



# Full wwPDB NMR Structure Validation Report ⓘ

Apr 26, 2016 – 03:02 PM BST

PDB ID : 1A66  
Title : SOLUTION NMR STRUCTURE OF THE CORE NFATC1/DNA COMPLEX, 18 STRUCTURES  
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Deposited on : 1998-03-06

This is a Full wwPDB NMR Structure Validation Report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](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  
Mogul : unknown  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
RCI : v\_1n\_11\_5\_13\_A (Berjanski et al., 2005)  
PANAV : Wang et al. (2010)  
ShiftChecker : rb-20027457  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : rb-20027457

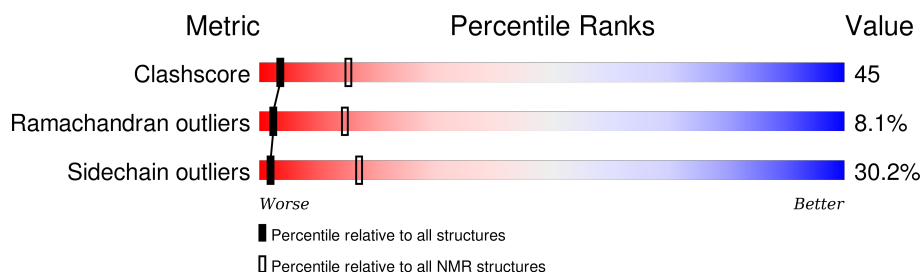
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*SOLUTION NMR*

The overall completeness of chemical shifts assignment was not calculated.

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



Metric	Whole archive (#Entries)	NMR archive (#Entries)
Clashscore	114402	11133
Ramachandran outliers	111179	9975
Sidechain outliers	111093	9958

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	B	12	
2	C	12	
3	A	178	

## 2 Ensemble composition and analysis

This entry contains 18 models. Model 3 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:10-A:40, A:45-A:177 (164)	0.77	3

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

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

The models can be grouped into 2 clusters and 3 single-model clusters were found.

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

### 3 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 3595 atoms, of which 1704 are hydrogens and 0 are deuteriums.

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

Mol	Chain	Residues	Atoms						Trace
1	B	12	Total	C	H	N	O	P	0
			385	119	136	52	67	11	

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

Mol	Chain	Residues	Atoms						Trace
2	C	12	Total	C	H	N	O	P	0
			376	116	139	37	73	11	

- Molecule 3 is a protein called CORE NFATC1.

Mol	Chain	Residues	Atoms						Trace
3	A	178	Total	C	H	N	O	S	0
			2834	875	1429	267	258	5	

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	ALA	ENGINEERED	UNP O95644
A	2	LYS	LEU	ENGINEERED	UNP O95644
A	28	ARG	HIS	ENGINEERED	UNP O95644

## 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: DNA (5'-D(\*CP\*GP\*AP\*GP\*GP\*AP\*AP\*AP\*AP\*TP\*TP\*G)-3')

Chain B: 

C315  
G316  
A317  
G318  
G319  
A320  
A321  
A322  
A323  
T324  
T325  
G326

- Molecule 2: DNA (5'-D(\*CP\*AP\*AP\*TP\*TP\*TP\*TP\*CP\*CP\*TP\*CP\*G)-3')

Chain C: 

C340  
A341  
A342  
T343  
T344  
T345  
T346  
C347  
C348  
T349  
C350  
G351

- Molecule 3: CORE NFATC1

Chain A: 

H1  
R2  
D3  
H4  
L5  
L6  
P7  
S8  
H9  
S10  
G11  
P12  
Y13  
E14  
L15  
R16  
I17  
H18  
R19  
Q20  
P21  
K22  
H25  
R26  
A27  
Y28  
R29  
E30  
T31  
E32  
R35  
G36  
A37  
V38  
K39  
A40  
S41  
A42  
G43  
G44  
R45  
P46  
L47  
V48  
Q49  
L50  
H51  
G52  
Y53  
E55  
N56  
E57  
P58  
L59  
N60  
L61  
Q62

L63  
F64  
L65  
G66  
T67  
R71  
L72  
L73  
R74  
P75  
H76  
A77  
F78  
Y79  
Q80  
H81  
V82  
R83  
I84  
T85  
G86  
K87  
T88  
V89  
T92  
S93  
H94  
E95  
G96  
I97  
L98  
S99  
N100  
T101  
K102  
V103  
L104  
L105  
I106  
P107  
L108  
L109  
P110  
M114  
V117  
I118  
D119  
C120  
I123  
L124  
K125  
L126  
R127  
N128  
S129

D130  
I131  
E132  
L133  
R134  
K135  
G136  
E137  
T138  
D139  
I140  
G141  
R142  
K143  
M144  
T145  
R146  
V147  
R148  
L149  
V150  
F151  
R152  
V153  
H154  
V155  
P156  
Q157  
P158  
S159  
G160  
R161  
T162  
L163  
S164  
L165  
Q166  
V167  
A168  
S169  
I172  
L173  
C174  
S175  
Q176  
R177  
S178

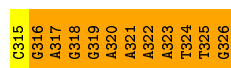
### 4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

#### 4.2.1 Score per residue for model 1

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

Chain B:  8% 92%



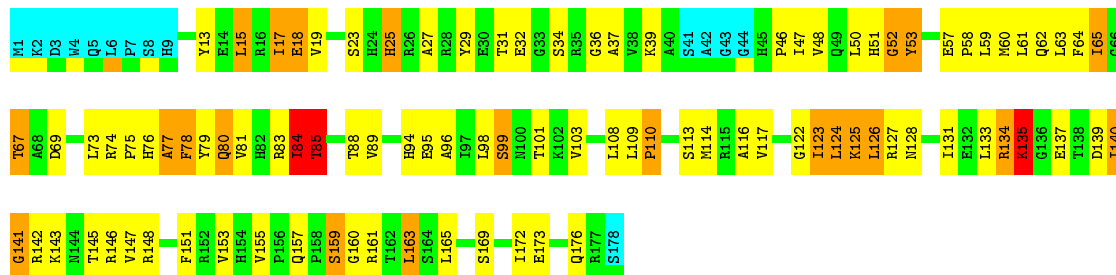
- Molecule 2: DNA (5'-D(\*CP\*AP\*AP\*TP\*TP\*TP\*TP\*CP\*CP\*TP\*CP\*G)-3')

Chain C:  8% 33% 58%



- Molecule 3: CORE NFATC1

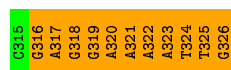
Chain A:  39% 39% 12% 8%



#### 4.2.2 Score per residue for model 2

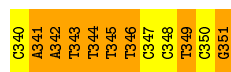
- Molecule 1: DNA (5'-D(\*CP\*GP\*AP\*GP\*GP\*AP\*AP\*AP\*AP\*TP\*TP\*G)-3')

Chain B:  8% 92%

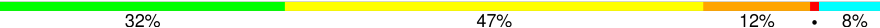


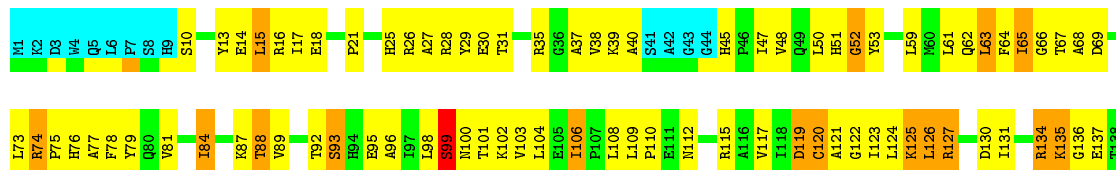
- Molecule 2: DNA (5'-D(\*CP\*AP\*AP\*TP\*TP\*TP\*TP\*CP\*CP\*TP\*CP\*G)-3')

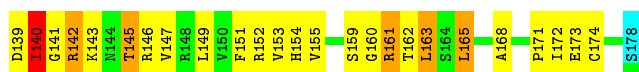
Chain C:  33% 67%



- Molecule 3: CORE NFATC1

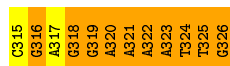
Chain A:  32% 47% 12% 8%





#### 4.2.3 Score per residue for model 3 (medoid)

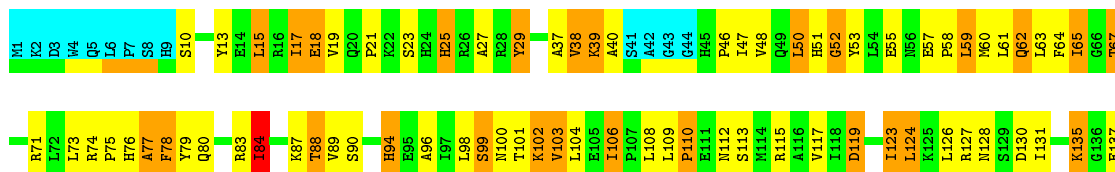
- Molecule 1: DNA (5'-D(\*CP\*GP\*AP\*GP\*GP\*AP\*AP\*AP\*AP\*TP\*TP\*G)-3')



- Molecule 2: DNA (5'-D(\*CP\*AP\*AP\*TP\*TP\*TP\*TP\*CP\*CP\*TP\*CP\*G)-3')

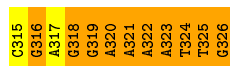


- Molecule 3: CORE NFATC1

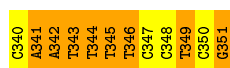


#### 4.2.4 Score per residue for model 4

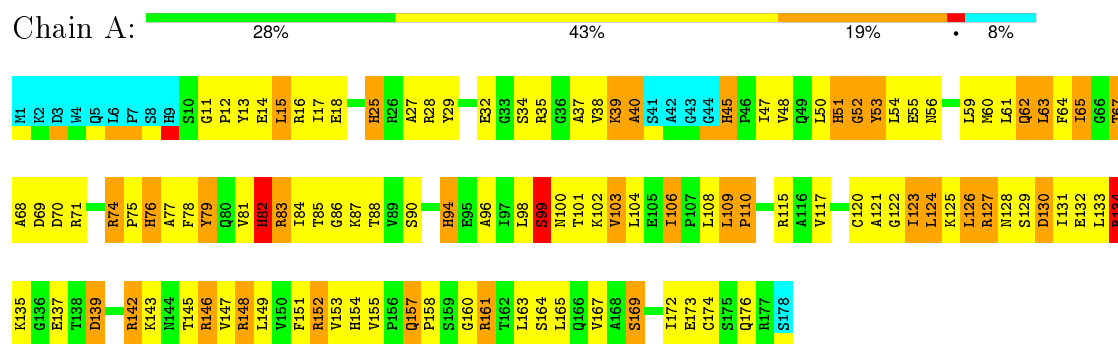
- Molecule 1: DNA (5'-D(\*CP\*GP\*AP\*GP\*GP\*AP\*AP\*AP\*AP\*TP\*TP\*G)-3')



- Molecule 2: DNA (5'-D(\*CP\*AP\*AP\*TP\*TP\*TP\*TP\*CP\*CP\*TP\*CP\*G)-3')



- Molecule 3: CORE NFATC1



#### 4.2.5 Score per residue for model 5

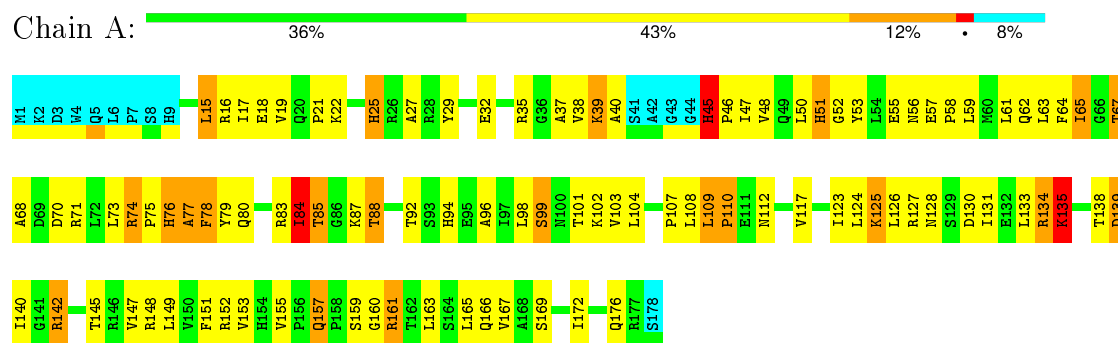
- Molecule 1: DNA (5'-D(\*CP\*GP\*AP\*GP\*GP\*AP\*AP\*AP\*AP\*TP\*TP\*G)-3')



- Molecule 2: DNA (5'-D(\*CP\*AP\*AP\*TP\*TP\*TP\*TP\*CP\*CP\*TP\*CP\*G)-3')



- Molecule 3: CORE NFATC1

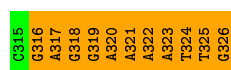


#### 4.2.6 Score per residue for model 6

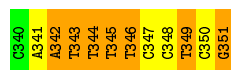
- Molecule 1: DNA (5'-D(\*CP\*GP\*AP\*GP\*GP\*AP\*AP\*AP\*AP\*TP\*TP\*G)-3')



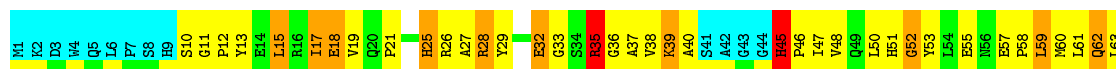




- Molecule 2: DNA (5'-D(\*CP\*AP\*AP\*TP\*TP\*TP\*TP\*CP\*CP\*TP\*CP\*G)-3')

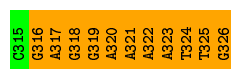


- Molecule 3: CORE NFATC1

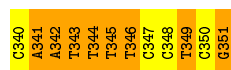


#### 4.2.7 Score per residue for model 7

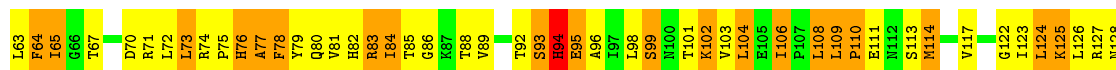
- Molecule 1: DNA (5'-D(\*CP\*GP\*AP\*GP\*GP\*AP\*AP\*AP\*AP\*TP\*TP\*G)-3')

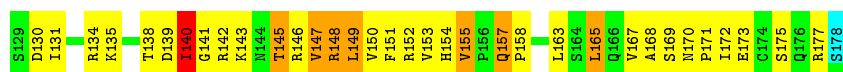


- Molecule 2: DNA (5'-D(\*CP\*AP\*AP\*TP\*TP\*TP\*TP\*CP\*CP\*TP\*CP\*G)-3')



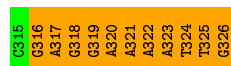
- Molecule 3: CORE NFATC1



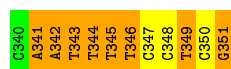


#### 4.2.8 Score per residue for model 8

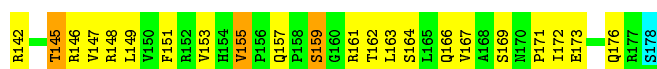
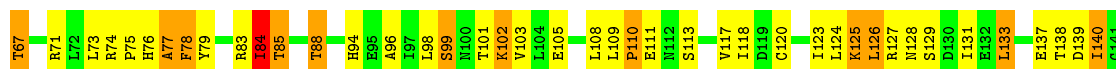
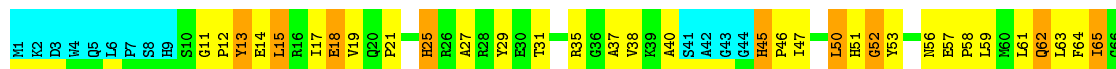
- Molecule 1: DNA (5'-D(\*CP\*GP\*AP\*GP\*GP\*AP\*AP\*AP\*AP\*TP\*TP\*G)-3')



- Molecule 2: DNA (5'-D(\*CP\*AP\*AP\*TP\*TP\*TP\*TP\*CP\*CP\*TP\*CP\*G)-3')

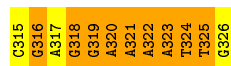


- Molecule 3: CORE NFATC1

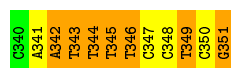


#### 4.2.9 Score per residue for model 9

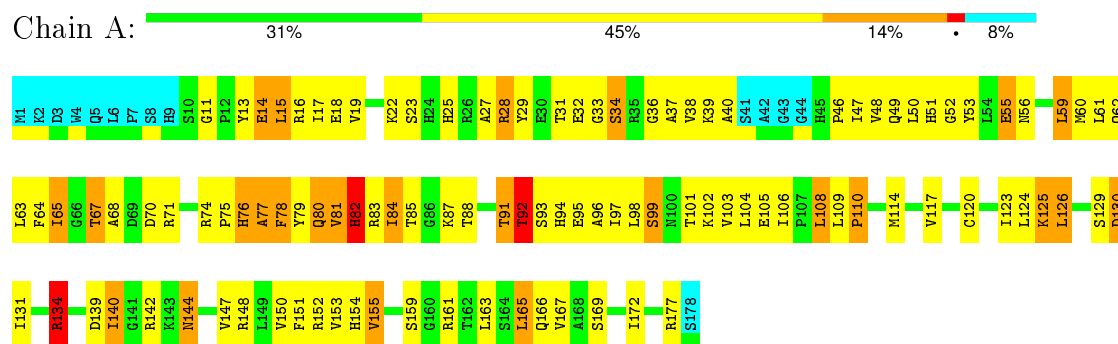
- Molecule 1: DNA (5'-D(\*CP\*GP\*AP\*GP\*GP\*AP\*AP\*AP\*AP\*TP\*TP\*G)-3')



- Molecule 2: DNA (5'-D(\*CP\*AP\*AP\*TP\*TP\*TP\*TP\*CP\*CP\*TP\*CP\*G)-3')



- Molecule 3: CORE NFATC1



#### 4.2.10 Score per residue for model 10

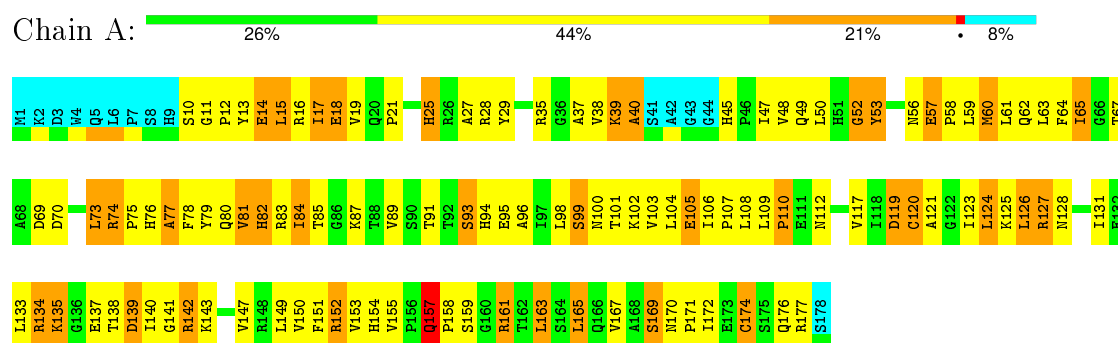
- Molecule 1: DNA (5'-D(\*CP\*GP\*AP\*GP\*GP\*AP\*AP\*AP\*AP\*TP\*TP\*G)-3')



- Molecule 2: DNA (5'-D(\*CP\*AP\*AP\*TP\*TP\*TP\*TP\*CP\*CP\*TP\*CP\*G)-3')



- Molecule 3: CORE NFATC1



#### 4.2.11 Score per residue for model 11

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




C315  
G316  
A317  
G318  
G319  
A320  
A321  
A322  
T323  
T324  
T325  
G326

- Molecule 2: DNA (5'-D(\*CP\*AP\*AP\*TP\*TP\*TP\*TP\*CP\*CP\*TP\*CP\*G)-3')

Chain C:  33% 67%

C340  
A341  
A342  
T343  
T344  
T345  
T346  
C347  
C348  
T349  
C350  
G351

- Molecule 3: CORE NFATC1

Chain A:  30% 46% 16% 8%

M1 K2 D3 W4 Q5 L6 P7 S8 H9 S10 Y13 Y14 L15 L16 I17 E18 V19 Q20 P21 E25 E26 A27 R28 Y29 E32 E37 V38 V39 A40 S41 A42 G43 G44 H45 P46 I47 V48 Q49 L50 H51 G52 Y53 L54 E55 N56 E57 F58 L59 M60 Q62 L61 Q63 F64 I65 T67

A68 D69 R74 P75 H76 A77 F78 Q80 V81 H82 R83 L84 T85 G86 K87 T88 V89 S90 T91 E95 S93 H94 R95 A96 I97 L98 S99 N100 T101 K102 V103 L104 E105 I106 P107 L108 L109 P110 I111 N112 V117 I118 D119 C120 A121 G122 I123 R124 K125 L126 R127 N128 I131 R135

G136 E137 T138 I140 G141 R142 K143 N144 R145 V146 V147 L148 L149 V150 F151 R152 V153 H154 V155 P156 Q157 P158 S159 G160 R161 T162 L163 S164 Q166 V167 A168 M170 P171 I172 E173 C174 S175 Q176 R177 S178

#### 4.2.12 Score per residue for model 12

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

Chain B:  8% 92%

C315  
G316  
A317  
G318  
G319  
A320  
A321  
A322  
T323  
T324  
T325  
G326

- Molecule 2: DNA (5'-D(\*CP\*AP\*AP\*TP\*TP\*TP\*TP\*CP\*CP\*TP\*CP\*G)-3')

Chain C:  8% 17% 75%

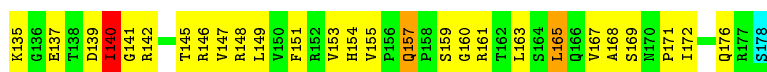
C340  
A341  
A342  
T343  
T344  
T345  
T346  
C347  
C348  
T349  
C350  
G351

- Molecule 3: CORE NFATC1

Chain A:  34% 47% 11% 8%

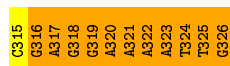
M1 K2 D3 W4 Q5 L6 P7 S8 H9 S10 Y13 Y14 L15 L16 I17 E18 V19 Q20 P21 E25 E26 A27 R28 Y29 E32 E37 V38 V39 A40 S41 A42 G43 G44 H45 P46 I47 L50 H51 G52 Y53 L54 E55 N56 L59 M60 Q62 L61 Q63 F64 I65 T67

A68 D69 R70 W71 L72 L73 R74 P75 H76 A77 F78 Q80 V81 H82 R83 T84 T85 T88 V89 S93 H94 R95 A96 I97 L98 S99 N100 T101 K102 V103 L104 E105 I106 P107 L108 L109 P110 M114 R115 A116 V117 I118 D119 C120 A121 G122 I123 L124 K125 L126 R127 M128 S129 D130 I131

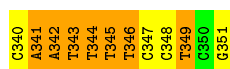


#### 4.2.13 Score per residue for model 13

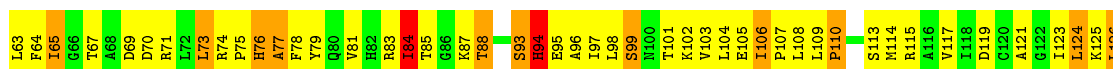
- Molecule 1: DNA (5'-D(\*CP\*GP\*AP\*GP\*GP\*AP\*AP\*AP\*AP\*TP\*TP\*G)-3')



- Molecule 2: DNA (5'-D(\*CP\*AP\*AP\*TP\*TP\*TP\*TP\*CP\*CP\*TP\*CP\*G)-3')

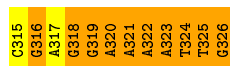


- Molecule 3: CORE NFATC1

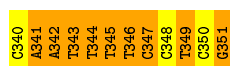


#### 4.2.14 Score per residue for model 14

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



- Molecule 2: DNA (5'-D(\*CP\*AP\*AP\*TP\*TP\*TP\*TP\*CP\*CP\*TP\*CP\*G)-3')



- Molecule 3: CORE NFATC1



#### 4.2.15 Score per residue for model 15

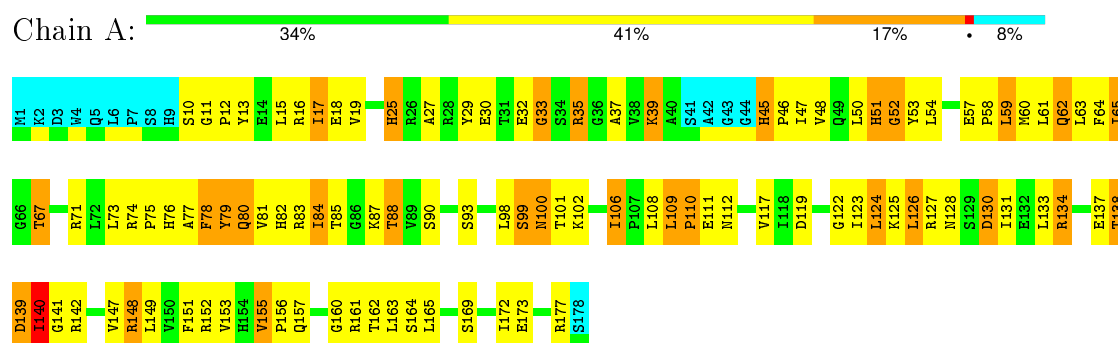
- Molecule 1: DNA (5'-D(\*CP\*GP\*AP\*GP\*GP\*AP\*AP\*AP\*AP\*TP\*TP\*G)-3')



- Molecule 2: DNA (5'-D(\*CP\*AP\*AP\*TP\*TP\*TP\*TP\*CP\*CP\*TP\*CP\*G)-3')



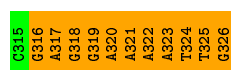
- Molecule 3: CORE NFATC1



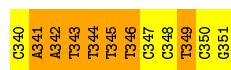
#### 4.2.16 Score per residue for model 16

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

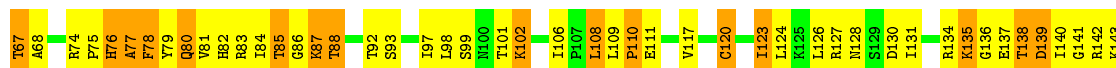




- Molecule 2: DNA (5'-D(\*CP\*AP\*AP\*TP\*TP\*TP\*TP\*CP\*CP\*TP\*CP\*G)-3')

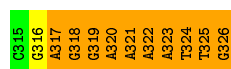


- Molecule 3: CORE NFATC1



#### 4.2.17 Score per residue for model 17

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



- Molecule 2: DNA (5'-D(\*CP\*AP\*AP\*TP\*TP\*TP\*TP\*CP\*CP\*TP\*CP\*G)-3')



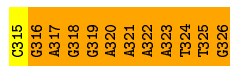
- Molecule 3: CORE NFATC1





#### 4.2.18 Score per residue for model 18

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



- Molecule 2: DNA (5'-D(\*CP\*AP\*AP\*TP\*TP\*TP\*TP\*CP\*CP\*TP\*CP\*G)-3')



- Molecule 3: CORE NFATC1





## 5 Refinement protocol and experimental data overview

The models were refined using the following method: *TORSION ANGLE DYNAMICS AND SIMULATED ANNEALING*.

Of the 18 calculated structures, 18 were deposited, based on the following criterion: *NOE VIOLATION  $\leq 0.4$  ANGSTROM, DIHEDRAL ANGLE VIOLATION  $\leq 5$  DEGREE*.

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

Software name	Classification	Version
X-PLOR	refinement	3.1
DYANA-1.4	structure solution	
X-PLOR	structure solution	3.1

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

### 6.1 Standard geometry

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#Z>5	RMSZ	#Z>5
1	B	1.28±0.02	2±0/281 (0.7±0.1%)	2.45±0.01	25±1/433 (5.8±0.3%)
2	C	1.23±0.01	1±0/263 (0.3±0.2%)	2.26±0.01	17±1/403 (4.3±0.3%)
3	A	1.02±0.01	0±0/1325 (0.0±0.0%)	0.80±0.01	0±0/1794 (0.0±0.0%)
All	All	1.10	51/33642 (0.2%)	1.49	765/47340 (1.6%)

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
1	B	325	DT	C5-C7	5.54	1.53	1.50	12	17
2	C	345	DT	C5-C7	5.49	1.53	1.50	1	15
1	B	324	DT	C5-C7	5.48	1.53	1.50	3	18
2	C	343	DT	C5-C7	5.11	1.53	1.50	13	1

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	B	326	DG	N7-C8-N9	9.71	117.95	113.10	8	18
1	B	316	DG	N7-C8-N9	9.38	117.79	113.10	16	18
2	C	351	DG	N7-C8-N9	9.23	117.71	113.10	5	18
1	B	319	DG	N7-C8-N9	9.15	117.68	113.10	17	18
1	B	318	DG	N7-C8-N9	8.94	117.57	113.10	11	18
2	C	341	DA	N7-C8-N9	8.31	117.95	113.80	5	18
2	C	342	DA	N7-C8-N9	7.79	117.69	113.80	2	18
1	B	317	DA	N7-C8-N9	7.65	117.62	113.80	4	18
1	B	323	DA	N7-C8-N9	7.64	117.62	113.80	15	18
1	B	321	DA	N7-C8-N9	7.63	117.61	113.80	5	18
1	B	320	DA	N7-C8-N9	7.45	117.53	113.80	13	18
1	B	322	DA	N7-C8-N9	7.44	117.52	113.80	7	18
2	C	343	DT	C6-C5-C7	-7.08	118.65	122.90	15	18

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
2	C	351	DG	C8-N9-C4	-6.95	103.62	106.40	5	18
1	B	326	DG	C8-N9-C4	-6.89	103.64	106.40	16	18
1	B	319	DG	C8-N9-C4	-6.87	103.65	106.40	9	18
1	B	318	DG	C8-N9-C4	-6.83	103.67	106.40	5	18
1	B	316	DG	C8-N9-C4	-6.72	103.71	106.40	18	18
2	C	344	DT	C6-C5-C7	-6.66	118.91	122.90	7	18
2	C	346	DT	C6-C5-C7	-6.30	119.12	122.90	16	16
2	C	345	DT	C6-C5-C7	-6.20	119.18	122.90	14	18
2	C	343	DT	O4'-C1'-N1	6.17	112.32	108.00	9	17
2	C	349	DT	C6-C5-C7	-6.10	119.24	122.90	14	18
1	B	317	DA	C8-N9-C4	-6.07	103.37	105.80	4	18
1	B	324	DT	C6-C5-C7	-6.05	119.27	122.90	14	18
2	C	342	DA	C8-N9-C4	-6.02	103.39	105.80	17	18
1	B	321	DA	C8-N9-C4	-5.89	103.44	105.80	14	18
2	C	345	DT	O4'-C1'-N1	5.84	112.09	108.00	1	6
1	B	325	DT	C6-C5-C7	-5.84	119.40	122.90	6	18
1	B	322	DA	C8-N9-C4	-5.83	103.47	105.80	16	18
1	B	319	DG	C5-N7-C8	-5.81	101.39	104.30	17	18
2	C	346	DT	C4-C5-C6	5.80	121.48	118.00	12	18
1	B	320	DA	C8-N9-C4	-5.63	103.55	105.80	15	18
1	B	323	DA	C8-N9-C4	-5.59	103.56	105.80	4	17
1	B	322	DA	O4'-C1'-N9	5.59	111.91	108.00	14	1
2	C	341	DA	O4'-C1'-N9	5.57	111.90	108.00	7	9
1	B	318	DG	C5-N7-C8	-5.52	101.54	104.30	2	18
1	B	324	DT	O4'-C1'-N1	5.52	111.86	108.00	17	4
1	B	319	DG	O4'-C1'-N9	5.45	111.81	108.00	11	3
1	B	326	DG	C5-N7-C8	-5.44	101.58	104.30	8	18
1	B	316	DG	O4'-C1'-N9	5.42	111.80	108.00	16	2
2	C	346	DT	C5-C6-N1	-5.40	120.46	123.70	7	2
2	C	347	DC	O4'-C1'-N1	5.36	111.75	108.00	12	2
1	B	316	DG	C5-N7-C8	-5.35	101.63	104.30	16	13
2	C	341	DA	C8-N9-C4	-5.35	103.66	105.80	5	7
2	C	344	DT	C4-C5-C6	5.31	121.19	118.00	11	15
2	C	343	DT	C4-C5-C6	5.29	121.18	118.00	17	12
1	B	317	DA	O4'-C1'-N9	5.29	111.70	108.00	6	5
1	B	323	DA	N1-C2-N3	-5.29	126.66	129.30	9	1
2	C	351	DG	C5-N7-C8	-5.22	101.69	104.30	5	14
2	C	349	DT	C4-C5-C6	5.19	121.11	118.00	14	18
2	C	341	DA	C5-N7-C8	-5.17	101.31	103.90	13	11
1	B	325	DT	O4'-C1'-N1	5.11	111.58	108.00	4	2
1	B	324	DT	C4-C5-C6	5.10	121.06	118.00	11	6

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
3	A	29	TYR	CB-CG-CD1	-5.08	117.95	121.00	7	1
1	B	320	DA	C5-N7-C8	-5.08	101.36	103.90	4	1
1	B	325	DT	C4-C5-C6	5.05	121.03	118.00	15	1
2	C	349	DT	O4'-C1'-N1	5.04	111.53	108.00	14	1
2	C	345	DT	C4-C5-C6	5.03	121.02	118.00	10	2

There are no chirality outliers.

There are no planarity outliers.

## 6.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	B	249	136	136	15±3
2	C	237	139	139	21±3
3	A	1300	1332	1332	127±13
All	All	32148	28926	28926	2773

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 45.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:A:61:LEU:HD13	3:A:153:VAL:HG22	1.11	1.11	14	18
3:A:15:LEU:HD13	3:A:153:VAL:HG21	1.09	1.23	10	18
3:A:37:ALA:HB2	3:A:123:ILE:HG22	1.05	1.17	14	6
3:A:79:TYR:CE2	3:A:126:LEU:HD21	1.04	1.87	13	7
3:A:47:ILE:HD12	3:A:117:VAL:HG13	1.00	1.34	17	12
3:A:59:LEU:HD21	3:A:153:VAL:HG11	0.99	1.26	11	10
3:A:47:ILE:HG23	3:A:117:VAL:HG22	0.98	1.29	8	15
3:A:96:ALA:HB3	3:A:103:VAL:HG23	0.97	1.37	18	15
2:C:344:DT:H2''	2:C:345:DT:O5'	0.96	1.60	17	18
3:A:79:TYR:CE1	3:A:126:LEU:HD22	0.95	1.97	10	2
3:A:59:LEU:HD21	3:A:153:VAL:HG13	0.94	1.40	7	8
3:A:25:HIS:CE1	3:A:172:ILE:HG23	0.94	1.97	7	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:A:37:ALA:CB	3:A:123:ILE:HG22	0.93	1.92	14	3
3:A:89:VAL:HG13	3:A:92:THR:HB	0.91	1.42	7	1
3:A:155:VAL:HG13	3:A:163:LEU:HB3	0.91	1.42	14	18
2:C:344:DT:H5"	3:A:142:ARG:O	0.90	1.66	14	11
3:A:15:LEU:HD13	3:A:153:VAL:CG2	0.88	1.98	15	14
3:A:59:LEU:HD21	3:A:153:VAL:CG1	0.88	1.98	15	13
3:A:147:VAL:HG23	3:A:172:ILE:HD12	0.87	1.44	8	13
3:A:15:LEU:HB3	3:A:165:LEU:HD22	0.86	1.44	2	8
3:A:147:VAL:CG2	3:A:172:ILE:HD12	0.86	2.01	10	13
3:A:93:SER:CB	3:A:106:ILE:HG22	0.85	2.01	14	3
3:A:94:HIS:HB3	3:A:106:ILE:HG23	0.85	1.45	4	2
3:A:79:TYR:CE2	3:A:147:VAL:HG11	0.85	2.07	7	1
3:A:78:PHE:CE2	3:A:131:ILE:HG23	0.85	2.07	16	2
3:A:59:LEU:HD11	3:A:153:VAL:HG12	0.84	1.47	11	9
3:A:15:LEU:CD1	3:A:153:VAL:HG21	0.83	2.03	2	11
3:A:48:VAL:HG21	3:A:151:PHE:CE2	0.83	2.09	9	2
3:A:15:LEU:CB	3:A:165:LEU:HD13	0.83	2.04	5	8
3:A:131:ILE:HG21	3:A:140:ILE:CG2	0.83	2.02	8	3
3:A:125:LYS:HE3	3:A:145:THR:HG22	0.83	1.49	8	1
3:A:27:ALA:HB2	3:A:123:ILE:CG1	0.82	2.04	6	7
3:A:27:ALA:HB2	3:A:123:ILE:HG23	0.82	1.52	16	1
3:A:157:GLN:HG2	3:A:163:LEU:HD23	0.82	1.50	17	1
3:A:27:ALA:HB2	3:A:123:ILE:HD12	0.81	1.51	4	2
3:A:17:ILE:HG23	3:A:47:ILE:O	0.80	1.77	4	18
3:A:61:LEU:HD13	3:A:153:VAL:CG2	0.80	2.01	14	3
3:A:59:LEU:HD13	3:A:155:VAL:HB	0.80	1.53	11	4
3:A:63:LEU:HD12	3:A:104:LEU:HD12	0.79	1.53	7	3
3:A:50:LEU:HD23	3:A:51:HIS:N	0.79	1.92	15	15
3:A:63:LEU:HD13	3:A:64:PHE:N	0.79	1.92	10	16
3:A:78:PHE:CE1	3:A:131:ILE:HD12	0.79	2.12	11	9
3:A:79:TYR:CD2	3:A:126:LEU:HD21	0.79	2.12	15	8
3:A:17:ILE:HG13	3:A:48:VAL:HG22	0.79	1.55	11	13
2:C:346:DT:H71	3:A:29:TYR:CE2	0.79	2.12	7	2
3:A:15:LEU:HB2	3:A:165:LEU:HD13	0.79	1.55	5	8
3:A:25:HIS:CD2	3:A:123:ILE:HG21	0.79	2.13	18	2
3:A:77:ALA:HB2	3:A:140:ILE:HD13	0.78	1.54	13	4
3:A:84:ILE:HG21	3:A:121:ALA:N	0.78	1.92	4	1
3:A:79:TYR:CE1	3:A:126:LEU:HD21	0.78	2.13	8	2
3:A:89:VAL:HG21	3:A:119:ASP:HB3	0.78	1.54	2	2
3:A:84:ILE:HG21	3:A:120:CYS:HA	0.78	1.53	9	4
3:A:25:HIS:NE2	3:A:123:ILE:HG21	0.78	1.92	3	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:A:127:ARG:O	3:A:131:ILE:HD12	0.78	1.77	5	2
3:A:47:ILE:HD12	3:A:117:VAL:HG22	0.77	1.55	16	12
3:A:78:PHE:CE2	3:A:131:ILE:HD12	0.77	2.14	16	3
3:A:37:ALA:HB2	3:A:123:ILE:CG2	0.77	2.10	13	4
2:C:346:DT:H71	3:A:29:TYR:HE2	0.76	1.38	7	2
3:A:38:VAL:HG13	3:A:45:HIS:HA	0.76	1.56	4	2
2:C:345:DT:H2''	2:C:346:DT:O5'	0.76	1.81	7	9
3:A:157:GLN:HG3	3:A:158:PRO:HD2	0.76	1.55	17	5
3:A:47:ILE:CD1	3:A:117:VAL:HG13	0.76	2.11	11	15
3:A:93:SER:C	3:A:106:ILE:HG21	0.76	2.01	13	1
3:A:126:LEU:N	3:A:126:LEU:HD13	0.76	1.96	6	4
3:A:15:LEU:HD23	3:A:167:VAL:CG2	0.75	2.10	9	8
3:A:15:LEU:HD12	3:A:50:LEU:HB2	0.75	1.55	12	7
3:A:47:ILE:HD13	3:A:117:VAL:HG22	0.75	1.57	4	2
3:A:27:ALA:HA	3:A:123:ILE:HG23	0.75	1.57	13	11
3:A:17:ILE:CG1	3:A:48:VAL:HG22	0.75	2.12	11	5
3:A:79:TYR:CD1	3:A:126:LEU:HD21	0.74	2.17	18	2
3:A:80:GLN:HB2	3:A:97:ILE:HD12	0.74	1.58	6	2
3:A:123:ILE:HD11	3:A:172:ILE:HG21	0.74	1.58	9	4
3:A:79:TYR:HA	3:A:126:LEU:HD21	0.74	1.56	3	2
3:A:126:LEU:HB2	3:A:145:THR:HG22	0.74	1.58	7	1
3:A:59:LEU:HD22	3:A:108:LEU:HD13	0.73	1.59	7	1
3:A:126:LEU:CB	3:A:145:THR:HG22	0.73	2.14	7	1
3:A:67:THR:HG22	3:A:147:VAL:HG12	0.73	1.58	13	1
3:A:124:LEU:HD23	3:A:125:LYS:N	0.73	1.97	9	2
3:A:17:ILE:HG12	3:A:48:VAL:HG22	0.72	1.60	13	3
3:A:59:LEU:HD23	3:A:108:LEU:CG	0.72	2.13	4	2
3:A:25:HIS:CD2	3:A:172:ILE:HG23	0.72	2.19	14	2
3:A:61:LEU:CD1	3:A:153:VAL:HG22	0.72	2.10	11	12
2:C:346:DT:H71	3:A:29:TYR:CE1	0.72	2.19	3	11
3:A:79:TYR:CD1	3:A:126:LEU:HD23	0.72	2.20	5	1
1:B:323:DA:H2''	1:B:324:DT:O5'	0.72	1.84	9	18
3:A:74:ARG:HD2	3:A:138:THR:HG21	0.72	1.59	8	1
3:A:157:GLN:HG3	3:A:158:PRO:CD	0.71	2.15	17	1
3:A:131:ILE:HG21	3:A:140:ILE:HG21	0.71	1.62	9	1
3:A:131:ILE:HG21	3:A:140:ILE:HG23	0.71	1.59	8	1
3:A:47:ILE:HG12	3:A:117:VAL:HG13	0.71	1.60	4	3
3:A:79:TYR:CD2	3:A:126:LEU:HD23	0.71	2.20	3	2
3:A:53:TYR:CE1	3:A:155:VAL:CG2	0.71	2.74	17	9
3:A:38:VAL:HG12	3:A:38:VAL:O	0.71	1.86	9	2
3:A:81:VAL:HG21	3:A:124:LEU:HB2	0.71	1.62	10	7

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:A:84:ILE:HD12	3:A:85:THR:N	0.71	2.00	1	1
3:A:94:HIS:CB	3:A:106:ILE:HG23	0.71	2.15	4	1
3:A:30:GLU:HB2	3:A:124:LEU:HD13	0.70	1.60	7	1
3:A:98:LEU:HD23	3:A:99:SER:N	0.70	2.02	11	17
3:A:140:ILE:HG23	3:A:141:GLY:N	0.70	2.02	15	4
3:A:63:LEU:HD21	3:A:151:PHE:CD1	0.70	2.22	2	1
3:A:59:LEU:HD23	3:A:108:LEU:HD12	0.69	1.64	11	1
3:A:108:LEU:HD23	3:A:108:LEU:N	0.69	2.02	11	2
3:A:157:GLN:CG	3:A:158:PRO:CD	0.69	2.69	10	2
3:A:34:SER:CB	3:A:81:VAL:HG21	0.69	2.17	9	1
3:A:27:ALA:HB2	3:A:123:ILE:HG13	0.69	1.64	9	5
3:A:80:GLN:O	3:A:81:VAL:HG23	0.69	1.88	15	7
3:A:63:LEU:HD23	3:A:151:PHE:CD2	0.69	2.23	13	14
3:A:53:TYR:CE1	3:A:155:VAL:HG21	0.69	2.23	17	10
3:A:78:PHE:CZ	3:A:131:ILE:HD12	0.69	2.23	15	9
3:A:79:TYR:CE1	3:A:126:LEU:HD13	0.68	2.23	7	2
3:A:27:ALA:HB2	3:A:123:ILE:HG12	0.68	1.65	6	7
3:A:94:HIS:HB2	3:A:104:LEU:HD22	0.68	1.65	7	1
3:A:131:ILE:HA	3:A:134:ARG:HG2	0.68	1.64	2	2
3:A:64:PHE:HA	3:A:103:VAL:HG12	0.68	1.65	18	7
3:A:169:SER:C	3:A:171:PRO:HD3	0.68	2.08	7	1
1:B:316:DG:H2''	1:B:317:DA:O5'	0.68	1.88	8	11
3:A:25:HIS:HB3	3:A:172:ILE:HG23	0.67	1.63	12	5
3:A:38:VAL:HG11	3:A:85:THR:OG1	0.67	1.88	18	1
3:A:123:ILE:HD11	3:A:172:ILE:CG2	0.67	2.20	13	2
3:A:63:LEU:HD22	3:A:64:PHE:H	0.67	1.50	13	1
3:A:27:ALA:HB1	3:A:124:LEU:C	0.67	2.10	6	5
3:A:59:LEU:HD12	3:A:155:VAL:HB	0.67	1.68	9	2
3:A:84:ILE:HG21	3:A:120:CYS:C	0.67	2.10	4	2
3:A:57:GLU:HG2	3:A:58:PRO:HD2	0.66	1.66	10	5
3:A:59:LEU:HD11	3:A:153:VAL:CG1	0.66	2.21	5	11
3:A:63:LEU:C	3:A:63:LEU:HD13	0.66	2.10	13	4
3:A:59:LEU:HD23	3:A:108:LEU:HG	0.66	1.68	4	7
3:A:46:PRO:O	3:A:47:ILE:HD13	0.66	1.90	17	12
3:A:126:LEU:HB2	3:A:140:ILE:HG21	0.66	1.68	1	1
3:A:59:LEU:HD23	3:A:108:LEU:CD1	0.66	2.21	11	2
3:A:27:ALA:CB	3:A:123:ILE:HG23	0.66	2.20	16	6
3:A:65:ILE:CG2	3:A:76:HIS:CD2	0.66	2.79	4	9
3:A:63:LEU:HD22	3:A:64:PHE:N	0.66	2.05	13	1
3:A:81:VAL:HG23	3:A:124:LEU:HB2	0.66	1.66	9	2
3:A:125:LYS:C	3:A:126:LEU:HD22	0.66	2.10	7	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:325:DT:H2''	1:B:326:DG:O5'	0.66	1.89	14	16
3:A:37:ALA:HB1	3:A:123:ILE:N	0.66	2.05	6	2
3:A:15:LEU:CD1	3:A:50:LEU:HD12	0.65	2.21	11	7
3:A:164:SER:O	3:A:165:LEU:HD22	0.65	1.91	4	2
3:A:53:TYR:CD1	3:A:155:VAL:HG21	0.65	2.25	17	1
3:A:124:LEU:HD23	3:A:125:LYS:O	0.65	1.91	12	2
3:A:38:VAL:HG13	3:A:38:VAL:O	0.65	1.90	14	3
3:A:155:VAL:HG23	3:A:156:PRO:HD2	0.65	1.67	17	2
3:A:109:LEU:HD12	3:A:110:PRO:HD2	0.65	1.67	13	2
3:A:63:LEU:HD12	3:A:64:PHE:N	0.65	2.07	4	1
3:A:25:HIS:NE2	3:A:37:ALA:HB1	0.65	2.06	7	1
2:C:344:DT:O3'	3:A:128:ASN:HB2	0.64	1.91	1	3
3:A:84:ILE:HD13	3:A:85:THR:N	0.64	2.08	12	8
3:A:17:ILE:HD11	3:A:151:PHE:CE1	0.64	2.27	9	1
3:A:25:HIS:CD2	3:A:37:ALA:HB1	0.64	2.27	7	2
3:A:96:ALA:HB3	3:A:103:VAL:CG2	0.64	2.22	8	1
3:A:78:PHE:HE2	3:A:131:ILE:HD12	0.64	1.52	16	2
3:A:15:LEU:HD12	3:A:50:LEU:HD12	0.64	1.69	11	4
3:A:89:VAL:O	3:A:92:THR:HG22	0.64	1.93	2	1
3:A:63:LEU:HD12	3:A:104:LEU:CD1	0.64	2.22	5	3
3:A:29:TYR:CE2	3:A:127:ARG:HB3	0.64	2.27	13	1
3:A:123:ILE:HD12	3:A:172:ILE:HD13	0.64	1.70	6	1
3:A:155:VAL:CG1	3:A:163:LEU:HB3	0.64	2.22	2	14
3:A:65:ILE:HD13	3:A:148:ARG:O	0.64	1.92	8	10
3:A:76:HIS:NE2	3:A:79:TYR:HB2	0.64	2.08	6	13
3:A:96:ALA:CB	3:A:103:VAL:HG23	0.64	2.18	4	2
3:A:126:LEU:HG	3:A:145:THR:HA	0.63	1.69	7	1
3:A:50:LEU:HD22	3:A:51:HIS:N	0.63	2.09	12	2
3:A:130:ASP:O	3:A:134:ARG:HG3	0.63	1.93	4	1
3:A:17:ILE:CD1	3:A:167:VAL:HG11	0.63	2.24	17	1
3:A:32:GLU:O	3:A:32:GLU:HG2	0.63	1.93	6	2
1:B:320:DA:H2''	1:B:321:DA:O5'	0.63	1.93	12	17
3:A:157:GLN:CG	3:A:163:LEU:HD23	0.63	2.24	17	1
3:A:59:LEU:HG	3:A:108:LEU:HD13	0.63	1.70	1	2
3:A:157:GLN:CG	3:A:158:PRO:HD2	0.63	2.24	10	2
3:A:59:LEU:HB3	3:A:108:LEU:HB2	0.62	1.69	7	10
3:A:131:ILE:HD13	3:A:131:ILE:N	0.62	2.09	17	2
3:A:88:THR:HG22	3:A:88:THR:O	0.62	1.93	4	2
3:A:63:LEU:HD13	3:A:64:PHE:H	0.62	1.52	2	1
3:A:63:LEU:HD12	3:A:104:LEU:HG	0.62	1.71	13	1
3:A:109:LEU:CD1	3:A:110:PRO:HD2	0.62	2.23	10	4

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:A:79:TYR:CE1	3:A:126:LEU:CD2	0.62	2.83	12	4
3:A:170:ASN:N	3:A:171:PRO:HD3	0.62	2.08	7	1
3:A:126:LEU:HD13	3:A:126:LEU:N	0.62	2.08	8	7
3:A:137:GLU:HG2	3:A:138:THR:N	0.62	2.08	11	1
3:A:74:ARG:HB2	3:A:75:PRO:HD2	0.62	1.72	13	2
3:A:131:ILE:N	3:A:131:ILE:HD13	0.62	2.09	14	4
3:A:92:THR:HG22	3:A:106:ILE:HG22	0.62	1.70	11	1
3:A:50:LEU:HD12	3:A:153:VAL:HG21	0.62	1.70	15	3
3:A:84:ILE:HG21	3:A:120:CYS:CA	0.62	2.25	12	3
3:A:123:ILE:HD11	3:A:172:ILE:HD13	0.62	1.70	2	3
3:A:61:LEU:CG	3:A:106:ILE:HD11	0.62	2.25	2	1
3:A:127:ARG:CD	3:A:130:ASP:HB2	0.62	2.25	13	1
3:A:47:ILE:CG2	3:A:117:VAL:HG22	0.62	2.21	14	6
3:A:128:ASN:HA	3:A:140:ILE:HG21	0.62	1.71	6	1
2:C:348:DC:H2''	2:C:349:DT:O5'	0.62	1.94	14	18
3:A:59:LEU:HD22	3:A:108:LEU:CD1	0.62	2.25	3	4
2:C:344:DT:H2'	2:C:345:DT:H71	0.61	1.70	11	10
3:A:37:ALA:HB3	3:A:123:ILE:HG22	0.61	1.71	18	1
1:B:318:DG:H2''	1:B:319:DG:O5'	0.61	1.94	14	12
3:A:15:LEU:HD23	3:A:167:VAL:HG23	0.61	1.71	13	5
3:A:109:LEU:HD13	3:A:110:PRO:HD2	0.61	1.71	5	2
3:A:37:ALA:HB3	3:A:123:ILE:CG2	0.61	2.25	18	1
3:A:74:ARG:HB3	3:A:75:PRO:HD2	0.61	1.73	8	13
3:A:65:ILE:CG1	3:A:149:LEU:HD23	0.61	2.26	13	2
3:A:65:ILE:HG21	3:A:76:HIS:CG	0.61	2.31	2	6
2:C:346:DT:OP2	3:A:29:TYR:CE2	0.60	2.54	3	3
2:C:343:DT:H2''	2:C:344:DT:O5'	0.60	1.95	9	5
3:A:76:HIS:NE2	3:A:79:TYR:N	0.60	2.47	12	2
3:A:27:ALA:CA	3:A:123:ILE:HG23	0.60	2.26	13	7
2:C:345:DT:OP1	3:A:128:ASN:N	0.60	2.35	12	15
3:A:106:ILE:N	3:A:106:ILE:HD13	0.60	2.11	13	1
3:A:98:LEU:HD22	3:A:101:THR:HB	0.60	1.71	7	10
3:A:78:PHE:CE1	3:A:131:ILE:HG23	0.60	2.31	11	3
3:A:78:PHE:CD2	3:A:126:LEU:HG	0.60	2.31	9	2
2:C:342:DA:H2''	2:C:343:DT:O5'	0.60	1.96	9	16
3:A:63:LEU:HD21	3:A:151:PHE:CE1	0.60	2.32	2	2
3:A:65:ILE:CG2	3:A:76:HIS:CG	0.60	2.84	17	11
1:B:317:DA:H2''	1:B:318:DG:O5'	0.60	1.93	17	5
3:A:98:LEU:HB3	3:A:101:THR:HB	0.60	1.73	2	13
3:A:126:LEU:HD23	3:A:140:ILE:CD1	0.60	2.27	10	1
3:A:126:LEU:CB	3:A:140:ILE:HD13	0.60	2.27	10	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:A:17:ILE:HG21	3:A:20:GLN:HB3	0.59	1.74	11	1
3:A:59:LEU:CG	3:A:108:LEU:HD13	0.59	2.27	17	2
2:C:343:DT:H1'	2:C:344:DT:O4'	0.59	1.97	9	1
2:C:346:DT:H72	3:A:29:TYR:CE1	0.59	2.32	4	5
3:A:78:PHE:CZ	3:A:131:ILE:HG23	0.59	2.31	6	7
3:A:88:THR:O	3:A:88:THR:HG23	0.59	1.96	1	6
3:A:25:HIS:HB2	3:A:172:ILE:HG23	0.59	1.72	1	2
3:A:59:LEU:HD12	3:A:60:MET:H	0.59	1.56	11	1
2:C:346:DT:H1'	2:C:347:DC:C6	0.59	2.33	7	4
3:A:137:GLU:O	3:A:138:THR:HG22	0.59	1.97	11	1
3:A:38:VAL:O	3:A:38:VAL:HG13	0.59	1.97	3	2
3:A:79:TYR:CE2	3:A:126:LEU:CD2	0.59	2.85	17	7
3:A:17:ILE:HD11	3:A:151:PHE:CD2	0.59	2.33	17	1
3:A:25:HIS:ND1	3:A:172:ILE:HG23	0.59	2.13	7	1
1:B:323:DA:C2	1:B:324:DT:C2	0.58	2.91	7	15
3:A:123:ILE:HD13	3:A:124:LEU:N	0.58	2.13	16	1
3:A:109:LEU:HD13	3:A:110:PRO:CD	0.58	2.28	14	2
3:A:73:LEU:HD12	3:A:74:ARG:O	0.58	1.97	10	2
3:A:157:GLN:HG3	3:A:158:PRO:HD3	0.58	1.73	10	1
2:C:346:DT:C7	3:A:29:TYR:CE1	0.58	2.87	2	14
3:A:63:LEU:HD22	3:A:151:PHE:CD2	0.58	2.33	4	1
3:A:65:ILE:HD11	3:A:149:LEU:HD23	0.58	1.75	17	3
3:A:85:THR:O	3:A:85:THR:HG23	0.58	1.98	9	5
3:A:53:TYR:CE2	3:A:155:VAL:CG2	0.58	2.86	2	1
3:A:78:PHE:CE1	3:A:131:ILE:HG21	0.58	2.34	7	3
3:A:37:ALA:CB	3:A:123:ILE:HB	0.58	2.29	4	3
1:B:321:DA:H2''	1:B:322:DA:O5'	0.58	1.99	2	16
3:A:164:SER:C	3:A:165:LEU:HD12	0.58	2.19	6	1
3:A:94:HIS:HB2	3:A:104:LEU:HD13	0.58	1.76	13	1
3:A:157:GLN:CB	3:A:158:PRO:CD	0.58	2.81	10	2
3:A:17:ILE:HD11	3:A:151:PHE:CE2	0.58	2.33	10	1
3:A:89:VAL:HG11	3:A:120:CYS:HB2	0.58	1.74	10	1
3:A:15:LEU:HD11	3:A:61:LEU:HD22	0.58	1.75	14	1
3:A:149:LEU:HD12	3:A:169:SER:CB	0.58	2.29	5	5
3:A:73:LEU:C	3:A:73:LEU:HD12	0.58	2.19	3	4
3:A:134:ARG:O	3:A:135:LYS:HG3	0.58	1.99	1	1
3:A:25:HIS:CB	3:A:172:ILE:HG23	0.58	2.28	8	3
3:A:89:VAL:HG21	3:A:119:ASP:CB	0.58	2.27	12	2
2:C:341:DA:H2''	2:C:342:DA:O5'	0.58	1.99	13	15
3:A:164:SER:C	3:A:165:LEU:HD22	0.58	2.19	4	3
3:A:17:ILE:HG21	3:A:20:GLN:HG3	0.58	1.76	17	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:A:21:PRO:HA	3:A:40:ALA:HB2	0.58	1.75	3	2
3:A:94:HIS:CG	3:A:106:ILE:HG23	0.58	2.34	4	1
3:A:81:VAL:HG13	3:A:122:GLY:N	0.58	2.14	4	1
3:A:25:HIS:CE1	3:A:172:ILE:CG2	0.57	2.86	3	2
3:A:29:TYR:CE1	3:A:127:ARG:HD2	0.57	2.35	7	1
3:A:84:ILE:HG23	3:A:84:ILE:O	0.57	1.99	18	5
3:A:29:TYR:HB2	3:A:32:GLU:HG2	0.57	1.77	15	5
3:A:126:LEU:CB	3:A:140:ILE:HG21	0.57	2.29	1	1
3:A:18:GLU:HB2	3:A:47:ILE:HB	0.57	1.75	13	3
3:A:92:THR:HG23	3:A:93:SER:N	0.57	2.14	9	1
3:A:79:TYR:CD1	3:A:124:LEU:O	0.57	2.58	17	6
3:A:84:ILE:C	3:A:84:ILE:HD13	0.57	2.20	3	3
3:A:147:VAL:CG2	3:A:172:ILE:HB	0.57	2.30	14	6
3:A:126:LEU:H	3:A:126:LEU:HD22	0.57	1.59	13	6
3:A:125:LYS:HG3	3:A:174:CYS:SG	0.57	2.40	2	2
3:A:50:LEU:HD22	3:A:50:LEU:C	0.57	2.20	12	1
3:A:51:HIS:CG	3:A:51:HIS:O	0.57	2.57	7	1
3:A:149:LEU:HD12	3:A:169:SER:HB3	0.57	1.76	4	3
3:A:53:TYR:CE1	3:A:155:VAL:HG22	0.56	2.35	16	5
3:A:13:TYR:CD1	3:A:52:GLY:HA2	0.56	2.35	13	3
3:A:147:VAL:HG22	3:A:172:ILE:HB	0.56	1.78	7	6
3:A:57:GLU:HG3	3:A:58:PRO:HD2	0.56	1.77	7	2
3:A:65:ILE:HG21	3:A:76:HIS:CD2	0.56	2.36	11	7
3:A:127:ARG:HG2	3:A:130:ASP:HB2	0.56	1.77	18	2
3:A:50:LEU:HD23	3:A:50:LEU:C	0.56	2.20	17	8
3:A:59:LEU:HD23	3:A:108:LEU:HD11	0.56	1.78	4	1
2:C:345:DT:H5"	3:A:129:SER:OG	0.56	2.01	4	1
3:A:79:TYR:HA	3:A:124:LEU:HB3	0.56	1.77	7	1
3:A:17:ILE:HD11	3:A:151:PHE:HD2	0.56	1.61	17	1
3:A:103:VAL:C	3:A:104:LEU:HD12	0.56	2.20	11	2
3:A:61:LEU:HG	3:A:106:ILE:HD11	0.56	1.76	2	1
3:A:94:HIS:HA	3:A:106:ILE:HD12	0.56	1.77	13	1
3:A:17:ILE:HD12	3:A:167:VAL:HG11	0.56	1.76	11	2
3:A:149:LEU:HB2	3:A:169:SER:CB	0.56	2.30	14	4
3:A:126:LEU:N	3:A:126:LEU:HD22	0.56	2.16	5	4
3:A:17:ILE:HD11	3:A:151:PHE:CD1	0.56	2.36	13	1
3:A:140:ILE:HG23	3:A:141:GLY:H	0.56	1.61	17	4
3:A:15:LEU:HD22	3:A:153:VAL:HG23	0.56	1.78	4	6
3:A:73:LEU:HD12	3:A:73:LEU:C	0.56	2.22	2	5
3:A:157:GLN:CB	3:A:158:PRO:HD2	0.56	2.31	10	1
3:A:67:THR:HG23	3:A:76:HIS:HA	0.55	1.78	5	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:A:74:ARG:CB	3:A:75:PRO:HD2	0.55	2.31	13	12
3:A:109:LEU:HD12	3:A:110:PRO:CD	0.55	2.30	13	2
3:A:63:LEU:CD2	3:A:151:PHE:CD1	0.55	2.89	2	2
2:C:344:DT:H4'	3:A:142:ARG:HD2	0.55	1.77	9	1
3:A:50:LEU:C	3:A:50:LEU:HD22	0.55	2.20	8	1
3:A:46:PRO:HD2	3:A:118:ILE:HB	0.55	1.76	14	1
3:A:78:PHE:N	3:A:78:PHE:CD1	0.55	2.75	15	6
3:A:37:ALA:C	3:A:123:ILE:HG22	0.55	2.22	6	1
3:A:37:ALA:HB1	3:A:122:GLY:CA	0.55	2.31	6	1
3:A:153:VAL:O	3:A:164:SER:HA	0.55	2.02	17	1
3:A:23:SER:HA	3:A:170:ASN:HB2	0.55	1.78	17	1
3:A:147:VAL:HG22	3:A:172:ILE:CB	0.55	2.31	7	1
1:B:319:DG:H2''	1:B:320:DA:O5'	0.55	2.01	17	18
3:A:21:PRO:HD3	3:A:46:PRO:HB3	0.55	1.78	11	3
3:A:126:LEU:HD22	3:A:126:LEU:H	0.55	1.62	15	5
3:A:148:ARG:HB2	3:A:170:ASN:HB3	0.55	1.79	7	1
3:A:109:LEU:CD1	3:A:110:PRO:CD	0.55	2.85	16	3
3:A:124:LEU:HG	3:A:125:LYS:N	0.55	2.17	7	3
3:A:94:HIS:HB2	3:A:104:LEU:CD2	0.55	2.31	7	1
3:A:28:ARG:HG3	3:A:35:ARG:HB3	0.55	1.77	7	1
3:A:61:LEU:HD12	3:A:62:GLN:H	0.55	1.61	7	11
1:B:315:DC:H2''	1:B:316:DG:O5'	0.55	2.01	18	10
3:A:78:PHE:CD1	3:A:78:PHE:N	0.55	2.75	8	8
3:A:47:ILE:HG23	3:A:117:VAL:HA	0.55	1.77	10	2
3:A:170:ASN:N	3:A:171:PRO:CD	0.55	2.70	7	1
3:A:13:TYR:CD2	3:A:163:LEU:HD23	0.55	2.37	15	2
3:A:94:HIS:O	3:A:104:LEU:HD23	0.55	2.01	10	2
3:A:37:ALA:CB	3:A:123:ILE:CG2	0.54	2.85	7	3
3:A:59:LEU:CB	3:A:108:LEU:HD12	0.54	2.32	6	2
3:A:174:CYS:O	3:A:175:SER:C	0.54	2.45	17	1
3:A:78:PHE:CD1	3:A:131:ILE:HD13	0.54	2.38	2	1
3:A:108:LEU:N	3:A:108:LEU:HD22	0.54	2.16	13	2
3:A:131:ILE:CA	3:A:134:ARG:HG2	0.54	2.32	2	1
3:A:15:LEU:HD12	3:A:50:LEU:HG	0.54	1.78	3	1
3:A:50:LEU:C	3:A:50:LEU:HD23	0.54	2.22	11	5
3:A:61:LEU:HD12	3:A:152:ARG:O	0.54	2.02	2	6
3:A:81:VAL:HG21	3:A:124:LEU:CB	0.54	2.31	10	1
3:A:107:PRO:C	3:A:108:LEU:HD22	0.54	2.23	5	3
1:B:324:DT:H2'	1:B:325:DT:H72	0.54	1.79	13	8
3:A:59:LEU:HG	3:A:60:MET:N	0.54	2.18	4	5
3:A:76:HIS:CE1	3:A:79:TYR:HB2	0.54	2.38	1	4

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:A:63:LEU:HD11	3:A:149:LEU:HD23	0.54	1.79	16	1
3:A:108:LEU:CD2	3:A:108:LEU:N	0.54	2.71	15	3
3:A:37:ALA:CB	3:A:123:ILE:N	0.54	2.70	14	1
3:A:45:HIS:CE1	3:A:121:ALA:HB3	0.54	2.37	6	1
3:A:93:SER:HB2	3:A:106:ILE:HG22	0.54	1.76	14	4
1:B:322:DA:H2''	1:B:323:DA:O5'	0.54	2.03	14	9
3:A:81:VAL:HG22	3:A:122:GLY:O	0.54	2.03	2	2
3:A:27:ALA:HB1	3:A:125:LYS:N	0.54	2.18	1	3
2:C:344:DT:C5'	3:A:142:ARG:O	0.54	2.52	14	2
3:A:63:LEU:CB	3:A:104:LEU:HB2	0.54	2.33	10	5
2:C:347:DC:H2''	2:C:348:DC:O5'	0.53	2.01	14	17
3:A:39:LYS:O	3:A:40:ALA:HB2	0.53	2.04	10	3
3:A:77:ALA:HB2	3:A:140:ILE:CD1	0.53	2.33	5	4
3:A:125:LYS:C	3:A:126:LEU:HD13	0.53	2.24	2	2
3:A:79:TYR:CE1	3:A:124:LEU:O	0.53	2.61	12	7
3:A:47:ILE:HD13	3:A:117:VAL:HG13	0.53	1.81	11	3
3:A:146:ARG:HG2	3:A:173:GLU:HG2	0.53	1.81	8	1
3:A:131:ILE:HG23	3:A:138:THR:HG22	0.53	1.79	14	1
3:A:155:VAL:O	3:A:163:LEU:N	0.53	2.41	17	1
3:A:81:VAL:HG22	3:A:124:LEU:HD12	0.53	1.80	9	1
3:A:63:LEU:HD12	3:A:104:LEU:HD23	0.53	1.80	3	1
3:A:37:ALA:HA	3:A:122:GLY:HA2	0.53	1.79	1	2
3:A:27:ALA:CB	3:A:123:ILE:HD12	0.53	2.28	4	1
3:A:163:LEU:HD13	3:A:163:LEU:C	0.53	2.24	11	3
3:A:63:LEU:CB	3:A:104:LEU:HD12	0.53	2.33	10	1
3:A:135:LYS:N	3:A:135:LYS:HD3	0.53	2.18	10	1
3:A:27:ALA:HA	3:A:123:ILE:CG2	0.53	2.34	12	4
3:A:79:TYR:CD2	3:A:126:LEU:CD2	0.53	2.91	9	3
3:A:50:LEU:HD12	3:A:153:VAL:HG11	0.53	1.79	4	1
3:A:19:VAL:HB	3:A:47:ILE:HG12	0.53	1.80	15	12
3:A:108:LEU:N	3:A:108:LEU:CD2	0.53	2.71	16	3
3:A:59:LEU:HD11	3:A:153:VAL:HG11	0.53	1.79	10	1
3:A:61:LEU:HD12	3:A:62:GLN:N	0.53	2.18	9	13
3:A:124:LEU:C	3:A:124:LEU:HD23	0.53	2.23	9	2
3:A:78:PHE:CE1	3:A:131:ILE:CG2	0.53	2.92	10	7
3:A:21:PRO:HA	3:A:40:ALA:CB	0.53	2.34	5	4
3:A:134:ARG:NH1	3:A:136:GLY:HA3	0.53	2.19	16	1
3:A:65:ILE:HD13	3:A:76:HIS:CD2	0.53	2.39	16	1
3:A:37:ALA:HA	3:A:122:GLY:CA	0.53	2.34	1	1
3:A:96:ALA:O	3:A:103:VAL:CG2	0.53	2.57	7	2
3:A:15:LEU:HD13	3:A:50:LEU:HD12	0.52	1.80	7	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:A:157:GLN:CG	3:A:158:PRO:HD3	0.52	2.34	10	1
2:C:350:DC:H2''	2:C:351:DG:O5'	0.52	2.04	11	14
3:A:15:LEU:CB	3:A:165:LEU:HD22	0.52	2.33	6	1
3:A:149:LEU:O	3:A:168:ALA:HA	0.52	2.04	7	6
3:A:169:SER:C	3:A:171:PRO:CD	0.52	2.77	7	1
3:A:137:GLU:O	3:A:138:THR:HG23	0.52	2.03	15	1
3:A:131:ILE:HA	3:A:134:ARG:CG	0.52	2.35	9	1
3:A:109:LEU:HD13	3:A:110:PRO:HD3	0.52	1.80	14	1
3:A:88:THR:HG23	3:A:88:THR:O	0.52	2.05	5	5
3:A:126:LEU:N	3:A:126:LEU:CD1	0.52	2.70	6	3
3:A:11:GLY:N	3:A:12:PRO:CD	0.52	2.73	7	6
3:A:79:TYR:CD2	3:A:123:ILE:HD11	0.52	2.39	18	1
3:A:65:ILE:HG21	3:A:76:HIS:CE1	0.52	2.40	17	3
3:A:61:LEU:CB	3:A:108:LEU:HD11	0.52	2.35	17	2
3:A:105:GLU:C	3:A:106:ILE:HD13	0.52	2.25	13	1
3:A:18:GLU:HB3	3:A:47:ILE:HB	0.52	1.82	10	3
3:A:61:LEU:CD2	3:A:106:ILE:HD11	0.52	2.33	2	2
3:A:67:THR:CG2	3:A:76:HIS:HA	0.52	2.34	9	1
3:A:25:HIS:CE1	3:A:27:ALA:HB2	0.52	2.40	7	1
2:C:341:DA:C6	2:C:342:DA:C6	0.52	2.98	16	3
3:A:84:ILE:C	3:A:84:ILE:HD12	0.52	2.25	1	1
3:A:78:PHE:CE1	3:A:131:ILE:HG13	0.52	2.39	7	2
3:A:15:LEU:HD23	3:A:167:VAL:HG21	0.52	1.79	9	1
3:A:38:VAL:CG1	3:A:38:VAL:O	0.52	2.58	14	3
3:A:77:ALA:HB3	3:A:79:TYR:CZ	0.52	2.40	7	1
2:C:345:DT:C5	2:C:346:DT:H73	0.52	2.39	14	1
3:A:53:TYR:CZ	3:A:155:VAL:CG2	0.52	2.93	18	3
3:A:125:LYS:O	3:A:126:LEU:HD22	0.52	2.04	7	1
3:A:47:ILE:HG23	3:A:117:VAL:CG2	0.52	2.23	14	3
3:A:87:LYS:O	3:A:88:THR:HB	0.52	2.05	3	7
2:C:346:DT:OP2	3:A:29:TYR:CD2	0.52	2.63	6	9
3:A:27:ALA:CB	3:A:123:ILE:CG1	0.52	2.88	12	2
3:A:134:ARG:CZ	3:A:136:GLY:HA3	0.52	2.35	16	1
3:A:151:PHE:CD1	3:A:151:PHE:N	0.51	2.78	10	2
3:A:104:LEU:N	3:A:104:LEU:HD22	0.51	2.20	3	1
3:A:124:LEU:HD21	3:A:126:LEU:HD13	0.51	1.83	3	2
3:A:57:GLU:CG	3:A:58:PRO:HD2	0.51	2.34	5	9
3:A:93:SER:OG	3:A:106:ILE:HG22	0.51	2.05	9	1
3:A:79:TYR:CD2	3:A:147:VAL:CG2	0.51	2.93	4	2
3:A:163:LEU:CD1	3:A:165:LEU:CD1	0.51	2.88	6	1
3:A:37:ALA:HB1	3:A:123:ILE:H	0.51	1.62	6	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:A:84:ILE:HD13	3:A:84:ILE:C	0.51	2.26	13	5
3:A:78:PHE:CZ	3:A:131:ILE:CG2	0.51	2.94	7	2
2:C:346:DT:O2	2:C:347:DC:C2	0.51	2.63	4	2
3:A:64:PHE:C	3:A:64:PHE:CD1	0.51	2.83	10	1
3:A:29:TYR:CE1	3:A:127:ARG:CD	0.51	2.93	7	1
3:A:124:LEU:HD23	3:A:124:LEU:C	0.51	2.25	15	3
3:A:163:LEU:C	3:A:163:LEU:HD13	0.51	2.26	15	6
3:A:76:HIS:CE1	3:A:102:LYS:HB2	0.51	2.41	7	3
3:A:15:LEU:N	3:A:165:LEU:HD22	0.51	2.20	11	1
3:A:65:ILE:HG23	3:A:66:GLY:N	0.51	2.20	2	1
3:A:53:TYR:CE2	3:A:55:GLU:HB3	0.51	2.41	13	7
3:A:89:VAL:HG21	3:A:119:ASP:OD2	0.51	2.06	11	1
2:C:346:DT:H2''	2:C:347:DC:OP2	0.51	2.05	6	1
3:A:11:GLY:N	3:A:12:PRO:HD2	0.51	2.21	7	6
3:A:28:ARG:CG	3:A:35:ARG:HB2	0.51	2.36	16	2
3:A:139:ASP:O	3:A:141:GLY:N	0.51	2.44	1	2
2:C:344:DT:C2'	2:C:345:DT:O5'	0.51	2.48	17	1
3:A:92:THR:HG21	3:A:107:PRO:O	0.51	2.05	5	1
2:C:344:DT:H2'	2:C:345:DT:C7	0.51	2.36	11	7
3:A:77:ALA:C	3:A:78:PHE:CD1	0.51	2.84	4	5
3:A:149:LEU:HB2	3:A:169:SER:HB3	0.51	1.82	16	5
3:A:93:SER:HB3	3:A:106:ILE:HG22	0.51	1.81	2	2
3:A:81:VAL:HG12	3:A:82:HIS:N	0.51	2.21	9	1
3:A:29:TYR:CE2	3:A:125:LYS:HD3	0.51	2.41	7	1
3:A:79:TYR:CG	3:A:147:VAL:HG21	0.50	2.42	5	1
3:A:149:LEU:HD12	3:A:169:SER:HB2	0.50	1.82	12	3
3:A:65:ILE:HG22	3:A:76:HIS:CG	0.50	2.42	5	6
1:B:319:DG:C2	1:B:320:DA:C4	0.50	2.99	11	5
3:A:81:VAL:CG2	3:A:124:LEU:HB2	0.50	2.36	9	3
3:A:15:LEU:CD2	3:A:167:VAL:CG2	0.50	2.89	11	2
3:A:163:LEU:CD1	3:A:165:LEU:HD23	0.50	2.35	16	1
3:A:92:THR:HG21	3:A:120:CYS:CB	0.50	2.36	2	2
3:A:37:ALA:HB1	3:A:123:ILE:HB	0.50	1.82	12	2
3:A:94:HIS:CA	3:A:104:LEU:HB3	0.50	2.36	7	1
3:A:15:LEU:HB3	3:A:165:LEU:HD13	0.50	1.78	5	2
1:B:323:DA:C2	2:C:344:DT:O2	0.50	2.64	10	14
3:A:81:VAL:HG21	3:A:123:ILE:CA	0.50	2.36	13	1
3:A:133:LEU:O	3:A:134:ARG:C	0.50	2.48	5	2
3:A:163:LEU:CD1	3:A:163:LEU:C	0.50	2.79	17	2
3:A:78:PHE:O	3:A:124:LEU:HD22	0.50	2.07	4	2
3:A:82:HIS:CG	3:A:82:HIS:O	0.50	2.64	4	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:A:82:HIS:O	3:A:83:ARG:CB	0.50	2.59	4	1
3:A:108:LEU:N	3:A:108:LEU:HD23	0.50	2.21	4	2
3:A:155:VAL:HG13	3:A:163:LEU:O	0.50	2.06	17	1
3:A:146:ARG:HA	3:A:172:ILE:O	0.50	2.07	7	6
3:A:93:SER:OG	3:A:106:ILE:HG21	0.50	2.07	10	1
3:A:63:LEU:HD23	3:A:151:PHE:CE2	0.50	2.42	9	1
3:A:39:LYS:HA	3:A:45:HIS:CE1	0.50	2.42	14	1
2:C:349:DT:H2''	2:C:350:DC:O5'	0.50	2.06	12	12
1:B:320:DA:C2	1:B:321:DA:C4	0.50	3.00	13	4
3:A:131:ILE:HG21	3:A:140:ILE:HG22	0.50	1.84	11	1
3:A:74:ARG:CB	3:A:75:PRO:CD	0.50	2.89	13	11
3:A:32:GLU:O	3:A:33:GLY:C	0.50	2.51	15	2
3:A:135:LYS:CD	3:A:135:LYS:C	0.50	2.80	6	1
3:A:109:LEU:CB	3:A:110:PRO:HD2	0.50	2.37	9	9
3:A:78:PHE:CE1	3:A:131:ILE:CD1	0.50	2.93	14	7
2:C:344:DT:H4'	3:A:142:ARG:HG2	0.50	1.83	7	3
3:A:34:SER:OG	3:A:81:VAL:HG21	0.49	2.07	9	1
3:A:62:GLN:HG2	3:A:63:LEU:N	0.49	2.21	4	1
3:A:79:TYR:CE1	3:A:123:ILE:HD11	0.49	2.42	4	1
3:A:45:HIS:O	3:A:45:HIS:CG	0.49	2.65	14	1
3:A:85:THR:HG23	3:A:85:THR:O	0.49	2.07	16	3
3:A:79:TYR:CE2	3:A:126:LEU:HD23	0.49	2.42	16	1
3:A:109:LEU:HD23	3:A:110:PRO:HD2	0.49	1.84	11	2
2:C:347:DC:OP2	3:A:32:GLU:HB3	0.49	2.07	9	1
3:A:15:LEU:H	3:A:165:LEU:HD22	0.49	1.66	7	2
2:C:346:DT:H71	3:A:29:TYR:CZ	0.49	2.42	16	6
3:A:63:LEU:HD13	3:A:63:LEU:C	0.49	2.28	10	3
3:A:48:VAL:HG21	3:A:151:PHE:CZ	0.49	2.42	9	1
3:A:29:TYR:HE1	3:A:127:ARG:CD	0.49	2.21	7	1
3:A:45:HIS:CB	3:A:46:PRO:HD2	0.49	2.38	6	1
3:A:140:ILE:CG2	3:A:141:GLY:N	0.49	2.73	15	3
3:A:63:LEU:HB3	3:A:104:LEU:HB2	0.49	1.82	3	2
3:A:15:LEU:HB2	3:A:50:LEU:HD23	0.49	1.83	8	2
3:A:74:ARG:HD2	3:A:75:PRO:HD2	0.49	1.83	9	1
3:A:36:GLY:CA	3:A:122:GLY:HA2	0.49	2.36	7	1
3:A:163:LEU:C	3:A:163:LEU:HD12	0.49	2.28	7	1
3:A:81:VAL:CG1	3:A:82:HIS:N	0.49	2.75	11	6
3:A:85:THR:HG23	3:A:120:CYS:HA	0.49	1.85	18	1
3:A:37:ALA:HB2	3:A:123:ILE:N	0.49	2.22	4	2
3:A:47:ILE:HG22	3:A:48:VAL:N	0.49	2.23	4	2
3:A:147:VAL:HG23	3:A:172:ILE:HB	0.49	1.84	5	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:A:123:ILE:CD1	3:A:172:ILE:HG21	0.49	2.38	6	3
3:A:93:SER:O	3:A:106:ILE:CG2	0.49	2.61	7	1
1:B:326:DG:C2	2:C:341:DA:C2	0.49	3.01	16	6
2:C:346:DT:H2''	2:C:347:DC:O5'	0.49	2.08	2	6
1:B:324:DT:H2''	1:B:325:DT:O5'	0.49	2.08	16	17
3:A:38:VAL:O	3:A:38:VAL:HG12	0.49	2.08	16	2
3:A:157:GLN:HB2	3:A:162:THR:HA	0.49	1.85	15	1
3:A:79:TYR:CD1	3:A:147:VAL:HG11	0.49	2.43	5	2
3:A:39:LYS:HD3	3:A:40:ALA:N	0.49	2.23	16	1
3:A:140:ILE:O	3:A:140:ILE:HG23	0.49	2.07	1	2
3:A:77:ALA:CB	3:A:140:ILE:HD13	0.49	2.37	3	3
3:A:163:LEU:CD1	3:A:165:LEU:HD11	0.49	2.38	6	1
3:A:39:LYS:CD	3:A:39:LYS:C	0.49	2.81	16	1
2:C:348:DC:H2'	2:C:349:DT:H72	0.49	1.85	17	1
3:A:13:TYR:CD1	3:A:13:TYR:N	0.49	2.80	4	3
3:A:134:ARG:O	3:A:135:LYS:C	0.48	2.52	5	1
3:A:127:ARG:HD2	3:A:130:ASP:HB2	0.48	1.85	15	3
2:C:342:DA:C5	2:C:343:DT:C4	0.48	3.01	1	6
3:A:134:ARG:HG3	3:A:134:ARG:O	0.48	2.07	2	1
3:A:123:ILE:CD1	3:A:172:ILE:HD13	0.48	2.38	5	1
1:B:318:DG:N2	2:C:349:DT:C2	0.48	2.80	6	5
3:A:137:GLU:O	3:A:138:THR:CB	0.48	2.60	11	1
3:A:124:LEU:HD21	3:A:126:LEU:CD1	0.48	2.39	3	2
3:A:65:ILE:HG12	3:A:149:LEU:HD23	0.48	1.84	6	3
3:A:127:ARG:HD3	3:A:130:ASP:HB2	0.48	1.84	13	1
3:A:15:LEU:HD12	3:A:50:LEU:CB	0.48	2.39	13	4
1:B:322:DA:C2	2:C:345:DT:O2	0.48	2.67	4	3
3:A:109:LEU:HD23	3:A:112:ASN:ND2	0.48	2.23	2	2
3:A:84:ILE:CG2	3:A:120:CYS:C	0.48	2.82	4	1
3:A:53:TYR:CE2	3:A:155:VAL:HG22	0.48	2.42	2	1
3:A:131:ILE:O	3:A:134:ARG:HG3	0.48	2.09	5	1
1:B:319:DG:C2	1:B:320:DA:N3	0.48	2.82	8	10
3:A:68:ALA:HB3	3:A:146:ARG:HG3	0.48	1.85	17	2
3:A:37:ALA:CB	3:A:122:GLY:HA2	0.48	2.38	15	1
3:A:126:LEU:HD21	3:A:147:VAL:HG13	0.48	1.86	12	1
3:A:50:LEU:CD1	3:A:153:VAL:HG11	0.48	2.39	9	2
3:A:59:LEU:HD12	3:A:60:MET:N	0.48	2.23	11	1
3:A:77:ALA:C	3:A:78:PHE:CG	0.48	2.86	10	12
3:A:63:LEU:HB2	3:A:104:LEU:HB2	0.48	1.86	17	1
3:A:124:LEU:CD2	3:A:126:LEU:CD1	0.48	2.91	17	2
3:A:47:ILE:HG22	3:A:48:VAL:H	0.48	1.69	10	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:A:84:ILE:HD12	3:A:120:CYS:HA	0.48	1.86	12	1
3:A:96:ALA:O	3:A:103:VAL:HG23	0.48	2.07	7	1
3:A:28:ARG:HG3	3:A:35:ARG:CB	0.48	2.37	7	1
3:A:38:VAL:HG13	3:A:45:HIS:CA	0.48	2.34	4	2
3:A:48:VAL:O	3:A:116:ALA:HB3	0.48	2.08	1	2
3:A:140:ILE:O	3:A:144:ASN:HB3	0.48	2.09	16	3
3:A:29:TYR:HB2	3:A:32:GLU:CB	0.48	2.38	5	1
3:A:30:GLU:CB	3:A:124:LEU:HD13	0.48	2.35	7	1
3:A:149:LEU:HB2	3:A:169:SER:HB2	0.48	1.84	3	3
3:A:79:TYR:HD1	3:A:126:LEU:HD21	0.48	1.65	18	1
3:A:13:TYR:HD2	3:A:163:LEU:HD23	0.48	1.68	15	1
3:A:84:ILE:HG21	3:A:121:ALA:CA	0.48	2.38	4	1
3:A:45:HIS:CB	3:A:46:PRO:CD	0.48	2.92	6	1
3:A:89:VAL:HG11	3:A:119:ASP:CB	0.48	2.38	18	1
3:A:65:ILE:CG2	3:A:76:HIS:HB3	0.48	2.38	9	1
3:A:10:SER:HB3	3:A:163:LEU:HD21	0.48	1.85	18	1
3:A:126:LEU:HD22	3:A:126:LEU:N	0.48	2.24	15	3
3:A:138:THR:O	3:A:139:ASP:HB2	0.48	2.09	18	2
3:A:94:HIS:HB2	3:A:104:LEU:HB3	0.48	1.86	3	2
3:A:13:TYR:HA	3:A:52:GLY:CA	0.47	2.39	8	4
3:A:154:HIS:CE1	3:A:162:THR:HG21	0.47	2.44	18	2
3:A:155:VAL:CG1	3:A:163:LEU:HG	0.47	2.39	7	1
3:A:29:TYR:CE1	3:A:125:LYS:HD2	0.47	2.44	11	1
3:A:155:VAL:HG12	3:A:163:LEU:O	0.47	2.08	4	1
3:A:109:LEU:CB	3:A:110:PRO:CD	0.47	2.92	9	9
3:A:155:VAL:HG23	3:A:156:PRO:CD	0.47	2.38	17	1
3:A:64:PHE:CD1	3:A:150:VAL:HB	0.47	2.44	10	1
3:A:27:ALA:HB3	3:A:174:CYS:SG	0.47	2.49	11	1
3:A:94:HIS:O	3:A:104:LEU:HD22	0.47	2.10	13	1
2:C:344:DT:H2'	2:C:345:DT:H72	0.47	1.86	15	4
3:A:59:LEU:HD23	3:A:108:LEU:HD22	0.47	1.85	17	1
3:A:68:ALA:HB1	3:A:171:PRO:HB3	0.47	1.86	12	1
1:B:318:DG:P	3:A:39:LYS:HE2	0.47	2.49	11	1
3:A:95:GLU:HA	3:A:104:LEU:HG	0.47	1.86	2	1
3:A:63:LEU:CD1	3:A:63:LEU:C	0.47	2.83	13	1
3:A:19:VAL:HB	3:A:47:ILE:CG1	0.47	2.39	14	3
3:A:25:HIS:N	3:A:25:HIS:ND1	0.47	2.63	14	1
3:A:89:VAL:HG12	3:A:92:THR:HB	0.47	1.86	14	1
2:C:344:DT:C5'	3:A:142:ARG:HG3	0.47	2.39	2	1
2:C:343:DT:H2''	2:C:344:DT:C6	0.47	2.44	10	9
3:A:109:LEU:HD12	3:A:112:ASN:ND2	0.47	2.25	5	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:A:98:LEU:HD23	3:A:98:LEU:C	0.47	2.29	15	1
3:A:59:LEU:CD2	3:A:153:VAL:HG13	0.47	2.40	4	1
3:A:53:TYR:CE2	3:A:155:VAL:HG21	0.47	2.44	2	1
2:C:344:DT:OP1	3:A:145:THR:HG23	0.47	2.08	5	1
3:A:147:VAL:O	3:A:171:PRO:HA	0.47	2.10	10	3
3:A:93:SER:HB3	3:A:105:GLU:O	0.47	2.10	12	1
3:A:27:ALA:HB1	3:A:124:LEU:CA	0.47	2.39	15	3
3:A:10:SER:HB2	3:A:13:TYR:HB2	0.47	1.85	16	1
3:A:13:TYR:HB3	3:A:52:GLY:HA3	0.47	1.86	2	4
1:B:317:DA:H5"	3:A:39:LYS:CD	0.47	2.40	15	1
3:A:28:ARG:HG3	3:A:35:ARG:HB2	0.47	1.87	2	2
3:A:127:ARG:HG3	3:A:127:ARG:O	0.47	2.10	10	1
3:A:78:PHE:CZ	3:A:131:ILE:HG21	0.47	2.45	7	2
3:A:80:GLN:HE21	3:A:97:ILE:HG21	0.47	1.69	9	1
2:C:346:DT:H71	3:A:29:TYR:HE1	0.47	1.65	3	2
3:A:137:GLU:O	3:A:138:THR:CG2	0.47	2.62	11	1
3:A:80:GLN:NE2	3:A:97:ILE:HG12	0.47	2.24	14	1
3:A:65:ILE:HG13	3:A:149:LEU:HD23	0.47	1.86	2	1
3:A:81:VAL:CG2	3:A:124:LEU:HD13	0.47	2.40	6	1
1:B:319:DG:C6	1:B:320:DA:C6	0.47	3.02	11	1
2:C:342:DA:C2'	2:C:343:DT:C6	0.47	2.98	11	4
3:A:76:HIS:HB3	3:A:101:THR:HA	0.47	1.87	1	1
3:A:77:ALA:HB1	3:A:140:ILE:HG22	0.47	1.87	1	1
3:A:84:ILE:HG21	3:A:122:GLY:N	0.47	2.24	2	1
3:A:138:THR:HG22	3:A:139:ASP:OD1	0.47	2.10	6	1
3:A:125:LYS:HE3	3:A:145:THR:HG21	0.47	1.86	11	1
3:A:142:ARG:HB2	3:A:142:ARG:NH1	0.47	2.25	2	1
3:A:26:ARG:O	3:A:37:ALA:HB2	0.46	2.10	18	1
3:A:130:ASP:O	3:A:134:ARG:HG2	0.46	2.10	15	2
3:A:109:LEU:HB3	3:A:112:ASN:HB2	0.46	1.87	10	1
3:A:77:ALA:HB3	3:A:126:LEU:CD1	0.46	2.39	12	1
3:A:94:HIS:CB	3:A:104:LEU:HB3	0.46	2.40	7	1
3:A:161:ARG:O	3:A:161:ARG:HD2	0.46	2.10	4	1
3:A:61:LEU:HD23	3:A:106:ILE:HD11	0.46	1.86	2	1
3:A:22:LYS:CG	3:A:40:ALA:HA	0.46	2.40	13	1
3:A:78:PHE:CD2	3:A:131:ILE:HD12	0.46	2.45	16	1
3:A:65:ILE:HG23	3:A:76:HIS:HB3	0.46	1.85	9	2
3:A:59:LEU:CD2	3:A:108:LEU:HD13	0.46	2.40	1	3
3:A:59:LEU:CD1	3:A:155:VAL:HB	0.46	2.38	1	1
3:A:79:TYR:CE2	3:A:147:VAL:CG1	0.46	2.93	7	1
3:A:78:PHE:CE1	3:A:131:ILE:HG12	0.46	2.46	4	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:A:66:GLY:HA3	3:A:73:LEU:HD22	0.46	1.87	2	1
3:A:15:LEU:CB	3:A:165:LEU:HG	0.46	2.41	4	3
3:A:65:ILE:HG22	3:A:76:HIS:HB2	0.46	1.87	7	3
3:A:68:ALA:HA	3:A:148:ARG:HB2	0.46	1.87	9	1
2:C:347:DC:N4	3:A:26:ARG:NH2	0.46	2.64	6	2
3:A:45:HIS:CG	3:A:46:PRO:HD2	0.46	2.45	6	1
3:A:15:LEU:CD1	3:A:153:VAL:CG2	0.46	2.86	15	4
3:A:79:TYR:CZ	3:A:124:LEU:O	0.46	2.68	12	1
3:A:139:ASP:O	3:A:140:ILE:C	0.46	2.54	7	1
3:A:148:ARG:HA	3:A:170:ASN:HA	0.46	1.88	7	1
3:A:25:HIS:HD2	3:A:172:ILE:HG23	0.46	1.66	14	1
3:A:79:TYR:CG	3:A:126:LEU:HD11	0.46	2.44	13	1
3:A:124:LEU:HD23	3:A:126:LEU:CD1	0.46	2.40	6	1
3:A:78:PHE:CZ	3:A:134:ARG:NH1	0.46	2.83	16	1
3:A:65:ILE:HD11	3:A:149:LEU:CD2	0.46	2.39	17	1
3:A:27:ALA:CB	3:A:123:ILE:HG13	0.46	2.41	12	2
3:A:68:ALA:HB2	3:A:147:VAL:C	0.46	2.31	4	1
1:B:318:DG:N2	2:C:349:DT:O2	0.46	2.49	7	13
3:A:115:ARG:NE	3:A:117:VAL:HG23	0.46	2.25	13	1
3:A:64:PHE:O	3:A:150:VAL:HB	0.46	2.11	9	5
3:A:93:SER:HB2	3:A:106:ILE:HG12	0.46	1.88	10	1
3:A:77:ALA:HB3	3:A:126:LEU:HD12	0.46	1.88	12	1
3:A:22:LYS:N	3:A:22:LYS:HD2	0.46	2.26	12	1
2:C:341:DA:H2"	2:C:342:DA:C8	0.46	2.46	2	1
3:A:45:HIS:CD2	3:A:45:HIS:N	0.46	2.84	5	2
3:A:134:ARG:O	3:A:135:LYS:CG	0.46	2.64	1	1
3:A:28:ARG:HG3	3:A:35:ARG:N	0.46	2.26	17	1
3:A:73:LEU:HD12	3:A:73:LEU:O	0.46	2.11	7	2
3:A:37:ALA:HA	3:A:123:ILE:HG23	0.46	1.87	6	1
3:A:78:PHE:C	3:A:126:LEU:HD11	0.46	2.31	17	2
3:A:81:VAL:CG2	3:A:124:LEU:CB	0.46	2.94	10	1
3:A:63:LEU:HB3	3:A:104:LEU:HD12	0.46	1.87	10	1
3:A:157:GLN:HB3	3:A:158:PRO:HD2	0.46	1.87	10	1
3:A:91:THR:O	3:A:92:THR:HG22	0.46	2.11	9	2
3:A:124:LEU:HD23	3:A:124:LEU:O	0.46	2.10	15	2
3:A:47:ILE:HD12	3:A:117:VAL:CG2	0.46	2.38	7	2
3:A:79:TYR:CD2	3:A:147:VAL:HG21	0.46	2.46	13	3
3:A:81:VAL:CG2	3:A:124:LEU:HD12	0.46	2.40	16	1
3:A:21:PRO:CB	3:A:40:ALA:HB2	0.46	2.41	10	1
3:A:36:GLY:HA2	3:A:84:ILE:HA	0.46	1.87	9	1
3:A:131:ILE:CG2	3:A:140:ILE:CG2	0.46	2.94	9	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:A:78:PHE:HZ	3:A:131:ILE:HG23	0.46	1.71	8	1
3:A:106:ILE:HD12	3:A:106:ILE:O	0.45	2.10	15	2
3:A:129:SER:HB3	3:A:142:ARG:NH1	0.45	2.27	9	1
3:A:76:HIS:CD2	3:A:77:ALA:N	0.45	2.84	18	1
3:A:22:LYS:CD	3:A:40:ALA:HB1	0.45	2.41	18	1
3:A:13:TYR:HA	3:A:52:GLY:HA2	0.45	1.89	8	2
3:A:93:SER:O	3:A:94:HIS:CB	0.45	2.65	7	1
3:A:105:GLU:O	3:A:106:ILE:HG23	0.45	2.12	10	2
2:C:345:DT:H3'	3:A:29:TYR:OH	0.45	2.11	14	3
3:A:77:ALA:O	3:A:78:PHE:CD1	0.45	2.69	9	1
3:A:25:HIS:NE2	3:A:123:ILE:HD13	0.45	2.25	3	1
3:A:131:ILE:CG2	3:A:138:THR:HG22	0.45	2.41	14	1
3:A:37:ALA:O	3:A:123:ILE:HG22	0.45	2.11	6	1
2:C:345:DT:OP1	3:A:127:ARG:HG2	0.45	2.11	3	2
3:A:65:ILE:HG21	3:A:76:HIS:NE2	0.45	2.26	8	2
3:A:125:LYS:CE	3:A:145:THR:HG22	0.45	2.30	8	1
3:A:59:LEU:CD2	3:A:108:LEU:HD11	0.45	2.40	4	1
3:A:132:GLU:CG	3:A:139:ASP:HB2	0.45	2.42	4	1
3:A:25:HIS:HD2	3:A:123:ILE:HG21	0.45	1.67	18	1
3:A:78:PHE:CD2	3:A:126:LEU:CD1	0.45	2.99	16	1
3:A:65:ILE:CD1	3:A:149:LEU:HD23	0.45	2.41	3	2
3:A:84:ILE:HG12	3:A:119:ASP:O	0.45	2.12	10	1
3:A:37:ALA:HB3	3:A:121:ALA:O	0.45	2.11	10	2
3:A:126:LEU:HD12	3:A:140:ILE:HG13	0.45	1.88	7	1
3:A:131:ILE:O	3:A:131:ILE:CG2	0.45	2.64	4	1
3:A:134:ARG:NH2	3:A:136:GLY:HA3	0.45	2.26	13	1
1:B:319:DG:N2	2:C:348:DC:C2	0.45	2.84	16	2
3:A:108:LEU:HD12	3:A:108:LEU:N	0.45	2.27	17	1
3:A:47:ILE:HG23	3:A:117:VAL:CA	0.45	2.42	10	1
3:A:84:ILE:HG13	3:A:120:CYS:HA	0.45	1.88	11	1
3:A:53:TYR:CE1	3:A:55:GLU:CB	0.45	2.99	4	1
3:A:92:THR:HG21	3:A:120:CYS:HB2	0.45	1.88	2	1
3:A:53:TYR:CZ	3:A:155:VAL:HG21	0.45	2.47	18	3
3:A:68:ALA:CB	3:A:146:ARG:HD2	0.45	2.41	2	1
3:A:53:TYR:CE1	3:A:157:GLN:NE2	0.45	2.84	5	3
3:A:61:LEU:HB3	3:A:108:LEU:HD21	0.45	1.88	13	1
3:A:106:ILE:HG13	3:A:106:ILE:O	0.45	2.12	9	1
3:A:102:LYS:HD3	3:A:102:LYS:N	0.45	2.26	14	1
3:A:29:TYR:HB2	3:A:32:GLU:HB3	0.45	1.89	5	1
3:A:125:LYS:CE	3:A:145:THR:HG21	0.45	2.42	11	1
3:A:79:TYR:CE2	3:A:124:LEU:O	0.45	2.70	8	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:A:74:ARG:CD	3:A:138:THR:HG21	0.45	2.37	8	1
3:A:106:ILE:O	3:A:106:ILE:HG13	0.45	2.12	14	1
3:A:14:GLU:HG3	3:A:51:HIS:O	0.45	2.11	14	1
3:A:128:ASN:O	3:A:129:SER:C	0.45	2.55	13	1
3:A:94:HIS:NE2	3:A:121:ALA:HB2	0.45	2.27	13	1
3:A:14:GLU:HB3	3:A:51:HIS:CE1	0.45	2.47	16	1
3:A:21:PRO:HG3	3:A:46:PRO:HB3	0.45	1.89	17	1
3:A:83:ARG:HA	3:A:122:GLY:HA3	0.45	1.89	7	1
3:A:104:LEU:HD12	3:A:104:LEU:N	0.45	2.27	4	1
3:A:127:ARG:O	3:A:131:ILE:HB	0.45	2.12	2	1
3:A:79:TYR:CA	3:A:126:LEU:HD21	0.44	2.42	5	2
3:A:39:LYS:CD	3:A:40:ALA:N	0.44	2.81	13	2
3:A:15:LEU:HB3	3:A:165:LEU:CD2	0.44	2.37	6	1
3:A:27:ALA:CB	3:A:123:ILE:HG12	0.44	2.40	6	1
3:A:15:LEU:HD22	3:A:153:VAL:CG2	0.44	2.42	4	2
2:C:340:DC:H2''	2:C:341:DA:O5'	0.44	2.11	14	9
2:C:344:DT:H5'	3:A:142:ARG:HD3	0.44	1.87	10	3
3:A:53:TYR:O	3:A:54:LEU:HD23	0.44	2.12	17	1
3:A:93:SER:C	3:A:94:HIS:CG	0.44	2.90	7	1
3:A:46:PRO:HG2	3:A:118:ILE:O	0.44	2.12	11	1
3:A:138:THR:O	3:A:139:ASP:CB	0.44	2.64	13	3
2:C:340:DC:H2''	2:C:341:DA:C8	0.44	2.47	13	1
3:A:23:SER:HA	3:A:170:ASN:HB3	0.44	1.88	13	1
3:A:45:HIS:CB	3:A:118:ILE:O	0.44	2.65	6	1
3:A:81:VAL:HG12	3:A:122:GLY:HA3	0.44	1.88	17	1
3:A:109:LEU:HB3	3:A:110:PRO:HD2	0.44	1.89	9	2
3:A:147:VAL:HG22	3:A:172:ILE:CG2	0.44	2.42	7	1
3:A:59:LEU:CD2	3:A:153:VAL:HG11	0.44	2.19	11	1
3:A:106:ILE:HD13	3:A:106:ILE:H	0.44	1.72	2	1
3:A:13:TYR:CB	3:A:52:GLY:HA3	0.44	2.42	2	1
3:A:128:ASN:O	3:A:131:ILE:N	0.44	2.50	13	1
3:A:98:LEU:CD2	3:A:99:SER:N	0.44	2.79	13	3
3:A:46:PRO:C	3:A:47:ILE:HD13	0.44	2.33	17	2
3:A:131:ILE:CD1	3:A:131:ILE:N	0.44	2.79	17	1
3:A:125:LYS:CE	3:A:174:CYS:HB3	0.44	2.41	10	1
3:A:79:TYR:HE1	3:A:126:LEU:HD22	0.44	1.67	12	1
3:A:78:PHE:O	3:A:126:LEU:HD11	0.44	2.13	3	1
3:A:84:ILE:O	3:A:84:ILE:CG2	0.44	2.65	3	1
3:A:15:LEU:CD1	3:A:50:LEU:HB2	0.44	2.37	8	1
3:A:25:HIS:CD2	3:A:40:ALA:HB1	0.44	2.48	14	1
3:A:61:LEU:HA	3:A:153:VAL:HG13	0.44	1.90	11	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:A:78:PHE:CE1	3:A:131:ILE:HD13	0.44	2.48	2	1
1:B:319:DG:N2	2:C:348:DC:O2	0.44	2.51	7	12
3:A:67:THR:CG2	3:A:74:ARG:HB2	0.44	2.42	1	1
3:A:98:LEU:O	3:A:100:ASN:N	0.44	2.51	15	3
3:A:28:ARG:HB2	3:A:34:SER:HA	0.44	1.88	9	1
3:A:79:TYR:CD2	3:A:147:VAL:HG11	0.44	2.48	3	1
3:A:29:TYR:HE1	3:A:127:ARG:HD2	0.44	1.70	7	1
3:A:151:PHE:O	3:A:167:VAL:HG23	0.44	2.11	11	1
3:A:161:ARG:O	3:A:161:ARG:CD	0.44	2.65	4	1
3:A:53:TYR:CE1	3:A:57:GLU:HB3	0.44	2.48	14	1
3:A:89:VAL:HG11	3:A:119:ASP:HB2	0.44	1.88	3	2
3:A:134:ARG:HB3	3:A:137:GLU:HB2	0.44	1.89	18	1
3:A:89:VAL:HG11	3:A:119:ASP:OD2	0.44	2.12	17	1
3:A:15:LEU:CD1	3:A:50:LEU:HG	0.44	2.43	3	1
3:A:61:LEU:HD23	3:A:106:ILE:HD12	0.44	1.88	3	1
3:A:68:ALA:N	3:A:147:VAL:HA	0.44	2.27	4	1
3:A:130:ASP:O	3:A:134:ARG:CG	0.44	2.64	4	1
3:A:135:LYS:O	3:A:135:LYS:HG3	0.44	2.12	16	1
3:A:37:ALA:CA	3:A:122:GLY:HA2	0.44	2.42	1	2
3:A:81:VAL:HB	3:A:122:GLY:HA3	0.44	1.89	12	1
3:A:63:LEU:C	3:A:63:LEU:HD12	0.44	2.33	4	1
3:A:94:HIS:N	3:A:94:HIS:CD2	0.44	2.85	4	1
3:A:34:SER:CB	3:A:83:ARG:HG2	0.44	2.42	4	1
3:A:10:SER:CB	3:A:13:TYR:HB2	0.44	2.42	16	2
3:A:125:LYS:HG3	3:A:126:LEU:N	0.44	2.28	12	1
3:A:155:VAL:HG13	3:A:163:LEU:HG	0.44	1.90	7	1
1:B:315:DC:H2'	1:B:316:DG:C8	0.44	2.48	11	1
3:A:61:LEU:HG	3:A:106:ILE:HG13	0.44	1.89	14	1
3:A:123:ILE:O	3:A:123:ILE:HG23	0.44	2.12	14	1
3:A:59:LEU:O	3:A:108:LEU:N	0.44	2.50	10	1
3:A:19:VAL:HB	3:A:47:ILE:HG13	0.44	1.89	10	1
3:A:80:GLN:HA	3:A:102:LYS:HG3	0.44	1.89	3	1
3:A:82:HIS:O	3:A:83:ARG:HB2	0.44	2.13	4	1
3:A:132:GLU:CG	3:A:139:ASP:CB	0.44	2.95	4	1
3:A:25:HIS:CG	3:A:40:ALA:HB2	0.44	2.48	14	1
1:B:318:DG:C2	1:B:319:DG:C4	0.43	3.06	13	2
3:A:98:LEU:CD2	3:A:101:THR:HB	0.43	2.42	4	3
3:A:15:LEU:HB3	3:A:165:LEU:HG	0.43	1.89	4	2
2:C:349:DT:C2	2:C:350:DC:C4	0.43	3.06	17	1
3:A:79:TYR:CD1	3:A:126:LEU:HD22	0.43	2.46	10	1
3:A:38:VAL:HG13	3:A:45:HIS:HB3	0.43	1.88	10	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:A:15:LEU:CA	3:A:50:LEU:HD23	0.43	2.43	12	2
1:B:315:DC:C2'	1:B:316:DG:C8	0.43	3.01	11	1
3:A:147:VAL:O	3:A:172:ILE:N	0.43	2.51	16	3
3:A:128:ASN:OD1	3:A:140:ILE:HG23	0.43	2.13	10	1
3:A:67:THR:HA	3:A:147:VAL:HA	0.43	1.89	13	2
3:A:19:VAL:O	3:A:46:PRO:HA	0.43	2.13	17	4
3:A:26:ARG:HD2	3:A:27:ALA:N	0.43	2.27	6	1
3:A:25:HIS:HA	3:A:39:LYS:CB	0.43	2.43	6	1
3:A:157:GLN:HG2	3:A:158:PRO:HD2	0.43	1.90	10	1
3:A:13:TYR:CD2	3:A:163:LEU:CD2	0.43	3.02	11	1
3:A:79:TYR:CD2	3:A:123:ILE:HG13	0.43	2.49	8	1
3:A:97:ILE:N	3:A:97:ILE:HD12	0.43	2.29	14	1
3:A:15:LEU:HB2	3:A:50:LEU:HG	0.43	1.90	3	4
3:A:21:PRO:CD	3:A:46:PRO:HB3	0.43	2.43	6	1
3:A:59:LEU:CD2	3:A:108:LEU:HG	0.43	2.43	9	1
3:A:126:LEU:N	3:A:126:LEU:CD2	0.43	2.81	7	1
3:A:129:SER:O	3:A:133:LEU:HD12	0.43	2.13	8	1
3:A:28:ARG:HB2	3:A:33:GLY:O	0.43	2.14	14	1
2:C:347:DC:OP2	3:A:32:GLU:CB	0.43	2.65	6	1
2:C:340:DC:C2'	2:C:341:DA:C8	0.43	3.01	16	1
3:A:157:GLN:NE2	3:A:157:GLN:HA	0.43	2.27	17	1
3:A:84:ILE:CG2	3:A:120:CYS:HA	0.43	2.41	12	3
3:A:128:ASN:ND2	3:A:145:THR:HG23	0.43	2.28	3	1
3:A:106:ILE:O	3:A:106:ILE:HG12	0.43	2.14	2	1
3:A:79:TYR:CD2	3:A:126:LEU:HD11	0.43	2.49	13	1
3:A:113:SER:O	3:A:114:MET:HG2	0.43	2.13	18	1
1:B:317:DA:O3'	3:A:39:LYS:HE3	0.43	2.13	16	1
3:A:25:HIS:CE1	3:A:39:LYS:HD3	0.43	2.48	4	1
3:A:76:HIS:CE1	3:A:79:TYR:H	0.43	2.31	13	1
3:A:96:ALA:N	3:A:103:VAL:O	0.43	2.51	10	1
3:A:84:ILE:HD13	3:A:84:ILE:O	0.43	2.14	11	1
3:A:151:PHE:HB2	3:A:167:VAL:HB	0.43	1.91	8	1
3:A:39:LYS:HE2	3:A:40:ALA:N	0.43	2.28	6	1
3:A:22:LYS:HD2	3:A:40:ALA:HB1	0.43	1.88	18	1
3:A:125:LYS:HD2	3:A:174:CYS:SG	0.43	2.54	18	2
3:A:135:LYS:N	3:A:135:LYS:HE3	0.43	2.28	18	1
2:C:344:DT:C5'	3:A:142:ARG:HG2	0.43	2.44	15	2
3:A:39:LYS:O	3:A:40:ALA:CB	0.43	2.67	4	2
3:A:77:ALA:HB1	3:A:78:PHE:CE1	0.43	2.49	7	1
3:A:148:ARG:HG2	3:A:149:LEU:N	0.43	2.29	7	1
3:A:149:LEU:CD1	3:A:169:SER:HB3	0.43	2.43	4	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:A:80:GLN:HB3	3:A:102:LYS:HG3	0.43	1.89	5	1
3:A:21:PRO:HB3	3:A:40:ALA:CB	0.43	2.43	6	1
3:A:81:VAL:HG23	3:A:124:LEU:HD12	0.43	1.91	16	1
3:A:64:PHE:CD1	3:A:64:PHE:C	0.43	2.92	15	3
3:A:148:ARG:HG2	3:A:171:PRO:HB3	0.43	1.90	17	1
1:B:316:DG:H5"	3:A:85:THR:HB	0.43	1.90	9	1
3:A:22:LYS:O	3:A:171:PRO:HB2	0.43	2.14	7	1
3:A:133:LEU:N	3:A:133:LEU:HD22	0.43	2.29	5	1
2:C:341:DA:C5	2:C:342:DA:C6	0.43	3.07	16	2
3:A:89:VAL:HB	3:A:119:ASP:HB3	0.43	1.91	6	1
3:A:77:ALA:CB	3:A:140:ILE:HG22	0.43	2.44	1	1
3:A:32:GLU:O	3:A:32:GLU:HG3	0.43	2.14	7	1
2:C:344:DT:C2'	2:C:345:DT:C6	0.42	3.02	15	5
3:A:133:LEU:HD22	3:A:133:LEU:N	0.42	2.29	6	1
3:A:93:SER:N	3:A:106:ILE:HG22	0.42	2.29	15	1
3:A:17:ILE:CG2	3:A:20:GLN:HB3	0.42	2.43	11	1
3:A:78:PHE:HE1	3:A:131:ILE:HG23	0.42	1.72	11	1
3:A:84:ILE:HG13	3:A:119:ASP:O	0.42	2.13	11	1
3:A:47:ILE:CG2	3:A:48:VAL:N	0.42	2.82	4	1
3:A:61:LEU:HG	3:A:106:ILE:CG1	0.42	2.44	14	1
3:A:109:LEU:CB	3:A:112:ASN:HB2	0.42	2.44	14	1
3:A:93:SER:HB2	3:A:106:ILE:CG2	0.42	2.44	2	1
1:B:317:DA:C2	1:B:318:DG:C2	0.42	3.07	17	1
3:A:124:LEU:CD2	3:A:126:LEU:HD13	0.42	2.44	17	1
3:A:149:LEU:HD21	3:A:172:ILE:HD11	0.42	1.90	12	1
3:A:65:ILE:CG2	3:A:102:LYS:HB3	0.42	2.44	9	1
3:A:45:HIS:CG	3:A:45:HIS:O	0.42	2.72	16	1
1:B:317:DA:C2	2:C:350:DC:O2	0.42	2.73	1	1
1:B:316:DG:N2	2:C:351:DG:C2	0.42	2.87	12	2
3:A:74:ARG:HD2	3:A:75:PRO:CD	0.42	2.44	9	1
3:A:68:ALA:HA	3:A:148:ARG:HG3	0.42	1.91	5	1
3:A:74:ARG:CG	3:A:75:PRO:HD2	0.42	2.44	5	1
3:A:13:TYR:HA	3:A:51:HIS:O	0.42	2.14	13	1
3:A:85:THR:O	3:A:88:THR:HG22	0.42	2.14	1	1
3:A:52:GLY:O	3:A:54:LEU:HG	0.42	2.15	15	1
3:A:128:ASN:HD21	3:A:145:THR:HG22	0.42	1.74	17	1
1:B:320:DA:C6	1:B:321:DA:C6	0.42	3.08	4	2
3:A:45:HIS:HB2	3:A:118:ILE:O	0.42	2.14	8	1
3:A:157:GLN:CB	3:A:161:ARG:O	0.42	2.68	5	1
3:A:109:LEU:CD1	3:A:110:PRO:HD3	0.42	2.44	16	2
3:A:146:ARG:CG	3:A:173:GLU:HG2	0.42	2.44	13	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:A:123:ILE:CD1	3:A:172:ILE:CG2	0.42	2.97	6	1
3:A:15:LEU:HD12	3:A:50:LEU:CG	0.42	2.45	9	1
3:A:79:TYR:CD2	3:A:124:LEU:O	0.42	2.72	8	1
3:A:125:LYS:HD3	3:A:174:CYS:SG	0.42	2.54	14	1
2:C:349:DT:H2"	2:C:350:DC:C6	0.42	2.49	17	2
3:A:53:TYR:CE1	3:A:155:VAL:HG23	0.42	2.49	17	1
3:A:77:ALA:HB3	3:A:126:LEU:HD21	0.42	1.92	10	1
1:B:326:DG:N1	2:C:341:DA:C2	0.42	2.88	10	1
3:A:13:TYR:HA	3:A:52:GLY:HA3	0.42	1.90	9	1
2:C:344:DT:H2"	2:C:345:DT:C6	0.42	2.50	3	1
3:A:79:TYR:CZ	3:A:126:LEU:CD1	0.42	3.03	7	1
3:A:74:ARG:HG2	3:A:75:PRO:HD2	0.42	1.91	4	1
3:A:94:HIS:CD2	3:A:121:ALA:HB2	0.42	2.50	13	1
3:A:32:GLU:CG	3:A:32:GLU:O	0.42	2.66	6	1
3:A:63:LEU:HG	3:A:104:LEU:HD12	0.42	1.92	6	1
3:A:79:TYR:CE2	3:A:123:ILE:CG1	0.42	3.02	18	1
1:B:319:DG:C2	1:B:320:DA:C2	0.42	3.08	17	4
3:A:126:LEU:O	3:A:128:ASN:N	0.42	2.53	14	2
3:A:61:LEU:CD2	3:A:106:ILE:CD1	0.42	2.98	9	1
3:A:45:HIS:CD2	3:A:119:ASP:HB3	0.42	2.50	11	1
3:A:99:SER:O	3:A:100:ASN:HB2	0.42	2.15	4	1
3:A:45:HIS:N	3:A:46:PRO:HD3	0.42	2.30	14	1
2:C:344:DT:H5'	3:A:142:ARG:HG3	0.42	1.92	2	1
3:A:97:ILE:HD12	3:A:97:ILE:N	0.42	2.30	13	2
3:A:29:TYR:HB2	3:A:32:GLU:CG	0.42	2.43	15	1
3:A:140:ILE:HD12	3:A:144:ASN:O	0.42	2.15	9	1
3:A:124:LEU:CG	3:A:125:LYS:N	0.42	2.83	7	1
3:A:18:GLU:CB	3:A:47:ILE:HB	0.41	2.45	5	2
3:A:25:HIS:NE2	3:A:37:ALA:HA	0.41	2.30	13	1
3:A:131:ILE:HG13	3:A:140:ILE:HG23	0.41	1.92	1	1
2:C:345:DT:OP2	3:A:127:ARG:HA	0.41	2.15	17	1
3:A:28:ARG:HG2	3:A:35:ARG:HB2	0.41	1.91	10	1
1:B:319:DG:N2	1:B:320:DA:N3	0.41	2.68	4	2
1:B:316:DG:N7	3:A:35:ARG:CZ	0.41	2.83	6	1
3:A:127:ARG:HD2	3:A:130:ASP:CG	0.41	2.36	17	1
3:A:131:ILE:HG21	3:A:140:ILE:CD1	0.41	2.44	17	1
3:A:154:HIS:C	3:A:154:HIS:CD2	0.41	2.92	10	1
3:A:38:VAL:O	3:A:38:VAL:CG1	0.41	2.68	3	1
1:B:318:DG:OP2	3:A:26:ARG:CB	0.41	2.68	2	1
3:A:123:ILE:HD11	3:A:172:ILE:HG23	0.41	1.90	13	1
3:A:79:TYR:CD1	3:A:126:LEU:CD2	0.41	2.97	18	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:A:134:ARG:HG2	3:A:135:LYS:N	0.41	2.30	17	1
3:A:89:VAL:HG21	3:A:119:ASP:O	0.41	2.15	10	1
3:A:29:TYR:CE2	3:A:125:LYS:HG2	0.41	2.50	12	1
3:A:81:VAL:HG21	3:A:123:ILE:N	0.41	2.30	12	1
3:A:127:ARG:C	3:A:131:ILE:HD12	0.41	2.35	4	1
3:A:131:ILE:HG21	3:A:140:ILE:HB	0.41	1.92	14	1
1:B:317:DA:OP1	3:A:38:VAL:HG12	0.41	2.15	6	1
3:A:138:THR:O	3:A:139:ASP:HB3	0.41	2.15	6	1
1:B:323:DA:N6	2:C:342:DA:N6	0.41	2.68	16	1
3:A:13:TYR:N	3:A:13:TYR:CD1	0.41	2.88	16	1
3:A:127:ARG:HD2	3:A:130:ASP:CB	0.41	2.45	17	1
3:A:124:LEU:O	3:A:124:LEU:HD23	0.41	2.15	17	2
3:A:25:HIS:NE2	3:A:123:ILE:CG2	0.41	2.77	3	1
3:A:74:ARG:HB3	3:A:75:PRO:CD	0.41	2.44	8	1
3:A:155:VAL:CG1	3:A:163:LEU:O	0.41	2.68	4	1
3:A:107:PRO:O	3:A:108:LEU:HD22	0.41	2.15	5	1
3:A:80:GLN:CB	3:A:102:LYS:HG3	0.41	2.45	5	1
3:A:38:VAL:O	3:A:38:VAL:HG22	0.41	2.15	18	1
3:A:78:PHE:H	3:A:126:LEU:HD11	0.41	1.76	16	1
3:A:79:TYR:CD1	3:A:126:LEU:HD13	0.41	2.50	12	1
3:A:154:HIS:CD2	3:A:154:HIS:C	0.41	2.94	9	1
3:A:101:THR:HG22	3:A:102:LYS:N	0.41	2.31	8	1
3:A:68:ALA:HB2	3:A:147:VAL:O	0.41	2.16	14	1
3:A:39:LYS:C	3:A:39:LYS:HD2	0.41	2.36	5	1
3:A:65:ILE:HG12	3:A:149:LEU:HA	0.41	1.92	13	1
3:A:21:PRO:HA	3:A:40:ALA:HB1	0.41	1.93	16	1
1:B:317:DA:H5"	3:A:39:LYS:HD3	0.41	1.93	15	1
2:C:342:DA:H2"	2:C:343:DT:C6	0.41	2.50	10	1
3:A:53:TYR:HB3	3:A:114:MET:CE	0.41	2.45	12	1
3:A:75:PRO:O	3:A:76:HIS:C	0.41	2.59	3	2
3:A:135:LYS:HD3	3:A:135:LYS:N	0.41	2.30	11	1
3:A:61:LEU:O	3:A:106:ILE:HD13	0.41	2.15	2	1
3:A:75:PRO:HG2	3:A:139:ASP:HB3	0.41	1.92	15	1
3:A:109:LEU:HD22	3:A:112:ASN:CG	0.41	2.36	11	1
3:A:27:ALA:HA	3:A:123:ILE:O	0.41	2.15	1	1
3:A:103:VAL:C	3:A:104:LEU:HD22	0.41	2.36	3	1
3:A:63:LEU:CD1	3:A:104:LEU:HD12	0.41	2.38	7	1
3:A:84:ILE:C	3:A:84:ILE:CD1	0.41	2.87	11	1
2:C:348:DC:H2"	2:C:349:DT:C5'	0.41	2.46	13	1
3:A:106:ILE:CD1	3:A:106:ILE:N	0.41	2.80	13	1
3:A:59:LEU:O	3:A:107:PRO:HA	0.41	2.16	13	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:A:25:HIS:HB3	3:A:123:ILE:HD13	0.41	1.92	6	1
3:A:77:ALA:HB1	3:A:78:PHE:CD1	0.41	2.51	6	1
3:A:100:ASN:ND2	3:A:137:GLU:HG2	0.41	2.31	6	1
3:A:127:ARG:O	3:A:131:ILE:HG12	0.41	2.15	16	2
3:A:94:HIS:HB2	3:A:105:GLU:O	0.41	2.14	18	1
1:B:317:DA:H4'	3:A:39:LYS:HE3	0.41	1.93	16	1
3:A:74:ARG:HD3	3:A:75:PRO:HD3	0.41	1.93	1	1
3:A:156:PRO:HB3	3:A:161:ARG:HG2	0.41	1.91	17	1
3:A:25:HIS:HB3	3:A:123:ILE:CD1	0.41	2.46	10	1
3:A:14:GLU:HG2	3:A:51:HIS:O	0.41	2.15	9	1
3:A:59:LEU:HB3	3:A:108:LEU:HG	0.41	1.91	9	1
3:A:124:LEU:CD2	3:A:125:LYS:O	0.41	2.68	9	1
3:A:163:LEU:HA	3:A:163:LEU:HD22	0.41	1.79	3	1
2:C:345:DT:H2'	3:A:29:TYR:CE2	0.41	2.51	7	1
3:A:172:ILE:HG22	3:A:172:ILE:O	0.41	2.15	7	1
3:A:25:HIS:CG	3:A:40:ALA:CB	0.41	3.03	14	1
3:A:37:ALA:HB2	3:A:123:ILE:HB	0.41	1.92	2	1
3:A:131:ILE:CG2	3:A:131:ILE:O	0.41	2.69	2	1
3:A:84:ILE:HG21	3:A:121:ALA:C	0.41	2.37	2	1
1:B:320:DA:C2	1:B:321:DA:C5	0.41	3.09	13	1
3:A:109:LEU:CG	3:A:110:PRO:HD2	0.41	2.45	15	1
3:A:35:ARG:C	3:A:84:ILE:HG21	0.40	2.37	18	1
3:A:134:ARG:CZ	3:A:135:LYS:HB2	0.40	2.46	17	1
3:A:169:SER:CB	3:A:171:PRO:HD3	0.40	2.47	7	1
3:A:79:TYR:CE2	3:A:123:ILE:HG13	0.40	2.50	8	1
3:A:160:GLY:C	3:A:161:ARG:HG3	0.40	2.36	4	1
3:A:125:LYS:HG2	3:A:174:CYS:SG	0.40	2.55	14	1
3:A:125:LYS:HE2	3:A:145:THR:HG22	0.40	1.92	2	1
2:C:340:DC:C4	2:C:341:DA:N6	0.40	2.89	16	1
2:C:347:DC:H2''	2:C:348:DC:C6	0.40	2.52	1	1
3:A:74:ARG:CD	3:A:75:PRO:HD2	0.40	2.47	1	2
1:B:318:DG:OP1	3:A:39:LYS:HE2	0.40	2.16	17	1
3:A:131:ILE:O	3:A:134:ARG:CG	0.40	2.69	5	1
3:A:80:GLN:HB2	3:A:102:LYS:HE3	0.40	1.93	5	1
3:A:93:SER:CA	3:A:106:ILE:HG21	0.40	2.45	13	1
3:A:84:ILE:CG2	3:A:84:ILE:O	0.40	2.69	13	1
1:B:316:DG:C8	3:A:35:ARG:HD3	0.40	2.51	6	1
2:C:348:DC:H2'	2:C:349:DT:H71	0.40	1.93	4	2
3:A:140:ILE:O	3:A:140:ILE:CG1	0.40	2.69	10	1
3:A:93:SER:HB2	3:A:107:PRO:HD2	0.40	1.93	12	1
3:A:59:LEU:HD22	3:A:108:LEU:HD11	0.40	1.93	9	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:A:72:LEU:HD23	3:A:72:LEU:HA	0.40	1.68	7	1
3:A:51:HIS:CD2	3:A:51:HIS:C	0.40	2.95	14	1
2:C:345:DT:H3'	3:A:29:TYR:CZ	0.40	2.51	14	1
3:A:28:ARG:HG2	3:A:32:GLU:CD	0.40	2.37	6	1
3:A:156:PRO:HA	3:A:162:THR:HG23	0.40	1.93	16	1
3:A:61:LEU:CB	3:A:108:LEU:HD12	0.40	2.47	7	1
3:A:113:SER:O	3:A:114:MET:C	0.40	2.59	7	1
3:A:23:SER:HA	3:A:170:ASN:CB	0.40	2.46	17	1
3:A:65:ILE:CG2	3:A:76:HIS:HB2	0.40	2.47	10	1
1:B:316:DG:OP1	3:A:84:ILE:HD11	0.40	2.15	3	1
3:A:125:LYS:C	3:A:126:LEU:CD2	0.40	2.88	7	1

## 6.3 Torsion angles [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	A	164/178 (92%)	114±5 (70±3%)	37±5 (22±3%)	13±3 (8±2%)	2	14
All	All	2952/3204 (92%)	2054 (70%)	659 (22%)	239 (8%)	2	14

All 49 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	99	SER	18
3	A	110	PRO	18
3	A	77	ALA	16
3	A	18	GLU	15
3	A	52	GLY	14
3	A	160	GLY	12
3	A	67	THR	10
3	A	88	THR	10
3	A	139	ASP	8
3	A	84	ILE	8
3	A	140	ILE	8

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Mol	Chain	Res	Type	Models (Total)
3	A	159	SER	8
3	A	141	GLY	7
3	A	127	ARG	7
3	A	134	ARG	6
3	A	33	GLY	6
3	A	135	LYS	4
3	A	45	HIS	4
3	A	38	VAL	4
3	A	136	GLY	3
3	A	82	HIS	3
3	A	76	HIS	3
3	A	53	TYR	3
3	A	86	GLY	3
3	A	85	THR	3
3	A	161	ARG	3
3	A	81	VAL	3
3	A	34	SER	3
3	A	92	THR	2
3	A	11	GLY	2
3	A	40	ALA	2
3	A	94	HIS	2
3	A	36	GLY	2
3	A	138	THR	2
3	A	35	ARG	2
3	A	91	THR	2
3	A	26	ARG	1
3	A	172	ILE	1
3	A	21	PRO	1
3	A	37	ALA	1
3	A	14	GLU	1
3	A	89	VAL	1
3	A	142	ARG	1
3	A	71	ARG	1
3	A	157	GLN	1
3	A	19	VAL	1
3	A	175	SER	1
3	A	95	GLU	1
3	A	83	ARG	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	145/156 (93%)	101±7 (70±5%)	44±7 (30±5%)	2	17
All	All	2610/2808 (93%)	1822 (70%)	788 (30%)	2	17

All 113 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	65	ILE	18
3	A	15	LEU	16
3	A	161	ARG	16
3	A	62	GLN	15
3	A	67	THR	15
3	A	83	ARG	15
3	A	157	GLN	14
3	A	135	LYS	14
3	A	78	PHE	14
3	A	84	ILE	14
3	A	16	ARG	13
3	A	124	LEU	13
3	A	39	LYS	13
3	A	102	LYS	13
3	A	137	GLU	13
3	A	126	LEU	13
3	A	25	HIS	12
3	A	130	ASP	12
3	A	94	HIS	11
3	A	56	ASN	11
3	A	125	LYS	11
3	A	143	LYS	11
3	A	31	THR	11
3	A	134	ARG	11
3	A	142	ARG	11
3	A	71	ARG	10
3	A	139	ASP	10
3	A	109	LEU	10
3	A	80	GLN	10

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Mol	Chain	Res	Type	Models (Total)
3	A	176	GLN	9
3	A	159	SER	9
3	A	45	HIS	9
3	A	74	ARG	9
3	A	145	THR	9
3	A	152	ARG	9
3	A	177	ARG	9
3	A	10	SER	9
3	A	60	MET	9
3	A	169	SER	8
3	A	69	ASP	8
3	A	17	ILE	8
3	A	14	GLU	8
3	A	173	GLU	8
3	A	138	THR	8
3	A	163	LEU	8
3	A	146	ARG	7
3	A	35	ARG	7
3	A	59	LEU	7
3	A	154	HIS	7
3	A	22	LYS	7
3	A	114	MET	7
3	A	155	VAL	7
3	A	87	LYS	7
3	A	119	ASP	7
3	A	165	LEU	7
3	A	82	HIS	7
3	A	90	SER	7
3	A	93	SER	7
3	A	70	ASP	7
3	A	106	ILE	7
3	A	85	THR	7
3	A	148	ARG	7
3	A	133	LEU	6
3	A	111	GLU	6
3	A	120	CYS	6
3	A	105	GLU	6
3	A	79	TYR	6
3	A	140	ILE	6
3	A	95	GLU	6
3	A	51	HIS	5
3	A	123	ILE	5

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Mol	Chain	Res	Type	Models (Total)
3	A	175	SER	5
3	A	166	GLN	5
3	A	73	LEU	4
3	A	115	ARG	4
3	A	103	VAL	4
3	A	113	SER	4
3	A	23	SER	4
3	A	28	ARG	4
3	A	29	TYR	4
3	A	76	HIS	4
3	A	49	GLN	4
3	A	127	ARG	4
3	A	55	GLU	4
3	A	18	GLU	3
3	A	50	LEU	3
3	A	108	LEU	3
3	A	99	SER	3
3	A	53	TYR	3
3	A	34	SER	3
3	A	30	GLU	3
3	A	63	LEU	3
3	A	162	THR	3
3	A	20	GLN	3
3	A	100	ASN	3
3	A	174	CYS	2
3	A	91	THR	2
3	A	54	LEU	2
3	A	170	ASN	2
3	A	104	LEU	2
3	A	92	THR	1
3	A	149	LEU	1
3	A	57	GLU	1
3	A	64	PHE	1
3	A	147	VAL	1
3	A	129	SER	1
3	A	32	GLU	1
3	A	38	VAL	1
3	A	26	ARG	1
3	A	13	TYR	1
3	A	164	SER	1
3	A	144	ASN	1
3	A	112	ASN	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