



Full wwPDB NMR Structure Validation Report ⓘ

Feb 12, 2017 – 05:27 pm GMT

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

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A user guide is available at

<http://wwpdb.org/validation/2016/NMRValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

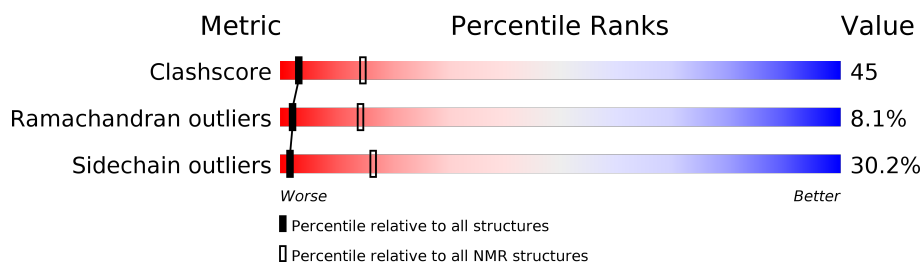
1 Overall quality at a glance

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 ≥ 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 [i](#)

4.1 Average score per residue in the NMR ensemble

These plots are provided for all protein, RNA and DNA chains in the entry. The first graphic is the same as shown in the summary in section 1 of this report. The second graphic shows the sequence where residues are colour-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outliers are shown as green connectors. Residues which are classified as ill-defined in the NMR ensemble, are shown in cyan with an underline colour-coded according to the previous scheme. Residues which were present in the experimental sample, but not modelled in the final structure are shown in grey.

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

Chain B: 

C315
C316
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: 

M1
K2
D3
W4
Q5
L6
P7
S8
H9
S10
G11
P12
Y13
E14
L15
R16
V17
I18
E19
V20
P21
K22
H25
R26
A27
R28
Y29
E30
T31
E32
R35
G36
A37
V38
K39
A40
S41
A42
G43
G44
H45
P46
L47
V48
Q49
L50
H51
G52
Y53
E54
E55
N56
E57
P58
L59
M60
L61
Q62

L63
F64
I65
G66
T67
R71
L72
L73
R74
P75
H76
A77
F78
Y79
Q80
V81
H82
R83
I84
T85
G86
K87
T88
V89
T92
S93
H94
E95
A96
I97
L98
S99
N100
V101
K102
V103
L104
E105
I106
P107
L108
L109
P110
M114
V117
I118
D119
C120
T123
L124
K125
L126
R127
N128
S129

D130
I131
E132
L133
R134
K135
G136
E137
T138
D139
I140
G141
R142
K143
N144
T145
R146
V147
L148
L149
V150
F151
R152
V153
H154
V155
P156
Q157
P158
S159
G160
R161
T162
L163
S164
L165
Q166
V167
A168
S169
I172
E173
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: 



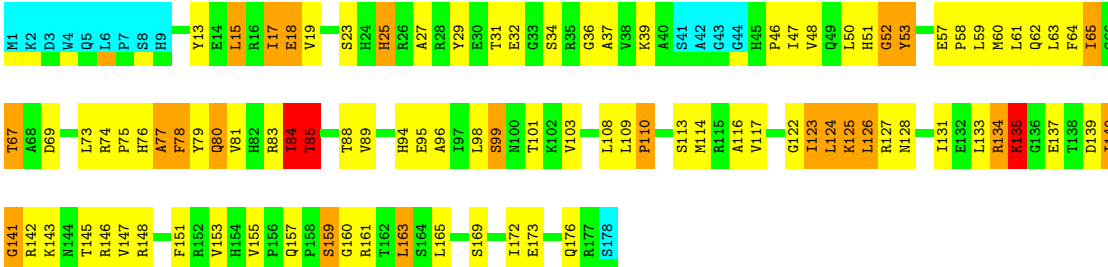
- Molecule 2: DNA (5'-D(*CP*AP*AP*TP*TP*TP*TP*CP*CP*TP*CP*G)-3')

Chain C: 



- Molecule 3: CORE NFATC1


Chain A: 



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: 

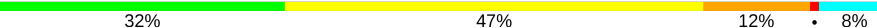


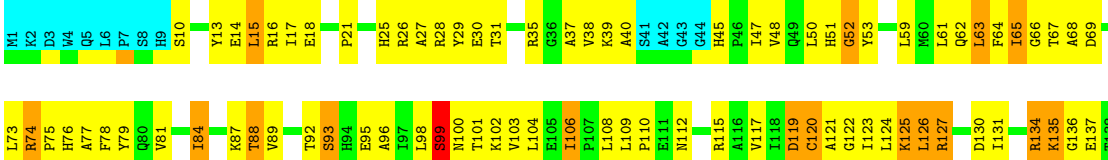
- Molecule 2: DNA (5'-D(*CP*AP*AP*TP*TP*TP*TP*CP*CP*TP*CP*G)-3')

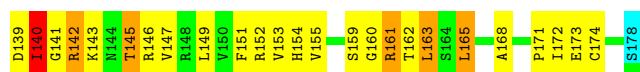
Chain C: 



- Molecule 3: CORE NFATC1

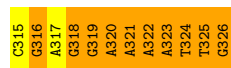
Chain A: 





4.2.3 Score per residue for model 3 (medoid)

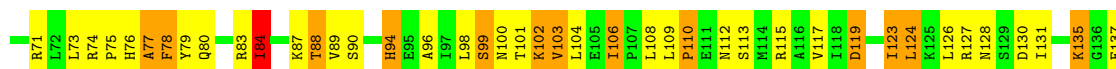
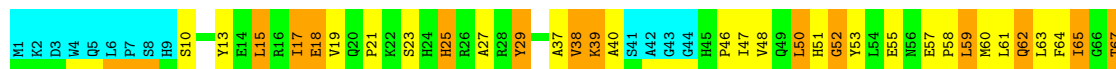
- Molecule 1: DNA (5'-D(*CP*GP*AP*GP*GP*AP*AP*AP*AP*TP*TP*G)-3')



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

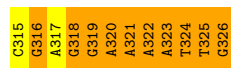


- Molecule 3: CORE NFATC1



4.2.4 Score per residue for model 4

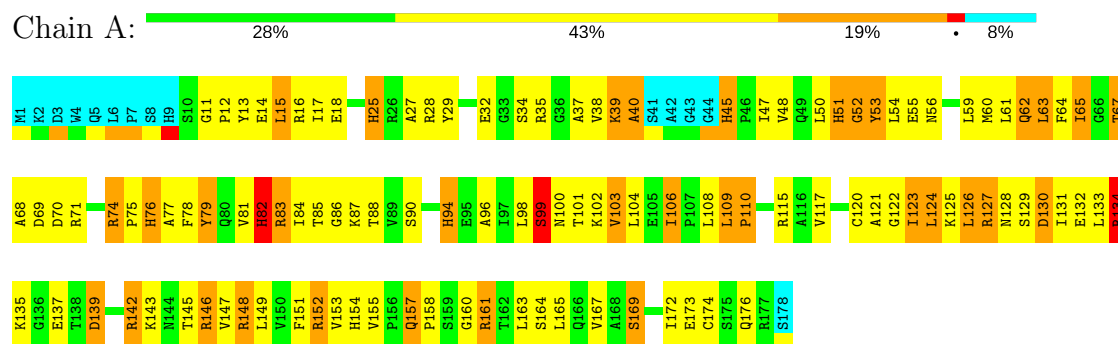
- Molecule 1: DNA (5'-D(*CP*GP*AP*GP*GP*AP*AP*AP*AP*TP*TP*G)-3')



- 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

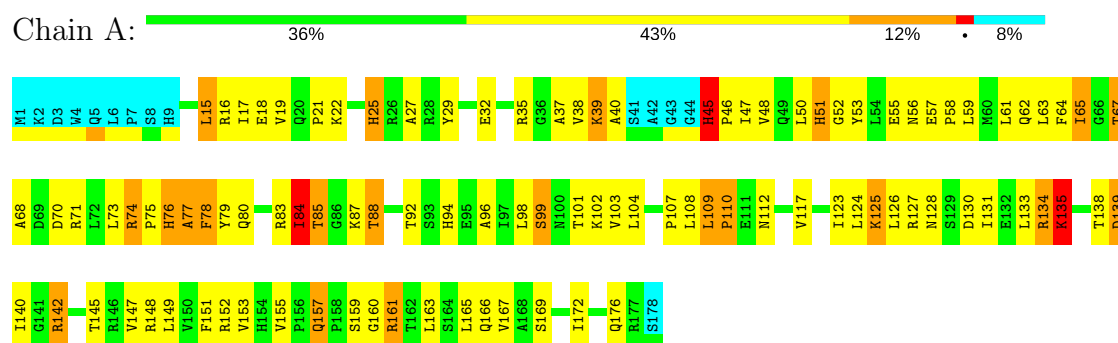
- Molecule 1: DNA (5'-D(*CP*GP*AP*GP*GP*AP*AP*AP*AP*TP*TP*G)-3')



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



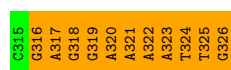
- Molecule 3: CORE NFATC1



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')

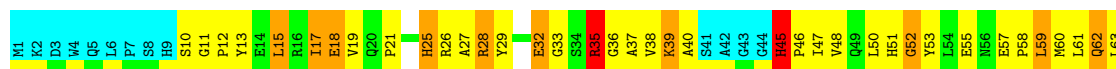
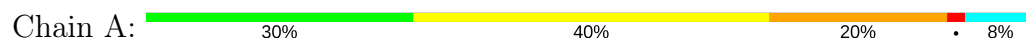




- Molecule 2: DNA (5'-D(*CP*AP*AP*TP*TP*TP*TP*CP*CP*TP*CP*G)-3')



- Molecule 3: CORE NFATC1



4.2.7 Score per residue for model 7

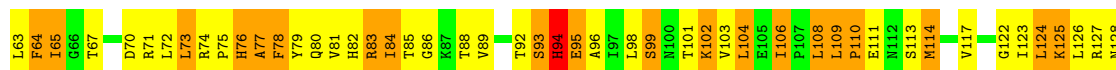
- Molecule 1: DNA (5'-D(*CP*GP*AP*GP*GP*AP*AP*AP*AP*TP*TP*G)-3')



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



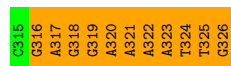
- Molecule 3: CORE NFATC1





4.2.8 Score per residue for model 8

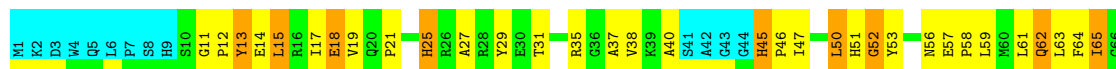
- Molecule 1: DNA (5'-D(*CP*GP*AP*GP*GP*AP*AP*AP*AP*TP*TP*G)-3')



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

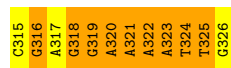


- Molecule 3: CORE NFATC1



4.2.9 Score per residue for model 9

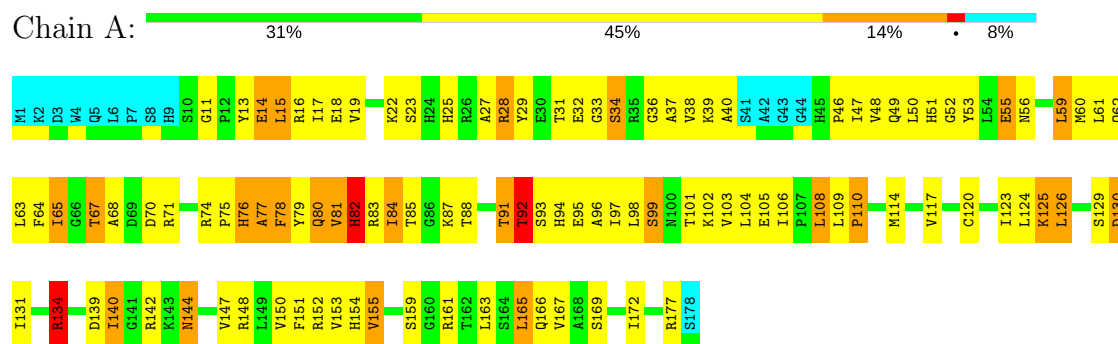
- Molecule 1: DNA (5'-D(*CP*GP*AP*GP*GP*AP*AP*AP*AP*TP*TP*G)-3')



- 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')



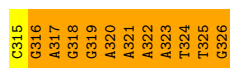
- Molecule 3: CORE NFATC1



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')

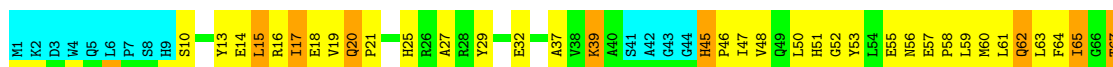




- Molecule 2: DNA (5'-D(*CP*AP*AP*TP*TP*TP*TP*CP*CP*TP*CP*G)-3')



- Molecule 3: CORE NFATC1

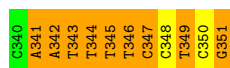


4.2.12 Score per residue for model 12

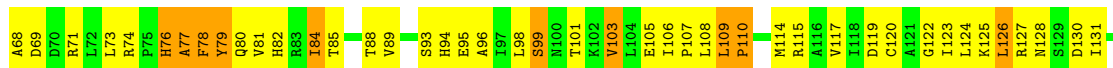
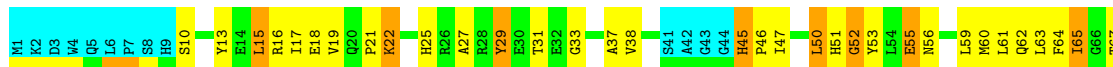
- Molecule 1: DNA (5'-D(*CP*GP*AP*GP*GP*AP*AP*AP*AP*TP*TP*G)-3')



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



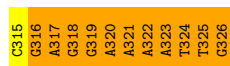
- Molecule 3: CORE NFATC1





4.2.13 Score per residue for model 13

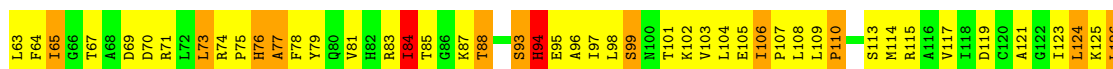
- Molecule 1: DNA (5'-D(*CP*GP*AP*GP*GP*AP*AP*AP*AP*TP*TP*G)-3')



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

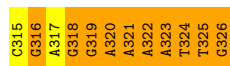


- Molecule 3: CORE NFATC1



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

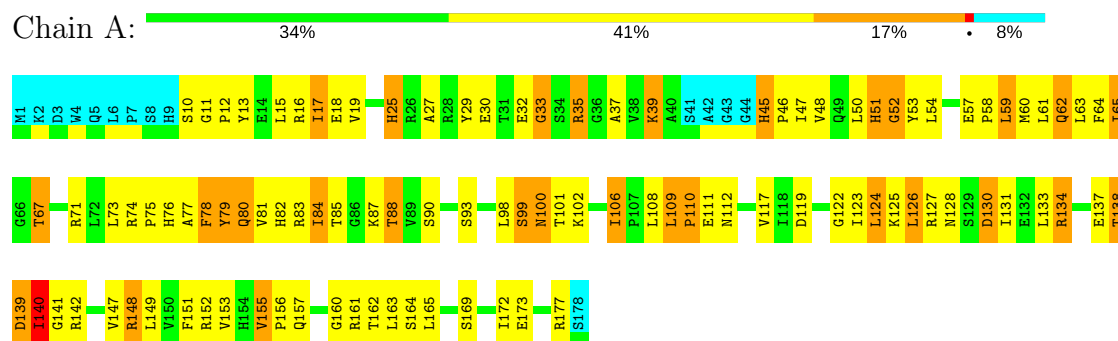
- Molecule 1: DNA (5'-D(*CP*GP*AP*GP*GP*AP*AP*AP*AP*TP*TP*G)-3')



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



- Molecule 3: CORE NFATC1



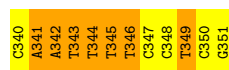
4.2.16 Score per residue for model 16

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

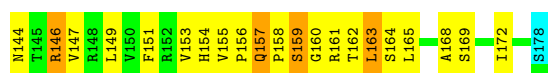
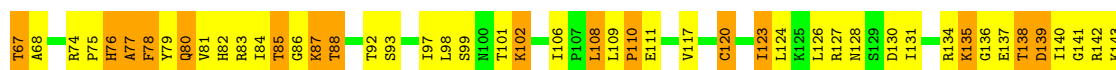




- Molecule 2: DNA (5'-D(*CP*AP*AP*TP*TP*TP*TP*CP*CP*TP*CP*G)-3')

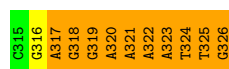


- Molecule 3: CORE NFATC1



4.2.17 Score per residue for model 17

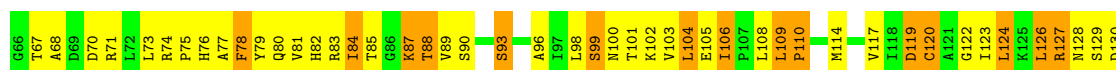
- Molecule 1: DNA (5'-D(*CP*GP*AP*GP*GP*AP*AP*AP*AP*TP*TP*G)-3')



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



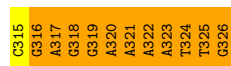
- Molecule 3: CORE NFATC1





4.2.18 Score per residue for model 18

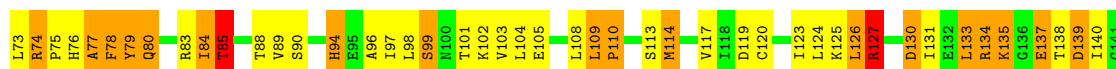
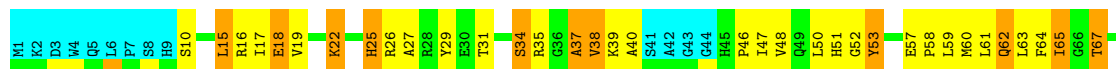
- Molecule 1: DNA (5'-D(*CP*GP*AP*GP*GP*AP*AP*AP*AP*TP*TP*G)-3')



- 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 ≤ 0.4 ANGSTROM, DIHEDRAL ANGLE VIOLATION ≤ 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: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:93:SER:CB	3:A:106:ILE:HG22	0.85	2.01	14	3
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:131:ILE:HG21	3:A:140:ILE:CG2	0.83	2.02	8	3
3:A:15:LEU:CB	3:A:165:LEU:HD13	0.83	2.04	5	8
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:50:LEU:HD23	3:A:51:HIS:N	0.79	1.92	15	15
3:A:63:LEU:HD12	3:A:104:LEU:HD12	0.79	1.53	7	3
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	3
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:126:LEU:HD13	3:A:126:LEU:N	0.74	1.98	13	8
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
1:B:323:DA:H2''	1:B:324:DT:O5'	0.72	1.84	9	18
3:A:79:TYR:CD1	3:A:126:LEU:HD23	0.72	2.20	5	1
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

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:A:81:VAL:HG21	3:A:124:LEU:HB2	0.71	1.62	10	7
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	1
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: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:63:LEU:HD23	3:A:151:PHE:CD2	0.69	2.23	13	14
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:84:ILE:HG21	3:A:120:CYS:C	0.67	2.10	4	2
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: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:HD13	3:A:63:LEU:C	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:59:LEU:HD23	3:A:108:LEU:CD1	0.66	2.21	11	2
3:A:126:LEU:HB2	3:A:140:ILE:HG21	0.66	1.68	1	1
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

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:A:125:LYS:C	3:A:126:LEU:HD22	0.66	2.10	7	1
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:124:LEU:HD23	3:A:125:LYS:O	0.65	1.91	12	2
3:A:53:TYR:CD1	3:A:155:VAL:HG21	0.65	2.25	17	1
3:A:164:SER:O	3:A:165:LEU:HD22	0.65	1.91	4	2
3:A:38:VAL:HG13	3:A:38:VAL:O	0.65	1.90	14	2
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:96:ALA:HB3	3:A:103:VAL:CG2	0.64	2.22	8	1
3:A:25:HIS:CD2	3:A:37:ALA:HB1	0.64	2.27	7	2
3:A:17:ILE:HD11	3:A:151:PHE:CE1	0.64	2.27	9	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:29:TYR:CE2	3:A:127:ARG:HB3	0.64	2.27	13	1
3:A:63:LEU:HD12	3:A:104:LEU:CD1	0.64	2.22	5	3
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	3
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:79:TYR:CE1	3:A:126:LEU:CD2	0.62	2.83	12	4

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
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
3:A:170:ASN:N	3:A:171:PRO:HD3	0.62	2.08	7	1
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	3
3:A:92:THR:HG22	3:A:106:ILE:HG22	0.62	1.70	11	1
3:A:84:ILE:HG21	3:A:120:CYS:CA	0.62	2.25	12	3
3:A:50:LEU:HD12	3:A:153:VAL:HG21	0.62	1.70	15	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:128:ASN:HA	3:A:140:ILE:HG21	0.62	1.71	6	1
3:A:47:ILE:CG2	3:A:117:VAL:HG22	0.62	2.21	14	6
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:65:ILE:CG1	3:A:149:LEU:HD23	0.61	2.26	13	2
3:A:74:ARG:HB3	3:A:75:PRO:HD2	0.61	1.73	8	13
3:A:65:ILE:HG21	3:A:76:HIS:CG	0.61	2.31	2	6
3:A:76:HIS:NE2	3:A:79:TYR:N	0.60	2.47	12	2
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
2:C:345:DT:OP1	3:A:128:ASN:N	0.60	2.35	12	15
3:A:98:LEU:HD22	3:A:101:THR:HB	0.60	1.71	7	10
3:A:106:ILE:N	3:A:106:ILE:HD13	0.60	2.11	13	1
3:A:27:ALA:CA	3:A:123:ILE:HG23	0.60	2.26	13	7
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	4
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	3
3:A:17:ILE:HD11	3:A:151:PHE:CD2	0.59	2.33	17	1
3:A:79:TYR:CE2	3:A:126:LEU:CD2	0.59	2.85	17	7
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:109:LEU:HD13	3:A:110:PRO:CD	0.58	2.28	14	2
3:A:123:ILE:HD13	3:A:124:LEU:N	0.58	2.13	16	1
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:89:VAL:HG21	3:A:119:ASP:CB	0.58	2.27	12	2
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	6
3:A:25:HIS:CB	3:A:172:ILE:HG23	0.58	2.28	8	3
3:A:134:ARG:O	3:A:135:LYS:HG3	0.58	1.99	1	1
2:C:341:DA:H2''	2:C:342:DA:O5'	0.58	1.99	13	15
3:A:17:ILE:HG21	3:A:20:GLN:HG3	0.58	1.76	17	1
3:A:21:PRO:HA	3:A:40:ALA:HB2	0.58	1.75	3	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:A:94:HIS:CG	3:A:106:ILE:HG23	0.58	2.34	4	1
3:A:164:SER:C	3:A:165:LEU:HD22	0.58	2.19	4	3
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:29:TYR:HB2	3:A:32:GLU:HG2	0.57	1.77	15	5
3:A:84:ILE:HG23	3:A:84:ILE:O	0.57	1.99	18	4
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	4
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	7
3:A:84:ILE:O	3:A:84:ILE:HG23	0.57	2.00	3	1
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:149:LEU:HD12	3:A:169:SER:HB3	0.57	1.76	4	3
3:A:51:HIS:CG	3:A:51:HIS:O	0.57	2.57	7	1
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:50:LEU:HD23	3:A:50:LEU:C	0.56	2.20	17	7
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:127:ARG:HG2	3:A:130:ASP:HB2	0.56	1.77	18	2
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:140:ILE:HG23	3:A:141:GLY:H	0.56	1.61	17	4
3:A:17:ILE:HD11	3:A:151:PHE:CD1	0.56	2.36	13	1
3:A:126:LEU:N	3:A:126:LEU:HD22	0.56	2.16	5	5
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	3
3:A:157:GLN:CB	3:A:158:PRO:HD2	0.56	2.31	10	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:A:109:LEU:HD12	3:A:110:PRO:CD	0.55	2.30	13	2
3:A:74:ARG:CB	3:A:75:PRO:HD2	0.55	2.31	13	12
3:A:50:LEU:C	3:A:50:LEU:HD22	0.55	2.20	8	1
3:A:67:THR:HG23	3:A:76:HIS:HA	0.55	1.78	5	3
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: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	7
3:A:37:ALA:C	3:A:123:ILE:HG22	0.55	2.22	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:37:ALA:HB1	3:A:122:GLY:CA	0.55	2.31	6	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: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:28:ARG:HG3	3:A:35:ARG:HB3	0.55	1.77	7	1
3:A:94:HIS:HB2	3:A:104:LEU:CD2	0.55	2.31	7	1
3:A:78:PHE:CD1	3:A:78:PHE:N	0.55	2.75	8	7
1:B:315:DC:H2''	1:B:316:DG:O5'	0.55	2.01	18	10
3:A:61:LEU:HD12	3:A:62:GLN:H	0.55	1.61	7	11
3:A:170:ASN:N	3:A:171:PRO:CD	0.55	2.70	7	1
3:A:47:ILE:HG23	3:A:117:VAL:HA	0.55	1.77	10	2
3:A:94:HIS:O	3:A:104:LEU:HD23	0.55	2.01	10	2
3:A:13:TYR:CD2	3:A:163:LEU:HD23	0.55	2.37	15	2
3:A:174:CYS:O	3:A:175:SER:C	0.54	2.45	17	1
3:A:59:LEU:CB	3:A:108:LEU:HD12	0.54	2.32	6	2
3:A:37:ALA:CB	3:A:123:ILE:CG2	0.54	2.85	7	3
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:88:THR:HG23	3:A:88:THR:O	0.54	2.02	9	7
3:A:50:LEU:C	3:A:50:LEU:HD23	0.54	2.22	11	6
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
1:B:324:DT:H2'	1:B:325:DT:H72	0.54	1.79	13	8
3:A:107:PRO:C	3:A:108:LEU:HD22	0.54	2.23	5	3
3:A:59:LEU:HG	3:A:60:MET:N	0.54	2.18	4	5

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:A:76:HIS:CE1	3:A:79:TYR:HB2	0.54	2.38	1	4
3:A:108:LEU:CD2	3:A:108:LEU:N	0.54	2.71	15	3
3:A:63:LEU:HD11	3:A:149:LEU:HD23	0.54	1.79	16	1
3:A:37:ALA:CB	3:A:123:ILE:N	0.54	2.70	14	1
3:A:93:SER:HB2	3:A:106:ILE:HG22	0.54	1.76	14	4
3:A:45:HIS:CE1	3:A:121:ALA:HB3	0.54	2.37	6	1
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:63:LEU:CB	3:A:104:LEU:HB2	0.54	2.33	10	5
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
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:79:TYR:CE1	3:A:124:LEU:O	0.53	2.61	12	7
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:146:ARG:HG2	3:A:173:GLU:HG2	0.53	1.81	8	1
3:A:47:ILE:HD13	3:A:117:VAL:HG13	0.53	1.81	11	3
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:27:ALA:CB	3:A:123:ILE:HD12	0.53	2.28	4	1
3:A:37:ALA:HA	3:A:122:GLY:HA2	0.53	1.79	1	2
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: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:61:LEU:HD12	3:A:62:GLN:N	0.53	2.18	9	13
3:A:21:PRO:HA	3:A:40:ALA:CB	0.53	2.34	5	4
3:A:96:ALA:O	3:A:103:VAL:CG2	0.53	2.57	7	2
3:A:37:ALA:HA	3:A:122:GLY:CA	0.53	2.34	1	1
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

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:A:15:LEU:HD13	3:A:50:LEU:HD12	0.52	1.80	7	3
3:A:157:GLN:CG	3:A:158:PRO:HD3	0.52	2.34	10	1
3:A:149:LEU:O	3:A:168:ALA:HA	0.52	2.04	7	6
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:169:SER:C	3:A:171:PRO:CD	0.52	2.77	7	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:137:GLU:O	3:A:138:THR:HG23	0.52	2.03	15	1
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:61:LEU:CB	3:A:108:LEU:HD11	0.52	2.35	17	2
3:A:65:ILE:HG21	3:A:76:HIS:CE1	0.52	2.40	17	3
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:67:THR:CG2	3:A:76:HIS:HA	0.52	2.34	9	1
3:A:61:LEU:CD2	3:A:106:ILE:HD11	0.52	2.33	2	2
3:A:25:HIS:CE1	3:A:27:ALA:HB2	0.52	2.40	7	1
3:A:78:PHE:CE1	3:A:131:ILE:HG13	0.52	2.39	7	2
2:C:341:DA:C6	2:C:342:DA:C6	0.52	2.98	16	3
3:A:77:ALA:HB3	3:A:79:TYR:CZ	0.52	2.40	7	1
3:A:15:LEU:HD23	3:A:167:VAL:HG21	0.52	1.79	9	1
3:A:84:ILE:C	3:A:84:ILE:HD12	0.52	2.25	1	1
3:A:38:VAL:O	3:A:38:VAL:CG1	0.52	2.58	14	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:27:ALA:CB	3:A:123:ILE:CG1	0.52	2.88	12	2
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:47:ILE:HG23	3:A:117:VAL:CG2	0.52	2.23	14	3
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:57:GLU:CG	3:A:58:PRO:HD2	0.51	2.34	5	9
3:A:124:LEU:HD21	3:A:126:LEU:HD13	0.51	1.83	3	2
3:A:79:TYR:CD2	3:A:147:VAL:CG2	0.51	2.93	4	2
3:A:93:SER:OG	3:A:106:ILE:HG22	0.51	2.05	9	1
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	4
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:29:TYR:CE1	3:A:127:ARG:CD	0.51	2.93	7	1
3:A:64:PHE:CD1	3:A:64:PHE:C	0.51	2.83	10	4
3:A:163:LEU:C	3:A:163:LEU:HD13	0.51	2.26	15	6
3:A:124:LEU:HD23	3:A:124:LEU:C	0.51	2.25	15	3
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
3:A:28:ARG:CG	3:A:35:ARG:HB2	0.51	2.36	16	2
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: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
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:92:THR:HG21	3:A:107:PRO:O	0.51	2.05	5	1
3:A:149:LEU:HB2	3:A:169:SER:HB3	0.51	1.82	16	5
3:A:29:TYR:CE2	3:A:125:LYS:HD3	0.51	2.41	7	1
3:A:81:VAL:HG12	3:A:82:HIS:N	0.51	2.21	9	1
3:A:93:SER:HB3	3:A:106:ILE:HG22	0.51	1.81	2	2
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
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:79:TYR:CG	3:A:147:VAL:HG21	0.50	2.42	5	1
1:B:319:DG:C2	1:B:320:DA:C4	0.50	2.99	11	5
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:92:THR:HG21	3:A:120:CYS:CB	0.50	2.36	2	2
3:A:163:LEU:CD1	3:A:165:LEU:HD23	0.50	2.35	16	1
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:15:LEU:HB3	3:A:165:LEU:HD13	0.50	1.78	5	2
3:A:163:LEU:CD1	3:A:163:LEU:C	0.50	2.79	17	2
3:A:133:LEU:O	3:A:134:ARG:C	0.50	2.48	5	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: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:108:LEU:N	3:A:108:LEU:HD23	0.50	2.21	4	3
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:109:LEU:CB	3:A:110:PRO:HD2	0.50	2.37	9	9
3:A:135:LYS:CD	3:A:135:LYS:C	0.50	2.80	6	1
3:A:78:PHE:CE1	3:A:131:ILE:CD1	0.50	2.93	14	7
3:A:38:VAL:CG1	3:A:38:VAL:O	0.50	2.58	9	3
2:C:344:DT:H4'	3:A:142:ARG:HG2	0.50	1.83	7	3
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:34:SER:OG	3:A:81:VAL:HG21	0.49	2.07	9	1
3:A:45:HIS:O	3:A:45:HIS:CG	0.49	2.65	14	1
3:A:109:LEU:HD23	3:A:110:PRO:HD2	0.49	1.84	11	2
3:A:85:THR:HG23	3:A:85:THR:O	0.49	2.07	16	3
3:A:15:LEU:H	3:A:165:LEU:HD22	0.49	1.66	7	2
2:C:347:DC:OP2	3:A:32:GLU:HB3	0.49	2.07	9	1
3:A:79:TYR:CE2	3:A:126:LEU:HD23	0.49	2.42	16	1
2:C:346:DT:H71	3:A:29:TYR:CZ	0.49	2.43	10	6
3:A:63:LEU:C	3:A:63:LEU:HD13	0.49	2.28	10	3
3:A:29:TYR:HE1	3:A:127:ARG:CD	0.49	2.21	7	1
3:A:48:VAL:HG21	3:A:151:PHE:CZ	0.49	2.42	9	1
3:A:15:LEU:HB2	3:A:50:LEU:HD23	0.49	1.83	8	2
3:A:140:ILE:CG2	3:A:141:GLY:N	0.49	2.73	15	3
3:A:45:HIS:CB	3:A:46:PRO:HD2	0.49	2.38	6	1
3:A:163:LEU:C	3:A:163:LEU:HD12	0.49	2.28	7	1
3:A:36:GLY:CA	3:A:122:GLY:HA2	0.49	2.36	7	1
3:A:63:LEU:HB3	3:A:104:LEU:HB2	0.49	1.82	3	2
3:A:74:ARG:HD2	3:A:75:PRO:HD2	0.49	1.83	9	1
3:A:37:ALA:HB2	3:A:123:ILE:N	0.49	2.22	4	2
3:A:81:VAL:CG1	3:A:82:HIS:N	0.49	2.75	11	6
3:A:47:ILE:HG22	3:A:48:VAL:N	0.49	2.23	4	2
3:A:85:THR:HG23	3:A:120:CYS:HA	0.49	1.85	18	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:147:VAL:HG23	3:A:172:ILE:HB	0.49	1.84	5	1
3:A:93:SER:O	3:A:106:ILE:CG2	0.49	2.61	7	1
1:B:324:DT:H2''	1:B:325:DT:O5'	0.49	2.08	16	17
2:C:346:DT:H2''	2:C:347:DC:O5'	0.49	2.08	2	6
1:B:326:DG:C2	2:C:341:DA:C2	0.49	3.01	16	6
3:A:126:LEU:HD22	3:A:126:LEU:H	0.49	1.68	8	4
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:77:ALA:CB	3:A:140:ILE:HD13	0.49	2.37	3	3
3:A:140:ILE:O	3:A:140:ILE:HG23	0.49	2.07	1	1
3:A:39:LYS:HD3	3:A:40:ALA:N	0.49	2.23	16	1
2:C:348:DC:H2'	2:C:349:DT:H72	0.49	1.85	17	1
3:A:163:LEU:CD1	3:A:165:LEU:HD11	0.49	2.38	6	1
3:A:13:TYR:CD1	3:A:13:TYR:N	0.49	2.80	4	3
3:A:39:LYS:CD	3:A:39:LYS:C	0.49	2.81	16	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:140:ILE:HG23	3:A:140:ILE:O	0.48	2.08	8	1
3:A:134:ARG:O	3:A:135:LYS:C	0.48	2.52	5	1
3:A:134:ARG:HG3	3:A:134:ARG:O	0.48	2.07	2	1
1:B:318:DG:N2	2:C:349:DT:C2	0.48	2.80	6	5
3:A:123:ILE:CD1	3:A:172:ILE:HD13	0.48	2.38	5	1
3:A:137:GLU:O	3:A:138:THR:CB	0.48	2.60	11	1
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
3:A:65:ILE:HG12	3:A:149:LEU:HD23	0.48	1.84	6	3
1:B:322:DA:C2	2:C:345:DT:O2	0.48	2.67	4	3
3:A:124:LEU:HD21	3:A:126:LEU:CD1	0.48	2.39	3	2
3:A:84:ILE:CG2	3:A:120:CYS:C	0.48	2.82	4	1
3:A:109:LEU:HD23	3:A:112:ASN:ND2	0.48	2.23	2	2
3:A:53:TYR:CE2	3:A:155:VAL:HG22	0.48	2.42	2	1
3:A:126:LEU:HD21	3:A:147:VAL:HG13	0.48	1.86	12	1
3:A:68:ALA:HB3	3:A:146:ARG:HG3	0.48	1.85	17	2
1:B:319:DG:C2	1:B:320:DA:N3	0.48	2.82	8	10
3:A:131:ILE:O	3:A:134:ARG:HG3	0.48	2.09	5	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:37:ALA:CB	3:A:122:GLY:HA2	0.48	2.38	15	1
3:A:84:ILE:HD12	3:A:120:CYS:HA	0.48	1.86	12	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
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:38:VAL:HG13	3:A:45:HIS:CA	0.48	2.34	4	2
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:47:ILE:HG22	3:A:48:VAL:H	0.48	1.69	10	1
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:84:ILE:HG21	3:A:121:ALA:CA	0.48	2.38	4	1
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: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:94:HIS:HB2	3:A:104:LEU:HB3	0.48	1.86	3	2
3:A:10:SER:HB3	3:A:163:LEU:HD21	0.48	1.85	18	1
3:A:138:THR:O	3:A:139:ASP:HB2	0.48	2.09	18	2
3:A:13:TYR:HA	3:A:52:GLY:CA	0.47	2.39	8	4
3:A:155:VAL:HG12	3:A:163:LEU:O	0.47	2.08	4	1
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:HG23	3:A:156:PRO:CD	0.47	2.38	17	1
3:A:109:LEU:CB	3:A:110:PRO:CD	0.47	2.92	4	9
3:A:27:ALA:HB3	3:A:174:CYS:SG	0.47	2.49	11	1
3:A:64:PHE:CD1	3:A:150:VAL:HB	0.47	2.44	10	1
3:A:68:ALA:HB1	3:A:171:PRO:HB3	0.47	1.86	12	1
2:C:344:DT:H2'	2:C:345:DT:H72	0.47	1.86	15	4
3:A:94:HIS:O	3:A:104:LEU:HD22	0.47	2.10	13	1
3:A:59:LEU:HD23	3:A:108:LEU:HD22	0.47	1.85	17	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
2:C:344:DT:C5'	3:A:142:ARG:HG3	0.47	2.39	2	1
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

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
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
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
3:A:98:LEU:HD23	3:A:98:LEU:C	0.47	2.29	15	1
3:A:93:SER:HB3	3:A:105:GLU:O	0.47	2.10	12	1
3:A:147:VAL:O	3:A:171:PRO:HA	0.47	2.10	10	3
2:C:344:DT:OP1	3:A:145:THR:HG23	0.47	2.08	5	1
3:A:27:ALA:HB1	3:A:124:LEU:CA	0.47	2.39	15	3
3:A:28:ARG:HG3	3:A:35:ARG:HB2	0.47	1.87	2	2
3:A:13:TYR:HB3	3:A:52:GLY:HA3	0.47	1.86	2	4
3:A:78:PHE:CZ	3:A:131:ILE:HG21	0.47	2.45	7	2
3:A:137:GLU:O	3:A:138:THR:CG2	0.47	2.62	11	1
3:A:127:ARG:HG3	3:A:127:ARG:O	0.47	2.10	10	1
3:A:80:GLN:HE21	3:A:97:ILE:HG21	0.47	1.69	9	1
3:A:65:ILE:HG13	3:A:149:LEU:HD23	0.47	1.86	2	1
3:A:80:GLN:NE2	3:A:97:ILE:HG12	0.47	2.24	14	1
2:C:346:DT:H71	3:A:29:TYR:HE1	0.47	1.65	3	2
1:B:317:DA:H5''	3:A:39:LYS:CD	0.47	2.40	15	1
3:A:10:SER:HB2	3:A:13:TYR:HB2	0.47	1.85	16	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:77:ALA:HB3	3:A:126:LEU:CD1	0.46	2.39	12	1
3:A:161:ARG:O	3:A:161:ARG:HD2	0.46	2.10	4	1
3:A:26:ARG:O	3:A:37:ALA:HB2	0.46	2.10	18	1
3:A:94:HIS:CB	3:A:104:LEU:HB3	0.46	2.40	7	1
3:A:109:LEU:HB3	3:A:112:ASN:HB2	0.46	1.87	10	1
3:A:130:ASP:O	3:A:134:ARG:HG2	0.46	2.09	9	2
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:59:LEU:CD2	3:A:108:LEU:HD13	0.46	2.40	1	3
3:A:78:PHE:CE1	3:A:131:ILE:HG12	0.46	2.46	4	1
3:A:79:TYR:CE2	3:A:147:VAL:CG1	0.46	2.93	7	1
3:A:65:ILE:HG23	3:A:76:HIS:HB3	0.46	1.85	9	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:A:59:LEU:CD1	3:A:155:VAL:HB	0.46	2.38	1	1
3:A:66:GLY:HA3	3:A:73:LEU:HD22	0.46	1.87	2	1
3:A:78:PHE:CD2	3:A:131:ILE:HD12	0.46	2.45	16	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
3:A:79:TYR:CZ	3:A:124:LEU:O	0.46	2.68	12	1
3:A:15:LEU:CD1	3:A:153:VAL:CG2	0.46	2.86	15	4
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: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:27:ALA:CB	3:A:123:ILE:HG13	0.46	2.41	12	2
3:A:79:TYR:CG	3:A:126:LEU:HD11	0.46	2.44	13	1
3:A:65:ILE:HD11	3:A:149:LEU:CD2	0.46	2.39	17	1
3:A:124:LEU:HD23	3:A:126:LEU:CD1	0.46	2.40	6	1
3:A:68:ALA:HB2	3:A:147:VAL:C	0.46	2.31	4	1
3:A:78:PHE:CZ	3:A:134:ARG:NH1	0.46	2.83	16	1
1:B:318:DG:N2	2:C:349:DT:O2	0.46	2.49	7	13
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
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
2:C:341:DA:H2"	2:C:342:DA:C8	0.46	2.46	2	1
3:A:28:ARG:HG3	3:A:35:ARG:N	0.46	2.26	17	1
3:A:45:HIS:CD2	3:A:45:HIS:N	0.46	2.84	5	2
3:A:73:LEU:O	3:A:73:LEU:HD12	0.46	2.11	7	1
3:A:134:ARG:O	3:A:135:LYS:CG	0.46	2.64	1	1
3:A:78:PHE:C	3:A:126:LEU:HD11	0.46	2.31	17	2
3:A:37:ALA:HA	3:A:123:ILE:HG23	0.46	1.87	6	1
3:A:63:LEU:HB3	3:A:104:LEU:HD12	0.46	1.87	10	1
3:A:81:VAL:CG2	3:A:124:LEU:CB	0.46	2.94	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:79:TYR:CD2	3:A:147:VAL:HG21	0.46	2.46	13	3
3:A:78:PHE:HZ	3:A:131:ILE:HG23	0.46	1.71	8	1
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:21:PRO:CB	3:A:40:ALA:HB2	0.46	2.41	10	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:A:131:ILE:CG2	3:A:140:ILE:CG2	0.46	2.94	9	1
3:A:36:GLY:HA2	3:A:84:ILE:HA	0.46	1.87	9	1
3:A:81:VAL:CG2	3:A:124:LEU:HD12	0.46	2.40	16	1
3:A:126:LEU:HD22	3:A:126:LEU:N	0.45	2.26	18	2
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:13:TYR:HA	3:A:52:GLY:HA2	0.45	1.89	8	2
3:A:22:LYS:CD	3:A:40:ALA:HB1	0.45	2.41	18	1
3:A:76:HIS:CD2	3:A:77:ALA:N	0.45	2.84	18	1
3:A:93:SER:O	3:A:94:HIS:CB	0.45	2.65	7	1
2:C:345:DT:H3'	3:A:29:TYR:OH	0.45	2.11	14	3
3:A:105:GLU:O	3:A:106:ILE:HG23	0.45	2.12	10	2
3:A:77:ALA:O	3:A:78:PHE:CD1	0.45	2.69	9	1
3:A:131:ILE:CG2	3:A:138:THR:HG22	0.45	2.41	14	1
3:A:25:HIS:NE2	3:A:123:ILE:HD13	0.45	2.25	3	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:125:LYS:CE	3:A:145:THR:HG22	0.45	2.30	8	1
3:A:65:ILE:HG21	3:A:76:HIS:NE2	0.45	2.26	8	2
3:A:132:GLU:CG	3:A:139:ASP:HB2	0.45	2.42	4	1
3:A:59:LEU:CD2	3:A:108:LEU:HD11	0.45	2.40	4	1
3:A:65:ILE:CD1	3:A:149:LEU:HD23	0.45	2.41	3	2
3:A:131:ILE:O	3:A:131:ILE:CG2	0.45	2.64	4	1
3:A:25:HIS:HD2	3:A:123:ILE:HG21	0.45	1.67	18	1
3:A:126:LEU:HD12	3:A:140:ILE:HG13	0.45	1.88	7	1
3:A:37:ALA:HB3	3:A:121:ALA:O	0.45	2.11	10	2
3:A:84:ILE:HG12	3:A:119:ASP:O	0.45	2.12	10	1
3:A:78:PHE:CD2	3:A:126:LEU:CD1	0.45	2.99	16	1
3:A:134:ARG:NH2	3:A:136:GLY:HA3	0.45	2.26	13	1
3:A:108:LEU:HD12	3:A:108:LEU:N	0.45	2.27	17	1
3:A:53:TYR:CE1	3:A:55:GLU:CB	0.45	2.99	4	1
3:A:84:ILE:HG13	3:A:120:CYS:HA	0.45	1.88	11	1
3:A:47:ILE:HG23	3:A:117:VAL:CA	0.45	2.42	10	1
1:B:319:DG:N2	2:C:348:DC:C2	0.45	2.84	16	2
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	2
3:A:102:LYS:HD3	3:A:102:LYS:N	0.45	2.26	14	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:A:79:TYR:CE2	3:A:124:LEU:O	0.45	2.70	8	1
3:A:74:ARG:CD	3:A:138:THR:HG21	0.45	2.37	8	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:14:GLU:HG3	3:A:51:HIS:O	0.45	2.11	14	1
3:A:94:HIS:NE2	3:A:121:ALA:HB2	0.45	2.27	13	1
3:A:128:ASN:O	3:A:129:SER:C	0.45	2.55	13	1
3:A:21:PRO:HG3	3:A:46:PRO:HB3	0.45	1.89	17	1
3:A:104:LEU:HD12	3:A:104:LEU:N	0.45	2.27	4	1
3:A:83:ARG:HA	3:A:122:GLY:HA3	0.45	1.89	7	1
3:A:127:ARG:O	3:A:131:ILE:HB	0.45	2.12	2	1
3:A:14:GLU:HB3	3:A:51:HIS:CE1	0.45	2.47	16	1
3:A:39:LYS:CD	3:A:40:ALA:N	0.44	2.81	13	2
3:A:53:TYR:O	3:A:54:LEU:HD23	0.44	2.12	17	1
2:C:344:DT:H5'	3:A:142:ARG:HD3	0.44	1.87	10	3
3:A:27:ALA:CB	3:A:123:ILE:HG12	0.44	2.40	6	1
3:A:15:LEU:HB3	3:A:165:LEU:CD2	0.44	2.37	6	1
3:A:79:TYR:CA	3:A:126:LEU:HD21	0.44	2.42	5	2
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
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
3:A:23:SER:HA	3:A:170:ASN:HB3	0.44	1.88	13	1
2:C:340:DC:H2''	2:C:341:DA:C8	0.44	2.47	13	1
3:A:81:VAL:HG12	3:A:122:GLY:HA3	0.44	1.88	17	1
3:A:45:HIS:CB	3:A:118:ILE:O	0.44	2.65	6	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:79:TYR:HE1	3:A:126:LEU:HD22	0.44	1.67	12	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:131:ILE:CD1	3:A:131:ILE:N	0.44	2.79	17	1
3:A:46:PRO:C	3:A:47:ILE:HD13	0.44	2.33	17	2
3:A:15:LEU:CD1	3:A:50:LEU:HB2	0.44	2.37	8	1
3:A:125:LYS:CE	3:A:174:CYS:HB3	0.44	2.41	10	1
3:A:25:HIS:CD2	3:A:40:ALA:HB1	0.44	2.48	14	1
3:A:78:PHE:O	3:A:126:LEU:HD11	0.44	2.13	3	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:A:84:ILE:O	3:A:84:ILE:CG2	0.44	2.65	3	1
3:A:61:LEU:HA	3:A:153:VAL:HG13	0.44	1.90	11	1
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:161:ARG:O	3:A:161:ARG:CD	0.44	2.65	4	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: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:67:THR:CG2	3:A:74:ARG:HB2	0.44	2.42	1	1
3:A:53:TYR:CE1	3:A:57:GLU:HB3	0.44	2.48	14	1
3:A:79:TYR:CD2	3:A:147:VAL:HG11	0.44	2.48	3	1
3:A:89:VAL:HG11	3:A:119:ASP:OD2	0.44	2.12	17	1
3:A:130:ASP:O	3:A:134:ARG:CG	0.44	2.64	4	1
3:A:68:ALA:N	3:A:147:VAL:HA	0.44	2.27	4	1
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:HB2	0.44	1.88	3	2
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: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:34:SER:CB	3:A:83:ARG:HG2	0.44	2.42	4	1
3:A:94:HIS:N	3:A:94:HIS:CD2	0.44	2.85	4	1
3:A:37:ALA:CA	3:A:122:GLY:HA2	0.44	2.42	1	2
3:A:135:LYS:O	3:A:135:LYS:HG3	0.44	2.12	16	1
3:A:125:LYS:HG3	3:A:126:LEU:N	0.44	2.28	12	1
3:A:10:SER:CB	3:A:13:TYR:HB2	0.44	2.42	16	2
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:123:ILE:O	3:A:123:ILE:HG23	0.44	2.12	14	1
3:A:61:LEU:HG	3:A:106:ILE:HG13	0.44	1.89	14	1
3:A:132:GLU:CG	3:A:139:ASP:CB	0.44	2.95	4	1
3:A:82:HIS:O	3:A:83:ARG:HB2	0.44	2.13	4	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:25:HIS:CG	3:A:40:ALA:HB2	0.44	2.48	14	1
3:A:80:GLN:HA	3:A:102:LYS:HG3	0.44	1.89	3	1
3:A:15:LEU:CA	3:A:50:LEU:HD23	0.43	2.43	12	2
1:B:318:DG:C2	1:B:319:DG:C4	0.43	3.06	13	2
2:C:349:DT:C2	2:C:350:DC:C4	0.43	3.06	17	1
3:A:98:LEU:CD2	3:A:101:THR:HB	0.43	2.42	4	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:A:15:LEU:HB3	3:A:165:LEU:HG	0.43	1.89	4	2
1:B:315:DC:C2'	1:B:316:DG:C8	0.43	3.01	11	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
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:25:HIS:HA	3:A:39:LYS:CB	0.43	2.43	6	1
3:A:26:ARG:HD2	3:A:27:ALA:N	0.43	2.27	6	1
3:A:79:TYR:CD2	3:A:123:ILE:HG13	0.43	2.49	8	1
3:A:13:TYR:CD2	3:A:163:LEU:CD2	0.43	3.02	11	1
3:A:157:GLN:HG2	3:A:158:PRO:HD2	0.43	1.90	10	1
3:A:97:ILE:HD12	3:A:97:ILE:N	0.43	2.29	14	2
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:129:SER:O	3:A:133:LEU:HD12	0.43	2.13	8	1
3:A:126:LEU:N	3:A:126:LEU:CD2	0.43	2.81	7	1
3:A:59:LEU:CD2	3:A:108:LEU:HG	0.43	2.43	9	1
3:A:28:ARG:HB2	3:A:33:GLY:O	0.43	2.14	14	1
3:A:84:ILE:CG2	3:A:120:CYS:HA	0.43	2.41	12	3
3:A:157:GLN:NE2	3:A:157:GLN:HA	0.43	2.27	17	1
2:C:347:DC:OP2	3:A:32:GLU:CB	0.43	2.65	6	1
3:A:106:ILE:HG12	3:A:106:ILE:O	0.43	2.14	2	1
3:A:128:ASN:ND2	3:A:145:THR:HG23	0.43	2.28	3	1
2:C:340:DC:C2'	2:C:341:DA:C8	0.43	3.01	16	1
3:A:79:TYR:CD2	3:A:126:LEU:HD11	0.43	2.49	13	1
3:A:25:HIS:CE1	3:A:39:LYS:HD3	0.43	2.48	4	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:76:HIS:CE1	3:A:79:TYR:H	0.43	2.31	13	1
3:A:151:PHE:HB2	3:A:167:VAL:HB	0.43	1.91	8	1
3:A:84:ILE:HD13	3:A:84:ILE:O	0.43	2.14	11	1
3:A:96:ALA:N	3:A:103:VAL:O	0.43	2.51	10	1
3:A:39:LYS:HE2	3:A:40:ALA:N	0.43	2.28	6	1
3:A:149:LEU:CD1	3:A:169:SER:HB3	0.43	2.43	4	1
3:A:39:LYS:O	3:A:40:ALA:CB	0.43	2.67	4	2
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
3:A:22:LYS:HD2	3:A:40:ALA:HB1	0.43	1.88	18	1
3:A:148:ARG:HG2	3:A:149:LEU:N	0.43	2.29	7	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:A:77:ALA:HB1	3:A:78:PHE:CE1	0.43	2.49	7	1
2:C:344:DT:C5'	3:A:142:ARG:HG2	0.43	2.44	15	2
3:A:148:ARG:HG2	3:A:171:PRO:HB3	0.43	1.90	17	1
3:A:21:PRO:HB3	3:A:40:ALA:CB	0.43	2.43	6	1
3:A:80:GLN:HB3	3:A:102:LYS:HG3	0.43	1.89	5	1
3:A:22:LYS:O	3:A:171:PRO:HB2	0.43	2.14	7	1
1:B:316:DG:H5''	3:A:85:THR:HB	0.43	1.90	9	1
3:A:81:VAL:HG23	3:A:124:LEU:HD12	0.43	1.91	16	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:133:LEU:N	3:A:133:LEU:HD22	0.43	2.29	5	1
3:A:32:GLU:O	3:A:32:GLU:HG3	0.43	2.14	7	1
3:A:77:ALA:CB	3:A:140:ILE:HG22	0.43	2.44	1	1
3:A:133:LEU:HD22	3:A:133:LEU:N	0.42	2.29	6	1
2:C:344:DT:C2'	2:C:345:DT:C6	0.42	3.02	15	5
3:A:47:ILE:CG2	3:A:48:VAL:N	0.42	2.82	4	1
3:A:78:PHE:HE1	3:A:131:ILE:HG23	0.42	1.72	11	1
3:A:17:ILE:CG2	3:A:20:GLN:HB3	0.42	2.43	11	1
3:A:84:ILE:HG13	3:A:119:ASP:O	0.42	2.13	11	1
3:A:93:SER:HB2	3:A:106:ILE:CG2	0.42	2.44	2	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:N	3:A:106:ILE:HG22	0.42	2.29	15	1
3:A:149:LEU:HD21	3:A:172:ILE:HD11	0.42	1.90	12	1
3:A:124:LEU:CD2	3:A:126:LEU:HD13	0.42	2.44	17	1
1:B:317:DA:C2	1:B:318:DG:C2	0.42	3.07	17	1
3:A:65:ILE:CG2	3:A:102:LYS:HB3	0.42	2.44	9	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
1:B:317:DA:C2	2:C:350:DC:O2	0.42	2.73	1	1
3:A:45:HIS:CG	3:A:45:HIS:O	0.42	2.72	16	1
3:A:13:TYR:HA	3:A:51:HIS:O	0.42	2.14	13	1
3:A:128:ASN:HD21	3:A:145:THR:HG22	0.42	1.74	17	1
3:A:45:HIS:HB2	3:A:118:ILE:O	0.42	2.14	8	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
1:B:320:DA:C6	1:B:321:DA:C6	0.42	3.08	4	2
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:146:ARG:CG	3:A:173:GLU:HG2	0.42	2.44	13	1
3:A:109:LEU:CD1	3:A:110:PRO:HD3	0.42	2.44	16	2

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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:79:TYR:CD2	3:A:124:LEU:O	0.42	2.72	8	1
3:A:157:GLN:CB	3:A:161:ARG:O	0.42	2.68	5	1
3:A:15:LEU:HD12	3:A:50:LEU:CG	0.42	2.45	9	1
3:A:125:LYS:HD3	3:A:174:CYS:SG	0.42	2.54	14	1
3:A:53:TYR:CE1	3:A:155:VAL:HG23	0.42	2.49	17	1
2:C:349:DT:H2''	2:C:350:DC:C6	0.42	2.49	17	2
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
3:A:74:ARG:HG2	3:A:75:PRO:HD2	0.42	1.91	4	1
3:A:79:TYR:CZ	3:A:126:LEU:CD1	0.42	3.03	7	1
2:C:344:DT:H2''	2:C:345:DT:C6	0.42	2.50	3	1
3:A:126:LEU:O	3:A:128:ASN:N	0.42	2.53	14	2
1:B:319:DG:C2	1:B:320:DA:C2	0.42	3.08	17	4
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:99:SER:O	3:A:100:ASN:HB2	0.42	2.15	4	1
3:A:79:TYR:CE2	3:A:123:ILE:CG1	0.42	3.02	18	1
3:A:45:HIS:CD2	3:A:119:ASP:HB3	0.42	2.50	11	1
3:A:61:LEU:CD2	3:A:106:ILE:CD1	0.42	2.98	9	1
2:C:344:DT:H5'	3:A:142:ARG:HG3	0.42	1.92	2	1
3:A:45:HIS:N	3:A:46:PRO:HD3	0.42	2.30	14	1
3:A:97:ILE:N	3:A:97:ILE:HD12	0.42	2.30	13	1
3:A:124:LEU:CG	3:A:125:LYS:N	0.42	2.83	7	1
3:A:140:ILE:HD12	3:A:144:ASN:O	0.42	2.15	9	1
3:A:29:TYR:HB2	3:A:32:GLU:CG	0.42	2.43	15	1
3:A:25:HIS:NE2	3:A:37:ALA:HA	0.41	2.30	13	1
2:C:345:DT:OP2	3:A:127:ARG:HA	0.41	2.15	17	1
3:A:18:GLU:CB	3:A:47:ILE:HB	0.41	2.45	8	2
1:B:319:DG:N2	1:B:320:DA:N3	0.41	2.68	4	2
3:A:28:ARG:HG2	3:A:35:ARG:HB2	0.41	1.91	10	1
3:A:131:ILE:HG13	3:A:140:ILE:HG23	0.41	1.92	1	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
1:B:316:DG:N7	3:A:35:ARG:CZ	0.41	2.83	6	1
3:A:154:HIS:C	3:A:154:HIS:CD2	0.41	2.92	10	1
3:A:73:LEU:HD12	3:A:73:LEU:O	0.41	2.15	2	1
1:B:318:DG:OP2	3:A:26:ARG:CB	0.41	2.68	2	1
3:A:81:VAL:HG21	3:A:123:ILE:N	0.41	2.30	12	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:A:29:TYR:CE2	3:A:125:LYS:HG2	0.41	2.50	12	1
3:A:123:ILE:HD11	3:A:172:ILE:HG23	0.41	1.90	13	1
3:A:134:ARG:HG2	3:A:135:LYS:N	0.41	2.30	17	1
3:A:127:ARG:C	3:A:131:ILE:HD12	0.41	2.35	4	1
3:A:79:TYR:CD1	3:A:126:LEU:CD2	0.41	2.97	18	1
3:A:89:VAL:HG21	3:A:119:ASP:O	0.41	2.15	10	1
3:A:131:ILE:HG21	3:A:140:ILE:HB	0.41	1.92	14	1
3:A:124:LEU:O	3:A:124:LEU:HD23	0.41	2.15	17	2
3:A:127:ARG:HD2	3:A:130:ASP:CB	0.41	2.45	17	1
3:A:138:THR:O	3:A:139:ASP:HB3	0.41	2.15	6	1
1:B:317:DA:OP1	3:A:38:VAL:HG12	0.41	2.15	6	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:25:HIS:NE2	3:A:123:ILE:CG2	0.41	2.77	3	1
3:A:13:TYR:N	3:A:13:TYR:CD1	0.41	2.88	16	1
1:B:323:DA:N6	2:C:342:DA:N6	0.41	2.68	16	1
3:A:79:TYR:CD1	3:A:126:LEU:HD13	0.41	2.50	12	1
3:A:101:THR:HG22	3:A:102:LYS:N	0.41	2.31	8	1
3:A:80:GLN:CB	3:A:102:LYS:HG3	0.41	2.45	5	1
3:A:107:PRO:O	3:A:108:LEU:HD22	0.41	2.15	5	1
3:A:38:VAL:O	3:A:38:VAL:HG22	0.41	2.15	18	1
3:A:154:HIS:CD2	3:A:154:HIS:C	0.41	2.94	9	1
3:A:68:ALA:HB2	3:A:147:VAL:O	0.41	2.16	14	1
3:A:78:PHE:H	3:A:126:LEU:HD11	0.41	1.76	16	1
3:A:53:TYR:HB3	3:A:114:MET:CE	0.41	2.45	12	1
3:A:65:ILE:HG12	3:A:149:LEU:HA	0.41	1.92	13	1
3:A:39:LYS:C	3:A:39:LYS:HD2	0.41	2.36	5	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
2:C:342:DA:H2''	2:C:343:DT:C6	0.41	2.50	10	1
3:A:61:LEU:O	3:A:106:ILE:HD13	0.41	2.15	2	1
1:B:317:DA:H5''	3:A:39:LYS:HD3	0.41	1.93	15	1
3:A:21:PRO:HA	3:A:40:ALA:HB1	0.41	1.93	16	1
3:A:109:LEU:HD22	3:A:112:ASN:CG	0.41	2.36	11	1
3:A:75:PRO:HG2	3:A:139:ASP:HB3	0.41	1.92	15	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
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:59:LEU:O	3:A:107:PRO:HA	0.41	2.16	13	1
2:C:348:DC:H2''	2:C:349:DT:C5'	0.41	2.46	13	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:A:106:ILE:CD1	3:A:106:ILE:N	0.41	2.80	13	1
3:A:156:PRO:HB3	3:A:161:ARG:HG2	0.41	1.91	17	1
3:A:100:ASN:ND2	3:A:137:GLU:HG2	0.41	2.31	6	1
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:94:HIS:HB2	3:A:105:GLU:O	0.41	2.14	18	1
3:A:127:ARG:O	3:A:131:ILE:HG12	0.41	2.15	16	2
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: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:74:ARG:HD3	3:A:75:PRO:HD3	0.41	1.93	1	1
3:A:37:ALA:HB2	3:A:123:ILE:HB	0.41	1.92	2	1
3:A:84:ILE:HG21	3:A:121:ALA:C	0.41	2.37	2	1
3:A:131:ILE:CG2	3:A:131:ILE:O	0.41	2.69	2	1
3:A:25:HIS:CG	3:A:40:ALA:CB	0.41	3.03	14	1
3:A:163:LEU:HA	3:A:163:LEU:HD22	0.41	1.79	3	1
1:B:317:DA:H4'	3:A:39:LYS:HE3	0.41	1.93	16	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:134:ARG:CZ	3:A:135:LYS:HB2	0.40	2.46	17	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:35:ARG:C	3:A:84:ILE:HG21	0.40	2.37	18	1
3:A:169:SER:CB	3:A:171:PRO:HD3	0.40	2.47	7	1
3:A:125:LYS:HE2	3:A:145:THR:HG22	0.40	1.92	2	1
3:A:125:LYS:HG2	3:A:174:CYS:SG	0.40	2.55	14	1
1:B:318:DG:OP1	3:A:39:LYS:HE2	0.40	2.16	17	1
3:A:74:ARG:CD	3:A:75:PRO:HD2	0.40	2.47	1	2
2:C:347:DC:H2''	2:C:348:DC:C6	0.40	2.52	1	1
2:C:340:DC:C4	2:C:341:DA:N6	0.40	2.89	16	1
3:A:93:SER:HB2	3:A:107:PRO:HD2	0.40	1.93	12	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
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
2:C:348:DC:H2'	2:C:349:DT:H71	0.40	1.93	4	2
3:A:72:LEU:HD23	3:A:72:LEU:HA	0.40	1.68	7	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:A:140:ILE:O	3:A:140:ILE:CG1	0.40	2.69	10	1
3:A:59:LEU:HD22	3:A:108:LEU:HD11	0.40	1.93	9	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: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:156:PRO:HA	3:A:162:THR:HG23	0.40	1.93	16	1
3:A:23:SER:HA	3:A:170:ASN:CB	0.40	2.46	17	1
3:A:125:LYS:C	3:A:126:LEU:CD2	0.40	2.88	7	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

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	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

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Mol	Chain	Res	Type	Models (Total)
3	A	140	ILE	8
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	16
All	All	2610/2808 (93%)	1822 (70%)	788 (30%)	2	16

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