



Full wwPDB NMR Structure Validation Report ⓘ

Feb 18, 2018 – 02:55 am GMT

PDB ID : 1J5N
Title : Solution Structure of the Non-Sequence-Specific HMGB protein NHP6A in complex with SRY DNA
Authors : Masse, J.E.; Wong, B.; Yen, Y.-M.; Allain, F.H.-T.; Johnson, R.C.; Feigon, J.
Deposited on : 2002-05-15

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

Cyrange : Kirchner and Güntert (2011)
NmrClust : Kelley et al. (1996)
MolProbity : 4.02b-467
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)
RCI : v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV : Wang et al. (2010)
ShiftChecker : trunk30686
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk30686

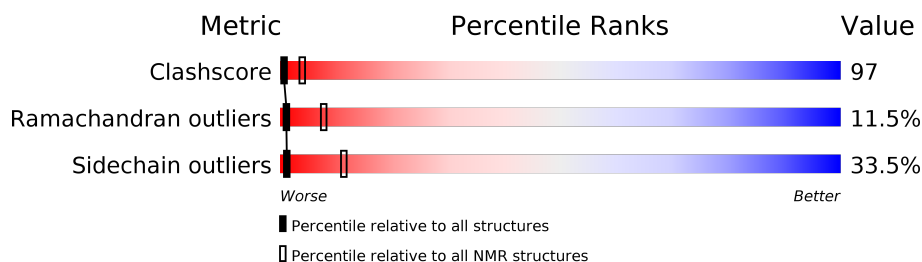
1 Overall quality at a glance

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	136279	12091
Ramachandran outliers	132675	10835
Sidechain outliers	132484	10811

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	15	<div> <div></div> <div>33%</div> <div>67%</div> </div>
2	C	15	<div> <div></div> <div>13%</div> <div>87%</div> </div>
3	A	93	<div> <div></div> <div>51%</div> <div>22%</div> <div></div> <div>23%</div> </div>

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:17-A:88 (72)	0.26	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 3 clusters and 2 single-model clusters were found.

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

3 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 2489 atoms, of which 1119 are hydrogens and 0 are deuteriums.

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

Mol	Chain	Residues	Atoms						Trace
1	B	15	Total	C	H	N	O	P	0
			484	149	172	58	91	14	

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

Mol	Chain	Residues	Atoms						Trace
2	C	15	Total	C	H	N	O	P	0
			466	143	169	55	85	14	

- Molecule 3 is a protein called Nonhistone chromosomal protein 6A.

Mol	Chain	Residues	Atoms						Trace
3	A	93	Total	C	H	N	O	S	0
			1539	478	778	138	143	2	

4 Residue-property plots

4.1 Average score per residue in the NMR ensemble

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

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

Chain B: 

G101	G102	G103	G104	T105	G106	A107	T108	T109	G110	T111	T112	C113	A114	G115
------	------	------	------	------	------	------	------	------	------	------	------	------	------	------

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

Chain C: 

C116	T117	G118	A119	A120	C121	A122	A123	T124	C125	A126	C127	C128	C129	C130
------	------	------	------	------	------	------	------	------	------	------	------	------	------	------

- Molecule 3: Nonhistone chromosomal protein 6A

Chain A: 

W1	W2	T3	P4	B5	E6	P7	K8	K9	R10	T11	T12	T13	K14	K15	K16	D17	P18	N19	A20	F21	K22	K23	A24	L25	S26	A27	Y28	M29	F30	F31	A32	N33	E34	N35	R36	D37	T38	V39	R40	S41	E42	N43	P44	D45	I46	T47	F48	G49	O50	N51	G52	K53	K54	L55	G56	E57	K58	N59	K60
----	----	----	----	----	----	----	----	----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

A61	L62	T63	P64	E65	E66	K67	Q68	P69	Y70	E71	A72	K73	A74	Q75	A76	D77	K78	K79	R80	Y81	E82	S83	E84	K85	E86	L87	Y88	N89	A90	T91	L92	A93
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

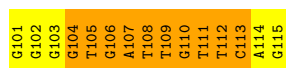
4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

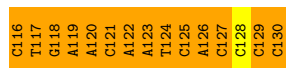
4.2.1 Score per residue for model 1 (medoid)

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

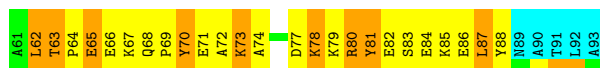
Chain B: 



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

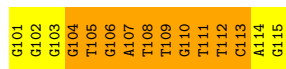


- Molecule 3: Nonhistone chromosomal protein 6A



4.2.2 Score per residue for model 2

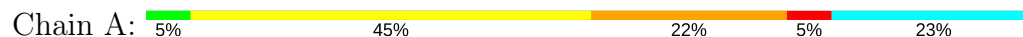
- Molecule 1: 5'-D(*GP*GP*GP*GP*TP*GP*AP*TP*TP*GP*TP*TP*CP*AP*G)-3'



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



- Molecule 3: Nonhistone chromosomal protein 6A



4.2.3 Score per residue for model 3

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

Chain B: 

G101
G102
G103
G104
T105
G106
A107
T108
T109
G110
T111
T112
C113
A114
G115

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

Chain C: 

C116
T117
G118
A119
A120
C121
A122
A123
T124
C125
A126
C127
C128
C129
C130

- Molecule 3: Nonhistone chromosomal protein 6A

Chain A: 

M1
V2
T3
P4
R5
E6
P7
K8
K9
R10
T11
T12
R13
K14
K15
K16
D17
P18
N19
A20
P21
K22
R23
A24
L25
S26
A27
Y28
M29
F30
F31
A32
N33
E34
N35
R36
D37
I38
V39
R40
S41
E42
N43
P44
D45
I46
T47
F48
G49
Q50
V51
G52
K53
K54
L55
G56
E57
K58
W59
K60

A61
L62
T63
P64
E65
E66
K67
Q68
P69
Y70
E71
A72
K73
A74
D77
K78
R79
R80
Y81
E82
S83
E84
K85
E86
L87
Y88
N89
A90
T91
L92
A93

4.2.4 Score per residue for model 4

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

Chain B: 

G101
G102
G103
G104
T105
G106
A107
T108
T109
G110
T111
T112
C113
A114
G115

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

Chain C: 

C116
T117
G118
A119
A120
C121
A122
A123
T124
C125
A126
C127
C128
C129
C130

- Molecule 3: Nonhistone chromosomal protein 6A

Chain A: 

M1
V2
T3
P4
R5
E6
P7
K8
K9
R10
T11
T12
R13
K14
K15
K16
D17
P18
N19
A20
P21
K22
R23
A24
L25
S26
A27
Y28
M29
F30
F31
A32
N33
E34
N35
R36
D37
I38
V39
R40
S41
E42
N43
P44
D45
I46
T47
F48
G49
Q50
V51
G52
K53
K54
L55
G56
E57
K58
W59
K60

A61
L62
T63
P64
E65
E66
K67
Q68
P69
Y70
E71
A72
K73
A74
D77
K78
R79
R80
Y81
E82
S83
E84
K85
E86
L87
Y88
N89
A90
T91
L92
A93

4.2.5 Score per residue for model 5

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

Chain B: 

G101 G102 G103 G104 G105 G106 A107 T108 T109 G110 T111 T112 C113 A114 G115

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

Chain C: 

C116 T117 G118 A119 A120 A121 A122 A123 T124 C125 A126 C127 C128 C129 C130

- Molecule 3: Nonhistone chromosomal protein 6A

Chain A: 

M1 V2 T3 P4 R5 E6 P7 K8 K9 R10 T11 T12 T13 K14 K15 K16 D17 P18 P19 A20 A21 P21 K22 K23 A24 L25 L26 S26 A27 Y28 M29 F30 F31 F32 A32 N33 E34 N35 R36 D37 I38 V39 R40 R41 S41 S42 N43 P44 P45 I46 T47 F48 G49 Q50 V51 G52 K53 K54 L55 G56 E57 K58 W59 K60

A61 L62 T63 P64 E65 E66 K67 Q68 P69 Y70 E71 A72 K73 K74 A74 D77 K78 K79 R80 A81 Y81 E82 S83 E84 K85 E86 L87 Y88 N89 T90 T91 T92 L92 A93

4.2.6 Score per residue for model 6

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

Chain B: 

G101 G102 G103 G104 G105 G106 A107 T108 T109 G110 T111 T112 C113 A114 G115

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

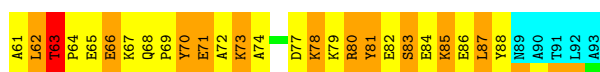
Chain C: 

C116 T117 G118 A119 A120 A121 A122 A123 T124 C125 A126 C127 C128 C129 C130

- Molecule 3: Nonhistone chromosomal protein 6A

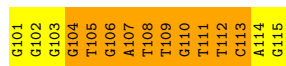
Chain A: 

M1 V2 T3 P4 R5 E6 P7 K8 K9 R10 T11 T12 T13 K14 K15 K16 D17 P18 P19 A20 A21 P21 K22 K23 A24 L25 L26 S26 A27 Y28 M29 F30 F31 F32 A32 N33 E34 N35 R36 D37 I38 V39 R40 R41 S41 S42 N43 P44 P45 I46 T47 F48 G49 Q50 V51 G52 K53 K54 L55 G56 E57 K58 W59 K60

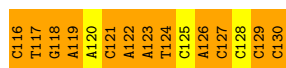


4.2.7 Score per residue for model 7

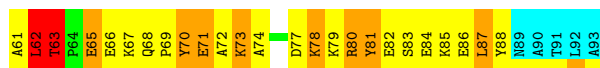
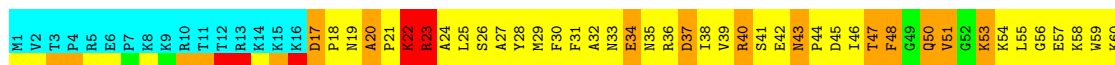
- Molecule 1: 5'-D(*GP*GP*GP*GP*TP*GP*AP*TP*TP*GP*TP*TP*CP*AP*G)-3'



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

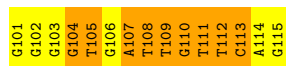


- Molecule 3: Nonhistone chromosomal protein 6A

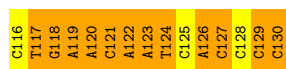


4.2.8 Score per residue for model 8

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

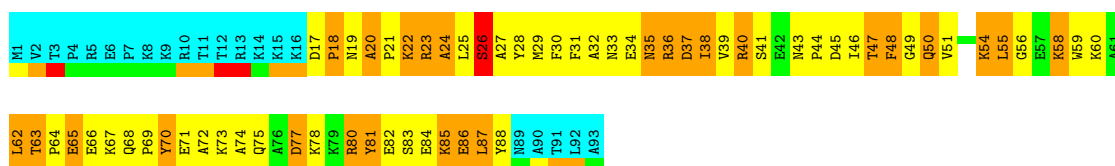


- Molecule 2: 5'-D(*CP*TP*GP*AP*AP*CP*AP*AP*TP*CP*AP*CP*CP*C)-3'



- Molecule 3: Nonhistone chromosomal protein 6A

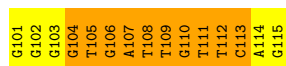




4.2.9 Score per residue for model 9

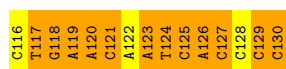
- Molecule 1: 5'-D(*GP*GP*GP*GP*TP*GP*AP*TP*TP*GP*TP*TP*CP*AP*G)-3'

Chain B: 33% 67%



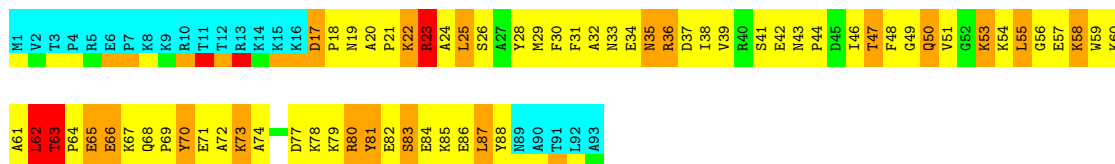
- Molecule 2: 5'-D(*CP*TP*GP*AP*AP*CP*AP*AP*TP*CP*AP*CP*CP*C)-3'

Chain C: 20% 80%



- Molecule 3: Nonhistone chromosomal protein 6A

Chain A: 6% 48% 19% 23%



4.2.10 Score per residue for model 10

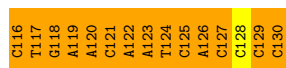
- Molecule 1: 5'-D(*GP*GP*GP*GP*TP*GP*AP*TP*TP*GP*TP*TP*CP*AP*G)-3'

Chain B: 53% 47%



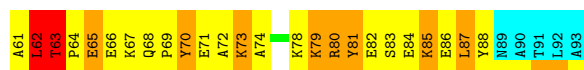
- Molecule 2: 5'-D(*CP*TP*GP*AP*AP*CP*AP*AP*TP*CP*AP*CP*CP*C)-3'

Chain C: 7% 93%



- Molecule 3: Nonhistone chromosomal protein 6A

Chain A: 44% 25% 23%



4.2.11 Score per residue for model 11

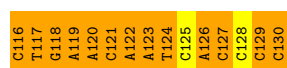
- Molecule 1: 5'-D(*GP*GP*GP*GP*TP*GP*AP*TP*TP*GP*TP*TP*CP*AP*G)-3'

Chain B: 47% 53%



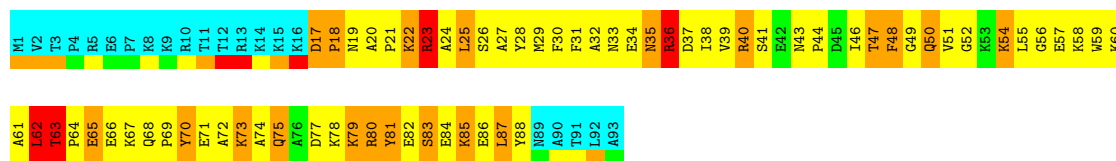
- Molecule 2: 5'-D(*CP*TP*GP*AP*AP*CP*AP*AP*TP*CP*AP*CP*CP*C)-3'

Chain C: 13% 87%



- Molecule 3: Nonhistone chromosomal protein 6A

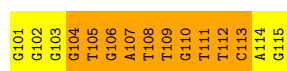
Chain A: 47% 22% 23%



4.2.12 Score per residue for model 12

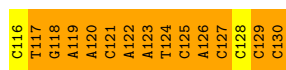
- Molecule 1: 5'-D(*GP*GP*GP*GP*TP*GP*AP*TP*TP*GP*TP*TP*CP*AP*G)-3'

Chain B: 33% 67%

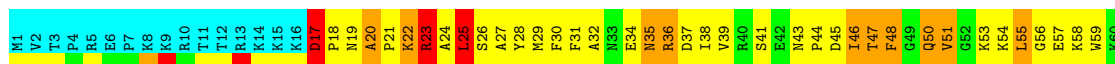


- Molecule 2: 5'-D(*CP*TP*GP*AP*AP*CP*AP*AP*TP*CP*AP*CP*CP*C)-3'

Chain C: 13% 87%



- Molecule 3: Nonhistone chromosomal protein 6A

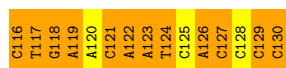


4.2.13 Score per residue for model 13

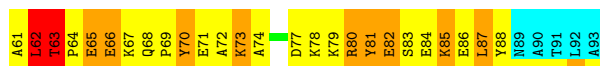
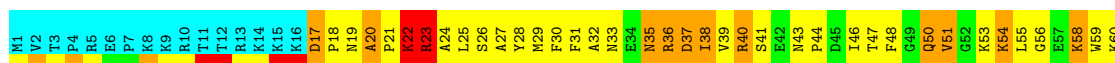
- Molecule 1: 5'-D(*GP*GP*GP*GP*TP*GP*AP*TP*TP*GP*TP*TP*CP*AP*G)-3'



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

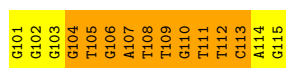


- Molecule 3: Nonhistone chromosomal protein 6A



4.2.14 Score per residue for model 14

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



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

Chain C:

C116
T117
G118
A119
A120
A121
A122
A123
T124
C125
A126
C127
C128
C129
C130

- Molecule 3: Nonhistone chromosomal protein 6A

Chain A:

M1
V2
T3
P4
R5
E6
P7
K8
Q9
R10
T11
T12
R13
K14
K15
K16
D17
P18
N19
A20
P21
K22
R23
S24
L25
S26
A27
Y28
M29
F30
F31
A32
N33
E34
N35
R36
D37
I38
V39
R40
S41
F42
N43
P44
D45
T46
T47
F48
G49
Q50
V51
G52
K53
K54
L55
G56
E57
K58
W59
K60

A61
L62
T63
P64
E65
E66
K67
Q68
P69
Y70
E71
A72
K73
A74
Q75
A76
D77
K78
K79
R80
Y81
E82
S83
E84
K85
E86
L87
Y88
M89
A90
T91
L92
A93

4.2.15 Score per residue for model 15

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

Chain B:

G101
G102
G103
G104
T105
G106
A107
T108
T109
G110
T111
T112
C113
A114
G115

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

Chain C:

C116
T117
G118
A119
A120
A121
A122
A123
T124
C125
A126
C127
C128
C129
C130

- Molecule 3: Nonhistone chromosomal protein 6A

Chain A:

M1
V2
T3
P4
R5
E6
P7
K8
Q9
R10
T11
T12
R13
K14
K15
K16
D17
P18
N19
A20
P21
K22
R23
S24
L25
S26
A27
Y28
M29
F30
F31
A32
N33
E34
N35
R36
D37
I38
V39
R40
S41
F42
N43
P44
D45
T46
T47
F48
G49
Q50
V51
G52
K53
K54
L55
G56
E57
K58
W59
K60

A61
L62
T63
P64
E65
E66
K67
Q68
P69
Y70
E71
A72
K73
A74
Q75
A76
D77
K78
K79
R80
Y81
E82
S83
E84
K85
E86
L87
Y88
M89
A90
T91
L92
A93

4.2.16 Score per residue for model 16

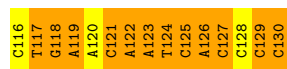
- Molecule 1: 5'-D(*GP*GP*GP*GP*TP*GP*AP*TP*TP*GP*TP*TP*CP*AP*G)-3'

Chain B:

G101
G102
G103
G104
T105
G106
A107
T108
T109
G110
T111
T112
C113
A114
G115

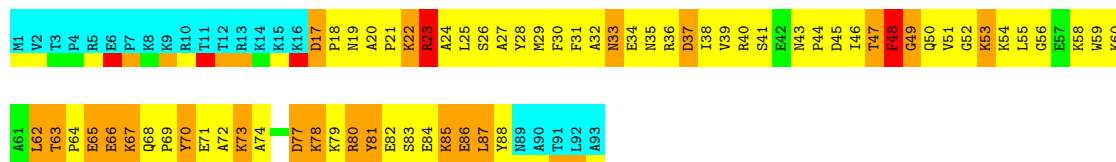
- Molecule 2: 5'-D(*CP*TP*GP*AP*AP*CP*AP*AP*TP*CP*AP*CP*CP*CP*C)-3'

Chain C: 



- Molecule 3: Nonhistone chromosomal protein 6A

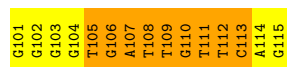
Chain A: 



4.2.17 Score per residue for model 17

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

Chain B: 



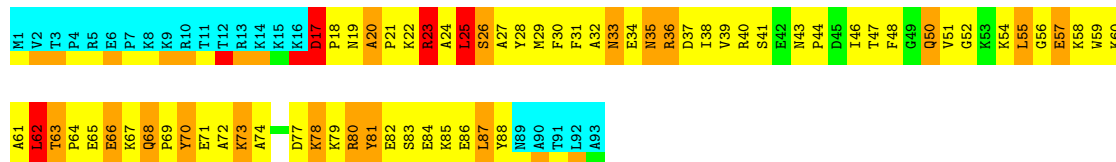
- Molecule 2: 5'-D(*CP*TP*GP*AP*AP*CP*AP*AP*TP*CP*AP*CP*CP*CP*C)-3'

Chain C: 



- Molecule 3: Nonhistone chromosomal protein 6A

Chain A: 



4.2.18 Score per residue for model 18

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

Chain B: 

G101
G102
G103
G104
T105
G106
A107
T108
T109
G110
T111
T112
C113
A114
G115

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

Chain C: 13% 87%

C116
T117
G118
A119
A120
C121
A122
A123
T124
C125
A126
C127
C128
C129
C130

- Molecule 3: Nonhistone chromosomal protein 6A

Chain A: 5% 48% 17% 6% 23%

M1
V2
T3
P4
R5
E6
P7
K8
Q9
K9
R10
T11
T12
R13
K14
K15
K16
D17
P18
N19
A20
P21
K22
R23
A24
L25
S26
A27
Y28
M29
F30
F31
A32
N33
E34
N35
R36
D37
I38
V39
R40
S41
E42
N43
P44
D45
I46
T47
F48
Q49
Q50
V51
G52
K53
K54
L55
G56
E57
K58
W59
K60

A61
L62
T63
P64
E65
E66
K67
Q68
P69
Y70
E71
A72
T73
K74
A75
K78
R79
Y81
E82
S83
K85
E86
L87
Y88
N89
A90
T91
L92
A93

4.2.19 Score per residue for model 19

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

Chain B: 40% 60%

G101
G102
G103
G104
T105
G106
A107
T108
T109
G110
T111
T112
C113
A114
G115

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

Chain C: 13% 87%

C116
T117
G118
A119
A120
C121
A122
A123
T124
C125
A126
C127
C128
C129
C130

- Molecule 3: Nonhistone chromosomal protein 6A

Chain A: 10% 44% 19% 23%

M1
V2
T3
P4
R5
E6
P7
K8
Q9
K9
R10
T11
T12
R13
K14
K15
K16
D17
P18
N19
A20
P21
K22
R23
A24
L25
S26
A27
Y28
M29
F30
F31
A32
N33
E34
N35
R36
D37
I38
V39
R40
S41
E42
N43
P44
D45
I46
T47
F48
Q49
Q50
V51
K54
L55
G56
E57
K58
W59
K60
A61
L62
T63
P64
E65
E66
K67
Q68
P69
Y70
E71
A72
T73
K74
A75
K78
R79
Y81
E82
S83
K85
E86
L87
Y88
N89
A90
T91
L92
A93

4.2.20 Score per residue for model 20

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

Chain B:  27% 73%

G101 G102 G103 G104 G105 G106 G107 T108 T109 G110 T111 T112 C113 A114 G115

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

Chain C:  20% 80%

C116 T117 G118 A119 A120 C121 A122 A123 T124 C125 A126 C127 C128 C129 C130

- Molecule 3: Nonhistone chromosomal protein 6A

Chain A:  6% 45% 22% 23%

M1 V2 T3 P4 R5 E6 P7 K8 R9 T10 T11 T12 T13 R14 K15 K16 D17 P18 N19 A20 P21 K22 R23 A24 L25 S26 A27 Y28 M29 F30 F31 A32 N33 E34 N35 R36 D37 I38 V39 R40 S41 E42 N43 P44 D45 I46 T47 F48 G49 Q50 V51 G52 K53 K54 L55 G56 E57 K58 W59 K60

A61 L62 T63 P64 E65 E66 K67 Q68 P69 Y70 E71 A72 K73 A74 Q75 A76 K78 K79 R80 Y81 E82 S83 E84 K85 E86 L87 Y88 N89 A90 T91 L92 A93

5 Refinement protocol and experimental data overview

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

Of the 100 calculated structures, 20 were deposited, based on the following criterion: *structures with acceptable covalent geometry*.

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

Software name	Classification	Version
X-PLOR	refinement	3.1

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

6 Model quality [i](#)

6.1 Standard geometry [i](#)

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	1.08±0.01	0±0/350 (0.0±0.1%)	2.24±0.02	35±1/541 (6.5±0.2%)
2	C	1.09±0.02	0±0/332 (0.0±0.0%)	2.22±0.02	25±1/508 (5.0±0.1%)
3	A	0.21±0.00	0±0/604 (0.0±0.0%)	0.32±0.00	0±0/812 (0.0±0.0%)
All	All	0.80	2/25720 (0.0%)	1.69	1208/37220 (3.2%)

All unique bond outliers are listed below.

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
1	B	109	DT	C5-C7	5.12	1.53	1.50	3	2

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
2	C	124	DT	O4'-C1'-N1	10.30	115.21	108.00	16	20
1	B	109	DT	O4'-C1'-N1	10.20	115.14	108.00	15	20
1	B	108	DT	O4'-C1'-N1	10.02	115.02	108.00	13	20
1	B	103	DG	O4'-C1'-N9	9.68	114.78	108.00	20	20
1	B	107	DA	O4'-C1'-N9	9.39	114.57	108.00	16	20
2	C	128	DC	O4'-C1'-N1	9.06	114.34	108.00	18	20
1	B	110	DG	O4'-C1'-N9	9.04	114.33	108.00	11	3
1	B	101	DG	O4'-C1'-N9	8.51	113.95	108.00	20	20
2	C	121	DC	O4'-C1'-N1	8.45	113.92	108.00	17	20
2	C	117	DT	C6-C5-C7	-8.36	117.88	122.90	7	20
2	C	122	DA	O4'-C1'-N9	8.25	113.78	108.00	16	20
2	C	116	DC	O4'-C4'-C3'	7.92	110.75	106.00	4	20
2	C	130	DC	O4'-C4'-C3'	7.87	110.72	106.00	4	20
2	C	127	DC	O4'-C1'-N1	7.60	113.32	108.00	17	20
2	C	125	DC	O4'-C1'-N1	7.54	113.28	108.00	9	20
2	C	119	DA	O4'-C4'-C3'	7.54	110.53	106.00	9	20
1	B	103	DG	O4'-C4'-C3'	7.39	110.43	106.00	3	20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	B	108	DT	C6-C5-C7	-7.37	118.48	122.90	10	20
1	B	106	DG	O4'-C4'-C3'	7.36	110.41	106.00	7	20
1	B	104	DG	O4'-C4'-C3'	7.34	110.41	106.00	4	20
1	B	101	DG	O4'-C4'-C3'	7.32	110.39	106.00	12	20
2	C	123	DA	O4'-C4'-C3'	7.17	110.30	106.00	11	20
1	B	108	DT	O4'-C4'-C3'	7.13	110.28	106.00	13	20
2	C	129	DC	O4'-C4'-C3'	7.10	110.26	106.00	9	20
2	C	128	DC	O4'-C4'-C3'	7.09	110.25	106.00	5	20
2	C	118	DG	O4'-C4'-C3'	7.07	110.24	106.00	3	20
1	B	102	DG	O4'-C4'-C3'	7.05	110.23	106.00	7	20
1	B	110	DG	O4'-C4'-C3'	7.01	110.21	106.00	13	20
1	B	115	DG	O4'-C4'-C3'	7.00	110.20	106.00	10	20
1	B	111	DT	O4'-C4'-C3'	7.00	110.20	106.00	15	20
1	B	107	DA	O4'-C4'-C3'	6.97	110.18	106.00	10	20
2	C	123	DA	O4'-C1'-N9	6.96	112.87	108.00	11	1
2	C	124	DT	O4'-C4'-C3'	6.94	110.16	106.00	2	20
2	C	122	DA	O4'-C4'-C3'	6.93	110.16	106.00	17	20
1	B	112	DT	O4'-C4'-C3'	6.92	110.15	106.00	11	20
1	B	102	DG	O4'-C1'-N9	6.87	112.81	108.00	5	20
2	C	121	DC	O4'-C4'-C3'	6.87	110.12	106.00	8	20
2	C	125	DC	O4'-C4'-C3'	6.81	110.09	106.00	2	20
1	B	105	DT	O4'-C4'-C3'	6.78	110.07	106.00	10	20
1	B	113	DC	O4'-C4'-C3'	6.76	110.06	106.00	14	20
2	C	126	DA	O4'-C4'-C3'	6.76	110.06	106.00	19	20
1	B	114	DA	O4'-C1'-N9	6.76	112.73	108.00	10	20
2	C	120	DA	O4'-C4'-C3'	6.76	110.05	106.00	16	20
2	C	117	DT	O4'-C4'-C3'	6.75	110.05	106.00	16	20
1	B	105	DT	O4'-C1'-N1	6.72	112.70	108.00	8	14
2	C	127	DC	O4'-C4'-C3'	6.68	110.01	106.00	6	20
1	B	114	DA	O4'-C4'-C3'	6.62	109.97	106.00	7	20
1	B	111	DT	O4'-C1'-N1	6.61	112.63	108.00	16	20
1	B	109	DT	O4'-C4'-C3'	6.58	109.95	106.00	16	20
1	B	109	DT	C6-C5-C7	-6.50	119.00	122.90	15	20
1	B	105	DT	C6-C5-C7	-6.39	119.07	122.90	10	20
2	C	126	DA	O4'-C1'-N9	6.21	112.34	108.00	10	4
2	C	124	DT	C6-C5-C7	-6.06	119.27	122.90	17	20
1	B	115	DG	O4'-C1'-N9	6.02	112.21	108.00	18	9
1	B	111	DT	C6-C5-C7	-6.00	119.30	122.90	16	20
1	B	108	DT	C4-C5-C6	5.86	121.52	118.00	10	20
1	B	109	DT	C4-C5-C6	5.65	121.39	118.00	16	20
2	C	117	DT	C4-C5-C6	5.62	121.38	118.00	18	20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
2	C	116	DC	C3'-C2'-C1'	5.61	109.23	102.50	14	3
2	C	124	DT	C4-C5-C6	5.57	121.34	118.00	11	15
1	B	111	DT	C4-C5-C6	5.52	121.31	118.00	16	20
1	B	105	DT	C4-C5-C6	5.49	121.29	118.00	3	20
1	B	104	DG	O4'-C1'-N9	5.46	111.82	108.00	5	16
1	B	112	DT	O4'-C1'-N1	5.40	111.78	108.00	5	11
2	C	120	DA	O4'-C1'-N9	5.38	111.77	108.00	17	1
1	B	113	DC	O4'-C1'-N1	5.36	111.75	108.00	20	18
1	B	112	DT	C6-C5-C7	-5.19	119.79	122.90	19	8
1	B	106	DG	O4'-C1'-N9	5.12	111.59	108.00	8	1
2	C	116	DC	C6-N1-C2	5.08	122.33	120.30	18	2
1	B	107	DA	C3'-C2'-C1'	5.07	108.59	102.50	2	1
1	B	112	DT	C4-C5-C6	5.00	121.00	118.00	1	1

There are no chirality outliers.

There are no planarity outliers.

6.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	B	312	172	172	28±4
2	C	297	169	169	38±7
3	A	590	579	579	170±9
All	All	23980	18400	18400	4125

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 97.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:A:47:THR:O	3:A:51:VAL:HG12	0.93	1.63	19	11
3:A:59:TRP:O	3:A:62:LEU:HD12	0.93	1.64	5	19
2:C:116:DC:H4'	2:C:117:DT:OP1	0.90	1.66	14	3
3:A:23:ARG:NH2	3:A:24:ALA:HB3	0.90	1.80	8	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:C:126:DA:H4'	2:C:127:DC:OP1	0.89	1.67	13	6
1:B:110:DG:C5'	3:A:25:LEU:HD21	0.88	1.98	2	20
3:A:34:GLU:O	3:A:38:ILE:HD13	0.88	1.68	18	16
1:B:110:DG:H5''	3:A:25:LEU:HD21	0.87	1.46	18	19
3:A:25:LEU:HD23	3:A:29:MET:HB2	0.86	1.47	18	20
1:B:110:DG:OP1	3:A:25:LEU:HD11	0.86	1.70	16	2
3:A:87:LEU:HD23	3:A:88:TYR:N	0.85	1.87	19	3
3:A:35:ASN:HB2	3:A:55:LEU:HD21	0.82	1.52	1	10
2:C:120:DA:H4'	2:C:121:DC:OP1	0.82	1.71	17	1
2:C:124:DT:H4'	2:C:125:DC:OP1	0.81	1.77	9	13
3:A:30:PHE:CE2	3:A:74:ALA:HA	0.80	2.11	15	20
1:B:110:DG:O5'	3:A:25:LEU:HD21	0.79	1.78	16	1
3:A:39:VAL:HG12	3:A:51:VAL:HG22	0.78	1.54	1	1
3:A:68:GLN:O	3:A:72:ALA:HB3	0.76	1.79	8	20
2:C:118:DG:C6	2:C:119:DA:C6	0.76	2.74	17	20
3:A:63:THR:HG23	3:A:64:PRO:HD2	0.76	1.56	8	17
2:C:126:DA:C2	2:C:127:DC:C2	0.75	2.75	13	20
3:A:25:LEU:HD23	3:A:29:MET:CB	0.74	2.11	18	20
3:A:46:ILE:O	3:A:47:THR:CB	0.74	2.36	7	11
3:A:31:PHE:CG	3:A:59:TRP:CE3	0.74	2.76	16	20
2:C:120:DA:C6	2:C:121:DC:C4	0.74	2.76	10	15
2:C:119:DA:N3	3:A:48:PHE:CE2	0.72	2.57	17	3
3:A:35:ASN:CB	3:A:55:LEU:HD21	0.72	2.14	1	3
2:C:126:DA:C4	2:C:127:DC:C5	0.72	2.77	17	17
3:A:35:ASN:C	3:A:39:VAL:HG12	0.72	2.04	17	1
1:B:104:DG:N2	1:B:105:DT:C2	0.71	2.58	11	16
3:A:71:GLU:O	3:A:74:ALA:HB3	0.71	1.85	8	20
3:A:46:ILE:C	3:A:47:THR:HG23	0.71	2.04	13	1
1:B:106:DG:C6	1:B:107:DA:N6	0.71	2.59	12	5
3:A:46:ILE:HD12	3:A:50:GLN:HB2	0.71	1.63	1	1
3:A:62:LEU:O	3:A:63:THR:CB	0.71	2.39	1	20
3:A:23:ARG:HH21	3:A:24:ALA:HB3	0.70	1.46	8	1
2:C:120:DA:C5	2:C:121:DC:C5	0.70	2.79	10	13
3:A:23:ARG:HA	3:A:81:TYR:CE2	0.70	2.22	7	20
3:A:28:TYR:O	3:A:32:ALA:HB3	0.70	1.87	7	14
2:C:126:DA:C2	2:C:127:DC:N3	0.69	2.60	10	16
2:C:121:DC:N4	2:C:122:DA:N6	0.69	2.40	15	3
3:A:31:PHE:CE2	3:A:35:ASN:OD1	0.69	2.45	12	15
3:A:46:ILE:HD12	3:A:51:VAL:CA	0.69	2.17	4	7
3:A:35:ASN:O	3:A:38:ILE:N	0.69	2.26	17	16
3:A:17:ASP:CG	3:A:20:ALA:HB2	0.68	2.08	10	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:A:47:THR:C	3:A:51:VAL:HG12	0.68	2.09	15	6
2:C:116:DC:C2'	2:C:117:DT:C6	0.67	2.77	18	9
3:A:68:GLN:O	3:A:72:ALA:CB	0.67	2.42	8	20
3:A:50:GLN:CD	3:A:50:GLN:N	0.67	2.45	8	8
1:B:110:DG:C4	3:A:29:MET:CE	0.67	2.78	15	5
3:A:17:ASP:CB	3:A:20:ALA:HB2	0.67	2.19	5	6
3:A:17:ASP:HB3	3:A:20:ALA:HB2	0.67	1.64	9	2
2:C:118:DG:C5	2:C:119:DA:C6	0.67	2.83	18	20
3:A:46:ILE:O	3:A:47:THR:HG23	0.67	1.90	13	1
3:A:68:GLN:N	3:A:69:PRO:CD	0.66	2.58	5	17
2:C:127:DC:P	3:A:85:LYS:CE	0.66	2.84	10	5
3:A:46:ILE:O	3:A:50:GLN:HG3	0.66	1.89	13	9
3:A:24:ALA:HB2	3:A:77:ASP:O	0.66	1.91	16	1
3:A:38:ILE:HG22	3:A:39:VAL:N	0.66	2.05	18	20
1:B:110:DG:N3	3:A:29:MET:CE	0.66	2.58	15	4
3:A:21:PRO:O	3:A:22:LYS:CB	0.66	2.44	8	16
3:A:35:ASN:O	3:A:36:ARG:C	0.66	2.35	17	16
3:A:31:PHE:CE1	3:A:62:LEU:HD11	0.66	2.26	6	4
1:B:109:DT:C2	1:B:110:DG:N7	0.65	2.64	16	1
1:B:110:DG:C4	3:A:29:MET:SD	0.65	2.90	4	15
1:B:110:DG:O4'	3:A:29:MET:HE2	0.65	1.90	16	1
2:C:116:DC:H2'	2:C:117:DT:C6	0.65	2.27	18	9
2:C:119:DA:C6	2:C:120:DA:N6	0.65	2.64	17	1
1:B:110:DG:N3	3:A:29:MET:HE1	0.65	2.06	16	5
3:A:28:TYR:O	3:A:32:ALA:CB	0.65	2.45	7	20
3:A:21:PRO:O	3:A:22:LYS:HB2	0.65	1.92	3	20
3:A:50:GLN:NE2	3:A:50:GLN:N	0.65	2.44	8	8
1:B:112:DT:O2	3:A:48:PHE:CG	0.65	2.50	1	12
3:A:23:ARG:CA	3:A:81:TYR:CE2	0.64	2.80	19	20
3:A:66:GLU:O	3:A:70:TYR:CE2	0.64	2.50	17	13
3:A:23:ARG:O	3:A:81:TYR:CD2	0.64	2.51	15	13
3:A:28:TYR:HB3	3:A:29:MET:HE2	0.64	1.67	11	9
2:C:126:DA:C5	2:C:127:DC:C4	0.64	2.86	7	16
3:A:48:PHE:O	3:A:50:GLN:N	0.64	2.31	18	6
3:A:39:VAL:CG1	3:A:51:VAL:HG22	0.64	2.22	1	1
3:A:87:LEU:HD23	3:A:88:TYR:H	0.64	1.50	19	2
3:A:50:GLN:O	3:A:54:LYS:CB	0.64	2.46	17	20
3:A:22:LYS:O	3:A:23:ARG:O	0.64	2.16	17	20
3:A:81:TYR:CD1	3:A:82:GLU:N	0.64	2.66	2	18
1:B:106:DG:C6	1:B:107:DA:C6	0.64	2.86	12	5
3:A:23:ARG:N	3:A:81:TYR:CE2	0.63	2.66	13	19

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:110:DG:N3	3:A:29:MET:SD	0.63	2.71	8	2
3:A:63:THR:HG22	3:A:65:GLU:H	0.63	1.52	5	2
2:C:126:DA:C8	2:C:126:DA:OP2	0.63	2.51	13	1
2:C:120:DA:N6	2:C:121:DC:N4	0.63	2.46	10	11
3:A:31:PHE:CD1	3:A:32:ALA:N	0.63	2.67	16	1
2:C:126:DA:N3	2:C:127:DC:C2	0.63	2.67	19	6
3:A:67:LYS:C	3:A:69:PRO:HD2	0.63	2.14	17	17
1:B:110:DG:C4	3:A:29:MET:HE1	0.62	2.28	15	5
2:C:123:DA:H4'	2:C:124:DT:OP1	0.62	1.93	11	2
3:A:70:TYR:O	3:A:73:LYS:N	0.62	2.32	8	20
3:A:87:LEU:HD12	3:A:88:TYR:N	0.62	2.09	5	1
2:C:121:DC:O2	3:A:28:TYR:CZ	0.62	2.52	3	20
3:A:31:PHE:CD2	3:A:59:TRP:CE3	0.62	2.88	5	19
3:A:48:PHE:CG	3:A:49:GLY:N	0.62	2.67	14	6
3:A:37:ASP:OD2	3:A:38:ILE:HD12	0.62	1.94	3	1
3:A:29:MET:SD	3:A:29:MET:N	0.62	2.73	15	4
3:A:66:GLU:O	3:A:70:TYR:CE1	0.62	2.53	8	7
3:A:37:ASP:O	3:A:41:SER:CB	0.62	2.48	20	20
3:A:32:ALA:HB1	3:A:36:ARG:NE	0.62	2.09	18	1
3:A:17:ASP:HB2	3:A:20:ALA:HB2	0.62	1.71	18	8
3:A:84:GLU:HA	3:A:87:LEU:HD22	0.62	1.71	19	2
1:B:112:DT:C4	1:B:113:DC:N4	0.61	2.68	15	17
1:B:108:DT:C4'	1:B:109:DT:OP1	0.61	2.48	13	1
3:A:46:ILE:HD12	3:A:51:VAL:HB	0.61	1.71	19	9
3:A:43:ASN:O	3:A:46:ILE:CG1	0.61	2.49	15	11
1:B:112:DT:O2	3:A:48:PHE:CD1	0.61	2.54	17	14
3:A:31:PHE:CD1	3:A:35:ASN:ND2	0.61	2.69	15	1
2:C:123:DA:C4'	2:C:124:DT:OP1	0.61	2.47	11	2
3:A:19:ASN:OD1	3:A:88:TYR:CD1	0.61	2.54	18	3
3:A:24:ALA:HB1	3:A:77:ASP:OD1	0.61	1.96	12	6
2:C:118:DG:C6	2:C:119:DA:N6	0.61	2.68	15	20
2:C:116:DC:C4'	2:C:117:DT:OP1	0.61	2.48	18	3
2:C:126:DA:C4	2:C:127:DC:C4	0.60	2.90	10	9
3:A:25:LEU:HB3	3:A:30:PHE:CZ	0.60	2.32	7	18
3:A:46:ILE:O	3:A:50:GLN:CG	0.60	2.50	2	8
3:A:31:PHE:CE1	3:A:35:ASN:ND2	0.60	2.69	15	2
2:C:127:DC:P	3:A:85:LYS:HE3	0.60	2.37	10	4
2:C:124:DT:C4'	2:C:125:DC:OP1	0.60	2.47	4	13
3:A:46:ILE:O	3:A:47:THR:HB	0.60	1.96	7	10
2:C:120:DA:C6	2:C:121:DC:N4	0.60	2.70	6	13
2:C:121:DC:O2	3:A:28:TYR:CE1	0.60	2.54	20	11

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:A:68:GLN:HG2	3:A:69:PRO:HD3	0.60	1.72	17	2
3:A:43:ASN:CB	3:A:46:ILE:CD1	0.59	2.80	13	5
3:A:35:ASN:OD1	3:A:55:LEU:HD21	0.59	1.96	8	8
3:A:26:SER:O	3:A:30:PHE:CE2	0.59	2.56	13	19
2:C:122:DA:O4'	3:A:28:TYR:CD2	0.59	2.55	1	5
3:A:25:LEU:CB	3:A:30:PHE:CE1	0.59	2.86	18	17
3:A:26:SER:O	3:A:30:PHE:CD2	0.59	2.55	3	19
3:A:32:ALA:O	3:A:36:ARG:CG	0.59	2.50	15	3
3:A:25:LEU:O	3:A:25:LEU:HD23	0.59	1.97	8	1
3:A:31:PHE:CD2	3:A:32:ALA:N	0.59	2.70	15	4
3:A:23:ARG:CZ	3:A:23:ARG:HB2	0.59	2.28	18	1
2:C:126:DA:OP1	3:A:78:LYS:CD	0.59	2.51	16	11
3:A:25:LEU:CB	3:A:30:PHE:CZ	0.59	2.86	5	13
3:A:23:ARG:CB	3:A:23:ARG:CZ	0.59	2.81	1	2
1:B:108:DT:O2	3:A:23:ARG:NE	0.59	2.36	10	4
3:A:23:ARG:HA	3:A:81:TYR:CD2	0.58	2.33	8	2
3:A:56:GLY:O	3:A:59:TRP:HB3	0.58	1.97	17	20
3:A:29:MET:O	3:A:33:ASN:ND2	0.58	2.36	7	11
3:A:83:SER:O	3:A:86:GLU:HG2	0.58	1.97	16	19
3:A:26:SER:C	3:A:30:PHE:CE2	0.58	2.76	15	19
3:A:35:ASN:O	3:A:39:VAL:HG23	0.58	1.98	19	4
1:B:109:DT:OP1	3:A:22:LYS:O	0.58	2.22	13	1
1:B:109:DT:O2	3:A:29:MET:CE	0.58	2.51	8	7
3:A:48:PHE:O	3:A:48:PHE:CD1	0.58	2.57	15	7
2:C:124:DT:OP2	3:A:27:ALA:HB3	0.58	1.98	19	2
3:A:80:ARG:CA	3:A:80:ARG:NE	0.58	2.67	17	6
2:C:123:DA:C8	2:C:124:DT:H71	0.57	2.34	19	20
1:B:109:DT:O3'	3:A:25:LEU:CD1	0.57	2.52	8	8
2:C:123:DA:C6	2:C:124:DT:C4	0.57	2.92	9	4
3:A:46:ILE:CG2	3:A:47:THR:N	0.57	2.67	8	4
1:B:108:DT:O2	3:A:23:ARG:CZ	0.57	2.52	14	3
3:A:28:TYR:CD1	3:A:28:TYR:O	0.57	2.57	4	6
1:B:111:DT:O3'	3:A:36:ARG:CD	0.57	2.52	14	13
3:A:50:GLN:N	3:A:50:GLN:NE2	0.57	2.53	3	2
3:A:25:LEU:HB3	3:A:30:PHE:CE1	0.57	2.34	14	14
1:B:110:DG:P	3:A:25:LEU:HD11	0.57	2.40	16	5
1:B:110:DG:O4'	3:A:29:MET:CE	0.57	2.53	16	1
3:A:85:LYS:HG3	3:A:86:GLU:N	0.57	2.14	16	10
3:A:51:VAL:HG13	3:A:52:GLY:N	0.57	2.15	18	6
2:C:129:DC:H2'	2:C:130:DC:C5	0.57	2.34	6	20
3:A:85:LYS:O	3:A:88:TYR:HB3	0.57	1.99	9	17

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:C:127:DC:OP1	3:A:85:LYS:CE	0.57	2.53	16	2
3:A:23:ARG:HB2	3:A:23:ARG:CZ	0.57	2.30	1	1
3:A:22:LYS:C	3:A:81:TYR:CD2	0.56	2.78	8	5
3:A:21:PRO:O	3:A:22:LYS:CG	0.56	2.53	8	8
3:A:80:ARG:NE	3:A:80:ARG:CA	0.56	2.68	18	4
2:C:123:DA:C8	2:C:124:DT:C7	0.56	2.88	19	19
3:A:28:TYR:O	3:A:28:TYR:CD1	0.56	2.58	14	3
3:A:43:ASN:CB	3:A:46:ILE:HD13	0.56	2.30	16	3
3:A:37:ASP:OD1	3:A:38:ILE:HD13	0.56	2.00	8	1
3:A:21:PRO:HB2	3:A:81:TYR:CE2	0.56	2.36	7	20
3:A:30:PHE:CE2	3:A:74:ALA:CA	0.56	2.88	6	20
3:A:46:ILE:HD12	3:A:51:VAL:HA	0.56	1.76	5	5
1:B:112:DT:OP1	3:A:36:ARG:CD	0.56	2.54	11	1
1:B:110:DG:C4'	1:B:111:DT:OP1	0.56	2.53	11	1
2:C:124:DT:OP2	3:A:27:ALA:CB	0.56	2.53	19	2
3:A:84:GLU:HA	3:A:87:LEU:HD21	0.56	1.75	5	1
3:A:31:PHE:CD2	3:A:35:ASN:ND2	0.56	2.74	16	1
3:A:46:ILE:CG1	3:A:51:VAL:HG23	0.56	2.30	1	1
2:C:121:DC:O5'	3:A:53:LYS:CD	0.56	2.52	7	1
1:B:110:DG:N3	3:A:36:ARG:NH2	0.56	2.52	18	1
1:B:111:DT:O2	3:A:36:ARG:CZ	0.56	2.53	16	1
2:C:119:DA:C5	2:C:120:DA:N6	0.56	2.73	17	1
3:A:68:GLN:HB2	3:A:69:PRO:HD3	0.56	1.78	15	15
2:C:125:DC:O5'	3:A:78:LYS:CD	0.56	2.54	19	4
3:A:51:VAL:O	3:A:55:LEU:HB2	0.56	2.00	20	11
3:A:23:ARG:NH1	3:A:24:ALA:O	0.56	2.39	13	5
2:C:126:DA:OP1	3:A:78:LYS:NZ	0.56	2.38	20	3
3:A:50:GLN:N	3:A:50:GLN:CD	0.56	2.57	3	3
3:A:67:LYS:C	3:A:69:PRO:CD	0.56	2.74	17	2
3:A:22:LYS:O	3:A:23:ARG:C	0.56	2.44	12	19
3:A:62:LEU:O	3:A:63:THR:HB	0.56	2.01	20	18
1:B:108:DT:H4'	1:B:109:DT:OP1	0.56	1.99	13	1
3:A:21:PRO:HD3	3:A:88:TYR:CD1	0.56	2.35	16	6
2:C:123:DA:OP1	3:A:60:LYS:CE	0.56	2.54	14	10
3:A:46:ILE:HG12	3:A:50:GLN:CB	0.56	2.31	8	3
3:A:36:ARG:NE	3:A:55:LEU:HD13	0.56	2.15	16	1
3:A:35:ASN:O	3:A:37:ASP:N	0.55	2.39	6	16
3:A:31:PHE:CE2	3:A:59:TRP:HB2	0.55	2.37	8	19
3:A:23:ARG:HA	3:A:81:TYR:CZ	0.55	2.35	16	18
3:A:48:PHE:CD1	3:A:48:PHE:C	0.55	2.79	3	9
3:A:31:PHE:HB2	3:A:70:TYR:CG	0.55	2.37	16	19

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:C:120:DA:C4	2:C:121:DC:C5	0.55	2.94	10	13
2:C:117:DT:C2'	2:C:118:DG:OP2	0.55	2.52	18	17
3:A:54:LYS:CE	3:A:58:LYS:CG	0.55	2.84	4	1
3:A:37:ASP:OD2	3:A:38:ILE:HD13	0.55	2.00	14	3
3:A:35:ASN:O	3:A:39:VAL:CG2	0.55	2.55	15	4
1:B:112:DT:OP1	3:A:36:ARG:NE	0.55	2.39	12	9
2:C:124:DT:O2	3:A:23:ARG:CZ	0.55	2.54	8	4
3:A:32:ALA:O	3:A:36:ARG:CB	0.55	2.54	11	2
1:B:109:DT:O3'	3:A:25:LEU:HD11	0.55	2.01	15	12
3:A:67:LYS:HA	3:A:70:TYR:CE2	0.55	2.37	5	13
3:A:24:ALA:HB1	3:A:77:ASP:OD2	0.55	2.01	14	1
3:A:43:ASN:CB	3:A:46:ILE:HD12	0.55	2.31	8	1
3:A:43:ASN:HB2	3:A:46:ILE:CD1	0.55	2.31	20	8
3:A:49:GLY:C	3:A:50:GLN:NE2	0.55	2.61	1	2
2:C:120:DA:C4'	2:C:121:DC:OP1	0.55	2.50	17	1
3:A:81:TYR:O	3:A:84:GLU:HG2	0.55	2.01	15	11
2:C:126:DA:C4'	2:C:127:DC:OP1	0.55	2.53	10	6
2:C:126:DA:OP1	3:A:78:LYS:CE	0.55	2.55	17	3
2:C:120:DA:C5	2:C:121:DC:C4	0.55	2.95	19	12
3:A:54:LYS:O	3:A:57:GLU:CG	0.55	2.55	6	2
3:A:36:ARG:O	3:A:40:ARG:CG	0.55	2.55	20	6
3:A:21:PRO:HA	3:A:84:GLU:CG	0.55	2.32	9	9
3:A:27:ALA:HB2	3:A:71:GLU:HA	0.55	1.78	5	4
1:B:111:DT:H2'	1:B:112:DT:C6	0.54	2.37	19	20
3:A:28:TYR:O	3:A:32:ALA:HB2	0.54	2.01	8	8
3:A:58:LYS:HA	3:A:61:ALA:HB3	0.54	1.79	2	17
3:A:25:LEU:N	3:A:77:ASP:OD2	0.54	2.40	14	1
1:B:109:DT:O2	1:B:110:DG:C8	0.54	2.60	16	1
3:A:81:TYR:CD1	3:A:81:TYR:C	0.54	2.80	12	8
3:A:81:TYR:C	3:A:81:TYR:CD1	0.54	2.81	11	11
3:A:51:VAL:CG1	3:A:52:GLY:N	0.54	2.70	16	5
3:A:46:ILE:C	3:A:47:THR:CG2	0.54	2.75	13	1
2:C:124:DT:O2	3:A:23:ARG:NH1	0.54	2.40	5	5
3:A:49:GLY:CA	3:A:50:GLN:NE2	0.54	2.70	8	2
1:B:110:DG:N2	3:A:28:TYR:CE1	0.54	2.76	11	7
3:A:31:PHE:CE2	3:A:35:ASN:ND2	0.54	2.76	16	1
3:A:37:ASP:OD2	3:A:38:ILE:CD1	0.54	2.56	1	4
3:A:62:LEU:O	3:A:63:THR:OG1	0.54	2.24	16	5
3:A:29:MET:HA	3:A:29:MET:HE3	0.54	1.79	16	1
3:A:43:ASN:HB2	3:A:46:ILE:HD11	0.54	1.78	12	5
3:A:34:GLU:O	3:A:38:ILE:CD1	0.54	2.56	9	8

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:A:23:ARG:NH2	3:A:24:ALA:O	0.54	2.41	14	6
3:A:85:LYS:CG	3:A:86:GLU:N	0.54	2.71	14	12
3:A:23:ARG:CZ	3:A:24:ALA:O	0.54	2.56	5	11
3:A:80:ARG:NE	3:A:80:ARG:O	0.54	2.41	15	3
2:C:119:DA:C2	3:A:48:PHE:CE2	0.54	2.96	12	4
3:A:35:ASN:N	3:A:35:ASN:ND2	0.54	2.55	13	11
1:B:112:DT:O4	2:C:118:DG:O6	0.54	2.25	14	18
3:A:48:PHE:CD1	3:A:48:PHE:O	0.54	2.61	6	6
3:A:57:GLU:CG	3:A:58:LYS:N	0.54	2.71	10	5
3:A:82:GLU:O	3:A:85:LYS:CG	0.54	2.55	8	6
3:A:82:GLU:O	3:A:85:LYS:HG3	0.54	2.03	16	2
3:A:80:ARG:CZ	3:A:80:ARG:O	0.54	2.56	15	3
2:C:125:DC:OP2	3:A:78:LYS:NZ	0.54	2.41	12	1
3:A:58:LYS:O	3:A:62:LEU:HG	0.54	2.03	8	20
2:C:122:DA:O4'	3:A:28:TYR:CE2	0.54	2.61	1	4
3:A:46:ILE:HB	3:A:50:GLN:CB	0.54	2.32	14	6
3:A:49:GLY:O	3:A:53:LYS:CD	0.54	2.56	10	4
2:C:123:DA:P	3:A:60:LYS:HD2	0.54	2.43	16	1
3:A:35:ASN:OD1	3:A:55:LEU:CD2	0.54	2.56	1	8
3:A:31:PHE:HA	3:A:70:TYR:CD2	0.54	2.38	1	7
3:A:50:GLN:O	3:A:54:LYS:CG	0.54	2.55	10	5
1:B:110:DG:H4'	1:B:111:DT:OP1	0.54	2.01	11	1
3:A:48:PHE:O	3:A:49:GLY:C	0.54	2.47	14	6
3:A:51:VAL:O	3:A:55:LEU:CG	0.54	2.56	14	3
3:A:23:ARG:NE	3:A:24:ALA:O	0.54	2.41	3	6
3:A:19:ASN:HB2	3:A:88:TYR:CD2	0.54	2.38	17	3
3:A:31:PHE:CE1	3:A:59:TRP:HB2	0.54	2.38	16	1
1:B:113:DC:OP2	3:A:40:ARG:CZ	0.54	2.55	16	1
3:A:67:LYS:HA	3:A:70:TYR:CD2	0.53	2.37	11	13
3:A:47:THR:O	3:A:51:VAL:CG1	0.53	2.53	17	6
2:C:126:DA:C6	2:C:127:DC:C4	0.53	2.96	2	13
3:A:21:PRO:CB	3:A:84:GLU:HG3	0.53	2.33	20	9
3:A:25:LEU:HB2	3:A:30:PHE:CE1	0.53	2.38	16	4
3:A:50:GLN:O	3:A:54:LYS:HB2	0.53	2.04	3	18
3:A:47:THR:O	3:A:49:GLY:N	0.53	2.41	15	3
3:A:31:PHE:HA	3:A:70:TYR:CD1	0.53	2.38	7	9
3:A:48:PHE:O	3:A:51:VAL:N	0.53	2.42	16	6
1:B:112:DT:OP1	3:A:36:ARG:CG	0.53	2.56	11	3
2:C:127:DC:OP2	3:A:85:LYS:CE	0.53	2.57	19	2
3:A:43:ASN:N	3:A:44:PRO:HD3	0.53	2.19	16	20
3:A:36:ARG:CZ	3:A:37:ASP:OD2	0.53	2.57	4	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:A:51:VAL:O	3:A:55:LEU:CB	0.53	2.57	14	1
2:C:128:DC:C2	2:C:129:DC:C5	0.53	2.97	6	1
3:A:37:ASP:OD1	3:A:38:ILE:CD1	0.53	2.56	8	1
3:A:80:ARG:O	3:A:80:ARG:NE	0.53	2.41	5	2
1:B:107:DA:C5	1:B:108:DT:C7	0.53	2.91	1	3
3:A:27:ALA:HA	3:A:30:PHE:CD2	0.53	2.39	8	7
3:A:24:ALA:CB	3:A:77:ASP:O	0.53	2.56	16	1
3:A:76:ALA:O	3:A:79:LYS:CG	0.53	2.57	20	1
3:A:22:LYS:O	3:A:81:TYR:CD2	0.53	2.62	2	5
2:C:116:DC:H2''	2:C:117:DT:C6	0.53	2.39	7	3
1:B:112:DT:P	3:A:36:ARG:HG3	0.53	2.44	11	4
2:C:119:DA:C2	3:A:48:PHE:CZ	0.53	2.97	20	3
3:A:21:PRO:O	3:A:22:LYS:CD	0.53	2.57	13	7
3:A:35:ASN:ND2	3:A:35:ASN:N	0.53	2.55	4	4
1:B:109:DT:O2	3:A:29:MET:HE3	0.53	2.04	8	1
3:A:23:ARG:NH2	3:A:25:LEU:O	0.53	2.42	2	4
3:A:19:ASN:OD1	3:A:87:LEU:HD21	0.53	2.03	12	1
1:B:112:DT:P	3:A:36:ARG:HD2	0.53	2.44	14	2
3:A:48:PHE:C	3:A:48:PHE:CD1	0.53	2.82	8	1
2:C:124:DT:H2''	2:C:125:DC:C6	0.52	2.40	12	11
3:A:66:GLU:OE1	3:A:66:GLU:CA	0.52	2.57	6	5
3:A:31:PHE:CG	3:A:59:TRP:CZ3	0.52	2.96	17	14
3:A:46:ILE:C	3:A:50:GLN:HG2	0.52	2.24	15	1
3:A:18:PRO:HG2	3:A:88:TYR:CE2	0.52	2.38	9	3
1:B:111:DT:O2	3:A:36:ARG:NH2	0.52	2.41	16	1
1:B:108:DT:O4'	3:A:23:ARG:HG2	0.52	2.05	12	7
3:A:82:GLU:O	3:A:85:LYS:HG2	0.52	2.04	20	9
3:A:54:LYS:O	3:A:58:LYS:CG	0.52	2.57	18	7
3:A:36:ARG:O	3:A:40:ARG:CB	0.52	2.57	8	4
3:A:46:ILE:HD12	3:A:51:VAL:CB	0.52	2.34	11	7
1:B:109:DT:O2	3:A:29:MET:SD	0.52	2.67	1	18
1:B:110:DG:N9	3:A:29:MET:SD	0.52	2.83	6	3
3:A:18:PRO:HG2	3:A:88:TYR:CE1	0.52	2.40	16	8
2:C:125:DC:P	3:A:78:LYS:HD2	0.52	2.43	14	2
3:A:51:VAL:O	3:A:55:LEU:HG	0.52	2.03	11	9
3:A:31:PHE:CD2	3:A:35:ASN:OD1	0.52	2.63	11	15
3:A:66:GLU:OE1	3:A:66:GLU:N	0.52	2.43	9	3
1:B:105:DT:C2'	1:B:106:DG:C8	0.52	2.93	17	2
3:A:83:SER:O	3:A:86:GLU:CG	0.52	2.57	5	1
1:B:113:DC:OP2	3:A:40:ARG:NH2	0.52	2.42	1	1
1:B:108:DT:O2	3:A:23:ARG:CD	0.52	2.57	11	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:C:125:DC:O4'	3:A:23:ARG:NH2	0.52	2.42	18	2
3:A:46:ILE:O	3:A:47:THR:OG1	0.52	2.28	20	11
1:B:108:DT:C2	3:A:23:ARG:HD3	0.52	2.40	17	2
3:A:31:PHE:CD1	3:A:59:TRP:CE3	0.52	2.98	15	11
3:A:66:GLU:N	3:A:66:GLU:OE1	0.52	2.43	6	1
3:A:80:ARG:C	3:A:80:ARG:CD	0.52	2.77	8	2
3:A:54:LYS:HD3	3:A:58:LYS:CG	0.51	2.35	14	6
3:A:21:PRO:HD3	3:A:88:TYR:CD2	0.51	2.40	17	2
3:A:46:ILE:O	3:A:47:THR:CG2	0.51	2.57	13	1
3:A:80:ARG:O	3:A:80:ARG:CZ	0.51	2.58	1	1
3:A:36:ARG:O	3:A:40:ARG:HG2	0.51	2.05	18	8
3:A:17:ASP:HB3	3:A:88:TYR:CE1	0.51	2.40	18	5
3:A:24:ALA:HB3	3:A:78:LYS:HA	0.51	1.81	16	2
1:B:110:DG:H5'	3:A:25:LEU:HD21	0.51	1.82	8	12
1:B:108:DT:O4'	3:A:23:ARG:CG	0.51	2.59	16	1
3:A:82:GLU:CG	3:A:85:LYS:CE	0.51	2.89	4	1
3:A:54:LYS:CD	3:A:58:LYS:CG	0.51	2.89	14	4
3:A:67:LYS:O	3:A:68:GLN:C	0.51	2.49	6	18
3:A:80:ARG:HG3	3:A:81:TYR:N	0.51	2.21	8	6
3:A:39:VAL:HG12	3:A:51:VAL:HG23	0.51	1.82	3	5
3:A:35:ASN:O	3:A:39:VAL:HG12	0.51	2.06	17	1
3:A:46:ILE:HB	3:A:50:GLN:CG	0.51	2.36	6	9
3:A:39:VAL:CG1	3:A:51:VAL:HG23	0.51	2.36	3	5
3:A:36:ARG:NH1	3:A:37:ASP:OD1	0.51	2.43	20	1
3:A:78:LYS:HZ3	3:A:78:LYS:HB3	0.51	1.66	20	1
3:A:31:PHE:O	3:A:35:ASN:ND2	0.51	2.43	3	10
3:A:23:ARG:HA	3:A:81:TYR:CG	0.51	2.41	8	2
3:A:50:GLN:O	3:A:54:LYS:HG3	0.51	2.06	1	5
3:A:23:ARG:NH2	3:A:25:LEU:C	0.51	2.64	17	2
3:A:31:PHE:HB2	3:A:70:TYR:CD2	0.51	2.41	11	8
3:A:82:GLU:CG	3:A:85:LYS:HE2	0.51	2.36	4	1
1:B:112:DT:O4'	3:A:36:ARG:NH1	0.50	2.45	15	1
1:B:108:DT:C2	3:A:23:ARG:HD2	0.50	2.41	11	1
3:A:34:GLU:N	3:A:34:GLU:OE1	0.50	2.45	7	1
3:A:19:ASN:OD1	3:A:88:TYR:O	0.50	2.29	1	2
3:A:24:ALA:CB	3:A:77:ASP:C	0.50	2.80	16	1
3:A:43:ASN:O	3:A:46:ILE:HG12	0.50	2.07	14	16
2:C:123:DA:N3	3:A:26:SER:OG	0.50	2.37	2	2
3:A:25:LEU:O	3:A:29:MET:HB2	0.50	2.05	8	1
1:B:110:DG:C5'	3:A:25:LEU:CD2	0.50	2.88	16	2
2:C:126:DA:C6	2:C:127:DC:N4	0.50	2.80	17	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:A:84:GLU:O	3:A:87:LEU:HD23	0.50	2.07	17	2
3:A:67:LYS:HA	3:A:70:TYR:CD1	0.50	2.41	16	7
3:A:75:GLN:CG	3:A:78:LYS:HZ2	0.50	2.19	2	1
3:A:68:GLN:N	3:A:69:PRO:HD2	0.50	2.22	14	4
1:B:104:DG:H4'	1:B:105:DT:OP1	0.50	2.07	20	17
3:A:43:ASN:HB3	3:A:46:ILE:HB	0.50	1.82	7	4
3:A:32:ALA:O	3:A:36:ARG:HG2	0.50	2.06	16	2
2:C:124:DT:P	3:A:27:ALA:HB3	0.50	2.46	11	1
1:B:111:DT:O4'	3:A:36:ARG:HD3	0.50	2.06	18	1
3:A:47:THR:OG1	3:A:50:GLN:NE2	0.50	2.45	17	1
3:A:21:PRO:HG3	3:A:88:TYR:CB	0.50	2.37	12	7
1:B:110:DG:N9	3:A:29:MET:HE2	0.49	2.22	19	3
3:A:46:ILE:CG2	3:A:50:GLN:HB2	0.49	2.36	15	5
3:A:54:LYS:CD	3:A:58:LYS:HG3	0.49	2.37	4	3
3:A:55:LEU:O	3:A:59:TRP:CB	0.49	2.59	16	4
3:A:80:ARG:NE	3:A:80:ARG:HA	0.49	2.22	17	2
1:B:109:DT:OP2	3:A:22:LYS:HB3	0.49	2.07	13	1
3:A:80:ARG:HA	3:A:80:ARG:NE	0.49	2.23	10	5
1:B:111:DT:C2'	1:B:112:DT:C6	0.49	2.95	16	20
3:A:23:ARG:O	3:A:81:TYR:CG	0.49	2.66	13	7
2:C:126:DA:H2''	2:C:127:DC:O5'	0.49	2.08	7	12
2:C:126:DA:O3'	3:A:85:LYS:NZ	0.49	2.43	8	2
1:B:107:DA:C6	1:B:108:DT:C4	0.49	2.99	1	2
3:A:47:THR:N	3:A:50:GLN:HG2	0.49	2.22	17	7
3:A:25:LEU:O	3:A:26:SER:O	0.49	2.29	8	1
3:A:35:ASN:O	3:A:39:VAL:HB	0.49	2.08	16	4
3:A:35:ASN:HB3	3:A:55:LEU:CD2	0.49	2.37	18	1
3:A:66:GLU:CA	3:A:66:GLU:OE1	0.49	2.58	19	1
3:A:20:ALA:O	3:A:22:LYS:NZ	0.49	2.46	12	1
3:A:79:LYS:HA	3:A:82:GLU:CB	0.49	2.38	10	10
1:B:108:DT:C1'	3:A:23:ARG:HD3	0.49	2.38	7	3
3:A:65:GLU:O	3:A:69:PRO:HD3	0.49	2.07	5	2
1:B:110:DG:C1'	3:A:29:MET:HE2	0.49	2.38	16	2
3:A:36:ARG:HG2	3:A:37:ASP:N	0.49	2.23	5	15
2:C:119:DA:N3	3:A:48:PHE:CZ	0.49	2.80	17	1
3:A:18:PRO:HD2	3:A:88:TYR:CE1	0.49	2.42	12	3
2:C:126:DA:C5	2:C:127:DC:C5	0.49	3.01	17	2
1:B:109:DT:O2	1:B:110:DG:C5	0.49	2.65	16	1
3:A:87:LEU:CD2	3:A:88:TYR:N	0.49	2.71	19	2
1:B:109:DT:OP2	3:A:22:LYS:CB	0.49	2.60	13	1
2:C:127:DC:P	3:A:85:LYS:HE2	0.49	2.48	12	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:A:80:ARG:HA	3:A:80:ARG:CZ	0.49	2.37	1	6
3:A:21:PRO:HD3	3:A:88:TYR:CG	0.49	2.43	16	1
1:B:109:DT:OP1	3:A:23:ARG:HG3	0.49	2.08	13	1
2:C:125:DC:OP2	3:A:78:LYS:CE	0.49	2.61	12	1
3:A:57:GLU:HG3	3:A:58:LYS:N	0.49	2.23	3	6
3:A:24:ALA:CB	3:A:78:LYS:HA	0.49	2.38	1	13
1:B:111:DT:O3'	3:A:36:ARG:HD3	0.49	2.08	6	6
3:A:62:LEU:HB3	3:A:66:GLU:CB	0.49	2.38	6	4
1:B:110:DG:O4'	3:A:29:MET:SD	0.49	2.71	10	3
2:C:126:DA:OP1	3:A:78:LYS:HD2	0.49	2.08	7	6
1:B:104:DG:N2	1:B:105:DT:N3	0.49	2.60	18	4
3:A:54:LYS:HE2	3:A:58:LYS:CD	0.49	2.37	4	1
3:A:19:ASN:O	3:A:20:ALA:O	0.49	2.30	2	6
3:A:29:MET:O	3:A:33:ASN:CB	0.49	2.61	18	2
1:B:106:DG:N1	1:B:107:DA:C6	0.48	2.81	12	2
3:A:38:ILE:CD1	3:A:38:ILE:N	0.48	2.76	16	5
3:A:63:THR:O	3:A:67:LYS:HG3	0.48	2.08	5	2
3:A:21:PRO:CG	3:A:85:LYS:HA	0.48	2.38	5	2
3:A:54:LYS:O	3:A:57:GLU:N	0.48	2.46	17	2
3:A:38:ILE:CG2	3:A:39:VAL:N	0.48	2.76	18	4
3:A:39:VAL:HG13	3:A:40:ARG:H	0.48	1.67	17	1
3:A:59:TRP:CZ2	3:A:67:LYS:HD2	0.48	2.43	1	16
3:A:23:ARG:HA	3:A:81:TYR:CE1	0.48	2.43	16	2
2:C:121:DC:O5'	3:A:53:LYS:HG2	0.48	2.07	7	3
3:A:24:ALA:HB2	3:A:78:LYS:HA	0.48	1.84	3	3
3:A:36:ARG:NH1	3:A:37:ASP:CG	0.48	2.67	20	1
1:B:108:DT:O2	3:A:23:ARG:HD3	0.48	2.08	19	8
1:B:111:DT:O3'	3:A:36:ARG:HD2	0.48	2.09	1	11
3:A:87:LEU:O	3:A:88:TYR:C	0.48	2.52	19	15
3:A:23:ARG:C	3:A:81:TYR:CD2	0.48	2.86	15	3
3:A:49:GLY:N	3:A:50:GLN:NE2	0.48	2.61	8	3
3:A:63:THR:HG23	3:A:64:PRO:CD	0.48	2.38	20	2
3:A:32:ALA:CB	3:A:36:ARG:NE	0.48	2.76	18	1
2:C:126:DA:OP1	3:A:78:LYS:HD3	0.48	2.08	10	6
3:A:21:PRO:HA	3:A:84:GLU:HG3	0.48	1.86	8	7
2:C:118:DG:C5	2:C:119:DA:N6	0.48	2.81	15	12
3:A:23:ARG:O	3:A:24:ALA:O	0.48	2.32	8	1
2:C:122:DA:C2	3:A:29:MET:CE	0.48	2.97	11	2
1:B:112:DT:OP1	3:A:36:ARG:HG3	0.48	2.09	11	5
2:C:127:DC:OP2	3:A:85:LYS:HE2	0.48	2.09	19	4
3:A:59:TRP:CH2	3:A:67:LYS:HB3	0.48	2.43	17	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:A:66:GLU:N	3:A:66:GLU:CD	0.48	2.67	17	2
3:A:63:THR:HB	3:A:66:GLU:HG2	0.48	1.85	8	14
2:C:127:DC:OP1	3:A:81:TYR:OH	0.48	2.28	19	2
2:C:126:DA:H1'	2:C:127:DC:C6	0.48	2.44	12	6
3:A:42:GLU:C	3:A:43:ASN:ND2	0.48	2.67	7	1
3:A:36:ARG:NE	3:A:37:ASP:OD1	0.48	2.47	17	1
2:C:123:DA:C5	2:C:124:DT:C5	0.48	3.02	9	4
2:C:123:DA:C4	2:C:124:DT:C5	0.48	3.01	19	4
3:A:46:ILE:O	3:A:50:GLN:HG2	0.48	2.09	10	7
3:A:23:ARG:CB	3:A:23:ARG:NH1	0.48	2.77	18	2
1:B:105:DT:C2'	1:B:106:DG:OP2	0.47	2.62	20	7
3:A:21:PRO:HB2	3:A:81:TYR:CD2	0.47	2.44	6	2
3:A:67:LYS:HA	3:A:70:TYR:CE1	0.47	2.44	1	7
2:C:125:DC:O5'	3:A:78:LYS:HD2	0.47	2.09	15	4
1:B:111:DT:C4'	3:A:36:ARG:HD3	0.47	2.39	18	1
3:A:37:ASP:O	3:A:41:SER:OG	0.47	2.32	16	7
3:A:27:ALA:HA	3:A:30:PHE:HD2	0.47	1.70	8	6
3:A:79:LYS:O	3:A:82:GLU:N	0.47	2.47	15	3
3:A:30:PHE:CZ	3:A:74:ALA:HA	0.47	2.43	5	7
1:B:110:DG:C5'	1:B:111:DT:OP1	0.47	2.61	11	1
3:A:46:ILE:HG13	3:A:51:VAL:HG23	0.47	1.84	1	1
3:A:72:ALA:HA	3:A:75:GLN:NE2	0.47	2.25	15	4
3:A:68:GLN:HB2	3:A:69:PRO:CD	0.47	2.39	11	3
3:A:47:THR:HG22	3:A:48:PHE:H	0.47	1.69	14	2
3:A:21:PRO:HB3	3:A:84:GLU:HG3	0.47	1.85	5	10
3:A:36:ARG:O	3:A:40:ARG:HB2	0.47	2.09	8	2
3:A:31:PHE:CE2	3:A:55:LEU:HD23	0.47	2.44	8	1
1:B:110:DG:OP1	3:A:25:LEU:CD1	0.47	2.55	16	1
3:A:34:GLU:O	3:A:37:ASP:OD1	0.47	2.31	3	4
3:A:80:ARG:CD	3:A:80:ARG:C	0.47	2.83	3	1
1:B:110:DG:C4	3:A:29:MET:HE2	0.47	2.45	19	4
1:B:103:DG:H4'	1:B:104:DG:OP1	0.47	2.09	20	1
2:C:125:DC:OP1	3:A:78:LYS:CE	0.47	2.62	2	1
3:A:50:GLN:O	3:A:54:LYS:HB3	0.47	2.10	7	8
3:A:31:PHE:CZ	3:A:35:ASN:OD1	0.47	2.67	11	9
3:A:33:ASN:O	3:A:37:ASP:OD2	0.47	2.33	8	1
3:A:43:ASN:HB3	3:A:46:ILE:CD1	0.47	2.39	13	1
3:A:59:TRP:HZ3	3:A:70:TYR:CD2	0.47	2.28	11	13
1:B:111:DT:O3'	3:A:36:ARG:CG	0.47	2.63	20	9
3:A:24:ALA:O	3:A:25:LEU:O	0.47	2.32	14	1
3:A:23:ARG:NH2	3:A:24:ALA:CB	0.47	2.68	8	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:A:77:ASP:O	3:A:77:ASP:OD1	0.47	2.33	17	5
2:C:122:DA:C2'	2:C:123:DA:OP2	0.47	2.62	16	5
3:A:35:ASN:O	3:A:39:VAL:CB	0.47	2.63	16	4
3:A:32:ALA:O	3:A:36:ARG:HB3	0.47	2.09	11	1
3:A:36:ARG:NH2	3:A:52:GLY:HA2	0.47	2.24	16	1
3:A:71:GLU:O	3:A:74:ALA:CB	0.47	2.62	8	16
3:A:37:ASP:O	3:A:41:SER:HB3	0.47	2.09	20	7
3:A:31:PHE:CZ	3:A:59:TRP:HA	0.47	2.45	15	3
3:A:82:GLU:CG	3:A:85:LYS:HE3	0.47	2.40	18	2
1:B:107:DA:H2''	1:B:108:DT:C5'	0.47	2.40	13	7
3:A:17:ASP:N	3:A:17:ASP:OD1	0.47	2.48	18	2
3:A:86:GLU:HG3	3:A:87:LEU:N	0.47	2.25	16	11
3:A:33:ASN:O	3:A:37:ASP:OD1	0.47	2.33	14	2
3:A:35:ASN:HB2	3:A:55:LEU:CD2	0.47	2.40	11	3
3:A:63:THR:CG2	3:A:64:PRO:HD2	0.47	2.37	1	3
3:A:46:ILE:HB	3:A:50:GLN:HB2	0.47	1.86	19	7
3:A:55:LEU:O	3:A:59:TRP:HB2	0.47	2.10	16	3
2:C:122:DA:O3'	3:A:60:LYS:HD2	0.47	2.10	16	1
3:A:46:ILE:CD1	3:A:51:VAL:HG23	0.47	2.40	1	1
3:A:30:PHE:O	3:A:33:ASN:HB2	0.46	2.11	18	14
3:A:29:MET:O	3:A:33:ASN:HB2	0.46	2.10	16	4
3:A:51:VAL:HG22	3:A:55:LEU:HD12	0.46	1.86	2	2
2:C:124:DT:OP1	3:A:26:SER:OG	0.46	2.31	19	1
3:A:80:ARG:CZ	3:A:80:ARG:HA	0.46	2.39	17	1
3:A:21:PRO:O	3:A:84:GLU:CD	0.46	2.53	12	4
3:A:54:LYS:O	3:A:57:GLU:HG2	0.46	2.10	6	5
3:A:23:ARG:CA	3:A:81:TYR:CD2	0.46	2.97	7	6
3:A:36:ARG:HG2	3:A:55:LEU:CD1	0.46	2.41	18	1
3:A:81:TYR:O	3:A:84:GLU:CG	0.46	2.63	10	1
3:A:84:GLU:O	3:A:84:GLU:OE1	0.46	2.33	2	1
3:A:37:ASP:O	3:A:41:SER:HB2	0.46	2.11	13	13
1:B:108:DT:H2''	1:B:109:DT:O5'	0.46	2.09	14	5
2:C:125:DC:O5'	3:A:78:LYS:HG3	0.46	2.11	19	3
3:A:43:ASN:CB	3:A:46:ILE:HG12	0.46	2.40	19	6
3:A:38:ILE:N	3:A:38:ILE:CD1	0.46	2.79	13	3
3:A:65:GLU:HA	3:A:68:GLN:HG3	0.46	1.87	8	16
1:B:110:DG:C2	3:A:29:MET:HE1	0.46	2.45	15	1
3:A:46:ILE:HG12	3:A:50:GLN:HB3	0.46	1.88	7	1
3:A:76:ALA:O	3:A:79:LYS:HG2	0.46	2.10	20	1
3:A:45:ASP:O	3:A:46:ILE:C	0.46	2.53	15	5
3:A:54:LYS:CE	3:A:58:LYS:CD	0.46	2.93	4	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:108:DT:O2	3:A:23:ARG:NH1	0.46	2.49	8	1
3:A:60:LYS:HA	3:A:67:LYS:NZ	0.46	2.26	5	2
2:C:124:DT:C5'	2:C:125:DC:OP1	0.46	2.64	19	3
3:A:84:GLU:O	3:A:88:TYR:HB2	0.46	2.11	15	3
3:A:43:ASN:O	3:A:46:ILE:HG13	0.46	2.11	9	7
1:B:113:DC:H4'	3:A:47:THR:HG22	0.46	1.87	19	2
3:A:67:LYS:CE	3:A:71:GLU:OE1	0.46	2.64	2	1
2:C:126:DA:C3'	3:A:85:LYS:HE3	0.46	2.40	12	1
3:A:70:TYR:O	3:A:74:ALA:N	0.46	2.49	17	20
2:C:120:DA:N3	3:A:48:PHE:CZ	0.46	2.84	15	1
3:A:79:LYS:HG3	3:A:80:ARG:N	0.46	2.26	20	2
3:A:23:ARG:HB3	3:A:23:ARG:NH1	0.46	2.25	1	2
3:A:81:TYR:O	3:A:84:GLU:N	0.46	2.49	16	2
3:A:17:ASP:OD1	3:A:88:TYR:OH	0.46	2.34	3	2
3:A:17:ASP:HB3	3:A:20:ALA:CB	0.46	2.39	9	1
2:C:126:DA:C2	2:C:127:DC:C4	0.46	3.04	10	1
3:A:77:ASP:OD1	3:A:77:ASP:O	0.46	2.34	12	7
1:B:111:DT:O3'	3:A:36:ARG:HG3	0.46	2.11	20	15
3:A:21:PRO:O	3:A:84:GLU:OE2	0.46	2.33	4	2
3:A:46:ILE:HG23	3:A:50:GLN:HB2	0.46	1.88	3	3
2:C:127:DC:OP1	3:A:85:LYS:HE2	0.46	2.09	16	2
2:C:119:DA:C2'	2:C:120:DA:C8	0.46	2.99	17	1
3:A:17:ASP:HB2	3:A:88:TYR:CE1	0.45	2.47	12	1
2:C:127:DC:OP1	3:A:85:LYS:HD2	0.45	2.11	10	7
3:A:60:LYS:NZ	3:A:60:LYS:HB3	0.45	2.27	16	1
3:A:54:LYS:CD	3:A:58:LYS:HG2	0.45	2.40	20	1
3:A:32:ALA:HA	3:A:35:ASN:OD1	0.45	2.11	1	13
3:A:46:ILE:CB	3:A:50:GLN:CG	0.45	2.94	6	6
3:A:21:PRO:HB3	3:A:84:GLU:CG	0.45	2.42	19	5
3:A:23:ARG:HA	3:A:81:TYR:CD1	0.45	2.46	8	2
3:A:46:ILE:HD11	3:A:51:VAL:HG23	0.45	1.88	1	1
3:A:46:ILE:CD1	3:A:51:VAL:HB	0.45	2.40	11	7
3:A:54:LYS:CE	3:A:58:LYS:HG3	0.45	2.41	4	1
2:C:126:DA:C4	2:C:127:DC:C6	0.45	3.04	8	8
3:A:23:ARG:O	3:A:24:ALA:C	0.45	2.55	8	1
3:A:31:PHE:O	3:A:34:GLU:N	0.45	2.50	15	2
3:A:62:LEU:HB3	3:A:66:GLU:CG	0.45	2.41	5	2
2:C:123:DA:OP1	3:A:60:LYS:HE3	0.45	2.12	4	6
3:A:23:ARG:HG3	3:A:24:ALA:N	0.45	2.26	15	2
3:A:17:ASP:CG	3:A:88:TYR:OH	0.45	2.55	5	8
3:A:81:TYR:CE1	3:A:85:LYS:HD2	0.45	2.46	5	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:112:DT:OP1	3:A:36:ARG:HD2	0.45	2.12	6	8
1:B:107:DA:C8	1:B:108:DT:H71	0.45	2.47	16	11
3:A:46:ILE:HG23	3:A:47:THR:N	0.45	2.27	7	3
1:B:113:DC:OP1	3:A:40:ARG:NE	0.45	2.49	16	1
2:C:124:DT:C2'	2:C:125:DC:C6	0.45	3.00	14	8
3:A:36:ARG:O	3:A:40:ARG:HB3	0.45	2.12	20	5
3:A:28:TYR:HB3	3:A:29:MET:HE1	0.45	1.88	7	1
3:A:78:LYS:HE2	3:A:78:LYS:CA	0.45	2.42	7	1
3:A:32:ALA:O	3:A:36:ARG:HG3	0.45	2.12	18	1
2:C:126:DA:C2'	2:C:127:DC:O5'	0.45	2.65	5	12
3:A:49:GLY:O	3:A:53:LYS:HB2	0.45	2.11	2	5
3:A:28:TYR:C	3:A:28:TYR:CD1	0.45	2.90	16	4
3:A:46:ILE:CG1	3:A:50:GLN:HB2	0.45	2.42	16	2
3:A:47:THR:N	3:A:50:GLN:CG	0.45	2.80	19	1
3:A:54:LYS:O	3:A:55:LEU:C	0.45	2.56	17	3
1:B:113:DC:O4'	3:A:48:PHE:HB2	0.45	2.12	2	3
3:A:43:ASN:CB	3:A:46:ILE:HB	0.45	2.40	7	1
3:A:40:ARG:NH2	3:A:44:PRO:HB3	0.45	2.27	18	2
2:C:124:DT:O2	3:A:23:ARG:NH2	0.45	2.50	18	1
3:A:79:LYS:HA	3:A:82:GLU:HB3	0.44	1.89	4	9
3:A:80:ARG:NE	3:A:80:ARG:C	0.44	2.70	15	4
2:C:125:DC:O5'	3:A:78:LYS:CG	0.44	2.65	19	1
3:A:43:ASN:HB3	3:A:46:ILE:HG12	0.44	1.89	6	9
2:C:123:DA:OP1	3:A:60:LYS:HD3	0.44	2.12	13	3
3:A:52:GLY:O	3:A:55:LEU:N	0.44	2.50	17	4
3:A:52:GLY:O	3:A:55:LEU:HB2	0.44	2.11	14	2
2:C:118:DG:C5	2:C:119:DA:C5	0.44	3.04	18	4
3:A:23:ARG:N	3:A:81:TYR:CD2	0.44	2.85	8	2
2:C:123:DA:OP1	3:A:60:LYS:HD2	0.44	2.12	3	3
3:A:49:GLY:O	3:A:53:LYS:HD2	0.44	2.13	18	2
3:A:46:ILE:C	3:A:50:GLN:CG	0.44	2.85	16	1
3:A:36:ARG:NH1	3:A:37:ASP:OD2	0.44	2.51	20	1
2:C:126:DA:OP1	3:A:78:LYS:HG2	0.44	2.12	19	1
2:C:125:DC:O5'	3:A:78:LYS:HD3	0.44	2.12	12	2
2:C:116:DC:H2'	2:C:117:DT:C5	0.44	2.47	18	3
2:C:124:DT:O2	3:A:23:ARG:NE	0.44	2.50	8	1
3:A:26:SER:HB3	3:A:29:MET:HG2	0.44	1.88	8	1
3:A:80:ARG:CG	3:A:81:TYR:N	0.44	2.80	8	1
3:A:48:PHE:C	3:A:50:GLN:N	0.44	2.71	10	3
1:B:110:DG:C1'	3:A:29:MET:CE	0.44	2.95	16	1
3:A:47:THR:O	3:A:48:PHE:C	0.44	2.56	12	4

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:A:18:PRO:HD2	3:A:88:TYR:OH	0.44	2.12	17	8
3:A:19:ASN:O	3:A:20:ALA:C	0.44	2.55	19	9
3:A:46:ILE:HG22	3:A:50:GLN:HG3	0.44	1.89	6	5
1:B:112:DT:O2	3:A:48:PHE:HB2	0.44	2.11	17	4
3:A:27:ALA:O	3:A:31:PHE:HB3	0.44	2.13	6	9
1:B:107:DA:H2''	1:B:108:DT:O5'	0.44	2.13	8	5
3:A:68:GLN:HG2	3:A:69:PRO:CD	0.44	2.42	17	2
3:A:32:ALA:O	3:A:36:ARG:HD2	0.44	2.13	18	1
1:B:109:DT:O2	1:B:110:DG:N7	0.44	2.50	16	1
3:A:54:LYS:O	3:A:58:LYS:HG2	0.44	2.12	19	3
3:A:59:TRP:CZ3	3:A:70:TYR:CD2	0.44	3.06	14	7
1:B:112:DT:H2''	1:B:113:DC:O5'	0.44	2.13	18	3
3:A:79:LYS:HD2	3:A:80:ARG:N	0.44	2.28	2	1
3:A:80:ARG:HA	3:A:80:ARG:NH1	0.44	2.27	1	1
1:B:111:DT:H2'	1:B:112:DT:H71	0.44	1.90	18	17
3:A:59:TRP:HZ3	3:A:70:TYR:CD1	0.44	2.31	9	5
3:A:75:GLN:HA	3:A:78:LYS:CE	0.44	2.43	14	1
2:C:126:DA:O3'	3:A:85:LYS:HE3	0.44	2.13	10	1
3:A:46:ILE:O	3:A:50:GLN:HB2	0.44	2.13	13	1
1:B:109:DT:O2	3:A:26:SER:HB2	0.44	2.13	8	1
3:A:59:TRP:O	3:A:62:LEU:HG	0.44	2.12	8	1
3:A:31:PHE:O	3:A:32:ALA:C	0.44	2.56	16	2
2:C:125:DC:H4'	2:C:126:DA:OP1	0.44	2.13	1	3
3:A:21:PRO:HA	3:A:84:GLU:HG2	0.44	1.89	20	5
1:B:107:DA:C5	1:B:108:DT:C5	0.44	3.06	1	2
3:A:46:ILE:HD11	3:A:51:VAL:CG2	0.44	2.42	1	1
3:A:78:LYS:HE3	3:A:78:LYS:O	0.43	2.12	6	1
3:A:85:LYS:HG2	3:A:86:GLU:N	0.43	2.27	19	3
2:C:126:DA:OP1	3:A:78:LYS:HE3	0.43	2.13	15	1
3:A:71:GLU:O	3:A:71:GLU:OE1	0.43	2.35	7	1
1:B:111:DT:C1'	3:A:36:ARG:HD3	0.43	2.42	18	1
3:A:38:ILE:O	3:A:41:SER:HB3	0.43	2.12	20	2
3:A:31:PHE:CE1	3:A:62:LEU:CD1	0.43	3.00	6	1
3:A:21:PRO:CA	3:A:84:GLU:HG3	0.43	2.43	4	7
3:A:35:ASN:ND2	3:A:35:ASN:H	0.43	2.10	11	3
3:A:79:LYS:O	3:A:82:GLU:HB3	0.43	2.13	15	10
3:A:36:ARG:NE	3:A:37:ASP:OD2	0.43	2.51	11	1
3:A:29:MET:O	3:A:33:ASN:CG	0.43	2.57	18	2
3:A:35:ASN:CB	3:A:55:LEU:CD2	0.43	2.96	18	1
3:A:49:GLY:O	3:A:53:LYS:HD3	0.43	2.13	9	3
2:C:123:DA:C5	2:C:124:DT:C7	0.43	3.01	16	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:C:125:DC:OP2	3:A:78:LYS:HE2	0.43	2.13	12	1
3:A:54:LYS:HE2	3:A:58:LYS:CG	0.43	2.43	4	2
3:A:47:THR:HG22	3:A:48:PHE:N	0.43	2.28	14	2
1:B:105:DT:H2''	1:B:106:DG:C8	0.43	2.47	17	4
3:A:36:ARG:CZ	3:A:55:LEU:CD1	0.43	2.96	16	1
2:C:122:DA:O3'	3:A:60:LYS:HE3	0.43	2.12	10	1
3:A:43:ASN:HB3	3:A:46:ILE:CG1	0.43	2.43	13	1
3:A:82:GLU:HG2	3:A:85:LYS:CE	0.43	2.43	4	1
1:B:110:DG:C5'	3:A:25:LEU:HD11	0.43	2.44	8	1
3:A:84:GLU:HA	3:A:87:LEU:CD2	0.43	2.41	5	1
1:B:110:DG:H5'	3:A:25:LEU:CD2	0.43	2.44	7	3
3:A:59:TRP:CZ3	3:A:70:TYR:CD1	0.43	3.07	16	1
3:A:49:GLY:CA	3:A:53:LYS:HD2	0.43	2.43	20	1
2:C:129:DC:C2'	2:C:130:DC:C5	0.43	3.02	19	19
3:A:65:GLU:O	3:A:68:GLN:HG3	0.43	2.13	6	12
3:A:19:ASN:ND2	3:A:19:ASN:N	0.43	2.66	4	1
3:A:28:TYR:CD1	3:A:28:TYR:C	0.43	2.92	15	3
2:C:119:DA:H2'	2:C:120:DA:C8	0.43	2.49	17	1
3:A:35:ASN:HB3	3:A:39:VAL:HG23	0.43	1.91	12	2
2:C:126:DA:O3'	3:A:85:LYS:HE2	0.43	2.13	8	2
3:A:21:PRO:O	3:A:84:GLU:OE1	0.43	2.36	3	1
3:A:35:ASN:H	3:A:35:ASN:ND2	0.43	2.10	20	4
1:B:103:DG:N2	2:C:129:DC:C2	0.43	2.87	20	1
2:C:125:DC:OP1	3:A:78:LYS:HD2	0.43	2.13	2	1
3:A:39:VAL:HG13	3:A:40:ARG:N	0.43	2.27	17	1
1:B:103:DG:H2''	1:B:104:DG:O5'	0.43	2.14	3	1
2:C:128:DC:C4	2:C:129:DC:N4	0.43	2.87	6	1
1:B:109:DT:O2	3:A:29:MET:CG	0.43	2.67	15	1
3:A:49:GLY:C	3:A:50:GLN:CD	0.43	2.78	1	1
3:A:46:ILE:CG2	3:A:50:GLN:HB3	0.43	2.44	12	1
3:A:72:ALA:O	3:A:75:GLN:HG2	0.43	2.14	12	3
3:A:26:SER:H	3:A:29:MET:HG2	0.43	1.72	14	3
3:A:79:LYS:O	3:A:80:ARG:C	0.43	2.56	15	8
3:A:54:LYS:O	3:A:54:LYS:HD2	0.43	2.14	2	2
2:C:125:DC:C3'	3:A:78:LYS:HD3	0.43	2.43	9	1
2:C:125:DC:C5'	3:A:23:ARG:NH2	0.43	2.81	4	2
3:A:66:GLU:O	3:A:69:PRO:HD2	0.43	2.14	1	6
3:A:27:ALA:CB	3:A:71:GLU:HA	0.43	2.44	16	2
1:B:106:DG:O6	1:B:107:DA:N6	0.42	2.52	12	2
1:B:111:DT:O4'	3:A:36:ARG:NH1	0.42	2.51	18	1
3:A:43:ASN:HB3	3:A:46:ILE:HD13	0.42	1.89	13	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:C:126:DA:O3'	3:A:85:LYS:HD2	0.42	2.14	1	1
3:A:71:GLU:OE1	3:A:74:ALA:HB3	0.42	2.14	15	1
3:A:82:GLU:HA	3:A:85:LYS:CD	0.42	2.44	5	1
2:C:125:DC:P	3:A:78:LYS:HE2	0.42	2.54	12	1
3:A:47:THR:C	3:A:51:VAL:CG1	0.42	2.87	6	2
3:A:31:PHE:CE1	3:A:35:ASN:CG	0.42	2.93	15	1
3:A:46:ILE:CD1	3:A:50:GLN:HB2	0.42	2.40	1	1
3:A:23:ARG:CG	3:A:24:ALA:N	0.42	2.82	15	2
3:A:54:LYS:HD3	3:A:58:LYS:HG2	0.42	1.90	20	3
3:A:21:PRO:O	3:A:22:LYS:HD3	0.42	2.14	1	2
3:A:39:VAL:HG11	3:A:51:VAL:HG13	0.42	1.91	1	1
3:A:40:ARG:NH1	3:A:44:PRO:HB3	0.42	2.30	7	1
2:C:122:DA:O3'	3:A:60:LYS:CD	0.42	2.68	16	1
2:C:121:DC:C5'	3:A:53:LYS:HG2	0.42	2.45	6	4
2:C:126:DA:O3'	3:A:85:LYS:CE	0.42	2.67	8	1
1:B:107:DA:N7	1:B:108:DT:C7	0.42	2.83	16	2
3:A:19:ASN:OD1	3:A:88:TYR:HA	0.42	2.15	1	1
3:A:31:PHE:O	3:A:35:ASN:CG	0.42	2.57	3	2
3:A:46:ILE:HG13	3:A:47:THR:N	0.42	2.30	16	1
3:A:54:LYS:O	3:A:57:GLU:HG3	0.42	2.15	6	1
3:A:70:TYR:O	3:A:71:GLU:C	0.42	2.58	8	1
3:A:48:PHE:HA	3:A:51:VAL:CG1	0.42	2.45	15	1
3:A:79:LYS:CG	3:A:80:ARG:N	0.42	2.82	3	1
3:A:43:ASN:ND2	3:A:43:ASN:N	0.42	2.68	7	1
2:C:120:DA:N3	3:A:48:PHE:CE1	0.42	2.88	12	1
2:C:121:DC:O2	3:A:28:TYR:OH	0.42	2.30	16	1
3:A:63:THR:CB	3:A:66:GLU:HG2	0.42	2.44	15	2
3:A:21:PRO:O	3:A:22:LYS:HD2	0.41	2.14	6	1
3:A:78:LYS:C	3:A:78:LYS:HE2	0.41	2.35	6	1
1:B:110:DG:O4'	3:A:29:MET:HB3	0.41	2.15	19	3
3:A:63:THR:HB	3:A:66:GLU:CG	0.41	2.44	8	1
3:A:28:TYR:HB3	3:A:29:MET:CE	0.41	2.46	20	2
3:A:21:PRO:O	3:A:22:LYS:HG3	0.41	2.15	9	1
3:A:25:LEU:HD13	3:A:77:ASP:OD2	0.41	2.16	7	3
2:C:118:DG:C2'	2:C:119:DA:C8	0.41	3.03	18	6
3:A:30:PHE:CE2	3:A:74:ALA:CB	0.41	3.03	3	1
3:A:17:ASP:HB2	3:A:20:ALA:CB	0.41	2.44	7	1
3:A:36:ARG:CG	3:A:55:LEU:HD13	0.41	2.45	18	1
3:A:35:ASN:HB3	3:A:39:VAL:CG2	0.41	2.46	12	2
3:A:40:ARG:CZ	3:A:44:PRO:HB3	0.41	2.46	7	1
3:A:36:ARG:NE	3:A:55:LEU:CD1	0.41	2.84	16	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:A:47:THR:CG2	3:A:48:PHE:N	0.41	2.83	20	1
3:A:80:ARG:CA	3:A:80:ARG:CZ	0.41	2.99	1	1
3:A:38:ILE:O	3:A:41:SER:HB2	0.41	2.16	12	2
3:A:26:SER:CB	3:A:29:MET:HG2	0.41	2.46	8	1
3:A:83:SER:HA	3:A:86:GLU:HG2	0.41	1.92	5	1
1:B:109:DT:C2	1:B:110:DG:C5	0.41	3.08	16	1
3:A:69:PRO:O	3:A:73:LYS:HB2	0.41	2.15	8	3
3:A:47:THR:HB	3:A:50:GLN:HG2	0.41	1.92	8	1
3:A:82:GLU:HA	3:A:85:LYS:HG2	0.41	1.91	11	2
3:A:54:LYS:O	3:A:58:LYS:HG3	0.41	2.16	10	1
3:A:17:ASP:HB3	3:A:20:ALA:CA	0.41	2.46	17	1
3:A:57:GLU:HA	3:A:57:GLU:OE1	0.41	2.15	17	1
3:A:30:PHE:HB2	3:A:70:TYR:HB3	0.41	1.91	11	1
2:C:121:DC:O5'	3:A:53:LYS:CG	0.41	2.69	7	1
3:A:78:LYS:O	3:A:78:LYS:HE2	0.41	2.16	16	1
3:A:68:GLN:CB	3:A:69:PRO:CD	0.41	2.99	11	2
1:B:110:DG:O4'	3:A:29:MET:HG3	0.41	2.15	8	1
3:A:58:LYS:CE	3:A:58:LYS:HA	0.41	2.46	7	1
3:A:75:GLN:CG	3:A:78:LYS:NZ	0.41	2.84	18	2
3:A:31:PHE:CB	3:A:59:TRP:CZ3	0.41	3.04	16	2
3:A:51:VAL:O	3:A:55:LEU:HD12	0.41	2.16	17	1
3:A:21:PRO:C	3:A:22:LYS:CG	0.41	2.89	7	1
3:A:46:ILE:HB	3:A:50:GLN:HB3	0.41	1.92	20	1
3:A:54:LYS:O	3:A:58:LYS:HB2	0.41	2.16	10	2
3:A:20:ALA:O	3:A:22:LYS:HG3	0.40	2.17	18	1
3:A:40:ARG:HG3	3:A:41:SER:N	0.40	2.30	18	1
3:A:54:LYS:O	3:A:58:LYS:CB	0.40	2.70	13	1
3:A:82:GLU:HG2	3:A:85:LYS:HE3	0.40	1.93	4	1
3:A:50:GLN:NE2	3:A:50:GLN:H	0.40	2.14	14	1
3:A:71:GLU:OE1	3:A:71:GLU:HA	0.40	2.16	15	1
3:A:78:LYS:O	3:A:82:GLU:HB2	0.40	2.17	3	1
1:B:108:DT:H2''	1:B:109:DT:C6	0.40	2.51	13	1
1:B:111:DT:C5'	3:A:33:ASN:ND2	0.40	2.85	15	1
3:A:77:ASP:O	3:A:80:ARG:HB3	0.40	2.16	11	1
3:A:36:ARG:CG	3:A:55:LEU:CD1	0.40	2.99	18	1
3:A:54:LYS:HD3	3:A:58:LYS:CD	0.40	2.47	20	1
2:C:129:DC:H2''	2:C:130:DC:C6	0.40	2.52	17	2
3:A:18:PRO:HD2	3:A:88:TYR:CZ	0.40	2.52	12	1
3:A:21:PRO:HG3	3:A:88:TYR:HB2	0.40	1.94	15	1
2:C:125:DC:O3'	3:A:78:LYS:HD3	0.40	2.16	9	1
3:A:47:THR:O	3:A:50:GLN:HG2	0.40	2.17	2	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:A:70:TYR:HA	3:A:73:LYS:HB2	0.40	1.94	8	1
1:B:109:DT:O2	3:A:29:MET:HG3	0.40	2.16	15	1
3:A:21:PRO:C	3:A:22:LYS:HG3	0.40	2.37	11	1
3:A:21:PRO:O	3:A:84:GLU:HG3	0.40	2.16	17	1
2:C:126:DA:C5'	3:A:78:LYS:HD3	0.40	2.46	1	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	72/93 (77%)	53±2 (73±3%)	11±2 (15±3%)	8±2 (12±3%)		
All	All	1440/1860 (77%)	1055 (73%)	219 (15%)	166 (12%)		

All 17 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	23	ARG	20
3	A	63	THR	20
3	A	17	ASP	18
3	A	62	LEU	18
3	A	36	ARG	16
3	A	22	LYS	16
3	A	20	ALA	14
3	A	47	THR	10
3	A	48	PHE	9
3	A	25	LEU	8
3	A	49	GLY	6
3	A	18	PRO	4
3	A	46	ILE	2
3	A	38	ILE	2
3	A	21	PRO	1
3	A	24	ALA	1
3	A	26	SER	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	61/80 (76%)	41±2 (66±3%)	20±2 (34±3%)	1	11
All	All	1220/1600 (76%)	811 (66%)	409 (34%)	1	11

All 48 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	81	TYR	20
3	A	80	ARG	20
3	A	70	TYR	20
3	A	23	ARG	19
3	A	87	LEU	19
3	A	73	LYS	18
3	A	62	LEU	18
3	A	65	GLU	18
3	A	35	ASN	15
3	A	63	THR	15
3	A	50	GLN	13
3	A	78	LYS	13
3	A	22	LYS	12
3	A	40	ARG	12
3	A	85	LYS	12
3	A	58	LYS	11
3	A	55	LEU	11
3	A	26	SER	11
3	A	45	ASP	10
3	A	48	PHE	10
3	A	54	LYS	9
3	A	79	LYS	8
3	A	25	LEU	8
3	A	66	GLU	8
3	A	47	THR	8
3	A	38	ILE	6
3	A	83	SER	6
3	A	37	ASP	6
3	A	71	GLU	5

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Mol	Chain	Res	Type	Models (Total)
3	A	82	GLU	5
3	A	53	LYS	4
3	A	19	ASN	4
3	A	51	VAL	4
3	A	33	ASN	4
3	A	77	ASP	3
3	A	46	ILE	3
3	A	75	GLN	3
3	A	17	ASP	3
3	A	29	MET	2
3	A	36	ARG	2
3	A	68	GLN	2
3	A	43	ASN	2
3	A	86	GLU	2
3	A	34	GLU	1
3	A	67	LYS	1
3	A	57	GLU	1
3	A	42	GLU	1
3	A	60	LYS	1

6.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

6.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.6 Ligand geometry ⓘ

There are no ligands in this entry.

6.7 Other polymers ⓘ

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