



# Full wwPDB NMR Structure Validation Report ⓘ

Feb 12, 2017 – 09:51 pm GMT

PDB ID : 2FF0  
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

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

with specific help available everywhere you see the ⓘ symbol.

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

Cyrange : Kirchner and Güntert (2011)  
NmrClust : Kelley et al. (1996)  
MolProbity : 4.02b-467  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
RCI : v\_1n\_11\_5\_13\_A (Berjanski et al., 2005)  
PANAV : Wang et al. (2010)  
ShiftChecker : trunk28760  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : recalc28949

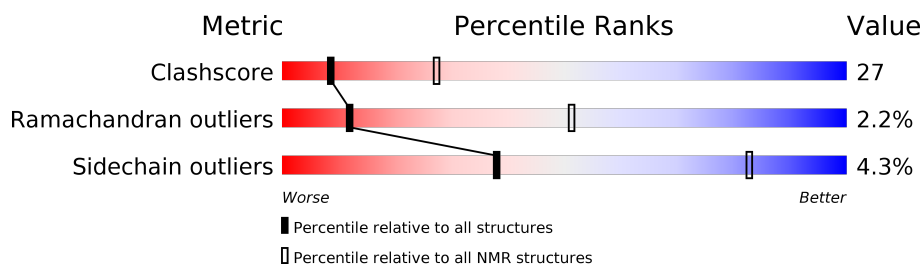
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*SOLUTION NMR*

The overall completeness of chemical shifts assignment was not calculated.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	NMR archive (#Entries)
Clashscore	125131	11601
Ramachandran outliers	121729	10391
Sidechain outliers	121581	10367

The table below summarises the geometric issues observed across the polymeric chains and their fit to the experimental data. The red, orange, yellow and green segments indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	73% 19% • 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)	0.71	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
1	B	15	Total	C	H	N	O	P	0
			475	145	168	62	86	14	

- Molecule 2 is a DNA chain called CTGTGGCCCTGAGCC.

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

- Molecule 3 is a protein called Steroidogenic factor 1.

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

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

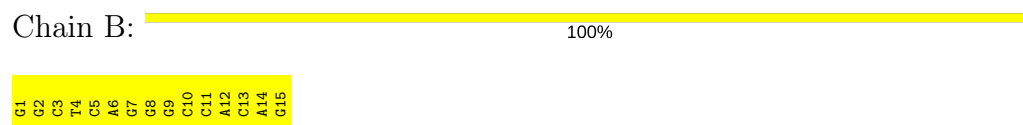
Mol	Chain	Residues	Atoms	
4	A	2	Total	Zn
			2	2

## 4 Residue-property plots [i](#)

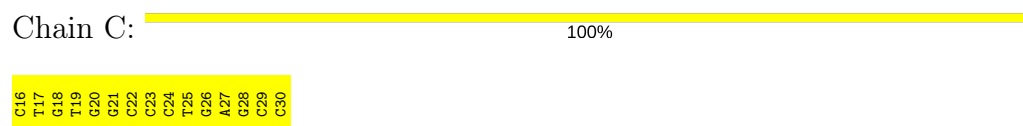
### 4.1 Average score per residue in the NMR ensemble

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

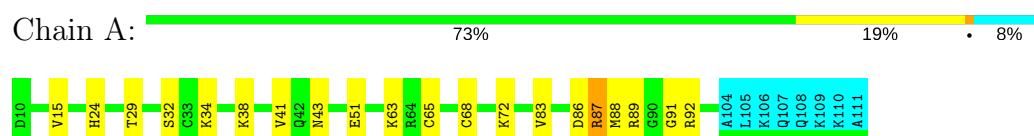
- Molecule 1: GGCTCAGGGCCACAG



- Molecule 2: CTGTGGCCCTGAGCC



- Molecule 3: Steroidogenic factor 1

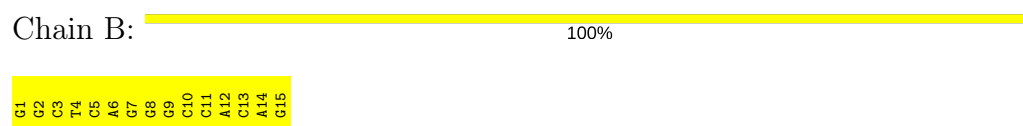


### 4.2 Scores per residue for each member of the ensemble


Colouring as in section 4.1 above.

#### 4.2.1 Score per residue for model 1 (medoid)

- Molecule 1: GGCTCAGGGCCACAG



- Molecule 2: CTGTGGCCCTGAGCC

Chain C:  100%

G16  
T17  
G18  
T19  
G20  
G21  
C22  
C23  
C24  
T25  
G26  
A27  
G28  
C29  
C30

- Molecule 3: Steroidogenic factor 1

Chain A:  61%  28%  8%

D10  
V15  
C16  
G17  
D18  
H24  
T29  
C30  
G20  
E31  
S32  
K38  
R39  
T40  
V41  
S52  
K59  
K63  
R64  
C65  
C68  
K72  
R79  
A82  
V83  
R84  
A85  
D86  
R87  
N88  
R89  
G90  
G91  
R92  
N93  
K94  
F95  
G96  
P97  
M98  
Y99  
K100  
A104  
L105  
K106  
Q107  
Q108  
K109  
K110

#### 4.2.2 Score per residue for model 2

- Molecule 1: GGCTCAGGGCCACAG

Chain B:  13%  87%

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

- Molecule 2: CTGTGGCCCTGAGCC

Chain C:  100%

G16  
T17  
G18  
T19  
G20  
G21  
C22  
C23  
C24  
T25  
G26  
A27  
G28  
C29  
C30

- Molecule 3: Steroidogenic factor 1

Chain A:  59%  31%  8%

D10  
V15  
K19  
V20  
Y23  
H24  
Y25  
L28  
T29  
R34  
K38  
V41  
G42  
M43  
E51  
S52  
C55  
R56  
I57  
K63  
R64  
C65  
C68  
R69  
F70  
Q71  
K72  
C73  
M78  
V83  
R87  
R88  
R89  
G90  
G91  
R92  
F95  
M98  
Y99  
K100  
R101  
A104  
L105

#### 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%

G16  
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  
H24  
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  
C10  
C11  
A12  
C13  
A14  
G15

- Molecule 2: CTGTGGCCCTGAGCC

Chain C:  7%  93%

G16  
T17  
G18  
T19  
G20  
G21  
C22  
C23  
C24  
T25  
G26  
A27  
G28  
C29  
C30

- Molecule 3: Steroidogenic factor 1

Chain A:  62%  25%  5%  8%

D10  
E11  
V15  
V23  
H24  
L28  
T29  
K34  
C35  
F36  
F37  
K38  
R39  
V41  
V42  
M43  
C49  
Q53  
R64  
C65  
P66  
P67  
C68  
K72  
L80  
V83  
R84  
R87  
M88  
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  
C10  
C11  
A14  
G15

- Molecule 2: CTGTGGCCCTGAGCC

Chain C:  7%  93%

G16  
T17  
G18  
T19  
G20  
G21  
C22  
C23  
C24  
T25  
G26  
A27  
G28  
C29  
G30

- Molecule 3: Steroidogenic factor 1

Chain A:  69% 24% 8%

D10  
E11  
D18  
K19  
V20  
H24  
Y25  
G26  
L27  
L28  
T29  
S32  
K38  
V41  
N44  
T50  
R62  
K63  
R64  
C65  
P66  
R69  
F70  
Q71  
V83  
R87  
H88  
R89  
G90  
G91  
R92  
A104  
L105  
K106  
Q107  
Q108  
K109  
K110  
A111

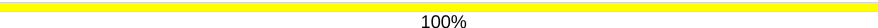
#### 4.2.6 Score per residue for model 6

- Molecule 1: GGCTCAGGGCCACAG

Chain B:  100%

G1  
G2  
C3  
T4  
C5  
A6  
G7  
G8  
C9  
C10  
C11  
A12  
C13  
A14  
G15

- Molecule 2: CTGTGGCCCTGAGCC

Chain C:  100%

G16  
T17  
G18  
T19  
G20  
G21  
C22  
C23  
C24  
T25  
G26  
A27  
G28  
C29  
G30

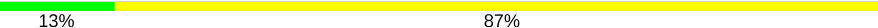
- Molecule 3: Steroidogenic factor 1

Chain A:  66% 25% 8%

D10  
P14  
V15  
C16  
H24  
T29  
C30  
E31  
K34  
K38  
S52  
I57  
R62  
K63  
C68  
R69  
F70  
C73  
L74  
V75  
V76  
G77  
M78  
E81  
R87  
H88  
R89  
G90  
G91  
R92  
Y99  
D102  
R103  
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  
C9  
C10  
C11  
A12  
C13  
A14  
G15

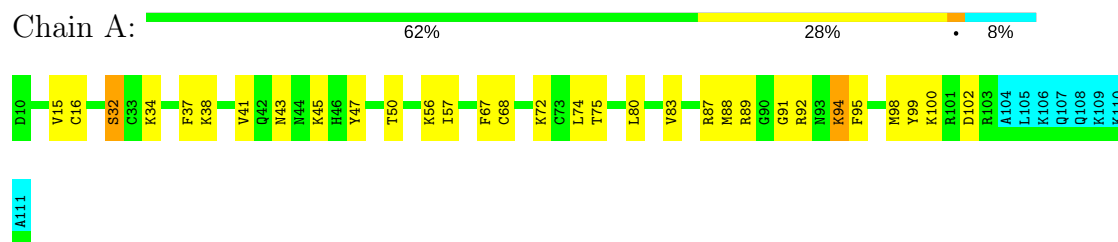
- Molecule 2: CTGTGGCCCTGAGCC

Chain C:  7% 93%

G16  
T17  
G18  
T19  
G20  
G21  
C22  
C23  
T25  
G26  
A27  
G28  
C29  
G30

- Molecule 3: Steroidogenic factor 1





#### 4.2.8 Score per residue for model 8

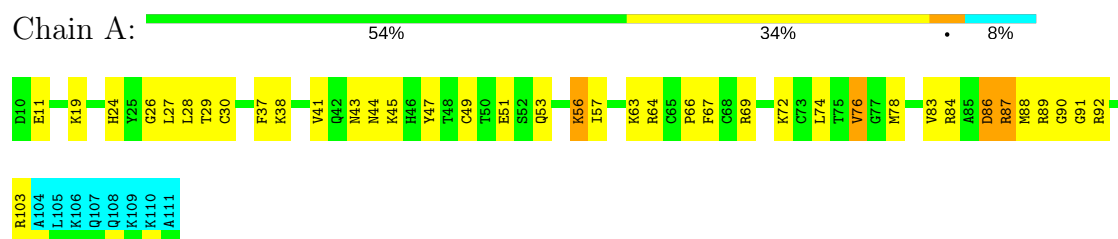
- Molecule 1: GGCTCAGGGCCACAG



- Molecule 2: CTGTGGCCCTGAGCC

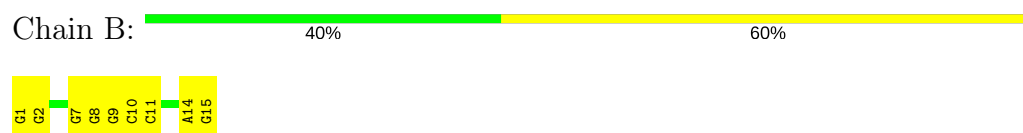


- Molecule 3: Steroidogenic factor 1



#### 4.2.9 Score per residue for model 9

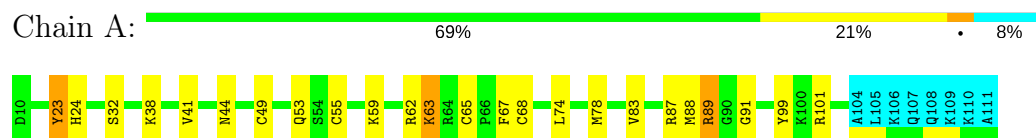
- Molecule 1: GGCTCAGGGCCACAG



- Molecule 2: CTGTGGCCCTGAGCC



- Molecule 3: Steroidogenic factor 1



#### 4.2.10 Score per residue for model 10

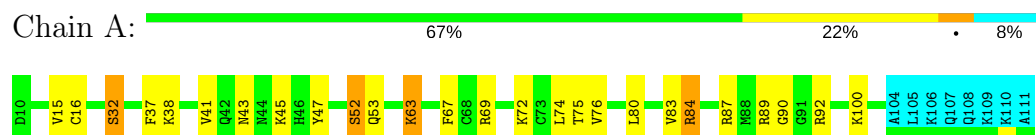
- Molecule 1: GGCTCAGGGCCACAG



- Molecule 2: CTGTGGCCCTGAGCC

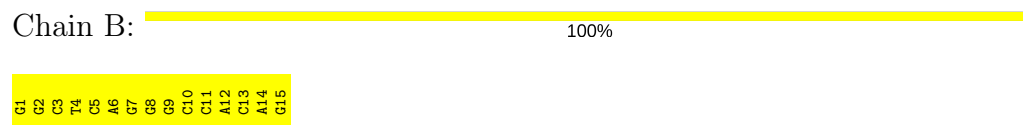


- Molecule 3: Steroidogenic factor 1



#### 4.2.11 Score per residue for model 11

- Molecule 1: GGCTCAGGGCCACAG

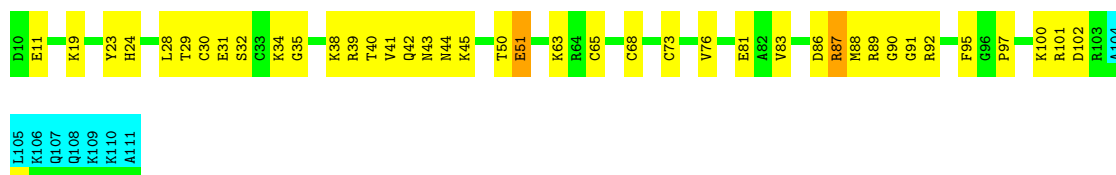


- Molecule 2: CTGTGGCCCTGAGCC



- Molecule 3: Steroidogenic factor 1

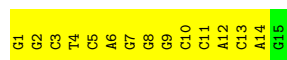




#### 4.2.12 Score per residue for model 12

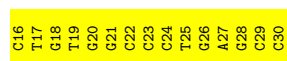
- Molecule 1: GGCTCAGGGCCACAG

Chain B: 7% 93%



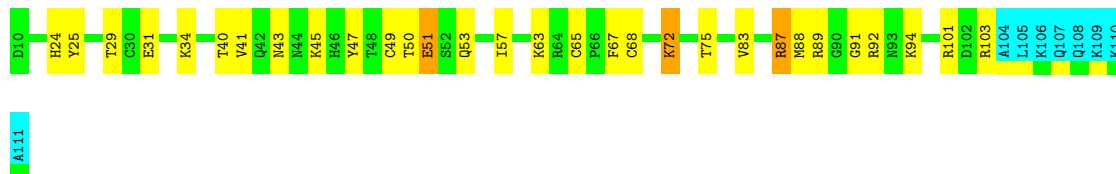
- Molecule 2: CTGTGGCCCTGAGCC

Chain C: 100%



- Molecule 3: Steroidogenic factor 1

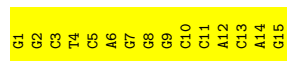
Chain A: 63% 26% 8%



#### 4.2.13 Score per residue for model 13

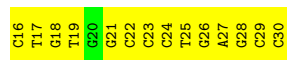
- Molecule 1: GGCTCAGGGCCACAG

Chain B: 100%

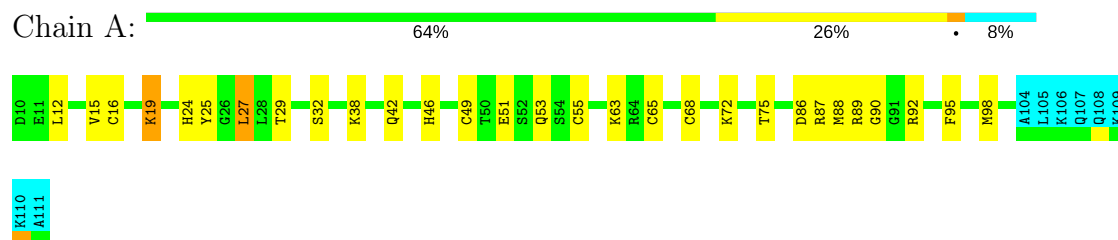


- Molecule 2: CTGTGGCCCTGAGCC

Chain C: 7% 93%



- Molecule 3: Steroidogenic factor 1



#### 4.2.14 Score per residue for model 14

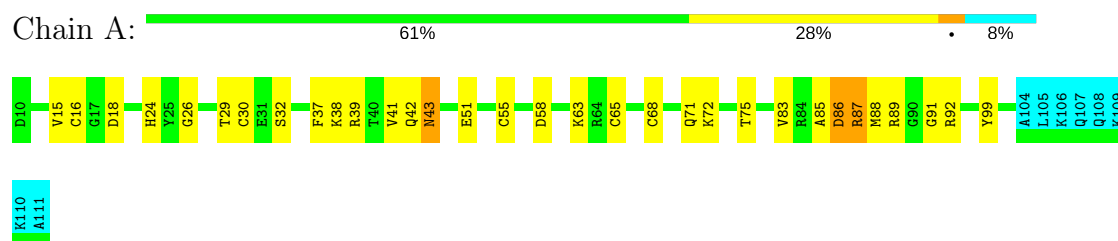
- Molecule 1: GGCTCAGGGCCACAG



- Molecule 2: CTGTGGCCCTGAGCC



- Molecule 3: Steroidogenic factor 1

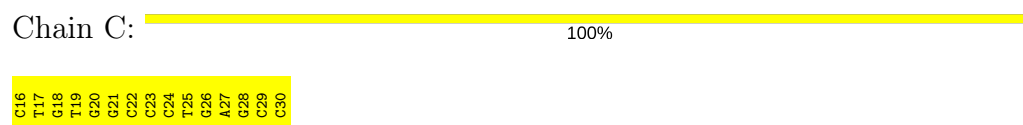


#### 4.2.15 Score per residue for model 15

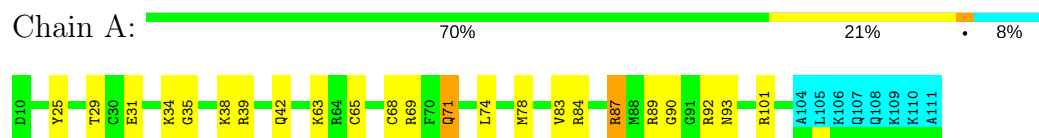
- Molecule 1: GGCTCAGGGCCACAG



- Molecule 2: CTGTGGCCCTGAGCC

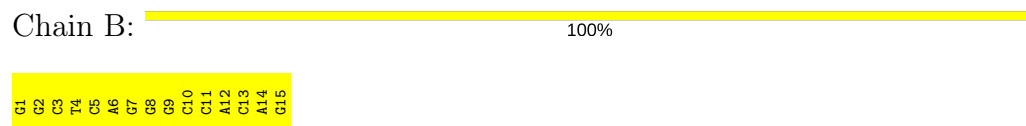


- Molecule 3: Steroidogenic factor 1

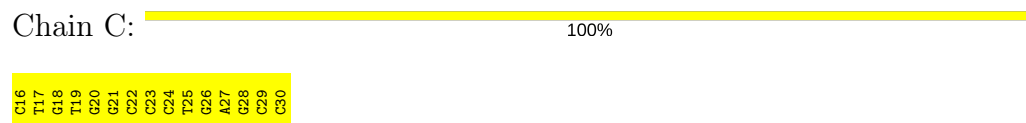


#### 4.2.16 Score per residue for model 16

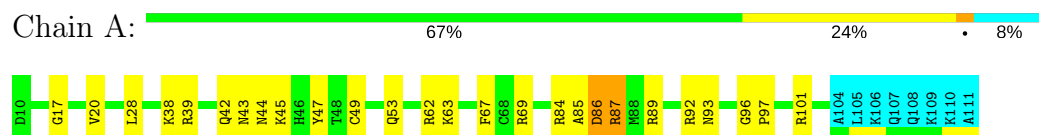
- Molecule 1: GGCTCAGGGCCACAG



- 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. No validations of the models with respect to experimental NMR restraints is performed at this time.

## 6 Model quality [i](#)

### 6.1 Standard geometry [i](#)

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

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	1051

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
2:C:18:DG:H2''	2:C:19:DT:H71	0.84	1.46	1	1
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
2:C:18:DG:C2'	2:C:19:DT:H71	0.76	2.11	1	1
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
1:B:14:DA:H2''	1:B:15:DG:C8	0.74	2.16	13	4
2:C:19:DT:H4'	3:A:63:LYS:HE3	0.74	1.59	1	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
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
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: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
1:B:7:DG:H2''	1:B:8:DG:OP2	0.69	1.87	1	7
2:C:28:DG:H5''	3:A:92:ARG:O	0.69	1.88	15	5
2:C:19:DT:H4'	3:A:63:LYS:HE2	0.69	1.64	11	2
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
2:C:16:DC:H6	2:C:16:DC:HO5'	0.67	1.31	12	1
1:B:11:DC:H1'	1:B:12:DA:H5'	0.67	1.66	4	2
3:A:94:LYS:HE3	3:A:94:LYS:HA	0.67	1.66	7	1
3:A:49:CYS:HB3	3:A:53:GLN:HG2	0.67	1.65	16	2
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:19:DT:H5''	3:A:63:LYS:HE2	0.65	1.68	14	1
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

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
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
2:C:16:DC:H2''	2:C:17:DT:H71	0.65	1.69	2	2
3:A:29:THR:HG21	3:A:78:MET:SD	0.64	2.33	6	2
1:B:8:DG:H1'	1:B:9:DG:H5'	0.64	1.68	14	10
2:C:28:DG:H4'	3:A:92:ARG:HB2	0.64	1.70	3	1
1:B:7:DG:H3'	3:A:25:TYR:CE1	0.64	2.27	13	1
1:B:8:DG:O4'	3:A:89:ARG:HG2	0.64	1.93	10	5
1:B:8:DG:H5''	3:A:88:MET:O	0.64	1.93	3	4
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:H3'	3:A:32:SER:OG	0.63	1.94	14	2
2:C:20:DG:H2'	3:A:32:SER:HB2	0.63	1.70	5	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
2:C:16:DC:C2'	2:C:17:DT:H72	0.62	2.24	5	4
2:C:27:DA:H1'	2:C:28:DG:C5'	0.62	2.23	16	2
1:B:10:DC:H2''	1:B:11:DC:C5	0.62	2.29	2	2
1:B:8:DG:H5''	3:A:84:ARG:HB2	0.62	1.71	15	1
2:C:26:DG:H1'	2:C:27:DA:C5'	0.62	2.24	13	3
1:B:1:DG:H2''	1:B:2:DG:H8	0.62	1.54	1	3
2:C:28:DG:H2''	2:C:29:DC:OP2	0.62	1.93	13	2
1:B:9:DG:C5'	3:A:87:ARG:HD2	0.62	2.24	12	1
2:C:20:DG:C1'	2:C:21:DG:H5'	0.62	2.20	9	1
3:A:71:GLN:HE21	3:A:71:GLN:HA	0.61	1.53	15	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
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
1:B:8:DG:H2''	3:A:38:LYS:HZ2	0.61	1.55	1	1
1:B:7:DG:H21	3:A:89:ARG:HD3	0.61	1.56	15	5
2:C:24:DC:H1'	2:C:25:DT:C5'	0.61	2.25	15	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:C:25:DT:H1'	2:C:26:DG:O4'	0.61	1.96	2	3
2:C:28:DG:H2''	2:C:29:DC:C5	0.61	2.31	10	5
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
2:C:27:DA:H2''	2:C:28:DG:C8	0.61	2.31	4	2
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
1:B:9:DG:N7	3:A:38:LYS:HE3	0.60	2.12	15	1
2:C:20:DG:H2''	2:C:21:DG:C8	0.60	2.32	7	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: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
1:B:1:DG:H2''	1:B:2:DG:OP2	0.59	1.97	4	2
2:C:16:DC:H2''	2:C:17:DT:C6	0.59	2.31	3	2
3:A:68:CYS:HA	3:A:71:GLN:HG3	0.59	1.74	2	1
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
1:B:6:DA:H5''	3:A:99:TYR:CD2	0.59	2.32	14	1
2:C:18:DG:H2''	2:C:19:DT:C6	0.59	2.33	2	2
1:B:8:DG:H2'	3:A:38:LYS:HG2	0.59	1.74	15	1
1:B:7:DG:H1'	1:B:8:DG:H5'	0.59	1.75	13	2
2:C:29:DC:H5''	3:A:100:LYS:HD3	0.59	1.74	1	1
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
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

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
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
3:A:51:GLU:HB2	3:A:55:CYS:SG	0.57	2.39	14	2
1:B:11:DC:H2''	1:B:12:DA:OP2	0.57	1.98	8	1
1:B:2:DG:H1'	1:B:3:DC:H5'	0.57	1.75	13	2
1:B:7:DG:C5'	3:A:91:GLY:HA2	0.57	2.30	8	1
3:A:72:LYS:CA	3:A:75:THR:HB	0.57	2.29	7	2
2:C:27:DA:C2'	2:C:28:DG:C8	0.57	2.87	4	1
3:A:31:GLU:HA	3:A:34:LYS:HG2	0.57	1.76	6	1
2:C:28:DG:H4'	3:A:92:ARG:NE	0.57	2.15	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	15	4
1:B:6:DA:H5''	3:A:99:TYR:HD2	0.56	1.60	14	1
2:C:19:DT:H4'	3:A:63:LYS:HG2	0.56	1.76	5	1
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:12:DA:H2''	1:B:13:DC:C5	0.56	2.36	2	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:5:DC:H1'	3:A:92:ARG:NH1	0.55	2.16	15	1
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
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	2.31	14	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
2:C:18:DG:H2''	2:C:19:DT:C7	0.55	2.25	1	4
1:B:3:DC:C2'	1:B:4:DT:H72	0.55	2.32	6	5
1:B:6:DA:H5''	3:A:99:TYR:CB	0.55	2.32	2	3
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

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
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:22:DC:H2''	2:C:23:DC:C6	0.54	2.37	13	2
2:C:28:DG:H2''	2:C:29:DC:H6	0.54	1.61	1	1
2:C:16:DC:O5'	2:C:16:DC:H6	0.54	1.85	12	1
2:C:19:DT:C4'	3:A:63:LYS:HG2	0.54	2.33	5	1
3:A:25:TYR:CE1	3:A:34:LYS:HG3	0.54	2.37	15	1
2:C:20:DG:H3'	3:A:32:SER:HB2	0.54	1.78	1	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
2:C:23:DC:H6	2:C:23:DC:O5'	0.54	1.86	16	2
1:B:7:DG:O4'	3:A:91:GLY:HA2	0.54	2.03	14	1
3:A:41:VAL:HG11	3:A:83:VAL:CG1	0.54	2.33	2	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:18:DG:C2'	2:C:19:DT:H72	0.53	2.33	11	3
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:HA	3:A:79:ARG:NE	0.53	2.18	1	1
2:C:18:DG:H2'	2:C:19:DT:H72	0.53	1.80	8	2
3:A:91:GLY:O	3:A:92:ARG:HD2	0.53	2.03	8	1
3:A:74:LEU:HG	3:A:80:LEU:HD21	0.53	1.79	7	1
2:C:27:DA:H4'	3:A:92:ARG:N	0.53	2.18	4	2
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
2:C:27:DA:H5''	3:A:91:GLY:CA	0.53	2.30	12	1
1:B:8:DG:H2'	3:A:38:LYS:HE3	0.53	1.78	10	1
1:B:8:DG:H2'	3:A:38:LYS:NZ	0.53	2.19	5	1
3:A:18:ASP:HB2	3:A:30:CYS:SG	0.52	2.45	14	2
1:B:9:DG:C1'	1:B:10:DC:H5'	0.52	2.31	14	1
1:B:9:DG:C5'	3:A:88:MET:H	0.52	2.15	12	1
1:B:3:DC:C6	1:B:4:DT:H72	0.52	2.39	12	1
1:B:6:DA:H2''	1:B:7:DG:N7	0.52	2.18	13	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
3:A:81:GLU:HG3	3:A:95:PHE:CZ	0.52	2.38	11	1
1:B:5:DC:O2	3:A:92:ARG:HD2	0.52	2.05	13	1
1:B:8:DG:C8	3:A:38:LYS:NZ	0.52	2.78	5	1
1:B:8:DG:H2'	3:A:38:LYS:HE2	0.52	1.81	6	1
3:A:49:CYS:HB3	3:A:53:GLN:HA	0.52	1.82	13	3
3:A:53:GLN:HB3	3:A:55:CYS:SG	0.52	2.44	9	1
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	5
1:B:5:DC:H1'	1:B:6:DA:C8	0.51	2.40	16	1
1:B:14:DA:H2''	1:B:15:DG:N7	0.51	2.20	14	2
3:A:37:PHE:O	3:A:41:VAL:HG22	0.51	2.06	14	5
3:A:81:GLU:HG3	3:A:95:PHE:HZ	0.51	1.65	11	1
2:C:20:DG:H2'	3:A:32:SER:CB	0.51	2.35	9	3
1:B:4:DT:H2''	1:B:5:DC:H6	0.51	1.63	5	1
1:B:3:DC:H2'	1:B:4:DT:H72	0.51	1.81	15	1
1:B:8:DG:H3'	3:A:42:GLN:HE22	0.51	1.66	14	1
1:B:3:DC:C1'	1:B:4:DT:H5'	0.51	2.25	1	1
2:C:18:DG:H2''	2:C:19:DT:H72	0.51	1.82	4	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
2:C:19:DT:H71	3:A:39:ARG:HG3	0.51	1.81	11	1
2:C:19:DT:H72	3:A:39:ARG:NE	0.51	2.20	1	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:9:DG:OP2	3:A:42:GLN:HG3	0.51	2.06	15	1
1:B:6:DA:H2''	1:B:7:DG:C8	0.51	2.41	13	1
1:B:6:DA:H5''	3:A:99:TYR:HB3	0.51	1.83	2	1
2:C:19:DT:H3'	3:A:69:ARG:HH22	0.51	1.65	10	1
3:A:38:LYS:HA	3:A:41:VAL:HG22	0.51	1.82	9	1
3:A:50:THR:HG22	3:A:51:GLU:HG3	0.51	1.81	11	2
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:43:ASN:HB2	3:A:45:LYS:HG3	0.50	1.83	7	5
1:B:8:DG:H5'	3:A:84:ARG:NH1	0.50	2.20	4	1
3:A:38:LYS:HG2	3:A:83:VAL:HG13	0.50	1.81	10	1
3:A:63:LYS:HA	3:A:69:ARG:NH2	0.50	2.20	10	1
1:B:9:DG:H1'	1:B:10:DC:O4'	0.50	2.06	9	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
2:C:19:DT:C5'	3:A:63:LYS:HE3	0.50	2.36	1	1
3:A:72:LYS:CA	3:A:72:LYS:HE3	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:18:DG:C2'	2:C:19:DT:C7	0.50	2.89	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:5:DC:H2''	1:B:6:DA:OP2	0.49	2.06	11	2
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
2:C:25:DT:H5'	3:A:89:ARG:NH1	0.49	2.22	16	2
2:C:29:DC:OP1	3:A:97:PRO:HG3	0.49	2.07	1	1
1:B:2:DG:C2'	1:B:3:DC:C5	0.49	2.92	12	1
2:C:27:DA:C4'	3:A:90:GLY:HA2	0.49	2.37	10	2
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
3:A:57:ILE:HD11	3:A:68:CYS:HB2	0.49	1.83	6	3
3:A:15:VAL:HG22	3:A:16:CYS:N	0.49	2.21	1	1
2:C:24:DC:C2'	2:C:25:DT:H72	0.49	2.37	7	1
3:A:41:VAL:CG2	3:A:83:VAL:HG21	0.49	2.38	4	1
2:C:23:DC:H2''	2:C:24:DC:OP2	0.49	2.07	16	7
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
2:C:22:DC:C2	2:C:23:DC:C5	0.49	3.01	11	3
1:B:7:DG:H2'	3:A:34:LYS:NZ	0.49	2.22	3	1
1:B:7:DG:H21	3:A:88:MET:HG2	0.49	1.68	12	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
2:C:28:DG:C2'	2:C:29:DC:C6	0.49	2.95	1	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

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:A:15:VAL:HG11	3:A:73:CYS:SG	0.48	2.48	6	1
3:A:56:LYS:HD3	3:A:56:LYS:N	0.48	2.24	8	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:9:DG:C4'	3:A:89:ARG:HG2	0.48	2.38	4	1
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
2:C:21:DG:OP2	3:A:32:SER:HB2	0.47	2.09	13	1
3:A:40:THR:HA	3:A:45:LYS:CE	0.47	2.35	11	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
1:B:11:DC:H6	1:B:11:DC:O5'	0.47	1.92	1	1
2:C:19:DT:H5''	3:A:63:LYS:HG2	0.47	1.86	2	1
1:B:9:DG:H5''	3:A:87:ARG:CD	0.47	2.38	13	3
3:A:82:ALA:HB2	3:A:95:PHE:CZ	0.47	2.43	1	1
2:C:25:DT:H2''	2:C:26:DG:N7	0.47	2.21	6	1
3:A:86:ASP:O	3:A:87:ARG:HB2	0.47	2.10	1	3
3:A:27:LEU:CD2	3:A:76:VAL:HG13	0.47	2.38	8	1
2:C:27:DA:H4'	3:A:92:ARG:H	0.47	1.70	4	2
2:C:16:DC:H2'	2:C:17:DT:H72	0.47	1.85	5	2
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:25:DT:H2''	2:C:26:DG:O5'	0.47	2.08	12	1
3:A:49:CYS:SG	3:A:53:GLN:HA	0.47	2.50	8	1
3:A:68:CYS:O	3:A:72:LYS:HB2	0.47	2.09	2	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
2:C:28:DG:OP1	3:A:93:ASN:HB3	0.47	2.10	16	1
1:B:8:DG:C2	1:B:9:DG:C4	0.47	3.03	14	5
3:A:35:GLY:HA2	3:A:38:LYS:NZ	0.46	2.25	11	1
1:B:9:DG:H5''	3:A:88:MET:N	0.46	2.21	12	1
2:C:18:DG:C2'	2:C:19:DT:OP2	0.46	2.62	5	1
2:C:19:DT:C3'	3:A:69:ARG:HH12	0.46	2.14	6	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
1:B:8:DG:O5'	1:B:8:DG:C8	0.46	2.69	6	1
3:A:96:GLY:N	3:A:97:PRO:HD2	0.46	2.25	16	1
1:B:10:DC:C2	1:B:11:DC:C5	0.46	3.03	16	1
2:C:19:DT:H3'	3:A:69:ARG:NH2	0.46	2.25	10	1
1:B:8:DG:C5'	3:A:84:ARG:HB2	0.46	2.38	15	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:8:DG:O5'	1:B:8:DG:H8	0.46	1.93	6	1
2:C:29:DC:C2	2:C:30:DC:C5	0.46	3.04	7	2
1:B:9:DG:H2''	1:B:10:DC:O5'	0.46	2.11	14	2
1:B:9:DG:N7	3:A:38:LYS:NZ	0.46	2.63	9	2
3:A:15:VAL:HG13	3:A:72:LYS:HB3	0.46	1.88	4	2
1:B:8:DG:H1'	1:B:9:DG:O5'	0.46	2.11	16	2
2:C:16:DC:C6	2:C:17:DT:H72	0.46	2.46	1	2
1:B:5:DC:H1'	3:A:92:ARG:HD2	0.46	1.87	14	1
3:A:14:PRO:HB2	3:A:76:VAL:HG11	0.46	1.87	6	1
2:C:19:DT:H71	3:A:39:ARG:NH1	0.46	2.26	16	1
2:C:25:DT:H4'	3:A:89:ARG:NH2	0.46	2.25	14	1
2:C:19:DT:O5'	2:C:19:DT:C6	0.45	2.69	11	1
3:A:84:ARG:HG2	3:A:88:MET:O	0.45	2.11	1	2
1:B:11:DC:O5'	1:B:11:DC:H6	0.45	1.94	9	1
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:38:LYS:O	3:A:42:GLN:HB2	0.45	2.11	13	1
2:C:19:DT:H6	2:C:19:DT:O5'	0.45	1.93	11	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
1:B:9:DG:C2'	1:B:10:DC:C6	0.45	2.99	9	1
1:B:8:DG:H2'	3:A:38:LYS:HD2	0.45	1.88	16	2
3:A:18:ASP:HB2	3:A:62:ARG:NH1	0.45	2.26	5	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
3:A:23:TYR:HB3	3:A:99:TYR:OH	0.45	2.12	9	1
2:C:21:DG:C2	2:C:22:DC:C2	0.45	3.04	7	1
3:A:38:LYS:O	3:A:42:GLN:HG3	0.45	2.11	11	1
2:C:19:DT:H5''	3:A:63:LYS:CB	0.45	2.42	9	1
2:C:19:DT:H5''	3:A:63:LYS:CA	0.45	2.35	6	1
2:C:16:DC:C2'	2:C:17:DT:H71	0.45	2.39	2	2
3:A:11:GLU:HG3	3:A:28:LEU:HD22	0.45	1.88	4	1
2:C:28:DG:H5''	3:A:92:ARG:HG3	0.45	1.89	10	1
1:B:7:DG:H21	3:A:89:ARG:HD2	0.45	1.71	14	1
2:C:16:DC:O5'	2:C:16:DC:C6	0.45	2.70	10	1
3:A:41:VAL:HB	3:A:83:VAL:HG11	0.45	1.88	1	2
3:A:80:LEU:O	3:A:83:VAL:HG22	0.44	2.12	7	1
3:A:15:VAL:HB	3:A:72:LYS:HG3	0.44	1.89	1	1
3:A:84:ARG:NE	3:A:84:ARG:HA	0.44	2.27	10	1
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

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:C:16:DC:C2'	2:C:17:DT:OP2	0.44	2.65	4	1
1:B:5:DC:C1'	3:A:92:ARG:HH12	0.44	2.26	16	3
1:B:3:DC:C2'	1:B:4:DT:C7	0.44	2.92	11	1
3:A:52:SER:HB2	3:A:55:CYS:SG	0.44	2.53	2	1
1:B:9:DG:C2'	1:B:10:DC:C5	0.44	2.99	10	1
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
3:A:95:PHE:O	3:A:98:MET:HG3	0.44	2.12	1	2
3:A:52:SER:O	3:A:53:GLN:HB2	0.44	2.12	10	1
2:C:20:DG:P	3:A:32:SER:HB3	0.44	2.53	7	1
3:A:41:VAL:HG21	3:A:83:VAL:CG2	0.44	2.42	11	1
3:A:37:PHE:O	3:A:41:VAL:HG23	0.44	2.12	10	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:8:DG:H2'	3:A:38:LYS:HZ2	0.44	1.71	5	1
1:B:14:DA:H1'	1:B:15:DG:C5'	0.44	2.42	9	1
3:A:62:ARG:O	3:A:69:ARG:HD2	0.44	2.13	16	1
2:C:22:DC:H2''	2:C:23:DC:OP2	0.44	2.13	2	2
2:C:19:DT:H73	2:C:19:DT:OP2	0.44	2.13	5	1
1:B:7:DG:C2	1:B:8:DG:C5	0.44	3.06	13	1
3:A:72:LYS:O	3:A:75:THR:HB	0.44	2.13	14	2
1:B:12:DA:H1'	1:B:13:DC:H5'	0.43	1.90	12	1
1:B:6:DA:H4'	3:A:92:ARG:HG2	0.43	1.88	13	1
1:B:7:DG:H5'	3:A:92:ARG:CZ	0.43	2.42	12	1
3:A:19:LYS:HD2	3:A:19:LYS:N	0.43	2.29	13	1
1:B:7:DG:H8	1:B:7:DG:O5'	0.43	1.95	13	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
3:A:40:THR:CA	3:A:45:LYS:HE2	0.43	2.37	11	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
1:B:1:DG:C6	1:B:2:DG:C6	0.43	3.06	11	2
1:B:2:DG:C2	1:B:3:DC:C2	0.43	3.06	13	1
3:A:11:GLU:HG3	3:A:28:LEU:HG	0.43	1.90	11	1
2:C:16:DC:HO5'	2:C:16:DC:H6	0.43	1.56	11	1
2:C:25:DT:O4'	3:A:89:ARG:HD2	0.43	2.14	5	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
2:C:27:DA:H4'	3:A:90:GLY:O	0.43	2.14	13	1
1:B:8:DG:H5'	3:A:89:ARG:HA	0.43	1.90	11	1
3:A:40:THR:HA	3:A:45:LYS:HD3	0.43	1.90	12	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
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
2:C:27:DA:O5'	2:C:27:DA:C8	0.43	2.72	4	1
1:B:9:DG:N7	3:A:38:LYS:HE2	0.43	2.28	13	1
3:A:64:ARG:O	3:A:66:PRO:HD3	0.43	2.14	5	3
2:C:17:DT:H2''	2:C:18:DG:OP2	0.43	2.13	3	1
1:B:9:DG:H4'	3:A:87:ARG:CD	0.43	2.44	12	1
3:A:57:ILE:HD11	3:A:68:CYS:CB	0.43	2.44	6	1
1:B:14:DA:C2	1:B:15:DG:C5	0.43	3.06	6	1
2:C:27:DA:N3	3:A:92:ARG:HD3	0.43	2.28	13	1
1:B:7:DG:OP1	3:A:24:HIS:HA	0.43	2.14	5	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
3:A:30:CYS:SG	3:A:32:SER:HB2	0.42	2.54	14	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
2:C:27:DA:C4'	3:A:91:GLY:H	0.42	2.26	7	2
2:C:18:DG:H1'	2:C:19:DT:O4'	0.42	2.14	14	1
1:B:8:DG:H2'	3:A:38:LYS:CE	0.42	2.44	10	1
1:B:1:DG:H8	1:B:1:DG:HO5'	0.42	1.54	2	1
1:B:1:DG:C2	1:B:2:DG:C5	0.42	3.08	13	1
3:A:11:GLU:HG2	3:A:28:LEU:HD22	0.42	1.91	8	1
2:C:18:DG:H8	2:C:18:DG:O5'	0.42	1.98	3	1
1:B:1:DG:C2'	1:B:2:DG:C8	0.42	2.98	15	1
1:B:5:DC:H4'	3:A:103:ARG:HH12	0.42	1.75	8	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
3:A:19:LYS:H	3:A:19:LYS:HD2	0.42	1.74	13	1
3:A:41:VAL:CG2	3:A:83:VAL:HG11	0.42	2.45	12	2
3:A:38:LYS:HA	3:A:41:VAL:CG2	0.42	2.45	9	1
3:A:15:VAL:O	3:A:57:ILE:HB	0.42	2.14	2	1
1:B:7:DG:N2	1:B:8:DG:C4	0.42	2.87	13	1
1:B:12:DA:C2	1:B:13:DC:C2	0.42	3.08	8	1
1:B:6:DA:C2'	1:B:7:DG:OP2	0.42	2.66	14	1
3:A:73:CYS:HB3	3:A:78:MET:SD	0.42	2.54	2	1
2:C:16:DC:C6	2:C:16:DC:O5'	0.42	2.72	2	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:C:16:DC:C2'	2:C:17:DT:C7	0.42	2.98	2	1
2:C:25:DT:H4'	3:A:89:ARG:CZ	0.42	2.44	3	1
1:B:13:DC:C1'	1:B:14:DA:H5'	0.41	2.36	15	1
1:B:8:DG:C2'	1:B:9:DG:OP2	0.41	2.68	13	2
1:B:5:DC:H1'	3:A:92:ARG:NH2	0.41	2.31	1	1
1:B:8:DG:H2'	3:A:38:LYS:CD	0.41	2.45	2	1
1:B:8:DG:H5''	3:A:84:ARG:CB	0.41	2.37	8	1
2:C:20:DG:C3'	3:A:32:SER:HB2	0.41	2.44	1	1
1:B:8:DG:C2'	3:A:38:LYS:NZ	0.41	2.82	1	1
2:C:27:DA:H4'	3:A:90:GLY:CA	0.41	2.45	10	1
1:B:10:DC:C2'	1:B:11:DC:OP2	0.41	2.68	5	1
3:A:42:GLN:OE1	3:A:42:GLN:HA	0.41	2.15	15	2
3:A:27:LEU:N	3:A:27:LEU:HD13	0.41	2.30	3	2
1:B:8:DG:C5'	3:A:88:MET:O	0.41	2.67	3	1
3:A:73:CYS:HB3	3:A:78:MET:HG3	0.41	1.93	6	1
3:A:15:VAL:HG23	3:A:72:LYS:HB3	0.41	1.93	13	1
1:B:4:DT:H1'	1:B:5:DC:C5'	0.41	2.45	7	1
2:C:16:DC:H2''	2:C:17:DT:H72	0.41	1.92	15	1
2:C:28:DG:C2'	2:C:29:DC:OP2	0.41	2.67	13	1
3:A:84:ARG:NE	3:A:86:ASP:HB3	0.41	2.31	8	1
2:C:20:DG:H2''	2:C:21:DG:O5'	0.41	2.15	3	1
2:C:21:DG:C5	2:C:22:DC:C4	0.41	3.08	15	1
3:A:73:CYS:O	3:A:76:VAL:HG22	0.41	2.16	11	1
1:B:12:DA:C2'	1:B:13:DC:OP2	0.41	2.66	10	1
3:A:15:VAL:HG13	3:A:16:CYS:N	0.41	2.31	7	1
3:A:56:LYS:NZ	3:A:56:LYS:HB2	0.41	2.30	7	1
3:A:23:TYR:HA	3:A:28:LEU:HA	0.41	1.93	2	1
1:B:8:DG:OP1	3:A:83:VAL:HA	0.41	2.14	3	1
2:C:28:DG:C4'	3:A:92:ARG:HB2	0.41	2.45	3	1
3:A:84:ARG:HA	3:A:84:ARG:NE	0.40	2.31	15	1
2:C:19:DT:O5'	2:C:19:DT:H6	0.40	1.99	7	1
1:B:5:DC:H2''	1:B:6:DA:O5'	0.40	2.15	4	1
2:C:26:DG:H2''	2:C:27:DA:H8	0.40	1.76	14	1
2:C:24:DC:H2''	2:C:25:DT:H72	0.40	1.93	11	1
2:C:16:DC:H6	2:C:16:DC:O5'	0.40	1.98	2	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
1:B:9:DG:C4	1:B:10:DC:C4	0.40	3.10	8	1
1:B:7:DG:C4'	3:A:91:GLY:HA2	0.40	2.47	8	1
2:C:22:DC:C6	2:C:22:DC:O5'	0.40	2.73	14	1
2:C:21:DG:C4	2:C:22:DC:C4	0.40	3.10	1	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:A:94:LYS:HZ3	3:A:94:LYS:HB3	0.40	1.77	12	1
2:C:26:DG:H1'	3:A:91:GLY:CA	0.40	2.46	9	1
3:A:12:LEU:HD12	3:A:12:LEU:N	0.40	2.32	13	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

## 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%)	12	51
All	All	1488/1632 (91%)	1326 (89%)	130 (9%)	32 (2%)	12	51

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	50	THR	2
3	A	25	TYR	2
3	A	26	GLY	2
3	A	93	ASN	2
3	A	88	MET	1
3	A	24	HIS	1
3	A	17	GLY	1
3	A	91	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%)	80±1 (96±2%)	4±1 (4±2%)	38	83
All	All	1344/1440 (93%)	1286 (96%)	58 (4%)	38	83

All 30 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	44	ASN	6
3	A	102	ASP	4
3	A	71	GLN	4
3	A	43	ASN	4
3	A	72	LYS	3
3	A	27	LEU	3
3	A	87	ARG	3
3	A	76	VAL	2
3	A	99	TYR	2
3	A	19	LYS	2
3	A	32	SER	2
3	A	63	LYS	2
3	A	94	LYS	2
3	A	29	THR	2
3	A	23	TYR	2
3	A	89	ARG	1
3	A	92	ARG	1
3	A	30	CYS	1
3	A	83	VAL	1
3	A	64	ARG	1
3	A	81	GLU	1
3	A	84	ARG	1
3	A	67	PHE	1
3	A	56	LYS	1
3	A	59	LYS	1
3	A	15	VAL	1
3	A	45	LYS	1
3	A	46	HIS	1
3	A	31	GLU	1
3	A	58	ASP	1

### 6.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 6.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

### 6.6 Ligand geometry [i](#)

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