



Full wwPDB NMR Structure Validation Report ⓘ

Mar 5, 2026 – 11:52 AM UTC

PDB ID : 1IG4 / pdb_00001ig4
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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

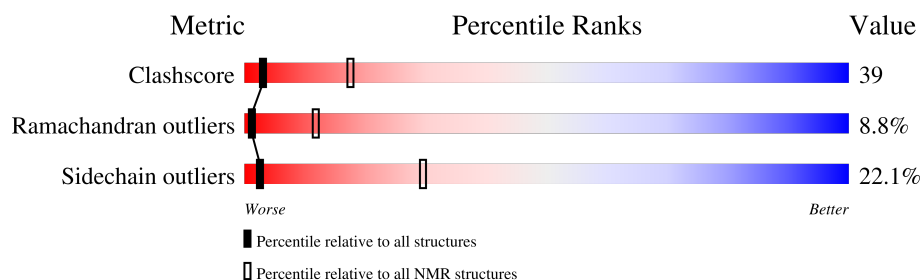
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment was not calculated.

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



Metric	Whole archive (#Entries)	NMR archive (#Entries)
Clashscore	229148	14424
Ramachandran outliers	224038	12848
Sidechain outliers	223484	12823

The table below summarises the geometric issues observed across the polymeric chains and their fit to the experimental data. The red, orange, yellow and green segments indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A cyan segment indicates the fraction of residues that are not part of the well-defined cores, and a grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	B	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)	0.47	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.

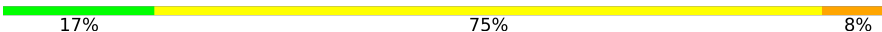
Mol	Chain	Residues	Atoms						Trace
2	A	75	Total	C	H	N	O	S	0
			1183	378	586	105	109	5	

4 Residue-property plots [i](#)

4.1 Average score per residue in the NMR ensemble

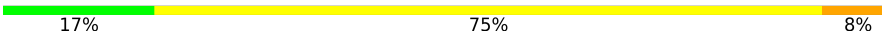
These plots are provided for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic is the same as shown in the summary in section 1 of this report. The second graphic shows the sequence where residues are colour-coded according to the number of geometric quality criteria for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

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

Chain B: 

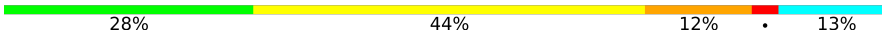


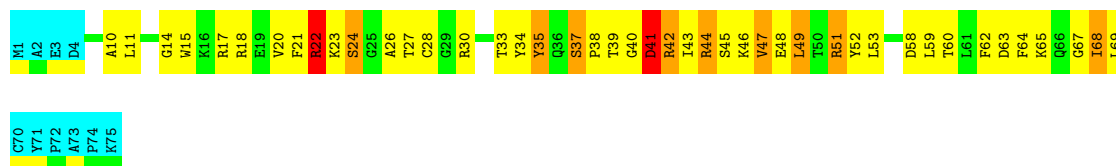
- Molecule 1: 5'-D(*GP*TP*AP*TP*CP*(5CM)P*GP*GP*AP*TP*AP*C)-3'

Chain C: 



- Molecule 2: Methyl-CpG Binding Protein

Chain A: 

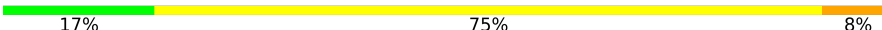


4.2 Scores per residue for each member of the ensemble

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'

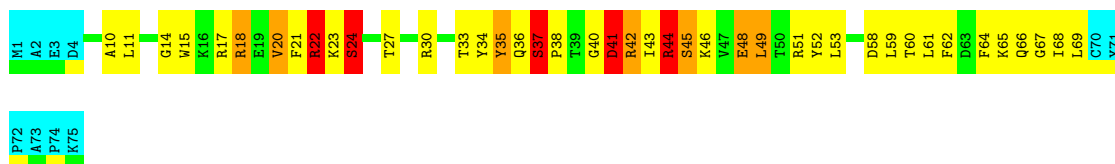
Chain B: 



- 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

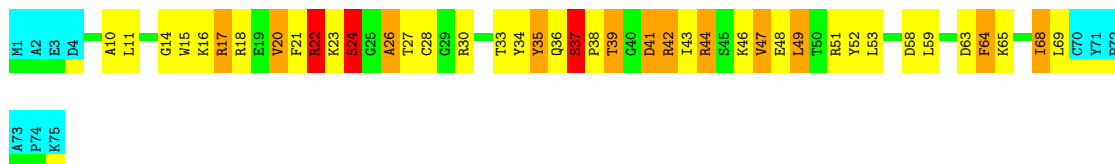
- Molecule 1: 5'-D(*GP*TP*AP*TP*CP*(5CM)P*GP*GP*AP*TP*AP*C)-3'



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

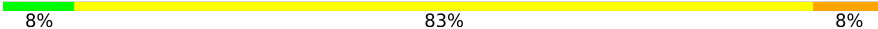


- Molecule 2: Methyl-CpG Binding Protein



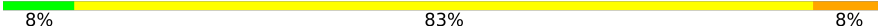
4.2.3 Score per residue for model 3

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

Chain B: 

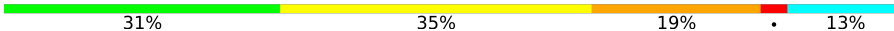
G101
T102
A103
T104
C105
G106
G107
G108
A109
T110
A111
C112

- 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
C124

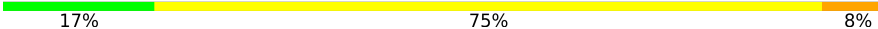
- Molecule 2: Methyl-CpG Binding Protein

Chain A: 

M1
A2
E3
D4
A10
L11
G14
W15
K16
R17
R18
E19
F20
F21
K22
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
D58
L59
T60
L61
F62
K65
Q66
G67
I68
L69
C70
Y71
P72
A73
P74
K75

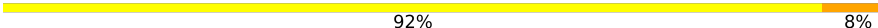
4.2.4 Score per residue for model 4

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

Chain B: 

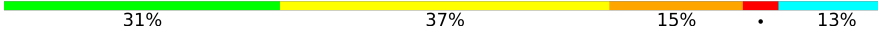
G101
T102
A103
T104
C105
G106
G107
G108
A109
T110
A111
C112

- 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
C124

- Molecule 2: Methyl-CpG Binding Protein

Chain A: 

M1
A2
E3
D4
V5
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
P72
A73
P74
K75

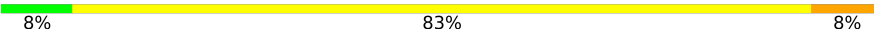
4.2.5 Score per residue for model 5

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

Chain B: 



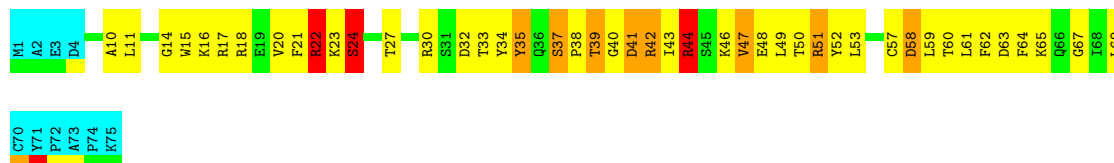
- Molecule 1: 5'-D(*GP*TP*AP*TP*CP*(5CM)P*GP*GP*AP*TP*AP*C)-3'

Chain C: 



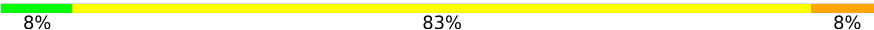
- Molecule 2: Methyl-CpG Binding Protein

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: 

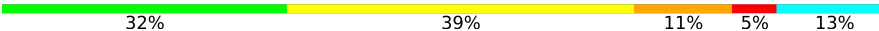


- Molecule 1: 5'-D(*GP*TP*AP*TP*CP*(5CM)P*GP*GP*AP*TP*AP*C)-3'

Chain C: 



- Molecule 2: Methyl-CpG Binding Protein

Chain A: 





4.2.7 Score per residue for model 7

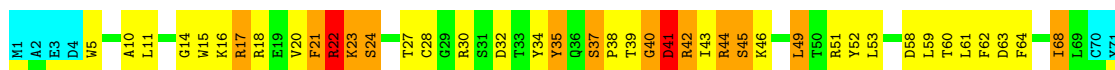
- Molecule 1: 5'-D(*GP*TP*AP*TP*CP*(5CM)P*GP*GP*AP*TP*AP*C)-3'



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



- Molecule 2: Methyl-CpG Binding Protein



4.2.8 Score per residue for model 8

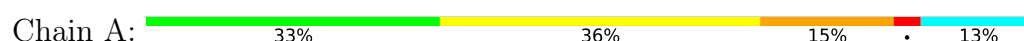
- Molecule 1: 5'-D(*GP*TP*AP*TP*CP*(5CM)P*GP*GP*AP*TP*AP*C)-3'

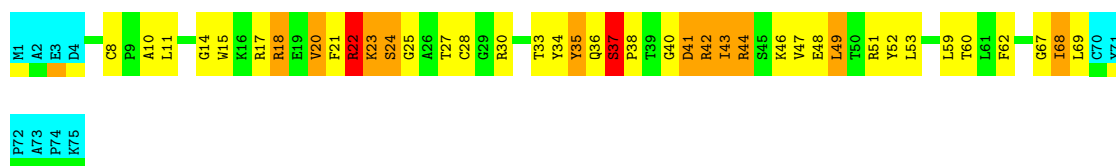


- Molecule 1: 5'-D(*GP*TP*AP*TP*CP*(5CM)P*GP*GP*AP*TP*AP*C)-3'



- Molecule 2: Methyl-CpG Binding Protein





4.2.9 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% 83% 8%



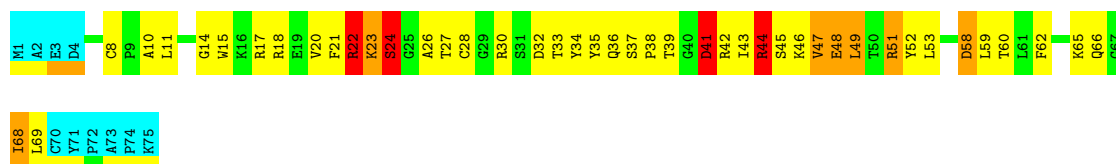
- Molecule 1: 5'-D(*GP*TP*AP*TP*CP*(5CM)P*GP*GP*AP*TP*AP*C)-3'

Chain C: 17% 75% 8%



- Molecule 2: Methyl-CpG Binding Protein

Chain A: 28% 44% 9% 5% 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: 17% 75% 8%

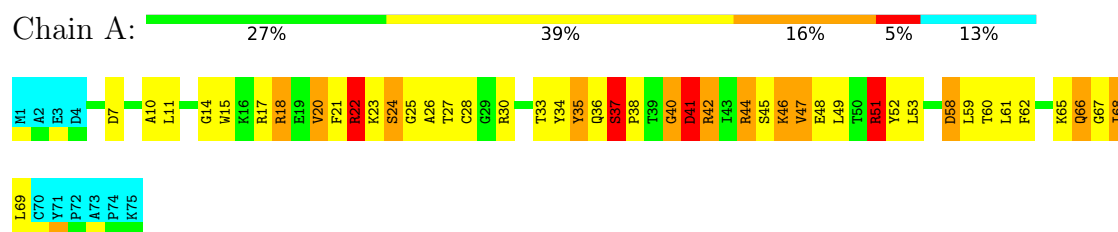


- Molecule 1: 5'-D(*GP*TP*AP*TP*CP*(5CM)P*GP*GP*AP*TP*AP*C)-3'

Chain C: 8% 83% 8%



- Molecule 2: Methyl-CpG Binding Protein

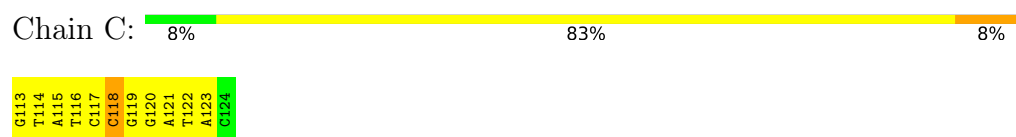


4.2.11 Score per residue for model 11

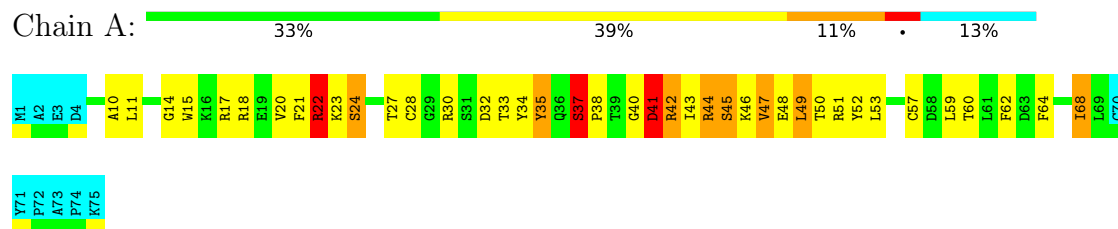
- Molecule 1: 5'-D(*GP*TP*AP*TP*CP*(5CM)P*GP*GP*AP*TP*AP*C)-3'



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

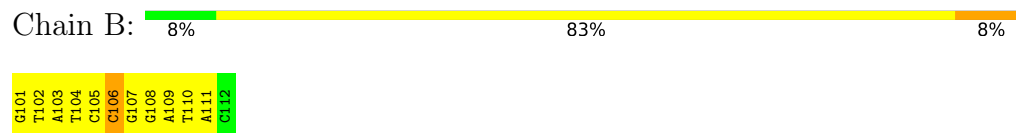


- Molecule 2: Methyl-CpG Binding Protein



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'

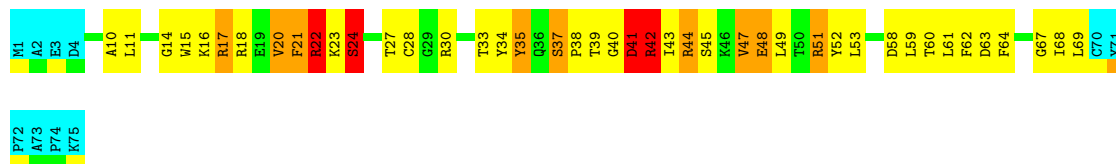


- Molecule 1: 5'-D(*GP*TP*AP*TP*CP*(5CM)P*GP*GP*AP*TP*AP*C)-3'





• Molecule 2: Methyl-CpG Binding Protein



4.2.13 Score per residue for model 13

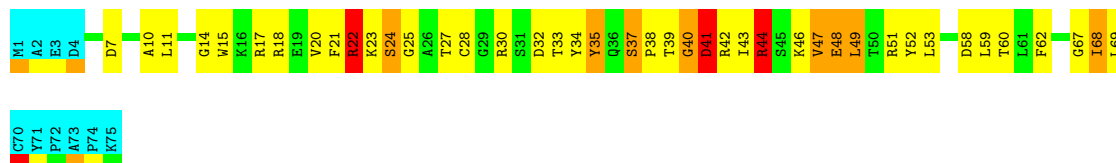
• Molecule 1: 5'-D(*GP*TP*AP*TP*CP*(5CM)P*GP*GP*AP*TP*AP*C)-3'



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



• Molecule 2: Methyl-CpG Binding Protein

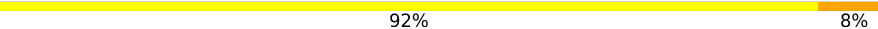


4.2.14 Score per residue for model 14

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

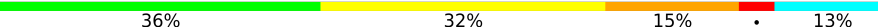


• Molecule 1: 5'-D(*GP*TP*AP*TP*CP*(5CM)P*GP*GP*AP*TP*AP*C)-3'

Chain C:  92% 8%

G113
T114
A115
T116
C117
G118
G119
G120
A121
T122
A123
C124

• Molecule 2: Methyl-CpG Binding Protein

Chain A:  36% 32% 15% 13%

M1 A2 E3 D4 A10 L11 G14 W15 K16 R17 R18 E19 V20 F21 R22 K23 S24 T27 C28 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 I68 L69 C70 Y71 P72 A73 P74
K75

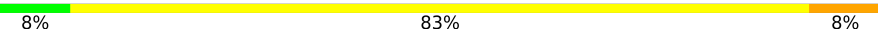
4.2.15 Score per residue for model 15

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

Chain B:  17% 75% 8%

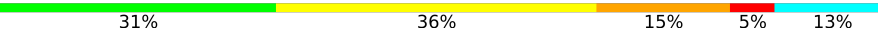
G101
T102
A103
T104
C105
G106
G107
G108
A109
T110
A111
C112

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

Chain C:  8% 83% 8%

G113
T114
A115
T116
C117
G118
G119
G120
A121
T122
A123
C124

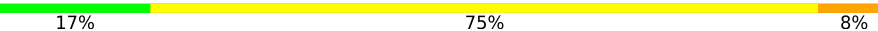
• Molecule 2: Methyl-CpG Binding Protein

Chain A:  31% 36% 15% 5% 13%

M1 A2 E3 D4 P9 A10 L11 G14 W15 K16 R17 R18 E19 V20 F21 R22 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 D58 L59 T60 L61 F62 D63 F64 G67 I68 L69 C70
Y71 P72 A73 P74 K75

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'

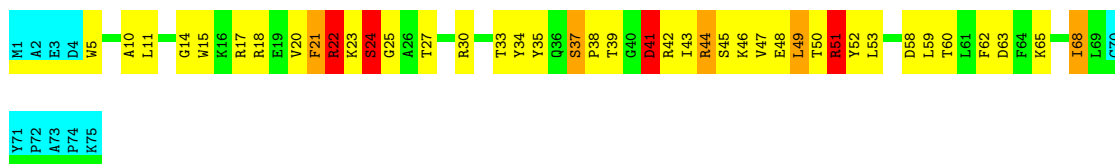
Chain B:  17% 75% 8%



- 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

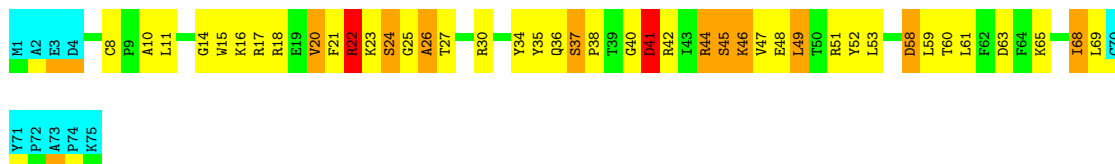
- Molecule 1: 5'-D(*GP*TP*AP*TP*CP*(5CM)P*GP*GP*AP*TP*AP*C)-3'



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

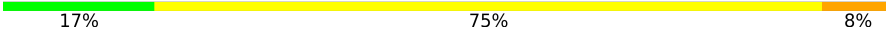


- Molecule 2: Methyl-CpG Binding Protein



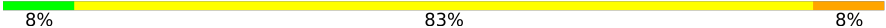
4.2.18 Score per residue for model 18

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

Chain B: 

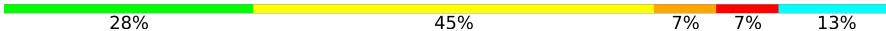
G101
T102
A103
T104
C105
G106
G107
G108
A109
T110
A111
G112

- 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
A121
T122
A123
G124

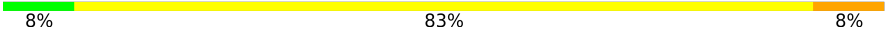
- Molecule 2: Methyl-CpG Binding Protein

Chain A: 

M1
A2
E3
D4
C8
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
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: 

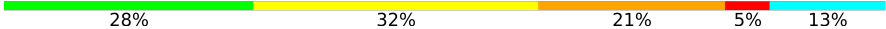
G101
T102
A103
T104
C105
G106
G107
G108
A109
T110
A111
G112

- 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
A121
T122
A123
G124

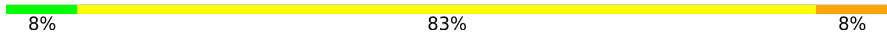
- Molecule 2: Methyl-CpG Binding Protein

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: 

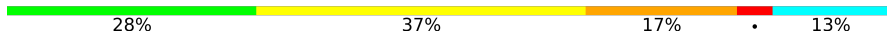
G101
T102
A103
T104
C105
G106
G107
G108
A109
T110
A111
G112

- 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
E19
V20
F21
R22
K23
S24
G25
A26
T27
C28
G29
R30
S31
D32
T33
Y34
Y35
Q36
S37
P38
T39
G40
D41
R42
T43
R44
V47
E48
L49
T50
R51
Y52
L53
D58
L59
T60
L61
F62
D63
F64
G67
R68
L69
G70

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.

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	0.56±0.00	0±0/250 (0.0± 0.0%)	1.27±0.00	0±0/382 (0.0± 0.0%)
1	C	0.56±0.00	0±0/250 (0.0± 0.0%)	1.27±0.00	0±0/382 (0.0± 0.0%)
2	A	1.44±0.01	0±0/534 (0.0± 0.0%)	1.53±0.01	2±0/722 (0.2± 0.1%)
All	All	1.11	0/20680 (0.0%)	1.40	33/29720 (0.1%)

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

There are no bond-length outliers.

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
2	A	47	VAL	N-CA-CB	-6.13	104.19	110.62	10	15
2	A	20	VAL	N-CA-CB	-5.95	105.27	112.35	17	18

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	30	ARG	Sidechain	20

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

6.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	B	244	139	139	19±2
1	C	244	139	139	12±2
2	A	520	516	516	48±4
All	All	20160	15880	15880	1396

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 39.

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
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:B:110:DT:H2''	1:B:111:DA:O5'	0.80	1.76	19	20
1:C:122:DT:H2''	1:C:123:DA:O5'	0.80	1.77	2	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:102:DT:H2''	1:B:103:DA:O5'	0.78	1.79	2	20
2:A:11:LEU:HD22	2:A:15:TRP:CE2	0.78	2.13	19	10

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
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
2:A:11:LEU:HD13	2:A:15:TRP:CE3	0.77	2.14	19	5
2:A:14:GLY:C	2:A:38:PRO:HA	0.77	2.04	8	20
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:10:ALA:HB2	2:A:67:GLY:C	0.76	2.05	20	8
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:106:5CM:OP2	1:B:106:5CM:H5A3	0.73	1.83	7	20
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: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:68:ILE:HD12	2:A:68:ILE:O	0.71	1.86	4	4
2:A:58:ASP:O	2:A:59:LEU:HD23	0.71	1.84	10	10
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
1:C:118:5CM:H5A2	2:A:44:ARG:HB3	0.69	1.64	16	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
2:A:11:LEU:HD21	2:A:49:LEU:HG	0.67	1.67	12	5
1:C:118:5CM:H5A1	2:A:44:ARG:CG	0.66	2.19	19	1
1:B:103:DA:H2'	1:B:104:DT:H72	0.66	1.65	19	11
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: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

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
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
1:C:117:DC:H3'	2:A:45:SER:CB	0.59	2.27	1	7
2:A:33:THR:HG22	2:A:35:TYR:CE2	0.59	2.32	19	14
2:A:42:ARG:C	2:A:43:ILE:HD12	0.58	2.24	7	4
1:C:118:5CM:H5A1	2:A:44:ARG:HG3	0.58	1.75	19	1
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
1:C:118:5CM:H5A1	2:A:44:ARG:HB2	0.57	1.76	3	15
2:A:10:ALA:HB1	2:A:62:PHE:HD2	0.56	1.61	13	4
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:CD1	2:A:35:TYR:N	0.54	2.76	16	17
2:A:37:SER:OG	2:A:41:ASP:HB3	0.54	2.02	9	3
2:A:11:LEU:HD21	2:A:49:LEU:HD11	0.54	1.78	6	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:20:VAL:HG21	2:A:34:TYR:CD1	0.53	2.38	10	10
2:A:11:LEU:CD1	2:A:49:LEU:HD21	0.53	2.30	19	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: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
1:C:118:5CM:H5A1	2:A:44:ARG:CB	0.52	2.34	4	2
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
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

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:A:5:TRP:O	2:A:6:LEU:HD23	0.51	2.05	4	1
2:A:43:ILE:HD13	2:A:48:GLU:OE2	0.51	2.05	13	1
1:B:101:DG:H2''	1:B:102:DT:O5'	0.51	2.05	12	4
1:C:118:5CM:H5A2	2:A:44:ARG:CB	0.51	2.35	16	1
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:45:SER:OG	2:A:46:LYS:N	0.51	2.42	7	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: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	3
2:A:34:TYR:N	2:A:34:TYR:CD1	0.49	2.81	2	5
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:B:107:DG:N7	2:A:22:ARG:NH1	0.48	2.61	2	9
1:B:103:DA:C2	1:C:123:DA:C2	0.48	3.02	5	1
2:A:15:TRP:CH2	2:A:43:ILE:HD13	0.48	2.43	8	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:O5'	1:B:106:5CM:H6	0.48	2.07	12	4
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

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
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:41:ASP:CG	2:A:52:TYR:CE1	0.46	2.94	16	6
2:A:23:LYS:O	2:A:24:SER:HB3	0.46	2.10	11	1
1:B:105:DC:O3'	2:A:23:LYS:CB	0.46	2.63	16	6
1:B:107:DG:N7	2:A:22:ARG:NH2	0.46	2.63	1	9
2:A:34:TYR:CD1	2:A:34:TYR:N	0.46	2.82	17	7
2:A:41:ASP:CG	2:A:52:TYR:CD1	0.46	2.94	11	8
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:OP2	1:B:106:5CM:H6	0.46	2.10	7	7
1:C:116:DT:H2''	1:C:117:DC:C6	0.46	2.46	10	5
2:A:22:ARG:NH1	2:A:27:THR:HB	0.46	2.25	12	2
2:A:22:ARG:HB3	2:A:28:CYS:HA	0.46	1.87	12	14
2:A:64:PHE:CD2	2:A:65:LYS:N	0.46	2.84	2	1
2:A:49:LEU:HD23	2:A:50:THR:N	0.46	2.26	16	1
1:B:111:DA:C2	1:C:115:DA:C2	0.46	3.03	18	1
2:A:22:ARG:NH2	2:A:27:THR:CB	0.45	2.79	9	9
2:A:62:PHE:CD1	2:A:62:PHE:C	0.45	2.94	16	6
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:52:TYR:C	2:A:52:TYR:CD1	0.45	2.95	14	2
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:15:TRP:CZ3	2:A:43:ILE:HD12	0.45	2.47	3	2
2:A:37:SER:CB	2:A:41:ASP:CB	0.45	2.94	15	3
2:A:37:SER:HB2	2:A:52:TYR:CD2	0.44	2.47	3	1
1:B:105:DC:C2'	1:B:106:5CM:H5A3	0.44	2.43	12	6
2:A:37:SER:CB	2:A:41:ASP:HB3	0.44	2.41	8	3
1:C:115:DA:H2'	1:C:116:DT:H71	0.44	1.90	10	2
2:A:63:ASP:O	2:A:67:GLY:N	0.44	2.51	20	1
2:A:37:SER:HB2	2:A:38:PRO:HD2	0.44	1.90	16	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
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
2:A:17:ARG:CZ	2:A:67:GLY:CA	0.43	2.96	12	1
1:C:118:5CM:O5'	1:C:118:5CM:H6	0.43	2.13	14	2
2:A:62:PHE:N	2:A:69:LEU:HD23	0.43	2.28	4	1
2:A:37:SER:HB3	2:A:38:PRO:CD	0.43	2.43	5	1
2:A:41:ASP:OD2	2:A:52:TYR:CG	0.43	2.71	8	2
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:C:121:DA:H2''	1:C:122:DT:C6	0.43	2.48	3	4
1:B:109:DA:H2'	1:B:110:DT:H71	0.43	1.88	3	2
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
2:A:22:ARG:HD2	2:A:27:THR:OG1	0.43	2.13	3	2
2:A:68:ILE:HD12	2:A:68:ILE:C	0.43	2.38	4	1
1:C:118:5CM:H6	1:C:118:5CM:O5'	0.43	2.13	6	2
2:A:64:PHE:CG	2:A:65:LYS:N	0.43	2.86	19	1
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
2:A:39:THR:HG22	2:A:52:TYR:OH	0.42	2.13	5	1
2:A:52:TYR:CD1	2:A:52:TYR:C	0.42	2.98	4	3
2:A:10:ALA:O	2:A:69:LEU:CD1	0.42	2.67	20	5
1:B:111:DA:H2''	1:B:112:DC:C6	0.42	2.50	14	3
1:C:121:DA:H2'	1:C:122:DT:H71	0.42	1.90	4	2
1:C:117:DC:H3'	2:A:45:SER:HB3	0.42	1.92	4	2
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
2:A:37:SER:HB3	2:A:52:TYR:CE2	0.42	2.49	14	1
2:A:37:SER:OG	2:A:41:ASP:CB	0.42	2.68	18	3
1:C:118:5CM:H5A1	2:A:44:ARG:HB3	0.42	1.90	4	1
2:A:61:LEU:O	2:A:69:LEU:HD23	0.42	2.14	10	1
2:A:11:LEU:HB3	2:A:15:TRP:CD1	0.42	2.49	19	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

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
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:35:TYR:OH	2:A:64:PHE:CD2	0.42	2.73	1	1
2:A:41:ASP:OD2	2:A:52:TYR:CD2	0.42	2.73	19	1
1:C:119:DG:H2''	1:C:120:DG:C8	0.41	2.50	5	2
1:C:117:DC:OP2	2:A:64:PHE:CD2	0.41	2.72	15	1
2:A:20:VAL:CG2	2:A:34:TYR:CD1	0.41	3.02	17	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: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
1:B:108:DG:C6	1:B:109:DA:C6	0.41	3.09	3	2
1:B:107:DG:OP2	2:A:27:THR:OG1	0.41	2.34	4	1
1:B:105:DC:O3'	2:A:23:LYS:HB3	0.41	2.15	11	2
2:A:61:LEU:C	2:A:69:LEU:HD23	0.41	2.39	17	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
2:A:64:PHE:CD1	2:A:64:PHE:C	0.41	2.98	1	4
1:C:123:DA:H2''	1:C:124:DC:C6	0.41	2.50	4	2
2:A:22:ARG:O	2:A:23:LYS:CE	0.41	2.68	6	2
2:A:41:ASP:HB2	2:A:52:TYR:CE2	0.41	2.51	6	2
2:A:43:ILE:N	2:A:43:ILE:CD1	0.41	2.84	12	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:11:LEU:CD2	2:A:49:LEU:HD21	0.41	2.37	13	1
2:A:27:THR:O	2:A:28:CYS:C	0.41	2.64	9	4
2:A:37:SER:CB	2:A:41:ASP:HB2	0.41	2.46	12	1
2:A:36:GLN:O	2:A:37:SER:O	0.41	2.38	2	1
2:A:25:GLY:O	2:A:26:ALA:HB2	0.41	2.15	3	1
2:A:32:ASP:HB3	2:A:34:TYR:CE1	0.41	2.51	5	4
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
2:A:41:ASP:HB3	2:A:52:TYR:CE2	0.41	2.51	19	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:14:GLY:CA	2:A:38:PRO:HA	0.40	2.45	6	1
2:A:21:PHE:O	2:A:21:PHE:CG	0.40	2.73	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:18:ARG:O	2:A:33:THR:HG23	0.40	2.16	1	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
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: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:107:DG:OP2	2:A:27:THR:HG23	0.40	2.17	15	1
1:B:103:DA:C2'	1:B:104:DT:H72	0.40	2.40	19	1
1:B:108:DG:H2''	1:B:109:DA:C8	0.40	2.51	3	1
2:A:15:TRP:CZ3	2:A:43:ILE:CD1	0.40	3.04	5	1
2:A:33:THR:CG2	2:A:35:TYR:CZ	0.40	3.05	19	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%)	10±2 (16±3%)	6±1 (9±2%)	1	12
All	All	1300/1500 (87%)	975 (75%)	210 (16%)	115 (9%)	1	12

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	24	SER	19
2	A	41	ASP	19
2	A	37	SER	18
2	A	39	THR	11
2	A	40	GLY	9
2	A	26	ALA	9
2	A	64	PHE	3
2	A	58	ASP	2
2	A	7	ASP	2
2	A	68	ILE	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%)	43±2 (78±3%)	12±2 (22±3%)	2	29
All	All	1100/1260 (87%)	857 (78%)	243 (22%)	2	29

All 29 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	41	ASP	18
2	A	60	THR	18
2	A	68	ILE	16
2	A	35	TYR	14
2	A	58	ASP	13
2	A	45	SER	12
2	A	49	LEU	12
2	A	42	ARG	12
2	A	48	GLU	11
2	A	24	SER	9
2	A	65	LYS	9
2	A	16	LYS	9
2	A	37	SER	8
2	A	44	ARG	8
2	A	23	LYS	8
2	A	63	ASP	7
2	A	21	PHE	6
2	A	46	LYS	6
2	A	51	ARG	6
2	A	17	ARG	4
2	A	8	CYS	4
2	A	66	GLN	3
2	A	18	ARG	3
2	A	43	ILE	3
2	A	36	GLN	1
2	A	7	ASP	1
2	A	47	VAL	1
2	A	11	LEU	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	18,21,22	0.53±0.01	0±0 (0±0%)
1	5CM	C	118	1	18,21,22	0.54±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	24,30,33	0.91±0.01	1±0 (4±0%)
1	5CM	C	118	1	24,30,33	1.00±0.01	1±0 (4±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±0,7,21,22	0±0,2,2,2
1	5CM	C	118	1	-	0±0,7,21,22	0±0,2,2,2

There are no bond-length outliers.

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	B	106	5CM	C5-C6-N1	2.58	120.51	123.31	13	20
1	C	118	5CM	C5-C6-N1	2.54	120.55	123.31	19	20

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

6.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.6 Ligand geometry [i](#)

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