	0.41	2.28	7	1
3:B:133:GLN:O	3:B:137:ARG:HB2	0.41	2.16	8	1
1:C:175:DA:C8	1:C:175:DA:O5'	0.41	2.74	10	1
2:D:189:DG:OP2	3:B:108:THR:HB	0.41	2.15	6	1
3:A:17:LEU:CD1	3:A:20:TYR:OH	0.41	2.68	15	1
3:B:110:ASP:HA	3:B:115:GLN:CD	0.41	2.36	15	1
3:B:122:VAL:O	3:B:123:ASN:CG	0.41	2.59	16	1
1:C:176:DT:OP2	3:B:102:LYS:HD3	0.41	2.16	17	1
3:A:17:LEU:HD23	3:B:132:MET:HA	0.41	1.92	18	1
3:B:112:ASP:C	3:B:114:TYR:H	0.41	2.17	6	1
3:B:114:TYR:CE1	3:B:118:LYS:CD	0.41	3.04	15	1
1:C:174:DT:C5	1:C:174:DT:OP1	0.41	2.74	12	1
2:D:190:DG:N7	3:A:4:ARG:NH2	0.41	2.69	5	1
1:C:177:DG:H8	3:B:104:ARG:NH2	0.41	2.13	1	1
1:C:179:DA:H2''	1:C:180:DT:C6	0.41	2.50	1	2
3:A:7:VAL:HB	3:B:105:ILE:HG22	0.41	1.92	9	1
1:C:178:DT:C7	3:A:6:THR:CG2	0.41	2.99	14	1
3:A:9:VAL:CG2	3:A:14:TYR:CB	0.41	2.83	18	1
1:C:179:DA:H2'	1:C:180:DT:C7	0.41	2.46	6	1
3:A:4:ARG:HD3	3:B:106:THR:OG1	0.41	2.16	15	1
2:D:190:DG:OP2	3:A:25:SER:CB	0.41	2.69	12	1
1:C:177:DG:OP2	3:A:7:VAL:HA	0.41	2.15	11	1
2:D:196:DA:C2	2:D:197:DT:C2	0.41	3.09	11	1
3:A:7:VAL:HB	3:B:105:ILE:CG2	0.41	2.46	9	1
3:A:7:VAL:HG11	3:B:128:VAL:HG21	0.41	1.92	14	1
2:D:188:DG:H2'	2:D:189:DG:C4'	0.41	2.46	16	1
2:D:192:DA:C2'	2:D:193:DT:C6	0.41	3.04	12	1
3:B:105:ILE:CD1	3:B:105:ILE:C	0.40	2.90	19	1
2:D:192:DA:O5'	2:D:192:DA:C8	0.40	2.74	10	1
3:A:32:MET:CB	3:B:114:TYR:HA	0.40	2.46	13	1
3:A:2:LYS:HB3	3:B:109:VAL:O	0.40	2.16	15	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:A:17:LEU:HD13	3:A:22:VAL:CG2	0.40	2.46	12	1
3:A:15:GLN:HA	3:A:18:LYS:HG2	0.40	1.91	8	1
3:B:124:ILE:HG23	3:B:127:LEU:HD13	0.40	1.92	20	1
3:A:2:LYS:NZ	3:B:109:VAL:O	0.40	2.43	13	1
3:A:17:LEU:HG	3:A:27:LEU:HD11	0.40	1.93	15	1
3:A:31:THR:HG22	3:B:127:LEU:HD11	0.40	1.94	16	1
3:B:122:VAL:C	3:B:124:ILE:N	0.40	2.74	7	1
3:A:28:VAL:HG11	3:B:107:VAL:HG11	0.40	1.93	3	1
1:C:173:DA:C2'	1:C:174:DT:OP1	0.40	2.69	20	1
1:C:181:DA:C5	1:C:182:DC:C4	0.40	3.10	20	1
3:A:12:ASP:O	3:B:129:SER:CB	0.40	2.70	1	1
3:B:117:LEU:HD13	3:B:127:LEU:CD2	0.40	2.46	2	1
3:A:33:GLN:OE1	3:A:37:ARG:NH2	0.40	2.47	14	1
3:A:9:VAL:C	3:A:11:SER:N	0.40	2.75	20	1
2:D:190:DG:C8	2:D:191:DT:H73	0.40	2.51	18	1
3:A:17:LEU:HG	3:A:27:LEU:HD22	0.40	1.93	7	1
2:D:190:DG:P	3:B:107:VAL:HA	0.40	2.56	11	1
3:B:124:ILE:HG23	3:B:127:LEU:HD23	0.40	1.92	19	1
1:C:177:DG:C5	1:C:178:DT:C4	0.40	3.10	10	1
2:D:191:DT:H73	3:A:4:ARG:HD3	0.40	1.92	10	1
1:C:179:DA:C6	2:D:194:DA:N1	0.40	2.89	10	1
3:A:23:ASN:OD1	3:A:23:ASN:N	0.40	2.53	6	1
3:A:28:VAL:HG13	3:A:32:MET:CG	0.40	2.46	6	1
3:A:7:VAL:HG21	3:B:124:ILE:C	0.40	2.37	16	1

## 6.3 Torsion angles ⓘ

### 6.3.1 Protein backbone ⓘ

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	A	37/72 (51%)	25±1 (66±2%)	6±1 (17±3%)	6±1 (16±3%)	0	4
3	B	37/72 (51%)	25±1 (68±3%)	6±2 (17±4%)	6±1 (15±3%)	1	4
All	All	1480/2880 (51%)	994 (67%)	251 (17%)	235 (16%)	0	4

All 21 unique Ramachandran outliers are listed below. They are sorted by the frequency of

occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
3	A	9	VAL	20
3	A	21	ASP	20
3	B	121	ASP	20
3	B	109	VAL	18
3	B	113	SER	18
3	A	13	SER	16
3	A	24	ILE	16
3	B	122	VAL	14
3	B	124	ILE	14
3	B	112	ASP	14
3	A	12	ASP	13
3	A	22	VAL	12
3	A	23	ASN	12
3	B	123	ASN	8
3	A	10	ASP	6
3	B	110	ASP	6
3	A	2	LYS	3
3	A	11	SER	2
3	A	28	VAL	1
3	B	128	VAL	1
3	B	108	THR	1

### 6.3.2 Protein sidechains ⓘ

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	A	34/64 (53%)	17±3 (49±7%)	17±3 (51±7%)	0	1
3	B	34/64 (53%)	17±2 (49±7%)	17±2 (51±7%)	0	1
All	All	1360/2560 (53%)	670 (49%)	690 (51%)	0	1

All 67 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)
3	A	6	THR	20
3	B	106	THR	20

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Mol	Chain	Res	Type	Models (Total)
3	A	24	ILE	20
3	A	14	TYR	19
3	B	116	LEU	19
3	B	114	TYR	18
3	A	17	LEU	18
3	A	16	LEU	18
3	B	124	ILE	17
3	A	20	TYR	17
3	B	133	GLN	16
3	B	120	TYR	16
3	B	137	ARG	16
3	A	33	GLN	16
3	B	117	LEU	16
3	B	107	VAL	16
3	A	7	VAL	15
3	A	37	ARG	15
3	B	105	ILE	15
3	A	5	ILE	15
3	A	38	ARG	14
3	A	21	ASP	14
3	B	112	ASP	14
3	B	125	SER	14
3	A	35	GLU	13
3	B	118	LYS	13
3	B	127	LEU	12
3	B	115	GLN	11
3	B	138	ARG	11
3	A	18	LYS	11
3	A	27	LEU	11
3	A	2	LYS	11
3	B	102	LYS	10
3	A	12	ASP	10
3	A	34	ASN	9
3	B	111	SER	9
3	A	4	ARG	9
3	B	130	THR	9
3	A	15	GLN	8
3	A	30	THR	8
3	B	131	THR	8
3	B	113	SER	8
3	A	13	SER	8
3	B	121	ASP	8

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Mol	Chain	Res	Type	Models (Total)
3	A	31	THR	7
3	A	25	SER	7
3	A	23	ASN	7
3	B	122	VAL	6
3	B	104	ARG	6
3	B	135	GLU	6
3	B	123	ASN	6
3	A	8	THR	6
3	B	134	ASN	5
3	A	11	SER	5
3	B	132	MET	5
3	B	103	GLN	5
3	A	32	MET	4
3	A	3	GLN	4
3	B	129	SER	3
3	B	108	THR	3
3	B	110	ASP	2
3	A	10	ASP	2
3	A	9	VAL	2
3	B	128	VAL	1
3	A	28	VAL	1
3	B	109	VAL	1
3	A	22	VAL	1

### 6.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 6.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

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

There are no ligands in this entry.

## 6.7 Other polymers [i](#)

There are no such molecules in this entry.

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

There are no chain breaks in this entry.



## 7 Chemical shift validation

No chemical shift data were provided