Full wwPDB NMR Structure Validation Report (i)

Mar 1, 2022 – 02:19 PM EST

PDB ID	:	2EZE
Title	:	SOLUTION STRUCTURE OF A COMPLEX OF THE SECOND DNA BINDING DOMAIN OF HUMAN HMG-I(Y) BOUND TO DNA DODECAMER CONTAINING THE PRDII SITE OF THE INTERFERON-BETA PROMOTER, NMR, 35 STRUCTURES
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Deposited on	:	1997-06-04

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 (i) symbol.

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

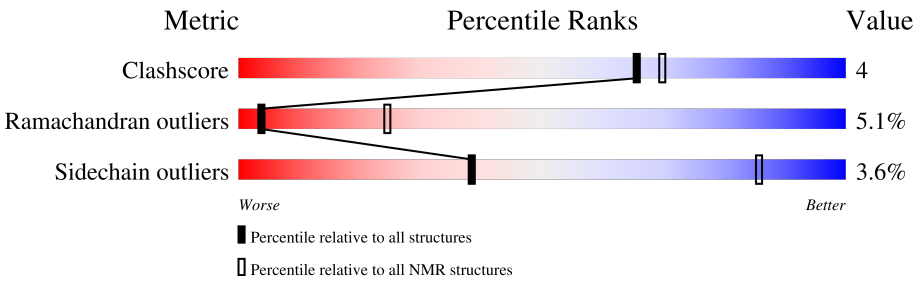
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
ShiftChecker	:	2.27
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.27

1 Overall quality at a glance (i)

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	158937	12864
Ramachandran outliers	154571	11451
Sidechain outliers	154315	11428

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 <=5%

Mol	Chain	Length	Quality of chain
1	B	12	67% 33%
2	C	12	67% 33%
3	A	25	32% 8% 60%

2 Ensemble composition and analysis (i)

This entry contains 35 models. Model 17 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:9-A:18 (10)	0.16	17

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 5 clusters. No single-model clusters were found.

Cluster number	Models
1	1, 4, 5, 6, 7, 8, 9, 11, 13, 14, 15, 16, 17, 20, 22, 23, 24, 25, 31, 32
2	2, 3, 10, 19, 26, 30, 34
3	21, 29, 33, 35
4	18, 28
5	12, 27

3 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 1168 atoms, of which 492 are hydrogens and 0 are deuteriums.

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

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	P	
1	B	12	380	117	137	45	70	11	0

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

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	P	
2	C	12	380	117	137	45	70	11	0

- Molecule 3 is a protein called HIGH MOBILITY GROUP PROTEIN HMG-I/HMG-Y.

Mol	Chain	Residues	Atoms					Trace
			Total	C	H	N	O	
3	A	25	408	116	218	44	30	0

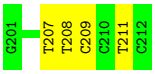
4 Residue-property plots (i)

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.

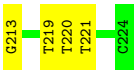
• Molecule 1: DNA (5'-D(*GP*GP*GP*AP*AP*AP*TP*TP*CP*CP*TP*C)-3')

Chain B: 67% 33%



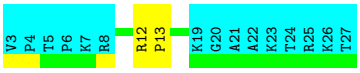
• Molecule 2: DNA (5'-D(*GP*AP*GP*GP*AP*AP*TP*TP*TP*CP*CP*C)-3')

Chain C: 67% 33%



• Molecule 3: HIGH MOBILITY GROUP PROTEIN HMG-I/HMG-Y

Chain A: 32% 8% 60%



4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

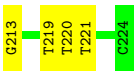
4.2.1 Score per residue for model 1

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

Chain B: 50% 50%

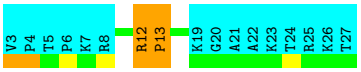
• Molecule 2: DNA (5'-D(*GP*AP*GP*GP*AP*AP*TP*TP*TP*CP*CP*C)-3')

Chain C: 67% 33%



• Molecule 3: HIGH MOBILITY GROUP PROTEIN HMG-I/HMG-Y

Chain A: 32% 8% 60%



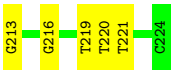
4.2.2 Score per residue for model 2

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

Chain B: 67% 33%

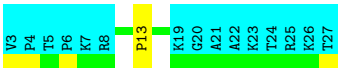
• Molecule 2: DNA (5'-D(*GP*AP*GP*GP*AP*AP*TP*TP*TP*CP*CP*C)-3')

Chain C: 58% 42%



• Molecule 3: HIGH MOBILITY GROUP PROTEIN HMG-I/HMG-Y

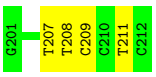
Chain A: 36% • 60%



4.2.3 Score per residue for model 3

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

Chain B: 67% 33%



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

Chain C: 58% 42%

G213 T219 T220 T221 C222 C223 C224

• Molecule 3: HIGH MOBILITY GROUP PROTEIN HMG-I/HMG-Y

Chain A: 36% • 60%

V3 P4 T5 P6 K7 R8 R12 K19 G20 A21 A22 K23 T24 R25 K26 T27

4.2.4 Score per residue for model 4

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

Chain B: 67% 33%

G201 G202 T207 T208 T211 C212

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

Chain C: 67% 25% 8%

G213 T219 T220 T221 C224

• Molecule 3: HIGH MOBILITY GROUP PROTEIN HMG-I/HMG-Y

Chain A: 40% 60%

V3 P4 T5 P6 K7 R8 K19 G20 A21 A22 K23 T24 R25 K26 T27

4.2.5 Score per residue for model 5

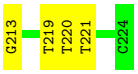
• Molecule 1: DNA (5'-D(*GP*GP*GP*AP*AP*AP*TP*TP*CP*CP*TP*C)-3')

Chain B: 67% 33%

G201 T207 T208 C209 C210 T211 C212

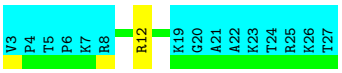
• Molecule 2: DNA (5'-D(*GP*AP*GP*GP*AP*AP*TP*TP*TP*CP*CP*C)-3')

Chain C: 67% 33%



• Molecule 3: HIGH MOBILITY GROUP PROTEIN HMG-I/HMG-Y

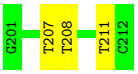
Chain A:



4.2.6 Score per residue for model 6

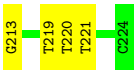
• Molecule 1: DNA (5'-D(*GP*GP*GP*AP*AP*AP*TP*TP*CP*CP*TP*C)-3')

Chain B:



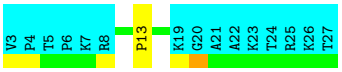
• Molecule 2: DNA (5'-D(*GP*AP*GP*GP*AP*AP*TP*TP*TP*CP*CP*C)-3')

Chain C:



• Molecule 3: HIGH MOBILITY GROUP PROTEIN HMG-I/HMG-Y

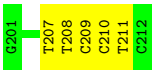
Chain A:



4.2.7 Score per residue for model 7

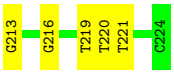
• Molecule 1: DNA (5'-D(*GP*GP*GP*AP*AP*AP*TP*TP*CP*CP*TP*C)-3')

Chain B:



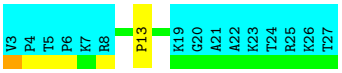
• Molecule 2: DNA (5'-D(*GP*AP*GP*GP*AP*AP*TP*TP*TP*CP*CP*C)-3')

Chain C:



• Molecule 3: HIGH MOBILITY GROUP PROTEIN HMG-I/HMG-Y

Chain A: 36% • 60%



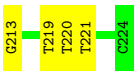
4.2.8 Score per residue for model 8

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

Chain B: 58% 42%

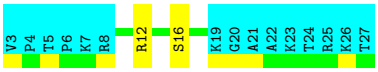
• Molecule 2: DNA (5'-D(*GP*AP*GP*GP*AP*AP*TP*TP*TP*CP*CP*C)-3')

Chain C: 67% 33%



• Molecule 3: HIGH MOBILITY GROUP PROTEIN HMG-I/HMG-Y

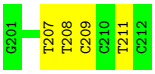
Chain A: 32% 8% 60%



4.2.9 Score per residue for model 9

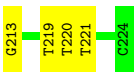
• Molecule 1: DNA (5'-D(*GP*GP*GP*AP*AP*AP*TP*TP*CP*CP*TP*C)-3')

Chain B: 67% 33%



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

Chain C: 67% 33%



• Molecule 3: HIGH MOBILITY GROUP PROTEIN HMG-I/HMG-Y

Chain A: 28% 12% 60%

V3 P4 T5 P6 K7 R8 R12 P13 S16 K19 G20 A21 A22 K23 T24 R25 K26 T27

4.2.10 Score per residue for model 10

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

Chain B: 58% 42%

G201 A206 T207 T208 T211 C212

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

Chain C: 67% 33%

G213 T219 T220 T221 C224

- Molecule 3: HIGH MOBILITY GROUP PROTEIN HMG-I/HMG-Y

Chain A: 40% 60%

V3 P4 T5 P6 K7 R8 K19 G20 A21 A22 K23 T24 R25 K26 T27

4.2.11 Score per residue for model 11

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

Chain B: 58% 42%

G201 G202 T207 T208 C209 C210 T211 C212

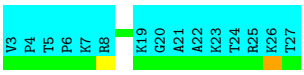
- Molecule 2: DNA (5'-D(*GP*AP*GP*GP*AP*AP*TP*TP*TP*CP*CP*C)-3')

Chain C: 75% 25%

G213 T219 T220 T221 C224

- Molecule 3: HIGH MOBILITY GROUP PROTEIN HMG-I/HMG-Y

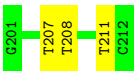
Chain A: 40% 60%



4.2.12 Score per residue for model 12

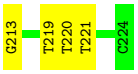
- Molecule 1: DNA (5'-D(*GP*GP*GP*AP*AP*AP*TP*TP*CP*CP*TP*C)-3')

Chain B: 75% 25%



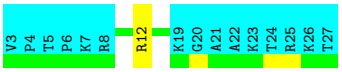
- Molecule 2: DNA (5'-D(*GP*AP*GP*GP*AP*AP*TP*TP*TP*CP*CP*C)-3')

Chain C: 67% 33%



- Molecule 3: HIGH MOBILITY GROUP PROTEIN HMG-I/HMG-Y

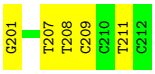
Chain A: 36% • 60%



4.2.13 Score per residue for model 13

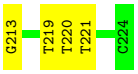
- Molecule 1: DNA (5'-D(*GP*GP*GP*AP*AP*AP*TP*TP*CP*CP*TP*C)-3')

Chain B: 58% 42%



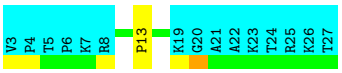
- Molecule 2: DNA (5'-D(*GP*AP*GP*GP*AP*AP*TP*TP*TP*CP*CP*C)-3')

Chain C: 67% 33%



- Molecule 3: HIGH MOBILITY GROUP PROTEIN HMG-I/HMG-Y

Chain A: 36% • 60%



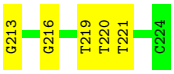
4.2.14 Score per residue for model 14

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

Chain B: 42% 58%

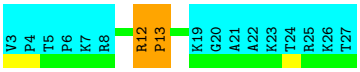
- Molecule 2: DNA (5'-D(*GP*AP*GP*GP*AP*AP*TP*TP*TP*CP*CP*C)-3')

Chain C: 58% 42%



- Molecule 3: HIGH MOBILITY GROUP PROTEIN HMG-I/HMG-Y

Chain A: 32% 8% 60%



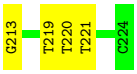
4.2.15 Score per residue for model 15

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

Chain B: 67% 33%

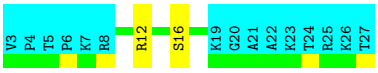
- Molecule 2: DNA (5'-D(*GP*AP*GP*GP*AP*AP*TP*TP*TP*CP*CP*C)-3')

Chain C: 67% 33%



- Molecule 3: HIGH MOBILITY GROUP PROTEIN HMG-I/HMG-Y

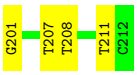
Chain A: 32% 8% 60%



4.2.16 Score per residue for model 16

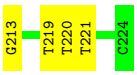
- Molecule 1: DNA (5'-D(*GP*GP*GP*AP*AP*AP*TP*TP*CP*CP*TP*C)-3')

Chain B: 67% 33%



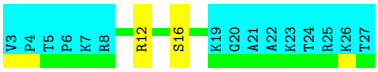
- Molecule 2: DNA (5'-D(*GP*AP*GP*GP*AP*AP*TP*TP*TP*CP*CP*C)-3')

Chain C: 67% 33%



- Molecule 3: HIGH MOBILITY GROUP PROTEIN HMG-I/HMG-Y

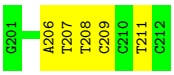
Chain A: 32% 8% 60%



4.2.17 Score per residue for model 17 (medoid)

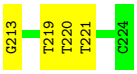
- Molecule 1: DNA (5'-D(*GP*GP*GP*AP*AP*AP*TP*TP*CP*CP*TP*C)-3')

Chain B: 58% 42%



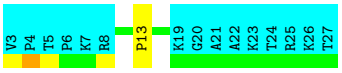
- Molecule 2: DNA (5'-D(*GP*AP*GP*GP*AP*AP*TP*TP*TP*CP*CP*C)-3')

Chain C: 67% 33%



- Molecule 3: HIGH MOBILITY GROUP PROTEIN HMG-I/HMG-Y

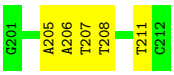
Chain A: 36% • 60%



4.2.18 Score per residue for model 18

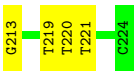
- Molecule 1: DNA (5'-D(*GP*GP*GP*AP*AP*AP*TP*TP*CP*CP*TP*C)-3')

Chain B: 58% 42%



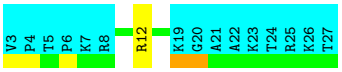
- Molecule 2: DNA (5'-D(*GP*AP*GP*GP*AP*AP*TP*TP*TP*CP*CP*C)-3')

Chain C: 67% 33%



- Molecule 3: HIGH MOBILITY GROUP PROTEIN HMG-I/HMG-Y

Chain A: 36% 60%



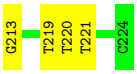
4.2.19 Score per residue for model 19

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

Chain B: 67% 33%

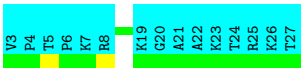
- Molecule 2: DNA (5'-D(*GP*AP*GP*GP*AP*AP*TP*TP*TP*CP*CP*C)-3')

Chain C: 67% 33%



- Molecule 3: HIGH MOBILITY GROUP PROTEIN HMG-I/HMG-Y

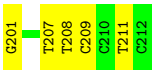
Chain A: 40% 60%



4.2.20 Score per residue for model 20

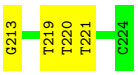
- Molecule 1: DNA (5'-D(*GP*GP*GP*AP*AP*AP*TP*TP*CP*CP*TP*C)-3')

Chain B: 58% 42%



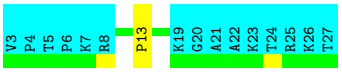
- Molecule 2: DNA (5'-D(*GP*AP*GP*GP*AP*AP*TP*TP*TP*CP*CP*C)-3')

Chain C: 67% 33%



- Molecule 3: HIGH MOBILITY GROUP PROTEIN HMG-I/HMG-Y

Chain A: 36% • 60%



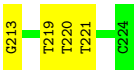
4.2.21 Score per residue for model 21

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

Chain B: 67% 33%

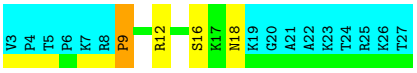
- Molecule 2: DNA (5'-D(*GP*AP*GP*GP*AP*AP*TP*TP*TP*CP*CP*C)-3')

Chain C: 67% 33%



- Molecule 3: HIGH MOBILITY GROUP PROTEIN HMG-I/HMG-Y

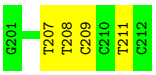
Chain A: 24% 12% • 60%



4.2.22 Score per residue for model 22

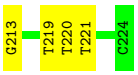
- Molecule 1: DNA (5'-D(*GP*GP*GP*AP*AP*AP*TP*TP*CP*CP*TP*C)-3')

Chain B: 67% 33%



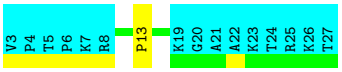
- Molecule 2: DNA (5'-D(*GP*AP*GP*GP*AP*AP*TP*TP*TP*CP*CP*C)-3')

Chain C: 67% 33%



- Molecule 3: HIGH MOBILITY GROUP PROTEIN HMG-I/HMG-Y

Chain A: 36% 60%



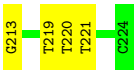
4.2.23 Score per residue for model 23

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

Chain B: 67% 33%

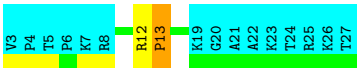
- Molecule 2: DNA (5'-D(*GP*AP*GP*GP*AP*AP*TP*TP*TP*CP*CP*C)-3')

Chain C: 67% 33%



- Molecule 3: HIGH MOBILITY GROUP PROTEIN HMG-I/HMG-Y

Chain A: 32% 60%



4.2.24 Score per residue for model 24

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

Chain B: 67% 33%

G201 T207 T208 C209 C210 T211 C212

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

Chain C: 67% 33%

G213 T219 T220 T221 C224

- Molecule 3: HIGH MOBILITY GROUP PROTEIN HMG-I/HMG-Y

Chain A: 32% 60%

V3 P4 T5 P6 K7 R8 R12 P13 K19 G20 A21 A22 K23 T24 R25 K26 T27

4.2.25 Score per residue for model 25

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

Chain B: 58% 42%

G201 T207 T208 C209 C210 T211 C212

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

Chain C: 58% 42%

G213 T219 T220 T221 C222 C223 C224

- Molecule 3: HIGH MOBILITY GROUP PROTEIN HMG-I/HMG-Y

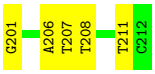
Chain A: 28% 8% 60%

V3 P4 T5 P6 K7 R8 R12 P13 K17 H18 K19 G20 A21 A22 K23 T24 R25 K26 T27

4.2.26 Score per residue for model 26

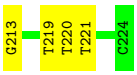
- Molecule 1: DNA (5'-D(*GP*GP*GP*AP*AP*AP*TP*TP*CP*CP*TP*C)-3')

Chain B: 58% 42%



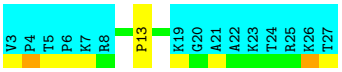
- Molecule 2: DNA (5'-D(*GP*AP*GP*GP*AP*AP*TP*TP*TP*CP*CP*C)-3')

Chain C: 67% 33%



- Molecule 3: HIGH MOBILITY GROUP PROTEIN HMG-I/HMG-Y

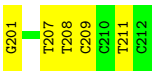
Chain A: 36% • 60%



4.2.27 Score per residue for model 27

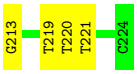
- Molecule 1: DNA (5'-D(*GP*GP*GP*AP*AP*AP*TP*TP*CP*CP*TP*C)-3')

Chain B: 58% 42%



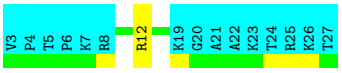
- Molecule 2: DNA (5'-D(*GP*AP*GP*GP*AP*AP*TP*TP*TP*CP*CP*C)-3')

Chain C: 67% 33%



- Molecule 3: HIGH MOBILITY GROUP PROTEIN HMG-I/HMG-Y

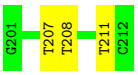
Chain A: 36% • 60%



4.2.28 Score per residue for model 28

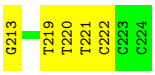
- Molecule 1: DNA (5'-D(*GP*GP*GP*AP*AP*AP*TP*TP*CP*CP*TP*C)-3')

Chain B: 75% 25%



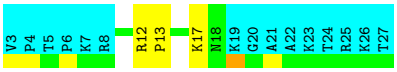
- Molecule 2: DNA (5'-D(*GP*AP*GP*GP*AP*AP*TP*TP*TP*CP*CP*C)-3')

Chain C: 58% 42%



- Molecule 3: HIGH MOBILITY GROUP PROTEIN HMG-I/HMG-Y

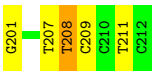
Chain A: 28% 12% 60%



4.2.29 Score per residue for model 29

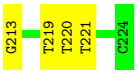
- Molecule 1: DNA (5'-D(*GP*GP*GP*AP*AP*AP*TP*TP*CP*CP*TP*C)-3')

Chain B: 58% 33% 8%



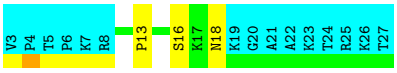
- Molecule 2: DNA (5'-D(*GP*AP*GP*GP*AP*AP*TP*TP*TP*CP*CP*C)-3')

Chain C: 67% 33%



- Molecule 3: HIGH MOBILITY GROUP PROTEIN HMG-I/HMG-Y

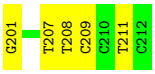
Chain A: 28% 12% 60%



4.2.30 Score per residue for model 30

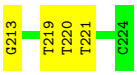
• Molecule 1: DNA (5'-D(*GP*GP*GP*AP*AP*AP*TP*TP*CP*CP*TP*C)-3')

Chain B: 58% 42%



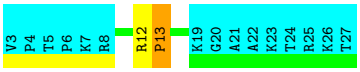
• Molecule 2: DNA (5'-D(*GP*AP*GP*GP*AP*AP*TP*TP*TP*CP*CP*C)-3')

Chain C: 67% 33%



• Molecule 3: HIGH MOBILITY GROUP PROTEIN HMG-I/HMG-Y

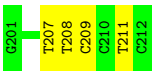
Chain A: 32% 60%



4.2.31 Score per residue for model 31

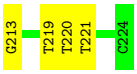
• Molecule 1: DNA (5'-D(*GP*GP*GP*AP*AP*AP*TP*TP*CP*CP*TP*C)-3')

Chain B: 67% 33%



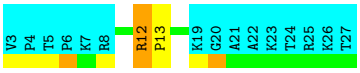
• Molecule 2: DNA (5'-D(*GP*AP*GP*GP*AP*AP*TP*TP*TP*CP*CP*C)-3')

Chain C: 67% 33%



• Molecule 3: HIGH MOBILITY GROUP PROTEIN HMG-I/HMG-Y

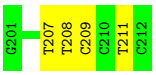
Chain A: 32% 60%



4.2.32 Score per residue for model 32

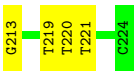
- Molecule 1: DNA (5'-D(*GP*GP*GP*AP*AP*AP*TP*TP*CP*CP*TP*C)-3')

Chain B: 67% 33%



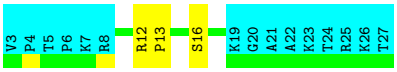
- Molecule 2: DNA (5'-D(*GP*AP*GP*GP*AP*AP*TP*TP*TP*CP*CP*C)-3')

Chain C: 67% 33%



- Molecule 3: HIGH MOBILITY GROUP PROTEIN HMG-I/HMG-Y

Chain A: 28% 12% 60%



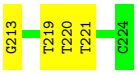
4.2.33 Score per residue for model 33

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

Chain B: 58% 42%

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

Chain C: 67% 33%



- Molecule 3: HIGH MOBILITY GROUP PROTEIN HMG-I/HMG-Y

Chain A: 28% 12% 60%

4.2.34 Score per residue for model 34

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

Chain B: 67% 33%

G201 T207 T208 C209 C210 T211 C212

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

Chain C: 58% 42%

G213 G216 T219 T220 T221 C224

- Molecule 3: HIGH MOBILITY GROUP PROTEIN HMG-I/HMG-Y

Chain A: 36% • 60%

V3 P4 T5 P6 K7 R8 P13 K19 G20 A21 A22 K23 T24 R25 K26 T27

4.2.35 Score per residue for model 35

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

Chain B: 67% 33%

G201 A206 T207 T208 T211 C212

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

Chain C: 67% 25% 8%

G213 T219 T220 T221 C224

- Molecule 3: HIGH MOBILITY GROUP PROTEIN HMG-I/HMG-Y

Chain A: 40% 60%

V3 P4 T5 P6 K7 R8 K19 G20 A21 A22 K23 T24 R25 K26 T27

5 Refinement protocol and experimental data overview (i)

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

Of the 35 calculated structures, 35 were deposited, based on the following criterion: *?*.

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

Software name	Classification	Version
X-PLOR	refinement	3.1
XPLOR MODIFIED	structure solution	MODIFIED

No chemical shift data was provided.

6 Model quality (i)

6.1 Standard geometry (i)

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the (average) root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#Z>5	RMSZ	#Z>5
1	B	1.18±0.05	2±1/272 (0.9± 0.3%)	1.65±0.02	5±1/418 (1.1± 0.3%)
2	C	1.20±0.05	2±1/272 (0.9± 0.2%)	1.64±0.03	5±1/418 (1.1± 0.3%)
3	A	1.09±0.04	0±0/78 (0.0± 0.0%)	0.87±0.03	0±0/102 (0.0± 0.0%)
All	All	1.18	168/21770 (0.8%)	1.58	324/32830 (1.0%)

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
2	C	219	DT	C5-C7	7.35	1.54	1.50	15	30
1	B	208	DT	C5-C7	7.24	1.54	1.50	16	28
2	C	221	DT	C5-C7	7.21	1.54	1.50	13	30
2	C	220	DT	C5-C7	7.07	1.54	1.50	21	25
1	B	207	DT	C5-C7	7.05	1.54	1.50	24	27
1	B	211	DT	C5-C7	6.92	1.54	1.50	11	28

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(^{o})	Ideal(^{o})	Models	
								Worst	Total
1	B	208	DT	C6-C5-C7	-7.18	118.59	122.90	9	25
2	C	219	DT	C6-C5-C7	-7.14	118.61	122.90	8	29
1	B	207	DT	C6-C5-C7	-6.83	118.80	122.90	21	31
1	B	211	DT	C6-C5-C7	-6.73	118.86	122.90	3	27
2	C	221	DT	C6-C5-C7	-6.52	118.99	122.90	26	21
2	C	220	DT	C6-C5-C7	-6.51	119.00	122.90	4	28
2	C	221	DT	C4-C5-C6	6.06	121.64	118.00	31	22
2	C	220	DT	C4-C5-C6	6.04	121.63	118.00	35	29
2	C	219	DT	C4-C5-C6	5.94	121.56	118.00	29	27
1	B	207	DT	C4-C5-C6	5.92	121.55	118.00	25	26
1	B	208	DT	C4-C5-C6	5.88	121.53	118.00	9	22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	B	211	DT	C4-C5-C6	5.81	121.48	118.00	3	26
1	B	202	DG	N7-C8-N9	5.38	115.79	113.10	11	2
1	B	202	DG	C8-N9-C4	-5.33	104.27	106.40	14	1
2	C	213	DG	N7-C8-N9	5.31	115.76	113.10	4	1
1	B	206	DA	N1-C2-N3	-5.31	126.64	129.30	18	4
1	B	201	DG	C8-N9-C4	-5.10	104.36	106.40	10	1
2	C	213	DG	C8-N9-C4	-5.06	104.38	106.40	35	1
1	B	205	DA	N1-C2-N3	-5.03	126.79	129.30	18	1

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	243	137	137	1±1
2	C	243	137	137	2±1
3	A	76	83	83	1±1
All	All	19670	12495	12495	131

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 4.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:C:213:DG:HO5'	2:C:213:DG:H8	0.92	0.97	21	31
2:C:213:DG:H8	2:C:213:DG:O5'	0.66	1.74	13	25
1:B:201:DG:HO5'	1:B:201:DG:H8	0.64	1.33	33	7
1:B:201:DG:H8	1:B:201:DG:O5'	0.56	1.83	33	3
1:B:201:DG:C8	1:B:201:DG:O5'	0.56	2.58	26	3
3:A:12:ARG:NE	3:A:16:SER:OG	0.55	2.40	15	4
1:B:201:DG:O5'	1:B:201:DG:H8	0.54	1.85	25	5
3:A:12:ARG:NH2	3:A:16:SER:O	0.54	2.40	8	2
2:C:213:DG:O5'	2:C:213:DG:H8	0.52	1.88	27	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:201:DG:H8	1:B:201:DG:HO5'	0.52	1.44	25	1
2:C:213:DG:H8	2:C:213:DG:HO5'	0.52	1.44	27	2
1:B:201:DG:O5'	1:B:201:DG:C8	0.51	2.62	14	5
3:A:12:ARG:CZ	3:A:16:SER:O	0.51	2.59	21	1
3:A:18:ASN:N	3:A:18:ASN:OD1	0.51	2.44	29	2
3:A:12:ARG:NH1	3:A:13:PRO:O	0.50	2.44	33	3
2:C:213:DG:O5'	2:C:213:DG:C8	0.50	2.59	29	14
1:B:210:DC:O2	2:C:216:DG:N2	0.50	2.45	34	4
2:C:223:DC:OP1	3:A:17:LYS:NZ	0.50	2.45	25	1
2:C:222:DC:O4'	3:A:12:ARG:NH2	0.48	2.46	28	2
1:B:205:DA:C6	1:B:206:DA:C6	0.47	3.02	1	1
3:A:12:ARG:O	3:A:13:PRO:O	0.46	2.34	1	5
3:A:12:ARG:NE	3:A:16:SER:O	0.45	2.49	33	1
1:B:210:DC:C2	2:C:216:DG:N2	0.44	2.86	7	1
3:A:13:PRO:O	3:A:16:SER:OG	0.43	2.37	29	1
3:A:12:ARG:CG	3:A:12:ARG:HH11	0.43	2.26	24	2
3:A:12:ARG:NH1	3:A:12:ARG:CG	0.42	2.83	33	3

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	10/25 (40%)	9±1 (91±7%)	0±1 (4±7%)	1±0 (5±5%)	4 24
All	All	350/875 (40%)	317 (91%)	15 (4%)	18 (5%)	4 24

All 2 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	13	PRO	17
3	A	9	PRO	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	8/20 (40%)	8±0 (96±6%)	0±0 (4±6%)	38 86
All	All	280/700 (40%)	270 (96%)	10 (4%)	38 86

All 2 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	12	ARG	9
3	A	17	LYS	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 monosaccharides 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 (i)

No chemical shift data were provided