



# Full wwPDB NMR Structure Validation Report ⓘ

Apr 26, 2016 – 03:33 PM BST

PDB ID : 1IG4  
Title : Solution Structure of the Methyl-CpG-Binding Domain of Human MBD1 in Complex with Methylated DNA  
Authors : Ohki, I.; Shimotake, N.; Fujita, N.; Jee, J.-G.; Ikegami, T.; Nakao, M.; Shirakawa, M.  
Deposited on : 2001-04-17

This is a Full wwPDB NMR Structure Validation Report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/NMRValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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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  
Mogul : 1.7.1 (RC1), CSD as537be (2016)  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
RCI : v\_1n\_11\_5\_13\_A (Berjanski et al., 2005)  
PANAV : Wang et al. (2010)  
ShiftChecker : rb-20027457  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : rb-20027457

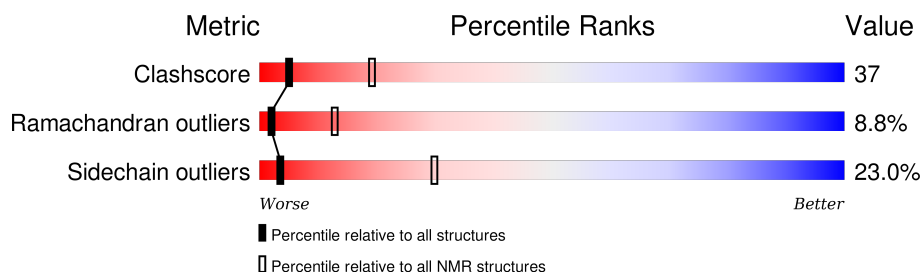
# 1 Overall quality at a glance

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	114402	11133
Ramachandran outliers	111179	9975
Sidechain outliers	111093	9958

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	12	
1	C	12	
2	A	75	

## 2 Ensemble composition and analysis

This entry contains 20 models. Model 6 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *lowest energy*.

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:5-A:69 (65)	0.27	6

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. No single-model clusters were found.

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

### 3 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 1949 atoms, of which 864 are hydrogens and 0 are deuteriums.

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

Mol	Chain	Residues	Atoms						Trace
1	B	12	Total	C	H	N	O	P	0
			383	118	139	45	70	11	
1	C	12	Total	C	H	N	O	P	0
			383	118	139	45	70	11	

- Molecule 2 is a protein called Methyl-CpG Binding Protein.

Mol	Chain	Residues	Atoms						Trace
2	A	75	Total	C	H	N	O	S	0
			1183	378	586	105	109	5	

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

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

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

- Molecule 1: 5'-D(\*GP\*TP\*AP\*TP\*CP\*(5CM)P\*GP\*GP\*AP\*TP\*AP\*C)-3'

Chain B: 



- Molecule 1: 5'-D(\*GP\*TP\*AP\*TP\*CP\*(5CM)P\*GP\*GP\*AP\*TP\*AP\*C)-3'

Chain C: 



- Molecule 2: Methyl-CpG Binding Protein

Chain A: 



### 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

- Molecule 1: 5'-D(\*GP\*TP\*AP\*TP\*CP\*(5CM)P\*GP\*GP\*AP\*TP\*AP\*C)-3'

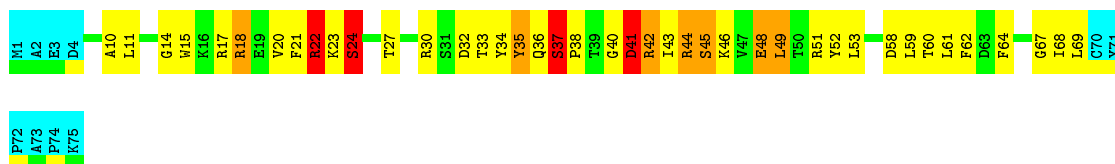
Chain B: 



- Molecule 1: 5'-D(\*GP\*TP\*AP\*TP\*CP\*(5CM)P\*GP\*GP\*AP\*TP\*AP\*C)-3'



- Molecule 2: Methyl-CpG Binding Protein



#### 4.2.2 Score per residue for model 2

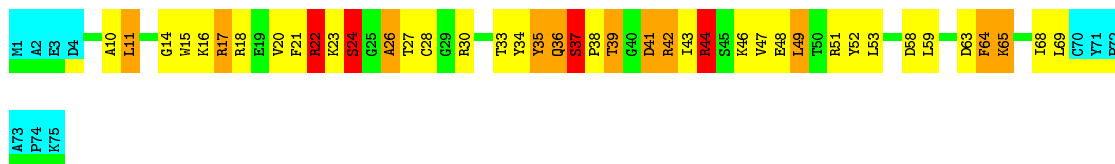
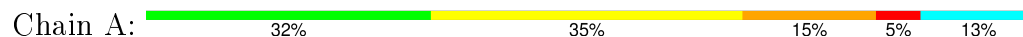
- Molecule 1: 5'-D(\*GP\*TP\*AP\*TP\*CP\*(5CM)P\*GP\*GP\*AP\*TP\*AP\*C)-3'



- Molecule 1: 5'-D(\*GP\*TP\*AP\*TP\*CP\*(5CM)P\*GP\*GP\*AP\*TP\*AP\*C)-3'



- Molecule 2: Methyl-CpG Binding Protein



#### 4.2.3 Score per residue for model 3

- Molecule 1: 5'-D(\*GP\*TP\*AP\*TP\*CP\*(5CM)P\*GP\*GP\*AP\*TP\*AP\*C)-3'

Chain B: 

G101  
T102  
A103  
T104  
C105  
G106  
G107  
G108  
A109  
T110  
A111  
G112

- Molecule 1: 5'-D(\*GP\*TP\*AP\*TP\*CP\*(5CM)P\*GP\*GP\*AP\*TP\*AP\*C)-3'

Chain C: 

G113  
T114  
A115  
T116  
C117  
G118  
G119  
G120  
A121  
T122  
A123  
G124

- Molecule 2: Methyl-CpG Binding Protein

Chain A: 

M1  
A2  
E3  
D4  
A10  
L11  
G14  
W15  
K16  
R17  
R18  
F21  
K23  
K23  
S24  
G25  
A26  
T27  
R30  
T33  
Y34  
Y35  
Q36  
S37  
P38  
T39  
G40  
D41  
R42  
I43  
R44  
S45  
K46  
V47  
E48  
L49  
T50  
R51  
Y52  
L53  
C57  
D58  
L59  
T60  
L61  
F62  
K65  
D66  
G67  
I68  
L69  
C70  
Y71  
Y72  
A73  
P74  
K75

#### 4.2.4 Score per residue for model 4

- Molecule 1: 5'-D(\*GP\*TP\*AP\*TP\*CP\*(5CM)P\*GP\*GP\*AP\*TP\*AP\*C)-3'

Chain B: 

G101  
T102  
A103  
T104  
C105  
G106  
G107  
G108  
A109  
T110  
A111  
G112

- Molecule 1: 5'-D(\*GP\*TP\*AP\*TP\*CP\*(5CM)P\*GP\*GP\*AP\*TP\*AP\*C)-3'

Chain C: 

G113  
T114  
A115  
T116  
C117  
G118  
G119  
G120  
A121  
T122  
A123  
G124

- Molecule 2: Methyl-CpG Binding Protein

Chain A: 

M1  
A2  
E3  
D4  
W5  
L6  
A10  
L11  
G14  
W15  
K16  
R17  
R18  
F21  
R22  
K23  
S24  
G25  
A26  
T27  
C28  
G29  
R30  
T33  
Y34  
Y35  
Q36  
S37  
P38  
T39  
G40  
D41  
R42  
I43  
R44  
S45  
K46  
V47  
E48  
L49  
T50  
R51  
Y52  
L53  
D58  
L59  
F62  
D63  
F64  
K65  
I68  
L69  
C70  
Y71  
Y72  
A73  
P74  
K75

### 4.2.5 Score per residue for model 5

- Molecule 1: 5'-D(\*GP\*TP\*AP\*TP\*CP\*(5CM)P\*GP\*GP\*AP\*TP\*AP\*C)-3'

Chain B: 



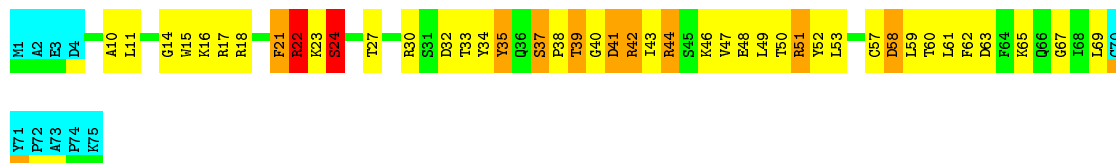
- Molecule 1: 5'-D(\*GP\*TP\*AP\*TP\*CP\*(5CM)P\*GP\*GP\*AP\*TP\*AP\*C)-3'

Chain C: 



- Molecule 2: Methyl-CpG Binding Protein

Chain A: 



### 4.2.6 Score per residue for model 6 (medoid)

- Molecule 1: 5'-D(\*GP\*TP\*AP\*TP\*CP\*(5CM)P\*GP\*GP\*AP\*TP\*AP\*C)-3'

Chain B: 



- Molecule 1: 5'-D(\*GP\*TP\*AP\*TP\*CP\*(5CM)P\*GP\*GP\*AP\*TP\*AP\*C)-3'

Chain C: 



- Molecule 2: Methyl-CpG Binding Protein

Chain A: 





K75

#### 4.2.7 Score per residue for model 7

- Molecule 1: 5'-D(\*GP\*TP\*AP\*TP\*CP\*(5CM)P\*GP\*GP\*AP\*TP\*AP\*C)-3'

Chain B: 

G101  
T102  
A103  
T104  
C105  
C106  
G107  
G108  
A109  
T110  
A111  
G112

- Molecule 1: 5'-D(\*GP\*TP\*AP\*TP\*CP\*(5CM)P\*GP\*GP\*AP\*TP\*AP\*C)-3'

Chain C: 

G113  
T114  
A115  
T116  
C117  
C118  
G119  
G120  
A121  
T122  
A123  
G124

- Molecule 2: Methyl-CpG Binding Protein

Chain A: 

M1  
A2  
E3  
D4  
W5  
A10  
L11  
G14  
W15  
K16  
R17  
R18  
F21  
R22  
K23  
S24  
T27  
C28  
G29  
R30  
S31  
D32  
T33  
Y34  
Y35  
Q36  
S37  
P38  
T39  
G40  
D41  
R42  
I43  
R44  
S45  
K46  
L49  
T50  
R51  
Y52  
L53  
D58  
L59  
T60  
L61  
F62  
D63  
F64  
I68  
L69  
C70  
Y71  
P72

A73  
P74  
K75

#### 4.2.8 Score per residue for model 8

- Molecule 1: 5'-D(\*GP\*TP\*AP\*TP\*CP\*(5CM)P\*GP\*GP\*AP\*TP\*AP\*C)-3'

Chain B: 

G101  
T102  
A103  
T104  
C105  
C106  
G107  
G108  
A109  
T110  
A111  
G112

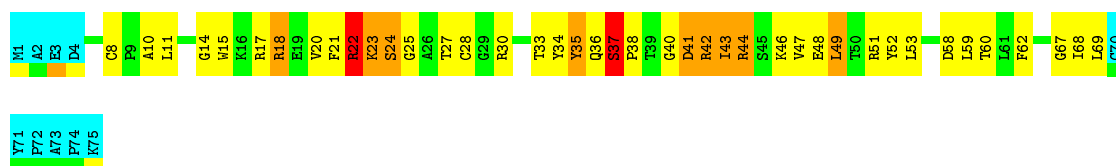
- Molecule 1: 5'-D(\*GP\*TP\*AP\*TP\*CP\*(5CM)P\*GP\*GP\*AP\*TP\*AP\*C)-3'

Chain C: 

G113  
T114  
A115  
T116  
C117  
C118  
G119  
G120  
A121  
T122  
A123  
G124

- Molecule 2: Methyl-CpG Binding Protein

Chain A: 



#### 4.2.9 Score per residue for model 9

- Molecule 1: 5'-D(\*GP\*TP\*AP\*TP\*CP\*(5CM)P\*GP\*GP\*AP\*TP\*AP\*C)-3'

Chain B: 8% 17% 75%



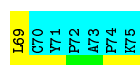
- Molecule 1: 5'-D(\*GP\*TP\*AP\*TP\*CP\*(5CM)P\*GP\*GP\*AP\*TP\*AP\*C)-3'

Chain C: 8% 25% 67%



- Molecule 2: Methyl-CpG Binding Protein

Chain A: 29% 41% 12% 13%



#### 4.2.10 Score per residue for model 10

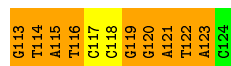
- Molecule 1: 5'-D(\*GP\*TP\*AP\*TP\*CP\*(5CM)P\*GP\*GP\*AP\*TP\*AP\*C)-3'

Chain B: 8% 25% 67%

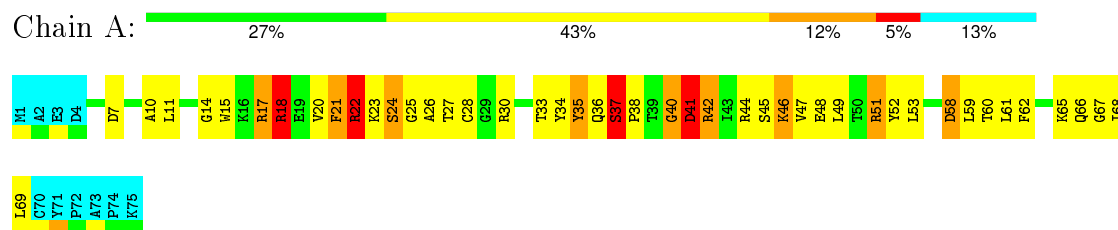


- Molecule 1: 5'-D(\*GP\*TP\*AP\*TP\*CP\*(5CM)P\*GP\*GP\*AP\*TP\*AP\*C)-3'

Chain C: 8% 17% 75%



- Molecule 2: Methyl-CpG Binding Protein



#### 4.2.11 Score per residue for model 11

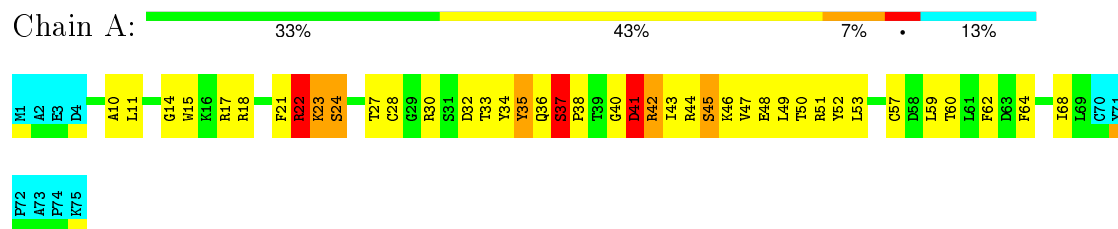
- Molecule 1: 5'-D(\*GP\*TP\*AP\*TP\*CP\*(5CM)P\*GP\*GP\*AP\*TP\*AP\*C)-3'



- Molecule 1: 5'-D(\*GP\*TP\*AP\*TP\*CP\*(5CM)P\*GP\*GP\*AP\*TP\*AP\*C)-3'



- Molecule 2: Methyl-CpG Binding Protein



#### 4.2.12 Score per residue for model 12

- Molecule 1: 5'-D(\*GP\*TP\*AP\*TP\*CP\*(5CM)P\*GP\*GP\*AP\*TP\*AP\*C)-3'

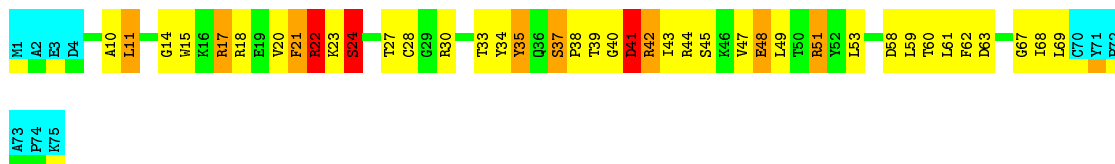


- Molecule 1: 5'-D(\*GP\*TP\*AP\*TP\*CP\*(5CM)P\*GP\*GP\*AP\*TP\*AP\*C)-3'





• Molecule 2: Methyl-CpG Binding Protein

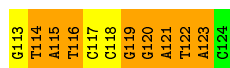


#### 4.2.13 Score per residue for model 13

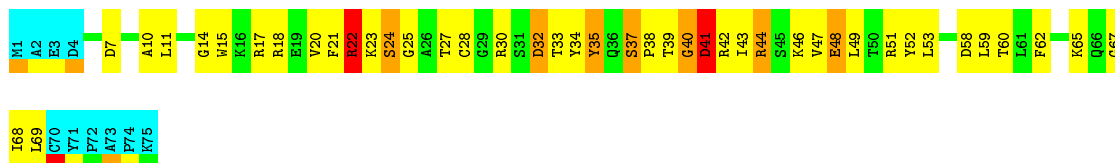
• Molecule 1: 5'-D(\*GP\*TP\*AP\*TP\*CP\*(5CM)P\*GP\*GP\*AP\*TP\*AP\*C)-3'



• Molecule 1: 5'-D(\*GP\*TP\*AP\*TP\*CP\*(5CM)P\*GP\*GP\*AP\*TP\*AP\*C)-3'



• Molecule 2: Methyl-CpG Binding Protein



#### 4.2.14 Score per residue for model 14

• Molecule 1: 5'-D(\*GP\*TP\*AP\*TP\*CP\*(5CM)P\*GP\*GP\*AP\*TP\*AP\*C)-3'



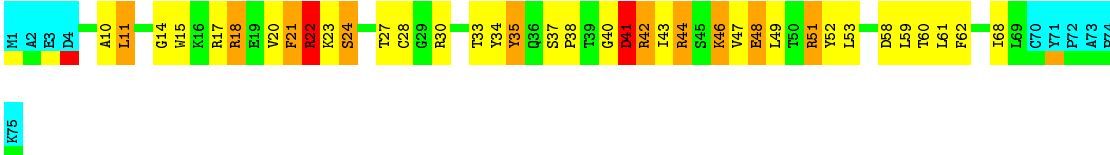
• Molecule 1: 5'-D(\*GP\*TP\*AP\*TP\*CP\*(5CM)P\*GP\*GP\*AP\*TP\*AP\*C)-3'

Chain C: 



• Molecule 2: Methyl-CpG Binding Protein

Chain A: 



#### 4.2.15 Score per residue for model 15

• Molecule 1: 5'-D(\*GP\*TP\*AP\*TP\*CP\*(5CM)P\*GP\*GP\*AP\*TP\*AP\*C)-3'

Chain B: 




• Molecule 1: 5'-D(\*GP\*TP\*AP\*TP\*CP\*(5CM)P\*GP\*GP\*AP\*TP\*AP\*C)-3'

Chain C: 



• Molecule 2: Methyl-CpG Binding Protein

Chain A: 



#### 4.2.16 Score per residue for model 16

• Molecule 1: 5'-D(\*GP\*TP\*AP\*TP\*CP\*(5CM)P\*GP\*GP\*AP\*TP\*AP\*C)-3'

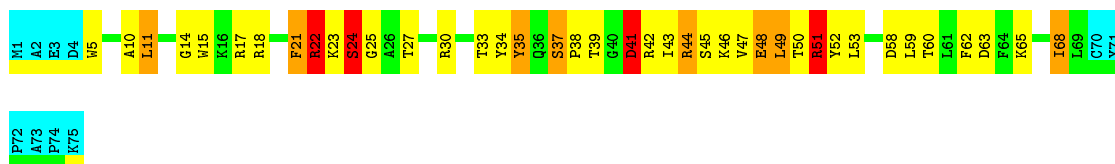
Chain B: 



- Molecule 1: 5'-D(\*GP\*TP\*AP\*TP\*CP\*(5CM)P\*GP\*GP\*AP\*TP\*AP\*C)-3'



- Molecule 2: Methyl-CpG Binding Protein



#### 4.2.17 Score per residue for model 17

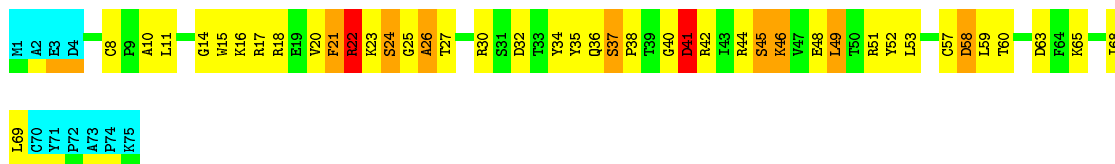
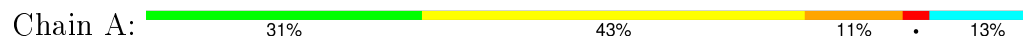
- Molecule 1: 5'-D(\*GP\*TP\*AP\*TP\*CP\*(5CM)P\*GP\*GP\*AP\*TP\*AP\*C)-3'



- Molecule 1: 5'-D(\*GP\*TP\*AP\*TP\*CP\*(5CM)P\*GP\*GP\*AP\*TP\*AP\*C)-3'



- Molecule 2: Methyl-CpG Binding Protein



#### 4.2.18 Score per residue for model 18

- Molecule 1: 5'-D(\*GP\*TP\*AP\*TP\*CP\*(5CM)P\*GP\*GP\*AP\*TP\*AP\*C)-3'

Chain B: 

G101  
T102  
A103  
T104  
C105  
G106  
G107  
G108  
A109  
T110  
A111  
G112

- Molecule 1: 5'-D(\*GP\*TP\*AP\*TP\*CP\*(5CM)P\*GP\*GP\*AP\*TP\*AP\*C)-3'

Chain C: 

G113  
T114  
A115  
T116  
C117  
G118  
G119  
G120  
T121  
T122  
A123  
G124

- Molecule 2: Methyl-CpG Binding Protein

Chain A: 

M1  
A2  
E3  
D4  
C8  
P9  
A10  
L11  
G14  
W15  
K16  
R17  
R18  
F21  
R22  
K23  
S24  
G25  
A26  
T27  
C28  
G29  
R30  
T33  
Y34  
Y35  
Q36  
S37  
P38  
T39  
G40  
D41  
R42  
I43  
R44  
S45  
K46  
V47  
E48  
L49  
T50  
R51  
Y52  
L53  
D58  
L59  
T60  
Q66  
G67  
I68  
L69  
C70  
Y71  
P72  
A73  
P74  
K75

#### 4.2.19 Score per residue for model 19

- Molecule 1: 5'-D(\*GP\*TP\*AP\*TP\*CP\*(5CM)P\*GP\*GP\*AP\*TP\*AP\*C)-3'

Chain B: 

G101  
T102  
A103  
T104  
C105  
G106  
G107  
G108  
A109  
T110  
A111  
G112

- Molecule 1: 5'-D(\*GP\*TP\*AP\*TP\*CP\*(5CM)P\*GP\*GP\*AP\*TP\*AP\*C)-3'

Chain C: 

G113  
T114  
A115  
T116  
C117  
G118  
G119  
G120  
T121  
T122  
A123  
G124

- Molecule 2: Methyl-CpG Binding Protein

Chain A: 

M1  
A2  
E3  
D4  
P9  
A10  
L11  
G14  
W15  
K16  
R17  
R18  
E19  
V20  
F21  
R22  
K23  
S24  
G25  
A26  
T27  
C28  
G29  
R30  
T33  
Y34  
Y35  
Q36  
S37  
P38  
T39  
G40  
D41  
R42  
I43  
R44  
S45  
K46  
V47  
E48  
L49  
T50  
R51  
Y52  
L53  
D58  
L59  
T60  
L61  
F62  
D63  
P64  
K65  
Q66  
G67  
I68  
I69  
C70  
Y71  
P72  
A73  
P74  
K75

#### 4.2.20 Score per residue for model 20

- Molecule 1: 5'-D(\*GP\*TP\*AP\*TP\*CP\*(5CM)P\*GP\*GP\*AP\*TP\*AP\*C)-3'

Chain B: 

G101  
T102  
A103  
T104  
C105  
G106  
G107  
G108  
A109  
T110  
A111  
G112

- Molecule 1: 5'-D(\*GP\*TP\*AP\*TP\*CP\*(5CM)P\*GP\*GP\*AP\*TP\*AP\*C)-3'

Chain C: 

G113  
T114  
A115  
T116  
C117  
G118  
G119  
G120  
A121  
T122  
A123  
G124

- Molecule 2: Methyl-CpG Binding Protein

Chain A: 

M1  
A2  
E3  
D4  
A10  
L11  
G14  
W15  
K16  
R17  
R18  
F21  
E22  
K23  
S24  
G25  
A26  
T27  
C28  
G29  
R30  
S31  
D32  
T33  
Y34  
Y35  
Q36  
S37  
P38  
T39  
G40  
D41  
R42  
I43  
I44  
V47  
E48  
L49  
T50  
R51  
T52  
L53  
D58  
L59  
T60  
L61  
F62  
D63  
G67  
I68  
L69  
C70  
Y71  
P72

A73  
P74  
K75



## 5 Refinement protocol and experimental data overview

The models were refined using the following method: *Structure calculations were performed following simulated annealing protocols using X-PLOR..*

Of the 200 calculated structures, 20 were deposited, based on the following criterion: *structures with the lowest energy.*

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

Software name	Classification	Version
X-PLOR	refinement	3.8

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 ⓘ

### 6.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: 5CM

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	1.29±0.01	0±0/250 (0.0±0.1%)	2.36±0.00	19±1/382 (4.9±0.2%)
1	C	1.29±0.01	0±0/250 (0.0±0.1%)	2.36±0.00	19±1/382 (5.0±0.2%)
2	A	1.03±0.00	0±0/534 (0.0±0.0%)	1.27±0.00	0±0/722 (0.0±0.0%)
All	All	1.16	3/20680 (0.0%)	1.91	751/29720 (2.5%)

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

Mol	Chain	Chirality	Planarity
2	A	0.0±0.0	6.9±0.3
All	All	0	138

All unique bond outliers are listed below. They are sorted according to the Z-score of the worst occurrence in the ensemble.

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
1	B	102	DT	C5-C7	5.08	1.53	1.50	4	1
1	C	116	DT	C5-C7	5.01	1.53	1.50	13	1
1	B	104	DT	C5-C7	5.01	1.53	1.50	14	1

All unique angle outliers are listed below. They are sorted according to the Z-score of the worst occurrence in the ensemble.

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	C	119	DG	N7-C8-N9	9.61	117.91	113.10	17	20
1	B	108	DG	N7-C8-N9	9.54	117.87	113.10	15	20
1	C	120	DG	N7-C8-N9	9.50	117.85	113.10	3	20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	B	107	DG	N7-C8-N9	9.45	117.82	113.10	12	20
1	B	101	DG	N7-C8-N9	9.40	117.80	113.10	15	20
1	C	113	DG	N7-C8-N9	9.35	117.78	113.10	4	20
1	C	121	DA	N7-C8-N9	8.12	117.86	113.80	3	20
1	B	109	DA	N7-C8-N9	8.12	117.86	113.80	12	20
1	B	103	DA	N7-C8-N9	8.09	117.84	113.80	12	20
1	C	123	DA	N7-C8-N9	8.00	117.80	113.80	1	20
1	B	111	DA	N7-C8-N9	7.87	117.73	113.80	7	20
1	C	115	DA	N7-C8-N9	7.78	117.69	113.80	20	20
1	C	113	DG	C8-N9-C4	-6.90	103.64	106.40	17	20
1	B	101	DG	C8-N9-C4	-6.83	103.67	106.40	10	20
1	B	108	DG	C8-N9-C4	-6.55	103.78	106.40	15	20
1	C	120	DG	C8-N9-C4	-6.47	103.81	106.40	13	20
1	B	107	DG	C8-N9-C4	-6.35	103.86	106.40	19	20
1	C	119	DG	C8-N9-C4	-6.14	103.94	106.40	8	20
1	C	122	DT	C6-C5-C7	-5.87	119.38	122.90	4	20
1	B	110	DT	C6-C5-C7	-5.84	119.39	122.90	13	20
1	B	104	DT	C6-C5-C7	-5.81	119.41	122.90	14	20
1	B	102	DT	C6-C5-C7	-5.80	119.42	122.90	11	20
1	C	114	DT	C6-C5-C7	-5.78	119.43	122.90	19	20
1	C	116	DT	C6-C5-C7	-5.75	119.45	122.90	1	20
1	C	119	DG	C5-N7-C8	-5.56	101.52	104.30	9	20
1	C	120	DG	C5-N7-C8	-5.47	101.56	104.30	7	20
1	B	107	DG	C5-N7-C8	-5.46	101.57	104.30	12	20
1	B	108	DG	C5-N7-C8	-5.41	101.59	104.30	3	20
1	B	101	DG	C5-N7-C8	-5.35	101.62	104.30	11	20
1	C	115	DA	C8-N9-C4	-5.34	103.66	105.80	12	18
1	C	113	DG	C5-N7-C8	-5.34	101.63	104.30	4	20
1	C	117	DC	O4'-C1'-N1	5.27	111.69	108.00	14	1
1	C	114	DT	C4-C5-C6	5.22	121.13	118.00	19	16
1	C	122	DT	C4-C5-C6	5.20	121.12	118.00	14	17
1	B	102	DT	C4-C5-C6	5.19	121.11	118.00	2	20
1	B	109	DA	C5-N7-C8	-5.18	101.31	103.90	12	9
1	B	110	DT	C4-C5-C6	5.18	121.11	118.00	6	14
1	B	104	DT	C4-C5-C6	5.17	121.10	118.00	1	15
1	C	116	DT	C4-C5-C6	5.17	121.10	118.00	4	7
1	C	123	DA	C8-N9-C4	-5.12	103.75	105.80	2	6
1	C	121	DA	C5-N7-C8	-5.12	101.34	103.90	13	10
1	B	103	DA	C8-N9-C4	-5.11	103.76	105.80	13	4
1	B	111	DA	C8-N9-C4	-5.10	103.76	105.80	13	4
1	B	103	DA	C5-N7-C8	-5.08	101.36	103.90	4	2

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	C	121	DA	C8-N9-C4	-5.07	103.77	105.80	18	4
1	B	111	DA	C5-N7-C8	-5.05	101.38	103.90	18	3
1	C	123	DA	C5-N7-C8	-5.02	101.39	103.90	13	1

There are no chirality outliers.

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

Mol	Chain	Res	Type	Group	Models (Total)
2	A	17	ARG	Sidechain	20
2	A	44	ARG	Sidechain	20
2	A	51	ARG	Sidechain	20
2	A	42	ARG	Sidechain	20
2	A	30	ARG	Sidechain	20
2	A	22	ARG	Sidechain	19
2	A	18	ARG	Sidechain	19

## 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	244	139	139	19±2
1	C	244	139	139	11±2
2	A	520	516	516	46±4
All	All	20160	15880	15880	1345

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 37.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:A:49:LEU:HD21	2:A:59:LEU:HD12	1.00	1.30	16	1
1:C:117:DC:H3'	2:A:45:SER:OG	0.98	1.58	1	6
2:A:11:LEU:HD11	2:A:49:LEU:HD21	0.97	1.30	9	11
2:A:43:ILE:HG21	2:A:49:LEU:HD12	0.88	1.44	20	8

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:A:11:LEU:HD22	2:A:15:TRP:CZ2	0.85	2.05	9	12
2:A:53:LEU:CD1	2:A:59:LEU:HD11	0.85	2.01	14	17
2:A:10:ALA:O	2:A:69:LEU:HD12	0.85	1.72	2	8
2:A:49:LEU:HD23	2:A:59:LEU:HD13	0.84	1.48	14	15
1:B:108:DG:H2''	1:B:109:DA:O5'	0.82	1.74	13	20
1:C:120:DG:H2''	1:C:121:DA:O5'	0.81	1.75	5	20
1:C:122:DT:H2''	1:C:123:DA:O5'	0.80	1.77	2	20
1:B:110:DT:H2''	1:B:111:DA:O5'	0.80	1.76	19	20
2:A:11:LEU:HD21	2:A:49:LEU:HD21	0.80	1.54	1	5
1:C:118:5CM:H2''	1:C:119:DG:O5'	0.79	1.77	6	20
1:B:106:5CM:H5A1	1:B:106:5CM:OP2	0.78	1.78	7	14
2:A:11:LEU:HD22	2:A:15:TRP:CE2	0.78	2.13	19	10
1:B:102:DT:H2''	1:B:103:DA:O5'	0.78	1.79	2	20
1:C:114:DT:H2''	1:C:115:DA:O5'	0.78	1.79	6	19
2:A:10:ALA:HB2	2:A:68:ILE:HA	0.78	1.55	17	16
1:B:106:5CM:OP2	1:B:106:5CM:H5A1	0.78	1.77	3	6
2:A:11:LEU:HD13	2:A:15:TRP:CE3	0.77	2.14	19	5
2:A:11:LEU:HD13	2:A:15:TRP:CD2	0.77	2.15	2	10
1:B:104:DT:H2''	1:B:105:DC:O5'	0.77	1.79	20	16
2:A:11:LEU:HD23	2:A:53:LEU:HD11	0.75	1.56	3	4
2:A:10:ALA:HB2	2:A:68:ILE:CA	0.75	2.11	10	15
2:A:11:LEU:HD21	2:A:49:LEU:CD2	0.75	2.12	1	7
2:A:53:LEU:HD13	2:A:59:LEU:HD11	0.74	1.57	3	6
2:A:50:THR:HG23	2:A:57:CYS:O	0.74	1.81	11	2
2:A:49:LEU:O	2:A:53:LEU:HD12	0.74	1.80	3	10
1:B:107:DG:H1'	1:B:108:DG:O4'	0.73	1.83	1	14
1:C:117:DC:H2''	1:C:118:5CM:O5'	0.73	1.84	19	17
2:A:14:GLY:C	2:A:38:PRO:HA	0.73	2.04	8	20
2:A:43:ILE:HG23	2:A:48:GLU:HB3	0.72	1.61	20	13
1:B:106:5CM:H2''	1:B:107:DG:O5'	0.71	1.84	17	20
2:A:15:TRP:CZ3	2:A:49:LEU:HD11	0.71	2.19	9	8
2:A:58:ASP:O	2:A:59:LEU:HD23	0.71	1.84	10	10
2:A:68:ILE:O	2:A:68:ILE:HD12	0.71	1.86	4	3
2:A:10:ALA:HB2	2:A:67:GLY:C	0.71	2.05	20	7
2:A:49:LEU:CD2	2:A:59:LEU:HD12	0.71	2.14	16	1
2:A:46:LYS:O	2:A:49:LEU:HD23	0.70	1.86	16	1
1:C:117:DC:H3'	2:A:45:SER:HG	0.69	1.47	18	1
2:A:11:LEU:CD2	2:A:53:LEU:HD11	0.69	2.17	3	15
2:A:49:LEU:HD23	2:A:59:LEU:CD1	0.68	2.18	17	14
2:A:11:LEU:CD2	2:A:49:LEU:HD11	0.68	2.19	10	4
2:A:15:TRP:CH2	2:A:49:LEU:HD13	0.67	2.24	11	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:A:11:LEU:HD21	2:A:49:LEU:HG	0.67	1.67	12	5
2:A:15:TRP:CH2	2:A:49:LEU:HD12	0.66	2.26	15	3
2:A:43:ILE:HG21	2:A:49:LEU:CD1	0.66	2.20	1	4
2:A:66:GLN:OE1	2:A:68:ILE:HD11	0.65	1.91	9	3
2:A:42:ARG:O	2:A:43:ILE:HD12	0.65	1.90	15	2
2:A:10:ALA:HB1	2:A:62:PHE:CD1	0.65	2.27	19	6
2:A:68:ILE:HD12	2:A:68:ILE:O	0.65	1.91	17	1
2:A:10:ALA:HB1	2:A:62:PHE:CD2	0.64	2.27	14	10
1:C:116:DT:H2''	1:C:117:DC:O5'	0.64	1.92	20	18
1:B:107:DG:OP2	2:A:27:THR:N	0.63	2.29	4	8
2:A:53:LEU:HD12	2:A:59:LEU:HD11	0.61	1.70	7	10
2:A:10:ALA:HB1	2:A:62:PHE:HD1	0.61	1.56	19	6
1:B:106:5CM:OP2	2:A:22:ARG:NE	0.60	2.33	11	20
2:A:10:ALA:HB2	2:A:68:ILE:N	0.60	2.11	19	9
1:B:105:DC:H2''	1:B:106:5CM:O5'	0.59	1.96	12	19
2:A:10:ALA:HB2	2:A:67:GLY:O	0.59	1.97	5	4
2:A:37:SER:OG	2:A:41:ASP:N	0.59	2.36	16	1
2:A:33:THR:HG22	2:A:35:TYR:CE2	0.59	2.32	19	14
1:C:117:DC:H3'	2:A:45:SER:CB	0.59	2.27	1	7
2:A:11:LEU:HD21	2:A:49:LEU:CG	0.57	2.30	13	6
2:A:49:LEU:HD22	2:A:62:PHE:CE2	0.57	2.35	3	1
2:A:40:GLY:O	2:A:41:ASP:CB	0.57	2.51	17	11
2:A:10:ALA:HB1	2:A:62:PHE:HD2	0.56	1.61	13	4
1:B:103:DA:H2'	1:B:104:DT:H72	0.55	1.78	11	10
1:C:116:DT:C4	1:C:117:DC:N4	0.55	2.75	14	5
2:A:43:ILE:HG23	2:A:48:GLU:CB	0.54	2.31	9	4
2:A:35:TYR:N	2:A:35:TYR:CD1	0.54	2.76	16	8
2:A:11:LEU:HD21	2:A:49:LEU:HD11	0.54	1.78	6	3
2:A:37:SER:OG	2:A:41:ASP:HB3	0.54	2.02	9	3
2:A:23:LYS:O	2:A:24:SER:CB	0.54	2.55	17	18
2:A:67:GLY:O	2:A:68:ILE:HG23	0.54	2.03	10	8
1:B:108:DG:C6	1:B:109:DA:N6	0.54	2.76	6	15
2:A:11:LEU:CD1	2:A:49:LEU:HD21	0.53	2.30	19	3
2:A:20:VAL:HG21	2:A:34:TYR:CD1	0.53	2.38	10	10
2:A:42:ARG:C	2:A:43:ILE:HD12	0.53	2.24	7	3
2:A:63:ASP:O	2:A:65:LYS:N	0.53	2.42	2	3
1:C:117:DC:O3'	2:A:47:VAL:HB	0.53	2.03	20	15
1:C:120:DG:C6	1:C:121:DA:N6	0.53	2.77	19	3
1:C:122:DT:C4	1:C:123:DA:N6	0.53	2.77	17	11
2:A:15:TRP:CH2	2:A:49:LEU:CD1	0.53	2.92	6	9
2:A:45:SER:OG	2:A:46:LYS:N	0.53	2.41	17	6

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:A:21:PHE:O	2:A:22:ARG:O	0.53	2.27	19	20
1:B:104:DT:C4	1:B:105:DC:N4	0.52	2.78	16	4
1:C:117:DC:C3'	2:A:45:SER:OG	0.52	2.48	11	1
2:A:37:SER:HB3	2:A:41:ASP:CB	0.52	2.35	10	8
2:A:15:TRP:CZ3	2:A:49:LEU:HD12	0.52	2.40	12	5
2:A:11:LEU:HD11	2:A:49:LEU:CD1	0.52	2.34	16	1
2:A:35:TYR:CD1	2:A:35:TYR:N	0.52	2.78	3	9
1:B:106:5CM:OP1	2:A:23:LYS:N	0.52	2.40	16	9
2:A:41:ASP:CB	2:A:52:TYR:CE1	0.52	2.92	17	1
1:B:109:DA:H2'	1:B:110:DT:H72	0.52	1.81	15	8
2:A:15:TRP:CZ3	2:A:49:LEU:CD1	0.51	2.93	14	12
2:A:43:ILE:HD13	2:A:48:GLU:OE2	0.51	2.05	13	1
2:A:5:TRP:O	2:A:6:LEU:HD23	0.51	2.05	4	1
1:B:101:DG:H2''	1:B:102:DT:O5'	0.51	2.05	12	4
1:B:110:DT:C4	1:B:111:DA:N6	0.51	2.78	5	5
2:A:48:GLU:O	2:A:51:ARG:HG3	0.51	2.06	16	1
1:B:107:DG:H2''	1:B:108:DG:O5'	0.51	2.04	6	6
2:A:11:LEU:HD13	2:A:15:TRP:CE2	0.51	2.41	20	3
2:A:38:PRO:HD2	2:A:52:TYR:CE2	0.51	2.41	10	3
2:A:9:PRO:HG2	2:A:68:ILE:HG22	0.51	1.83	19	2
2:A:24:SER:OG	2:A:25:GLY:N	0.50	2.44	8	7
2:A:17:ARG:NH2	2:A:35:TYR:CE2	0.50	2.79	12	1
1:B:107:DG:OP2	2:A:26:ALA:N	0.50	2.43	4	6
2:A:11:LEU:HD22	2:A:15:TRP:CH2	0.50	2.42	3	1
1:C:118:5CM:C5A	2:A:44:ARG:HG3	0.50	2.36	19	1
2:A:11:LEU:HD22	2:A:49:LEU:HD11	0.50	1.82	10	1
1:C:118:5CM:H5A3	2:A:44:ARG:CB	0.50	2.36	8	3
1:B:104:DT:C2'	1:B:105:DC:C6	0.50	2.94	11	4
2:A:37:SER:OG	2:A:52:TYR:CD2	0.49	2.65	18	4
1:C:117:DC:OP1	2:A:46:LYS:HB3	0.49	2.07	10	4
2:A:43:ILE:CD1	2:A:43:ILE:N	0.49	2.75	1	1
2:A:34:TYR:CD1	2:A:34:TYR:N	0.49	2.81	2	9
1:B:105:DC:O3'	2:A:23:LYS:HB2	0.49	2.07	12	6
1:C:113:DG:H2''	1:C:114:DT:O5'	0.49	2.07	10	3
2:A:15:TRP:CE2	2:A:38:PRO:HD3	0.49	2.42	18	15
1:B:107:DG:C8	2:A:27:THR:HG21	0.49	2.43	17	9
2:A:49:LEU:HD11	2:A:53:LEU:HD11	0.49	1.84	11	2
1:C:117:DC:OP1	2:A:46:LYS:CB	0.48	2.61	2	7
1:C:118:5CM:H5A3	2:A:44:ARG:HB3	0.48	1.85	4	3
1:B:107:DG:N7	2:A:22:ARG:NH1	0.48	2.61	2	9
2:A:15:TRP:CH2	2:A:43:ILE:HD13	0.48	2.43	8	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:103:DA:C2	1:C:123:DA:C2	0.48	3.02	5	1
1:B:109:DA:H2''	1:B:110:DT:O5'	0.48	2.09	10	7
2:A:23:LYS:O	2:A:24:SER:HB2	0.48	2.08	4	5
2:A:15:TRP:CZ2	2:A:49:LEU:CD1	0.48	2.97	18	2
1:B:106:5CM:H6	1:B:106:5CM:O5'	0.48	2.07	12	3
2:A:47:VAL:O	2:A:51:ARG:HG2	0.47	2.09	14	2
2:A:11:LEU:HD21	2:A:53:LEU:HD11	0.47	1.85	2	4
1:B:105:DC:H2''	1:B:106:5CM:OP2	0.47	2.10	20	2
1:B:108:DG:C2'	1:B:109:DA:C8	0.47	2.97	3	1
2:A:33:THR:HG22	2:A:35:TYR:CZ	0.47	2.44	19	1
2:A:11:LEU:HB2	2:A:15:TRP:CD1	0.47	2.44	13	12
2:A:37:SER:CB	2:A:38:PRO:CD	0.47	2.93	19	13
2:A:15:TRP:CZ2	2:A:49:LEU:HD13	0.47	2.43	11	1
1:B:107:DG:H8	2:A:27:THR:HG21	0.47	1.70	17	9
2:A:34:TYR:CD2	2:A:44:ARG:HB3	0.47	2.45	19	1
2:A:23:LYS:O	2:A:24:SER:HB3	0.46	2.10	11	1
1:B:107:DG:N7	2:A:22:ARG:NH2	0.46	2.63	1	9
1:B:105:DC:O3'	2:A:23:LYS:CB	0.46	2.63	16	6
2:A:34:TYR:N	2:A:34:TYR:CD1	0.46	2.82	17	3
2:A:49:LEU:CD1	2:A:53:LEU:HD11	0.46	2.40	18	2
1:B:102:DT:C4	1:B:103:DA:N6	0.46	2.84	15	2
2:A:33:THR:CG2	2:A:35:TYR:CE2	0.46	2.98	19	1
2:A:22:ARG:HG3	2:A:30:ARG:HB2	0.46	1.88	3	2
1:B:106:5CM:H3'	2:A:24:SER:O	0.46	2.11	18	10
1:B:106:5CM:H6	1:B:106:5CM:OP2	0.46	2.10	7	4
2:A:22:ARG:HB3	2:A:28:CYS:HA	0.46	1.87	12	14
2:A:22:ARG:NH1	2:A:27:THR:HB	0.46	2.25	12	2
1:C:116:DT:H2''	1:C:117:DC:C6	0.46	2.46	10	5
2:A:64:PHE:CD2	2:A:65:LYS:N	0.46	2.84	2	1
1:B:111:DA:C2	1:C:115:DA:C2	0.46	3.03	18	1
2:A:49:LEU:HD23	2:A:50:THR:N	0.46	2.26	16	1
2:A:22:ARG:NH2	2:A:27:THR:CB	0.45	2.79	9	9
2:A:11:LEU:CB	2:A:15:TRP:CD1	0.45	2.99	16	2
2:A:22:ARG:NH1	2:A:27:THR:CB	0.45	2.80	2	7
2:A:15:TRP:CE3	2:A:36:GLN:O	0.45	2.70	8	8
1:B:107:DG:OP1	2:A:26:ALA:HB3	0.45	2.11	15	1
1:B:106:5CM:C2'	1:B:107:DG:O5'	0.45	2.63	11	5
2:A:41:ASP:HB2	2:A:52:TYR:CE1	0.45	2.47	17	3
1:B:106:5CM:N4	2:A:34:TYR:OH	0.45	2.50	4	6
1:B:107:DG:H2''	1:B:108:DG:OP2	0.45	2.11	5	1
2:A:37:SER:CB	2:A:41:ASP:CB	0.45	2.94	15	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:A:15:TRP:CZ3	2:A:43:ILE:HD12	0.45	2.47	3	2
2:A:37:SER:HB2	2:A:52:TYR:CD2	0.44	2.47	3	1
2:A:37:SER:CB	2:A:41:ASP:HB3	0.44	2.41	8	3
2:A:63:ASP:O	2:A:67:GLY:N	0.44	2.51	20	1
1:C:118:5CM:H5A3	2:A:44:ARG:HB2	0.44	1.90	8	1
2:A:37:SER:HB2	2:A:38:PRO:HD2	0.44	1.90	16	1
1:B:105:DC:H2'	1:B:106:5CM:H5A2	0.44	1.89	7	3
2:A:41:ASP:CB	2:A:52:TYR:CD1	0.44	3.00	17	1
2:A:32:ASP:HB3	2:A:34:TYR:CE2	0.44	2.48	7	2
1:B:104:DT:H2''	1:B:105:DC:C6	0.44	2.48	9	1
2:A:33:THR:O	2:A:35:TYR:CZ	0.44	2.71	2	5
1:C:121:DA:H2''	1:C:122:DT:O5'	0.43	2.13	19	2
1:C:118:5CM:H6	1:C:118:5CM:O5'	0.43	2.13	14	2
2:A:17:ARG:CZ	2:A:67:GLY:CA	0.43	2.96	12	1
2:A:41:ASP:OD2	2:A:52:TYR:CG	0.43	2.71	8	2
2:A:37:SER:HB3	2:A:38:PRO:CD	0.43	2.43	5	1
2:A:62:PHE:N	2:A:69:LEU:HD23	0.43	2.28	4	1
1:C:113:DG:H2''	1:C:114:DT:C6	0.43	2.48	3	4
2:A:37:SER:HB3	2:A:52:TYR:CD2	0.43	2.47	5	1
1:B:106:5CM:OP2	1:B:106:5CM:H6	0.43	2.13	8	3
1:C:121:DA:H2''	1:C:122:DT:C6	0.43	2.48	3	4
1:B:103:DA:C2'	1:B:104:DT:H71	0.43	2.44	19	1
2:A:36:GLN:CG	2:A:41:ASP:O	0.43	2.67	2	1
1:C:117:DC:OP2	2:A:64:PHE:CD1	0.43	2.72	11	1
1:C:123:DA:C2'	1:C:124:DC:C6	0.43	3.01	14	1
2:A:37:SER:CB	2:A:52:TYR:CE2	0.43	3.02	2	1
1:C:118:5CM:O5'	1:C:118:5CM:H6	0.43	2.13	6	2
2:A:64:PHE:CG	2:A:65:LYS:N	0.43	2.86	19	1
2:A:43:ILE:N	2:A:43:ILE:CD1	0.43	2.81	7	3
2:A:22:ARG:HD2	2:A:27:THR:OG1	0.43	2.13	3	2
1:C:119:DG:N7	2:A:44:ARG:NH1	0.43	2.67	20	1
2:A:41:ASP:OD2	2:A:52:TYR:CD1	0.43	2.72	18	5
2:A:37:SER:HB3	2:A:41:ASP:HB3	0.43	1.91	19	1
2:A:41:ASP:OD1	2:A:52:TYR:CE1	0.42	2.72	18	3
1:B:109:DA:H2'	1:B:110:DT:H71	0.42	1.91	10	2
2:A:39:THR:HG22	2:A:52:TYR:OH	0.42	2.13	5	1
1:C:118:5CM:C5A	2:A:44:ARG:CG	0.42	2.98	19	1
1:B:111:DA:H2''	1:B:112:DC:C6	0.42	2.50	14	3
2:A:10:ALA:O	2:A:69:LEU:CD1	0.42	2.67	20	5
1:C:121:DA:H2'	1:C:122:DT:H71	0.42	1.90	4	2
2:A:37:SER:HB3	2:A:52:TYR:CE2	0.42	2.49	14	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:A:22:ARG:NH2	2:A:27:THR:HB	0.42	2.29	7	2
2:A:35:TYR:OH	2:A:64:PHE:CD1	0.42	2.72	7	1
1:C:117:DC:H3'	2:A:45:SER:HB3	0.42	1.92	4	2
2:A:37:SER:OG	2:A:41:ASP:CB	0.42	2.68	18	3
2:A:11:LEU:HB3	2:A:15:TRP:CD1	0.42	2.49	19	1
2:A:61:LEU:O	2:A:69:LEU:HD23	0.42	2.14	10	1
2:A:50:THR:HA	2:A:53:LEU:HD12	0.42	1.91	11	1
1:B:101:DG:H2''	1:B:102:DT:C6	0.42	2.50	19	5
2:A:33:THR:O	2:A:35:TYR:CE1	0.42	2.73	11	3
2:A:11:LEU:HD21	2:A:49:LEU:CD1	0.42	2.44	16	1
2:A:41:ASP:CG	2:A:52:TYR:CE1	0.42	2.94	16	1
2:A:41:ASP:OD2	2:A:52:TYR:CD2	0.42	2.73	19	1
2:A:35:TYR:OH	2:A:64:PHE:CD2	0.42	2.73	1	1
1:C:117:DC:OP2	2:A:64:PHE:CD2	0.41	2.72	15	1
1:C:119:DG:H2''	1:C:120:DG:C8	0.41	2.50	5	2
2:A:20:VAL:CG2	2:A:34:TYR:CD1	0.41	3.02	17	1
2:A:41:ASP:CG	2:A:52:TYR:CD1	0.41	2.94	11	1
1:B:103:DA:H2''	1:B:104:DT:C6	0.41	2.50	14	2
1:B:111:DA:H2'	1:B:112:DC:C5	0.41	2.51	14	1
2:A:47:VAL:O	2:A:51:ARG:HG3	0.41	2.15	5	2
1:B:105:DC:O3'	2:A:23:LYS:CG	0.41	2.68	9	2
1:B:108:DG:C6	1:B:109:DA:C6	0.41	3.09	3	2
1:B:105:DC:O3'	2:A:23:LYS:HB3	0.41	2.15	11	2
1:B:107:DG:OP2	2:A:27:THR:OG1	0.41	2.34	4	1
2:A:37:SER:HB3	2:A:38:PRO:HD2	0.41	1.92	8	3
2:A:47:VAL:O	2:A:51:ARG:CG	0.41	2.68	3	2
2:A:53:LEU:HD13	2:A:59:LEU:CD1	0.41	2.40	3	1
1:C:123:DA:H2''	1:C:124:DC:C6	0.41	2.50	4	2
2:A:41:ASP:HB2	2:A:52:TYR:CE2	0.41	2.51	6	2
2:A:22:ARG:O	2:A:23:LYS:CE	0.41	2.68	6	2
2:A:11:LEU:CD2	2:A:49:LEU:HD21	0.41	2.37	13	1
2:A:37:SER:HB2	2:A:41:ASP:CB	0.41	2.46	11	2
2:A:15:TRP:CH2	2:A:43:ILE:CD1	0.41	3.03	5	2
2:A:37:SER:CB	2:A:41:ASP:HB2	0.41	2.46	12	1
2:A:38:PRO:O	2:A:39:THR:HB	0.41	2.16	2	1
2:A:36:GLN:O	2:A:37:SER:O	0.41	2.38	2	1
2:A:32:ASP:HB3	2:A:34:TYR:CE1	0.41	2.51	5	4
2:A:41:ASP:HB3	2:A:52:TYR:CE2	0.41	2.51	19	1
2:A:62:PHE:CD1	2:A:62:PHE:C	0.41	2.94	16	1
2:A:24:SER:HA	2:A:28:CYS:HB3	0.41	1.93	7	1
2:A:17:ARG:CZ	2:A:67:GLY:HA3	0.41	2.46	12	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:A:25:GLY:O	2:A:26:ALA:HB2	0.41	2.15	3	1
2:A:49:LEU:CD2	2:A:59:LEU:HD13	0.41	2.43	3	1
1:C:123:DA:H2'	1:C:124:DC:C5	0.40	2.51	5	2
2:A:21:PHE:CG	2:A:21:PHE:O	0.40	2.73	6	1
2:A:14:GLY:CA	2:A:38:PRO:HA	0.40	2.45	6	1
2:A:49:LEU:HD22	2:A:62:PHE:CZ	0.40	2.50	10	1
2:A:15:TRP:CD1	2:A:38:PRO:HB3	0.40	2.52	11	1
2:A:15:TRP:NE1	2:A:38:PRO:HD3	0.40	2.32	2	1
2:A:39:THR:O	2:A:39:THR:HG23	0.40	2.16	2	1
1:B:107:DG:OP2	2:A:27:THR:HG23	0.40	2.17	15	1
2:A:18:ARG:O	2:A:33:THR:HG23	0.40	2.16	1	2
1:B:107:DG:C2'	1:B:108:DG:OP2	0.40	2.69	5	1
2:A:40:GLY:O	2:A:41:ASP:HB2	0.40	2.17	5	1
1:B:106:5CM:H5A1	2:A:22:ARG:HE	0.40	1.77	20	1
2:A:52:TYR:C	2:A:52:TYR:CD1	0.40	2.95	14	1
2:A:33:THR:CG2	2:A:35:TYR:CZ	0.40	3.05	19	1
2:A:15:TRP:CZ3	2:A:43:ILE:CD1	0.40	3.04	5	1
1:B:106:5CM:O5'	1:B:106:5CM:H6	0.40	2.16	6	1
1:B:108:DG:H2''	1:B:109:DA:C8	0.40	2.51	3	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	
2	A	65/75 (87%)	49±2 (75±2%)	11±2 (16±3%)	6±1 (9±2%)	2	13
All	All	1300/1500 (87%)	975 (75%)	210 (16%)	115 (9%)	2	13

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)
2	A	22	ARG	20
2	A	41	ASP	19
2	A	24	SER	19

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Mol	Chain	Res	Type	Models (Total)
2	A	37	SER	18
2	A	39	THR	11
2	A	26	ALA	9
2	A	40	GLY	9
2	A	64	PHE	3
2	A	7	ASP	2
2	A	68	ILE	2
2	A	58	ASP	2
2	A	66	GLN	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	
2	A	55/63 (87%)	42±2 (77±3%)	13±2 (23±3%)	3	30
All	All	1100/1260 (87%)	847 (77%)	253 (23%)	3	30

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)
2	A	22	ARG	20
2	A	60	THR	18
2	A	41	ASP	18
2	A	35	TYR	17
2	A	58	ASP	14
2	A	42	ARG	13
2	A	45	SER	12
2	A	48	GLU	12
2	A	21	PHE	11
2	A	44	ARG	10
2	A	65	LYS	10
2	A	23	LYS	9
2	A	24	SER	9
2	A	37	SER	8
2	A	63	ASP	8
2	A	49	LEU	8

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Mol	Chain	Res	Type	Models (Total)
2	A	16	LYS	8
2	A	68	ILE	7
2	A	11	LEU	7
2	A	46	LYS	6
2	A	17	ARG	5
2	A	8	CYS	4
2	A	18	ARG	4
2	A	32	ASP	4
2	A	36	GLN	3
2	A	51	ARG	3
2	A	57	CYS	2
2	A	66	GLN	1
2	A	7	ASP	1
2	A	43	ILE	1

### 6.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

2 non-standard protein/DNA/RNA residues are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths		
					Counts	RMSZ	#Z>2
1	5CM	B	106	1	13,21,22	0.83±0.01	0±0 (0±0%)
1	5CM	C	118	1	13,21,22	0.82±0.01	0±0 (0±0%)

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

the bond angles.

Mol	Type	Chain	Res	Link	Bond angles		
					Counts	RMSZ	#Z>2
1	5CM	B	106	1	17,30,33	0.91±0.01	0±0 (0±0%)
1	5CM	C	118	1	17,30,33	1.04±0.01	0±0 (0±0%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	5CM	B	106	1	-	0±0,3,21,22	0±0,2,2,2
1	5CM	C	118	1	-	0±0,3,21,22	0±0,2,2,2

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 6.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.6 Ligand geometry [i](#)

There are no ligands in this entry.

## 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