



Full wwPDB NMR Structure Validation Report ⓘ

Mar 8, 2026 – 10:38 AM UTC

PDB ID : 2FF0 / pdb_00002ff0
Title : Solution Structure of Steroidogenic Factor 1 DNA Binding Domain Bound to its Target Sequence in the Inhibin alpha-subunit Promoter
Authors : Little, T.H.; Zhang, Y.; Matulis, C.K.; Weck, J.; Zhang, Z.; Ramachandran, A.; Mayo, K.E.; Radhakrishnan, I.
Deposited on : 2005-12-17

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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
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

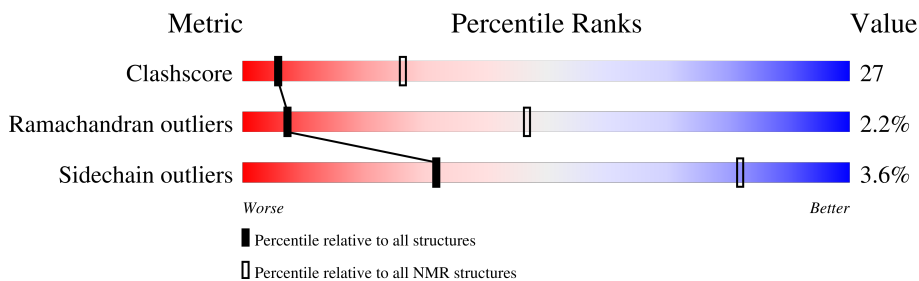
1 Overall quality at a glance

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	15	100%
2	C	15	100%
3	A	102	75% 18% 8%

2 Ensemble composition and analysis

This entry contains 16 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:10-A:103 (94)	1.24	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 3 single-model clusters were found.

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

3 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 2613 atoms, of which 1178 are hydrogens and 0 are deuteriums.

- Molecule 1 is a DNA chain called GGCTCAGGGCCACAG.

Mol	Chain	Residues	Atoms					Trace	
			Total	C	H	N	O		P
1	B	15	475	145	168	62	86	14	0

- Molecule 2 is a DNA chain called CTGTGGCCCTGAGCC.

Mol	Chain	Residues	Atoms					Trace	
			Total	C	H	N	O		P
2	C	15	472	144	170	54	90	14	0

- Molecule 3 is a protein called Steroidogenic factor 1.

Mol	Chain	Residues	Atoms					Trace	
			Total	C	H	N	O		S
3	A	102	1664	507	840	161	144	12	0

- Molecule 4 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	
			Total	Zn
4	A	2	2	2

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: GGCTCAGGGCCACAG

Chain B:  100%


G1
G2
C3
T4
C5
A6
G7
G8
G9
C10
C11
A12
C13
A14
G15

- Molecule 2: CTGTGGCCCTGAGCC

Chain C:  100%

C16
T17
G18
T19
G20
G21
C22
C23
C24
T25
G26
A27
G28
C29
C30

- Molecule 3: Steroidogenic factor 1

Chain A:  75% 18% 8%

D10
V15
H24
T29
S32
K38
V41
Q42
N43
K63
R64
C65
C68
K72
V83
D86
R87
M88
R89
G90
G91
R92
A104
L105
K106
Q107
Q108
K109
K110
A111

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: GGCTCAGGGCCACAG

Chain B:  100%

G1
G2
C3
T4
C5
A6
G7
G8
G9
C10
C11
A12
C13
A14
G15

- Molecule 2: CTGTGGCCCTGAGCC

Chain C: 100%

C16
T17
G18
T19
G20
G21
G22
C23
C24
T25
G26
A27
G28
C29
C30

- Molecule 3: Steroidogenic factor 1

Chain A: 60% 29% 8%

B10
V15
C16
G17
D18
H24
T29
C30
E31
S32
K38
R39
T40
V41
S52
K56
K59
K63
R64
C65
C68
K72
R79
A82
V83
R84
R86
D86
R87
M88
R89
G90
G91
R92
N93
K94
F95
G96
P97
M98
Y99
K100
A104
L105
K106
Q107
Q108

K109
K110
A111

4.2.2 Score per residue for model 2

- Molecule 1: GGCTCAGGGCCACAG

Chain B: 13% 87%

G1
G2
C3
T4
C5
A6
C7
G8
G9
C10
C11
A12
C13
A14
G15

- Molecule 2: CTGTGGCCCTGAGCC

Chain C: 100%

C16
T17
G18
T19
G20
G21
G22
C23
C24
T25
G26
A27
G28
C29
C30

- Molecule 3: Steroidogenic factor 1

Chain A: 58% 32% 8%

B10
V15
K19
V20
Y23
H24
Y25
L28
T29
R34
K38
V41
R42
M43
E51
S52
R53
S54
C55
R56
I57
K63
R64
C65
C68
R69
F70
Q71
K72
C73
M78
V83
R87
M88
R89
G90
G91
R92
F95
M98
Y99
K100
R101
A104

L105
K106
Q107
Q108
K109
K110
A111

4.2.3 Score per residue for model 3

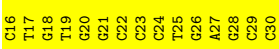
- Molecule 1: GGCTCAGGGCCACAG

Chain B: 33% 67%

G1
G2
C3
T4
C5
A6
G7
G8
G9
A12
C13
A14
G15


- Molecule 2: CTGTGGCCCTGAGCC

Chain C:  100%

 C16
T17
G18
T19
G20
G21
C22
C23
C24
T25
G26
A27
G28
C29
C30

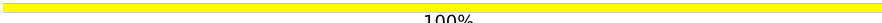
- Molecule 3: Steroidogenic factor 1

Chain A:  71% 21% 8%

 D10
V20
R24
L27
L28
T29
K34
F37
V41
Q42
M43
M44
K59
C65
C68
L74
L80
V83
D86
R87
M88
R89
R92
D102
R103
A104
L105
K106
Q107
Q108
K109
K110
A111


4.2.4 Score per residue for model 4

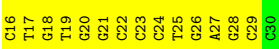
- Molecule 1: GGCTCAGGGCCACAG

Chain B:  100%

 G1
G2
C3
T4
C5
A6
G7
G8
G9
C10
C11
A12
C13
A14
G15

- Molecule 2: CTGTGGCCCTGAGCC

Chain C:  7% 93%

 C16
T17
G18
T19
G20
G21
C22
C23
C24
T25
G26
A27
G28
C29
C30


- Molecule 3: Steroidogenic factor 1

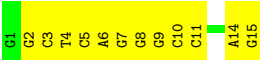
Chain A:  62% 26% 8%

 D10
E11
V15
Y23
H24
L28
T29
K34
G35
F36
F37
K38
R39
T40
V41
M42
M43
C49
Q53
R64
C65
P66
F67
C68
K72
L80
V83
R84
R87
R88
R89
G90
G91
R92
R93
Y99
R103
A104
L105
K106
Q107
Q108
K109
K110
A111

4.2.5 Score per residue for model 5

- Molecule 1: GGCTCAGGGCCACAG

Chain B:  20% 80%

 G1
G2
C3
T4
C5
A6
G7
G8
G9
C10
C11
A14
G15

- Molecule 2: CTGTGGCCCTGAGCC

Chain C:  7% 93%

C16
T17
G18
T19
G20
G21
C22
C23
C24
T25
T26
A27
G28
C29
C30

- Molecule 3: Steroidogenic factor 1

Chain A:  70% 23% 8%

D10
E11
D18
T4
K19
V20
H24
Y25
G26
L27
L28
T29
S32
K38
V41
T50
R62
K63
R64
C65
P66
R69
F70
Q71
V83
R87
M88
R89
G90
G91
R92
A104
L105
K106
Q107
Q108
K109
K110
A111

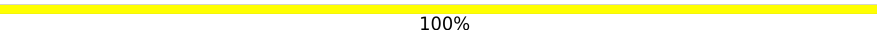
4.2.6 Score per residue for model 6

- Molecule 1: GGCTCAGGGCCACAG

Chain B:  100%

G1
G2
C3
T4
C5
A6
G7
G8
G9
C10
C11
A12
C13
A14
G15

- Molecule 2: CTGTGGCCCTGAGCC

Chain C:  100%

C16
T17
G18
T19
G20
G21
C22
C23
C24
T25
T26
A27
G28
C29
C30

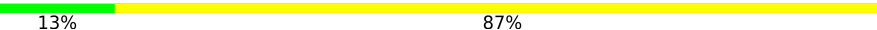
- Molecule 3: Steroidogenic factor 1

Chain A:  69% 22% 8%

D10
P14
V15
C16
H24
T29
C30
E31
K34
K38
S52
I57
R62
K63
C68
R69
F70
C73
L74
T75
V76
G77
M78
R87
M88
R89
G90
G91
R92
A104
L105
K106
Q107
Q108
K109
K110
A111

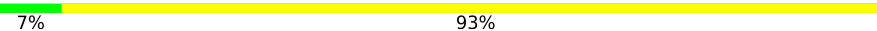
4.2.7 Score per residue for model 7

- Molecule 1: GGCTCAGGGCCACAG

Chain B:  13% 87%

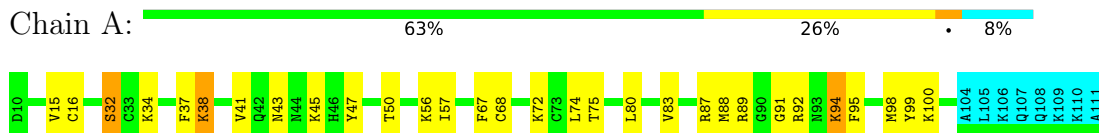
G1
G2
C3
T4
C5
A6
G7
G8
G9
C10
C11
A12
C13
A14
G15

- Molecule 2: CTGTGGCCCTGAGCC

Chain C:  7% 93%

C16
T17
G18
T19
G20
G21
C22
C23
C24
T25
T26
A27
G28
C29
C30

- Molecule 3: Steroidogenic factor 1



4.2.8 Score per residue for model 8

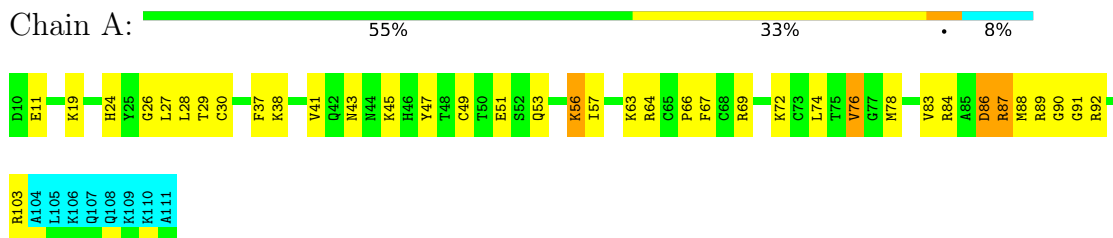
- Molecule 1: GGCTCAGGGCCACAG



- Molecule 2: CTGTGGCCCTGAGCC



- Molecule 3: Steroidogenic factor 1



4.2.9 Score per residue for model 9

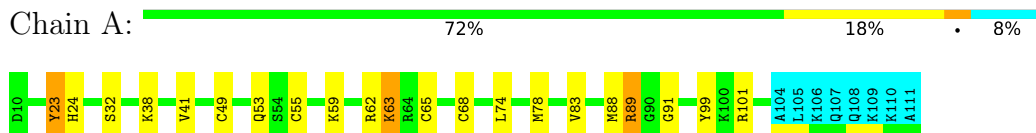
- Molecule 1: GGCTCAGGGCCACAG



- Molecule 2: CTGTGGCCCTGAGCC



- Molecule 3: Steroidogenic factor 1



4.2.10 Score per residue for model 10

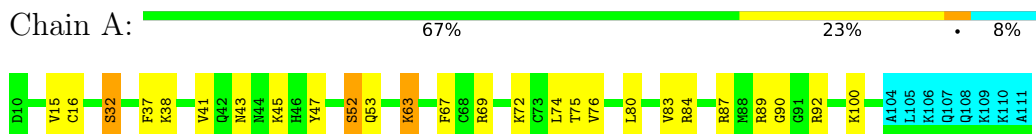
- Molecule 1: GGCTCAGGGCCACAG



- Molecule 2: CTGTGGCCCTGAGCC

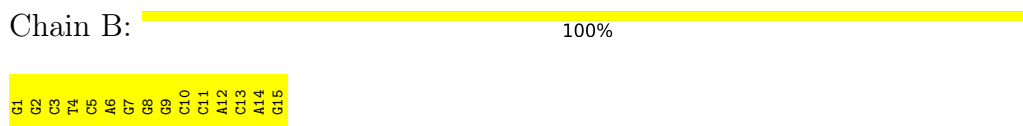


- Molecule 3: Steroidogenic factor 1



4.2.11 Score per residue for model 11

- Molecule 1: GGCTCAGGGCCACAG

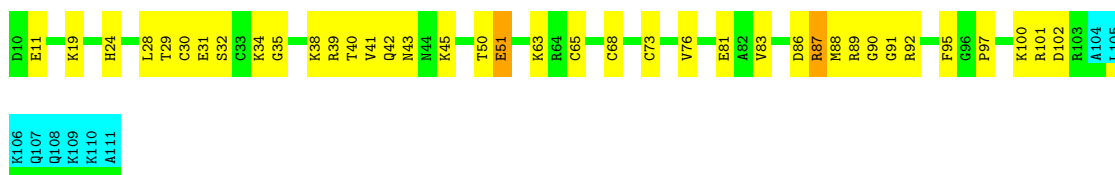


- Molecule 2: CTGTGGCCCTGAGCC



- Molecule 3: Steroidogenic factor 1





K106
Q107
Q108
K109
K110
A111

4.2.12 Score per residue for model 12

- Molecule 1: GGCTCAGGGCCACAG

Chain B: 7% 93%

G1
G2
C3
T4
C5
A6
G7
G8
G9
C10
C11
A12
C13
A14
G15

- Molecule 2: CTGTGGCCCTGAGCC

Chain C: 100%

C16
T17
G18
T19
G20
G21
C22
C23
C24
T25
G26
A27
G28
C29
C30

- Molecule 3: Steroidogenic factor 1

Chain A: 63% 26% 8%

D10
H24
Y25
T29
C30
E31
K34
T40
V41
Q42
N43
N44
K45
R46
V47
T48
C49
T50
E51
S52
Q53
I57
K63
R64
C65
P66
F67
C68
K72
T75
V83
R87
M88
R89
G90
G91
R92
R93
K94
R101
D102
R103
A104
L105
K106
Q107
Q108
K109
K110

A111

4.2.13 Score per residue for model 13

- Molecule 1: GGCTCAGGGCCACAG

Chain B: 100%

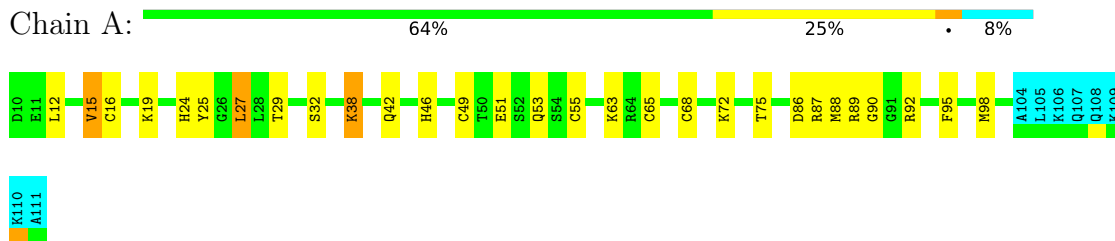
G1
G2
C3
T4
C5
A6
G7
G8
G9
C10
C11
A12
C13
A14
G15

- Molecule 2: CTGTGGCCCTGAGCC

Chain C: 7% 93%

C16
T17
G18
T19
G20
C21
C22
C23
C24
T25
G26
A27
G28
C29
C30

- Molecule 3: Steroidogenic factor 1



4.2.14 Score per residue for model 14

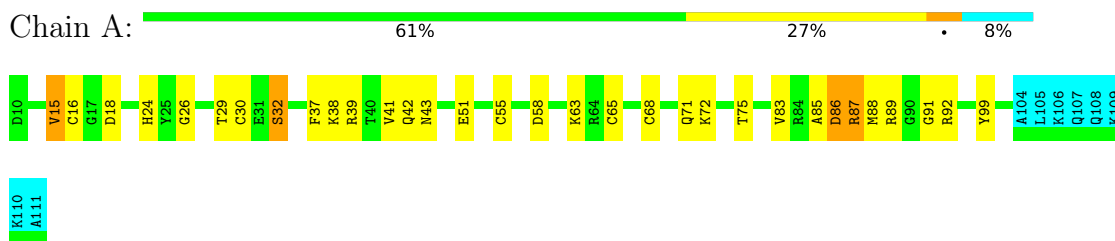
- Molecule 1: GGCTCAGGGCCACAG



- Molecule 2: CTGTGGCCCTGAGCC



- Molecule 3: Steroidogenic factor 1



4.2.15 Score per residue for model 15

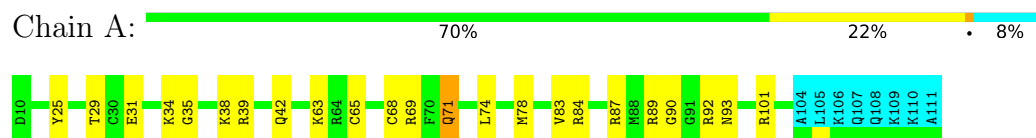
- Molecule 1: GGCTCAGGGCCACAG



- Molecule 2: CTGTGGCCCTGAGCC



- Molecule 3: Steroidogenic factor 1

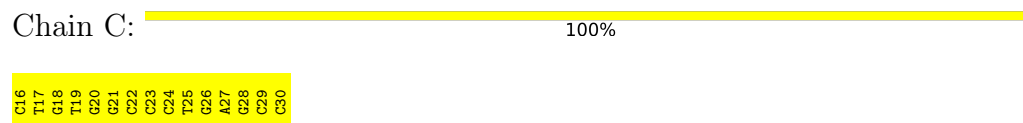


4.2.16 Score per residue for model 16

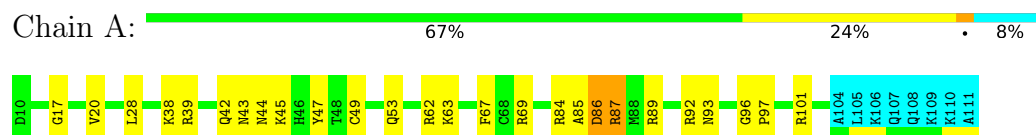
- Molecule 1: GGCTCAGGGCCACAG



- Molecule 2: CTGTGGCCCTGAGCC



- Molecule 3: Steroidogenic factor 1



5 Refinement protocol and experimental data overview

The models were refined using the following method: *Simulated annealing and cartesian molecular dynamics*.

Of the 200 calculated structures, 16 were deposited, based on the following criterion: *lowest restraint energies, restraint violations, and RMS deviations from ideal covalent geometry*.

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

Software name	Classification	Version
ARIA	refinement	1.2
CNS	refinement	1.1

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

There are no covalent bond-length or bond-angle outliers.

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

There are no planarity outliers.

6.2 Too-close contacts i

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	B	307	168	168	25±5
2	C	302	170	170	29±5
3	A	760	764	753	30±6
All	All	21936	17632	17456	1054

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 27.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:C:18:DG:H1'	2:C:19:DT:H5'	1.10	1.23	7	6
2:C:27:DA:H4'	3:A:91:GLY:H	0.97	1.18	6	3
2:C:20:DG:H1'	2:C:21:DG:H5'	0.96	1.34	9	9
1:B:3:DC:H1'	1:B:4:DT:H5'	0.93	1.36	1	2
2:C:19:DT:H3'	3:A:69:ARG:HH12	0.93	1.24	15	4
2:C:28:DG:H5''	3:A:92:ARG:HB2	0.92	1.42	5	2
2:C:27:DA:H4'	3:A:91:GLY:HA2	0.89	1.44	7	3
1:B:9:DG:H5''	3:A:87:ARG:HD3	0.87	1.42	16	6
2:C:29:DC:H5''	3:A:100:LYS:HE3	0.87	1.43	10	1
2:C:25:DT:H2''	2:C:26:DG:C8	0.86	2.04	6	5

Continued on next page...

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:C:18:DG:H1'	2:C:19:DT:C5'	0.86	2.01	7	4
2:C:22:DC:H1'	2:C:23:DC:H5'	0.86	1.46	9	8
2:C:29:DC:H2''	2:C:30:DC:C5	0.85	2.05	15	8
2:C:27:DA:H1'	2:C:28:DG:H5'	0.85	1.48	16	8
2:C:27:DA:H5''	3:A:91:GLY:HA2	0.85	1.47	12	1
1:B:4:DT:H1'	1:B:5:DC:H5'	0.85	1.48	13	2
2:C:28:DG:H2''	2:C:29:DC:C6	0.85	2.06	5	10
2:C:21:DG:H1'	2:C:22:DC:H5'	0.84	1.47	6	6
1:B:6:DA:H1'	1:B:7:DG:H5'	0.83	1.46	8	2
2:C:26:DG:H1'	2:C:27:DA:H5'	0.83	1.50	4	4
1:B:3:DC:H2''	1:B:4:DT:H71	0.82	1.48	11	1
2:C:25:DT:H1'	2:C:26:DG:H5'	0.82	1.51	12	1
2:C:20:DG:H2'	3:A:32:SER:HB3	0.81	1.50	10	1
1:B:7:DG:H2''	1:B:8:DG:C8	0.81	2.11	15	3
2:C:26:DG:H2''	2:C:27:DA:C8	0.81	2.11	3	7
2:C:23:DC:H2''	2:C:24:DC:C5	0.80	2.11	8	5
2:C:17:DT:H2''	2:C:18:DG:C8	0.80	2.12	8	2
1:B:8:DG:H2''	1:B:9:DG:OP2	0.80	1.76	14	11
1:B:2:DG:H2''	1:B:3:DC:C5	0.79	2.13	12	7
3:A:40:THR:HA	3:A:45:LYS:HE2	0.79	1.54	11	1
3:A:72:LYS:HA	3:A:75:THR:HB	0.78	1.55	7	3
1:B:8:DG:H3'	3:A:42:GLN:HE21	0.78	1.37	15	1
1:B:13:DC:H2''	1:B:14:DA:C8	0.78	2.14	11	2
2:C:26:DG:H5''	3:A:89:ARG:HA	0.77	1.56	12	1
1:B:4:DT:H2''	1:B:5:DC:C5	0.77	2.14	3	3
1:B:3:DC:H1'	1:B:4:DT:C5'	0.77	2.09	1	1
2:C:16:DC:H2''	2:C:17:DT:OP2	0.76	1.80	7	5
1:B:8:DG:H5''	3:A:84:ARG:HB3	0.76	1.56	8	3
1:B:13:DC:H1'	1:B:14:DA:H5'	0.76	1.57	15	2
2:C:19:DT:H3'	3:A:69:ARG:NH1	0.75	1.96	6	3
2:C:27:DA:C5'	3:A:91:GLY:HA2	0.75	2.10	12	1
1:B:1:DG:H2''	1:B:2:DG:C8	0.75	2.16	15	4
2:C:20:DG:H3'	3:A:32:SER:HB3	0.75	1.58	11	1
2:C:24:DC:H1'	2:C:25:DT:H5'	0.75	1.57	15	5
2:C:28:DG:H4'	3:A:92:ARG:HD2	0.74	1.58	5	2
1:B:3:DC:H2''	1:B:4:DT:H72	0.74	1.57	2	3
1:B:10:DC:H1'	1:B:11:DC:H5'	0.74	1.59	13	3
2:C:19:DT:H4'	3:A:63:LYS:HE3	0.74	1.59	1	1
1:B:14:DA:H2''	1:B:15:DG:C8	0.74	2.16	13	4
1:B:5:DC:H2''	1:B:6:DA:C8	0.74	2.17	6	2
1:B:9:DG:H1'	1:B:10:DC:H5'	0.74	1.59	14	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:C:25:DT:C1'	2:C:26:DG:H5'	0.74	2.11	12	1
1:B:9:DG:H5''	3:A:88:MET:H	0.73	1.41	12	1
2:C:24:DC:H2''	2:C:25:DT:C6	0.73	2.18	3	2
2:C:19:DT:H5''	3:A:63:LYS:HA	0.73	1.57	6	1
1:B:12:DA:H2''	1:B:13:DC:C6	0.73	2.19	1	3
1:B:9:DG:H5''	3:A:87:ARG:HD2	0.73	1.61	10	6
2:C:27:DA:H4'	3:A:91:GLY:N	0.72	1.98	2	4
2:C:18:DG:H2''	2:C:19:DT:H71	0.72	1.61	11	1
2:C:22:DC:H1'	2:C:23:DC:C5'	0.72	2.13	9	2
2:C:20:DG:H2'	3:A:32:SER:HA	0.72	1.61	11	2
2:C:18:DG:C1'	2:C:19:DT:H5'	0.72	2.14	14	1
1:B:6:DA:H2''	1:B:7:DG:OP2	0.72	1.83	1	7
1:B:10:DC:H2''	1:B:11:DC:C6	0.72	2.19	2	2
2:C:16:DC:H2''	2:C:17:DT:C5	0.71	2.20	3	3
2:C:27:DA:C5'	3:A:90:GLY:HA2	0.71	2.15	8	2
1:B:4:DT:H2''	1:B:5:DC:C6	0.71	2.20	5	5
3:A:27:LEU:HD22	3:A:76:VAL:HG13	0.70	1.62	8	1
2:C:18:DG:H2''	2:C:19:DT:OP2	0.70	1.85	5	7
1:B:3:DC:H2''	1:B:4:DT:C7	0.70	2.17	11	4
2:C:16:DC:H2''	2:C:17:DT:H71	0.70	1.63	5	3
1:B:7:DG:H2''	1:B:8:DG:OP2	0.69	1.87	1	7
2:C:18:DG:C2'	2:C:19:DT:H72	0.69	2.18	1	3
2:C:19:DT:H4'	3:A:63:LYS:HE2	0.69	1.64	11	2
2:C:28:DG:H5''	3:A:92:ARG:O	0.69	1.88	15	5
3:A:72:LYS:HA	3:A:72:LYS:HE3	0.69	1.64	2	1
1:B:9:DG:C8	3:A:38:LYS:HE2	0.69	2.22	8	2
2:C:27:DA:H4'	3:A:91:GLY:CA	0.68	2.16	7	3
3:A:16:CYS:HB2	3:A:62:ARG:HD2	0.68	1.65	6	1
2:C:17:DT:H2''	2:C:18:DG:H8	0.68	1.46	8	2
1:B:14:DA:H1'	1:B:15:DG:H5'	0.68	1.65	9	5
1:B:9:DG:H2''	1:B:10:DC:C5	0.67	2.24	10	2
1:B:12:DA:H2''	1:B:13:DC:OP2	0.67	1.90	10	4
1:B:11:DC:H1'	1:B:12:DA:H5'	0.67	1.66	4	2
3:A:94:LYS:HA	3:A:94:LYS:HE3	0.67	1.66	7	1
3:A:49:CYS:HB3	3:A:53:GLN:HG2	0.67	1.65	16	2
1:B:8:DG:H2''	3:A:38:LYS:HZ2	0.67	1.48	1	1
2:C:28:DG:H5''	3:A:92:ARG:HB3	0.66	1.67	11	2
1:B:6:DA:H5''	3:A:99:TYR:CG	0.66	2.25	7	2
1:B:3:DC:H2''	1:B:4:DT:C6	0.66	2.25	4	2
2:C:16:DC:HO5'	2:C:16:DC:H6	0.66	1.33	12	2
2:C:19:DT:H5''	3:A:63:LYS:HE2	0.65	1.68	14	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:C:20:DG:H1'	2:C:21:DG:C5'	0.65	2.16	9	4
3:A:41:VAL:HG21	3:A:83:VAL:HG21	0.65	1.68	11	5
2:C:26:DG:H5''	3:A:89:ARG:CA	0.65	2.20	12	1
1:B:7:DG:OP2	3:A:24:HIS:HA	0.65	1.92	8	5
1:B:8:DG:H2''	3:A:38:LYS:NZ	0.65	2.06	1	2
1:B:8:DG:H1'	1:B:9:DG:H5'	0.64	1.68	14	10
3:A:29:THR:HG21	3:A:78:MET:SD	0.64	2.33	6	2
2:C:28:DG:H4'	3:A:92:ARG:HB2	0.64	1.70	3	1
1:B:8:DG:O4'	3:A:89:ARG:HG2	0.64	1.93	10	5
1:B:7:DG:H3'	3:A:25:TYR:CE1	0.64	2.27	13	1
1:B:8:DG:H5''	3:A:88:MET:O	0.64	1.93	3	4
2:C:19:DT:H71	3:A:39:ARG:CZ	0.63	2.23	1	1
1:B:2:DG:H2''	1:B:3:DC:C6	0.63	2.28	15	7
1:B:1:DG:H1'	1:B:2:DG:H5'	0.63	1.70	10	1
2:C:29:DC:H2''	2:C:30:DC:C6	0.63	2.27	8	4
2:C:25:DT:H4'	3:A:87:ARG:NH2	0.63	2.09	12	1
2:C:19:DT:H5''	3:A:63:LYS:HE3	0.63	1.71	13	2
1:B:9:DG:H4'	3:A:89:ARG:HG2	0.63	1.70	4	1
2:C:25:DT:H1'	3:A:89:ARG:O	0.63	1.91	4	1
1:B:10:DC:H2''	1:B:11:DC:OP2	0.63	1.94	5	6
2:C:20:DG:H2'	3:A:32:SER:HB2	0.63	1.70	5	2
2:C:20:DG:H3'	3:A:32:SER:OG	0.63	1.94	14	2
3:A:24:HIS:HB2	3:A:29:THR:OG1	0.63	1.94	13	9
2:C:16:DC:H1'	2:C:17:DT:H5'	0.62	1.70	9	3
2:C:17:DT:H1'	2:C:18:DG:H5'	0.62	1.71	10	1
2:C:24:DC:H2''	2:C:25:DT:OP2	0.62	1.94	2	11
1:B:10:DC:H2''	1:B:11:DC:C5	0.62	2.29	2	2
2:C:27:DA:H1'	2:C:28:DG:C5'	0.62	2.23	16	2
1:B:1:DG:H2''	1:B:2:DG:H8	0.62	1.54	1	3
2:C:26:DG:H1'	2:C:27:DA:C5'	0.62	2.24	13	3
1:B:8:DG:H5''	3:A:84:ARG:HB2	0.62	1.71	15	1
2:C:18:DG:H2''	2:C:19:DT:C7	0.62	2.25	1	3
2:C:28:DG:H2''	2:C:29:DC:OP2	0.62	1.93	13	2
2:C:20:DG:C1'	2:C:21:DG:H5'	0.62	2.20	9	1
1:B:9:DG:C5'	3:A:87:ARG:HD2	0.62	2.24	12	1
1:B:14:DA:H2''	1:B:15:DG:OP2	0.61	1.95	11	7
2:C:25:DT:H1'	2:C:26:DG:C5'	0.61	2.25	12	1
3:A:71:GLN:HE21	3:A:71:GLN:HA	0.61	1.53	15	1
1:B:15:DG:H4'	3:A:63:LYS:HE3	0.61	1.70	6	1
1:B:8:DG:H1'	1:B:9:DG:C5'	0.61	2.25	14	3
2:C:25:DT:H1'	2:C:26:DG:O4'	0.61	1.96	2	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:C:24:DC:H1'	2:C:25:DT:C5'	0.61	2.25	15	3
1:B:7:DG:H21	3:A:89:ARG:HD3	0.61	1.56	15	5
2:C:28:DG:H2''	2:C:29:DC:C5	0.61	2.31	10	5
2:C:27:DA:H2''	2:C:28:DG:C8	0.61	2.31	4	2
2:C:23:DC:H2''	2:C:24:DC:C6	0.61	2.29	8	5
2:C:27:DA:H5''	3:A:90:GLY:HA2	0.61	1.71	8	1
1:B:8:DG:O4'	3:A:88:MET:HB2	0.60	1.96	12	1
2:C:19:DT:C4'	3:A:63:LYS:HE3	0.60	2.26	1	1
2:C:18:DG:H2''	2:C:19:DT:C5	0.60	2.32	4	1
2:C:19:DT:H5''	3:A:63:LYS:HB2	0.60	1.73	10	1
2:C:26:DG:H2''	2:C:27:DA:OP2	0.60	1.95	4	5
3:A:34:LYS:O	3:A:38:LYS:HG3	0.60	1.95	11	2
2:C:20:DG:H2''	2:C:21:DG:C8	0.60	2.32	7	1
1:B:9:DG:N7	3:A:38:LYS:HE3	0.60	2.12	15	1
2:C:19:DT:C5'	3:A:63:LYS:HG2	0.60	2.26	5	2
1:B:3:DC:C2'	1:B:4:DT:H71	0.60	2.27	11	2
1:B:8:DG:C5'	3:A:89:ARG:HA	0.60	2.26	11	1
2:C:16:DC:C2'	2:C:17:DT:H71	0.60	2.26	5	3
2:C:27:DA:H4'	3:A:92:ARG:HG3	0.60	1.74	12	1
2:C:24:DC:H2'	2:C:25:DT:H72	0.59	1.74	3	1
1:B:8:DG:H5'	3:A:88:MET:HB2	0.59	1.74	9	1
3:A:68:CYS:HA	3:A:71:GLN:HG3	0.59	1.74	2	1
2:C:16:DC:H2''	2:C:17:DT:C6	0.59	2.31	3	2
1:B:1:DG:H2''	1:B:2:DG:OP2	0.59	1.97	4	2
2:C:29:DC:H2''	2:C:30:DC:OP2	0.59	1.96	10	2
2:C:27:DA:H1'	2:C:28:DG:O4'	0.59	1.98	5	1
2:C:20:DG:OP2	3:A:32:SER:HB3	0.59	1.97	14	1
2:C:18:DG:H2''	2:C:19:DT:C6	0.59	2.33	2	2
1:B:6:DA:H5''	3:A:99:TYR:CD2	0.59	2.32	14	1
1:B:8:DG:H2'	3:A:38:LYS:HG2	0.59	1.74	15	1
2:C:29:DC:H5''	3:A:100:LYS:HD3	0.59	1.74	1	1
1:B:7:DG:H1'	1:B:8:DG:H5'	0.59	1.75	13	2
3:A:47:TYR:HB2	3:A:67:PHE:HB2	0.59	1.74	12	5
2:C:23:DC:H1'	2:C:24:DC:H5'	0.59	1.74	13	2
2:C:28:DG:H4'	3:A:92:ARG:CB	0.58	2.28	3	1
3:A:65:CYS:HB3	3:A:68:CYS:SG	0.58	2.37	14	10
2:C:28:DG:C5'	3:A:92:ARG:HB3	0.58	2.28	11	2
1:B:6:DA:H5''	3:A:103:ARG:NH1	0.58	2.12	12	1
2:C:28:DG:H4'	3:A:92:ARG:HB3	0.58	1.75	6	2
3:A:42:GLN:HG2	3:A:85:ALA:HA	0.58	1.75	14	2
1:B:13:DC:H2''	1:B:14:DA:OP2	0.58	1.99	12	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:C:28:DG:H4'	3:A:92:ARG:CD	0.58	2.28	3	1
1:B:9:DG:H3'	3:A:87:ARG:NH1	0.58	2.14	5	1
1:B:6:DA:H1'	1:B:7:DG:C5'	0.58	2.27	8	2
3:A:72:LYS:HA	3:A:75:THR:CB	0.58	2.27	7	3
2:C:27:DA:C1'	2:C:28:DG:H5'	0.58	2.28	11	4
1:B:4:DT:H2''	1:B:5:DC:OP2	0.57	1.99	16	3
1:B:11:DC:H2''	1:B:12:DA:OP2	0.57	1.98	8	1
3:A:51:GLU:HB2	3:A:55:CYS:SG	0.57	2.39	14	2
2:C:18:DG:C2'	2:C:19:DT:H71	0.57	2.30	11	1
1:B:2:DG:H1'	1:B:3:DC:H5'	0.57	1.75	13	2
3:A:72:LYS:CA	3:A:75:THR:HB	0.57	2.29	7	2
1:B:7:DG:C5'	3:A:91:GLY:HA2	0.57	2.30	8	1
2:C:27:DA:C2'	2:C:28:DG:C8	0.57	2.87	4	1
2:C:28:DG:H4'	3:A:92:ARG:NE	0.57	2.15	6	1
3:A:31:GLU:HA	3:A:34:LYS:HG2	0.57	1.76	6	1
1:B:9:DG:C4'	3:A:87:ARG:HD2	0.57	2.30	12	1
1:B:11:DC:H2''	1:B:12:DA:C8	0.56	2.35	1	4
2:C:19:DT:H4'	3:A:63:LYS:HG2	0.56	1.76	5	1
1:B:6:DA:H5''	3:A:99:TYR:HD2	0.56	1.60	14	1
1:B:12:DA:H2''	1:B:13:DC:C5	0.56	2.36	2	2
1:B:8:DG:O4'	3:A:89:ARG:HG3	0.56	2.00	6	1
1:B:2:DG:H2''	1:B:3:DC:OP2	0.56	2.00	14	2
1:B:8:DG:C3'	3:A:42:GLN:HE21	0.56	2.12	15	1
2:C:21:DG:H1'	2:C:22:DC:C5'	0.56	2.26	6	4
1:B:7:DG:H4'	3:A:91:GLY:O	0.56	2.01	4	1
2:C:25:DT:H2''	2:C:26:DG:H8	0.56	1.60	5	3
2:C:28:DG:C4'	3:A:92:ARG:HD2	0.56	2.30	3	2
1:B:7:DG:N2	3:A:89:ARG:HD3	0.55	2.15	16	3
3:A:25:TYR:HE1	3:A:34:LYS:HG3	0.55	1.60	2	1
1:B:5:DC:H1'	3:A:92:ARG:NH1	0.55	2.16	15	1
2:C:21:DG:H2''	2:C:22:DC:C5	0.55	2.36	1	2
2:C:20:DG:C2'	3:A:32:SER:HB2	0.55	2.31	9	2
2:C:27:DA:C3'	3:A:92:ARG:H	0.55	2.13	12	1
1:B:9:DG:H2''	1:B:10:DC:C6	0.55	2.37	11	3
2:C:27:DA:H2''	2:C:28:DG:OP2	0.55	2.00	5	2
1:B:8:DG:C1'	1:B:9:DG:H5'	0.55	2.32	11	3
2:C:21:DG:H2''	2:C:22:DC:C6	0.55	2.36	11	3
1:B:8:DG:H1'	1:B:9:DG:O4'	0.55	2.01	6	1
3:A:41:VAL:HG21	3:A:83:VAL:HG11	0.55	1.78	7	4
1:B:6:DA:H5''	3:A:99:TYR:CB	0.55	2.32	2	3
1:B:3:DC:C2'	1:B:4:DT:H72	0.55	2.32	6	5

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:C:20:DG:H2''	2:C:21:DG:OP2	0.54	2.01	9	3
2:C:28:DG:H4'	3:A:92:ARG:HE	0.54	1.62	6	2
3:A:63:LYS:HA	3:A:69:ARG:HH21	0.54	1.61	10	1
3:A:74:LEU:HD21	3:A:80:LEU:HD13	0.54	1.79	10	1
2:C:28:DG:H2''	2:C:29:DC:H6	0.54	1.61	1	1
2:C:16:DC:H6	2:C:16:DC:O5'	0.54	1.85	12	1
2:C:22:DC:H2''	2:C:23:DC:C6	0.54	2.37	13	2
2:C:19:DT:C4'	3:A:63:LYS:HG2	0.54	2.33	5	1
2:C:20:DG:H3'	3:A:32:SER:HB2	0.54	1.78	1	1
3:A:25:TYR:CE1	3:A:34:LYS:HG3	0.54	2.37	15	1
1:B:8:DG:OP1	3:A:84:ARG:HG2	0.54	2.02	15	1
2:C:27:DA:H2''	2:C:28:DG:O5'	0.54	2.02	3	2
2:C:26:DG:C1'	2:C:27:DA:H5'	0.54	2.28	4	1
1:B:9:DG:H4'	3:A:87:ARG:NH1	0.54	2.18	12	2
3:A:41:VAL:HG11	3:A:83:VAL:CG1	0.54	2.33	2	2
1:B:7:DG:O4'	3:A:91:GLY:HA2	0.54	2.03	14	1
2:C:23:DC:H6	2:C:23:DC:O5'	0.54	1.86	16	2
3:A:82:ALA:HB2	3:A:95:PHE:HZ	0.54	1.63	1	1
3:A:57:ILE:HG13	3:A:69:ARG:HA	0.53	1.79	2	2
2:C:26:DG:H5''	3:A:88:MET:SD	0.53	2.42	4	1
1:B:9:DG:OP1	3:A:87:ARG:HA	0.53	2.02	8	2
3:A:30:CYS:SG	3:A:32:SER:HB3	0.53	2.44	1	1
3:A:79:ARG:NE	3:A:79:ARG:HA	0.53	2.18	1	1
2:C:18:DG:H2'	2:C:19:DT:H72	0.53	1.80	8	3
2:C:27:DA:H4'	3:A:92:ARG:N	0.53	2.18	4	2
3:A:74:LEU:HG	3:A:80:LEU:HD21	0.53	1.79	7	1
3:A:91:GLY:O	3:A:92:ARG:HD2	0.53	2.03	8	1
3:A:47:TYR:CB	3:A:67:PHE:HB2	0.53	2.33	12	1
2:C:21:DG:H2''	2:C:22:DC:OP2	0.53	2.02	8	2
2:C:19:DT:H1'	2:C:20:DG:H5'	0.53	1.80	12	1
3:A:95:PHE:O	3:A:98:MET:HG2	0.53	2.03	7	2
1:B:14:DA:C2	2:C:18:DG:C2	0.53	2.97	14	9
2:C:27:DA:H4'	3:A:92:ARG:O	0.53	2.04	4	1
1:B:8:DG:H2'	3:A:38:LYS:NZ	0.53	2.19	5	1
1:B:8:DG:H2'	3:A:38:LYS:HE3	0.53	1.78	10	1
2:C:27:DA:H5''	3:A:91:GLY:CA	0.53	2.30	12	1
3:A:18:ASP:HB2	3:A:30:CYS:SG	0.52	2.45	14	2
1:B:9:DG:C5'	3:A:88:MET:H	0.52	2.15	12	1
1:B:9:DG:C1'	1:B:10:DC:H5'	0.52	2.31	14	1
1:B:3:DC:C6	1:B:4:DT:H72	0.52	2.39	12	1
1:B:7:DG:H21	3:A:89:ARG:HB3	0.52	1.64	2	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:6:DA:H2''	1:B:7:DG:N7	0.52	2.18	13	1
3:A:81:GLU:HG3	3:A:95:PHE:CZ	0.52	2.38	11	1
1:B:8:DG:C8	3:A:38:LYS:NZ	0.52	2.78	5	1
1:B:5:DC:O2	3:A:92:ARG:HD2	0.52	2.05	13	1
3:A:49:CYS:HB3	3:A:53:GLN:HA	0.52	1.82	13	3
1:B:8:DG:H2'	3:A:38:LYS:HE2	0.52	1.81	6	1
3:A:53:GLN:HB3	3:A:55:CYS:SG	0.52	2.44	9	1
2:C:18:DG:H2''	2:C:19:DT:H72	0.52	1.82	1	2
1:B:10:DC:H1'	1:B:11:DC:C5'	0.52	2.34	13	2
3:A:23:TYR:OH	3:A:103:ARG:HD3	0.52	2.04	4	1
2:C:16:DC:H2''	2:C:17:DT:C7	0.52	2.34	2	4
3:A:37:PHE:O	3:A:41:VAL:HG22	0.51	2.06	14	5
1:B:4:DT:H2''	1:B:5:DC:H6	0.51	1.63	5	1
2:C:20:DG:H2'	3:A:32:SER:CB	0.51	2.35	9	3
3:A:81:GLU:HG3	3:A:95:PHE:HZ	0.51	1.65	11	1
1:B:14:DA:H2''	1:B:15:DG:N7	0.51	2.20	14	2
1:B:5:DC:H1'	1:B:6:DA:C8	0.51	2.40	16	1
1:B:8:DG:H3'	3:A:42:GLN:HE22	0.51	1.66	14	1
1:B:3:DC:H2'	1:B:4:DT:H72	0.51	1.81	15	1
1:B:3:DC:C1'	1:B:4:DT:H5'	0.51	2.25	1	1
1:B:11:DC:H2''	1:B:12:DA:O5'	0.51	2.06	4	1
2:C:28:DG:C5'	3:A:92:ARG:HB2	0.51	2.27	5	2
1:B:9:DG:H3'	3:A:87:ARG:HH11	0.51	1.66	5	1
1:B:8:DG:O4'	3:A:89:ARG:HA	0.51	2.06	5	2
3:A:59:LYS:HA	3:A:62:ARG:NE	0.51	2.20	9	1
1:B:6:DA:H5''	3:A:99:TYR:HB3	0.51	1.83	2	1
3:A:38:LYS:HA	3:A:41:VAL:HG22	0.51	1.82	9	1
2:C:19:DT:H3'	3:A:69:ARG:HH22	0.51	1.65	10	1
1:B:6:DA:H2''	1:B:7:DG:C8	0.51	2.41	13	1
1:B:9:DG:OP2	3:A:42:GLN:HG3	0.51	2.06	15	1
2:C:28:DG:H5''	3:A:92:ARG:CB	0.51	2.36	10	1
2:C:28:DG:H5''	3:A:92:ARG:CG	0.51	2.36	10	1
3:A:50:THR:HG22	3:A:51:GLU:HG3	0.51	1.81	11	2
1:B:8:DG:H5'	3:A:84:ARG:NH1	0.50	2.20	4	1
3:A:43:ASN:HB2	3:A:45:LYS:HG3	0.50	1.83	7	5
3:A:38:LYS:HG2	3:A:83:VAL:HG13	0.50	1.81	10	1
1:B:9:DG:H1'	1:B:10:DC:O4'	0.50	2.06	9	1
3:A:63:LYS:HA	3:A:69:ARG:NH2	0.50	2.20	10	1
2:C:19:DT:C5'	3:A:63:LYS:HE3	0.50	2.36	1	1
2:C:19:DT:C5'	3:A:63:LYS:HA	0.50	2.33	6	1
2:C:29:DC:C2'	2:C:30:DC:C5	0.50	2.94	8	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:A:72:LYS:HE3	3:A:72:LYS:CA	0.50	2.34	2	1
2:C:27:DA:C4'	3:A:92:ARG:H	0.50	2.20	12	1
1:B:8:DG:C4'	3:A:89:ARG:HA	0.50	2.37	1	2
2:C:29:DC:H4'	3:A:100:LYS:HD2	0.50	1.82	7	1
2:C:24:DC:C2'	2:C:25:DT:H71	0.50	2.37	12	1
3:A:74:LEU:HA	3:A:78:MET:O	0.50	2.06	9	3
1:B:7:DG:H3'	3:A:25:TYR:HE1	0.50	1.65	13	1
1:B:15:DG:H8	1:B:15:DG:O5'	0.50	1.89	6	2
1:B:8:DG:N7	3:A:34:LYS:HE2	0.50	2.22	12	1
2:C:28:DG:C2'	2:C:29:DC:C5	0.50	2.95	14	3
1:B:12:DA:C2	2:C:20:DG:C2	0.49	3.00	7	3
2:C:22:DC:H6	2:C:22:DC:O5'	0.49	1.90	14	2
1:B:5:DC:H2''	1:B:6:DA:OP2	0.49	2.06	11	2
2:C:29:DC:OP1	3:A:97:PRO:HG3	0.49	2.07	1	1
2:C:25:DT:H5'	3:A:89:ARG:NH1	0.49	2.22	16	2
1:B:2:DG:C2'	1:B:3:DC:C5	0.49	2.92	12	1
3:A:41:VAL:HG11	3:A:83:VAL:HG11	0.49	1.82	2	2
3:A:74:LEU:HD11	3:A:80:LEU:HG	0.49	1.83	3	1
2:C:27:DA:C4'	3:A:90:GLY:HA2	0.49	2.37	10	2
3:A:15:VAL:HG22	3:A:16:CYS:N	0.49	2.21	1	1
3:A:57:ILE:HD11	3:A:68:CYS:HB2	0.49	1.83	6	3
3:A:41:VAL:CG2	3:A:83:VAL:HG21	0.49	2.38	4	1
2:C:24:DC:C2'	2:C:25:DT:H72	0.49	2.37	7	1
2:C:23:DC:H2''	2:C:24:DC:OP2	0.49	2.07	16	7
1:B:7:DG:H2'	3:A:34:LYS:NZ	0.49	2.22	3	1
2:C:22:DC:C2	2:C:23:DC:C5	0.49	3.01	11	3
1:B:9:DG:H2''	1:B:10:DC:OP2	0.49	2.08	8	3
1:B:8:DG:H5'	3:A:88:MET:O	0.49	2.07	14	1
1:B:7:DG:H21	3:A:88:MET:HG2	0.49	1.68	12	1
2:C:28:DG:C2'	2:C:29:DC:C6	0.49	2.95	1	1
1:B:9:DG:OP1	3:A:87:ARG:HG2	0.49	2.08	7	1
1:B:7:DG:H4'	3:A:90:GLY:HA2	0.49	1.85	11	1
1:B:3:DC:H2''	1:B:4:DT:OP2	0.49	2.08	8	1
3:A:39:ARG:O	3:A:43:ASN:HB2	0.48	2.08	4	2
2:C:25:DT:H4'	3:A:87:ARG:HH22	0.48	1.68	12	1
2:C:18:DG:C2	2:C:19:DT:C2	0.48	3.01	8	3
3:A:15:VAL:HG13	3:A:16:CYS:H	0.48	1.68	14	4
2:C:22:DC:C1'	2:C:23:DC:H5'	0.48	2.36	14	3
1:B:8:DG:C5'	3:A:84:ARG:HB3	0.48	2.33	8	1
3:A:15:VAL:HG11	3:A:73:CYS:SG	0.48	2.48	6	1
3:A:56:LYS:N	3:A:56:LYS:HD3	0.48	2.24	8	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:9:DG:C4'	3:A:89:ARG:HG2	0.48	2.38	4	1
2:C:19:DT:H2''	2:C:20:DG:O5'	0.48	2.09	15	2
3:A:31:GLU:HA	3:A:34:LYS:HB3	0.48	1.86	11	3
1:B:7:DG:N2	3:A:89:ARG:HB3	0.48	2.24	13	1
2:C:19:DT:H2''	2:C:20:DG:C8	0.48	2.43	16	1
3:A:20:VAL:HG11	3:A:28:LEU:HB3	0.47	1.84	16	3
3:A:40:THR:HA	3:A:45:LYS:CE	0.47	2.35	11	1
2:C:21:DG:OP2	3:A:32:SER:HB2	0.47	2.09	13	1
1:B:11:DC:O5'	1:B:11:DC:H6	0.47	1.92	1	2
2:C:19:DT:H5''	3:A:63:LYS:HG2	0.47	1.86	2	1
2:C:23:DC:C2'	2:C:24:DC:C5	0.47	2.98	15	2
1:B:11:DC:C2'	1:B:12:DA:C8	0.47	2.98	16	2
3:A:82:ALA:HB2	3:A:95:PHE:CZ	0.47	2.43	1	1
1:B:9:DG:H5''	3:A:87:ARG:CD	0.47	2.38	13	3
3:A:86:ASP:O	3:A:87:ARG:HB2	0.47	2.10	1	3
2:C:25:DT:H2''	2:C:26:DG:N7	0.47	2.21	6	1
2:C:27:DA:H4'	3:A:92:ARG:H	0.47	1.70	4	2
3:A:27:LEU:CD2	3:A:76:VAL:HG13	0.47	2.38	8	1
3:A:25:TYR:OH	3:A:38:LYS:HG3	0.47	2.10	2	1
2:C:27:DA:H8	2:C:27:DA:O5'	0.47	1.92	4	1
2:C:16:DC:C2'	2:C:17:DT:H72	0.47	2.39	12	3
2:C:25:DT:H2''	2:C:26:DG:O5'	0.47	2.08	12	1
3:A:68:CYS:O	3:A:72:LYS:HB2	0.47	2.09	2	1
3:A:49:CYS:SG	3:A:53:GLN:HA	0.47	2.50	8	1
2:C:19:DT:O3'	3:A:63:LYS:HE3	0.47	2.09	12	1
2:C:25:DT:H4'	3:A:89:ARG:HB3	0.47	1.87	9	1
1:B:8:DG:C2	1:B:9:DG:C4	0.47	3.03	14	5
2:C:28:DG:OP1	3:A:93:ASN:HB3	0.47	2.10	16	1
3:A:35:GLY:HA2	3:A:38:LYS:NZ	0.46	2.25	11	1
2:C:18:DG:C2'	2:C:19:DT:OP2	0.46	2.62	5	1
1:B:9:DG:H5''	3:A:88:MET:N	0.46	2.21	12	1
3:A:59:LYS:HB2	3:A:59:LYS:NZ	0.46	2.25	3	1
1:B:7:DG:P	3:A:24:HIS:HA	0.46	2.51	5	2
2:C:19:DT:C3'	3:A:69:ARG:HH12	0.46	2.14	6	1
1:B:8:DG:O5'	1:B:8:DG:C8	0.46	2.69	6	1
2:C:19:DT:H3'	3:A:69:ARG:NH2	0.46	2.25	10	1
1:B:10:DC:C2	1:B:11:DC:C5	0.46	3.03	16	1
3:A:96:GLY:N	3:A:97:PRO:HD2	0.46	2.25	16	1
2:C:29:DC:C2	2:C:30:DC:C5	0.46	3.04	7	2
3:A:15:VAL:HG13	3:A:72:LYS:HB3	0.46	1.88	4	2
1:B:8:DG:O5'	1:B:8:DG:H8	0.46	1.93	6	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:9:DG:N7	3:A:38:LYS:NZ	0.46	2.63	9	2
1:B:9:DG:H2''	1:B:10:DC:O5'	0.46	2.11	14	2
1:B:8:DG:C5'	3:A:84:ARG:HB2	0.46	2.38	15	1
2:C:16:DC:C6	2:C:17:DT:H72	0.46	2.46	1	2
2:C:18:DG:C2'	2:C:19:DT:C7	0.46	2.93	8	2
1:B:5:DC:H1'	3:A:92:ARG:HD2	0.46	1.87	14	1
1:B:8:DG:H1'	1:B:9:DG:O5'	0.46	2.11	16	2
3:A:14:PRO:HB2	3:A:76:VAL:HG11	0.46	1.87	6	1
2:C:25:DT:H4'	3:A:89:ARG:NH2	0.46	2.25	14	1
2:C:19:DT:H71	3:A:39:ARG:NH1	0.46	2.26	16	1
2:C:19:DT:C6	2:C:19:DT:O5'	0.45	2.69	11	1
3:A:84:ARG:HG2	3:A:88:MET:O	0.45	2.11	1	2
2:C:27:DA:H5'	3:A:91:GLY:HA3	0.45	1.87	4	1
2:C:27:DA:H4'	3:A:92:ARG:CG	0.45	2.40	12	1
3:A:68:CYS:HA	3:A:71:GLN:CG	0.45	2.40	2	1
1:B:4:DT:C2'	1:B:5:DC:C5	0.45	2.96	3	1
2:C:19:DT:O5'	2:C:19:DT:H6	0.45	1.93	11	2
1:B:9:DG:C2'	1:B:10:DC:C6	0.45	2.99	9	1
3:A:38:LYS:O	3:A:42:GLN:HB2	0.45	2.11	13	1
3:A:18:ASP:HB2	3:A:62:ARG:NH1	0.45	2.26	5	1
1:B:8:DG:H2'	3:A:38:LYS:HD2	0.45	1.88	16	2
3:A:23:TYR:HB3	3:A:99:TYR:OH	0.45	2.12	9	1
2:C:19:DT:H72	3:A:39:ARG:HG3	0.45	1.87	11	1
1:B:6:DA:N3	3:A:91:GLY:HA3	0.45	2.26	14	1
1:B:8:DG:H3'	3:A:42:GLN:NE2	0.45	2.26	14	1
2:C:21:DG:C2	2:C:22:DC:C2	0.45	3.04	7	1
2:C:19:DT:H5''	3:A:63:LYS:CB	0.45	2.42	9	1
3:A:38:LYS:O	3:A:42:GLN:HG3	0.45	2.11	11	1
3:A:11:GLU:HG3	3:A:28:LEU:HD22	0.45	1.88	4	1
2:C:19:DT:H5''	3:A:63:LYS:CA	0.45	2.35	6	1
2:C:28:DG:H5''	3:A:92:ARG:HG3	0.45	1.89	10	1
2:C:16:DC:C6	2:C:16:DC:O5'	0.45	2.70	10	2
1:B:7:DG:H21	3:A:89:ARG:HD2	0.45	1.71	14	1
3:A:41:VAL:HB	3:A:83:VAL:HG11	0.45	1.88	1	2
3:A:15:VAL:HB	3:A:72:LYS:HG3	0.44	1.89	1	1
3:A:80:LEU:O	3:A:83:VAL:HG22	0.44	2.12	7	1
3:A:84:ARG:NE	3:A:84:ARG:HA	0.44	2.27	10	2
2:C:27:DA:H5'	3:A:90:GLY:HA3	0.44	1.88	15	2
1:B:10:DC:C2'	1:B:11:DC:C5	0.44	3.00	2	1
2:C:16:DC:C2'	2:C:17:DT:OP2	0.44	2.65	4	1
3:A:52:SER:HB2	3:A:55:CYS:SG	0.44	2.53	2	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:5:DC:C1'	3:A:92:ARG:HH12	0.44	2.26	16	3
1:B:9:DG:C2'	1:B:10:DC:C5	0.44	2.99	10	1
1:B:3:DC:C2'	1:B:4:DT:C7	0.44	2.92	11	1
3:A:95:PHE:O	3:A:98:MET:HG3	0.44	2.12	1	2
2:C:21:DG:H1'	2:C:22:DC:O5'	0.44	2.12	8	1
3:A:19:LYS:O	3:A:30:CYS:HB3	0.44	2.13	11	2
2:C:20:DG:P	3:A:32:SER:HB3	0.44	2.53	7	1
3:A:37:PHE:O	3:A:41:VAL:HG23	0.44	2.12	10	1
3:A:41:VAL:HG21	3:A:83:VAL:CG2	0.44	2.42	11	1
2:C:26:DG:C2	2:C:27:DA:C4	0.44	3.06	6	2
1:B:4:DT:H1'	1:B:5:DC:O5'	0.44	2.12	7	2
1:B:14:DA:H1'	1:B:15:DG:C5'	0.44	2.42	9	1
2:C:22:DC:H2''	2:C:23:DC:OP2	0.44	2.13	2	2
2:C:19:DT:OP2	2:C:19:DT:H73	0.44	2.13	5	1
3:A:62:ARG:O	3:A:69:ARG:HD2	0.44	2.13	16	1
3:A:72:LYS:O	3:A:75:THR:HB	0.44	2.13	14	2
1:B:7:DG:C2	1:B:8:DG:C5	0.44	3.06	13	1
1:B:12:DA:H1'	1:B:13:DC:H5'	0.43	1.90	12	1
1:B:7:DG:H5'	3:A:92:ARG:CZ	0.43	2.42	12	1
1:B:6:DA:H4'	3:A:92:ARG:HG2	0.43	1.88	13	1
2:C:16:DC:H2'	2:C:17:DT:H72	0.43	1.90	16	1
3:A:80:LEU:O	3:A:83:VAL:HG12	0.43	2.11	4	1
1:B:8:DG:H1'	3:A:89:ARG:HG2	0.43	1.90	5	1
1:B:7:DG:H8	1:B:7:DG:O5'	0.43	1.95	13	1
3:A:19:LYS:N	3:A:19:LYS:HD2	0.43	2.29	13	1
3:A:20:VAL:HG21	3:A:28:LEU:HD12	0.43	1.91	2	1
2:C:19:DT:H4'	3:A:63:LYS:CG	0.43	2.43	5	1
3:A:40:THR:CA	3:A:45:LYS:HE2	0.43	2.37	11	1
2:C:25:DT:O4'	3:A:89:ARG:HD2	0.43	2.14	5	1
1:B:1:DG:C6	1:B:2:DG:C6	0.43	3.06	11	2
3:A:11:GLU:HG3	3:A:28:LEU:HG	0.43	1.90	11	1
1:B:2:DG:C2	1:B:3:DC:C2	0.43	3.06	13	1
3:A:35:GLY:O	3:A:39:ARG:HG2	0.43	2.13	15	2
3:A:70:PHE:O	3:A:74:LEU:HD13	0.43	2.13	6	1
1:B:8:DG:H5'	3:A:89:ARG:HA	0.43	1.90	11	1
2:C:27:DA:H4'	3:A:90:GLY:O	0.43	2.14	13	1
3:A:52:SER:O	3:A:53:GLN:HB2	0.43	2.12	10	1
3:A:40:THR:HA	3:A:45:LYS:HD3	0.43	1.90	12	1
2:C:27:DA:O5'	2:C:27:DA:C8	0.43	2.72	4	1
1:B:11:DC:H2''	1:B:12:DA:H8	0.43	1.74	11	2
3:A:97:PRO:HA	3:A:100:LYS:HE2	0.43	1.90	11	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:15:DG:H4'	3:A:63:LYS:NZ	0.43	2.29	16	1
2:C:17:DT:H2''	2:C:18:DG:OP2	0.43	2.13	3	1
3:A:64:ARG:O	3:A:66:PRO:HD3	0.43	2.14	5	3
1:B:9:DG:H4'	3:A:87:ARG:CD	0.43	2.44	12	1
1:B:9:DG:N7	3:A:38:LYS:HE2	0.43	2.28	13	1
1:B:7:DG:OP1	3:A:24:HIS:HA	0.43	2.14	5	1
1:B:14:DA:C2	1:B:15:DG:C5	0.43	3.06	6	1
3:A:57:ILE:HD11	3:A:68:CYS:CB	0.43	2.44	6	1
2:C:27:DA:N3	3:A:92:ARG:HD3	0.43	2.28	13	1
3:A:11:GLU:O	3:A:20:VAL:HG22	0.42	2.14	5	1
1:B:9:DG:C8	3:A:38:LYS:NZ	0.42	2.87	9	1
2:C:16:DC:H1'	2:C:17:DT:C5'	0.42	2.41	9	1
1:B:15:DG:H4'	3:A:63:LYS:HZ2	0.42	1.75	16	1
1:B:8:DG:N7	3:A:34:LYS:HD2	0.42	2.29	4	1
1:B:8:DG:H2''	1:B:9:DG:O5'	0.42	2.13	4	1
2:C:29:DC:H6	2:C:29:DC:O5'	0.42	1.96	4	1
3:A:49:CYS:SG	3:A:53:GLN:HG3	0.42	2.54	9	1
3:A:30:CYS:SG	3:A:32:SER:HB2	0.42	2.54	14	1
2:C:27:DA:C4'	3:A:91:GLY:H	0.42	2.26	7	2
1:B:8:DG:H2'	3:A:38:LYS:CE	0.42	2.44	10	1
2:C:18:DG:H1'	2:C:19:DT:O4'	0.42	2.14	14	1
1:B:1:DG:HO5'	1:B:1:DG:H8	0.42	1.54	2	1
2:C:18:DG:O5'	2:C:18:DG:H8	0.42	1.98	3	1
3:A:11:GLU:HG2	3:A:28:LEU:HD22	0.42	1.91	8	1
1:B:1:DG:C2	1:B:2:DG:C5	0.42	3.08	13	1
2:C:21:DG:C2'	2:C:22:DC:C5	0.42	3.02	1	1
1:B:9:DG:OP1	3:A:87:ARG:HD3	0.42	2.15	4	1
2:C:19:DT:C2	2:C:20:DG:C8	0.42	3.07	4	1
1:B:5:DC:H4'	3:A:103:ARG:HH12	0.42	1.75	8	1
1:B:1:DG:C2'	1:B:2:DG:C8	0.42	2.98	15	1
3:A:38:LYS:HA	3:A:41:VAL:CG2	0.42	2.45	9	1
3:A:41:VAL:CG2	3:A:83:VAL:HG11	0.42	2.45	12	2
3:A:19:LYS:HD2	3:A:19:LYS:H	0.42	1.74	13	1
3:A:15:VAL:O	3:A:57:ILE:HB	0.42	2.14	2	1
2:C:16:DC:C2'	2:C:17:DT:C7	0.42	2.98	2	1
3:A:73:CYS:HB3	3:A:78:MET:SD	0.42	2.54	2	1
2:C:25:DT:H4'	3:A:89:ARG:CZ	0.42	2.44	3	1
1:B:12:DA:C2	1:B:13:DC:C2	0.42	3.08	8	1
1:B:7:DG:N2	1:B:8:DG:C4	0.42	2.87	13	1
1:B:6:DA:C2'	1:B:7:DG:OP2	0.42	2.66	14	1
1:B:5:DC:H1'	3:A:92:ARG:NH2	0.41	2.31	1	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:8:DG:H2'	3:A:38:LYS:CD	0.41	2.45	2	1
1:B:8:DG:C2'	1:B:9:DG:OP2	0.41	2.67	3	2
1:B:13:DC:C1'	1:B:14:DA:H5'	0.41	2.36	15	1
1:B:8:DG:C2'	3:A:38:LYS:NZ	0.41	2.82	1	1
2:C:20:DG:C3'	3:A:32:SER:HB2	0.41	2.44	1	1
1:B:10:DC:C2'	1:B:11:DC:OP2	0.41	2.68	5	1
1:B:8:DG:H5''	3:A:84:ARG:CB	0.41	2.37	8	1
2:C:27:DA:H4'	3:A:90:GLY:CA	0.41	2.45	10	1
1:B:8:DG:C5'	3:A:88:MET:O	0.41	2.67	3	1
3:A:27:LEU:HD13	3:A:27:LEU:N	0.41	2.30	3	1
3:A:42:GLN:HA	3:A:42:GLN:OE1	0.41	2.15	15	2
3:A:73:CYS:HB3	3:A:78:MET:HG3	0.41	1.93	6	1
1:B:4:DT:H1'	1:B:5:DC:C5'	0.41	2.45	7	1
3:A:15:VAL:HG23	3:A:72:LYS:HB3	0.41	1.93	13	1
2:C:20:DG:H2''	2:C:21:DG:O5'	0.41	2.15	3	1
3:A:84:ARG:NE	3:A:86:ASP:HB3	0.41	2.31	8	1
2:C:28:DG:C2'	2:C:29:DC:OP2	0.41	2.67	13	1
2:C:16:DC:H2''	2:C:17:DT:H72	0.41	1.92	15	1
1:B:12:DA:C2'	1:B:13:DC:OP2	0.41	2.66	10	1
3:A:73:CYS:O	3:A:76:VAL:HG22	0.41	2.16	11	1
2:C:21:DG:C5	2:C:22:DC:C4	0.41	3.08	15	1
3:A:23:TYR:HA	3:A:28:LEU:HA	0.41	1.93	2	1
3:A:52:SER:C	3:A:54:SER:H	0.41	2.24	2	1
1:B:8:DG:OP1	3:A:83:VAL:HA	0.41	2.14	3	1
3:A:15:VAL:HG13	3:A:16:CYS:N	0.41	2.31	7	1
3:A:56:LYS:HB2	3:A:56:LYS:NZ	0.41	2.30	7	1
2:C:28:DG:C4'	3:A:92:ARG:HB2	0.41	2.45	3	1
1:B:5:DC:H2''	1:B:6:DA:O5'	0.40	2.15	4	1
2:C:16:DC:O5'	2:C:16:DC:H6	0.40	1.98	2	1
2:C:24:DC:H2''	2:C:25:DT:H72	0.40	1.93	11	1
3:A:27:LEU:N	3:A:27:LEU:HD13	0.40	2.31	13	1
1:B:8:DG:C2'	3:A:38:LYS:HZ3	0.40	2.29	14	1
2:C:26:DG:H2''	2:C:27:DA:H8	0.40	1.76	14	1
1:B:7:DG:C2'	1:B:8:DG:OP2	0.40	2.69	6	1
1:B:13:DC:H2''	1:B:14:DA:N7	0.40	2.30	11	1
2:C:21:DG:C4	2:C:22:DC:C4	0.40	3.10	1	1
1:B:7:DG:C4'	3:A:91:GLY:HA2	0.40	2.47	8	1
1:B:9:DG:C4	1:B:10:DC:C4	0.40	3.10	8	1
2:C:26:DG:H1'	3:A:91:GLY:CA	0.40	2.46	9	1
3:A:94:LYS:HB3	3:A:94:LYS:HZ3	0.40	1.77	12	1
2:C:22:DC:O5'	2:C:22:DC:C6	0.40	2.73	14	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:A:31:GLU:H	3:A:31:GLU:CD	0.40	2.24	6	1
2:C:19:DT:O3'	3:A:63:LYS:HE2	0.40	2.16	8	1
1:B:9:DG:C4'	3:A:87:ARG:CD	0.40	3.00	12	1
3:A:12:LEU:N	3:A:12:LEU:HD12	0.40	2.32	13	1

6.3 Torsion angles [i](#)

6.3.1 Protein backbone [i](#)

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	A	93/102 (91%)	83±3 (89±3%)	8±3 (9±3%)	2±1 (2±1%)	7	47
All	All	1488/1632 (91%)	1326 (89%)	130 (9%)	32 (2%)	7	47

All 12 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	86	ASP	7
3	A	87	ARG	6
3	A	51	GLU	4
3	A	52	SER	3
3	A	93	ASN	2
3	A	25	TYR	2
3	A	50	THR	2
3	A	26	GLY	2
3	A	24	HIS	1
3	A	88	MET	1
3	A	91	GLY	1
3	A	17	GLY	1

6.3.2 Protein sidechains [i](#)

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

was analysed and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
3	A	84/90 (93%)	81±1 (96±1%)	3±1 (4±1%)	32 82
All	All	1344/1440 (93%)	1295 (96%)	49 (4%)	32 82

All 28 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	71	GLN	4
3	A	15	VAL	3
3	A	72	LYS	3
3	A	27	LEU	3
3	A	38	LYS	3
3	A	32	SER	3
3	A	56	LYS	2
3	A	94	LYS	2
3	A	43	ASN	2
3	A	44	ASN	2
3	A	102	ASP	2
3	A	29	THR	2
3	A	76	VAL	2
3	A	63	LYS	2
3	A	59	LYS	1
3	A	19	LYS	1
3	A	64	ARG	1
3	A	92	ARG	1
3	A	99	TYR	1
3	A	30	CYS	1
3	A	31	GLU	1
3	A	23	TYR	1
3	A	89	ARG	1
3	A	45	LYS	1
3	A	87	ARG	1
3	A	46	HIS	1
3	A	58	ASP	1
3	A	83	VAL	1

6.3.3 RNA [i](#)

There are no RNA molecules in this entry.

6.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.6 Ligand geometry [i](#)

Of 2 ligands modelled in this entry, 2 are 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