



Full wwPDB NMR Structure Validation Report ⓘ

Mar 12, 2026 – 02:36 AM UTC

PDB ID : 1ZGW / pdb_00001zgw
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

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
wwPDB-RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
wwPDB-ShiftChecker	:	v1.2
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

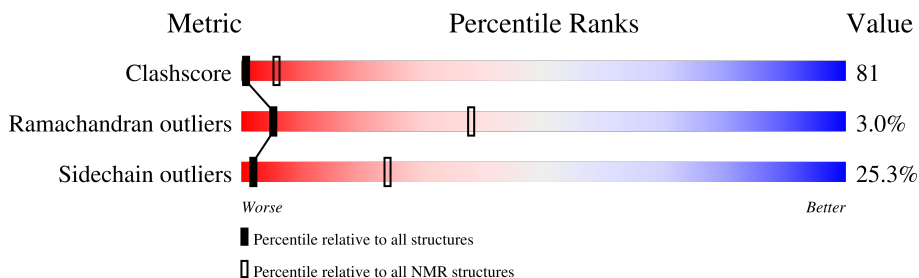
1 Overall quality at a glance

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	229148	14424
Ramachandran outliers	224038	12848
Sidechain outliers	223484	12823

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	6% 89% 6%
2	C	18	22% 72% 6%
3	A	139	16% 55% 22% 6%

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)	1.04	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 (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	
4	A	1	Total	Zn
			1	1

4 Residue-property plots

4.1 Average score per residue in the NMR ensemble

These plots are provided for all protein, RNA, DNA and oligosaccharide 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
K4
T5
G6
L7
T8
D9
Q10
Q11
R12
V13
Q14
S15
V16
L17
A18
R19
D20
P21
M22
A23
D24
G25
E26
F27
V28
F29
A30
L31
V32
T33
T34
G35
I36
P37
C38
R39
P40
S41
C42
R43
R44
R45
H46
A47
L48
R49
F50
N51
V52
S53
F54
V55
A56
N57
A58
S59
E60

A61
L62
A63
F66
G67
P68
K69
K70
R71
Q72
Q73
P74
D75
K76
A77
N78
P79
R80
L84
D85
K86
I87
T88
H89
A90
C91
R92
L93
L94
E95
Q96
E97
T98
P99
V100
T101
L102
L105
A106
V109
A110
M111
S112
P113
F114
H115
L116
H117
R118
L119
F120
K121
A122
T123
T124
G125

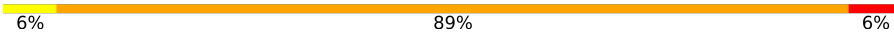
M126
T127
P128
K129
A130
V131
Q132
Q133
A134
W135
R136
R139

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: 

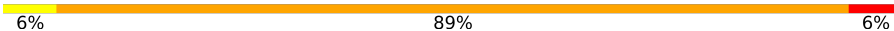
M1
K2
K3
A4
T5
C6
L7
T8
D9
Q10
Q11
R12
W13
Q14
S15
V16
L17
A18
R19
R20
F21
R22
A23
D24
D25
E26
F27
V28
F29
A30
V31
R32
T33
T34
G35
G36
F37
C38
R39
P40
S41
C42
R43
R44
R45
H46
A47
L48
R49
E50
H51
Y52
F53
F54
Y55
A56
N57
A58
S59
E60

A61
L62
A63
A64
G65
G66
R67
P68
C69
R70
K71
C72
Q73
P74
D75
K76
A77
N78
P79
R80
Q81
H82
R83
L84
D85
K86
I87
T88
H89
A90
C91
R92
L93
L94
E95
Q96
E97
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
Q133
A134
W135
R136
R139

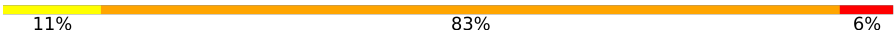
4.2.2 Score per residue for model 2

- 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

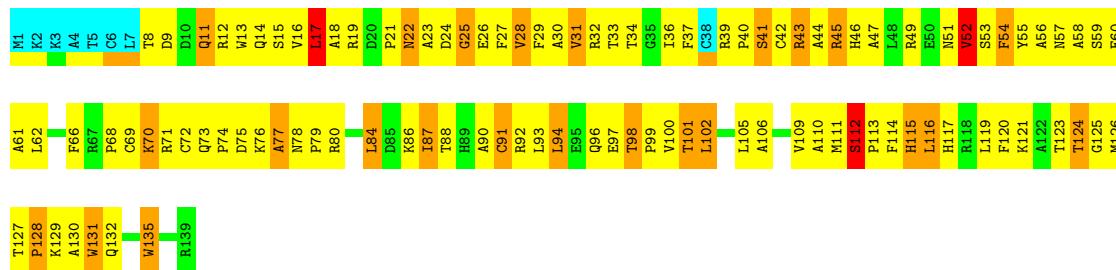
- Molecule 2: 5'-D(*TP*CP*TP*TP*GP*CP*GP*CP*TP*TP*TP*AP*AP*TP*TP*TP*GP*C)-3'

Chain C: 

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

- Molecule 3: Ada polypeptide

Chain A: 19% 55% 17% 6%



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'

Chain B: 6% 89% 6%



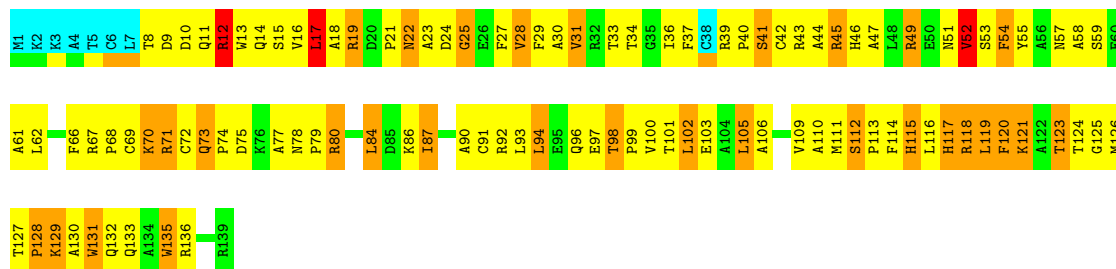
- Molecule 2: 5'-D(*TP*CP*TP*TP*GP*CP*GP*CP*TP*TP*TP*AP*AP*TP*TP*TP*GP*C)-3'

Chain C: 28% 67% 6%



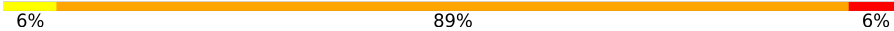
- Molecule 3: Ada polypeptide

Chain A: 19% 50% 22% 6%



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: 

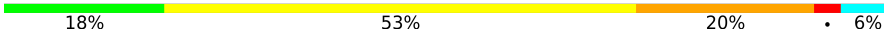
G190
C191
A192
A193
A194
T195
T196
A197
A198
A199
G200
C201
G202
C203
A204
A205
G206
G207

- 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
G226
G227
C228
T229
T230
T231
A232
A233
T234
T235
T236
G237
C238

- Molecule 3: Ada polypeptide

Chain A: 

H1
K2
K3
A4
T5
O6
L7
T8
D9
D10
Q11
R12
H13
Q14
S15
V16
L17
A18
R19
D20
F21
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
F50
H51
V52
S53
F54
Y55
A56
H57
A58
S59
E60

A61
L62
A63
A64
G65
F66
R67
P68
C69
K70
D71
Q72
Q73
P74
D75
K76
A77
N78
P79
R80
R83
L84
D85
K86
I87
T88
H89
A90
C91
R92
L93
L94
E95
Q96
E97
T98
P99
V100
T101
L102
L105
A106
D107
Q108
V109
A110
M111
F114
H115
L116
H117
R118
L119
F120
K121
A122
S123

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: 

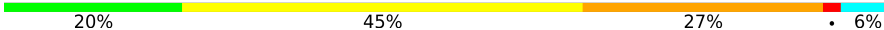
G190
C191
A192
A193
A194
T195
T196
A197
A198
A199
G200
C201
G202
C203
A204
A205
G206
G207

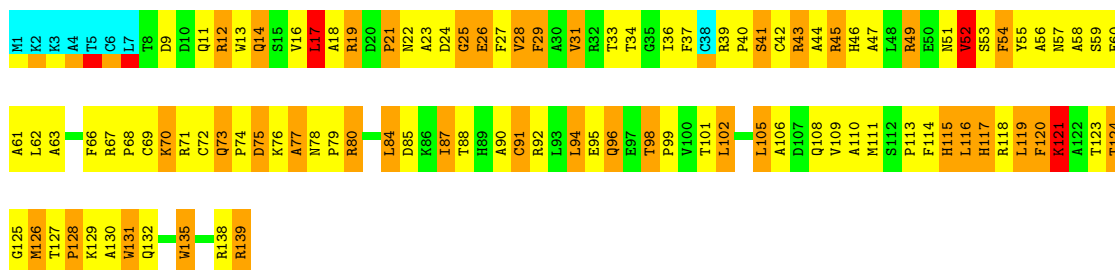
- Molecule 2: 5'-D(*TP*CP*TP*TP*GP*CP*GP*CP*TP*TP*TP*AP*AP*TP*TP*TP*GP*C)-3'

Chain C: 

T221
C222
T223
T224
G225
G226
G227
C228
T229
T230
T231
A232
A233
T234
T235
T236
G237
C238

- Molecule 3: Ada polypeptide

Chain A: 

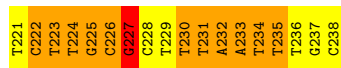


4.2.6 Score per residue for model 6

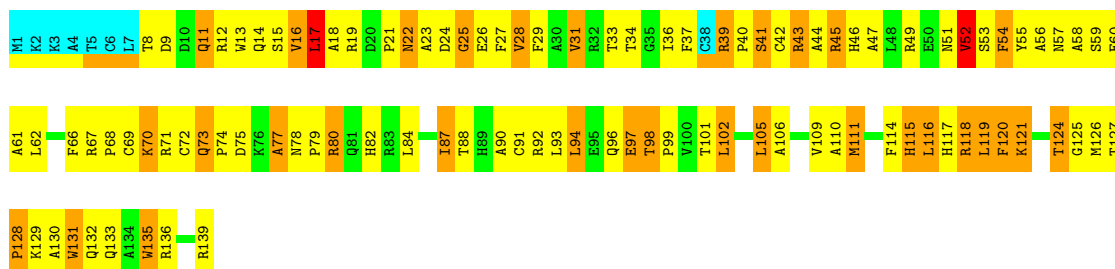
- Molecule 1: 5'-D(*GP*CP*AP*AP*AP*TP*TP*AP*AP*AP*GP*CP*GP*CP*AP*AP*GP*A)-3'



- 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 polyprotein

Chain A: 14% 58% 19% 6%

M1
K2
K3
A4
T5
O6
L7
T8
D9
D10
Q11
R12
W13
Q14
S15
V16
L17
L18
R19
D20
P21
N22
A23
D24
G25
E26
F27
V28
F29
A30
A31
V32
R33
T34
G35
I36
F37
C38
R39
P40
S41
C42
R43
R44
R45
H46
A47
P48
L49
E50
N51
V52
S53
F54
Y55
A56
N57
A58
S59
E60

A61
L62
F66
P68
C69
K70
R71
C72
Q73
W74
D75
K76
A77
N78
P79
R80
L84
D85
K86
I87
T88
H89
A90
C91
R92
L93
L94
E95
Q96
E97
T98
P99
V100
T101
L102
L105
D107
A108
Q109
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'

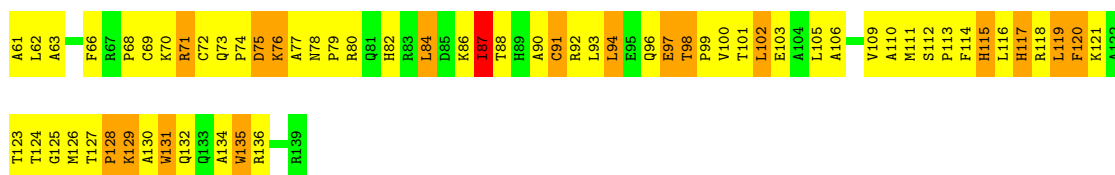
Chain C: 22% 72% 6%

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

- Molecule 3: Ada polyprotein

Chain A: 15% 55% 21% 6%

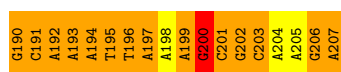
M1
K2
K3
A4
T5
O6
L7
T8
D9
D10
Q11
R12
W13
Q14
S15
V16
L17
L18
R19
D20
P21
N22
A23
D24
G25
E26
F27
V28
F29
A30
A31
V32
R33
T34
G35
I36
F37
C38
R39
P40
S41
C42
R43
R44
R45
H46
A47
P48
L49
E50
N51
V52
S53
F54
Y55
A56
N57
A58
S59
E60



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'

Chain B: 17% 78% 6%



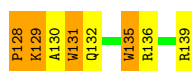
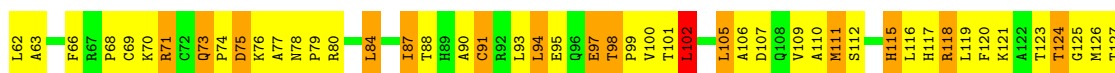
- Molecule 2: 5'-D(*TP*CP*TP*TP*GP*CP*GP*CP*TP*TP*TP*AP*AP*TP*TP*TP*GP*C)-3'

Chain C: 33% 61% 6%



- Molecule 3: Ada polypeptide

Chain A: 20% 52% 20% 6%



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'

Chain B: 6% 89% 6%

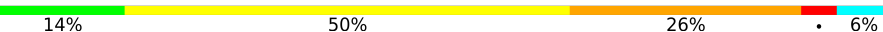


- Molecule 2: 5'-D(*TP*CP*TP*TP*GP*CP*GP*CP*TP*TP*TP*AP*AP*TP*TP*TP*GP*C)-3'

Chain C: 



- Molecule 3: Ada polypeptide

Chain A: 



4.2.11 Score per residue for model 11

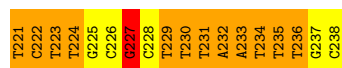
- Molecule 1: 5'-D(*GP*CP*AP*AP*AP*TP*TP*AP*AP*AP*GP*CP*GP*CP*AP*AP*GP*A)-3'

Chain B: 

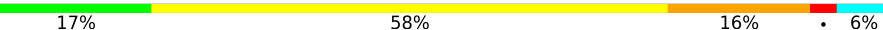


- Molecule 2: 5'-D(*TP*CP*TP*TP*GP*CP*GP*CP*TP*TP*TP*AP*AP*TP*TP*TP*GP*C)-3'

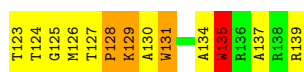
Chain C: 



- Molecule 3: Ada polypeptide

Chain A: 





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'



- 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



4.2.13 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'



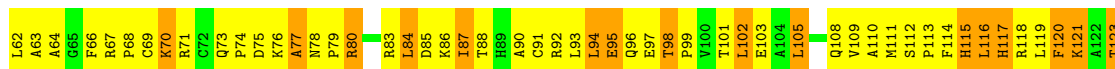
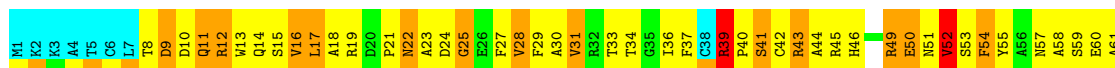
- Molecule 2: 5'-D(*TP*CP*TP*TP*GP*CP*GP*CP*TP*TP*TP*AP*AP*TP*TP*TP*GP*C)-3'





• Molecule 3: Ada polypeptide

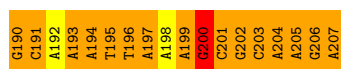
Chain A: 15% 53% 24% 6%



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'

Chain B: 11% 83% 6%



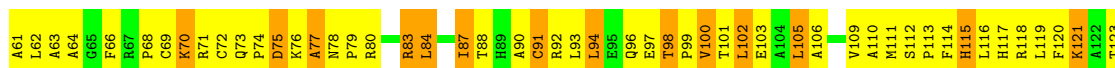
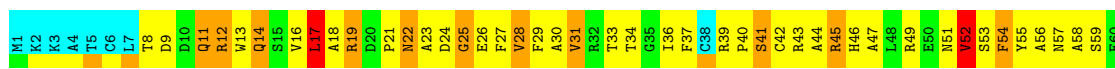
• Molecule 2: 5'-D(*TP*CP*TP*TP*GP*CP*GP*CP*TP*TP*TP*AP*AP*TP*TP*TP*GP*C)-3'

Chain C: 22% 72% 6%



• Molecule 3: Ada polypeptide

Chain A: 18% 55% 20% 6%



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: 

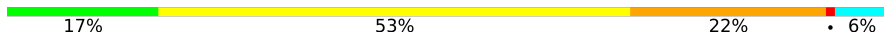
G190
C191
A192
A193
A194
T195
T196
A197
A198
A199
G200
C201
G202
C203
A204
A205
G206
A207

- 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: 

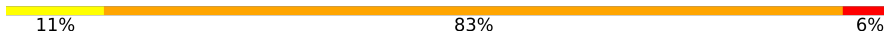
M1
K2
K3
A4
T5
C6
L7
T8
Q11
R12
W13
Q14
S15
V16
L17
A18
R19
D20
P21
N22
A23
D24
G25
E26
F27
V28
F29
A30
V31
R32
T33
T34
I35
I36
F37
C38
R39
P40
S41
C42
R43
R44
R45
H46
A47
E50
N51
Y52
S53
F54
Y55
A56
N57
A58
S59
E60
A61
L62

A63
A64
S65
F66
R67
P68
C69
K70
R71
C72
Q73
P74
D75
K76
A77
M78
P79
R80
L84
D85
K86
T87
T88
H89
A90
C91
R92
L93
L94
F95
Q96
E97
T98
P99
V100
T101
L102
E103
A104
L105
A106
V109
A110
M111
P113
F114
H115
L116
H117
R118
L119
F120
K121
A122
T123
T124
G125

M126
T127
P128
K129
A130
W131
Q132
Q133
A134
W135
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: 

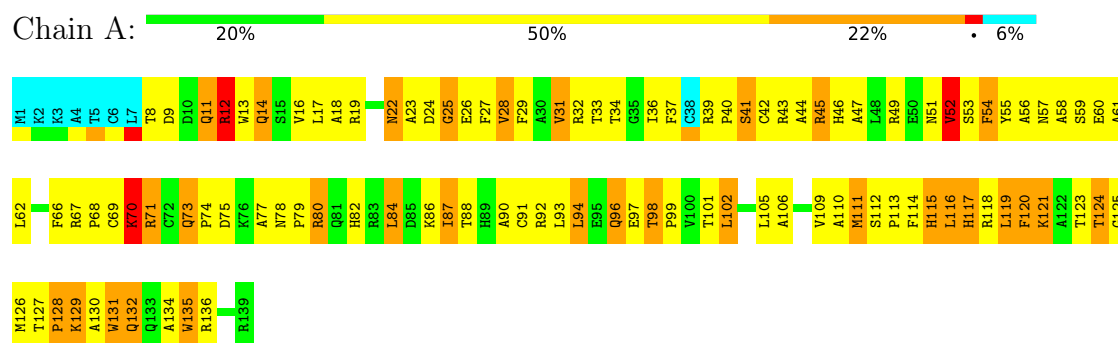
G190
C191
A192
A193
A194
T195
T196
A197
A198
A199
G200
C201
G202
C203
A204
A205
G206
A207

- 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: 

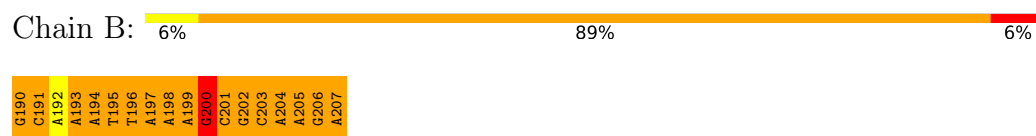
T221
C222
T223
T224
G225
C226
G227
C228
T229
T230
T231
A232
A233
T234
T235
T236
G237
C238

- Molecule 3: Ada polypeptide



4.2.17 Score per residue for model 17

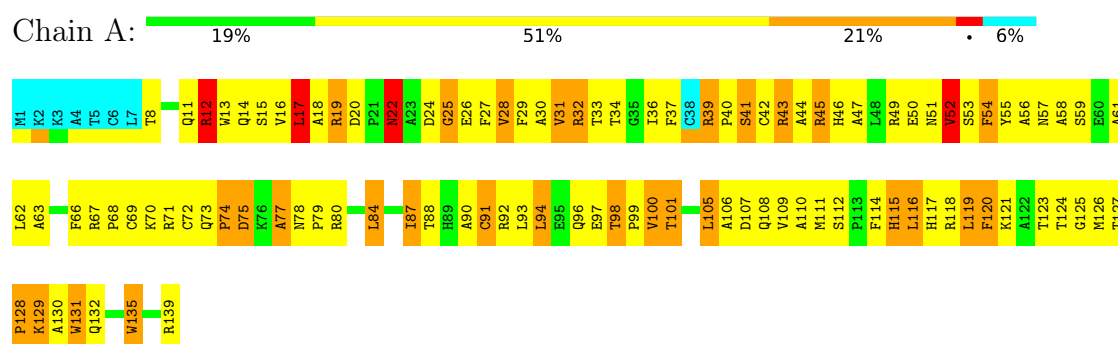
- Molecule 1: 5'-D(*GP*CP*AP*AP*AP*TP*TP*AP*AP*AP*GP*CP*GP*CP*AP*AP*GP*A)-3'



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

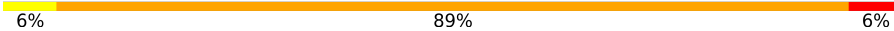


- Molecule 3: Ada polypeptide



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: 

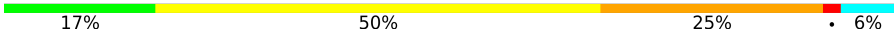
G190 C191
A192 A193
A194 T195
T196 A197
A198 A199
G200 C201
C202 C203
A204 A205
G206 A207

- 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: 

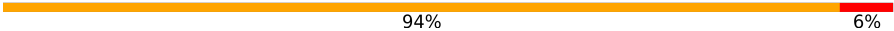
M1 K2 K3 K4
T5 T6 T7 T8
D9 D10
D11 D12
R13 R14
Q15 Q16
S17 S18
L19 L20
A21 A22
N23 N24
D25 D26
E27 E28
F29 F30
V31 V32
R33 R34
T35 T36
G37 G38
F39 F40
R41 R42
S43 S44
A45 A46
R47 R48
H49 H50
L51 L52
R53 R54
Y55 Y56
A57 A58
S59 S60
A61

L62 A63
A64 A65
P66 P67
R68 R69
K70 K71
R72 R73
P74 P75
D76 D77
N78 N79
P80 P81
Q82 Q83
L84 L85
K86 K87
T88 T89
R90 R91
C92 C93
L94 L95
E97 E98
T99 T100
V101 V102
L103 L104
A105 A106
D107 D108
Q109 Q110
M111 M112
S113 S114
F115 F116
H117 H118
R119 R120
L121 L122
T123 T124

G125 M126
T127 T128
P129 P130
K131 K132
Q133 Q134
W135 W136
R137 R138
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: 

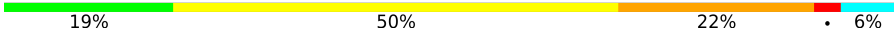
G190 C191
A192 A193
A194 T195
T196 A197
A198 A199
G200 C201
C202 C203
A204 A205
G206 A207

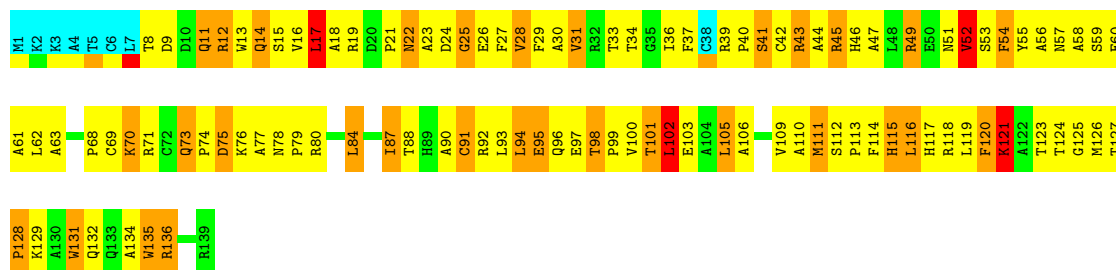
- Molecule 2: 5'-D(*TP*CP*TP*TP*GP*CP*GP*CP*TP*TP*TP*AP*AP*TP*TP*TP*GP*C)-3'

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%



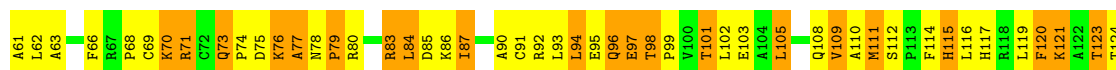
- Molecule 2: 5'-D(*TP*CP*TP*TP*GP*CP*GP*CP*TP*TP*TP*AP*AP*TP*TP*TP*GP*C)-3'

Chain C: 44% 50% 6%



- Molecule 3: Ada polypeptide

Chain A: 19% 47% 27% 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.

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	1.54±0.00	18±0/419 (4.3± 0.0%)	1.80±0.00	18±0/645 (2.8± 0.0%)
2	C	1.55±0.00	18±0/401 (4.5± 0.0%)	1.86±0.00	18±0/617 (2.9± 0.0%)
3	A	1.40±0.01	0±1/1080 (0.0± 0.1%)	1.70±0.01	12±1/1459 (0.8± 0.1%)
All	All	1.46	727/38000 (1.9%)	1.76	955/54420 (1.8%)

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
3	A	77	ALA	N-CA	6.86	1.50	1.46	13	2
3	A	39	ARG	C-N	-6.38	1.27	1.33	13	1
1	B	191	DC	C3'-C2'	-6.23	1.40	1.52	19	20
2	C	233	DA	C3'-C2'	-6.20	1.40	1.52	16	20
1	B	190	DG	C3'-C2'	-6.09	1.40	1.52	12	20
2	C	221	DT	C3'-C2'	-6.08	1.40	1.52	6	20
1	B	201	DC	C3'-C2'	-5.96	1.41	1.52	7	20
2	C	231	DT	C3'-C2'	-5.96	1.41	1.52	3	20
2	C	234	DT	C3'-C2'	-5.91	1.41	1.52	7	20
1	B	196	DT	C3'-C2'	-5.91	1.41	1.52	12	20
1	B	194	DA	C3'-C2'	-5.89	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	202	DG	C3'-C2'	-5.87	1.41	1.52	18	20
1	B	199	DA	C3'-C2'	-5.87	1.41	1.52	3	20
2	C	237	DG	C3'-C2'	-5.83	1.41	1.52	20	20
1	B	205	DA	C3'-C2'	-5.80	1.41	1.52	9	20
2	C	235	DT	C3'-C2'	-5.77	1.41	1.52	13	20
1	B	203	DC	C3'-C2'	-5.76	1.41	1.52	3	20
2	C	229	DT	C3'-C2'	-5.68	1.41	1.52	13	20
2	C	224	DT	C3'-C2'	-5.66	1.41	1.52	16	20
1	B	204	DA	C3'-C2'	-5.63	1.41	1.52	7	20
2	C	227	DG	C3'-C2'	-5.60	1.41	1.52	10	20
2	C	238	DC	C3'-C2'	-5.60	1.41	1.52	1	20
2	C	236	DT	C3'-C2'	-5.59	1.41	1.52	3	20
1	B	193	DA	C3'-C2'	-5.58	1.41	1.52	7	20
2	C	222	DC	C3'-C2'	-5.58	1.41	1.52	10	20
2	C	232	DA	C3'-C2'	-5.57	1.41	1.52	14	20
1	B	207	DA	C3'-C2'	-5.55	1.41	1.52	6	20
1	B	200	DG	C3'-C2'	-5.54	1.41	1.52	13	20
2	C	226	DC	C3'-C2'	-5.52	1.42	1.52	16	20
1	B	192	DA	C3'-C2'	-5.51	1.42	1.52	9	20
2	C	223	DT	C3'-C2'	-5.51	1.42	1.52	2	20
2	C	225	DG	C3'-C2'	-5.50	1.42	1.52	13	20
1	B	197	DA	C3'-C2'	-5.50	1.42	1.52	11	20
3	A	101	THR	C-N	-5.48	1.26	1.33	4	1
2	C	230	DT	C3'-C2'	-5.46	1.42	1.52	10	20
1	B	195	DT	C3'-C2'	-5.45	1.42	1.52	6	20
1	B	198	DA	C3'-C2'	-5.43	1.42	1.52	11	20
2	C	228	DC	C3'-C2'	-5.33	1.42	1.52	5	20
1	B	206	DG	C3'-C2'	-5.32	1.42	1.52	3	20
3	A	121	LYS	N-CA	5.06	1.52	1.46	3	1
3	A	120	PHE	N-CA	5.05	1.52	1.46	3	1
3	A	16	VAL	C-N	-5.02	1.26	1.33	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
3	A	115	HIS	CA-CB-CG	-10.46	103.34	113.80	5	20
1	B	204	DA	C3'-C2'-C1'	9.52	115.88	101.60	15	20
2	C	235	DT	C3'-C2'-C1'	9.37	115.66	101.60	6	20
1	B	199	DA	C3'-C2'-C1'	9.16	115.34	101.60	7	20
2	C	227	DG	C3'-C2'-C1'	9.14	115.31	101.60	15	20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	B	192	DA	C3'-C2'-C1'	9.11	115.26	101.60	7	20
2	C	232	DA	C3'-C2'-C1'	9.07	115.20	101.60	5	20
1	B	193	DA	C3'-C2'-C1'	9.03	115.14	101.60	9	20
2	C	225	DG	C3'-C2'-C1'	9.02	115.13	101.60	3	20
2	C	224	DT	C3'-C2'-C1'	8.98	115.07	101.60	2	20
1	B	205	DA	C3'-C2'-C1'	8.97	115.06	101.60	5	20
1	B	197	DA	C3'-C2'-C1'	8.93	115.00	101.60	4	20
1	B	203	DC	C3'-C2'-C1'	8.91	114.96	101.60	7	20
2	C	231	DT	C3'-C2'-C1'	8.91	114.97	101.60	19	20
2	C	234	DT	C3'-C2'-C1'	8.91	114.97	101.60	12	20
1	B	194	DA	C3'-C2'-C1'	8.88	114.92	101.60	2	20
2	C	229	DT	C3'-C2'-C1'	8.88	114.92	101.60	20	20
1	B	206	DG	C3'-C2'-C1'	8.87	114.90	101.60	19	20
2	C	233	DA	C3'-C2'-C1'	8.87	114.90	101.60	2	20
1	B	198	DA	C3'-C2'-C1'	8.85	114.87	101.60	20	20
2	C	236	DT	C3'-C2'-C1'	8.85	114.87	101.60	3	20
1	B	190	DG	C3'-C2'-C1'	8.83	114.85	101.60	7	20
1	B	201	DC	C3'-C2'-C1'	8.83	114.84	101.60	3	20
2	C	223	DT	C3'-C2'-C1'	8.83	114.84	101.60	12	20
1	B	207	DA	C3'-C2'-C1'	8.81	114.82	101.60	16	20
2	C	230	DT	C3'-C2'-C1'	8.81	114.82	101.60	9	20
2	C	228	DC	C3'-C2'-C1'	8.80	114.80	101.60	19	20
2	C	237	DG	C3'-C2'-C1'	8.78	114.76	101.60	11	20
1	B	200	DG	C3'-C2'-C1'	8.77	114.75	101.60	8	20
1	B	202	DG	C3'-C2'-C1'	8.73	114.70	101.60	13	20
2	C	222	DC	C3'-C2'-C1'	8.71	114.67	101.60	3	20
2	C	226	DC	C3'-C2'-C1'	8.66	114.60	101.60	9	20
2	C	221	DT	C3'-C2'-C1'	8.60	114.50	101.60	11	20
1	B	195	DT	C3'-C2'-C1'	8.56	114.44	101.60	13	20
1	B	196	DT	C3'-C2'-C1'	8.53	114.39	101.60	2	20
2	C	238	DC	C3'-C2'-C1'	8.51	114.36	101.60	11	20
1	B	191	DC	C3'-C2'-C1'	8.17	113.86	101.60	13	20
3	A	102	LEU	N-CA-C	-7.28	105.32	114.56	12	10
3	A	25	GLY	N-CA-C	-7.14	106.19	114.69	5	18
3	A	52	VAL	N-CA-CB	-7.06	102.56	111.46	18	20
3	A	87	ILE	N-CA-CB	-6.89	102.87	110.51	15	8
3	A	22	ASN	N-CA-CB	-6.71	100.79	110.65	6	20
3	A	54	PHE	CA-CB-CG	-6.63	107.17	113.80	17	20
3	A	120	PHE	N-CA-CB	-6.62	100.14	110.06	10	14
3	A	117	HIS	CA-CB-CG	-6.25	107.55	113.80	10	6
3	A	31	VAL	N-CA-CB	-6.09	104.72	111.66	10	18

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
3	A	12	ARG	N-CA-C	-6.06	104.68	111.28	15	16
3	A	17	LEU	N-CA-CB	-5.87	101.89	110.47	6	18
3	A	39	ARG	N-CA-CB	-5.81	100.62	110.50	20	5
3	A	21	PRO	N-CA-C	-5.64	108.81	114.68	5	1
3	A	41	SER	N-CA-CB	-5.59	102.67	111.39	2	19
3	A	71	ARG	N-CA-CB	-5.53	103.24	110.59	11	3
3	A	135	TRP	N-CA-CB	-5.45	101.82	109.94	11	1
3	A	79	PRO	N-CA-C	-5.38	107.05	113.98	18	4
3	A	121	LYS	N-CA-CB	-5.29	102.39	110.07	3	3
3	A	71	ARG	N-CA-C	-5.25	107.42	113.88	11	1
3	A	16	VAL	N-CA-CB	-5.21	103.90	110.57	13	1
3	A	50	GLU	N-CA-CB	-5.20	101.71	110.49	15	2
3	A	100	VAL	N-CA-CB	-5.13	102.76	111.23	4	1
3	A	75	ASP	N-CA-CB	-5.08	103.34	110.25	8	1
3	A	100	VAL	CA-C-N	-5.07	115.63	123.14	17	1
3	A	100	VAL	C-N-CA	-5.07	115.63	123.14	17	1
3	A	112	SER	CA-C-N	5.01	124.79	119.28	2	1
3	A	112	SER	C-N-CA	5.01	124.79	119.28	2	1
3	A	8	THR	N-CA-CB	-5.00	104.43	110.53	8	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

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±4
2	C	361	209	209	37±6
3	A	1055	1034	1034	230±16
All	All	35760	28900	28900	5250

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 81.

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:24:ASP:O	3:A:78:ASN:CG	0.97	2.07	7	20
3:A:109:VAL:HG11	3:A:111:MET:HE2	0.97	1.34	4	2
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:12:ARG:O	3:A:16:VAL:HG23	0.93	1.64	18	20
3:A:31:VAL:HG12	3:A:33:THR:HG22	0.93	1.40	12	20
3:A:105:LEU:C	3:A:105:LEU:HD13	0.92	1.90	17	4
3:A:84:LEU:HD21	3:A:123:THR:C	0.92	1.90	2	10
2:C:234:DT:OP2	3:A:36:ILE:HD12	0.91	1.66	8	17
3:A:111:MET:HE3	3:A:115:HIS:HB3	0.90	1.44	3	1
2:C:224:DT:OP1	3:A:130:ALA:HB2	0.89	1.67	5	7
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:23:ALA:HB1	3:A:27:PHE:CE2	0.87	2.05	20	12
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

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
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:93:LEU:HD23	3:A:101:THR:HB	0.82	1.51	1	1
3:A:127:THR:O	3:A:131:TRP:HB2	0.82	1.74	6	20
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
2:C:224:DT:H71	2:C:224:DT:OP2	0.79	1.77	17	3
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
3:A:116:LEU:O	3:A:116:LEU:HD12	0.79	1.77	11	3
3:A:90:ALA:O	3:A:94:LEU:HD13	0.78	1.79	7	5
3:A:24:ASP:C	3:A:77:ALA:HB1	0.78	2.03	3	19
3:A:102:LEU:HD23	3:A:116:LEU:HD12	0.78	1.56	2	1
3:A:109:VAL:HG11	3:A:111:MET:HE3	0.78	1.55	10	4
3:A:13:TRP:CD1	3:A:17:LEU:HD11	0.78	2.13	18	5
3:A:94:LEU:HD22	3:A:132:GLN:CD	0.77	2.04	17	7
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: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

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:A:77:ALA:C	3:A:79:PRO:HD2	0.76	2.06	16	20
3:A:121:LYS:HB2	3:A:128:PRO:CD	0.76	2.11	12	19
3:A:132:GLN:HA	3:A:135:TRP:CD1	0.76	2.16	14	4
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:101:THR:C	3:A:102:LEU:HD12	0.75	2.05	2	1
3:A:105:LEU:HD22	3:A:116:LEU:HD13	0.75	1.57	6	1
3:A:124:THR:HG1	3:A:131:TRP:CD1	0.74	2.00	19	6
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:111:MET:HE1	3:A:112:SER:O	0.74	1.83	3	1
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: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:37:PHE:CG	3:A:61:ALA:HB1	0.72	2.20	11	20
3:A:109:VAL:O	3:A:110:ALA:HB3	0.72	1.84	16	19
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
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:119:LEU:C	3:A:119:LEU:HD22	0.71	2.10	16	7
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:18:ALA:O	3:A:19:ARG:HG2	0.70	1.87	14	7
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:58:ALA:O	3:A:62:LEU:HG	0.70	1.86	3	20
3:A:109:VAL:HG11	3:A:111:MET:CE	0.70	2.16	6	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:A:100:VAL:CG1	3:A:102:LEU:HD12	0.70	2.17	11	1
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:97:GLU:C	3:A:97:GLU:CD	0.69	2.59	20	3
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
3:A:62:LEU:HD21	3:A:68:PRO:HG3	0.68	1.65	13	20
2:C:235:DT:OP1	3:A:47:ALA:HA	0.68	1.89	2	9
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:O	3:A:105:LEU:HD22	0.68	1.88	17	1
3:A:8:THR:O	3:A:12:ARG:HD2	0.68	1.88	4	1
3:A:102:LEU:CD2	3:A:117:HIS:NE2	0.68	2.57	19	5
3:A:84:LEU:CD2	3:A:124:THR:HA	0.68	2.18	6	1
3:A:93:LEU:HD13	3:A:97:GLU:OE1	0.68	1.89	9	1
2:C:223:DT:H72	3:A:114:PHE:CE2	0.67	2.24	6	5
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	2.28	1	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: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	1
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:109:VAL:CG1	3:A:111:MET:HE3	0.66	2.19	10	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
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:109:VAL:HG12	3:A:111:MET:HE3	0.66	1.67	17	2
3:A:77:ALA:O	3:A:80:ARG:CB	0.65	2.44	12	18
3:A:116:LEU:HD13	3:A:116:LEU:C	0.65	2.16	2	14
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:116:LEU:HD12	3:A:116:LEU:C	0.65	2.16	19	3
3:A:28:VAL:HG21	3:A:61:ALA:HB2	0.65	1.69	10	20
3:A:119:LEU:HD22	3:A:119:LEU:O	0.65	1.90	8	5
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:97:GLU:OE1	3:A:99:PRO:O	0.65	2.14	14	3
3:A:111:MET:SD	3:A:115:HIS:HB2	0.65	2.31	2	1
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:111:MET:HE3	3:A:116:LEU:HA	0.64	1.69	12	3
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:84:LEU:CD2	3:A:123:THR:HG21	0.64	2.21	4	1
2:C:234:DT:H4'	3:A:45:ARG:CB	0.64	2.23	13	1
3:A:102:LEU:HD12	3:A:106:ALA:HB2	0.64	1.70	3	2
3:A:90:ALA:HA	3:A:93:LEU:HD21	0.64	1.70	6	2
3:A:43:ARG:H	3:A:43:ARG:HD2	0.64	1.53	13	1
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:24:ASP:OD1	3:A:77:ALA:CB	0.64	2.46	18	4
3:A:131:TRP:CE3	3:A:131:TRP:HA	0.64	2.28	4	17
3:A:105:LEU:HD22	3:A:116:LEU:HD11	0.64	1.68	9	5
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
1:B:201:DC:OP1	3:A:111:MET:HE1	0.63	1.94	20	1
3:A:116:LEU:C	3:A:116:LEU:HD12	0.63	2.18	7	3
3:A:94:LEU:HG	3:A:100:VAL:HG12	0.63	1.69	3	2
3:A:102:LEU:HD11	3:A:113:PRO:HA	0.63	1.69	8	1
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:CD1	3:A:37:PHE:O	0.63	2.52	6	20
3:A:76:LYS:O	3:A:80:ARG:HB2	0.63	1.92	7	4

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:A:111:MET:HE1	3:A:116:LEU:HA	0.63	1.70	19	1
3:A:94:LEU:HD23	3:A:132:GLN:HG3	0.63	1.68	4	1
3:A:119:LEU:HD13	3:A:119:LEU:C	0.62	2.19	4	11
3:A:12:ARG:HD2	3:A:12:ARG:N	0.62	2.09	16	7
2:C:224:DT:OP2	2:C:224:DT:H73	0.62	1.94	15	10
3:A:98:THR:HB	3:A:99:PRO:CD	0.62	2.23	11	20
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
3:A:17:LEU:HD23	3:A:17:LEU:N	0.62	2.10	3	15
3:A:109:VAL:CG2	3:A:111:MET:HE2	0.62	2.25	1	1
2:C:233:DA:OP1	3:A:70:LYS:CB	0.62	2.47	6	2
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:109:VAL:HG21	3:A:111:MET:HE2	0.62	1.70	1	1
3:A:105:LEU:C	3:A:105:LEU:CD1	0.62	2.73	5	3
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:H6	1:B:201:DC:O5'	0.61	1.78	7	10
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:116:LEU:HD12	3:A:116:LEU:O	0.61	1.94	1	2
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:37:PHE:CD2	3:A:61:ALA:HB1	0.61	2.31	20	20
3:A:109:VAL:CB	3:A:111:MET:HE2	0.61	2.26	1	1
3:A:97:GLU:CD	3:A:99:PRO:O	0.61	2.44	2	6
3:A:16:VAL:HG12	3:A:46:HIS:CE1	0.61	2.29	13	13
3:A:111:MET:HE3	3:A:115:HIS:CB	0.61	2.23	3	1
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
1:B:201:DC:H2''	1:B:202:DG:O5'	0.61	1.96	3	20
3:A:93:LEU:O	3:A:97:GLU:OE1	0.61	2.17	10	2
3:A:102:LEU:HD22	3:A:117:HIS:NE2	0.61	2.11	19	1
3:A:109:VAL:CG1	3:A:111:MET:HE2	0.61	2.21	4	1
2:C:234:DT:O4'	3:A:45:ARG:CD	0.61	2.49	15	1
3:A:27:PHE:CD1	3:A:27:PHE:C	0.60	2.78	20	12
3:A:97:GLU:HG2	3:A:98:THR:N	0.60	2.11	8	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:A:105:LEU:CD2	3:A:116:LEU:HD21	0.60	2.26	10	2
3:A:97:GLU:HG3	3:A:99:PRO:O	0.60	1.96	16	7
3:A:55:TYR:CD2	3:A:61:ALA:HB2	0.60	2.30	8	10
3:A:100:VAL:CG1	3:A:102:LEU:HD11	0.60	2.26	19	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:111:MET:CE	3:A:115:HIS:HB3	0.60	2.22	3	1
3:A:31:VAL:CG1	3:A:33:THR:HG22	0.60	2.27	3	20
3:A:116:LEU:HD13	3:A:116:LEU:O	0.60	1.97	14	10
3:A:16:VAL:C	3:A:17:LEU:HD23	0.59	2.21	8	15
3:A:24:ASP:OD1	3:A:39:ARG:NE	0.59	2.35	18	5
3:A:84:LEU:HD13	3:A:87:ILE:CD1	0.59	2.28	4	1
3:A:24:ASP:OD1	3:A:40:PRO:HD2	0.59	1.97	17	2
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:23:ALA:HB1	3:A:27:PHE:HE2	0.59	1.57	1	4
3:A:58:ALA:O	3:A:62:LEU:CG	0.59	2.50	2	20
3:A:90:ALA:C	3:A:94:LEU:HD12	0.59	2.22	9	3
3:A:94:LEU:HG	3:A:100:VAL:HG13	0.59	1.75	19	6
3:A:121:LYS:HG3	3:A:128:PRO:HD3	0.59	1.74	7	5
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
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:39:ARG:NH2	3:A:76:LYS:C	0.59	2.61	20	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:62:LEU:HD21	3:A:68:PRO:CG	0.58	2.28	6	20
3:A:24:ASP:OD1	3:A:39:ARG:HD3	0.58	1.98	2	2
3:A:94:LEU:HD11	3:A:102:LEU:CD1	0.58	2.24	7	1
3:A:39:ARG:NH2	3:A:75:ASP:CG	0.58	2.61	20	6
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

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
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: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:119:LEU:C	3:A:119:LEU:HD23	0.58	2.24	11	4
3:A:125:GLY:O	3:A:126:MET:HG2	0.58	1.99	12	6
3:A:84:LEU:CD1	3:A:87:ILE:HD12	0.58	2.27	4	1
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:29:PHE:CD1	3:A:52:VAL:HG22	0.58	2.33	13	20
3:A:97:GLU:N	3:A:97:GLU:OE1	0.58	2.37	20	2
3:A:121:LYS:HD2	3:A:126:MET:HA	0.58	1.76	19	1
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
2:C:234:DT:H4'	3:A:45:ARG:C	0.57	2.23	6	2
1:B:202:DG:C2	1:B:203:DC:C2	0.57	2.91	13	19
3:A:14:GLN:O	3:A:18:ALA:CB	0.57	2.53	4	19
3:A:87:ILE:HG21	3:A:120:PHE:CD1	0.57	2.33	2	14
3:A:8:THR:C	3:A:12:ARG:HD2	0.57	2.25	18	2
3:A:24:ASP:CG	3:A:77:ALA:CB	0.57	2.78	8	2
3:A:127:THR:HB	3:A:131:TRP:CE3	0.57	2.34	8	1
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:24:ASP:OD1	3:A:39:ARG:CG	0.57	2.53	9	17
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:HB3	0.57	2.00	4	14
3:A:39:ARG:NH1	3:A:75:ASP:CG	0.57	2.63	2	9
3:A:118:ARG:HA	3:A:128:PRO:HB3	0.57	1.76	7	6
3:A:94:LEU:HD11	3:A:100:VAL:HG13	0.57	1.75	4	1
3:A:71:ARG:O	3:A:75:ASP:HB3	0.57	1.98	6	1
1:B:202:DG:N2	2:C:227:DG:C2	0.57	2.72	12	16
3:A:84:LEU:CD2	3:A:123:THR:CG2	0.57	2.82	4	5
2:C:231:DT:O2	3:A:71:ARG:NH2	0.57	2.38	9	4
1:B:190:DG:C5	1:B:191:DC:N4	0.57	2.73	10	20
3:A:28:VAL:HG23	3:A:29:PHE:N	0.56	2.15	16	20
3:A:72:CYS:HA	3:A:75:ASP:OD2	0.56	1.99	14	5
3:A:121:LYS:CD	3:A:126:MET:HA	0.56	2.30	3	3
3:A:114:PHE:CD1	3:A:129:LYS:HE2	0.56	2.35	4	2
2:C:224:DT:H71	3:A:129:LYS:CD	0.56	2.29	7	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:A:105:LEU:HD11	3:A:116:LEU:CB	0.56	2.31	17	1
2:C:235:DT:P	3:A:46:HIS:O	0.56	2.63	13	16
3:A:91:CYS:SG	3:A:135:TRP:CB	0.56	2.93	3	7
3:A:125:GLY:O	3:A:126:MET:CG	0.56	2.54	9	19
2:C:224:DT:OP1	3:A:130:ALA:CA	0.56	2.53	11	6
3:A:16:VAL:HG13	3:A:29:PHE:CD2	0.56	2.35	13	2
3:A:102:LEU:HB3	3:A:116:LEU:HD23	0.56	1.78	19	1
3:A:29:PHE:CE1	3:A:52:VAL:HG22	0.56	2.35	8	20
2:C:232:DA:C5	2:C:233:DA:C6	0.56	2.93	3	5
1:B:197:DA:C2	2:C:232:DA:C2	0.56	2.93	13	5
3:A:19:ARG:CG	3:A:19:ARG:O	0.56	2.53	13	5
2:C:224:DT:O5'	2:C:224:DT:H6	0.56	1.84	18	6
3:A:93:LEU:HD11	3:A:97:GLU:OE2	0.56	2.00	4	1
3:A:127:THR:HB	3:A:131:TRP:CG	0.56	2.36	15	8
2:C:223:DT:OP2	3:A:114:PHE:CZ	0.56	2.59	2	9
3:A:127:THR:CG2	3:A:131:TRP:CE3	0.56	2.88	19	9
3:A:73:GLN:HB3	3:A:74:PRO:HD3	0.56	1.77	2	3
3:A:131:TRP:O	3:A:135:TRP:CG	0.56	2.59	11	7
3:A:101:THR:O	3:A:102:LEU:HD12	0.56	2.01	4	2
3:A:102:LEU:HD23	3:A:113:PRO:CA	0.56	2.31	5	1
3:A:94:LEU:HD22	3:A:132:GLN:CG	0.56	2.31	9	2
3:A:18:ALA:O	3:A:19:ARG:HB3	0.56	1.99	13	1
3:A:78:ASN:C	3:A:80:ARG:N	0.56	2.63	10	3
3:A:131:TRP:CD1	3:A:135:TRP:CZ2	0.56	2.94	9	5
3:A:117:HIS:CE1	3:A:129:LYS:HE3	0.56	2.36	19	1
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	3
2:C:223:DT:OP1	3:A:129:LYS:HE3	0.55	2.00	13	2
3:A:13:TRP:HZ3	3:A:16:VAL:HG11	0.55	1.62	16	16
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:39:ARG:NH2	3:A:72:CYS:O	0.55	2.39	3	2
3:A:13:TRP:O	3:A:17:LEU:HD12	0.55	2.02	11	5
3:A:68:PRO:HB2	3:A:73:GLN:HB2	0.55	1.79	20	10
3:A:126:MET:C	3:A:127:THR:OG1	0.55	2.50	4	19
1:B:202:DG:N7	3:A:115:HIS:CE1	0.55	2.74	8	5
3:A:93:LEU:HD21	3:A:97:GLU:CD	0.55	2.27	4	1
3:A:121:LYS:CD	3:A:128:PRO:HD3	0.55	2.32	4	1
3:A:97:GLU:OE1	3:A:97:GLU:N	0.55	2.40	10	1
2:C:223:DT:P	3:A:129:LYS:CE	0.55	2.95	13	1
3:A:84:LEU:HD13	3:A:87:ILE:HG13	0.55	1.79	14	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:A:28:VAL:HG21	3:A:37:PHE:CD1	0.55	2.36	8	20
3:A:75:ASP:OD1	3:A:75:ASP:C	0.55	2.49	17	2
1:B:202:DG:O6	3:A:118:ARG:CD	0.55	2.54	10	4
3:A:78:ASN:C	3:A:80:ARG:H	0.55	2.09	10	1
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:77:ALA:O	3:A:80:ARG:N	0.55	2.38	10	4
1:B:195:DT:O2	3:A:45:ARG:NH2	0.55	2.35	11	8
3:A:119:LEU:C	3:A:119:LEU:CD2	0.55	2.80	17	6
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
1:B:202:DG:H2''	1:B:203:DC:O5'	0.55	2.02	18	18
3:A:13:TRP:O	3:A:17:LEU:HG	0.55	2.02	8	15
3:A:73:GLN:N	3:A:74:PRO:HD2	0.55	2.15	20	12
3:A:39:ARG:NE	3:A:72:CYS:O	0.55	2.40	2	4
3:A:102:LEU:HD12	3:A:102:LEU:C	0.55	2.27	8	1
3:A:91:CYS:SG	3:A:135:TRP:HB3	0.55	2.42	11	1
3:A:29:PHE:CE1	3:A:31:VAL:CG2	0.55	2.90	8	20
3:A:77:ALA:C	3:A:79:PRO:CD	0.55	2.80	5	19
2:C:235:DT:OP2	3:A:47:ALA:HB2	0.55	2.01	2	1
3:A:116:LEU:HD22	3:A:116:LEU:O	0.55	2.02	17	2
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
2:C:222:DC:H2'	2:C:223:DT:H71	0.54	1.78	6	5
3:A:37:PHE:CD1	3:A:37:PHE:C	0.54	2.85	13	20
3:A:111:MET:HE1	3:A:119:LEU:HD12	0.54	1.78	1	2
3:A:113:PRO:O	3:A:117:HIS:CD2	0.54	2.60	11	4
3:A:39:ARG:CZ	3:A:75:ASP:CG	0.54	2.80	20	9
3:A:27:PHE:CE1	3:A:40:PRO:HB3	0.54	2.37	13	1
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
1:B:206:DG:C6	1:B:207:DA:C6	0.54	2.96	20	20
3:A:102:LEU:HD12	3:A:102:LEU:N	0.54	2.17	2	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:58:ALA:HB1	3:A:73:GLN:NE2	0.54	2.16	8	1
3:A:131:TRP:CD2	3:A:135:TRP:CZ2	0.54	2.96	2	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:C:224:DT:OP1	3:A:130:ALA:CB	0.54	2.54	9	3
1:B:206:DG:C6	1:B:207:DA:N6	0.54	2.76	7	16
2:C:234:DT:O4'	3:A:45:ARG:HB3	0.54	2.02	6	3
3:A:12:ARG:HA	3:A:12:ARG:NE	0.54	2.17	3	1
1:B:199:DA:H2''	1:B:200:DG:O5'	0.54	2.02	5	20
3:A:55:TYR:CE2	3:A:61:ALA:HA	0.54	2.38	3	20
2:C:222:DC:H2'	2:C:223:DT:H72	0.54	1.78	16	12
3:A:131:TRP:CG	3:A:135:TRP:CZ2	0.54	2.96	4	3
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
3:A:102:LEU:HD23	3:A:117:HIS:HE2	0.54	1.62	3	1
3:A:43:ARG:NH1	3:A:71:ARG:CD	0.54	2.71	7	1
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:87:ILE:CG2	3:A:120:PHE:CE1	0.54	2.91	8	15
3:A:8:THR:HG22	3:A:8:THR:O	0.54	2.03	20	3
3:A:16:VAL:CA	3:A:40:PRO:HA	0.54	2.31	6	1
3:A:43:ARG:HD2	3:A:43:ARG:N	0.54	2.17	13	1
3:A:119:LEU:HD23	3:A:119:LEU:O	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: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:71:ARG:O	3:A:75:ASP:CG	0.53	2.51	6	1
3:A:117:HIS:ND1	3:A:129:LYS:HG3	0.53	2.18	7	1
2:C:223:DT:H73	3:A:114:PHE:CE2	0.53	2.38	17	6
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
3:A:95:GLU:HB3	3:A:139:ARG:C	0.53	2.28	7	2
2:C:223:DT:OP2	3:A:114:PHE:CE1	0.53	2.62	6	8
3:A:117:HIS:O	3:A:128:PRO:CB	0.53	2.56	12	13
3:A:93:LEU:HD13	3:A:93:LEU:O	0.53	2.04	4	1
2:C:235:DT:C5'	3:A:45:ARG:HG2	0.53	2.34	13	1
3:A:105:LEU:HD22	3:A:116:LEU:CD1	0.53	2.32	6	1
3:A:72:CYS:HA	3:A:75:ASP:HB3	0.53	1.79	8	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

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
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
2:C:223:DT:P	3:A:129:LYS:HD3	0.53	2.44	10	1
3:A:84:LEU:HD13	3:A:123:THR:HB	0.53	1.79	7	1
3:A:117:HIS:HB3	3:A:129:LYS:CA	0.53	2.34	7	2
3:A:98:THR:HB	3:A:99:PRO:HD3	0.53	1.80	13	2
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
2:C:224:DT:H3'	3:A:130:ALA:HB2	0.53	1.80	7	1
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
2:C:225:DG:N7	3:A:118:ARG:NH1	0.53	2.57	16	2
1:B:196:DT:H2''	1:B:197:DA:O5'	0.52	2.04	20	20
3:A:37:PHE:CE1	3:A:58:ALA:HA	0.52	2.38	13	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
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
1:B:202:DG:N3	1:B:203:DC:C2	0.52	2.77	3	5
3:A:119:LEU:O	3:A:119:LEU:HD22	0.52	2.05	7	2
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:CG	3:A:100:VAL:HG12	0.51	2.35	3	1
3:A:94:LEU:HD13	3:A:132:GLN:HG3	0.51	1.82	8	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
2:C:223:DT:H3'	3:A:129:LYS:HB3	0.51	1.82	5	1
3:A:77:ALA:O	3:A:80:ARG:HB3	0.51	2.06	14	1
3:A:29:PHE:HD1	3:A:52:VAL:HG13	0.51	1.65	12	20
3:A:37:PHE:CG	3:A:37:PHE:O	0.51	2.64	12	20
2:C:232:DA:C6	2:C:233:DA:C6	0.51	2.99	2	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:A:117:HIS:CE1	3:A:132:GLN:HB2	0.51	2.40	5	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	2.58	4	14
3:A:29:PHE:CD1	3:A:52:VAL:HG13	0.51	2.41	12	14
3:A:111:MET:HE1	3:A:116:LEU:HD23	0.51	1.83	9	1
3:A:13:TRP:CZ3	3:A:52:VAL:HG11	0.51	2.41	14	17
3:A:55:TYR:CD2	3:A:61:ALA:CB	0.51	2.94	8	10
2:C:223:DT:H3'	3:A:129:LYS:HG2	0.51	1.82	9	1
3:A:94:LEU:HD23	3:A:100:VAL:HG13	0.51	1.83	9	1
1:B:201:DC:O5'	3:A:115:HIS:CE1	0.51	2.64	19	1
3:A:93:LEU:HD23	3:A:101:THR:CB	0.51	2.31	1	1
3:A:12:ARG:HD2	3:A:12:ARG:H	0.51	1.66	10	2
3:A:102:LEU:HD13	3:A:102:LEU:C	0.51	2.31	14	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:23:ALA:C	3:A:40:PRO:HG3	0.51	2.30	20	9
3:A:9:ASP:HA	3:A:12:ARG:HB2	0.50	1.82	20	8
2:C:224:DT:OP2	3:A:129:LYS:C	0.50	2.54	7	1
3:A:114:PHE:HA	3:A:117:HIS:ND1	0.50	2.21	19	1
1:B:201:DC:C2	1:B:202:DG:C5	0.50	2.99	9	4
3:A:70:LYS:O	3:A:74:PRO:CD	0.50	2.60	6	1
3:A:12:ARG:HD3	3:A:27:PHE:CE2	0.50	2.42	1	1
3:A:116:LEU:HD13	3:A:117:HIS:N	0.50	2.21	5	2
3:A:11:GLN:O	3:A:12:ARG:C	0.50	2.53	10	20
3:A:37:PHE:CG	3:A:61:ALA:CB	0.50	2.95	11	20
3:A:90:ALA:O	3:A:94:LEU:CD1	0.50	2.60	4	16
3:A:97:GLU:OE1	3:A:98:THR:N	0.50	2.45	2	2
2:C:224:DT:O4	3:A:118:ARG:NH2	0.50	2.44	8	1
3:A:93:LEU:HD13	3:A:101:THR:OG1	0.50	2.05	18	1
3:A:117:HIS:ND1	3:A:129:LYS:HD3	0.50	2.21	9	2
1:B:201:DC:O5'	3:A:115:HIS:HE1	0.50	1.89	10	1
1:B:202:DG:O6	3:A:118:ARG:HD3	0.50	2.07	16	3
3:A:87:ILE:HG21	3:A:120:PHE:CG	0.50	2.41	2	3
3:A:105:LEU:O	3:A:109:VAL:HG23	0.50	2.06	20	6
3:A:127:THR:CG2	3:A:130:ALA:HB3	0.50	2.35	8	2
1:B:204:DA:C2	2:C:225:DG:C2	0.50	2.99	16	1
2:C:223:DT:C7	3:A:114:PHE:CZ	0.50	2.95	16	1
1:B:201:DC:P	3:A:115:HIS:HE1	0.50	2.29	19	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:202:DG:C6	1:B:203:DC:N4	0.50	2.79	13	7
3:A:91:CYS:HA	3:A:135:TRP:CD1	0.50	2.42	4	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:70:LYS:HD2	3:A:70:LYS:O	0.50	2.07	12	1
2:C:225:DG:H2''	2:C:226:DC:O5'	0.50	2.07	3	6
3:A:94:LEU:HD23	3:A:132:GLN:CG	0.50	2.36	4	2
3:A:24:ASP:O	3:A:78:ASN:CA	0.50	2.60	4	3
2:C:234:DT:C3'	3:A:46:HIS:O	0.50	2.60	18	1
3:A:111:MET:HE1	3:A:116:LEU:CA	0.50	2.35	19	1
3:A:64:ALA:HB3	3:A:66:PHE:CD2	0.50	2.42	18	7
3:A:105:LEU:HD12	3:A:116:LEU:HB2	0.50	1.84	1	1
2:C:232:DA:N3	3:A:43:ARG:NH2	0.50	2.60	2	2
3:A:109:VAL:HG11	3:A:119:LEU:HG	0.50	1.84	20	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
2:C:224:DT:OP2	2:C:224:DT:C7	0.49	2.61	19	11
2:C:225:DG:C2	2:C:226:DC:C2	0.49	3.00	2	3
3:A:102:LEU:HD13	3:A:102:LEU:O	0.49	2.06	3	3
3:A:93:LEU:HG	3:A:101:THR:OG1	0.49	2.05	4	1
3:A:105:LEU:CD2	3:A:116:LEU:HD22	0.49	2.37	11	1
3:A:111:MET:HE1	3:A:119:LEU:HB2	0.49	1.84	4	3
3:A:13:TRP:CG	3:A:49:ARG:CD	0.49	2.94	10	1
1:B:198:DA:H4'	3:A:43:ARG:CG	0.49	2.38	13	1
3:A:28:VAL:CG2	3:A:37:PHE:CD1	0.49	2.96	8	20
3:A:31:VAL:CG1	3:A:47:ALA:CB	0.49	2.90	9	17
3:A:121:LYS:O	3:A:125:GLY:N	0.49	2.45	14	18
3:A:25:GLY:HA3	3:A:78:ASN:H	0.49	1.68	12	5
3:A:24:ASP:CG	3:A:77:ALA:HB1	0.49	2.33	6	2
3:A:102:LEU:CG	3:A:116:LEU:HD21	0.49	2.36	7	1
3:A:114:PHE:O	3:A:118:ARG:HG2	0.49	2.07	14	2
3:A:16:VAL:CA	3:A:40:PRO:O	0.49	2.49	13	1
3:A:27:PHE:CZ	3:A:40:PRO:CB	0.49	2.92	13	1
3:A:105:LEU:CD1	3:A:116:LEU:HG	0.49	2.37	17	1
3:A:87:ILE:HB	3:A:120:PHE:CE1	0.49	2.43	12	10
3:A:117:HIS:HB3	3:A:129:LYS:N	0.49	2.22	2	2
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

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:A:57:ASN:OD1	3:A:60:GLU:N	0.49	2.45	9	10
3:A:39:ARG:CD	3:A:77:ALA:HB2	0.49	2.37	14	3
3:A:19:ARG:O	3:A:19:ARG:HG3	0.49	2.07	13	2
3:A:43:ARG:O	3:A:43:ARG:NE	0.49	2.45	12	1
3:A:24:ASP:HA	3:A:40:PRO:HD2	0.49	1.85	6	4
3:A:93:LEU:HB3	3:A:101:THR:OG1	0.49	2.07	4	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
2:C:233:DA:O4'	3:A:44:ALA:CB	0.49	2.60	4	5
1:B:202:DG:N3	2:C:227:DG:N2	0.49	2.60	13	6
1:B:197:DA:C6	1:B:198:DA:C6	0.49	3.01	4	3
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:193:DA:N6	2:C:234:DT:O4	0.49	2.46	8	12
3:A:131:TRP:O	3:A:135:TRP:CD2	0.49	2.66	14	4
3:A:77:ALA:HB3	3:A:79:PRO:HD2	0.49	1.84	8	4
3:A:18:ALA:O	3:A:19:ARG:CD	0.49	2.61	18	1
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
3:A:121:LYS:CG	3:A:128:PRO:HD3	0.48	2.38	2	5
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:116:LEU:C	3:A:116:LEU:CD1	0.48	2.86	16	14
3:A:87:ILE:HG23	3:A:120:PHE:CD2	0.48	2.43	16	7
3:A:111:MET:HE2	3:A:115:HIS:HB3	0.48	1.84	7	1
3:A:94:LEU:HD23	3:A:100:VAL:HG11	0.48	1.82	14	2
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
2:C:223:DT:P	3:A:129:LYS:HE3	0.48	2.48	13	2
3:A:84:LEU:CD2	3:A:123:THR:C	0.48	2.83	9	1
3:A:93:LEU:O	3:A:97:GLU:HG3	0.48	2.08	14	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
1:B:199:DA:H5'	3:A:43:ARG:CB	0.48	2.39	20	3
1:B:193:DA:H2''	1:B:194:DA:O5'	0.48	2.09	9	16
1:B:204:DA:H2''	1:B:205:DA:O5'	0.48	2.09	10	17
3:A:8:THR:O	3:A:9:ASP:C	0.48	2.56	11	16
3:A:36:ILE:CG2	3:A:37:PHE:N	0.48	2.77	11	20

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
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:109:VAL:HB	3:A:111:MET:HE2	0.48	1.85	1	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:112:SER:CB	3:A:113:PRO:HD2	0.48	2.39	2	1
3:A:116:LEU:C	3:A:116:LEU:HD22	0.48	2.32	17	2
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:93:LEU:HD13	3:A:93:LEU:C	0.48	2.33	4	1
3:A:39:ARG:NH1	3:A:77:ALA:N	0.48	2.62	2	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:87:ILE:CG2	3:A:120:PHE:CD2	0.47	2.97	1	8
3:A:102:LEU:C	3:A:102:LEU:CD1	0.47	2.87	14	2
3:A:87:ILE:CG2	3:A:120:PHE:CZ	0.47	2.96	18	4
3:A:105:LEU:CB	3:A:116:LEU:HD22	0.47	2.38	19	1
2:C:227:DG:C8	2:C:228:DC:C4	0.47	3.02	5	1
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
3:A:13:TRP:CD1	3:A:17:LEU:CD1	0.47	2.96	16	5
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	3
2:C:223:DT:OP1	3:A:129:LYS:HD3	0.47	2.09	4	2
3:A:8:THR:O	3:A:11:GLN:N	0.47	2.46	4	5
3:A:12:ARG:HB3	3:A:27:PHE:CE2	0.47	2.44	6	2
3:A:16:VAL:CG2	3:A:27:PHE:CZ	0.47	2.97	14	2
3:A:43:ARG:CZ	3:A:71:ARG:NH2	0.47	2.77	2	1
3:A:54:PHE:CD1	3:A:54:PHE:N	0.47	2.81	2	1
3:A:94:LEU:HD22	3:A:132:GLN:HG3	0.47	1.85	12	2
3:A:70:LYS:O	3:A:70:LYS:CD	0.47	2.63	7	1
3:A:16:VAL:HG22	3:A:27:PHE:HE1	0.47	1.69	20	2
3:A:105:LEU:CG	3:A:116:LEU:HD13	0.47	2.36	19	1
3:A:113:PRO:O	3:A:117:HIS:ND1	0.47	2.48	3	3
3:A:117:HIS:CE1	3:A:132:GLN:OE1	0.47	2.67	7	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:A:102:LEU:HD13	3:A:116:LEU:HG	0.47	1.87	8	1
3:A:54:PHE:CD2	3:A:54:PHE:N	0.47	2.82	1	3
2:C:223:DT:OP1	3:A:129:LYS:CE	0.47	2.63	13	4
3:A:9:ASP:OD1	3:A:9:ASP:N	0.47	2.46	5	5
3:A:117:HIS:O	3:A:128:PRO:HB3	0.47	2.09	8	7
3:A:121:LYS:HB2	3:A:128:PRO:HD3	0.47	1.86	4	1
3:A:124:THR:OG1	3:A:131:TRP:CD1	0.47	2.65	6	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
1:B:201:DC:P	3:A:115:HIS:CE1	0.47	3.07	19	1
3:A:109:VAL:HG12	3:A:111:MET:SD	0.47	2.49	20	1
1:B:198:DA:C4'	3:A:43:ARG:O	0.47	2.63	7	4
3:A:16:VAL:HA	3:A:40:PRO:C	0.47	2.35	4	11
3:A:117:HIS:CD2	3:A:129:LYS:NZ	0.47	2.82	5	1
3:A:102:LEU:CD1	3:A:102:LEU:C	0.47	2.87	13	2
3:A:13:TRP:CD1	3:A:49:ARG:CD	0.47	2.97	10	1
3:A:84:LEU:HA	3:A:87:ILE:HG13	0.47	1.86	4	1
3:A:91:CYS:SG	3:A:135:TRP:CD2	0.47	3.08	7	4
3:A:94:LEU:HG	3:A:100:VAL:CG1	0.47	2.40	1	4
3:A:120:PHE:O	3:A:124:THR:CG2	0.47	2.63	4	11
3:A:97:GLU:OE1	3:A:99:PRO:N	0.47	2.48	14	2
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:31:VAL:HG22	3:A:52:VAL:CG2	0.46	2.40	6	3
3:A:105:LEU:CD1	3:A:105:LEU:C	0.46	2.88	7	1
3:A:111:MET:CG	3:A:115:HIS:HB3	0.46	2.40	18	2
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
1:B:200:DG:C2'	1:B:201:DC:C5	0.46	2.98	7	4
2:C:233:DA:C1'	3:A:44:ALA:HB1	0.46	2.40	2	1
3:A:121:LYS:CE	3:A:128:PRO:HD3	0.46	2.41	4	1
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
1:B:201:DC:H2'	3:A:115:HIS:CD2	0.46	2.45	4	3
3:A:69:CYS:C	3:A:71:ARG:H	0.46	2.18	12	16
3:A:127:THR:CG2	3:A:131:TRP:CD2	0.46	2.99	4	1
2:C:227:DG:C4	2:C:228:DC:N3	0.46	2.83	5	1
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
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

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:C:233:DA:H3'	3:A:36:ILE:CD1	0.46	2.40	3	3
3:A:13:TRP:HA	3:A:13:TRP:CE3	0.46	2.45	18	8
3:A:102:LEU:C	3:A:102:LEU:HD13	0.46	2.35	13	1
3:A:105:LEU:C	3:A:105:LEU:HD12	0.46	2.35	19	1
3:A:94:LEU:CD2	3:A:100:VAL:CG1	0.46	2.93	3	2
3:A:117:HIS:CD2	3:A:129:LYS:CD	0.46	2.98	5	1
3:A:121:LYS:HD3	3:A:126:MET:HA	0.46	1.86	5	1
3:A:12:ARG:HD2	3:A:27:PHE:CD1	0.46	2.45	12	2
3:A:24:ASP:CG	3:A:77:ALA:HA	0.46	2.36	7	5
3:A:72:CYS:C	3:A:75:ASP:OD1	0.46	2.59	3	2
3:A:105:LEU:HD11	3:A:116:LEU:CG	0.46	2.41	17	1
3:A:113:PRO:O	3:A:117:HIS:CE1	0.46	2.68	19	1
3:A:39:ARG:NH2	3:A:75:ASP:C	0.46	2.73	20	1
3:A:13:TRP:CD1	3:A:49:ARG:HG3	0.46	2.45	6	3
3:A:84:LEU:HD13	3:A:123:THR:CG2	0.46	2.39	7	1
3:A:132:GLN:O	3:A:135:TRP:HB2	0.46	2.10	14	1
2:C:223:DT:H72	3:A:114:PHE:HE2	0.46	1.70	12	4
3:A:37:PHE:CZ	3:A:58:ALA:HB1	0.46	2.46	3	9
2:C:233:DA:C5'	3:A:69:CYS:SG	0.46	3.04	3	4
3:A:121:LYS:CE	3:A:126:MET:HA	0.46	2.41	3	1
3:A:30:ALA:HB2	3:A:55:TYR:HE2	0.46	1.71	15	4
1:B:196:DT:O4'	3:A:45:ARG:NH2	0.46	2.49	15	1
3:A:135:TRP:O	3:A:139:ARG:N	0.46	2.49	18	2
3:A:114:PHE:CD1	3:A:114:PHE:N	0.46	2.84	18	2
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:41:SER:O	3:A:42:CYS:C	0.46	2.58	16	4
3:A:135:TRP:N	3:A:135:TRP:CE3	0.46	2.84	2	2
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
2:C:233:DA:H3'	3:A:36:ILE:HD13	0.45	1.88	3	4
3:A:29:PHE:CE1	3:A:52:VAL:CG2	0.45	2.99	11	18
3:A:54:PHE:C	3:A:55:TYR:CD1	0.45	2.95	1	10
3:A:9:ASP:OD1	3:A:10:ASP:N	0.45	2.49	3	1
3:A:95:GLU:CG	3:A:139:ARG:OXT	0.45	2.65	11	3
3:A:106:ALA:HA	3:A:111:MET:HE1	0.45	1.87	9	1
2:C:231:DT:H2''	2:C:232:DA:C5'	0.45	2.40	2	3
3:A:37:PHE:CD2	3:A:61:ALA:CB	0.45	2.99	20	7
1:B:201:DC:N4	3:A:118:ARG:NH2	0.45	2.64	4	1
2:C:226:DC:N4	3:A:118:ARG:HH12	0.45	2.08	6	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:A:39:ARG:NH2	3:A:77:ALA:CB	0.45	2.78	6	1
2:C:225:DG:C6	2:C:226:DC:N4	0.45	2.84	7	1
3:A:127:THR:HB	3:A:131:TRP:HB2	0.45	1.88	8	1
2:C:224:DT:O5'	2:C:224:DT:C6	0.45	2.69	18	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:31:VAL:HG11	3:A:47:ALA:HB1	0.45	1.86	6	1
3:A:121:LYS:HG3	3:A:127:THR:N	0.45	2.26	9	2
2:C:235:DT:P	3:A:46:HIS:C	0.45	2.99	13	1
3:A:19:ARG:O	3:A:19:ARG:CD	0.45	2.64	13	1
1:B:202:DG:N7	3:A:115:HIS:CD2	0.45	2.84	4	5
2:C:225:DG:N7	3:A:118:ARG:NH2	0.45	2.64	12	2
3:A:17:LEU:N	3:A:17:LEU:CD2	0.45	2.80	12	3
2:C:224:DT:H2''	2:C:225:DG:O5'	0.45	2.10	7	1
3:A:127:THR:OG1	3:A:131:TRP:CE3	0.45	2.66	8	1
3:A:87:ILE:HG22	3:A:120:PHE:CD2	0.45	2.46	12	4
3:A:111:MET:CE	3:A:116:LEU:HB2	0.45	2.40	9	1
3:A:131:TRP:NE1	3:A:135:TRP:CZ2	0.45	2.85	18	2
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
2:C:234:DT:C2'	2:C:235:DT:H71	0.45	2.39	15	2
3:A:70:LYS:O	3:A:70:LYS:HD3	0.45	2.11	7	1
1:B:201:DC:N3	1:B:202:DG:C6	0.45	2.84	9	1
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
2:C:223:DT:P	3:A:129:LYS:HG2	0.45	2.51	5	1
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	13	3
3:A:87:ILE:O	3:A:90:ALA:N	0.45	2.50	2	12
2:C:233:DA:C4'	3:A:44:ALA:CB	0.45	2.95	4	2
2:C:225:DG:C5	3:A:118:ARG:NH1	0.45	2.84	6	2
2:C:235:DT:OP1	3:A:46:HIS:C	0.45	2.49	13	2
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
3:A:16:VAL:CG2	3:A:27:PHE:CE1	0.45	3.00	1	8
3:A:121:LYS:CD	3:A:121:LYS:C	0.45	2.88	5	1
2:C:232:DA:OP1	3:A:70:LYS:HE2	0.45	2.12	7	1
3:A:117:HIS:ND1	3:A:129:LYS:CD	0.45	2.80	14	1
3:A:59:SER:HA	3:A:62:LEU:HB2	0.45	1.89	2	20
3:A:97:GLU:OE2	3:A:101:THR:CB	0.45	2.61	1	1
3:A:24:ASP:HA	3:A:40:PRO:CD	0.45	2.41	8	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:A:69:CYS:O	3:A:73:GLN:N	0.45	2.50	4	1
3:A:43:ARG:NH2	3:A:71:ARG:CZ	0.45	2.79	6	1
2:C:222:DC:H2''	2:C:223:DT:O5'	0.45	2.11	7	1
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
2:C:234:DT:H4'	3:A:45:ARG:HG2	0.45	1.89	1	2
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:94:LEU:HG	3:A:100:VAL:HG22	0.45	1.88	4	1
3:A:102:LEU:HD21	3:A:117:HIS:CD2	0.45	2.46	4	2
1:B:201:DC:O2	1:B:202:DG:C4	0.45	2.70	6	5
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
3:A:106:ALA:CA	3:A:111:MET:O	0.45	2.64	16	1
2:C:235:DT:H2''	2:C:236:DT:O5'	0.44	2.11	8	6
3:A:121:LYS:HB2	3:A:128:PRO:CB	0.44	2.42	11	3
3:A:39:ARG:HG2	3:A:77:ALA:HB2	0.44	1.90	4	1
2:C:233:DA:H2''	2:C:234:DT:OP2	0.44	2.11	6	2
3:A:75:ASP:OD2	3:A:77:ALA:HB2	0.44	2.13	8	1
3:A:101:THR:C	3:A:102:LEU:HG	0.44	2.35	19	1
3:A:87:ILE:C	3:A:120:PHE:CZ	0.44	2.95	3	2
3:A:84:LEU:HD13	3:A:123:THR:CB	0.44	2.43	7	1
3:A:39:ARG:CG	3:A:75:ASP:OD2	0.44	2.64	8	1
2:C:223:DT:P	3:A:129:LYS:HZ3	0.44	2.35	11	1
3:A:102:LEU:CD1	3:A:113:PRO:HA	0.44	2.42	14	1
2:C:223:DT:C7	3:A:114:PHE:CE2	0.44	3.00	18	1
2:C:234:DT:OP1	3:A:36:ILE:HG21	0.44	2.12	6	1
2:C:225:DG:OP2	3:A:130:ALA:HB2	0.44	2.12	7	1
3:A:69:CYS:O	3:A:71:ARG:N	0.44	2.50	8	10
3:A:133:GLN:OE1	3:A:136:ARG:NH1	0.44	2.50	3	1
3:A:87:ILE:CG2	3:A:120:PHE:CE2	0.44	2.99	15	6
3:A:49:ARG:O	3:A:52:VAL:HB	0.44	2.13	6	1
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
1:B:197:DA:C2	3:A:43:ARG:NH2	0.44	2.86	12	1
3:A:93:LEU:CD2	3:A:101:THR:HG21	0.44	2.43	15	1
3:A:102:LEU:HD11	3:A:116:LEU:HB2	0.44	1.89	18	1
3:A:31:VAL:N	3:A:36:ILE:O	0.44	2.50	17	13
3:A:73:GLN:CB	3:A:74:PRO:HD3	0.44	2.43	6	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:C:224:DT:P	3:A:129:LYS:C	0.44	3.00	7	1
3:A:117:HIS:CD2	3:A:129:LYS:HE2	0.44	2.47	10	1
3:A:19:ARG:CZ	3:A:41:SER:O	0.44	2.66	13	1
3:A:93:LEU:HD21	3:A:101:THR:HG21	0.44	1.90	15	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:N	3:A:66:PHE:CD1	0.44	2.86	7	11
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:24:ASP:CG	3:A:39:ARG:HD3	0.44	2.38	17	1
3:A:55:TYR:CD1	3:A:55:TYR:N	0.44	2.85	6	9
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:131:TRP:NE1	3:A:135:TRP:CH2	0.44	2.85	8	1
3:A:116:LEU:CD1	3:A:116:LEU:C	0.44	2.91	12	1
3:A:43:ARG:HH11	3:A:44:ALA:HB2	0.44	1.70	20	1
2:C:223:DT:OP1	3:A:129:LYS:HE2	0.43	2.13	12	4
3:A:32:ARG:N	3:A:51:ASN:O	0.43	2.51	2	6
3:A:59:SER:O	3:A:63:ALA:N	0.43	2.51	8	12
3:A:118:ARG:NH1	3:A:121:LYS:CD	0.43	2.81	7	1
3:A:121:LYS:HA	3:A:124:THR:CG2	0.43	2.42	8	3
1:B:192:DA:H2''	1:B:193:DA:O5'	0.43	2.13	19	5
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:43:ARG:CD	3:A:43:ARG:C	0.43	2.92	20	2
3:A:111:MET:HE2	3:A:115:HIS:CB	0.43	2.43	7	1
3:A:16:VAL:O	3:A:46:HIS:CE1	0.43	2.72	8	2
2:C:233:DA:H4'	3:A:44:ALA:CB	0.43	2.42	16	1
3:A:39:ARG:NH2	3:A:72:CYS:C	0.43	2.76	17	1
3:A:19:ARG:HA	3:A:41:SER:CA	0.43	2.43	20	1
1:B:197:DA:H2''	1:B:198:DA:O5'	0.43	2.12	13	2
3:A:111:MET:CE	3:A:115:HIS:CB	0.43	2.93	3	1
3:A:95:GLU:OE1	3:A:95:GLU:HA	0.43	2.12	7	2
3:A:10:ASP:O	3:A:13:TRP:HB3	0.43	2.14	7	1
3:A:97:GLU:CG	3:A:98:THR:N	0.43	2.80	7	3
3:A:102:LEU:O	3:A:105:LEU:N	0.43	2.52	8	1
2:C:223:DT:OP1	3:A:129:LYS:HD2	0.43	2.13	18	1
3:A:121:LYS:HB3	3:A:128:PRO:HB3	0.43	1.91	3	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:A:14:GLN:O	3:A:18:ALA:HB3	0.43	2.12	4	1
3:A:92:ARG:HA	3:A:139:ARG:O	0.43	2.13	7	1
1:B:190:DG:C4	1:B:191:DC:C4	0.43	3.06	13	8
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:80:ARG:NH2	3:A:123:THR:O	0.43	2.52	14	1
3:A:93:LEU:CD2	3:A:101:THR:HB	0.43	2.34	1	1
3:A:75:ASP:OD1	3:A:75:ASP:N	0.43	2.50	2	1
3:A:109:VAL:HG12	3:A:111:MET:CG	0.43	2.43	3	1
3:A:24:ASP:C	3:A:78:ASN:N	0.43	2.75	4	1
3:A:89:HIS:NE2	3:A:92:ARG:NH2	0.43	2.65	4	1
2:C:225:DG:N7	3:A:118:ARG:CZ	0.43	2.82	16	2
2:C:225:DG:C4	2:C:226:DC:C5	0.43	3.06	7	1
2:C:234:DT:O2	3:A:45:ARG:NH2	0.43	2.52	17	2
1:B:202:DG:N7	3:A:115:HIS:ND1	0.43	2.67	11	1
3:A:118:ARG:CA	3:A:118:ARG:NE	0.43	2.81	19	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:69:CYS:C	3:A:71:ARG:N	0.43	2.77	13	16
3:A:134:ALA:O	3:A:135:TRP:C	0.43	2.62	10	9
3:A:119:LEU:C	3:A:119:LEU:CD1	0.43	2.92	12	2
3:A:111:MET:HE2	3:A:112:SER:O	0.43	2.14	9	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:71:ARG:C	3:A:74:PRO:HD2	0.43	2.38	17	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
2:C:224:DT:C7	3:A:129:LYS:CE	0.43	2.96	7	1
3:A:15:SER:OG	3:A:23:ALA:CB	0.43	2.67	7	1
3:A:43:ARG:NH1	3:A:43:ARG:HG2	0.43	2.28	7	1
3:A:72:CYS:O	3:A:75:ASP:CG	0.43	2.62	8	1
3:A:8:THR:C	3:A:10:ASP:N	0.43	2.76	20	3
3:A:91:CYS:O	3:A:92:ARG:C	0.43	2.59	10	5
3:A:117:HIS:CD2	3:A:117:HIS:N	0.43	2.87	11	2
3:A:20:ASP:C	3:A:22:ASN:H	0.43	2.21	20	5
3:A:112:SER:HB3	3:A:113:PRO:HD2	0.43	1.90	3	1
3:A:24:ASP:C	3:A:78:ASN:H	0.43	2.22	4	2
3:A:92:ARG:HD2	3:A:139:ARG:NE	0.43	2.28	6	1
3:A:50:GLU:C	3:A:50:GLU:OE1	0.43	2.62	8	1
3:A:120:PHE:CE1	3:A:131:TRP:HB3	0.43	2.49	8	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:201:DC:H42	2:C:226:DC:N4	0.43	2.12	9	1
3:A:39:ARG:NH1	3:A:76:LYS:C	0.43	2.77	13	1
3:A:18:ALA:C	3:A:19:ARG:CG	0.42	2.92	4	1
3:A:105:LEU:HD11	3:A:111:MET:HE3	0.42	1.91	5	1
1:B:201:DC:H41	3:A:118:ARG:HH11	0.42	1.56	7	1
3:A:94:LEU:CD2	3:A:100:VAL:HG12	0.42	2.41	14	1
3:A:95:GLU:HG3	3:A:136:ARG:HG3	0.42	1.90	20	2
3:A:127:THR:HB	3:A:131:TRP:CD2	0.42	2.49	19	1
3:A:105:LEU:HD13	3:A:105:LEU:O	0.42	2.14	1	2
2:C:233:DA:H4'	3:A:44:ALA:HB3	0.42	1.91	4	1
1:B:199:DA:O4'	3:A:43:ARG:NH1	0.42	2.52	17	2
3:A:9:ASP:HB2	3:A:54:PHE:CD2	0.42	2.49	14	3
3:A:84:LEU:HD13	3:A:124:THR:N	0.42	2.29	6	1
2:C:234:DT:H72	3:A:34:THR:OG1	0.42	2.14	7	1
1:B:201:DC:C2'	3:A:115:HIS:CE1	0.42	2.93	8	1
3:A:105:LEU:C	3:A:105:LEU:HD22	0.42	2.38	17	1
3:A:83:ARG:O	3:A:87:ILE:HG13	0.42	2.13	20	1
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:135:TRP:CE3	3:A:135:TRP:CA	0.42	3.02	2	4
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
1:B:202:DG:N2	1:B:203:DC:O2	0.42	2.52	16	2
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:118:ARG:NH2	3:A:128:PRO:CG	0.42	2.82	12	1
3:A:68:PRO:CB	3:A:73:GLN:NE2	0.42	2.83	18	1
3:A:119:LEU:O	3:A:119:LEU:HD23	0.42	2.15	1	1
1:B:193:DA:N1	1:B:194:DA:C6	0.42	2.88	2	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:39:ARG:NH2	3:A:76:LYS:O	0.42	2.52	18	1
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:102:LEU:HD11	3:A:116:LEU:CG	0.42	2.45	3	1
3:A:111:MET:HG3	3:A:115:HIS:HB3	0.42	1.92	9	1
3:A:39:ARG:HB3	3:A:40:PRO:HD2	0.42	1.90	10	1
3:A:79:PRO:O	3:A:80:ARG:C	0.42	2.63	10	2
3:A:75:ASP:OD1	3:A:76:LYS:N	0.42	2.53	5	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:A:93:LEU:O	3:A:97:GLU:CD	0.42	2.62	7	2
3:A:76:LYS:HE2	3:A:83:ARG:CD	0.42	2.44	14	1
1:B:193:DA:C2	1:B:194:DA:C6	0.42	3.07	2	1
3:A:62:LEU:CD2	3:A:68:PRO:HG3	0.42	2.44	2	4
3:A:114:PHE:N	3:A:114:PHE:CD1	0.42	2.87	6	4
3:A:18:ALA:C	3:A:19:ARG:HG2	0.42	2.40	8	1
3:A:43:ARG:C	3:A:43:ARG:HD2	0.42	2.40	9	1
3:A:34:THR:HG23	3:A:36:ILE:HB	0.42	1.92	11	2
3:A:105:LEU:HD12	3:A:105:LEU:O	0.42	2.14	19	1
2:C:223:DT:OP1	3:A:129:LYS:NZ	0.42	2.50	17	2
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:24:ASP:OD2	3:A:41:SER:OG	0.42	2.36	6	1
3:A:94:LEU:HD23	3:A:132:GLN:HG2	0.42	1.90	7	1
3:A:11:GLN:HG3	3:A:14:GLN:HB3	0.42	1.91	8	1
3:A:129:LYS:O	3:A:129:LYS:CD	0.42	2.68	20	1
1:B:193:DA:C2	1:B:194:DA:C4	0.42	3.08	2	1
2:C:230:DT:C2'	2:C:231:DT:H71	0.42	2.45	10	3
3:A:9:ASP:HA	3:A:12:ARG:CD	0.42	2.44	7	1
3:A:84:LEU:HD13	3:A:84:LEU:HA	0.42	1.67	14	2
3:A:111:MET:CE	3:A:116:LEU:HD22	0.42	2.45	13	2
3:A:106:ALA:HA	3:A:111:MET:SD	0.42	2.55	18	1
3:A:114:PHE:CD1	3:A:129:LYS:CE	0.41	3.03	4	1
3:A:111:MET:HE2	3:A:116:LEU:HB2	0.41	1.92	18	1
2:C:225:DG:O6	3:A:118:ARG:NH1	0.41	2.53	19	1
3:A:117:HIS:HB3	3:A:128:PRO:HB2	0.41	1.90	6	1
3:A:98:THR:HB	3:A:99:PRO:HD2	0.41	1.91	11	1
3:A:9:ASP:HA	3:A:12:ARG:CG	0.41	2.45	13	1
3:A:13:TRP:CD1	3:A:49:ARG:NE	0.41	2.88	18	1
2:C:234:DT:OP2	2:C:234:DT:H73	0.41	2.15	2	1
3:A:109:VAL:HB	3:A:111:MET:HG2	0.41	1.93	4	1
3:A:13:TRP:CE2	3:A:17:LEU:CD1	0.41	3.00	14	4
3:A:91:CYS:SG	3:A:139:ARG:OXT	0.41	2.72	7	1
1:B:198:DA:C2	1:B:199:DA:C6	0.41	3.09	13	1
2:C:224:DT:H71	3:A:118:ARG:HH22	0.41	1.73	15	1
3:A:13:TRP:CE3	3:A:13:TRP:HA	0.41	2.51	8	2
3:A:102:LEU:HD23	3:A:116:LEU:CG	0.41	2.46	2	1
3:A:94:LEU:CD1	3:A:132:GLN:NE2	0.41	2.83	6	1
3:A:109:VAL:CG1	3:A:111:MET:SD	0.41	3.09	20	2
3:A:119:LEU:HD13	3:A:120:PHE:N	0.41	2.30	7	1
3:A:102:LEU:HD11	3:A:106:ALA:HB2	0.41	1.92	8	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:A:117:HIS:ND1	3:A:129:LYS:CE	0.41	2.84	11	1
3:A:43:ARG:NH1	3:A:75:ASP:OD2	0.41	2.53	18	1
1:B:190:DG:C5	1:B:191:DC:C4	0.41	3.09	4	1
3:A:100:VAL:HG12	3:A:101:THR:N	0.41	2.31	11	1
3:A:44:ALA:O	3:A:45:ARG:CB	0.41	2.69	20	2
3:A:105:LEU:HD22	3:A:116:LEU:HD21	0.41	1.93	2	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
3:A:105:LEU:HD12	3:A:116:LEU:CD1	0.41	2.32	7	1
1:B:198:DA:H2''	1:B:199:DA:C8	0.41	2.51	13	1
3:A:97:GLU:OE2	3:A:98:THR:C	0.41	2.63	20	1
1:B:198:DA:H4'	3:A:43:ARG:HB2	0.41	1.90	2	1
3:A:102:LEU:HD23	3:A:113:PRO:HB3	0.41	1.92	5	1
2:C:224:DT:OP2	3:A:129:LYS:HD2	0.41	2.11	7	1
3:A:131:TRP:CD1	3:A:135:TRP:HZ2	0.41	2.33	7	1
3:A:31:VAL:HB	3:A:34:THR:CG2	0.41	2.46	10	1
3:A:93:LEU:CD2	3:A:101:THR:OG1	0.41	2.65	11	1
1:B:198:DA:C5'	3:A:43:ARG:HG2	0.41	2.45	13	1
3:A:42:CYS:O	3:A:46:HIS:NE2	0.41	2.50	13	1
3:A:109:VAL:HB	3:A:111:MET:HG3	0.41	1.92	19	1
1:B:193:DA:C6	1:B:194:DA:N6	0.41	2.89	2	1
3:A:86:LYS:O	3:A:89:HIS:HB3	0.41	2.15	4	1
3:A:124:THR:CG2	3:A:131:TRP:CE3	0.41	3.03	8	1
3:A:33:THR:CG2	3:A:34:THR:N	0.41	2.84	9	2
3:A:24:ASP:HA	3:A:40:PRO:CG	0.41	2.45	13	1
3:A:19:ARG:HG3	3:A:19:ARG:O	0.41	2.16	15	1
3:A:114:PHE:O	3:A:118:ARG:NH2	0.41	2.53	19	1
3:A:97:GLU:OE2	3:A:101:THR:CG2	0.41	2.69	1	1
3:A:43:ARG:NH1	3:A:71:ARG:HD3	0.41	2.31	7	1
3:A:50:GLU:OE2	3:A:51:ASN:ND2	0.41	2.54	7	1
3:A:135:TRP:HA	3:A:135:TRP:CE3	0.41	2.51	11	1
3:A:109:VAL:HG21	3:A:111:MET:CE	0.41	2.45	1	1
1:B:199:DA:H5'	3:A:43:ARG:HB2	0.41	1.93	5	1
3:A:29:PHE:HB2	3:A:54:PHE:CE1	0.41	2.51	5	1
2:C:224:DT:OP2	3:A:129:LYS:O	0.41	2.39	7	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
3:A:12:ARG:O	3:A:27:PHE:CZ	0.41	2.74	10	2
3:A:93:LEU:N	3:A:93:LEU:CD2	0.41	2.84	13	1
3:A:55:TYR:CD2	3:A:61:ALA:N	0.41	2.89	20	1
3:A:129:LYS:O	3:A:129:LYS:HD3	0.41	2.16	20	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:A:60:GLU:OE1	3:A:60:GLU:HA	0.40	2.17	5	1
3:A:97:GLU:CD	3:A:97:GLU:N	0.40	2.78	6	1
3:A:68:PRO:HB2	3:A:73:GLN:CD	0.40	2.41	8	1
2:C:234:DT:C1'	3:A:45:ARG:HD3	0.40	2.46	15	1
3:A:62:LEU:HD23	3:A:68:PRO:HD3	0.40	1.93	18	1
3:A:94:LEU:CD2	3:A:132:GLN:CG	0.40	2.98	2	1
3:A:91:CYS:CB	3:A:135:TRP:CD1	0.40	3.03	4	1
3:A:12:ARG:HD3	3:A:27:PHE:CE1	0.40	2.51	6	1
3:A:97:GLU:OE1	3:A:98:THR:C	0.40	2.64	6	1
3:A:13:TRP:CZ3	3:A:17:LEU:HD21	0.40	2.51	7	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: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:111:MET:HG3	3:A:112:SER:N	0.40	2.32	2	1
3:A:24:ASP:CB	3:A:77:ALA:HB1	0.40	2.46	6	1
3:A:117:HIS:HB3	3:A:129:LYS:HA	0.40	1.93	7	1
3:A:106:ALA:HA	3:A:111:MET:CE	0.40	2.46	9	1
3:A:95:GLU:CG	3:A:136:ARG:HG3	0.40	2.46	13	1
2:C:224:DT:OP1	3:A:129:LYS:O	0.40	2.39	7	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
3:A:23:ALA:HB3	3:A:40:PRO:HG3	0.40	1.92	18	1
3:A:25:GLY:CA	3:A:78:ASN:H	0.40	2.29	4	1
3:A:117:HIS:C	3:A:128:PRO:CB	0.40	2.95	4	1
2:C:232:DA:C4	2:C:233:DA:C5	0.40	3.10	5	1
3:A:12:ARG:NH1	3:A:27:PHE:CB	0.40	2.85	5	1
3:A:25:GLY:HA3	3:A:78:ASN:HB2	0.40	1.93	6	1
3:A:68:PRO:CB	3:A:73:GLN:CD	0.40	2.95	8	1
3:A:95:GLU:HG2	3:A:136:ARG:HG3	0.40	1.92	15	1
3:A:11:GLN:O	3:A:14:GLN:HB3	0.40	2.17	19	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	130/139 (94%)	113±2 (87±1%)	13±2 (10±1%)	4±1 (3±1%)	5	38
All	All	2600/2780 (94%)	2266 (87%)	256 (10%)	78 (3%)	5	38

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	98	THR	20
3	A	128	PRO	20
3	A	70	LYS	16
3	A	77	ALA	9
3	A	9	ASP	4
3	A	45	ARG	3
3	A	19	ARG	3
3	A	97	GLU	1
3	A	110	ALA	1
3	A	74	PRO	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	108/114 (95%)	81±4 (75±4%)	27±4 (25±4%)	2	24
All	All	2160/2280 (95%)	1613 (75%)	547 (25%)	2	24

All 64 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	28	VAL	20
3	A	52	VAL	20
3	A	101	THR	20
3	A	131	TRP	20
3	A	135	TRP	20
3	A	94	LEU	18
3	A	22	ASN	17
3	A	84	LEU	17

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Mol	Chain	Res	Type	Models (Total)
3	A	43	ARG	16
3	A	17	LEU	15
3	A	105	LEU	15
3	A	45	ARG	14
3	A	102	LEU	14
3	A	121	LYS	13
3	A	87	ILE	12
3	A	91	CYS	12
3	A	112	SER	12
3	A	116	LEU	11
3	A	119	LEU	11
3	A	11	GLN	11
3	A	15	SER	10
3	A	86	LYS	9
3	A	129	LYS	9
3	A	124	THR	9
3	A	71	ARG	9
3	A	73	GLN	9
3	A	118	ARG	9
3	A	12	ARG	8
3	A	70	LYS	8
3	A	75	ASP	8
3	A	19	ARG	8
3	A	67	ARG	8
3	A	14	GLN	8
3	A	76	LYS	7
3	A	49	ARG	7
3	A	103	GLU	7
3	A	39	ARG	7
3	A	111	MET	7
3	A	108	GLN	7
3	A	83	ARG	6
3	A	80	ARG	6
3	A	85	ASP	6
3	A	97	GLU	6
3	A	26	GLU	5
3	A	82	HIS	5
3	A	93	LEU	5
3	A	107	ASP	5
3	A	96	GLN	5
3	A	50	GLU	5
3	A	139	ARG	4

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Mol	Chain	Res	Type	Models (Total)
3	A	132	GLN	4
3	A	123	THR	3
3	A	109	VAL	3
3	A	29	PHE	2
3	A	126	MET	2
3	A	100	VAL	2
3	A	136	ARG	2
3	A	95	GLU	2
3	A	32	ARG	2
3	A	138	ARG	1
3	A	133	GLN	1
3	A	92	ARG	1
3	A	41	SER	1
3	A	81	GLN	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	5,6,7	0.65±0.10	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	2.01±0.05	1±0 (33±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	-

There are no bond-length outliers.

All unique angle outliers are listed below.

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
3	A	38	SMC	CA-CB-SG	3.43	108.50	114.04	13	20

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

6.5 Carbohydrates [i](#)

There are no oligosaccharides 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 [i](#)

There are no chain breaks in this entry.

7 Chemical shift validation

No chemical shift data were provided