



Full wwPDB NMR Structure Validation Report ⓘ

Feb 12, 2017 – 08:58 pm GMT

PDB ID : 1ZGW
Title : NMR structure of E. Coli Ada protein in complex with DNA
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Deposited on : 2005-04-22

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

We welcome your comments at validation@mail.wwpdb.org

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
Mogul	:	1.7.2 (RC1), CSD as538be (2017)
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

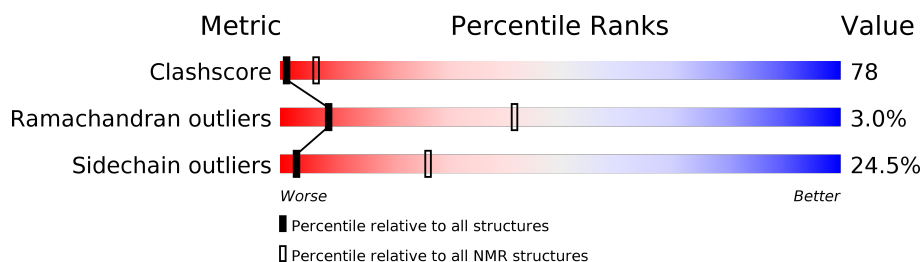
1 Overall quality at a glance

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	18	
2	C	18	
3	A	139	

2 Ensemble composition and analysis

This entry contains 20 models. Model 1 is the overall representative, medoid model (most similar to other models).

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

Well-defined (core) protein residues			
Well-defined core	Residue range (total)	Backbone RMSD (Å)	Medoid model
1	A:8-A:37, A:39-A:139 (131)	0.60	1

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

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

The models can be grouped into 6 clusters and 1 single-model cluster was found.

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

3 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 3364 atoms, of which 1517 are hydrogens and 0 are deuteriums.

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

Mol	Chain	Residues	Atoms						Trace
1	B	18	Total	C	H	N	O	P	0
			573	177	202	78	99	17	

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

Mol	Chain	Residues	Atoms						Trace
2	C	18	Total	C	H	N	O	P	0
			570	176	209	55	113	17	

- Molecule 3 is a protein called Ada polypeptide.

Mol	Chain	Residues	Atoms						Trace
3	A	139	Total	C	H	N	O	S	0
			2220	692	1106	219	194	9	

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	38	SMC	CYS	MODIFIED RESIDUE	UNP P06134

- Molecule 4 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	
4	A	1	Total	Zn
			1	1

4 Residue-property plots [i](#)

4.1 Average score per residue in the NMR ensemble

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

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

Chain B: 

G190
C191
A192
A193
A194
T195
T196
A197
A198
A199
G200
C201
G202
C203
A204
A205
G206
A207

- Molecule 2: 5'-D(*TP*CP*TP*TP*GP*CP*GP*CP*TP*TP*TP*AP*AP*TP*TP*TP*GP*C)-3'

Chain C: 

T221
C222
T223
T224
G225
C226
G227
C228
T229
T230
T231
A232
A233
T234
T235
T236
G237
C238

- Molecule 3: Ada polypeptide

Chain A: 

M1
K2
K3
A4
T5
G6
L7
T8
D9
D10
Q11
R12
V13
Q14
S15
V16
L17
A18
R19
D20
P21
M22
A23
D24
G25
E26
F27
V28
F29
A30
V31
R32
T33
G34
G35
I36
F37
C38
R39
P40
S41
A42
R43
A44
R45
H46
A47
L48
R49
E50
N51
V52
S53
F54
Y55
A56
N57
A58
S59
E60

A61
L62
A63
F64
R65
P66
P68
C69
K70
R71
C72
Q73
P74
D75
K76
A77
N78
P79
R80
L84
I87
T88
H89
A90
C91
R92
L93
L94
E95
Q96
T98
P99
V100
T101
L102
L105
A106
V109
A110
M111
S112
P113
F114
H115
L116
H117
R118
L119
F120
K121
A122
T123
T124
G125
M126

T127
P128
K129
A130
W131
Q132
W135
R136
R139

4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1 (medoid)

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

Chain B: 

G190
C191
A192
A193
A194
T195
T196
A197
A198
A199
G200
C201
G202
C203
A204
A205
G206
A207

- Molecule 2: 5'-D(*TP*CP*TP*TP*GP*CP*GP*CP*TP*TP*TP*AP*AP*TP*TP*TP*GP*C)-3'

Chain C: 

T221
C222
T223
T224
G225
C226
G227
C228
T229
T230
T231
A232
A233
T234
T235
T236
G237
C238

- Molecule 3: Ada polypeptide

Chain A: 

M1
K2
K3
A4
T5
C6
L7
T8
D9
Q11
D10
R12
M13
Q14
S15
V16
L17
A18
R19
N22
A23
D24
D25
G26
E26
F27
V28
F29
A30
V31
R32
T33
T34
G35
I36
F37
C38
R39
P40
S41
C42
R43
R44
R45
H46
A47
L48
R49
E50
N51
V52
S53
F54
Y55
A56
N57
A58
S59
E60
A61

L62
A63
A64
G65
F66
R67
P68
C69
R70
R71
C72
Q73
P74
D75
K76
A77
N78
P79
R80
R81
H82
R83
L84
D85
K86
T87
T88
H89
A90
C91
R92
L93
L94
E95
Q96
E97
T98
P99
V100
T101
L102
L105
A106
D107
Q108
V109
A110
M111
S112
F113
F114
H115
L116
H117
R118
L119
F120
K121
A122

T123
T124
G125
M126
T127
P128
K129
A130
M131
Q132
M135
R136
R139

4.2.2 Score per residue for model 2

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

Chain B: 

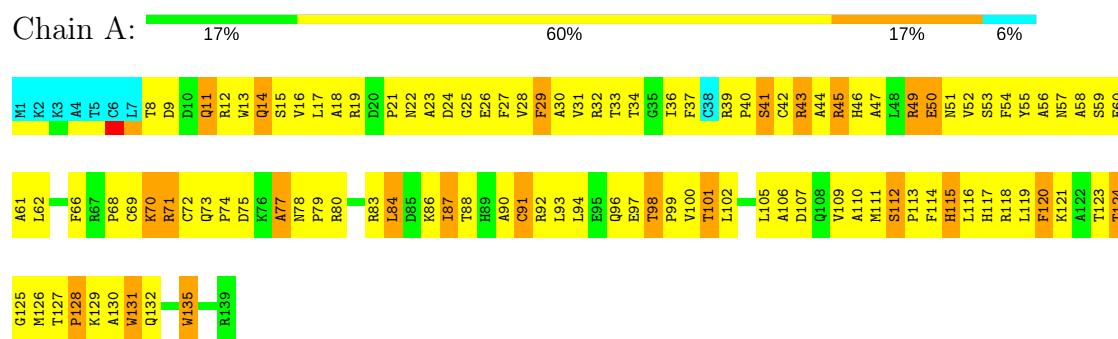
G190
C191
A192
A193
A194
T195
T196
A197
A198
A199
G200
C201
G202
C203
A204
A205
G206
A207

- Molecule 2: 5'-D(*TP*CP*TP*TP*GP*CP*GP*CP*TP*TP*TP*AP*AP*TP*TP*TP*GP*C)-3'

Chain C: 

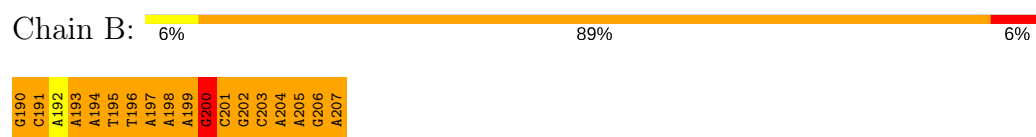
T221
C222
T223
T224
G225
C226
G227
C228
T229
T230
T231
A232
A233
T234
T235
T236
G237
C238

- Molecule 3: Ada polypeptide



4.2.3 Score per residue for model 3

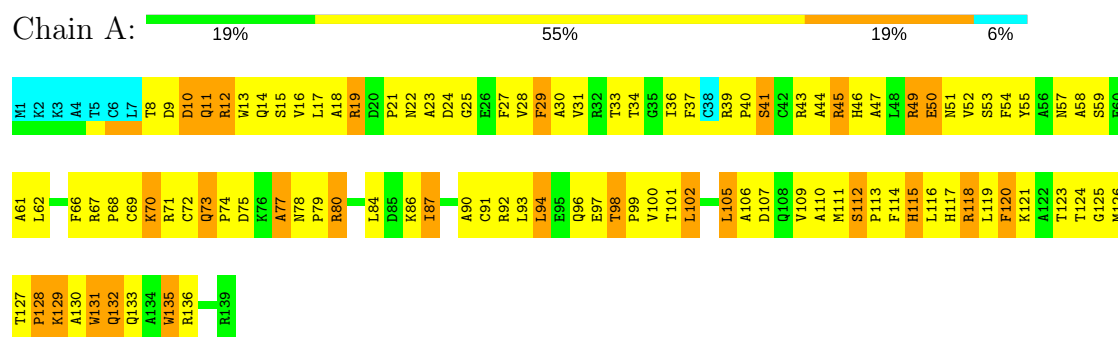
- Molecule 1: 5'-D(*GP*CP*AP*AP*AP*TP*TP*AP*AP*AP*GP*CP*GP*CP*AP*AP*GP*A)-3'



- Molecule 2: 5'-D(*TP*CP*TP*TP*GP*CP*GP*CP*TP*TP*TP*AP*AP*TP*TP*TP*GP*C)-3'



- Molecule 3: Ada polypeptide



4.2.4 Score per residue for model 4

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

Chain B: 

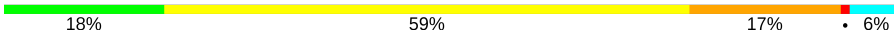
G190
C191
A192
A193
A194
T195
T196
A197
A198
A199
G200
C201
G202
C203
A204
A205
G206
A207

- Molecule 2: 5'-D(*TP*CP*TP*TP*GP*CP*GP*CP*TP*TP*TP*AP*AP*TP*TP*TP*GP*C)-3'

Chain C: 

T221
C222
T223
T224
G225
C226
G227
C228
T229
T230
T231
A232
A233
T234
T235
T236
G237
C238

- Molecule 3: Ada polypeptide

Chain A: 

M1
K2
K3
A4
T5
C6
L7
T8
Q11
R12
W13
Q14
S15
V16
L17
A18
R19
D20
P21
N22
A23
D24
G25
E26
F27
V28
F29
A30
V31
R32
T33
T34
Q35
I36
F37
C38
R39
P40
S41
A44
R45
H46
A47
L48
R49
E50
N51
V52
S53
F54
Y55
A56
N57
A58
S59
E60
A61
L62

A63
A64
G65
F66
R67
P68
C69
K70
R71
C72
P74
D75
K76
A77
R78
P79
B80
R83
L84
D85
K86
T87
T88
H89
A90
C91
R92
L93
L94
E95
Q96
E97
T98
P99
V100
T101
L102
L105
A106
D107
Q108
V109
M110
M111
S112
P113
F114
H115
L116
H117
R118
L119
F120
K121
A122
T123
T124

G125
M126
T127
P128
K129
A130
W131
Q132
W135
R139

4.2.5 Score per residue for model 5

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

Chain B: 


G190
C191
A192
A193
A194
T195
T196
A197
A198
A199
G200
C201
G202
C203
A204
A205
G206
A207

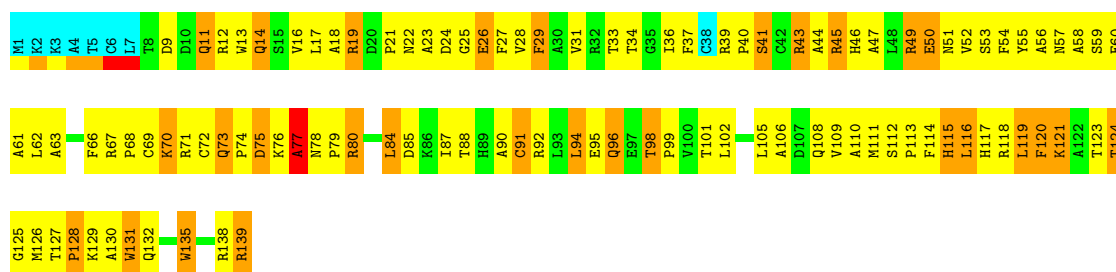
- Molecule 2: 5'-D(*TP*CP*TP*TP*GP*CP*GP*CP*TP*TP*TP*AP*AP*TP*TP*TP*GP*C)-3'

Chain C: 

T221
C222
T223
T224
G225
C226
G227
C228
T229
T230
T231
A232
A233
T234
T235
T236
G237
C238

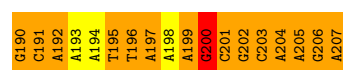
- Molecule 3: Ada polypeptide

Chain A: 



4.2.6 Score per residue for model 6

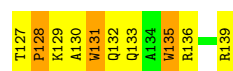
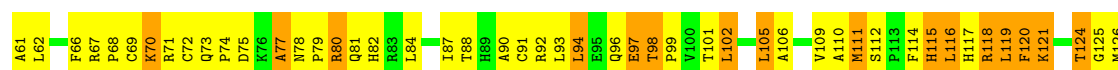
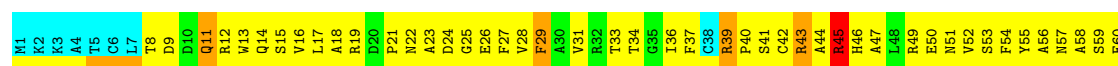
- Molecule 1: 5'-D(*GP*CP*AP*AP*AP*TP*TP*AP*AP*AP*GP*CP*GP*CP*AP*AP*GP*A)-3'



- Molecule 2: 5'-D(*TP*CP*TP*TP*GP*CP*GP*CP*TP*TP*TP*AP*AP*TP*TP*TP*GP*C)-3'



- Molecule 3: Ada polypeptide



4.2.7 Score per residue for model 7

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



G190
C191
A192
A193
A194
T195
T196
A197
A198
A199
G200
C201
G202
C203
A204
A205
G206
A207

- Molecule 2: 5'-D(*TP*CP*TP*TP*GP*CP*GP*CP*TP*TP*TP*AP*AP*TP*TP*TP*GP*C)-3'

Chain C: 22% 72% 6%

T221
C222
T223
T224
G225
C226
G227
C228
T229
T230
T231
A232
A233
T234
T235
T236
G237
C238

- Molecule 3: Ada polypeptide

Chain A: 14% 62% 17% 6%

M1
K2
K3
A4
T5
G6
L7
T8
D9
D10
Q11
Q12
W13
W14
Q15
S16
V16
L17
L18
R19
D20
P21
N22
A23
D24
D25
E26
F27
V28
F29
A30
V31
R32
T33
T34
G35
I36
F37
C38
R39
P40
S41
C42
R43
A44
R45
R46
A47
L48
R49
E50
N51
V52
S53
F54
Y55
A56
N57
A58
S59
E60

A61
L62
F66
P68
C69
K70
R71
C72
C73
Q74
D75
W76
A77
N78
P79
R80
L84
D85
K86
I87
T88
H89
A90
C91
R92
L93
L94
E95
Q96
E97
P99
V100
T101
L102
L105
D107
Q108
V109
A110
M111
S112
P113
F114
H115
L116
H117
R118
L119
F120
K121
A122
T123
G125

M126
T127
P128
K129
A130
W131
Q132
Q133
A134
W135
R136
A137
R138
A139

4.2.8 Score per residue for model 8

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

Chain B: 11% 83% 6%

G190
C191
A192
A193
A194
T195
T196
A197
A198
A199
G200
C201
G202
C203
A204
A205
G206
A207

- Molecule 2: 5'-D(*TP*CP*TP*TP*GP*CP*GP*CP*TP*TP*TP*AP*AP*TP*TP*TP*GP*C)-3'

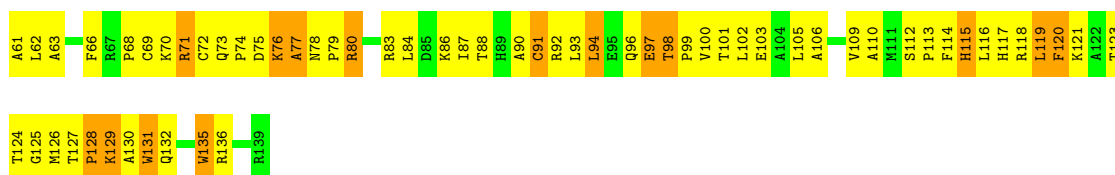
Chain C: 22% 72% 6%

T221
C222
T223
T224
G225
C226
G227
C228
T229
T230
T231
A232
A233
T234
T235
T236
G237
C238

- Molecule 3: Ada polypeptide

Chain A: 17% 61% 15% 6%

M1
K2
K3
A4
T5
G6
L7
T8
D9
D10
Q11
Q12
W13
W14
Q15
S16
V16
L17
L18
R19
D20
P21
N22
A23
D24
D25
E26
F27
V28
F29
A30
V31
R32
T33
T34
G35
I36
F37
C38
R39
P40
S41
C42
R43
A44
R45
R46
A47
L48
R49
E50
N51
V52
S53
F54
Y55
A56
N57
A58
S59
E60



4.2.9 Score per residue for model 9

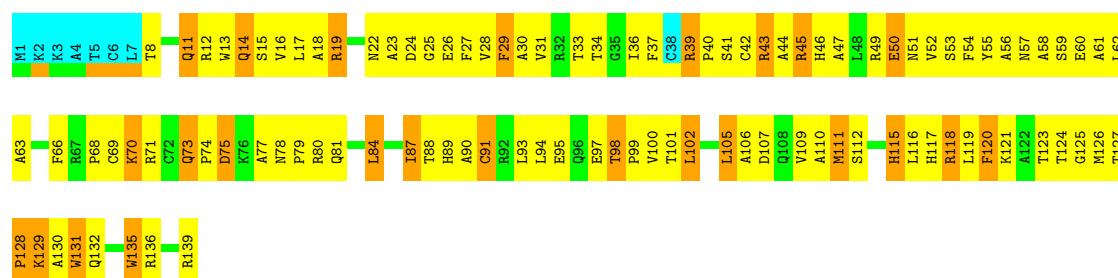
- Molecule 1: 5'-D(*GP*CP*AP*AP*AP*TP*TP*AP*AP*AP*GP*CP*GP*CP*AP*AP*GP*A)-3'



- Molecule 2: 5'-D(*TP*CP*TP*TP*GP*CP*GP*CP*TP*TP*TP*AP*AP*TP*TP*TP*GP*C)-3'

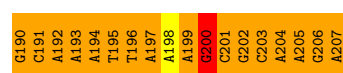


- Molecule 3: Ada polypeptide



4.2.10 Score per residue for model 10

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

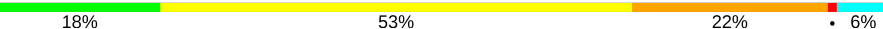


- Molecule 2: 5'-D(*TP*CP*TP*TP*GP*CP*GP*CP*TP*TP*TP*AP*AP*TP*TP*TP*GP*C)-3'

Chain C: 

T221 C222 T223 T224 T225 C226 C227 C228 T229 T230 T231 A232 A233 T234 T235 T236 C237 C238

- Molecule 3: Ada polypeptide

Chain A: 

M1 K2 K3 A4 T5 C6 C7 L7 T8 D9 D10 Q11 R12 R13 Q14 R15 S16 V16 L17 L18 R19 R20 P21 N22 A23 D24 D25 G26 E26 F27 V28 F29 A30 V31 R32 T33 T34 R35 G36 G37 I36 F37 C38 R39 P40 P41 S41 C42 C43 R44 A44 R45 H46 A47 L48 R49 E50 N51 V52 S53 F54 Y55 A56 N57 A58 S59 E60

A61 L62 A63 A64 G65 G66 F66 P67 P68 C69 R70 R71 R72 Q73 Q74 D75 K76 K77 N78 P79 R80 R81 H82 H83 L84 L87 T88 H89 A90 C91 R92 L93 L94 E95 E96 Q96 E97 T98 P99 V100 T101 L102 L105 A106 D107 Q108 V109 M110 M111 S112 P113 F114 H115 L116 H117 R118 L119 F120 K121 A122

T123 T124 G125 M126 T127 P128 K129 A130 Q132 M135 R136 R139

4.2.11 Score per residue for model 11

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

Chain B: 

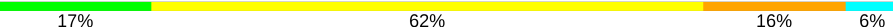
G190 C191 A192 A193 A194 T195 T196 A197 A198 A199 G200 C201 G202 C203 A204 A205 G206 A207

- Molecule 2: 5'-D(*TP*CP*TP*TP*GP*CP*GP*CP*TP*TP*TP*AP*AP*TP*TP*TP*GP*C)-3'

Chain C: 

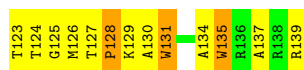
T221 C222 T223 T224 T225 C226 C227 C228 T229 T230 T231 A232 A233 T234 T235 T236 C237 C238

- Molecule 3: Ada polypeptide

Chain A: 

M1 K2 K3 A4 T5 C6 C7 L7 T8 D9 D10 Q11 R12 R13 Q14 R15 S16 V16 L17 L18 R19 R20 P21 N22 A23 D24 D25 G26 E26 F27 V28 F29 A30 V31 R32 T33 T34 R35 G36 G37 I36 F37 C38 R39 P40 P41 S41 C42 C43 R44 A44 R45 H46 A47 L48 R49 E50 N51 V52 S53 F54 Y55 A56 N57 A58 S59 E60

A61 L62 A63 A64 G65 G66 F66 P67 P68 C69 R70 R71 R72 Q73 Q74 D75 K76 K77 N78 P79 R80 R81 H82 H83 L84 L87 T88 H89 A90 C91 R92 L93 L94 E95 E96 Q96 E97 T98 P99 V100 T101 L102 L105 A106 D107 Q108 V109 M110 M111 S112 P113 F114 H115 L116 H117 R118 L119 F120 K121 A122



4.2.12 Score per residue for model 12

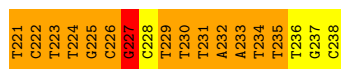
- Molecule 1: 5'-D(*GP*CP*AP*AP*AP*TP*TP*AP*AP*AP*GP*CP*GP*CP*AP*AP*GP*A)-3'

Chain B: 6% 89% 6%



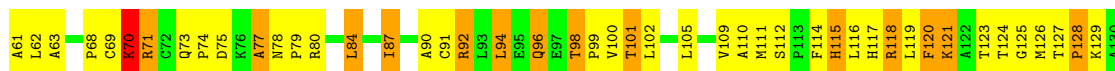
- Molecule 2: 5'-D(*TP*CP*TP*TP*GP*CP*GP*CP*TP*TP*TP*AP*AP*TP*TP*TP*GP*C)-3'

Chain C: 22% 72% 6%



- Molecule 3: Ada polypeptide

Chain A: 27% 51% 16% 6%



4.2.13 Score per residue for model 13

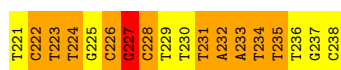
- Molecule 1: 5'-D(*GP*CP*AP*AP*AP*TP*TP*AP*AP*AP*GP*CP*GP*CP*AP*AP*GP*A)-3'

Chain B: 6% 89% 6%

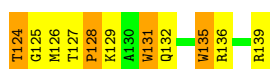
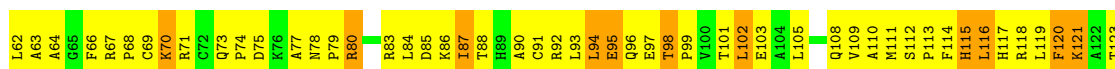


- Molecule 2: 5'-D(*TP*CP*TP*TP*GP*CP*GP*CP*TP*TP*TP*AP*AP*TP*TP*TP*GP*C)-3'

Chain C: 39% 56% 6%

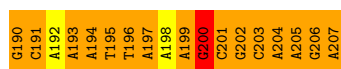


• Molecule 3: Ada polypeptide



4.2.14 Score per residue for model 14

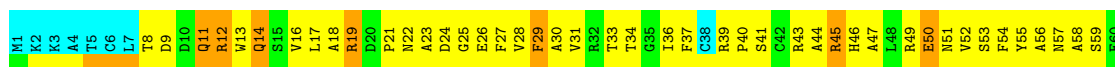
• Molecule 1: 5'-D(*GP*CP*AP*AP*AP*TP*TP*AP*AP*AP*GP*CP*GP*CP*AP*AP*GP*A)-3'



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



• Molecule 3: Ada polypeptide



4.2.15 Score per residue for model 15

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

Chain B: 

G190
C191
A192
A193
A194
T195
T196
A197
A198
A199
G200
C201
G202
C203
A204
A205
G206
A207

- Molecule 2: 5'-D(*TP*CP*TP*TP*GP*CP*GP*CP*TP*TP*TP*AP*AP*TP*TP*TP*GP*C)-3'

Chain C: 

T221
C222
T223
T224
G225
C226
G227
C228
T229
T230
T231
A232
A233
T234
T235
T236
G237
C238

- Molecule 3: Ada polypeptide

Chain A: 

M1
K2
K3
A4
T5
C6
L7
T8
Q11
R12
W13
Q14
S15
V16
L17
A18
R19
D20
P21
N22
A23
D24
G25
E26
F27
V28
F29
A30
V31
R32
T33
T34
G35
I36
F37
C38
R39
P40
S41
C42
R43
A44
R45
H46
A47

A64
S65
F66
R67
P68
C69
K70
R71
C72
Q73
P74
D75
K76
A77
W78
P79
R80
L84
R85
R86
T87
T88
H89
A90
C91
R92
L93
L94
E95
Q96
E97
T98
P99
V100
T101
L102
E103
A104
L105
A106
D107
V108
V109
A110
M111
S112
P113
F114
H115
L116
H117
R118
L119
F120
K121
A122
T123
T124
L125

M126
T127
P128
K129
A130
W131
Q132
M135
R136
R139

4.2.16 Score per residue for model 16

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

Chain B: 

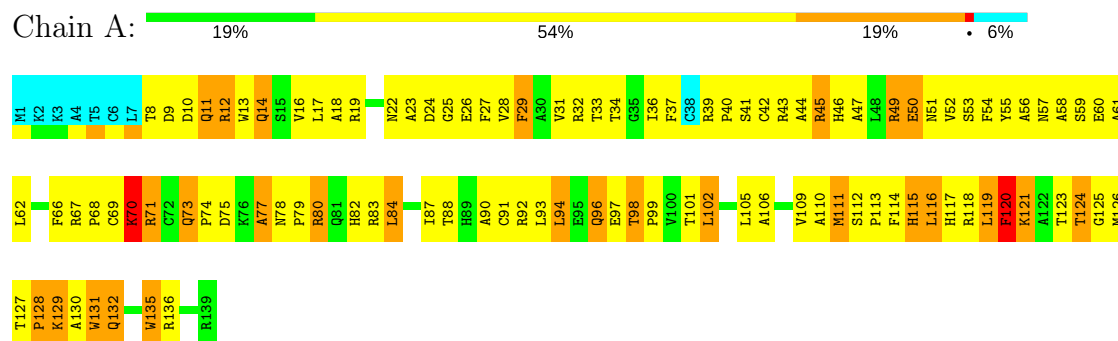
G190
C191
A192
A193
A194
T195
T196
A197
A198
A199
G200
C201
G202
C203
A204
A205
G206
A207

- Molecule 2: 5'-D(*TP*CP*TP*TP*GP*CP*GP*CP*TP*TP*TP*AP*AP*TP*TP*TP*GP*C)-3'

Chain C: 

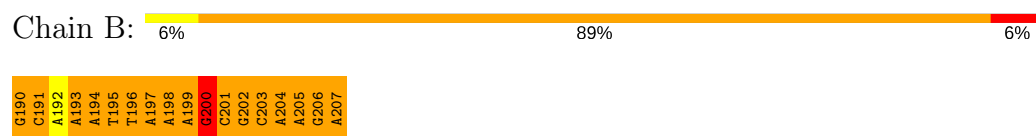
T221
C222
T223
T224
G225
C226
G227
C228
T229
T230
T231
A232
A233
T234
T235
T236
G237
C238

- Molecule 3: Ada polypeptide

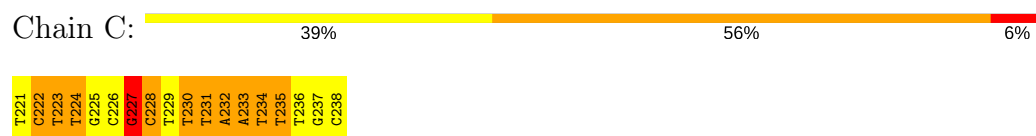


4.2.17 Score per residue for model 17

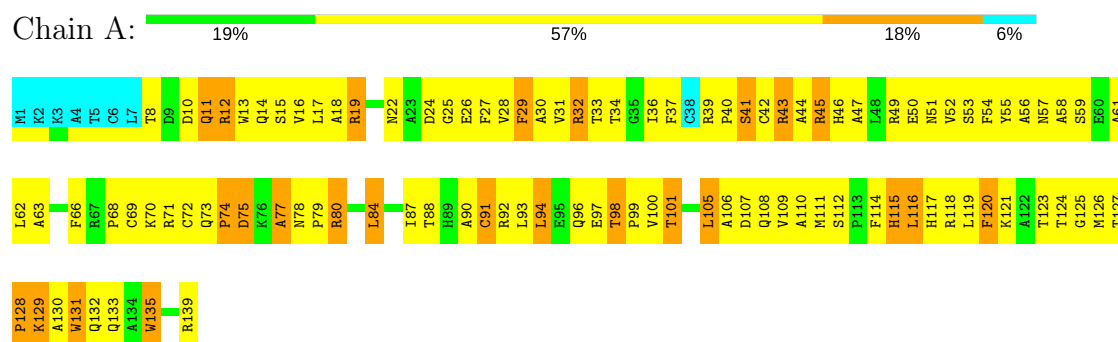
- Molecule 1: 5'-D(*GP*CP*AP*AP*AP*TP*TP*AP*AP*AP*GP*CP*GP*CP*AP*AP*GP*A)-3'



- Molecule 2: 5'-D(*TP*CP*TP*TP*GP*CP*GP*CP*TP*TP*TP*AP*AP*TP*TP*TP*GP*C)-3'



- Molecule 3: Ada polypeptide



4.2.18 Score per residue for model 18

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

Chain B: 

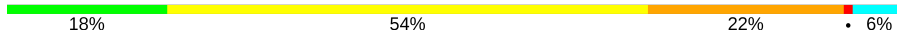
G190
C191
A192
A193
A194
T195
T196
A197
A198
A199
G200
C201
G202
C203
A204
A205
G206
A207

- Molecule 2: 5'-D(*TP*CP*TP*TP*GP*CP*GP*CP*TP*TP*TP*AP*AP*TP*TP*TP*GP*C)-3'

Chain C: 

T221
C222
T223
T224
G225
C226
G227
C228
T229
T230
T231
A232
A233
T234
T235
T236
G237
C238

- Molecule 3: Ada polypeptide

Chain A: 

M1
K2
K3
A4
T5
C6
L7
T8
D9
D10
Q11
R12
W13
Q14
S15
V16
L17
A18
R19
N22
A23
D24
G25
E26
F27
V28
F29
A30
V31
R32
T33
T34
G35
I36
F37
C38
R39
P40
S41
C42
R43
A44
R45
H46
A47
L48
R49
E50
M51
V52
S53
F54
Y55
A56
M57
A58
S59
E60
A61

L62
A63
A64
G65
F66
A67
P68
C69
K70
R71
C72
Q73
P74
D75
K76
A77
N78
P79
R80
L84
D85
K86
T87
T88
H89
A90
C91
R92
L93
L94
E97
T98
P99
V100
T101
L102
L105
A106
D107
Q108
V109
A110
M111
S112
P113
F114
H115
L116
H117
R118
L119
F120
K121
A122
T123
T124
G125

M126
T127
P128
K129
A130
W131
Q132
W135
R136
R139

4.2.19 Score per residue for model 19

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

Chain B: 

G190
C191
A192
A193
A194
T195
T196
A197
A198
A199
G200
C201
G202
C203
A204
A205
G206
A207

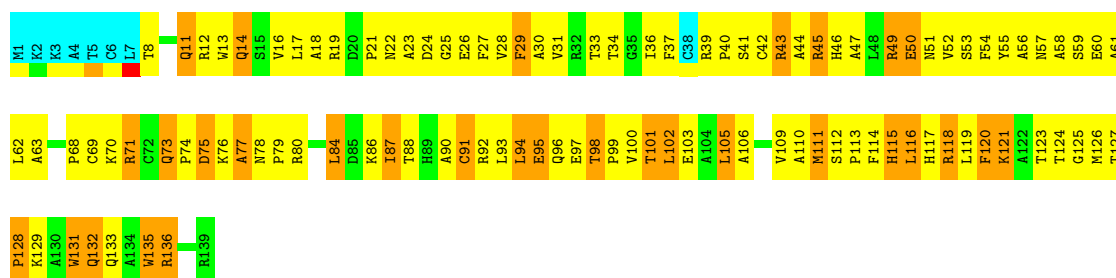
- Molecule 2: 5'-D(*TP*CP*TP*TP*GP*CP*GP*CP*TP*TP*TP*AP*AP*TP*TP*TP*GP*C)-3'

Chain C: 

T221
C222
T223
T224
G225
C226
G227
C228
T229
T230
T231
A232
A233
T234
T235
T236
G237
C238

- Molecule 3: Ada polypeptide

Chain A: 



4.2.20 Score per residue for model 20

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

Chain B: 6% 89% 6%



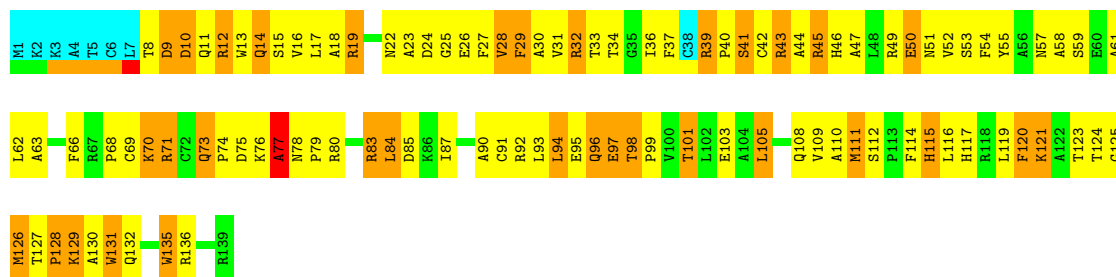
- Molecule 2: 5'-D(*TP*CP*TP*TP*GP*CP*GP*CP*TP*TP*TP*AP*AP*TP*TP*TP*GP*C)-3'

Chain C: 44% 50% 6%



- Molecule 3: Ada polypeptide

Chain A: 20% 50% 24% 6%



5 Refinement protocol and experimental data overview ⓘ

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

Of the 40 calculated structures, 20 were deposited, based on the following criterion: *The submitted conformer models have no restraint violations and lowest energies*.

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

Software name	Classification	Version
X-PLOR	refinement	3.851
Procheck nmr	structure solution	3.5.4

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

6 Model quality (i)

6.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, SMC

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	2.70±0.01	37±0/419 (8.8±0.1%)	2.86±0.00	55±1/645 (8.6±0.1%)
2	C	2.74±0.01	37±1/401 (9.1±0.2%)	2.75±0.01	53±2/617 (8.6±0.3%)
3	A	1.02±0.01	0±0/1080 (0.0±0.0%)	1.34±0.01	4±1/1459 (0.3±0.1%)
All	All	1.95	1469/38000 (3.9%)	2.15	2250/54420 (4.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	Chirality	Planarity
1	B	0.0±0.0	1.0±0.0
2	C	0.0±0.0	1.0±0.0
All	All	0	40

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	191	DC	C3'-C2'	-9.80	1.40	1.52	19	20
2	C	233	DA	C3'-C2'	-9.75	1.40	1.52	16	20
1	B	190	DG	C3'-C2'	-9.57	1.40	1.52	12	20
2	C	221	DT	C3'-C2'	-9.55	1.40	1.52	6	20
1	B	201	DC	C3'-C2'	-9.35	1.41	1.52	7	20
2	C	231	DT	C3'-C2'	-9.35	1.41	1.52	3	20
2	C	234	DT	C3'-C2'	-9.27	1.41	1.52	7	20
1	B	196	DT	C3'-C2'	-9.26	1.41	1.52	12	20
1	B	194	DA	C3'-C2'	-9.24	1.41	1.52	19	20
1	B	202	DG	C3'-C2'	-9.21	1.41	1.52	18	20
1	B	199	DA	C3'-C2'	-9.20	1.41	1.52	3	20

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
1	B	190	DG	C2'-C1'	-9.15	1.43	1.52	16	20
2	C	237	DG	C3'-C2'	-9.14	1.41	1.52	20	20
1	B	193	DA	C2'-C1'	-9.13	1.43	1.52	18	20
1	B	205	DA	C3'-C2'	-9.08	1.41	1.52	9	20
2	C	235	DT	C3'-C2'	-9.04	1.41	1.52	13	20
1	B	203	DC	C3'-C2'	-9.03	1.41	1.52	3	20
2	C	229	DT	C3'-C2'	-8.88	1.41	1.52	13	20
1	B	201	DC	C2'-C1'	-8.86	1.43	1.52	19	20
2	C	234	DT	C2'-C1'	-8.86	1.43	1.52	13	20
2	C	224	DT	C3'-C2'	-8.84	1.41	1.52	16	20
1	B	204	DA	C2'-C1'	-8.83	1.43	1.52	10	20
1	B	204	DA	C3'-C2'	-8.79	1.41	1.52	7	20
2	C	225	DG	C2'-C1'	-8.77	1.43	1.52	13	20
2	C	227	DG	C3'-C2'	-8.75	1.41	1.52	10	20
2	C	238	DC	C3'-C2'	-8.75	1.41	1.52	1	20
2	C	236	DT	C3'-C2'	-8.73	1.41	1.52	3	20
1	B	193	DA	C3'-C2'	-8.71	1.41	1.52	7	20
2	C	222	DC	C3'-C2'	-8.71	1.41	1.52	10	20
2	C	232	DA	C3'-C2'	-8.71	1.41	1.52	14	20
1	B	206	DG	C2'-C1'	-8.67	1.43	1.52	6	20
1	B	207	DA	C3'-C2'	-8.67	1.41	1.52	6	20
1	B	200	DG	C3'-C2'	-8.65	1.41	1.52	13	20
2	C	226	DC	C3'-C2'	-8.61	1.42	1.52	16	20
1	B	192	DA	C3'-C2'	-8.60	1.42	1.52	9	20
2	C	223	DT	C3'-C2'	-8.60	1.42	1.52	2	20
2	C	225	DG	C3'-C2'	-8.58	1.42	1.52	13	20
1	B	197	DA	C3'-C2'	-8.58	1.42	1.52	11	20
2	C	230	DT	C3'-C2'	-8.53	1.42	1.52	10	20
1	B	195	DT	C3'-C2'	-8.50	1.42	1.52	6	20
1	B	198	DA	C3'-C2'	-8.46	1.42	1.52	11	20
2	C	235	DT	C2'-C1'	-8.44	1.43	1.52	3	20
1	B	207	DA	C2'-C1'	-8.41	1.43	1.52	13	20
2	C	224	DT	C2'-C1'	-8.37	1.43	1.52	1	20
2	C	228	DC	C3'-C2'	-8.29	1.42	1.52	5	20
1	B	206	DG	C3'-C2'	-8.28	1.42	1.52	3	20
2	C	223	DT	C2'-C1'	-8.13	1.44	1.52	3	20
2	C	228	DC	C2'-C1'	-7.78	1.44	1.52	3	20
2	C	227	DG	C2'-C1'	-7.74	1.44	1.52	3	20
2	C	230	DT	C2'-C1'	-7.74	1.44	1.52	12	20
1	B	197	DA	C2'-C1'	-7.66	1.44	1.52	6	20
2	C	224	DT	C5-C7	7.43	1.54	1.50	4	19

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
1	B	205	DA	C2'-C1'	-7.42	1.44	1.52	19	20
2	C	229	DT	C2'-C1'	-7.41	1.44	1.52	11	20
1	B	191	DC	C2'-C1'	-7.23	1.45	1.52	14	20
2	C	226	DC	C2'-C1'	-7.23	1.45	1.52	9	20
1	B	203	DC	C2'-C1'	-7.18	1.45	1.52	18	20
2	C	236	DT	C2'-C1'	-7.16	1.45	1.52	17	20
2	C	222	DC	C2'-C1'	-7.13	1.45	1.52	3	20
2	C	231	DT	C2'-C1'	-7.04	1.45	1.52	16	20
1	B	198	DA	C2'-C1'	-6.98	1.45	1.52	11	20
1	B	192	DA	C2'-C1'	-6.97	1.45	1.52	15	20
1	B	194	DA	C2'-C1'	-6.80	1.45	1.52	12	20
1	B	199	DA	C2'-C1'	-6.55	1.45	1.52	3	20
2	C	233	DA	C2'-C1'	-6.48	1.45	1.52	6	20
1	B	200	DG	C2'-C1'	-6.39	1.45	1.52	13	20
2	C	232	DA	C2'-C1'	-6.38	1.45	1.52	9	20
1	B	195	DT	C5-C7	6.16	1.53	1.50	6	20
1	B	196	DT	C5-C7	6.12	1.53	1.50	10	20
2	C	238	DC	C2'-C1'	-6.02	1.46	1.52	11	20
2	C	237	DG	C2'-C1'	-6.01	1.46	1.52	11	20
1	B	195	DT	C2'-C1'	-5.52	1.46	1.52	8	20
1	B	202	DG	C2'-C1'	-5.48	1.46	1.52	15	19
2	C	236	DT	C5-C7	5.17	1.53	1.50	19	1
2	C	235	DT	C5-C7	5.17	1.53	1.50	16	6
2	C	231	DT	C5-C7	5.11	1.53	1.50	6	1
2	C	221	DT	C5-C7	5.07	1.53	1.50	15	1
2	C	221	DT	C2'-C1'	-5.04	1.47	1.52	18	1
2	C	229	DT	C5-C7	5.04	1.53	1.50	6	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	204	DA	C3'-C2'-C1'	11.15	115.88	102.50	15	20
2	C	235	DT	C3'-C2'-C1'	10.97	115.66	102.50	6	20
1	B	199	DA	C3'-C2'-C1'	10.70	115.34	102.50	7	20
2	C	227	DG	C3'-C2'-C1'	10.68	115.31	102.50	15	20
1	B	192	DA	C3'-C2'-C1'	10.63	115.26	102.50	7	20
2	C	232	DA	C3'-C2'-C1'	10.59	115.20	102.50	5	20
1	B	193	DA	C3'-C2'-C1'	10.53	115.14	102.50	9	20
2	C	225	DG	C3'-C2'-C1'	10.53	115.13	102.50	3	20
2	C	224	DT	C3'-C2'-C1'	10.47	115.07	102.50	2	20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	B	205	DA	C3'-C2'-C1'	10.47	115.06	102.50	5	20
1	B	197	DA	C3'-C2'-C1'	10.41	115.00	102.50	4	20
2	C	231	DT	C3'-C2'-C1'	10.39	114.97	102.50	19	20
2	C	234	DT	C3'-C2'-C1'	10.39	114.97	102.50	12	20
1	B	203	DC	C3'-C2'-C1'	10.39	114.96	102.50	7	20
1	B	194	DA	C3'-C2'-C1'	10.35	114.92	102.50	2	20
2	C	229	DT	C3'-C2'-C1'	10.35	114.92	102.50	20	20
1	B	206	DG	C3'-C2'-C1'	10.34	114.90	102.50	19	20
2	C	233	DA	C3'-C2'-C1'	10.33	114.90	102.50	2	20
2	C	236	DT	C3'-C2'-C1'	10.31	114.87	102.50	3	20
1	B	198	DA	C3'-C2'-C1'	10.31	114.87	102.50	20	20
1	B	190	DG	C3'-C2'-C1'	10.29	114.85	102.50	7	20
1	B	201	DC	C3'-C2'-C1'	10.29	114.84	102.50	3	20
2	C	223	DT	C3'-C2'-C1'	10.28	114.84	102.50	12	20
1	B	207	DA	C3'-C2'-C1'	10.27	114.82	102.50	16	20
2	C	230	DT	C3'-C2'-C1'	10.26	114.82	102.50	9	20
2	C	228	DC	C3'-C2'-C1'	10.25	114.80	102.50	19	20
2	C	237	DG	C3'-C2'-C1'	10.22	114.76	102.50	11	20
1	B	200	DG	C3'-C2'-C1'	10.21	114.75	102.50	8	20
1	B	202	DG	C3'-C2'-C1'	10.17	114.70	102.50	13	20
2	C	222	DC	C3'-C2'-C1'	10.14	114.67	102.50	3	20
2	C	227	DG	N7-C8-N9	10.12	118.16	113.10	17	20
2	C	226	DC	C3'-C2'-C1'	10.08	114.60	102.50	9	20
2	C	221	DT	C3'-C2'-C1'	10.00	114.50	102.50	11	20
1	B	195	DT	C3'-C2'-C1'	9.95	114.44	102.50	13	20
1	B	196	DT	C3'-C2'-C1'	9.91	114.39	102.50	2	20
2	C	238	DC	C3'-C2'-C1'	9.88	114.36	102.50	11	20
2	C	225	DG	N7-C8-N9	9.66	117.93	113.10	4	20
2	C	237	DG	N7-C8-N9	9.57	117.89	113.10	9	20
1	B	191	DC	C3'-C2'-C1'	9.47	113.86	102.50	13	20
1	B	190	DG	N7-C8-N9	9.40	117.80	113.10	13	20
1	B	206	DG	N7-C8-N9	9.34	117.77	113.10	14	20
1	B	200	DG	N7-C8-N9	9.32	117.76	113.10	9	20
1	B	202	DG	N7-C8-N9	8.98	117.59	113.10	14	20
1	B	200	DG	C8-N9-C4	-8.90	102.84	106.40	5	20
1	B	192	DA	N7-C8-N9	8.30	117.95	113.80	12	20
1	B	204	DA	N7-C8-N9	8.26	117.93	113.80	4	20
1	B	197	DA	N7-C8-N9	8.14	117.87	113.80	20	20
2	C	232	DA	N7-C8-N9	7.95	117.78	113.80	3	20
1	B	198	DA	N7-C8-N9	7.90	117.75	113.80	14	20
2	C	233	DA	N7-C8-N9	7.84	117.72	113.80	5	20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	B	193	DA	N7-C8-N9	7.78	117.69	113.80	7	20
1	B	199	DA	N7-C8-N9	7.70	117.65	113.80	13	20
1	B	205	DA	N7-C8-N9	7.69	117.65	113.80	9	20
1	B	202	DG	C8-N9-C4	-7.67	103.33	106.40	8	20
1	B	207	DA	N7-C8-N9	7.62	117.61	113.80	18	20
1	B	194	DA	N7-C8-N9	7.56	117.58	113.80	20	20
1	B	191	DC	O4'-C1'-N1	7.47	113.23	108.00	11	20
2	C	227	DG	C8-N9-C4	-7.45	103.42	106.40	17	20
1	B	206	DG	C8-N9-C4	-7.43	103.43	106.40	13	20
2	C	225	DG	C8-N9-C4	-7.09	103.56	106.40	1	20
1	B	205	DA	O4'-C1'-N9	6.99	112.89	108.00	16	20
2	C	237	DG	C8-N9-C4	-6.87	103.65	106.40	16	20
1	B	206	DG	O4'-C1'-N9	6.84	112.79	108.00	9	20
1	B	190	DG	C8-N9-C4	-6.70	103.72	106.40	17	20
1	B	197	DA	C8-N9-C4	-6.66	103.14	105.80	20	20
1	B	199	DA	C8-N9-C4	-6.38	103.25	105.80	2	20
1	B	207	DA	C8-N9-C4	-6.33	103.27	105.80	5	20
1	B	198	DA	C8-N9-C4	-6.26	103.29	105.80	9	20
2	C	224	DT	C6-C5-C7	-6.26	119.14	122.90	19	18
2	C	232	DA	C8-N9-C4	-6.23	103.31	105.80	19	20
1	B	193	DA	C8-N9-C4	-6.20	103.32	105.80	15	20
2	C	234	DT	O4'-C1'-N1	6.20	112.34	108.00	13	7
2	C	229	DT	C6-C5-C7	-6.16	119.20	122.90	6	20
1	B	197	DA	O4'-C1'-N9	6.14	112.30	108.00	13	20
1	B	204	DA	C8-N9-C4	-6.12	103.35	105.80	20	20
1	B	192	DA	C8-N9-C4	-6.11	103.36	105.80	12	20
1	B	194	DA	C8-N9-C4	-6.09	103.36	105.80	13	20
2	C	232	DA	O4'-C1'-N9	6.09	112.26	108.00	2	16
2	C	236	DT	C6-C5-C7	-6.08	119.25	122.90	10	20
2	C	233	DA	C8-N9-C4	-6.08	103.37	105.80	5	20
2	C	234	DT	C6-C5-C7	-6.08	119.25	122.90	20	20
3	A	115	HIS	CA-CB-CG	-6.04	103.34	113.60	5	20
2	C	223	DT	C6-C5-C7	-6.01	119.29	122.90	19	20
2	C	230	DT	C6-C5-C7	-6.00	119.30	122.90	1	20
1	B	203	DC	O4'-C1'-N1	5.99	112.19	108.00	18	20
2	C	231	DT	C6-C5-C7	-5.95	119.33	122.90	12	20
2	C	235	DT	C6-C5-C7	-5.92	119.35	122.90	17	20
2	C	236	DT	O4'-C1'-N1	5.92	112.14	108.00	15	20
1	B	204	DA	O4'-C1'-N9	5.88	112.11	108.00	5	15
2	C	221	DT	C6-C5-C7	-5.86	119.38	122.90	14	20
2	C	228	DC	O4'-C1'-N1	5.82	112.07	108.00	13	19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
3	A	120	PHE	N-CA-CB	-5.81	100.14	110.60	10	4
2	C	221	DT	O4'-C1'-N1	5.78	112.04	108.00	19	20
2	C	229	DT	C4-C5-C6	5.78	121.47	118.00	7	20
1	B	205	DA	C8-N9-C4	-5.76	103.50	105.80	7	20
2	C	226	DC	O4'-C1'-N1	5.75	112.02	108.00	9	3
1	B	195	DT	O4'-C1'-N1	5.74	112.02	108.00	11	14
2	C	236	DT	C4-C5-C6	5.59	121.35	118.00	2	20
2	C	223	DT	C4-C5-C6	5.58	121.35	118.00	18	18
1	B	207	DA	O4'-C1'-N9	5.58	111.90	108.00	18	20
3	A	39	ARG	N-CA-CB	-5.54	100.62	110.60	20	3
2	C	230	DT	C4-C5-C6	5.54	121.32	118.00	4	20
2	C	234	DT	C4-C5-C6	5.53	121.32	118.00	7	20
2	C	235	DT	C4-C5-C6	5.52	121.31	118.00	7	20
2	C	233	DA	O4'-C1'-N9	5.47	111.83	108.00	13	3
3	A	22	ASN	N-CA-CB	-5.45	100.79	110.60	6	20
3	A	77	ALA	N-CA-CB	-5.40	102.54	110.10	1	12
1	B	190	DG	C5-N7-C8	-5.36	101.62	104.30	3	20
2	C	224	DT	C4-C5-C6	5.32	121.19	118.00	7	1
1	B	196	DT	C4-C5-C6	5.32	121.19	118.00	19	20
1	B	198	DA	O4'-C1'-N9	5.32	111.72	108.00	12	4
2	C	225	DG	C5-N7-C8	-5.31	101.64	104.30	13	16
1	B	195	DT	C4-C5-C6	5.29	121.17	118.00	16	20
2	C	237	DG	C5-N7-C8	-5.28	101.66	104.30	19	19
3	A	50	GLU	N-CA-CB	-5.25	101.14	110.60	13	19
2	C	227	DG	C5-N7-C8	-5.25	101.68	104.30	3	20
2	C	221	DT	C4-C5-C6	5.25	121.15	118.00	10	17
2	C	231	DT	O4'-C1'-N1	5.22	111.66	108.00	11	8
3	A	41	SER	N-CA-CB	-5.22	102.67	110.50	2	9
2	C	238	DC	O4'-C1'-N1	5.20	111.64	108.00	11	5
2	C	231	DT	C4-C5-C6	5.19	121.11	118.00	6	20
2	C	235	DT	O4'-C1'-N1	5.16	111.61	108.00	8	3
2	C	237	DG	O4'-C1'-N9	5.14	111.60	108.00	17	5
1	B	200	DG	O4'-C1'-N9	5.13	111.59	108.00	11	2
1	B	206	DG	C5-N7-C8	-5.12	101.74	104.30	6	9
1	B	193	DA	O4'-C1'-N9	5.01	111.50	108.00	2	1

There are no chirality outliers.

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

Mol	Chain	Res	Type	Group	Models (Total)
1	B	200	DG	Sidechain	20
2	C	227	DG	Sidechain	20

6.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	B	371	202	202	28±5
2	C	361	209	209	36±6
3	A	1055	1034	1034	221±17
All	All	35760	28900	28900	5071

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 78.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:C:235:DT:OP1	3:A:46:HIS:O	1.18	1.62	13	5
3:A:97:GLU:OE2	3:A:101:THR:OG1	1.12	1.65	1	3
2:C:224:DT:OP2	3:A:129:LYS:HB3	1.06	1.50	11	19
2:C:234:DT:O3'	3:A:46:HIS:O	1.05	1.75	18	17
3:A:102:LEU:HD23	3:A:116:LEU:HD23	1.02	1.23	1	3
3:A:102:LEU:HD23	3:A:116:LEU:HD21	1.00	1.32	7	1
3:A:127:THR:HG21	3:A:131:TRP:CE3	1.00	1.92	15	18
3:A:84:LEU:HD22	3:A:123:THR:HG22	1.00	1.29	5	12
3:A:78:ASN:N	3:A:79:PRO:HD2	0.98	1.73	20	20
3:A:13:TRP:NE1	3:A:17:LEU:HD11	0.96	1.74	16	20
3:A:13:TRP:CZ2	3:A:17:LEU:HD21	0.95	1.95	6	20
3:A:16:VAL:HA	3:A:40:PRO:O	0.95	1.62	13	20
3:A:94:LEU:HD11	3:A:102:LEU:HD13	0.94	1.40	7	1
3:A:84:LEU:HD21	3:A:123:THR:HG22	0.94	1.37	14	5
3:A:90:ALA:O	3:A:94:LEU:HD12	0.93	1.62	9	13
3:A:24:ASP:O	3:A:78:ASN:CG	0.93	2.07	7	20
3:A:31:VAL:HG12	3:A:33:THR:HG22	0.93	1.40	12	20
3:A:12:ARG:O	3:A:16:VAL:HG23	0.93	1.64	18	20
2:C:234:DT:OP2	3:A:36:ILE:HD12	0.91	1.66	8	17
2:C:224:DT:OP1	3:A:130:ALA:HB2	0.89	1.67	5	7

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:A:105:LEU:HD23	3:A:116:LEU:HD13	0.89	1.40	16	1
1:B:201:DC:C6	3:A:115:HIS:NE2	0.88	2.41	10	20
3:A:105:LEU:HD13	3:A:105:LEU:C	0.88	1.90	17	1
3:A:23:ALA:HB1	3:A:27:PHE:CE2	0.87	2.05	20	12
3:A:84:LEU:HD21	3:A:123:THR:C	0.87	1.90	2	10
3:A:88:THR:O	3:A:91:CYS:HB3	0.87	1.70	11	17
3:A:105:LEU:HD23	3:A:116:LEU:HD11	0.86	1.45	12	3
3:A:24:ASP:OD1	3:A:39:ARG:HG2	0.86	1.70	20	14
3:A:84:LEU:HD21	3:A:124:THR:HA	0.86	1.46	8	4
2:C:224:DT:OP2	3:A:129:LYS:CB	0.85	2.24	11	17
3:A:105:LEU:HD13	3:A:106:ALA:N	0.85	1.86	17	1
3:A:13:TRP:CE2	3:A:17:LEU:HD11	0.85	2.07	11	20
3:A:16:VAL:HA	3:A:40:PRO:HA	0.85	1.48	6	19
3:A:84:LEU:HD21	3:A:123:THR:HG21	0.85	1.46	4	1
3:A:24:ASP:O	3:A:78:ASN:N	0.84	2.11	6	20
3:A:94:LEU:HD23	3:A:100:VAL:CG1	0.84	2.02	14	4
3:A:105:LEU:HD12	3:A:116:LEU:HD13	0.84	1.48	7	1
3:A:84:LEU:CD2	3:A:123:THR:HG22	0.84	2.03	14	11
3:A:121:LYS:HB2	3:A:128:PRO:N	0.84	1.87	13	20
2:C:234:DT:H4'	3:A:45:ARG:HB3	0.84	1.49	13	3
2:C:233:DA:OP1	3:A:69:CYS:HA	0.83	1.74	7	12
1:B:201:DC:H2'	3:A:115:HIS:CE1	0.83	2.08	8	18
2:C:224:DT:OP1	3:A:130:ALA:N	0.83	2.11	8	13
2:C:224:DT:OP2	2:C:224:DT:H71	0.83	1.73	8	3
3:A:31:VAL:HG11	3:A:47:ALA:CB	0.83	2.04	6	18
3:A:13:TRP:CH2	3:A:17:LEU:HD21	0.82	2.09	14	15
3:A:127:THR:O	3:A:131:TRP:HB2	0.82	1.74	6	20
3:A:93:LEU:HD23	3:A:101:THR:HB	0.82	1.51	1	1
3:A:102:LEU:HD21	3:A:116:LEU:HD12	0.82	1.47	18	2
3:A:87:ILE:HG22	3:A:120:PHE:CZ	0.82	2.10	5	17
3:A:102:LEU:CD2	3:A:116:LEU:HD23	0.82	2.05	11	2
3:A:102:LEU:HD23	3:A:116:LEU:CD2	0.81	2.06	1	2
3:A:18:ALA:O	3:A:19:ARG:CG	0.80	2.29	7	10
3:A:16:VAL:HA	3:A:40:PRO:CA	0.80	2.06	6	19
2:C:224:DT:OP1	3:A:130:ALA:HA	0.80	1.75	7	3
3:A:78:ASN:N	3:A:79:PRO:CD	0.79	2.44	4	20
1:B:201:DC:H2'	3:A:115:HIS:NE2	0.79	1.92	1	15
3:A:84:LEU:HD21	3:A:124:THR:N	0.79	1.92	17	10
3:A:84:LEU:HG	3:A:124:THR:HA	0.79	1.53	13	8
3:A:31:VAL:HA	3:A:51:ASN:O	0.79	1.77	7	20
3:A:16:VAL:HG12	3:A:46:HIS:HE1	0.79	1.37	16	20

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:A:116:LEU:O	3:A:116:LEU:HD12	0.79	1.77	11	4
3:A:90:ALA:O	3:A:94:LEU:HD13	0.78	1.79	7	5
3:A:102:LEU:HD23	3:A:116:LEU:HD12	0.78	1.56	2	1
3:A:13:TRP:CD1	3:A:17:LEU:HD11	0.78	2.13	18	5
2:C:224:DT:H71	2:C:224:DT:OP2	0.77	1.79	11	3
3:A:39:ARG:HD3	3:A:77:ALA:HB2	0.77	1.55	3	2
2:C:234:DT:C4'	3:A:45:ARG:HB3	0.77	2.10	13	17
3:A:102:LEU:CD2	3:A:116:LEU:HD21	0.77	2.08	7	1
3:A:105:LEU:C	3:A:105:LEU:HD13	0.77	2.01	5	3
3:A:102:LEU:CD2	3:A:116:LEU:HD12	0.77	2.09	2	2
3:A:84:LEU:HD21	3:A:123:THR:CG2	0.76	2.09	4	6
3:A:27:PHE:CZ	3:A:40:PRO:HB3	0.76	2.14	13	17
2:C:233:DA:C5'	3:A:71:ARG:HB2	0.76	2.09	6	1
3:A:25:GLY:N	3:A:77:ALA:HB1	0.76	1.95	12	19
3:A:132:GLN:HA	3:A:135:TRP:CD1	0.76	2.16	14	4
3:A:121:LYS:HB2	3:A:128:PRO:CD	0.76	2.11	12	19
3:A:100:VAL:CG1	3:A:102:LEU:HD13	0.76	2.11	4	1
2:C:224:DT:OP2	3:A:129:LYS:CG	0.76	2.34	7	7
3:A:102:LEU:HD21	3:A:117:HIS:NE2	0.75	1.96	15	5
3:A:97:GLU:OE2	3:A:99:PRO:O	0.75	2.05	20	3
3:A:91:CYS:SG	3:A:135:TRP:HB2	0.75	2.21	3	10
3:A:29:PHE:HA	3:A:53:SER:O	0.75	1.81	8	20
3:A:105:LEU:HD22	3:A:116:LEU:HD13	0.75	1.57	6	1
3:A:102:LEU:HD12	3:A:102:LEU:O	0.74	1.82	8	1
3:A:105:LEU:HD23	3:A:116:LEU:HD21	0.74	1.59	10	5
2:C:233:DA:H5''	3:A:69:CYS:SG	0.74	2.23	11	18
3:A:24:ASP:C	3:A:77:ALA:HB1	0.73	2.03	3	19
3:A:106:ALA:HB1	3:A:111:MET:O	0.73	1.83	15	12
3:A:84:LEU:HD13	3:A:87:ILE:HD12	0.73	1.60	4	2
3:A:87:ILE:HG22	3:A:120:PHE:CE1	0.73	2.19	5	10
3:A:13:TRP:CZ3	3:A:16:VAL:HG11	0.73	2.19	13	20
3:A:94:LEU:HD22	3:A:132:GLN:CD	0.73	2.04	17	7
3:A:113:PRO:HA	3:A:116:LEU:HD23	0.73	1.60	7	2
3:A:94:LEU:CD1	3:A:100:VAL:HG13	0.72	2.14	4	1
3:A:31:VAL:HG11	3:A:47:ALA:HB3	0.72	1.61	18	16
3:A:87:ILE:O	3:A:90:ALA:HB3	0.72	1.84	3	20
3:A:93:LEU:HD23	3:A:101:THR:OG1	0.72	1.84	11	2
3:A:109:VAL:O	3:A:110:ALA:HB3	0.72	1.84	16	19
3:A:37:PHE:CG	3:A:61:ALA:HB1	0.72	2.20	11	20
3:A:102:LEU:HD23	3:A:113:PRO:CB	0.72	2.13	5	1
3:A:77:ALA:O	3:A:80:ARG:HB2	0.72	1.85	10	19

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:A:109:VAL:O	3:A:110:ALA:HB2	0.72	1.85	15	1
1:B:201:DC:C6	3:A:115:HIS:CE1	0.72	2.78	4	17
3:A:94:LEU:HD22	3:A:132:GLN:OE1	0.71	1.85	1	3
3:A:94:LEU:HD22	3:A:132:GLN:NE2	0.71	2.01	18	3
2:C:234:DT:OP2	3:A:36:ILE:CD1	0.71	2.37	16	7
3:A:77:ALA:C	3:A:79:PRO:HD2	0.71	2.06	16	20
3:A:18:ALA:O	3:A:19:ARG:HG2	0.70	1.87	14	7
3:A:101:THR:C	3:A:102:LEU:HD12	0.70	2.05	2	1
2:C:234:DT:H2'	2:C:235:DT:H71	0.70	1.61	15	19
3:A:24:ASP:OD1	3:A:39:ARG:HG3	0.70	1.86	8	1
3:A:39:ARG:NH2	3:A:75:ASP:OD2	0.70	2.25	14	10
3:A:109:VAL:HG11	3:A:111:MET:HE2	0.70	1.62	6	3
3:A:58:ALA:O	3:A:62:LEU:HG	0.70	1.86	3	20
3:A:100:VAL:CG1	3:A:102:LEU:HD12	0.70	2.17	11	1
3:A:109:VAL:HG11	3:A:111:MET:CE	0.70	2.16	6	3
3:A:39:ARG:CZ	3:A:75:ASP:OD1	0.70	2.40	17	12
3:A:39:ARG:HD2	3:A:77:ALA:HB2	0.70	1.64	13	3
3:A:93:LEU:CG	3:A:101:THR:OG1	0.70	2.39	4	1
2:C:233:DA:H5''	3:A:71:ARG:HB2	0.70	1.64	6	1
3:A:109:VAL:O	3:A:110:ALA:CB	0.69	2.39	15	20
3:A:29:PHE:O	3:A:37:PHE:HA	0.69	1.87	17	20
2:C:234:DT:H2''	2:C:235:DT:O5'	0.69	1.88	6	9
3:A:24:ASP:OD1	3:A:39:ARG:CD	0.69	2.40	3	3
2:C:224:DT:OP2	3:A:129:LYS:CD	0.69	2.40	7	1
3:A:39:ARG:NH1	3:A:75:ASP:OD1	0.69	2.26	16	10
3:A:84:LEU:HD22	3:A:123:THR:CG2	0.69	2.14	5	3
3:A:91:CYS:HB2	3:A:135:TRP:CD1	0.69	2.23	9	7
3:A:111:MET:CE	3:A:112:SER:O	0.69	2.41	3	2
3:A:73:GLN:N	3:A:74:PRO:CD	0.68	2.56	17	18
2:C:235:DT:P	3:A:47:ALA:HA	0.68	2.27	15	15
2:C:235:DT:OP1	3:A:47:ALA:HA	0.68	1.89	2	9
3:A:62:LEU:HD21	3:A:68:PRO:HG3	0.68	1.65	13	20
3:A:93:LEU:HD12	3:A:101:THR:OG1	0.68	1.88	4	1
2:C:233:DA:O4'	3:A:44:ALA:HB1	0.68	1.89	4	15
2:C:223:DT:H3'	3:A:129:LYS:HD2	0.68	1.65	19	2
3:A:39:ARG:NH2	3:A:75:ASP:OD1	0.68	2.27	5	10
3:A:105:LEU:HD22	3:A:105:LEU:O	0.68	1.88	17	1
3:A:102:LEU:CD2	3:A:117:HIS:NE2	0.68	2.57	19	5
3:A:93:LEU:HD13	3:A:97:GLU:OE1	0.68	1.89	9	1
3:A:84:LEU:CD2	3:A:124:THR:HA	0.68	2.18	6	1
3:A:8:THR:O	3:A:12:ARG:HD2	0.68	1.88	4	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:A:43:ARG:NH1	3:A:44:ALA:HB2	0.67	2.03	20	1
3:A:39:ARG:NH1	3:A:75:ASP:OD2	0.67	2.27	10	10
3:A:100:VAL:HG12	3:A:102:LEU:CD1	0.67	2.20	2	2
3:A:105:LEU:CD1	3:A:116:LEU:HD13	0.67	2.18	7	1
3:A:105:LEU:HD11	3:A:116:LEU:HB2	0.67	1.66	17	1
3:A:95:GLU:HB3	3:A:139:ARG:OXT	0.67	1.90	9	2
3:A:105:LEU:CD2	3:A:116:LEU:HD11	0.67	2.20	12	2
3:A:119:LEU:HD22	3:A:119:LEU:C	0.66	2.10	16	4
3:A:86:LYS:HE3	3:A:105:LEU:HD13	0.66	1.66	8	1
3:A:131:TRP:HA	3:A:131:TRP:CE3	0.66	2.24	2	7
3:A:105:LEU:HG	3:A:116:LEU:HD13	0.66	1.65	19	2
2:C:234:DT:OP2	3:A:36:ILE:HD13	0.66	1.90	6	1
3:A:102:LEU:HD23	3:A:113:PRO:HB2	0.66	1.67	16	1
3:A:16:VAL:CG1	3:A:29:PHE:CD2	0.66	2.79	13	19
3:A:77:ALA:O	3:A:80:ARG:CB	0.65	2.44	12	18
3:A:44:ALA:O	3:A:45:ARG:HB2	0.65	1.91	2	20
3:A:24:ASP:O	3:A:78:ASN:ND2	0.65	2.30	6	11
3:A:105:LEU:CD2	3:A:116:LEU:HD13	0.65	2.18	16	2
3:A:28:VAL:HG21	3:A:61:ALA:HB2	0.65	1.69	10	20
3:A:119:LEU:O	3:A:119:LEU:HD22	0.65	1.90	8	4
3:A:94:LEU:HD23	3:A:100:VAL:HG12	0.65	1.69	14	1
3:A:135:TRP:O	3:A:139:ARG:O	0.65	2.15	9	3
3:A:102:LEU:HD11	3:A:116:LEU:CB	0.65	2.21	14	5
3:A:111:MET:SD	3:A:115:HIS:HB2	0.65	2.31	2	1
3:A:97:GLU:OE1	3:A:99:PRO:O	0.65	2.14	14	3
3:A:28:VAL:HG22	3:A:55:TYR:HB2	0.64	1.69	10	20
3:A:93:LEU:HD21	3:A:97:GLU:OE1	0.64	1.91	4	1
3:A:100:VAL:HG12	3:A:102:LEU:HD11	0.64	1.68	1	2
2:C:224:DT:OP2	3:A:129:LYS:HG2	0.64	1.92	11	3
3:A:111:MET:CE	3:A:115:HIS:HB3	0.64	2.22	3	1
3:A:119:LEU:C	3:A:119:LEU:HD22	0.64	2.11	8	2
2:C:234:DT:H4'	3:A:45:ARG:CB	0.64	2.23	13	1
3:A:84:LEU:CD2	3:A:123:THR:HG21	0.64	2.21	4	1
3:A:90:ALA:HA	3:A:93:LEU:HD21	0.64	1.70	6	2
3:A:102:LEU:HD12	3:A:106:ALA:HB2	0.64	1.70	3	2
3:A:43:ARG:HD2	3:A:43:ARG:H	0.64	1.53	13	1
3:A:24:ASP:OD1	3:A:77:ALA:CB	0.64	2.46	18	4
2:C:234:DT:OP2	3:A:34:THR:HG21	0.64	1.93	3	8
3:A:121:LYS:HB2	3:A:128:PRO:CA	0.64	2.23	7	10
3:A:105:LEU:HD22	3:A:116:LEU:HD11	0.64	1.68	9	5
3:A:131:TRP:CE3	3:A:131:TRP:HA	0.64	2.28	4	11

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:A:111:MET:HE3	3:A:115:HIS:HB3	0.64	1.69	3	1
3:A:127:THR:HG22	3:A:130:ALA:HB3	0.64	1.68	8	4
3:A:87:ILE:HG22	3:A:120:PHE:CE2	0.63	2.28	1	14
3:A:102:LEU:HD11	3:A:113:PRO:HA	0.63	1.69	8	1
3:A:94:LEU:HG	3:A:100:VAL:HG12	0.63	1.69	3	2
2:C:223:DT:H73	3:A:114:PHE:CZ	0.63	2.28	18	7
3:A:84:LEU:HD22	3:A:124:THR:HA	0.63	1.69	6	1
3:A:37:PHE:O	3:A:37:PHE:CD1	0.63	2.52	6	10
3:A:76:LYS:O	3:A:80:ARG:HB2	0.63	1.92	7	4
3:A:94:LEU:HD23	3:A:132:GLN:HG3	0.63	1.68	4	1
3:A:12:ARG:N	3:A:12:ARG:HD2	0.62	2.09	16	3
3:A:98:THR:HB	3:A:99:PRO:CD	0.62	2.23	11	20
2:C:224:DT:H73	2:C:224:DT:OP2	0.62	1.94	15	5
3:A:127:THR:HG21	3:A:131:TRP:CD2	0.62	2.30	9	7
3:A:88:THR:HG23	3:A:135:TRP:CD1	0.62	2.30	13	1
3:A:13:TRP:CE2	3:A:17:LEU:HD21	0.62	2.30	1	15
2:C:233:DA:OP1	3:A:70:LYS:CB	0.62	2.47	6	2
3:A:17:LEU:HD23	3:A:17:LEU:N	0.62	2.10	3	5
3:A:105:LEU:HD23	3:A:116:LEU:CD1	0.62	2.25	12	2
2:C:233:DA:OP1	3:A:70:LYS:N	0.62	2.33	11	7
3:A:93:LEU:HD12	3:A:101:THR:N	0.62	2.10	4	1
3:A:93:LEU:CD1	3:A:101:THR:OG1	0.62	2.48	4	1
3:A:31:VAL:HG22	3:A:52:VAL:HG22	0.61	1.70	18	20
1:B:198:DA:H4'	3:A:43:ARG:O	0.61	1.95	3	3
3:A:94:LEU:HD22	3:A:132:GLN:HG2	0.61	1.71	16	2
1:B:201:DC:O5'	1:B:201:DC:H6	0.61	1.78	7	8
3:A:39:ARG:NH2	3:A:77:ALA:HB2	0.61	2.10	6	1
3:A:29:PHE:CE1	3:A:31:VAL:HG22	0.61	2.30	8	20
3:A:105:LEU:HB3	3:A:116:LEU:HD22	0.61	1.70	19	2
3:A:98:THR:CB	3:A:99:PRO:CD	0.61	2.78	11	19
3:A:12:ARG:HD2	3:A:12:ARG:N	0.61	2.08	3	4
3:A:37:PHE:CD2	3:A:61:ALA:HB1	0.61	2.31	20	20
3:A:16:VAL:HG12	3:A:46:HIS:CE1	0.61	2.29	13	13
1:B:202:DG:C2	1:B:203:DC:N3	0.61	2.68	7	20
3:A:102:LEU:HD21	3:A:116:LEU:CD1	0.61	2.25	18	1
3:A:116:LEU:HD13	3:A:116:LEU:C	0.61	2.16	2	8
1:B:201:DC:H2''	1:B:202:DG:O5'	0.61	1.96	3	20
3:A:102:LEU:HD22	3:A:117:HIS:NE2	0.61	2.11	19	1
3:A:111:MET:HE1	3:A:116:LEU:HD23	0.61	1.73	9	1
3:A:93:LEU:O	3:A:97:GLU:OE1	0.61	2.17	10	2
3:A:17:LEU:N	3:A:17:LEU:HD23	0.61	2.11	1	10

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:C:234:DT:O4'	3:A:45:ARG:CD	0.61	2.49	15	1
3:A:116:LEU:HD12	3:A:116:LEU:C	0.60	2.16	19	3
3:A:97:GLU:HG2	3:A:98:THR:N	0.60	2.11	8	2
3:A:105:LEU:CD2	3:A:116:LEU:HD21	0.60	2.26	10	2
3:A:97:GLU:C	3:A:97:GLU:CD	0.60	2.59	20	2
3:A:55:TYR:CD2	3:A:61:ALA:HB2	0.60	2.30	8	10
3:A:97:GLU:HG3	3:A:99:PRO:O	0.60	1.96	16	7
3:A:100:VAL:CG1	3:A:102:LEU:HD11	0.60	2.26	19	2
3:A:105:LEU:CD1	3:A:105:LEU:C	0.60	2.66	17	2
3:A:27:PHE:O	3:A:40:PRO:HD3	0.60	1.97	13	1
3:A:84:LEU:HD21	3:A:124:THR:CA	0.60	2.26	8	7
3:A:126:MET:O	3:A:127:THR:OG1	0.60	2.19	2	20
3:A:23:ALA:HB1	3:A:27:PHE:HE1	0.60	1.57	15	7
2:C:224:DT:H71	3:A:129:LYS:HD2	0.60	1.74	7	1
1:B:200:DG:H2''	1:B:201:DC:C5	0.60	2.31	7	9
3:A:84:LEU:HD21	3:A:123:THR:CB	0.60	2.26	20	4
3:A:31:VAL:CG1	3:A:33:THR:HG22	0.60	2.27	3	20
3:A:116:LEU:O	3:A:116:LEU:HD13	0.60	1.97	14	5
3:A:24:ASP:OD1	3:A:39:ARG:NE	0.59	2.35	18	5
3:A:24:ASP:OD1	3:A:40:PRO:HD2	0.59	1.97	17	2
3:A:116:LEU:C	3:A:116:LEU:HD12	0.59	2.17	11	3
3:A:116:LEU:HD12	3:A:116:LEU:O	0.59	1.96	6	1
3:A:84:LEU:HD13	3:A:87:ILE:CD1	0.59	2.28	4	1
3:A:92:ARG:O	3:A:96:GLN:N	0.59	2.35	16	16
3:A:102:LEU:HD22	3:A:113:PRO:CB	0.59	2.27	10	3
3:A:58:ALA:HB1	3:A:73:GLN:HE22	0.59	1.57	8	1
3:A:37:PHE:CD1	3:A:37:PHE:O	0.59	2.54	2	10
3:A:58:ALA:O	3:A:62:LEU:CG	0.59	2.50	2	20
3:A:23:ALA:HB1	3:A:27:PHE:HE2	0.59	1.57	1	4
3:A:116:LEU:C	3:A:116:LEU:HD13	0.59	2.18	8	6
3:A:94:LEU:HG	3:A:100:VAL:HG13	0.59	1.75	19	6
3:A:18:ALA:O	3:A:19:ARG:CB	0.59	2.51	18	6
3:A:109:VAL:HB	3:A:111:MET:SD	0.59	2.37	9	2
3:A:121:LYS:HG3	3:A:128:PRO:HD3	0.59	1.74	7	5
1:B:195:DT:H2''	1:B:196:DT:O5'	0.59	1.98	15	18
3:A:95:GLU:HB3	3:A:139:ARG:O	0.59	1.98	7	1
3:A:31:VAL:HG12	3:A:33:THR:CG2	0.59	2.24	12	15
3:A:94:LEU:HD13	3:A:132:GLN:OE1	0.59	1.98	18	2
2:C:231:DT:H2''	2:C:232:DA:O5'	0.58	1.97	7	20
3:A:25:GLY:N	3:A:77:ALA:CB	0.58	2.67	4	14
3:A:24:ASP:OD1	3:A:39:ARG:HD3	0.58	1.98	2	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:A:62:LEU:HD21	3:A:68:PRO:CG	0.58	2.28	6	20
3:A:94:LEU:HD11	3:A:102:LEU:CD1	0.58	2.24	7	1
3:A:84:LEU:HG	3:A:124:THR:CA	0.58	2.26	13	2
3:A:31:VAL:HB	3:A:34:THR:HG22	0.58	1.74	3	20
3:A:109:VAL:HG11	3:A:111:MET:HE3	0.58	1.74	10	3
3:A:13:TRP:CD1	3:A:49:ARG:HD3	0.58	2.33	10	1
2:C:224:DT:P	3:A:129:LYS:HB3	0.58	2.39	20	9
3:A:135:TRP:O	3:A:139:ARG:OXT	0.58	2.22	7	2
3:A:119:LEU:HD13	3:A:119:LEU:C	0.58	2.19	4	6
3:A:105:LEU:HD21	3:A:116:LEU:HD23	0.58	1.75	17	1
3:A:19:ARG:HA	3:A:41:SER:HA	0.58	1.76	15	19
3:A:125:GLY:O	3:A:126:MET:HG2	0.58	1.99	12	6
3:A:100:VAL:HG12	3:A:102:LEU:HD12	0.58	1.74	11	1
1:B:194:DA:N1	2:C:233:DA:N1	0.58	2.51	13	1
3:A:84:LEU:CD1	3:A:87:ILE:HD12	0.58	2.27	4	1
3:A:29:PHE:CD1	3:A:52:VAL:HG22	0.58	2.33	13	20
3:A:121:LYS:HD2	3:A:126:MET:HA	0.58	1.76	19	1
3:A:97:GLU:N	3:A:97:GLU:OE1	0.58	2.37	20	2
3:A:30:ALA:HB3	3:A:53:SER:OG	0.57	1.98	2	2
3:A:84:LEU:HD11	3:A:124:THR:N	0.57	2.14	3	6
3:A:69:CYS:HB3	3:A:72:CYS:HB2	0.57	1.75	8	1
3:A:87:ILE:HG21	3:A:120:PHE:CD1	0.57	2.33	2	14
3:A:14:GLN:O	3:A:18:ALA:CB	0.57	2.53	4	19
1:B:202:DG:C2	1:B:203:DC:C2	0.57	2.91	13	19
3:A:127:THR:HB	3:A:131:TRP:CE3	0.57	2.34	8	1
3:A:119:LEU:C	3:A:119:LEU:HD13	0.57	2.20	2	5
2:C:232:DA:H2''	2:C:233:DA:O5'	0.57	1.99	11	11
3:A:16:VAL:HG23	3:A:27:PHE:CZ	0.57	2.35	17	3
3:A:105:LEU:HB3	3:A:116:LEU:HD23	0.57	1.76	2	1
3:A:24:ASP:OD1	3:A:39:ARG:CG	0.57	2.53	9	17
3:A:24:ASP:OD1	3:A:39:ARG:HB3	0.57	2.00	4	14
3:A:118:ARG:HA	3:A:128:PRO:HB3	0.57	1.76	7	6
3:A:71:ARG:O	3:A:75:ASP:HB3	0.57	1.98	6	1
3:A:94:LEU:HD11	3:A:100:VAL:HG13	0.57	1.75	4	1
1:B:202:DG:N2	2:C:227:DG:C2	0.57	2.72	12	16
2:C:231:DT:O2	3:A:71:ARG:NH2	0.57	2.38	9	4
3:A:84:LEU:CD2	3:A:123:THR:CG2	0.57	2.82	4	5
1:B:190:DG:C5	1:B:191:DC:N4	0.57	2.73	10	20
3:A:119:LEU:HD22	3:A:119:LEU:O	0.57	2.00	18	3
3:A:28:VAL:HG23	3:A:29:PHE:N	0.56	2.15	16	20
3:A:97:GLU:CD	3:A:99:PRO:O	0.56	2.44	2	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:C:224:DT:OP2	2:C:224:DT:H73	0.56	1.99	19	5
3:A:121:LYS:CD	3:A:126:MET:HA	0.56	2.30	3	3
3:A:72:CYS:HA	3:A:75:ASP:OD2	0.56	1.99	14	5
2:C:224:DT:H71	3:A:129:LYS:CD	0.56	2.29	7	1
3:A:114:PHE:CD1	3:A:129:LYS:HE2	0.56	2.35	4	2
3:A:105:LEU:C	3:A:105:LEU:CD1	0.56	2.73	5	2
3:A:105:LEU:HD11	3:A:116:LEU:CB	0.56	2.31	17	1
3:A:125:GLY:O	3:A:126:MET:CG	0.56	2.54	9	19
2:C:235:DT:P	3:A:46:HIS:O	0.56	2.63	13	16
2:C:224:DT:OP1	3:A:130:ALA:CA	0.56	2.53	11	6
3:A:102:LEU:HB3	3:A:116:LEU:HD23	0.56	1.78	19	1
3:A:91:CYS:SG	3:A:135:TRP:CB	0.56	2.93	3	7
3:A:16:VAL:HG13	3:A:29:PHE:CD2	0.56	2.35	13	2
3:A:29:PHE:CE1	3:A:52:VAL:HG22	0.56	2.36	19	20
2:C:232:DA:C5	2:C:233:DA:C6	0.56	2.93	3	5
2:C:224:DT:H6	2:C:224:DT:O5'	0.56	1.84	18	2
3:A:19:ARG:CG	3:A:19:ARG:O	0.56	2.53	13	4
1:B:197:DA:C2	2:C:232:DA:C2	0.56	2.93	13	5
3:A:127:THR:HB	3:A:131:TRP:CG	0.56	2.36	15	8
3:A:27:PHE:CD1	3:A:27:PHE:C	0.56	2.78	20	9
3:A:93:LEU:HD11	3:A:97:GLU:OE2	0.56	2.00	4	1
3:A:73:GLN:HB3	3:A:74:PRO:HD3	0.56	1.77	2	3
2:C:223:DT:OP2	3:A:114:PHE:CZ	0.56	2.59	2	9
3:A:131:TRP:O	3:A:135:TRP:CG	0.56	2.59	11	7
3:A:127:THR:CG2	3:A:131:TRP:CE3	0.56	2.88	19	9
3:A:94:LEU:HD22	3:A:132:GLN:CG	0.56	2.31	9	2
3:A:102:LEU:HD23	3:A:113:PRO:CA	0.56	2.31	5	1
3:A:101:THR:O	3:A:102:LEU:HD12	0.56	2.01	4	2
3:A:18:ALA:O	3:A:19:ARG:HB3	0.56	1.99	13	1
3:A:117:HIS:CE1	3:A:129:LYS:HE3	0.56	2.36	19	1
3:A:131:TRP:CD1	3:A:135:TRP:CZ2	0.56	2.94	9	5
3:A:102:LEU:HD23	3:A:116:LEU:CD1	0.55	2.28	2	1
3:A:131:TRP:HA	3:A:131:TRP:HE3	0.55	1.61	2	2
2:C:223:DT:OP1	3:A:129:LYS:HE3	0.55	2.00	13	2
3:A:27:PHE:HA	3:A:55:TYR:O	0.55	2.00	20	18
3:A:31:VAL:CG1	3:A:47:ALA:HB3	0.55	2.31	9	14
3:A:13:TRP:HZ3	3:A:16:VAL:HG11	0.55	1.62	16	16
3:A:13:TRP:O	3:A:17:LEU:HD12	0.55	2.01	18	5
3:A:39:ARG:NH2	3:A:72:CYS:O	0.55	2.39	3	2
1:B:202:DG:N7	3:A:115:HIS:CE1	0.55	2.74	8	5
3:A:68:PRO:HB2	3:A:73:GLN:HB2	0.55	1.79	20	10

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:C:223:DT:H73	3:A:114:PHE:CE2	0.55	2.37	6	10
3:A:84:LEU:HD13	3:A:87:ILE:HG13	0.55	1.79	14	1
2:C:223:DT:P	3:A:129:LYS:CE	0.55	2.95	13	1
3:A:121:LYS:CD	3:A:128:PRO:HD3	0.55	2.32	4	1
3:A:28:VAL:HG21	3:A:37:PHE:CD1	0.55	2.36	8	20
1:B:202:DG:O6	3:A:118:ARG:CD	0.55	2.54	10	4
3:A:116:LEU:HG	3:A:117:HIS:N	0.55	2.17	16	1
3:A:26:GLU:O	3:A:56:ALA:O	0.55	2.24	9	16
3:A:16:VAL:C	3:A:17:LEU:HD23	0.55	2.21	8	15
3:A:77:ALA:O	3:A:80:ARG:N	0.55	2.38	10	4
3:A:105:LEU:HD22	3:A:116:LEU:CD2	0.55	2.31	2	1
3:A:117:HIS:CE1	3:A:129:LYS:CE	0.55	2.89	19	1
3:A:116:LEU:HD13	3:A:116:LEU:O	0.55	2.02	13	5
1:B:195:DT:O2	3:A:45:ARG:NH2	0.55	2.35	11	8
3:A:39:ARG:NE	3:A:72:CYS:O	0.55	2.40	2	4
3:A:13:TRP:O	3:A:17:LEU:HG	0.55	2.02	8	15
1:B:202:DG:H2''	1:B:203:DC:O5'	0.55	2.02	18	18
3:A:73:GLN:N	3:A:74:PRO:HD2	0.55	2.15	20	12
3:A:91:CYS:SG	3:A:135:TRP:HB3	0.55	2.42	11	1
2:C:235:DT:OP2	3:A:47:ALA:HB2	0.55	2.01	2	1
3:A:29:PHE:CE1	3:A:31:VAL:CG2	0.55	2.90	8	20
3:A:116:LEU:HD22	3:A:116:LEU:O	0.55	2.02	17	1
3:A:87:ILE:CG2	3:A:120:PHE:CG	0.54	2.90	1	10
3:A:91:CYS:HA	3:A:132:GLN:OE1	0.54	2.02	1	2
1:B:200:DG:N1	2:C:227:DG:C6	0.54	2.75	20	20
2:C:221:DT:C4	2:C:222:DC:N4	0.54	2.76	16	9
3:A:113:PRO:O	3:A:117:HIS:CD2	0.54	2.60	11	4
3:A:27:PHE:CE1	3:A:40:PRO:HB3	0.54	2.37	13	1
3:A:27:PHE:C	3:A:27:PHE:CD1	0.54	2.81	18	3
1:B:202:DG:C2	2:C:227:DG:N2	0.54	2.75	20	14
3:A:30:ALA:HB2	3:A:55:TYR:CE2	0.54	2.38	15	4
3:A:105:LEU:HD11	3:A:111:MET:CE	0.54	2.32	5	1
3:A:127:THR:HG21	3:A:131:TRP:HE3	0.54	1.62	17	5
3:A:102:LEU:HD12	3:A:102:LEU:N	0.54	2.17	2	1
1:B:206:DG:C6	1:B:207:DA:C6	0.54	2.96	20	20
3:A:58:ALA:HB1	3:A:73:GLN:NE2	0.54	2.16	8	1
2:C:234:DT:O4'	3:A:45:ARG:HG2	0.54	2.03	9	2
2:C:226:DC:N4	3:A:118:ARG:NH1	0.54	2.55	16	2
3:A:131:TRP:CD2	3:A:135:TRP:CZ2	0.54	2.96	2	1
2:C:224:DT:OP1	3:A:130:ALA:CB	0.54	2.54	9	3
2:C:234:DT:O4'	3:A:45:ARG:HB3	0.54	2.02	6	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:206:DG:C6	1:B:207:DA:N6	0.54	2.76	7	16
3:A:12:ARG:HA	3:A:12:ARG:NE	0.54	2.17	3	1
3:A:131:TRP:CG	3:A:135:TRP:CZ2	0.54	2.96	4	3
3:A:55:TYR:CE2	3:A:61:ALA:HA	0.54	2.38	3	20
1:B:199:DA:H2''	1:B:200:DG:O5'	0.54	2.02	5	20
2:C:222:DC:H2'	2:C:223:DT:H72	0.54	1.78	16	15
3:A:39:ARG:NH2	3:A:75:ASP:CG	0.54	2.61	20	4
3:A:18:ALA:O	3:A:19:ARG:HG3	0.54	2.02	7	5
3:A:59:SER:HA	3:A:62:LEU:HD12	0.54	1.79	3	17
2:C:223:DT:P	3:A:129:LYS:HE2	0.54	2.43	9	1
2:C:226:DC:N3	2:C:227:DG:C6	0.54	2.75	9	1
3:A:43:ARG:NH1	3:A:71:ARG:CD	0.54	2.71	7	1
3:A:87:ILE:CG2	3:A:120:PHE:CE1	0.54	2.91	8	15
3:A:43:ARG:HD2	3:A:43:ARG:N	0.54	2.17	13	1
3:A:8:THR:O	3:A:8:THR:HG22	0.54	2.03	20	1
3:A:16:VAL:CA	3:A:40:PRO:HA	0.54	2.31	6	1
3:A:109:VAL:CB	3:A:111:MET:HE3	0.54	2.33	4	1
3:A:119:LEU:O	3:A:119:LEU:HD23	0.53	2.03	11	2
1:B:198:DA:C2	1:B:199:DA:C2	0.53	2.95	13	1
3:A:131:TRP:CD2	3:A:135:TRP:CH2	0.53	2.96	2	1
3:A:117:HIS:ND1	3:A:129:LYS:HG3	0.53	2.18	7	1
3:A:15:SER:OG	3:A:23:ALA:HB3	0.53	2.03	7	2
3:A:94:LEU:CG	3:A:100:VAL:HG13	0.53	2.33	4	1
3:A:121:LYS:HD3	3:A:128:PRO:HD3	0.53	1.79	4	1
3:A:36:ILE:HG22	3:A:37:PHE:N	0.53	2.18	2	20
3:A:121:LYS:HA	3:A:124:THR:HG22	0.53	1.80	18	19
3:A:102:LEU:HD23	3:A:117:HIS:NE2	0.53	2.18	3	1
3:A:91:CYS:SG	3:A:135:TRP:CG	0.53	3.02	4	7
3:A:94:LEU:HD13	3:A:132:GLN:NE2	0.53	2.18	6	1
2:C:234:DT:H4'	3:A:45:ARG:C	0.53	2.23	6	2
3:A:117:HIS:O	3:A:128:PRO:CB	0.53	2.56	12	13
2:C:223:DT:OP2	3:A:114:PHE:CE1	0.53	2.62	6	8
2:C:235:DT:C5'	3:A:45:ARG:HG2	0.53	2.34	13	1
3:A:93:LEU:HD13	3:A:93:LEU:O	0.53	2.04	4	1
3:A:72:CYS:HA	3:A:75:ASP:HB3	0.53	1.79	8	1
3:A:39:ARG:NH2	3:A:76:LYS:C	0.53	2.61	20	1
3:A:105:LEU:HD22	3:A:116:LEU:CD1	0.53	2.32	6	1
3:A:87:ILE:CG2	3:A:120:PHE:CD1	0.53	2.92	6	20
3:A:8:THR:HG22	3:A:11:GLN:H	0.53	1.64	2	9
3:A:127:THR:HG22	3:A:131:TRP:N	0.53	2.19	11	10
2:C:223:DT:H2''	2:C:224:DT:O5'	0.53	2.04	3	4

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:201:DC:H6	1:B:201:DC:O5'	0.53	1.86	8	2
3:A:119:LEU:C	3:A:119:LEU:HD23	0.53	2.24	11	2
2:C:223:DT:P	3:A:129:LYS:HD3	0.53	2.44	10	1
3:A:8:THR:C	3:A:12:ARG:HD2	0.53	2.25	18	2
3:A:98:THR:HB	3:A:99:PRO:HD3	0.53	1.80	13	2
3:A:117:HIS:HB3	3:A:129:LYS:CA	0.53	2.34	7	2
3:A:84:LEU:HD13	3:A:123:THR:HB	0.53	1.79	7	1
3:A:102:LEU:HB3	3:A:113:PRO:HB3	0.53	1.80	16	1
3:A:28:VAL:O	3:A:54:PHE:HA	0.53	2.03	9	20
3:A:39:ARG:CZ	3:A:75:ASP:OD2	0.53	2.57	7	4
3:A:91:CYS:HA	3:A:132:GLN:HG2	0.53	1.81	8	2
3:A:24:ASP:CG	3:A:77:ALA:CB	0.53	2.78	8	2
2:C:225:DG:N7	3:A:118:ARG:NH1	0.53	2.57	16	2
2:C:224:DT:H3'	3:A:130:ALA:HB2	0.53	1.80	7	1
3:A:37:PHE:CE1	3:A:58:ALA:HA	0.52	2.38	13	20
1:B:196:DT:H2''	1:B:197:DA:O5'	0.52	2.04	20	20
3:A:93:LEU:CB	3:A:101:THR:OG1	0.52	2.58	4	1
2:C:226:DC:H41	3:A:118:ARG:NH2	0.52	2.00	7	4
1:B:202:DG:C2	2:C:227:DG:C2	0.52	2.97	13	11
3:A:102:LEU:CD1	3:A:106:ALA:HB2	0.52	2.34	8	2
3:A:95:GLU:HB2	3:A:136:ARG:HA	0.52	1.82	9	1
3:A:39:ARG:NH1	3:A:75:ASP:CG	0.52	2.63	2	4
2:C:226:DC:H2''	2:C:227:DG:O5'	0.52	2.03	5	10
3:A:111:MET:HB2	3:A:115:HIS:HB3	0.52	1.80	5	2
2:C:230:DT:H2'	2:C:231:DT:H71	0.52	1.82	11	14
3:A:23:ALA:HB1	3:A:27:PHE:CE1	0.52	2.38	8	6
2:C:232:DA:H2''	2:C:233:DA:C8	0.52	2.40	19	11
3:A:127:THR:CB	3:A:131:TRP:CE3	0.52	2.93	8	1
3:A:16:VAL:O	3:A:40:PRO:O	0.52	2.28	16	11
3:A:90:ALA:C	3:A:94:LEU:HD12	0.52	2.22	9	3
1:B:202:DG:N3	1:B:203:DC:C2	0.52	2.77	3	5
1:B:198:DA:H4'	3:A:43:ARG:HG3	0.52	1.81	13	1
3:A:13:TRP:CZ3	3:A:16:VAL:CG1	0.52	2.92	13	20
2:C:225:DG:C2	2:C:226:DC:N3	0.52	2.77	7	2
2:C:225:DG:C6	3:A:118:ARG:NH1	0.52	2.78	6	1
3:A:94:LEU:HD13	3:A:132:GLN:HG3	0.51	1.82	8	1
3:A:94:LEU:CG	3:A:100:VAL:HG12	0.51	2.35	3	1
3:A:116:LEU:O	3:A:116:LEU:HD22	0.51	2.04	5	1
3:A:57:ASN:OD1	3:A:59:SER:HB3	0.51	2.05	9	20
3:A:16:VAL:HG22	3:A:27:PHE:CE1	0.51	2.40	20	8
3:A:77:ALA:O	3:A:80:ARG:HB3	0.51	2.06	14	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:C:223:DT:H3'	3:A:129:LYS:HB3	0.51	1.82	5	1
2:C:232:DA:C6	2:C:233:DA:C6	0.51	2.99	2	1
3:A:29:PHE:HD1	3:A:52:VAL:HG13	0.51	1.65	12	20
3:A:37:PHE:O	3:A:37:PHE:CG	0.51	2.64	12	7
3:A:117:HIS:CE1	3:A:132:GLN:HB2	0.51	2.40	5	1
3:A:78:ASN:C	3:A:80:ARG:H	0.51	2.09	10	1
3:A:93:LEU:HD12	3:A:94:LEU:N	0.51	2.20	6	1
3:A:24:ASP:O	3:A:78:ASN:CB	0.51	2.59	7	14
3:A:29:PHE:CD1	3:A:52:VAL:HG13	0.51	2.41	12	14
3:A:78:ASN:C	3:A:80:ARG:N	0.51	2.63	10	3
3:A:55:TYR:CD2	3:A:61:ALA:CB	0.51	2.94	8	10
3:A:13:TRP:CZ3	3:A:52:VAL:HG11	0.51	2.41	14	17
1:B:201:DC:O5'	3:A:115:HIS:CE1	0.51	2.64	19	1
3:A:94:LEU:HD23	3:A:100:VAL:HG13	0.51	1.83	9	1
2:C:223:DT:H3'	3:A:129:LYS:HG2	0.51	1.82	9	1
2:C:223:DT:H72	3:A:114:PHE:CE2	0.51	2.41	8	1
3:A:12:ARG:H	3:A:12:ARG:HD2	0.51	1.66	10	2
3:A:109:VAL:HG21	3:A:111:MET:HE1	0.51	1.83	1	1
3:A:93:LEU:HD23	3:A:101:THR:CB	0.51	2.31	1	1
3:A:125:GLY:O	3:A:126:MET:HG3	0.51	2.06	15	3
2:C:223:DT:P	3:A:129:LYS:NZ	0.51	2.84	11	1
3:A:11:GLN:O	3:A:14:GLN:N	0.51	2.44	7	14
3:A:102:LEU:HD22	3:A:113:PRO:HB2	0.51	1.82	10	2
3:A:77:ALA:N	3:A:79:PRO:HG2	0.51	2.21	5	8
3:A:9:ASP:HA	3:A:12:ARG:HB2	0.50	1.82	20	8
3:A:114:PHE:HA	3:A:117:HIS:ND1	0.50	2.21	19	1
3:A:93:LEU:HD21	3:A:97:GLU:CD	0.50	2.27	4	1
3:A:8:THR:HG22	3:A:8:THR:O	0.50	2.06	17	2
1:B:201:DC:C2	1:B:202:DG:C5	0.50	2.99	9	4
3:A:75:ASP:OD1	3:A:75:ASP:C	0.50	2.49	17	1
3:A:70:LYS:O	3:A:74:PRO:CD	0.50	2.60	6	1
3:A:37:PHE:CG	3:A:37:PHE:O	0.50	2.65	10	13
3:A:126:MET:C	3:A:127:THR:OG1	0.50	2.50	18	18
3:A:116:LEU:HD13	3:A:117:HIS:N	0.50	2.21	5	2
3:A:12:ARG:HD3	3:A:27:PHE:CE2	0.50	2.42	1	1
3:A:97:GLU:OE1	3:A:98:THR:N	0.50	2.45	2	2
3:A:90:ALA:O	3:A:94:LEU:CD1	0.50	2.59	18	16
3:A:37:PHE:CG	3:A:61:ALA:CB	0.50	2.95	11	20
3:A:93:LEU:HD13	3:A:101:THR:OG1	0.50	2.05	18	1
2:C:224:DT:O4	3:A:118:ARG:NH2	0.50	2.44	8	1
3:A:117:HIS:ND1	3:A:129:LYS:HD3	0.50	2.21	9	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:202:DG:O6	3:A:118:ARG:HD3	0.50	2.07	16	3
3:A:119:LEU:C	3:A:119:LEU:CD2	0.50	2.80	17	3
1:B:201:DC:O5'	3:A:115:HIS:HE1	0.50	1.89	10	1
3:A:87:ILE:HG21	3:A:120:PHE:CG	0.50	2.41	2	3
3:A:77:ALA:C	3:A:79:PRO:CD	0.50	2.79	10	17
1:B:201:DC:P	3:A:115:HIS:HE1	0.50	2.29	19	1
3:A:102:LEU:HD12	3:A:102:LEU:C	0.50	2.27	8	1
3:A:127:THR:CG2	3:A:130:ALA:HB3	0.50	2.35	8	2
3:A:105:LEU:O	3:A:109:VAL:HG23	0.50	2.06	20	6
2:C:223:DT:C7	3:A:114:PHE:CZ	0.50	2.95	16	1
1:B:204:DA:C2	2:C:225:DG:C2	0.50	2.99	16	1
1:B:202:DG:C6	1:B:203:DC:N4	0.50	2.79	13	7
3:A:70:LYS:HD2	3:A:70:LYS:O	0.50	2.07	12	1
2:C:234:DT:P	3:A:36:ILE:HD13	0.50	2.47	6	1
3:A:71:ARG:O	3:A:75:ASP:CB	0.50	2.59	6	1
3:A:91:CYS:HA	3:A:135:TRP:CD1	0.50	2.42	4	1
3:A:94:LEU:HD23	3:A:132:GLN:CG	0.50	2.36	4	2
2:C:225:DG:H2''	2:C:226:DC:O5'	0.50	2.07	3	6
2:C:234:DT:C3'	3:A:46:HIS:O	0.50	2.60	18	1
3:A:24:ASP:O	3:A:78:ASN:CA	0.50	2.60	4	3
2:C:232:DA:N3	3:A:43:ARG:NH2	0.50	2.60	2	2
3:A:39:ARG:CZ	3:A:75:ASP:CG	0.50	2.80	20	3
3:A:37:PHE:CD1	3:A:37:PHE:C	0.50	2.85	13	14
3:A:64:ALA:HB3	3:A:66:PHE:CD2	0.50	2.42	18	7
3:A:109:VAL:HG11	3:A:119:LEU:HG	0.50	1.84	20	1
3:A:105:LEU:HD12	3:A:116:LEU:HB2	0.50	1.84	1	1
3:A:91:CYS:SG	3:A:136:ARG:N	0.49	2.85	19	8
1:B:202:DG:C5	1:B:203:DC:C4	0.49	3.00	13	5
3:A:105:LEU:HD11	3:A:116:LEU:HD23	0.49	1.83	5	1
3:A:97:GLU:CD	3:A:97:GLU:C	0.49	2.71	6	1
2:C:225:DG:C2	2:C:226:DC:C2	0.49	3.00	2	3
2:C:224:DT:OP2	2:C:224:DT:C7	0.49	2.61	19	7
3:A:102:LEU:HD13	3:A:102:LEU:O	0.49	2.06	3	3
3:A:105:LEU:CD2	3:A:116:LEU:HD22	0.49	2.37	11	1
3:A:71:ARG:O	3:A:75:ASP:CG	0.49	2.51	6	1
3:A:93:LEU:HG	3:A:101:THR:OG1	0.49	2.05	4	1
1:B:198:DA:H4'	3:A:43:ARG:CG	0.49	2.38	13	1
3:A:13:TRP:CG	3:A:49:ARG:CD	0.49	2.94	10	1
3:A:28:VAL:CG2	3:A:37:PHE:CD1	0.49	2.96	8	20
3:A:121:LYS:O	3:A:125:GLY:N	0.49	2.45	14	18
3:A:31:VAL:CG1	3:A:47:ALA:CB	0.49	2.90	9	17

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:A:114:PHE:O	3:A:118:ARG:HG2	0.49	2.07	14	2
3:A:102:LEU:CG	3:A:116:LEU:HD21	0.49	2.36	7	1
3:A:25:GLY:HA3	3:A:78:ASN:H	0.49	1.68	12	5
3:A:119:LEU:CD2	3:A:119:LEU:C	0.49	2.80	5	1
3:A:27:PHE:CZ	3:A:40:PRO:CB	0.49	2.92	13	1
3:A:16:VAL:CA	3:A:40:PRO:O	0.49	2.49	13	1
3:A:105:LEU:CD1	3:A:116:LEU:HG	0.49	2.37	17	1
3:A:117:HIS:HB3	3:A:129:LYS:N	0.49	2.22	2	2
3:A:87:ILE:HB	3:A:120:PHE:CE1	0.49	2.43	12	10
3:A:121:LYS:HD3	3:A:127:THR:N	0.49	2.22	19	2
2:C:226:DC:H41	3:A:118:ARG:CZ	0.49	2.19	7	2
3:A:102:LEU:HD11	3:A:116:LEU:HB3	0.49	1.83	14	1
3:A:49:ARG:HA	3:A:52:VAL:HB	0.49	1.85	10	19
3:A:57:ASN:OD1	3:A:60:GLU:N	0.49	2.45	9	10
3:A:19:ARG:HG3	3:A:19:ARG:O	0.49	2.07	13	2
3:A:39:ARG:CD	3:A:77:ALA:HB2	0.49	2.37	14	3
3:A:43:ARG:NE	3:A:43:ARG:O	0.49	2.45	12	1
3:A:93:LEU:HB3	3:A:101:THR:OG1	0.49	2.07	4	4
3:A:24:ASP:HA	3:A:40:PRO:HD2	0.49	1.85	6	4
3:A:90:ALA:O	3:A:93:LEU:HG	0.49	2.08	6	1
3:A:84:LEU:HD21	3:A:123:THR:O	0.49	2.08	19	3
2:C:226:DC:N4	3:A:118:ARG:NH2	0.49	2.60	4	2
1:B:202:DG:N3	2:C:227:DG:N2	0.49	2.60	13	6
2:C:233:DA:O4'	3:A:44:ALA:CB	0.49	2.60	4	5
3:A:109:VAL:CG1	3:A:111:MET:HE3	0.49	2.37	4	1
2:C:233:DA:H1'	3:A:44:ALA:HB1	0.49	1.85	2	1
3:A:120:PHE:O	3:A:124:THR:HG22	0.49	2.08	8	8
1:B:191:DC:H2''	1:B:192:DA:OP2	0.49	2.08	6	6
1:B:197:DA:C6	1:B:198:DA:C6	0.49	3.01	4	3
3:A:131:TRP:O	3:A:135:TRP:CD2	0.49	2.66	14	4
3:A:18:ALA:O	3:A:19:ARG:CD	0.49	2.61	18	1
3:A:77:ALA:HB3	3:A:79:PRO:HD2	0.49	1.84	8	4
1:B:193:DA:N6	2:C:234:DT:O4	0.49	2.46	8	12
3:A:121:LYS:CG	3:A:128:PRO:HD3	0.48	2.38	2	5
3:A:37:PHE:CE2	3:A:62:LEU:HG	0.48	2.43	8	19
3:A:87:ILE:O	3:A:90:ALA:CB	0.48	2.60	17	18
1:B:202:DG:C5	1:B:203:DC:N4	0.48	2.81	8	5
3:A:97:GLU:CG	3:A:99:PRO:O	0.48	2.61	10	3
3:A:23:ALA:O	3:A:40:PRO:HG3	0.48	2.07	13	1
3:A:87:ILE:HG23	3:A:120:PHE:CD2	0.48	2.43	16	7
3:A:94:LEU:HD23	3:A:100:VAL:HG11	0.48	1.82	14	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:A:94:LEU:HA	3:A:100:VAL:HG22	0.48	1.84	11	1
3:A:98:THR:H	3:A:99:PRO:HD2	0.48	1.68	19	8
3:A:95:GLU:HB3	3:A:139:ARG:C	0.48	2.28	7	2
3:A:93:LEU:O	3:A:97:GLU:HG3	0.48	2.08	14	2
2:C:223:DT:P	3:A:129:LYS:HE3	0.48	2.48	13	2
3:A:105:LEU:HD11	3:A:116:LEU:HG	0.48	1.85	17	1
3:A:30:ALA:HA	3:A:36:ILE:O	0.48	2.08	17	7
3:A:9:ASP:N	3:A:9:ASP:OD1	0.48	2.46	5	3
1:B:199:DA:H5'	3:A:43:ARG:CB	0.48	2.39	20	3
3:A:36:ILE:CG2	3:A:37:PHE:N	0.48	2.77	11	20
1:B:204:DA:H2''	1:B:205:DA:O5'	0.48	2.09	10	17
1:B:193:DA:H2''	1:B:194:DA:O5'	0.48	2.09	9	16
2:C:232:DA:C5	2:C:233:DA:N6	0.48	2.82	5	1
2:C:234:DT:H5'	3:A:45:ARG:HB3	0.48	1.85	9	5
3:A:112:SER:CB	3:A:113:PRO:HD2	0.48	2.39	2	1
3:A:16:VAL:HG11	3:A:29:PHE:CD2	0.48	2.43	16	18
3:A:70:LYS:O	3:A:74:PRO:HG3	0.48	2.09	14	8
3:A:29:PHE:HE1	3:A:31:VAL:HG22	0.48	1.69	3	14
3:A:13:TRP:NE1	3:A:17:LEU:CD1	0.48	2.75	6	6
3:A:102:LEU:HD11	3:A:116:LEU:HG	0.48	1.86	3	1
3:A:117:HIS:ND1	3:A:129:LYS:HD2	0.48	2.24	3	1
3:A:131:TRP:CE2	3:A:135:TRP:CZ2	0.48	3.02	17	4
3:A:39:ARG:NH1	3:A:77:ALA:N	0.48	2.62	2	1
3:A:111:MET:HE2	3:A:112:SER:N	0.48	2.24	3	1
1:B:198:DA:C2	1:B:199:DA:N1	0.48	2.81	13	1
3:A:8:THR:O	3:A:12:ARG:HD3	0.48	2.07	17	1
1:B:193:DA:C2	1:B:194:DA:C5	0.48	3.02	2	1
1:B:194:DA:H2''	1:B:195:DT:O5'	0.48	2.09	2	7
3:A:109:VAL:HG11	3:A:111:MET:HE1	0.48	1.85	1	1
3:A:87:ILE:CG2	3:A:120:PHE:CZ	0.47	2.96	18	4
3:A:87:ILE:CG2	3:A:120:PHE:CD2	0.47	2.97	1	8
3:A:105:LEU:CB	3:A:116:LEU:HD22	0.47	2.38	19	1
3:A:13:TRP:CD1	3:A:17:LEU:CD1	0.47	2.95	18	5
3:A:95:GLU:CB	3:A:136:ARG:HA	0.47	2.40	9	1
1:B:197:DA:N3	3:A:43:ARG:NH2	0.47	2.62	12	3
2:C:227:DG:C8	2:C:228:DC:C4	0.47	3.02	5	1
3:A:131:TRP:CE3	3:A:135:TRP:CH2	0.47	3.02	2	1
3:A:43:ARG:NE	3:A:71:ARG:HD3	0.47	2.23	9	1
3:A:12:ARG:N	3:A:12:ARG:CD	0.47	2.77	20	2
3:A:8:THR:O	3:A:11:GLN:N	0.47	2.46	4	5
3:A:16:VAL:CG2	3:A:27:PHE:CZ	0.47	2.97	14	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:A:12:ARG:HB3	3:A:27:PHE:CE2	0.47	2.44	6	2
2:C:223:DT:OP1	3:A:129:LYS:HD3	0.47	2.09	4	2
3:A:54:PHE:CD1	3:A:54:PHE:N	0.47	2.81	2	1
3:A:43:ARG:CZ	3:A:71:ARG:NH2	0.47	2.77	2	1
3:A:105:LEU:CG	3:A:116:LEU:HD13	0.47	2.36	19	1
3:A:111:MET:HE3	3:A:112:SER:O	0.47	2.10	9	1
3:A:70:LYS:O	3:A:70:LYS:CD	0.47	2.63	7	1
3:A:94:LEU:HD22	3:A:132:GLN:HG3	0.47	1.85	12	2
3:A:16:VAL:HG22	3:A:27:PHE:HE1	0.47	1.69	20	2
3:A:102:LEU:HD13	3:A:116:LEU:HG	0.47	1.87	8	1
3:A:117:HIS:CE1	3:A:132:GLN:OE1	0.47	2.67	7	1
3:A:91:CYS:SG	3:A:139:ARG:OXT	0.47	2.72	7	1
3:A:113:PRO:O	3:A:117:HIS:ND1	0.47	2.48	3	3
2:C:223:DT:OP1	3:A:129:LYS:CE	0.47	2.63	13	4
3:A:117:HIS:O	3:A:128:PRO:HB3	0.47	2.09	8	7
1:B:201:DC:P	3:A:115:HIS:CE1	0.47	3.07	19	1
3:A:54:PHE:CD2	3:A:54:PHE:N	0.47	2.82	1	2
3:A:92:ARG:O	3:A:96:GLN:CB	0.47	2.63	10	3
1:B:195:DT:O4	2:C:233:DA:N1	0.47	2.48	13	1
3:A:109:VAL:HG12	3:A:111:MET:SD	0.47	2.49	20	1
3:A:121:LYS:HB2	3:A:128:PRO:HD3	0.47	1.86	4	1
1:B:198:DA:C4'	3:A:43:ARG:O	0.47	2.63	7	4
3:A:117:HIS:CD2	3:A:129:LYS:NZ	0.47	2.82	5	1
3:A:13:TRP:CD1	3:A:49:ARG:CD	0.47	2.97	10	1
3:A:91:CYS:SG	3:A:135:TRP:CD2	0.47	3.08	7	4
3:A:84:LEU:HA	3:A:87:ILE:HG13	0.47	1.86	4	1
3:A:97:GLU:OE1	3:A:99:PRO:N	0.47	2.48	14	2
3:A:120:PHE:O	3:A:124:THR:CG2	0.47	2.63	4	11
3:A:94:LEU:HG	3:A:100:VAL:CG1	0.47	2.40	1	4
3:A:91:CYS:HB2	3:A:135:TRP:CG	0.47	2.45	9	2
2:C:234:DT:O4'	3:A:45:ARG:HD2	0.47	2.09	15	2
3:A:111:MET:CE	3:A:115:HIS:CB	0.47	2.93	3	1
3:A:111:MET:CG	3:A:115:HIS:HB3	0.46	2.40	18	2
3:A:31:VAL:HG22	3:A:52:VAL:CG2	0.46	2.40	6	3
2:C:230:DT:C2	2:C:231:DT:C4	0.46	3.03	10	2
3:A:91:CYS:SG	3:A:132:GLN:O	0.46	2.71	20	1
2:C:233:DA:C1'	3:A:44:ALA:HB1	0.46	2.40	2	1
1:B:200:DG:C2'	1:B:201:DC:C5	0.46	2.98	7	4
3:A:39:ARG:NE	3:A:77:ALA:HB2	0.46	2.24	11	1
3:A:43:ARG:NH1	3:A:44:ALA:CB	0.46	2.75	20	1
3:A:121:LYS:CE	3:A:128:PRO:HD3	0.46	2.41	4	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:A:16:VAL:CG2	3:A:27:PHE:CE2	0.46	2.98	8	5
3:A:134:ALA:O	3:A:137:ALA:HB3	0.46	2.11	11	2
1:B:201:DC:H2'	3:A:115:HIS:CD2	0.46	2.45	4	3
2:C:227:DG:C4	2:C:228:DC:N3	0.46	2.83	5	1
2:C:235:DT:H5''	3:A:45:ARG:HG2	0.46	1.87	13	1
3:A:117:HIS:CE1	3:A:132:GLN:NE2	0.46	2.84	16	1
3:A:127:THR:CG2	3:A:131:TRP:CD2	0.46	2.99	4	1
3:A:13:TRP:HA	3:A:13:TRP:CE3	0.46	2.45	18	8
2:C:233:DA:H3'	3:A:36:ILE:CD1	0.46	2.40	3	3
3:A:94:LEU:CD2	3:A:100:VAL:CG1	0.46	2.93	3	2
3:A:12:ARG:HD2	3:A:27:PHE:CD1	0.46	2.45	12	2
3:A:121:LYS:HD3	3:A:126:MET:HA	0.46	1.86	5	1
3:A:117:HIS:CD2	3:A:129:LYS:CD	0.46	2.98	5	1
3:A:23:ALA:C	3:A:40:PRO:HG3	0.46	2.30	20	4
3:A:113:PRO:O	3:A:117:HIS:CE1	0.46	2.68	19	1
3:A:105:LEU:HD11	3:A:116:LEU:CG	0.46	2.41	17	1
3:A:13:TRP:CD1	3:A:49:ARG:HG3	0.46	2.45	6	3
3:A:102:LEU:HD13	3:A:102:LEU:C	0.46	2.31	14	1
3:A:132:GLN:O	3:A:135:TRP:HB2	0.46	2.10	14	1
3:A:84:LEU:HD13	3:A:123:THR:CG2	0.46	2.39	7	1
3:A:37:PHE:CZ	3:A:58:ALA:HB1	0.46	2.46	3	9
3:A:114:PHE:CD1	3:A:114:PHE:N	0.46	2.84	18	2
3:A:135:TRP:O	3:A:139:ARG:N	0.46	2.49	18	2
3:A:30:ALA:HB2	3:A:55:TYR:HE2	0.46	1.71	15	4
2:C:224:DT:OP2	3:A:129:LYS:C	0.46	2.54	7	1
2:C:233:DA:C5'	3:A:69:CYS:SG	0.46	3.04	3	4
1:B:196:DT:O4'	3:A:45:ARG:NH2	0.46	2.49	15	1
3:A:121:LYS:CE	3:A:126:MET:HA	0.46	2.41	3	1
3:A:105:LEU:HD11	3:A:111:MET:HE3	0.46	1.86	5	1
3:A:24:ASP:OD1	3:A:39:ARG:HD2	0.46	2.11	19	3
3:A:13:TRP:CE3	3:A:52:VAL:HG11	0.46	2.45	14	1
3:A:135:TRP:CE3	3:A:135:TRP:N	0.46	2.84	2	1
3:A:14:GLN:O	3:A:18:ALA:HB2	0.46	2.10	14	4
1:B:198:DA:C5'	3:A:43:ARG:CG	0.46	2.94	13	1
3:A:84:LEU:HD21	3:A:123:THR:HB	0.46	1.87	20	1
3:A:29:PHE:CE1	3:A:52:VAL:CG2	0.45	2.99	11	18
2:C:233:DA:H3'	3:A:36:ILE:HD13	0.45	1.88	3	4
3:A:11:GLN:O	3:A:12:ARG:C	0.45	2.53	10	13
3:A:95:GLU:CG	3:A:139:ARG:OXT	0.45	2.65	11	3
3:A:9:ASP:OD1	3:A:10:ASP:N	0.45	2.49	3	1
2:C:231:DT:H2''	2:C:232:DA:C5'	0.45	2.40	2	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:A:37:PHE:CD2	3:A:61:ALA:CB	0.45	2.99	20	7
2:C:224:DT:O5'	2:C:224:DT:C6	0.45	2.69	18	1
3:A:127:THR:HB	3:A:131:TRP:HB2	0.45	1.88	8	1
3:A:75:ASP:C	3:A:75:ASP:OD1	0.45	2.53	9	1
2:C:225:DG:C6	2:C:226:DC:N4	0.45	2.84	7	1
2:C:226:DC:N4	3:A:118:ARG:HH12	0.45	2.08	6	1
3:A:39:ARG:NH2	3:A:77:ALA:CB	0.45	2.78	6	1
1:B:201:DC:N4	3:A:118:ARG:NH2	0.45	2.64	4	1
2:C:235:DT:OP1	3:A:47:ALA:CA	0.45	2.61	2	1
1:B:202:DG:C4	1:B:203:DC:C4	0.45	3.03	3	3
3:A:121:LYS:HG3	3:A:127:THR:N	0.45	2.26	9	2
3:A:19:ARG:CD	3:A:19:ARG:O	0.45	2.64	13	1
3:A:31:VAL:HG11	3:A:47:ALA:HB1	0.45	1.86	6	1
3:A:131:TRP:NE1	3:A:135:TRP:CZ2	0.45	2.85	18	2
3:A:87:ILE:HG22	3:A:120:PHE:CD2	0.45	2.46	12	4
3:A:127:THR:OG1	3:A:131:TRP:CE3	0.45	2.66	8	1
3:A:111:MET:CE	3:A:116:LEU:HB2	0.45	2.40	9	1
1:B:202:DG:N7	3:A:115:HIS:CD2	0.45	2.84	4	5
2:C:224:DT:H2''	2:C:225:DG:O5'	0.45	2.10	7	1
2:C:225:DG:N7	3:A:118:ARG:NH2	0.45	2.64	12	2
3:A:17:LEU:CD2	3:A:17:LEU:N	0.45	2.80	12	1
2:C:224:DT:C7	2:C:224:DT:OP2	0.45	2.64	20	4
3:A:135:TRP:N	3:A:135:TRP:CE3	0.45	2.85	4	1
3:A:70:LYS:O	3:A:74:PRO:CG	0.45	2.64	13	5
3:A:120:PHE:O	3:A:124:THR:HB	0.45	2.12	18	6
3:A:37:PHE:C	3:A:37:PHE:CD1	0.45	2.90	19	6
1:B:201:DC:N3	1:B:202:DG:C6	0.45	2.84	9	1
3:A:70:LYS:O	3:A:70:LYS:HD3	0.45	2.11	7	1
2:C:234:DT:C2'	2:C:235:DT:H71	0.45	2.39	15	2
3:A:117:HIS:CE1	3:A:129:LYS:HE2	0.45	2.46	11	1
3:A:102:LEU:HB3	3:A:113:PRO:CB	0.45	2.41	16	1
3:A:17:LEU:N	3:A:17:LEU:CD2	0.45	2.79	6	2
3:A:8:THR:O	3:A:10:ASP:N	0.45	2.50	8	5
3:A:109:VAL:HG11	3:A:111:MET:SD	0.45	2.51	15	3
2:C:224:DT:O5'	2:C:224:DT:H6	0.45	1.94	17	4
2:C:223:DT:P	3:A:129:LYS:HG2	0.45	2.51	5	1
3:A:87:ILE:O	3:A:90:ALA:N	0.45	2.50	2	12
2:C:224:DT:P	3:A:129:LYS:O	0.45	2.75	7	1
3:A:94:LEU:HD11	3:A:101:THR:O	0.45	2.12	15	1
2:C:225:DG:C5	3:A:118:ARG:NH1	0.45	2.84	6	2
2:C:233:DA:C4'	3:A:44:ALA:CB	0.45	2.95	4	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:A:16:VAL:CG2	3:A:27:PHE:CE1	0.45	3.00	1	8
3:A:117:HIS:ND1	3:A:129:LYS:CD	0.45	2.80	14	1
2:C:232:DA:OP1	3:A:70:LYS:HE2	0.45	2.12	7	1
3:A:59:SER:HA	3:A:62:LEU:HB2	0.45	1.89	2	20
3:A:24:ASP:HA	3:A:40:PRO:CD	0.45	2.41	8	2
2:C:222:DC:H2''	2:C:223:DT:O5'	0.45	2.11	7	1
3:A:13:TRP:CE3	3:A:13:TRP:HA	0.45	2.47	15	2
2:C:221:DT:H2''	2:C:222:DC:O5'	0.45	2.10	11	1
3:A:129:LYS:HD2	3:A:129:LYS:O	0.45	2.12	16	2
3:A:43:ARG:NH2	3:A:71:ARG:CZ	0.45	2.79	6	1
3:A:69:CYS:O	3:A:73:GLN:N	0.45	2.50	4	1
3:A:97:GLU:OE2	3:A:101:THR:CB	0.45	2.61	1	1
1:B:206:DG:H2''	1:B:207:DA:O5'	0.45	2.12	5	6
2:C:227:DG:H2''	2:C:228:DC:O5'	0.45	2.12	17	11
3:A:19:ARG:O	3:A:21:PRO:HD3	0.45	2.12	3	14
3:A:91:CYS:CB	3:A:135:TRP:CG	0.45	3.00	9	2
3:A:43:ARG:NE	3:A:43:ARG:H	0.45	2.09	9	1
3:A:43:ARG:NE	3:A:71:ARG:CD	0.45	2.80	9	1
1:B:201:DC:O2	1:B:202:DG:C4	0.45	2.70	6	5
3:A:102:LEU:HD21	3:A:117:HIS:CD2	0.45	2.46	4	2
2:C:234:DT:H4'	3:A:45:ARG:HG2	0.45	1.89	1	2
3:A:106:ALA:CA	3:A:111:MET:O	0.45	2.64	16	1
3:A:54:PHE:N	3:A:54:PHE:CD2	0.45	2.85	10	1
3:A:94:LEU:HG	3:A:100:VAL:HG22	0.45	1.88	4	1
2:C:235:DT:H2''	2:C:236:DT:O5'	0.44	2.11	8	6
3:A:75:ASP:OD2	3:A:77:ALA:HB2	0.44	2.13	8	1
3:A:121:LYS:HB2	3:A:128:PRO:CB	0.44	2.42	11	3
2:C:233:DA:H2''	2:C:234:DT:OP2	0.44	2.11	6	2
3:A:24:ASP:CG	3:A:77:ALA:HB1	0.44	2.33	6	1
3:A:39:ARG:HG2	3:A:77:ALA:HB2	0.44	1.90	4	1
2:C:223:DT:C7	3:A:114:PHE:CE2	0.44	3.00	18	2
3:A:114:PHE:N	3:A:114:PHE:CD1	0.44	2.86	19	4
3:A:39:ARG:CG	3:A:75:ASP:OD2	0.44	2.64	8	1
3:A:102:LEU:CD1	3:A:113:PRO:HA	0.44	2.42	14	1
3:A:84:LEU:HD13	3:A:123:THR:CB	0.44	2.43	7	1
2:C:225:DG:OP2	3:A:130:ALA:HB2	0.44	2.12	7	1
2:C:234:DT:OP1	3:A:36:ILE:HG21	0.44	2.12	6	1
3:A:75:ASP:OD1	3:A:75:ASP:N	0.44	2.50	2	1
3:A:69:CYS:O	3:A:71:ARG:N	0.44	2.50	8	10
3:A:102:LEU:HD11	3:A:116:LEU:HB2	0.44	1.89	18	1
3:A:87:ILE:CG2	3:A:120:PHE:CE2	0.44	3.00	18	6

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:A:43:ARG:NH2	3:A:71:ARG:HB3	0.44	2.27	7	1
3:A:95:GLU:OE1	3:A:136:ARG:O	0.44	2.35	7	1
3:A:93:LEU:CD2	3:A:101:THR:HG21	0.44	2.43	15	1
3:A:133:GLN:OE1	3:A:136:ARG:NH1	0.44	2.50	3	1
1:B:197:DA:C2	3:A:43:ARG:NH2	0.44	2.86	12	1
3:A:12:ARG:CD	3:A:12:ARG:N	0.44	2.80	10	1
3:A:49:ARG:O	3:A:52:VAL:HB	0.44	2.13	6	1
3:A:31:VAL:N	3:A:36:ILE:O	0.44	2.50	17	13
3:A:84:LEU:CD2	3:A:123:THR:C	0.44	2.83	9	1
3:A:93:LEU:HD21	3:A:101:THR:HG21	0.44	1.90	15	1
3:A:19:ARG:CZ	3:A:41:SER:O	0.44	2.66	13	1
3:A:117:HIS:CD2	3:A:129:LYS:HE2	0.44	2.47	10	1
3:A:73:GLN:CB	3:A:74:PRO:HD3	0.44	2.43	6	1
3:A:13:TRP:CZ2	3:A:17:LEU:CD2	0.44	2.88	2	6
3:A:24:ASP:OD2	3:A:77:ALA:HA	0.44	2.13	2	2
3:A:24:ASP:OD1	3:A:77:ALA:HB1	0.44	2.11	18	2
3:A:37:PHE:HZ	3:A:58:ALA:HB1	0.44	1.72	3	5
3:A:66:PHE:CD1	3:A:66:PHE:N	0.44	2.86	7	4
2:C:223:DT:P	3:A:129:LYS:HZ3	0.44	2.36	11	1
3:A:109:VAL:HG12	3:A:111:MET:HG3	0.44	1.90	3	1
2:C:234:DT:C4'	3:A:45:ARG:HG2	0.44	2.43	5	1
3:A:116:LEU:CD1	3:A:116:LEU:C	0.44	2.86	16	4
3:A:60:GLU:O	3:A:63:ALA:HB3	0.44	2.13	19	6
3:A:11:GLN:O	3:A:15:SER:N	0.44	2.48	15	5
3:A:93:LEU:O	3:A:97:GLU:OE2	0.44	2.35	6	3
3:A:55:TYR:CD1	3:A:55:TYR:N	0.44	2.85	6	4
3:A:111:MET:HE3	3:A:116:LEU:HA	0.44	1.88	12	1
3:A:131:TRP:NE1	3:A:135:TRP:CH2	0.44	2.85	8	1
3:A:43:ARG:HH11	3:A:44:ALA:HB2	0.44	1.70	20	1
3:A:32:ARG:N	3:A:51:ASN:O	0.43	2.51	2	6
2:C:223:DT:OP1	3:A:129:LYS:HE2	0.43	2.13	12	4
1:B:192:DA:H2''	1:B:193:DA:O5'	0.43	2.13	19	5
3:A:59:SER:O	3:A:63:ALA:N	0.43	2.51	8	12
3:A:121:LYS:HA	3:A:124:THR:CG2	0.43	2.42	8	3
3:A:118:ARG:NH1	3:A:121:LYS:CD	0.43	2.81	7	1
3:A:111:MET:HE1	3:A:112:SER:O	0.43	2.12	3	1
3:A:109:VAL:HG21	3:A:111:MET:HE2	0.43	1.90	5	1
3:A:19:ARG:NE	3:A:41:SER:O	0.43	2.51	13	1
3:A:27:PHE:CE1	3:A:40:PRO:CB	0.43	3.00	13	1
3:A:8:THR:O	3:A:9:ASP:C	0.43	2.56	11	10
3:A:16:VAL:O	3:A:46:HIS:CE1	0.43	2.72	8	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:C:233:DA:H4'	3:A:44:ALA:CB	0.43	2.42	16	1
3:A:19:ARG:HA	3:A:41:SER:CA	0.43	2.43	20	1
2:C:223:DT:OP1	3:A:129:LYS:HD2	0.43	2.13	18	1
3:A:102:LEU:O	3:A:105:LEU:N	0.43	2.52	8	1
3:A:97:GLU:CG	3:A:98:THR:N	0.43	2.80	7	3
3:A:10:ASP:O	3:A:13:TRP:HB3	0.43	2.14	7	1
3:A:95:GLU:HA	3:A:95:GLU:OE1	0.43	2.12	7	1
1:B:197:DA:H2''	1:B:198:DA:O5'	0.43	2.12	13	2
3:A:92:ARG:HA	3:A:139:ARG:O	0.43	2.13	7	1
3:A:121:LYS:HB3	3:A:128:PRO:HB3	0.43	1.91	3	1
3:A:14:GLN:O	3:A:18:ALA:HB3	0.43	2.12	4	1
1:B:190:DG:C4	1:B:191:DC:C4	0.43	3.06	13	8
3:A:80:ARG:NH2	3:A:123:THR:O	0.43	2.52	14	1
3:A:30:ALA:HA	3:A:37:PHE:HA	0.43	1.90	1	5
3:A:94:LEU:CG	3:A:100:VAL:CG1	0.43	2.96	3	1
2:C:223:DT:OP2	3:A:129:LYS:CE	0.43	2.66	5	1
3:A:55:TYR:N	3:A:55:TYR:CD1	0.43	2.86	1	5
3:A:118:ARG:CA	3:A:118:ARG:NE	0.43	2.81	19	1
2:C:234:DT:O2	3:A:45:ARG:NH2	0.43	2.52	17	2
2:C:225:DG:C4	2:C:226:DC:C5	0.43	3.06	7	1
1:B:202:DG:N7	3:A:115:HIS:ND1	0.43	2.67	11	1
3:A:109:VAL:HG12	3:A:111:MET:CG	0.43	2.43	3	1
2:C:225:DG:N7	3:A:118:ARG:CZ	0.43	2.82	16	2
3:A:89:HIS:NE2	3:A:92:ARG:NH2	0.43	2.65	4	1
3:A:93:LEU:HD13	3:A:93:LEU:C	0.43	2.33	4	1
3:A:93:LEU:CD2	3:A:101:THR:HB	0.43	2.34	1	1
1:B:205:DA:H2''	1:B:206:DG:O5'	0.43	2.14	16	8
3:A:28:VAL:HG21	3:A:61:ALA:CB	0.43	2.43	6	5
3:A:95:GLU:OE1	3:A:95:GLU:HA	0.43	2.14	5	1
1:B:198:DA:H5''	3:A:43:ARG:CG	0.43	2.44	13	1
3:A:39:ARG:NH1	3:A:72:CYS:HA	0.43	2.29	17	1
3:A:15:SER:OG	3:A:23:ALA:CB	0.43	2.67	7	1
2:C:224:DT:C7	3:A:129:LYS:CE	0.43	2.96	7	1
3:A:26:GLU:HB2	3:A:78:ASN:OD1	0.43	2.13	6	1
3:A:87:ILE:HD11	3:A:119:LEU:HD11	0.43	1.90	6	1
3:A:117:HIS:N	3:A:117:HIS:CD2	0.43	2.87	11	2
3:A:43:ARG:HG2	3:A:43:ARG:NH1	0.43	2.28	7	1
3:A:9:ASP:OD1	3:A:9:ASP:N	0.43	2.52	2	2
3:A:120:PHE:CE1	3:A:131:TRP:HB3	0.43	2.49	8	1
1:B:201:DC:H42	2:C:226:DC:N4	0.43	2.12	9	1
3:A:112:SER:HB3	3:A:113:PRO:HD2	0.43	1.90	3	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:A:116:LEU:HD22	3:A:116:LEU:C	0.43	2.32	17	1
3:A:92:ARG:HD2	3:A:139:ARG:NE	0.43	2.28	6	1
3:A:127:THR:HB	3:A:131:TRP:CD2	0.42	2.49	19	1
3:A:95:GLU:HG3	3:A:136:ARG:HG3	0.42	1.90	20	2
3:A:94:LEU:CD2	3:A:100:VAL:HG12	0.42	2.41	14	1
3:A:116:LEU:C	3:A:116:LEU:CD1	0.42	2.87	4	3
1:B:201:DC:H41	3:A:118:ARG:HH11	0.42	1.56	7	1
3:A:109:VAL:CG1	3:A:111:MET:HE2	0.42	2.39	6	1
1:B:201:DC:C2'	3:A:115:HIS:CE1	0.42	2.93	8	1
3:A:9:ASP:HB2	3:A:54:PHE:CD2	0.42	2.49	14	3
2:C:234:DT:H72	3:A:34:THR:OG1	0.42	2.14	7	1
1:B:199:DA:O4'	3:A:43:ARG:NH1	0.42	2.52	17	2
3:A:83:ARG:O	3:A:87:ILE:HG13	0.42	2.13	20	1
3:A:24:ASP:OD2	3:A:41:SER:OG	0.42	2.36	6	1
3:A:84:LEU:HD13	3:A:124:THR:N	0.42	2.29	6	1
2:C:233:DA:H4'	3:A:44:ALA:HB3	0.42	1.91	4	1
3:A:105:LEU:O	3:A:105:LEU:HD13	0.42	2.14	1	1
3:A:135:TRP:CE3	3:A:135:TRP:CA	0.42	3.02	2	2
1:B:200:DG:H2''	1:B:201:DC:C6	0.42	2.50	2	5
3:A:24:ASP:OD1	3:A:39:ARG:CB	0.42	2.67	11	5
3:A:68:PRO:CB	3:A:73:GLN:NE2	0.42	2.83	18	1
3:A:72:CYS:O	3:A:75:ASP:OD1	0.42	2.37	8	4
3:A:62:LEU:CD2	3:A:68:PRO:HD3	0.42	2.44	11	5
3:A:13:TRP:CZ2	3:A:17:LEU:HD11	0.42	2.49	14	2
3:A:102:LEU:HG	3:A:113:PRO:CB	0.42	2.45	3	1
3:A:118:ARG:NH2	3:A:128:PRO:CG	0.42	2.82	12	1
1:B:202:DG:N2	1:B:203:DC:O2	0.42	2.52	16	2
1:B:193:DA:N1	1:B:194:DA:C6	0.42	2.88	2	1
3:A:39:ARG:NH2	3:A:76:LYS:O	0.42	2.52	18	1
3:A:68:PRO:CB	3:A:73:GLN:OE1	0.42	2.67	8	2
3:A:102:LEU:HD21	3:A:116:LEU:HD23	0.42	1.84	11	1
3:A:117:HIS:HB3	3:A:129:LYS:HB2	0.42	1.91	12	1
3:A:119:LEU:HD23	3:A:119:LEU:O	0.42	2.15	1	1
3:A:66:PHE:N	3:A:66:PHE:CD1	0.42	2.87	14	7
3:A:139:ARG:CZ	3:A:139:ARG:CB	0.42	2.98	14	1
3:A:139:ARG:CZ	3:A:139:ARG:HB2	0.42	2.45	14	1
2:C:229:DT:H2''	2:C:230:DT:O5'	0.42	2.14	2	5
3:A:111:MET:HG3	3:A:115:HIS:HB3	0.42	1.92	9	1
3:A:102:LEU:C	3:A:102:LEU:CD1	0.42	2.87	14	1
3:A:102:LEU:HD11	3:A:116:LEU:CG	0.42	2.45	3	1
3:A:16:VAL:HA	3:A:40:PRO:C	0.42	2.35	4	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:A:102:LEU:CD1	3:A:102:LEU:C	0.42	2.87	13	1
3:A:39:ARG:HB3	3:A:40:PRO:HD2	0.42	1.90	10	1
3:A:76:LYS:HE2	3:A:83:ARG:CD	0.42	2.44	14	1
3:A:75:ASP:OD1	3:A:76:LYS:N	0.42	2.53	5	3
3:A:62:LEU:CD2	3:A:68:PRO:HG3	0.42	2.44	2	4
1:B:193:DA:C2	1:B:194:DA:C6	0.42	3.07	2	1
3:A:105:LEU:HD12	3:A:105:LEU:O	0.42	2.14	19	1
3:A:34:THR:HG23	3:A:36:ILE:HB	0.42	1.92	11	2
2:C:223:DT:OP1	3:A:129:LYS:NZ	0.42	2.50	17	2
3:A:69:CYS:C	3:A:71:ARG:H	0.42	2.18	12	5
3:A:11:GLN:HG3	3:A:14:GLN:HB3	0.42	1.91	8	1
3:A:94:LEU:HD23	3:A:132:GLN:HG2	0.42	1.90	7	1
3:A:121:LYS:CB	3:A:128:PRO:HB3	0.42	2.45	3	1
3:A:106:ALA:CB	3:A:111:MET:O	0.42	2.68	5	3
3:A:116:LEU:C	3:A:116:LEU:HD22	0.42	2.34	5	1
3:A:129:LYS:CD	3:A:129:LYS:O	0.42	2.68	20	1
1:B:193:DA:C2	1:B:194:DA:C4	0.42	3.08	2	1
3:A:106:ALA:HA	3:A:111:MET:SD	0.42	2.55	18	1
3:A:97:GLU:OE1	3:A:97:GLU:N	0.42	2.53	8	1
3:A:84:LEU:HA	3:A:84:LEU:HD13	0.42	1.67	14	1
3:A:111:MET:CE	3:A:116:LEU:HD22	0.42	2.45	13	2
3:A:9:ASP:HA	3:A:12:ARG:CD	0.42	2.44	7	1
2:C:230:DT:C2'	2:C:231:DT:H71	0.42	2.45	10	3
2:C:225:DG:O6	3:A:118:ARG:NH1	0.41	2.53	19	1
3:A:41:SER:O	3:A:42:CYS:C	0.41	2.58	16	1
3:A:114:PHE:CD1	3:A:129:LYS:CE	0.41	3.03	4	1
3:A:13:TRP:CD1	3:A:49:ARG:NE	0.41	2.88	18	1
3:A:105:LEU:HD12	3:A:105:LEU:C	0.41	2.35	19	1
3:A:98:THR:HB	3:A:99:PRO:HD2	0.41	1.91	11	1
3:A:102:LEU:C	3:A:102:LEU:HD13	0.41	2.35	13	1
3:A:9:ASP:HA	3:A:12:ARG:CG	0.41	2.45	13	1
3:A:117:HIS:HB3	3:A:128:PRO:HB2	0.41	1.90	6	1
3:A:111:MET:HE1	3:A:119:LEU:HD12	0.41	1.91	1	1
2:C:234:DT:OP2	2:C:234:DT:H73	0.41	2.15	2	1
3:A:13:TRP:CE2	3:A:17:LEU:CD1	0.41	3.00	14	4
3:A:135:TRP:CA	3:A:135:TRP:CE3	0.41	3.03	7	2
2:C:224:DT:H71	3:A:118:ARG:HH22	0.41	1.73	15	1
1:B:198:DA:C2	1:B:199:DA:C6	0.41	3.09	13	1
3:A:109:VAL:HB	3:A:111:MET:HG2	0.41	1.93	4	1
3:A:102:LEU:HD23	3:A:116:LEU:CG	0.41	2.46	2	1
3:A:72:CYS:C	3:A:75:ASP:OD1	0.41	2.59	3	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:A:43:ARG:NH1	3:A:75:ASP:OD2	0.41	2.53	18	1
3:A:102:LEU:HD11	3:A:106:ALA:HB2	0.41	1.92	8	1
3:A:24:ASP:CG	3:A:77:ALA:HA	0.41	2.36	7	4
3:A:119:LEU:HD13	3:A:120:PHE:N	0.41	2.30	7	1
3:A:109:VAL:CG1	3:A:111:MET:SD	0.41	3.09	20	2
3:A:117:HIS:ND1	3:A:129:LYS:CE	0.41	2.84	11	1
3:A:39:ARG:NH2	3:A:75:ASP:C	0.41	2.73	20	1
3:A:94:LEU:CD1	3:A:132:GLN:NE2	0.41	2.83	6	1
3:A:44:ALA:O	3:A:45:ARG:CB	0.41	2.69	20	2
3:A:100:VAL:HG12	3:A:101:THR:N	0.41	2.31	11	1
1:B:190:DG:C5	1:B:191:DC:C4	0.41	3.09	4	1
3:A:105:LEU:HD22	3:A:116:LEU:HD21	0.41	1.93	2	1
3:A:105:LEU:HD12	3:A:116:LEU:CD1	0.41	2.32	7	1
2:C:232:DA:H5''	3:A:70:LYS:HB3	0.41	1.92	3	1
1:B:199:DA:C4'	3:A:43:ARG:NH1	0.41	2.84	5	1
1:B:198:DA:H2''	1:B:199:DA:C8	0.41	2.51	13	1
1:B:198:DA:H4'	3:A:43:ARG:HB2	0.41	1.90	2	1
3:A:109:VAL:HB	3:A:111:MET:HG3	0.41	1.92	19	1
3:A:131:TRP:CD1	3:A:135:TRP:HZ2	0.41	2.33	7	1
2:C:224:DT:OP2	3:A:129:LYS:HD2	0.41	2.11	7	1
3:A:93:LEU:CD2	3:A:101:THR:OG1	0.41	2.65	11	1
3:A:102:LEU:HD23	3:A:113:PRO:HB3	0.41	1.92	5	1
3:A:42:CYS:O	3:A:46:HIS:NE2	0.41	2.50	13	1
1:B:198:DA:C5'	3:A:43:ARG:HG2	0.41	2.45	13	1
3:A:31:VAL:HB	3:A:34:THR:CG2	0.41	2.46	10	1
1:B:193:DA:C6	1:B:194:DA:N6	0.41	2.89	2	1
3:A:33:THR:CG2	3:A:34:THR:N	0.41	2.84	9	2
3:A:114:PHE:O	3:A:118:ARG:NH2	0.41	2.53	19	1
3:A:124:THR:CG2	3:A:131:TRP:CE3	0.41	3.03	8	1
3:A:111:MET:HE2	3:A:115:HIS:HB3	0.41	1.91	7	1
3:A:19:ARG:O	3:A:19:ARG:HG3	0.41	2.16	15	1
3:A:131:TRP:HE3	3:A:131:TRP:HA	0.41	1.72	5	1
3:A:24:ASP:HA	3:A:40:PRO:CG	0.41	2.45	13	1
3:A:86:LYS:O	3:A:89:HIS:HB3	0.41	2.15	4	1
3:A:50:GLU:OE2	3:A:51:ASN:ND2	0.41	2.54	7	1
3:A:43:ARG:NH1	3:A:71:ARG:HD3	0.41	2.31	7	1
3:A:135:TRP:HA	3:A:135:TRP:CE3	0.41	2.51	11	1
3:A:54:PHE:C	3:A:55:TYR:CD1	0.41	2.95	1	3
3:A:97:GLU:OE2	3:A:101:THR:CG2	0.41	2.69	1	1
3:A:68:PRO:HB2	3:A:73:GLN:CG	0.41	2.46	8	1
3:A:93:LEU:CD1	3:A:97:GLU:OE1	0.41	2.65	9	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:C:224:DT:OP2	3:A:129:LYS:O	0.41	2.39	7	1
3:A:29:PHE:HB2	3:A:54:PHE:CE1	0.41	2.51	5	1
1:B:199:DA:H5'	3:A:43:ARG:HB2	0.41	1.93	5	1
2:C:235:DT:P	3:A:46:HIS:C	0.41	2.99	13	1
3:A:93:LEU:N	3:A:93:LEU:CD2	0.41	2.84	13	1
3:A:116:LEU:CG	3:A:117:HIS:N	0.41	2.84	16	1
3:A:12:ARG:O	3:A:27:PHE:CZ	0.41	2.74	10	2
3:A:84:LEU:HD13	3:A:84:LEU:HA	0.41	1.62	10	1
3:A:129:LYS:HD3	3:A:129:LYS:O	0.41	2.16	20	1
3:A:55:TYR:CD2	3:A:61:ALA:N	0.41	2.89	20	1
3:A:109:VAL:HG21	3:A:111:MET:CE	0.41	2.45	1	1
3:A:62:LEU:HD23	3:A:68:PRO:HD3	0.40	1.93	18	1
2:C:234:DT:C1'	3:A:45:ARG:HD3	0.40	2.46	15	1
3:A:60:GLU:HA	3:A:60:GLU:OE1	0.40	2.17	5	1
3:A:124:THR:OG1	3:A:131:TRP:CD1	0.40	2.65	6	1
3:A:94:LEU:CD2	3:A:132:GLN:CG	0.40	2.98	2	1
2:C:223:DT:H2''	2:C:224:DT:C6	0.40	2.51	8	1
2:C:234:DT:H2'	2:C:235:DT:C7	0.40	2.43	9	1
3:A:13:TRP:CZ3	3:A:17:LEU:HD21	0.40	2.51	7	1
3:A:105:LEU:HD13	3:A:105:LEU:O	0.40	2.15	5	1
3:A:15:SER:O	3:A:40:PRO:O	0.40	2.39	13	1
3:A:19:ARG:HD3	3:A:41:SER:HB2	0.40	1.93	13	1
3:A:12:ARG:HD3	3:A:27:PHE:CE1	0.40	2.51	6	1
3:A:91:CYS:CB	3:A:135:TRP:CD1	0.40	3.03	4	1
3:A:111:MET:HG3	3:A:112:SER:N	0.40	2.32	2	1
3:A:101:THR:C	3:A:102:LEU:HG	0.40	2.35	19	1
3:A:106:ALA:HA	3:A:111:MET:CE	0.40	2.46	9	1
3:A:117:HIS:HB3	3:A:129:LYS:HA	0.40	1.93	7	1
3:A:19:ARG:O	3:A:19:ARG:CG	0.40	2.69	7	1
3:A:95:GLU:CG	3:A:136:ARG:HG3	0.40	2.46	13	1
3:A:24:ASP:CB	3:A:77:ALA:HB1	0.40	2.46	6	1
3:A:23:ALA:HB3	3:A:40:PRO:HG3	0.40	1.92	18	1
3:A:121:LYS:CA	3:A:124:THR:HG22	0.40	2.47	8	1
3:A:43:ARG:CZ	3:A:71:ARG:CD	0.40	3.00	9	1
3:A:64:ALA:HB3	3:A:66:PHE:CD1	0.40	2.52	14	1
2:C:224:DT:OP1	3:A:129:LYS:O	0.40	2.39	7	1
2:C:235:DT:OP1	3:A:46:HIS:C	0.40	2.49	13	1
3:A:124:THR:HG1	3:A:131:TRP:HE1	0.40	1.58	17	1
3:A:11:GLN:O	3:A:14:GLN:HB3	0.40	2.17	19	1
2:C:222:DC:H2'	2:C:223:DT:H71	0.40	1.91	8	1
3:A:95:GLU:HG2	3:A:136:ARG:HG3	0.40	1.92	15	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:A:121:LYS:C	3:A:121:LYS:CD	0.40	2.88	5	1
3:A:12:ARG:NH1	3:A:27:PHE:CB	0.40	2.85	5	1
2:C:232:DA:C4	2:C:233:DA:C5	0.40	3.10	5	1
3:A:25:GLY:HA3	3:A:78:ASN:HB2	0.40	1.93	6	1
3:A:25:GLY:CA	3:A:78:ASN:H	0.40	2.29	4	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	130/139 (94%)	113±2 (87±1%)	13±2 (10±1%)	4±1 (3±1%)	9	42
All	All	2600/2780 (94%)	2266 (87%)	256 (10%)	78 (3%)	9	42

All 10 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	128	PRO	20
3	A	98	THR	20
3	A	70	LYS	16
3	A	77	ALA	9
3	A	9	ASP	4
3	A	19	ARG	3
3	A	45	ARG	3
3	A	110	ALA	1
3	A	97	GLU	1
3	A	74	PRO	1

6.3.2 Protein sidechains [i](#)

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	A	108/114 (95%)	82±4 (76±4%)	26±4 (24±4%)	3	26
All	All	2160/2280 (95%)	1631 (76%)	529 (24%)	3	26

All 60 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	120	PHE	20
3	A	131	TRP	20
3	A	29	PHE	20
3	A	135	TRP	20
3	A	101	THR	20
3	A	11	GLN	18
3	A	112	SER	17
3	A	43	ARG	16
3	A	50	GLU	16
3	A	45	ARG	16
3	A	94	LEU	15
3	A	71	ARG	15
3	A	121	LYS	13
3	A	84	LEU	13
3	A	118	ARG	12
3	A	91	CYS	12
3	A	14	GLN	11
3	A	102	LEU	11
3	A	105	LEU	11
3	A	87	ILE	10
3	A	116	LEU	10
3	A	80	ARG	10
3	A	12	ARG	10
3	A	49	ARG	9
3	A	107	ASP	9
3	A	15	SER	9
3	A	129	LYS	9
3	A	67	ARG	8
3	A	70	LYS	8
3	A	19	ARG	8
3	A	75	ASP	8
3	A	119	LEU	8
3	A	73	GLN	8
3	A	86	LYS	7
3	A	83	ARG	7
3	A	111	MET	7

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Mol	Chain	Res	Type	Models (Total)
3	A	124	THR	7
3	A	108	GLN	7
3	A	103	GLU	6
3	A	132	GLN	6
3	A	85	ASP	6
3	A	39	ARG	5
3	A	96	GLN	5
3	A	97	GLU	5
3	A	10	ASP	4
3	A	26	GLU	4
3	A	93	LEU	4
3	A	139	ARG	4
3	A	76	LYS	4
3	A	82	HIS	4
3	A	133	GLN	3
3	A	81	GLN	2
3	A	92	ARG	2
3	A	95	GLU	2
3	A	136	ARG	2
3	A	32	ARG	2
3	A	28	VAL	1
3	A	138	ARG	1
3	A	126	MET	1
3	A	89	HIS	1

6.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

1 non-standard protein/DNA/RNA residue is modelled in this entry.

In the following table, the Counts columns list the number of bonds for which Mogul statistics could be retrieved, the number of bonds that are observed in the model and the number of bonds that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length is the number of standard deviations the observed value is removed from the expected value. A bond length with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the average root-mean-square of all Z scores of the bond lengths.

Mol	Type	Chain	Res	Link	Bond lengths		
					Counts	RMSZ	#Z>2
3	SMC	A	38	3,4	6,6,7	0.75±0.11	0±0 (0±0%)

In the following table, the Counts columns list the number of angles for which Mogul statistics could be retrieved, the number of angles that are observed in the model and the number of angles that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond angle is the number of standard deviations the observed value is removed from the expected value. A bond angle with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the average root-mean-square of all Z scores of the bond angles.

Mol	Type	Chain	Res	Link	Counts	Bond angles	
						RMSZ	#Z>2
3	SMC	A	38	3,4	3,6,8	2.82±0.10	0±0 (0±0%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	SMC	A	38	3,4	-	0±0,3,5,7	0±0,0,0,0

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

6.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.6 Ligand geometry [i](#)

Of 1 ligands modelled in this entry, 1 is monoatomic - leaving 0 for Mogul analysis.

6.7 Other polymers [i](#)

There are no such molecules in this entry.

6.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

7 Chemical shift validation

No chemical shift data were provided