



# Full wwPDB NMR Structure Validation Report ⓘ

Apr 27, 2016 – 06:41 AM BST

PDB ID : 3GAT  
Title : SOLUTION NMR STRUCTURE OF THE C-TERMINAL DOMAIN OF CHICKEN GATA-1 BOUND TO DNA, 34 STRUCTURES  
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Deposited on : 1997-11-07

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 : unknown  
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

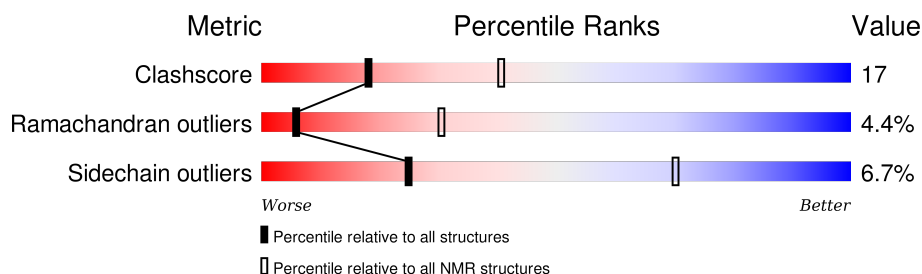
# 1 Overall quality at a glance

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	16	
2	C	16	
3	A	66	

## 2 Ensemble composition and analysis

This entry contains 34 models. Model 22 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:3-A:58 (56)	0.30	22

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 6 clusters and 3 single-model clusters were found.

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

### 3 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 2088 atoms, of which 913 are hydrogens and 0 are deuteriums.

- Molecule 1 is a DNA chain called DNA (5'-D(\*GP\*TP\*TP\*GP\*CP\*AP\*GP\*AP\*TP\*AP\*AP\*AP\*CP\*AP\*TP\*T)-3').

Mol	Chain	Residues	Atoms						Trace
1	B	16	Total	C	H	N	O	P	0
			510	158	183	61	93	15	

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

Mol	Chain	Residues	Atoms						Trace
2	C	16	Total	C	H	N	O	P	0
			507	157	184	56	95	15	

- Molecule 3 is a protein called ERYTHROID TRANSCRIPTION FACTOR GATA-1.

Mol	Chain	Residues	Atoms						Trace
3	A	66	Total	C	H	N	O	S	0
			1070	316	546	110	92	6	

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

Mol	Chain	Residues	Atoms	
4	A	1	Total	Zn
			1	1

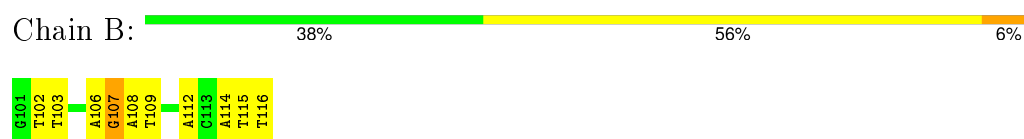


## 4 Residue-property plots [i](#)

### 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.

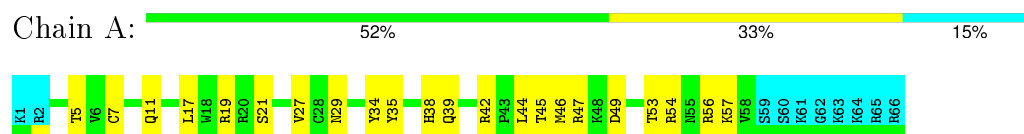
- Molecule 1: DNA (5'-D(\*GP\*TP\*TP\*GP\*CP\*AP\*GP\*AP\*TP\*AP\*AP\*AP\*CP\*AP\*TP\*T)-3')



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



- Molecule 3: ERYTHROID TRANSCRIPTION FACTOR GATA-1



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

Colouring as in section 4.1 above.

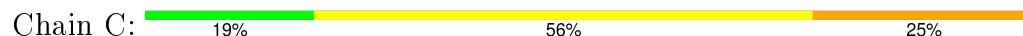
#### 4.2.1 Score per residue for model 1

- Molecule 1: DNA (5'-D(\*GP\*TP\*TP\*GP\*CP\*AP\*GP\*AP\*TP\*AP\*AP\*AP\*CP\*AP\*TP\*T)-3')

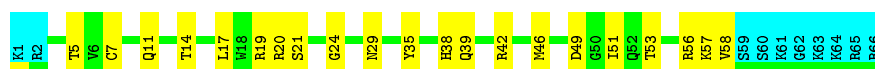




- Molecule 2: DNA (5'-D(\*AP\*AP\*TP\*GP\*TP\*TP\*TP\*AP\*TP\*CP\*TP\*GP\*CP\*AP\*AP\*C)-3')



- Molecule 3: ERYTHROID TRANSCRIPTION FACTOR GATA-1

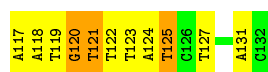


#### 4.2.2 Score per residue for model 2

- Molecule 1: DNA (5'-D(\*GP\*TP\*TP\*GP\*CP\*AP\*GP\*AP\*TP\*AP\*AP\*AP\*CP\*AP\*TP\*T)-3')



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



- Molecule 3: ERYTHROID TRANSCRIPTION FACTOR GATA-1



#### 4.2.3 Score per residue for model 3

- Molecule 1: DNA (5'-D(\*GP\*TP\*TP\*GP\*CP\*AP\*GP\*AP\*TP\*AP\*AP\*AP\*CP\*AP\*TP\*T)-3')

Chain B: 



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

Chain C: 



- Molecule 3: ERYTHROID TRANSCRIPTION FACTOR GATA-1

Chain A: 



#### 4.2.4 Score per residue for model 4

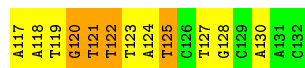
- Molecule 1: DNA (5'-D(\*GP\*TP\*TP\*GP\*CP\*AP\*GP\*AP\*TP\*AP\*AP\*AP\*CP\*AP\*TP\*T)-3')

Chain B: 



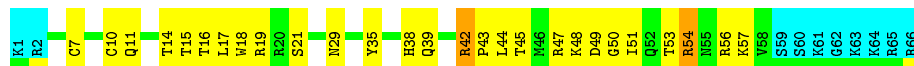
- Molecule 2: DNA (5'-D(\*AP\*AP\*TP\*GP\*TP\*TP\*TP\*AP\*TP\*CP\*TP\*GP\*CP\*AP\*AP\*C)-3')

Chain C: 



- Molecule 3: ERYTHROID TRANSCRIPTION FACTOR GATA-1

Chain A: 



### 4.2.5 Score per residue for model 5

- Molecule 1: DNA (5'-D(\*GP\*TP\*TP\*GP\*CP\*AP\*GP\*AP\*TP\*AP\*AP\*AP\*CP\*AP\*TP\*T)-3')

Chain B: 



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

Chain C: 



- Molecule 3: ERYTHROID TRANSCRIPTION FACTOR GATA-1

Chain A: 



### 4.2.6 Score per residue for model 6

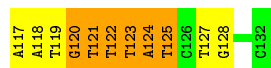
- Molecule 1: DNA (5'-D(\*GP\*TP\*TP\*GP\*CP\*AP\*GP\*AP\*TP\*AP\*AP\*AP\*CP\*AP\*TP\*T)-3')

Chain B: 

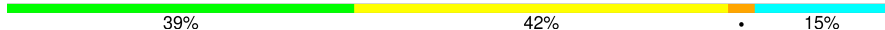


- Molecule 2: DNA (5'-D(\*AP\*AP\*TP\*GP\*TP\*TP\*TP\*AP\*TP\*CP\*TP\*GP\*CP\*AP\*AP\*C)-3')

Chain C: 



- Molecule 3: ERYTHROID TRANSCRIPTION FACTOR GATA-1

Chain A: 



### 4.2.7 Score per residue for model 7

- Molecule 1: DNA (5'-D(\*GP\*TP\*TP\*GP\*CP\*AP\*GP\*AP\*TP\*AP\*AP\*AP\*CP\*AP\*TP\*T)-3')

Chain B: 



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

Chain C: 



- Molecule 3: ERYTHROID TRANSCRIPTION FACTOR GATA-1

Chain A: 



### 4.2.8 Score per residue for model 8

- Molecule 1: DNA (5'-D(\*GP\*TP\*TP\*GP\*CP\*AP\*GP\*AP\*TP\*AP\*AP\*AP\*CP\*AP\*TP\*T)-3')

Chain B: 



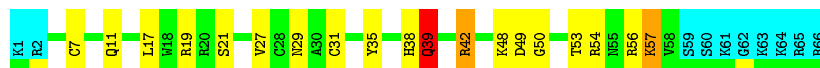
- Molecule 2: DNA (5'-D(\*AP\*AP\*TP\*GP\*TP\*TP\*TP\*AP\*TP\*CP\*TP\*GP\*CP\*AP\*AP\*C)-3')

Chain C: 



- Molecule 3: ERYTHROID TRANSCRIPTION FACTOR GATA-1

Chain A: 



### 4.2.9 Score per residue for model 9

- Molecule 1: DNA (5'-D(\*GP\*TP\*TP\*GP\*CP\*AP\*GP\*AP\*TP\*AP\*AP\*AP\*CP\*AP\*TP\*T)-3')

Chain B: 



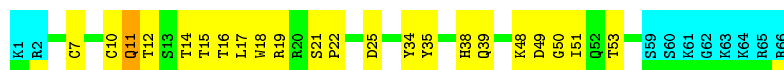
- Molecule 2: DNA (5'-D(\*AP\*AP\*TP\*GP\*TP\*TP\*TP\*AP\*TP\*CP\*TP\*GP\*CP\*AP\*AP\*C)-3')

Chain C: 



- Molecule 3: ERYTHROID TRANSCRIPTION FACTOR GATA-1

Chain A: 



### 4.2.10 Score per residue for model 10

- Molecule 1: DNA (5'-D(\*GP\*TP\*TP\*GP\*CP\*AP\*GP\*AP\*TP\*AP\*AP\*AP\*CP\*AP\*TP\*T)-3')

Chain B: 



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

Chain C: 



- Molecule 3: ERYTHROID TRANSCRIPTION FACTOR GATA-1

Chain A: 



### 4.2.11 Score per residue for model 11

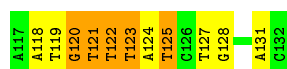
- Molecule 1: DNA (5'-D(\*GP\*TP\*TP\*GP\*CP\*AP\*GP\*AP\*TP\*AP\*AP\*AP\*CP\*AP\*TP\*T)-3')

Chain B: 



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

Chain C: 



- Molecule 3: ERYTHROID TRANSCRIPTION FACTOR GATA-1

Chain A: 



### 4.2.12 Score per residue for model 12

- Molecule 1: DNA (5'-D(\*GP\*TP\*TP\*GP\*CP\*AP\*GP\*AP\*TP\*AP\*AP\*AP\*CP\*AP\*TP\*T)-3')

Chain B: 



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

Chain C: 



- Molecule 3: ERYTHROID TRANSCRIPTION FACTOR GATA-1

Chain A: 



### 4.2.13 Score per residue for model 13

- Molecule 1: DNA (5'-D(\*GP\*TP\*TP\*GP\*CP\*AP\*GP\*AP\*TP\*AP\*AP\*AP\*CP\*AP\*TP\*T)-3')

Chain B: 



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

Chain C: 



- Molecule 3: ERYTHROID TRANSCRIPTION FACTOR GATA-1

Chain A: 



### 4.2.14 Score per residue for model 14

- Molecule 1: DNA (5'-D(\*GP\*TP\*TP\*GP\*CP\*AP\*GP\*AP\*TP\*AP\*AP\*AP\*CP\*AP\*TP\*T)-3')

Chain B: 



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

Chain C: 



- Molecule 3: ERYTHROID TRANSCRIPTION FACTOR GATA-1

Chain A: 





#### 4.2.15 Score per residue for model 15

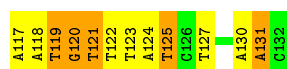
- Molecule 1: DNA (5'-D(\*GP\*TP\*TP\*GP\*CP\*AP\*GP\*AP\*TP\*AP\*AP\*AP\*CP\*AP\*TP\*T)-3')

Chain B: 



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

Chain C: 



- Molecule 3: ERYTHROID TRANSCRIPTION FACTOR GATA-1

Chain A: 



#### 4.2.16 Score per residue for model 16

- Molecule 1: DNA (5'-D(\*GP\*TP\*TP\*GP\*CP\*AP\*GP\*AP\*TP\*AP\*AP\*AP\*CP\*AP\*TP\*T)-3')

Chain B: 



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

Chain C: 



- Molecule 3: ERYTHROID TRANSCRIPTION FACTOR GATA-1

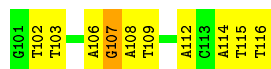
Chain A: 



#### 4.2.17 Score per residue for model 17

- Molecule 1: DNA (5'-D(\*GP\*TP\*TP\*GP\*CP\*AP\*GP\*AP\*TP\*AP\*AP\*AP\*CP\*AP\*TP\*T)-3')

Chain B: 



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

Chain C: 



- Molecule 3: ERYTHROID TRANSCRIPTION FACTOR GATA-1

Chain A: 



#### 4.2.18 Score per residue for model 18

- Molecule 1: DNA (5'-D(\*GP\*TP\*TP\*GP\*CP\*AP\*GP\*AP\*TP\*AP\*AP\*AP\*CP\*AP\*TP\*T)-3')

Chain B: 



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

Chain C: 



- Molecule 3: ERYTHROID TRANSCRIPTION FACTOR GATA-1

Chain A: 



#### 4.2.19 Score per residue for model 19

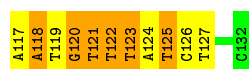
- Molecule 1: DNA (5'-D(\*GP\*TP\*TP\*GP\*CP\*AP\*GP\*AP\*TP\*AP\*AP\*AP\*CP\*AP\*TP\*T)-3')

Chain B: 



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

Chain C: 



- Molecule 3: ERYTHROID TRANSCRIPTION FACTOR GATA-1

Chain A: 



#### 4.2.20 Score per residue for model 20

- Molecule 1: DNA (5'-D(\*GP\*TP\*TP\*GP\*CP\*AP\*GP\*AP\*TP\*AP\*AP\*AP\*CP\*AP\*TP\*T)-3')

Chain B: 



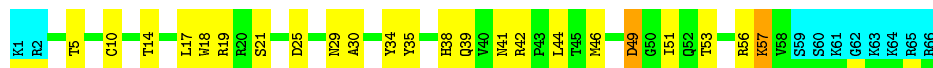
- Molecule 2: DNA (5'-D(\*AP\*AP\*TP\*GP\*TP\*TP\*TP\*AP\*TP\*CP\*TP\*GP\*CP\*AP\*AP\*C)-3')

Chain C: 



- Molecule 3: ERYTHROID TRANSCRIPTION FACTOR GATA-1

Chain A: 



#### 4.2.21 Score per residue for model 21

- Molecule 1: DNA (5'-D(\*GP\*TP\*TP\*GP\*CP\*AP\*GP\*AP\*TP\*AP\*AP\*AP\*CP\*AP\*TP\*T)-3')

Chain B: 



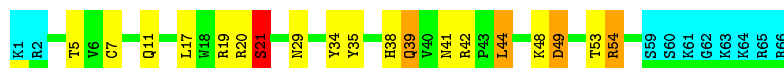
- Molecule 2: DNA (5'-D(\*AP\*AP\*TP\*GP\*TP\*TP\*TP\*AP\*TP\*CP\*TP\*GP\*CP\*AP\*AP\*C)-3')

Chain C: 



- Molecule 3: ERYTHROID TRANSCRIPTION FACTOR GATA-1

Chain A: 



#### 4.2.22 Score per residue for model 22 (medoid)

- Molecule 1: DNA (5'-D(\*GP\*TP\*TP\*GP\*CP\*AP\*GP\*AP\*TP\*AP\*AP\*AP\*CP\*AP\*TP\*T)-3')

Chain B: 



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

Chain C: 



- Molecule 3: ERYTHROID TRANSCRIPTION FACTOR GATA-1

Chain A: 



### 4.2.23 Score per residue for model 23

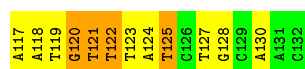
- Molecule 1: DNA (5'-D(\*GP\*TP\*TP\*GP\*CP\*AP\*GP\*AP\*TP\*AP\*AP\*AP\*CP\*AP\*TP\*T)-3')

Chain B: 



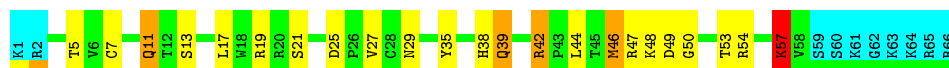
- Molecule 2: DNA (5'-D(\*AP\*AP\*TP\*GP\*TP\*TP\*TP\*AP\*TP\*CP\*TP\*GP\*CP\*AP\*AP\*C)-3')

Chain C: 



- Molecule 3: ERYTHROID TRANSCRIPTION FACTOR GATA-1

Chain A: 



### 4.2.24 Score per residue for model 24

- Molecule 1: DNA (5'-D(\*GP\*TP\*TP\*GP\*CP\*AP\*GP\*AP\*TP\*AP\*AP\*AP\*CP\*AP\*TP\*T)-3')

Chain B: 



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

Chain C: 



- Molecule 3: ERYTHROID TRANSCRIPTION FACTOR GATA-1

Chain A: 



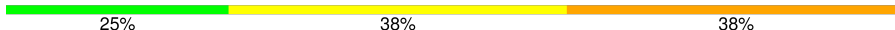
#### 4.2.25 Score per residue for model 25

- Molecule 1: DNA (5'-D(\*GP\*TP\*TP\*GP\*CP\*AP\*GP\*AP\*TP\*AP\*AP\*AP\*CP\*AP\*TP\*T)-3')

Chain B: 



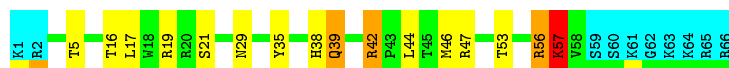
- Molecule 2: DNA (5'-D(\*AP\*AP\*TP\*GP\*TP\*TP\*TP\*AP\*TP\*CP\*TP\*GP\*CP\*AP\*AP\*C)-3')

Chain C: 



- Molecule 3: ERYTHROID TRANSCRIPTION FACTOR GATA-1

Chain A: 



#### 4.2.26 Score per residue for model 26

- Molecule 1: DNA (5'-D(\*GP\*TP\*TP\*GP\*CP\*AP\*GP\*AP\*TP\*AP\*AP\*AP\*CP\*AP\*TP\*T)-3')

Chain B: 



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

Chain C: 



- Molecule 3: ERYTHROID TRANSCRIPTION FACTOR GATA-1

Chain A: 



#### 4.2.27 Score per residue for model 27

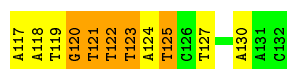
- Molecule 1: DNA (5'-D(\*GP\*TP\*TP\*GP\*CP\*AP\*GP\*AP\*TP\*AP\*AP\*AP\*CP\*AP\*TP\*T)-3')

Chain B: 



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

Chain C: 



- Molecule 3: ERYTHROID TRANSCRIPTION FACTOR GATA-1

Chain A: 



#### 4.2.28 Score per residue for model 28

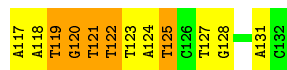
- Molecule 1: DNA (5'-D(\*GP\*TP\*TP\*GP\*CP\*AP\*GP\*AP\*TP\*AP\*AP\*AP\*CP\*AP\*TP\*T)-3')

Chain B: 



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

Chain C: 



- Molecule 3: ERYTHROID TRANSCRIPTION FACTOR GATA-1

Chain A: 



#### 4.2.29 Score per residue for model 29

- Molecule 1: DNA (5'-D(\*GP\*TP\*TP\*GP\*CP\*AP\*GP\*AP\*TP\*AP\*AP\*AP\*CP\*AP\*TP\*T)-3')

Chain B: 



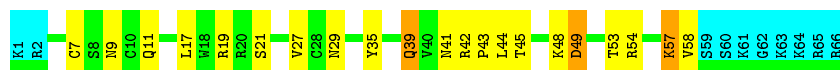
- Molecule 2: DNA (5'-D(\*AP\*AP\*TP\*GP\*TP\*TP\*TP\*AP\*TP\*CP\*TP\*GP\*CP\*AP\*AP\*C)-3')

Chain C: 



- Molecule 3: ERYTHROID TRANSCRIPTION FACTOR GATA-1

Chain A: 



#### 4.2.30 Score per residue for model 30

- Molecule 1: DNA (5'-D(\*GP\*TP\*TP\*GP\*CP\*AP\*GP\*AP\*TP\*AP\*AP\*AP\*CP\*AP\*TP\*T)-3')

Chain B: 



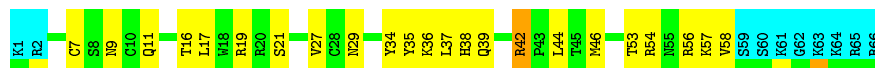
- Molecule 2: DNA (5'-D(\*AP\*AP\*TP\*GP\*TP\*TP\*TP\*AP\*TP\*CP\*TP\*GP\*CP\*AP\*AP\*C)-3')

Chain C: 



- Molecule 3: ERYTHROID TRANSCRIPTION FACTOR GATA-1

Chain A: 





#### 4.2.31 Score per residue for model 31

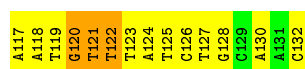
- Molecule 1: DNA (5'-D(\*GP\*TP\*TP\*GP\*CP\*AP\*GP\*AP\*TP\*AP\*AP\*AP\*CP\*AP\*TP\*T)-3')

Chain B: 



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

Chain C: 



- Molecule 3: ERYTHROID TRANSCRIPTION FACTOR GATA-1

Chain A: 



#### 4.2.32 Score per residue for model 32

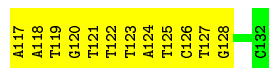
- Molecule 1: DNA (5'-D(\*GP\*TP\*TP\*GP\*CP\*AP\*GP\*AP\*TP\*AP\*AP\*AP\*CP\*AP\*TP\*T)-3')

Chain B: 



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

Chain C: 



- Molecule 3: ERYTHROID TRANSCRIPTION FACTOR GATA-1

Chain A: 



### 4.2.33 Score per residue for model 33

- Molecule 1: DNA (5'-D(\*GP\*TP\*TP\*GP\*CP\*AP\*GP\*AP\*TP\*AP\*AP\*AP\*CP\*AP\*TP\*T)-3')

Chain B: 



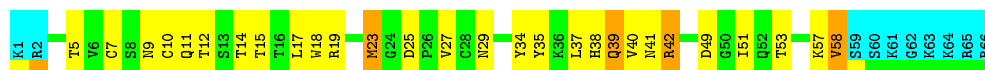
- Molecule 2: DNA (5'-D(\*AP\*AP\*TP\*GP\*TP\*TP\*TP\*AP\*TP\*CP\*TP\*GP\*CP\*AP\*AP\*C)-3')

Chain C: 



- Molecule 3: ERYTHROID TRANSCRIPTION FACTOR GATA-1

Chain A: 



### 4.2.34 Score per residue for model 34

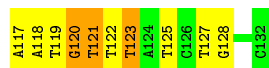
- Molecule 1: DNA (5'-D(\*GP\*TP\*TP\*GP\*CP\*AP\*GP\*AP\*TP\*AP\*AP\*AP\*CP\*AP\*TP\*T)-3')

Chain B: 



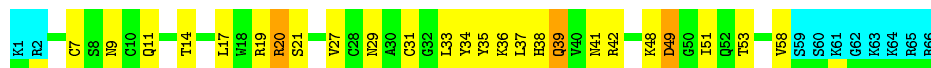
- Molecule 2: DNA (5'-D(\*AP\*AP\*TP\*GP\*TP\*TP\*TP\*AP\*TP\*CP\*TP\*GP\*CP\*AP\*AP\*C)-3')

Chain C: 



- Molecule 3: ERYTHROID TRANSCRIPTION FACTOR GATA-1

Chain A: 



## 5 Refinement protocol and experimental data overview

The models were refined using the following method: *SIMULATED ANNEALING*.

Of the 34 calculated structures, 34 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
X-PLOR MODIFIED	structure solution	MODIFIED

No chemical shift data was provided. No validations of the models with respect to experimental NMR restraints is performed at this time.

## 6 Model quality i

### 6.1 Standard geometry i

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

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	1.38±0.02	5±0/367 (1.4±0.0%)	1.90±0.01	5±2/565 (0.8±0.3%)
2	C	1.39±0.03	5±1/361 (1.4±0.2%)	1.94±0.01	10±2/555 (1.8±0.4%)
3	A	1.06±0.01	0±0/446 (0.0±0.0%)	0.96±0.01	0±0/604 (0.0±0.0%)
All	All	1.27	347/39916 (0.9%)	1.65	495/58616 (0.8%)

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
1	B	0.0±0.0	0.0±0.2
All	All	0	1

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	7.83	1.54	1.50	30	34
2	C	123	DT	C5-C7	7.22	1.54	1.50	30	34
2	C	121	DT	C5-C7	6.64	1.54	1.50	4	25
1	B	109	DT	C5-C7	6.63	1.54	1.50	15	34
2	C	122	DT	C5-C7	6.60	1.54	1.50	9	34
2	C	127	DT	C5-C7	6.57	1.53	1.50	24	34
1	B	116	DT	C5-C7	6.56	1.53	1.50	19	34
1	B	115	DT	C5-C7	6.53	1.53	1.50	30	34
2	C	119	DT	C5-C7	6.37	1.53	1.50	33	34
1	B	103	DT	C5-C7	6.36	1.53	1.50	14	34
2	C	125	DT	C5-C7	5.92	1.53	1.50	28	16

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	C	120	DG	O4'-C1'-N9	7.54	113.28	108.00	32	23
2	C	125	DT	O4'-C1'-N1	7.31	113.12	108.00	25	33
1	B	107	DG	O4'-C1'-N9	7.17	113.02	108.00	9	34
2	C	121	DT	O4'-C1'-N1	6.94	112.86	108.00	26	32
1	B	112	DA	O4'-C1'-N9	6.60	112.62	108.00	32	33
2	C	121	DT	C6-C5-C7	-6.45	119.03	122.90	14	26
1	B	108	DA	O4'-C1'-N9	6.39	112.47	108.00	4	3
1	B	115	DT	O4'-C1'-N1	6.29	112.40	108.00	10	11
2	C	125	DT	C6-C5-C7	-6.16	119.20	122.90	34	19
2	C	123	DT	O4'-C1'-N1	6.01	112.21	108.00	1	14
2	C	125	DT	C4-C5-C6	5.94	121.56	118.00	20	34
1	B	110	DA	O4'-C1'-N9	5.93	112.15	108.00	22	13
1	B	107	DG	C8-N9-C4	-5.81	104.08	106.40	28	32
2	C	127	DT	O4'-C1'-N1	5.80	112.06	108.00	5	10
2	C	122	DT	O4'-C1'-N1	5.65	111.96	108.00	14	4
2	C	119	DT	O4'-C1'-N1	5.63	111.94	108.00	23	8
2	C	131	DA	O4'-C1'-N9	5.55	111.88	108.00	2	5
2	C	123	DT	C4-C5-C6	5.53	121.32	118.00	15	32
1	B	104	DG	O4'-C1'-N9	5.50	111.85	108.00	30	6
2	C	121	DT	C4-C5-C6	5.49	121.30	118.00	24	28
2	C	130	DA	O4'-C1'-N9	5.45	111.82	108.00	14	7
1	B	116	DT	C6-C5-C7	-5.39	119.67	122.90	9	3
1	B	103	DT	O4'-C1'-N1	5.39	111.77	108.00	30	2
2	C	132	DC	O4'-C1'-N1	5.36	111.75	108.00	31	3
1	B	114	DA	O4'-C1'-N9	5.34	111.74	108.00	22	7
1	B	109	DT	O4'-C1'-N1	5.34	111.74	108.00	18	1
2	C	120	DG	N7-C8-N9	5.31	115.75	113.10	14	12
2	C	119	DT	C6-C5-C7	-5.31	119.71	122.90	23	4
2	C	123	DT	C6-C5-C7	-5.30	119.72	122.90	32	2
2	C	118	DA	O4'-C1'-N9	5.29	111.71	108.00	8	4
2	C	119	DT	C4-C5-C6	5.24	121.14	118.00	15	5
1	B	102	DT	C6-C5-C7	-5.23	119.76	122.90	30	3
2	C	122	DT	C6-C5-C7	-5.23	119.76	122.90	24	2
1	B	102	DT	O4'-C1'-N1	5.22	111.65	108.00	5	2
2	C	122	DT	C4-C5-C6	5.19	121.12	118.00	26	10
2	C	127	DT	C4-C5-C6	5.18	121.11	118.00	22	13
1	B	102	DT	C4-C5-C6	5.16	121.09	118.00	29	5
1	B	108	DA	N1-C2-N3	-5.15	126.72	129.30	25	2
1	B	115	DT	C6-C5-C7	-5.11	119.83	122.90	7	4
2	C	124	DA	O4'-C1'-N9	5.07	111.55	108.00	6	3

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	B	116	DT	O4'-C1'-N1	5.01	111.50	108.00	2	1

There are no chirality outliers.

All unique planar outliers are listed below.

Mol	Chain	Res	Type	Group	Models (Total)
1	B	108	DA	Sidechain	1

## 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	327	183	183	9±3
2	C	323	184	184	11±3
3	A	438	440	440	23±5
All	All	37026	27438	27438	1114

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 17.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:A:38:HIS:O	3:A:40:VAL:N	0.97	1.96	33	1
3:A:17:LEU:HD23	3:A:19:ARG:NH1	0.86	1.85	11	30
2:C:117:DA:H8	2:C:117:DA:HO5'	0.85	1.12	25	8
3:A:10:CYS:O	3:A:12:THR:N	0.83	2.11	32	3
2:C:117:DA:HO5'	2:C:117:DA:H8	0.82	1.13	20	15
1:B:106:DA:N7	3:A:17:LEU:HD21	0.80	1.91	12	27
3:A:38:HIS:O	3:A:40:VAL:HG22	0.72	1.83	33	1
3:A:19:ARG:HH21	3:A:29:ASN:ND2	0.72	1.83	6	20
3:A:35:TYR:O	3:A:39:GLN:N	0.71	2.23	10	33
3:A:42:ARG:H	3:A:42:ARG:NE	0.71	1.82	33	3
3:A:42:ARG:H	3:A:42:ARG:HE	0.71	1.27	33	1
3:A:42:ARG:NE	3:A:42:ARG:H	0.70	1.84	23	2
2:C:122:DT:P	3:A:38:HIS:HE2	0.67	2.11	19	9

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:106:DA:C5	3:A:17:LEU:HD21	0.66	2.25	27	20
3:A:19:ARG:NH2	3:A:29:ASN:HD22	0.66	1.86	15	1
3:A:31:CYS:SG	3:A:42:ARG:NE	0.64	2.70	34	1
3:A:34:TYR:CD2	3:A:42:ARG:NH1	0.64	2.66	16	1
3:A:19:ARG:NH2	3:A:29:ASN:ND2	0.63	2.46	15	10
2:C:122:DT:P	3:A:38:HIS:NE2	0.63	2.72	19	17
3:A:14:THR:O	3:A:51:ILE:HD11	0.63	1.93	18	10
3:A:28:CYS:SG	3:A:47:ARG:NH2	0.62	2.72	19	1
1:B:107:DG:N7	3:A:17:LEU:CD2	0.61	2.63	29	34
2:C:117:DA:H8	2:C:117:DA:O5'	0.61	1.79	20	10
3:A:31:CYS:SG	3:A:47:ARG:NH2	0.61	2.74	15	4
3:A:34:TYR:CE2	3:A:42:ARG:NH1	0.60	2.70	16	1
3:A:10:CYS:O	3:A:10:CYS:SG	0.60	2.59	32	1
3:A:5:THR:O	3:A:18:TRP:CH2	0.60	2.54	17	1
3:A:17:LEU:HD23	3:A:19:ARG:HH12	0.60	1.57	13	7
3:A:37:LEU:HD12	3:A:37:LEU:N	0.60	2.11	33	1
3:A:34:TYR:CD1	3:A:42:ARG:NH1	0.60	2.70	20	1
2:C:126:DC:P	3:A:56:ARG:HE	0.59	2.20	26	1
1:B:114:DA:N6	2:C:118:DA:N6	0.59	2.51	14	34
2:C:117:DA:O5'	2:C:117:DA:H8	0.59	1.79	28	11
3:A:42:ARG:N	3:A:42:ARG:NE	0.58	2.51	33	2
3:A:34:TYR:CE1	3:A:38:HIS:CD2	0.58	2.91	24	6
3:A:34:TYR:CZ	3:A:42:ARG:NE	0.58	2.72	15	1
3:A:38:HIS:O	3:A:39:GLN:CB	0.58	2.52	14	6
1:B:107:DG:C6	1:B:108:DA:N6	0.57	2.72	15	26
3:A:9:ASN:O	3:A:42:ARG:NH1	0.57	2.37	33	1
3:A:19:ARG:HH21	3:A:29:ASN:HD21	0.57	1.40	17	2
3:A:42:ARG:NH2	3:A:47:ARG:CZ	0.57	2.67	18	1
1:B:114:DA:C2	2:C:120:DG:N2	0.57	2.73	6	14
3:A:11:GLN:NE2	3:A:11:GLN:O	0.57	2.38	27	1
2:C:120:DG:C5	2:C:121:DT:C4	0.56	2.92	17	31
3:A:34:TYR:CD1	3:A:38:HIS:CD2	0.56	2.93	24	2
1:B:106:DA:C2	2:C:128:DG:N2	0.56	2.73	30	25
3:A:44:LEU:O	3:A:46:MET:N	0.56	2.39	5	11
3:A:47:ARG:N	3:A:47:ARG:HE	0.56	1.98	6	1
3:A:7:CYS:O	3:A:11:GLN:N	0.56	2.37	15	28
1:B:106:DA:C8	3:A:17:LEU:HD21	0.56	2.36	34	13
3:A:42:ARG:CZ	3:A:47:ARG:NH2	0.56	2.69	18	1
1:B:107:DG:O6	3:A:17:LEU:HD22	0.55	2.01	28	9
3:A:38:HIS:O	3:A:39:GLN:CG	0.55	2.55	15	2
3:A:37:LEU:CD1	3:A:37:LEU:N	0.55	2.70	33	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:108:DA:N6	2:C:124:DA:N6	0.55	2.54	18	4
2:C:124:DA:C5	2:C:125:DT:C4	0.55	2.95	26	6
2:C:120:DG:C2	2:C:121:DT:C2	0.55	2.95	15	21
3:A:47:ARG:O	3:A:47:ARG:NE	0.55	2.40	5	2
2:C:122:DT:OP1	3:A:38:HIS:CD2	0.55	2.60	16	13
1:B:107:DG:N2	1:B:108:DA:C2	0.54	2.75	30	7
3:A:31:CYS:SG	3:A:42:ARG:NH1	0.54	2.80	3	1
2:C:124:DA:C2	2:C:125:DT:N3	0.54	2.75	24	20
3:A:48:LYS:O	3:A:50:GLY:N	0.54	2.41	11	6
3:A:23:MET:N	3:A:23:MET:SD	0.54	2.81	6	2
3:A:42:ARG:NH1	3:A:46:MET:SD	0.54	2.81	27	2
2:C:122:DT:OP2	3:A:38:HIS:NE2	0.54	2.41	26	9
1:B:107:DG:N7	3:A:17:LEU:HD23	0.54	2.18	27	9
3:A:42:ARG:H	3:A:42:ARG:CD	0.54	2.15	23	2
3:A:14:THR:O	3:A:51:ILE:CG1	0.54	2.56	4	2
2:C:125:DT:O3'	3:A:56:ARG:NH1	0.53	2.42	6	2
1:B:113:DC:OP1	3:A:54:ARG:NH1	0.53	2.41	32	3
3:A:42:ARG:CG	3:A:42:ARG:HH11	0.53	2.17	3	5
1:B:107:DG:C8	3:A:19:ARG:NH1	0.53	2.76	7	7
3:A:20:ARG:NH2	3:A:24:GLY:O	0.53	2.42	1	2
3:A:54:ARG:NH1	3:A:54:ARG:CG	0.53	2.72	31	4
2:C:117:DA:C8	2:C:117:DA:O5'	0.53	2.61	18	9
3:A:42:ARG:CG	3:A:42:ARG:NH1	0.53	2.71	3	5
3:A:36:LYS:NZ	3:A:37:LEU:CD1	0.53	2.71	30	1
3:A:42:ARG:CZ	3:A:42:ARG:O	0.53	2.57	33	1
3:A:42:ARG:HH11	3:A:42:ARG:CG	0.53	2.16	30	4
3:A:17:LEU:HD23	3:A:19:ARG:CZ	0.52	2.34	22	9
3:A:54:ARG:HH11	3:A:54:ARG:CG	0.52	2.16	21	3
3:A:42:ARG:O	3:A:44:LEU:N	0.52	2.40	6	2
3:A:34:TYR:CE2	3:A:42:ARG:CZ	0.52	2.92	16	1
3:A:9:ASN:O	3:A:42:ARG:NH2	0.52	2.43	33	1
2:C:117:DA:O5'	2:C:117:DA:C8	0.52	2.61	29	6
3:A:47:ARG:HE	3:A:47:ARG:N	0.52	2.03	16	1
3:A:4:GLY:O	3:A:6:VAL:N	0.52	2.43	17	1
3:A:46:MET:CG	3:A:47:ARG:HH21	0.52	2.18	6	1
2:C:123:DT:OP1	3:A:47:ARG:NH2	0.52	2.43	6	1
3:A:14:THR:O	3:A:51:ILE:CD1	0.52	2.58	33	15
3:A:19:ARG:HH21	3:A:29:ASN:HD22	0.52	1.45	15	1
3:A:42:ARG:NH1	3:A:42:ARG:CG	0.52	2.72	30	5
2:C:123:DT:OP1	3:A:42:ARG:NH1	0.52	2.43	29	4
1:B:114:DA:C2	1:B:115:DT:C2	0.52	2.98	12	4

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:A:25:ASP:N	3:A:25:ASP:OD1	0.52	2.41	9	4
3:A:19:ARG:CZ	3:A:29:ASN:HD22	0.52	2.18	15	1
3:A:36:LYS:HZ2	3:A:37:LEU:CD1	0.52	2.18	30	1
3:A:9:ASN:ND2	3:A:27:VAL:HG11	0.51	2.20	18	10
3:A:44:LEU:N	3:A:44:LEU:HD12	0.51	2.20	31	4
3:A:10:CYS:O	3:A:47:ARG:NH1	0.51	2.44	4	1
2:C:123:DT:OP1	3:A:30:ALA:HB1	0.51	2.05	20	1
3:A:39:GLN:O	3:A:39:GLN:CG	0.51	2.59	15	2
3:A:30:ALA:HB3	3:A:47:ARG:HH21	0.51	1.65	19	1
3:A:54:ARG:CG	3:A:54:ARG:NH1	0.51	2.73	4	2
3:A:10:CYS:CB	3:A:47:ARG:HH11	0.51	2.19	18	2
2:C:126:DC:OP1	3:A:56:ARG:NE	0.50	2.45	32	3
2:C:122:DT:OP1	3:A:38:HIS:NE2	0.50	2.44	11	9
2:C:130:DA:C6	2:C:131:DA:C6	0.50	3.00	15	3
3:A:42:ARG:CB	3:A:42:ARG:HH11	0.50	2.20	16	1
3:A:30:ALA:HB3	3:A:47:ARG:HH12	0.50	1.67	7	1
2:C:125:DT:C4	2:C:126:DC:N4	0.50	2.80	25	2
3:A:42:ARG:NE	3:A:47:ARG:NH2	0.50	2.59	18	1
3:A:44:LEU:C	3:A:46:MET:N	0.49	2.64	13	12
3:A:54:ARG:CG	3:A:54:ARG:HH11	0.49	2.19	4	1
3:A:20:ARG:O	3:A:21:SER:O	0.49	2.30	21	4
2:C:125:DT:N3	2:C:126:DC:N3	0.49	2.60	25	1
1:B:112:DA:O3'	3:A:54:ARG:NH2	0.49	2.46	6	2
1:B:106:DA:N7	3:A:17:LEU:HD11	0.49	2.22	34	2
3:A:58:VAL:O	3:A:58:VAL:HG22	0.49	2.07	26	1
3:A:19:ARG:NH2	3:A:29:ASN:HD21	0.49	2.03	17	1
2:C:125:DT:C3'	3:A:56:ARG:NH1	0.49	2.76	6	1
1:B:112:DA:C4'	3:A:54:ARG:HH21	0.49	2.21	8	1
2:C:126:DC:OP1	3:A:56:ARG:NH1	0.49	2.46	3	2
1:B:112:DA:O4'	3:A:54:ARG:NH2	0.49	2.45	29	1
3:A:44:LEU:HD12	3:A:44:LEU:N	0.49	2.23	18	7
3:A:34:TYR:CE1	3:A:38:HIS:CG	0.49	3.00	33	2
3:A:42:ARG:CD	3:A:42:ARG:H	0.49	2.20	5	2
3:A:38:HIS:CD2	3:A:38:HIS:N	0.48	2.81	15	1
3:A:47:ARG:O	3:A:47:ARG:CZ	0.48	2.61	5	2
3:A:15:THR:HG21	3:A:18:TRP:CH2	0.48	2.44	4	4
3:A:43:PRO:O	3:A:45:THR:N	0.48	2.46	6	4
3:A:19:ARG:NH1	3:A:29:ASN:HD22	0.48	2.07	16	4
3:A:25:ASP:OD1	3:A:25:ASP:N	0.48	2.45	23	6
3:A:9:ASN:O	3:A:42:ARG:CZ	0.48	2.61	33	1
3:A:42:ARG:CD	3:A:42:ARG:N	0.48	2.77	25	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:A:42:ARG:N	3:A:42:ARG:CD	0.48	2.76	23	3
3:A:20:ARG:CZ	3:A:24:GLY:O	0.48	2.62	1	1
1:B:101:DG:H8	1:B:101:DG:HO5'	0.48	1.51	21	3
1:B:107:DG:N1	1:B:108:DA:C6	0.48	2.82	6	8
2:C:124:DA:C6	2:C:125:DT:O4	0.47	2.67	3	18
2:C:122:DT:OP1	3:A:34:TYR:CE2	0.47	2.67	22	3
3:A:57:LYS:CG	3:A:58:VAL:N	0.47	2.78	10	3
3:A:57:LYS:NZ	3:A:57:LYS:CB	0.47	2.77	10	2
2:C:123:DT:OP1	3:A:42:ARG:NH2	0.47	2.48	27	1
3:A:48:LYS:C	3:A:50:GLY:H	0.47	2.13	6	6
2:C:120:DG:C6	2:C:121:DT:C4	0.47	3.03	17	3
3:A:41:ASN:OD1	3:A:41:ASN:O	0.47	2.32	19	7
2:C:124:DA:C4	2:C:125:DT:C4	0.47	3.02	19	3
3:A:33:LEU:O	3:A:37:LEU:HD13	0.47	2.10	34	1
3:A:34:TYR:CD1	3:A:34:TYR:C	0.46	2.88	7	5
2:C:122:DT:OP1	3:A:34:TYR:CD2	0.46	2.68	7	1
3:A:6:VAL:HG21	3:A:11:GLN:NE2	0.46	2.25	32	1
3:A:10:CYS:O	3:A:44:LEU:HD21	0.46	2.10	20	1
2:C:123:DT:OP1	3:A:46:MET:SD	0.46	2.74	19	3
3:A:43:PRO:C	3:A:45:THR:H	0.46	2.14	17	10
1:B:107:DG:C8	3:A:19:ARG:NH2	0.46	2.83	19	2
3:A:34:TYR:C	3:A:34:TYR:CD1	0.46	2.88	9	3
3:A:57:LYS:O	3:A:58:VAL:O	0.46	2.34	33	1
2:C:119:DT:N3	2:C:120:DG:C6	0.46	2.84	15	2
3:A:41:ASN:OD1	3:A:41:ASN:N	0.46	2.48	28	1
2:C:119:DT:C4	2:C:120:DG:C6	0.46	3.04	15	2
3:A:19:ARG:O	3:A:27:VAL:HG22	0.46	2.11	6	7
3:A:19:ARG:HB2	3:A:27:VAL:HG23	0.46	1.87	31	5
3:A:15:THR:HG21	3:A:18:TRP:CZ3	0.46	2.46	4	9
1:B:107:DG:C2	1:B:108:DA:C6	0.46	3.03	8	6
3:A:34:TYR:CB	3:A:42:ARG:NH1	0.46	2.79	21	1
2:C:125:DT:C7	3:A:16:THR:OG1	0.45	2.64	19	8
2:C:126:DC:OP1	3:A:56:ARG:CZ	0.45	2.64	18	5
3:A:20:ARG:CG	3:A:20:ARG:NH1	0.45	2.79	34	2
1:B:107:DG:C8	3:A:19:ARG:CZ	0.45	2.99	16	7
1:B:109:DT:O2	3:A:57:LYS:NZ	0.45	2.46	3	3
3:A:34:TYR:OH	3:A:42:ARG:NE	0.45	2.49	19	1
3:A:55:ASN:O	3:A:55:ASN:OD1	0.45	2.34	16	1
1:B:101:DG:HO5'	1:B:101:DG:H8	0.45	1.55	27	3
3:A:56:ARG:CG	3:A:56:ARG:HH11	0.45	2.25	16	1
2:C:124:DA:C6	2:C:125:DT:C4	0.45	3.05	2	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:111:DA:N6	2:C:121:DT:O4	0.45	2.49	26	1
1:B:114:DA:N6	2:C:118:DA:C6	0.45	2.85	21	2
2:C:125:DT:C2	2:C:126:DC:C4	0.44	3.05	25	1
3:A:56:ARG:CG	3:A:56:ARG:NH1	0.44	2.77	30	1
3:A:10:CYS:O	3:A:11:GLN:C	0.44	2.56	11	1
3:A:39:GLN:O	3:A:40:VAL:HG13	0.44	2.12	33	1
3:A:44:LEU:C	3:A:46:MET:H	0.44	2.16	31	4
3:A:29:ASN:OD1	3:A:29:ASN:O	0.44	2.35	25	5
3:A:13:SER:O	3:A:13:SER:OG	0.44	2.36	22	1
2:C:125:DT:N3	2:C:126:DC:C4	0.44	2.86	25	1
1:B:107:DG:C6	1:B:108:DA:C6	0.44	3.06	27	7
2:C:124:DA:C2	2:C:125:DT:C2	0.44	3.06	2	2
3:A:23:MET:SD	3:A:25:ASP:OD2	0.44	2.76	5	1
1:B:106:DA:H2''	1:B:107:DG:O5'	0.43	2.12	30	2
3:A:54:ARG:CG	3:A:55:ASN:N	0.43	2.82	7	1
1:B:107:DG:N2	2:C:127:DT:O2	0.43	2.51	26	1
3:A:38:HIS:O	3:A:40:VAL:CG2	0.43	2.62	33	1
3:A:19:ARG:NE	3:A:29:ASN:HD22	0.43	2.11	15	1
1:B:113:DC:OP1	3:A:54:ARG:NH2	0.43	2.51	23	1
3:A:11:GLN:CD	3:A:11:GLN:N	0.43	2.71	21	1
3:A:41:ASN:N	3:A:41:ASN:OD1	0.43	2.52	10	3
2:C:130:DA:C6	2:C:131:DA:N6	0.43	2.86	1	2
3:A:8:SER:N	3:A:26:PRO:O	0.43	2.40	3	1
3:A:9:ASN:OD1	3:A:27:VAL:HG11	0.43	2.13	24	2
3:A:44:LEU:H	3:A:44:LEU:HD12	0.43	1.74	31	1
1:B:114:DA:C2	2:C:120:DG:C2	0.43	3.06	6	1
1:B:112:DA:N6	2:C:120:DG:O6	0.43	2.51	30	4
3:A:48:LYS:C	3:A:50:GLY:N	0.43	2.72	11	5
3:A:42:ARG:NH2	3:A:46:MET:SD	0.43	2.92	16	2
2:C:122:DT:OP1	3:A:34:TYR:CE1	0.43	2.72	24	1
3:A:42:ARG:NE	3:A:42:ARG:N	0.43	2.65	25	1
3:A:20:ARG:O	3:A:21:SER:C	0.43	2.57	21	4
1:B:109:DT:O4	2:C:124:DA:N1	0.43	2.51	30	1
3:A:29:ASN:C	3:A:29:ASN:OD1	0.43	2.57	18	1
3:A:31:CYS:SG	3:A:42:ARG:CZ	0.43	3.07	8	1
2:C:124:DA:H8	2:C:124:DA:O5'	0.43	1.97	24	2
3:A:6:VAL:CG2	3:A:11:GLN:NE2	0.43	2.82	32	1
3:A:46:MET:C	3:A:47:ARG:HE	0.43	2.16	16	1
3:A:35:TYR:O	3:A:39:GLN:CA	0.42	2.68	21	4
3:A:56:ARG:O	3:A:57:LYS:O	0.42	2.37	25	2
3:A:42:ARG:HG2	3:A:42:ARG:HH11	0.42	1.73	18	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:A:29:ASN:OD1	3:A:29:ASN:C	0.42	2.58	24	3
1:B:112:DA:C4'	3:A:54:ARG:NH2	0.42	2.83	14	1
3:A:10:CYS:SG	3:A:12:THR:HG22	0.42	2.54	9	2
3:A:38:HIS:O	3:A:39:GLN:C	0.42	2.58	25	7
3:A:48:LYS:O	3:A:49:ASP:C	0.42	2.58	29	8
3:A:57:LYS:O	3:A:58:VAL:C	0.42	2.58	1	1
1:B:106:DA:OP1	3:A:20:ARG:NH1	0.42	2.53	17	1
3:A:56:ARG:O	3:A:57:LYS:C	0.41	2.58	8	1
3:A:42:ARG:O	3:A:42:ARG:NE	0.41	2.35	25	1
1:B:106:DA:C2	2:C:128:DG:C2	0.41	3.08	11	2
3:A:29:ASN:O	3:A:29:ASN:OD1	0.41	2.38	30	1
3:A:30:ALA:HB3	3:A:47:ARG:NH2	0.41	2.30	19	1
2:C:126:DC:OP1	3:A:56:ARG:NH2	0.41	2.53	16	1
3:A:31:CYS:O	3:A:35:TYR:CB	0.41	2.68	6	1
3:A:31:CYS:CA	3:A:42:ARG:HH21	0.41	2.28	11	1
1:B:107:DG:N7	3:A:19:ARG:NH1	0.41	2.68	7	1
3:A:47:ARG:CA	3:A:47:ARG:NE	0.41	2.83	6	1
1:B:108:DA:N1	2:C:126:DC:N3	0.41	2.69	8	1
3:A:44:LEU:O	3:A:45:THR:C	0.41	2.58	5	5
2:C:117:DA:H2'	2:C:118:DA:N7	0.41	2.30	5	1
3:A:10:CYS:SG	3:A:47:ARG:CZ	0.41	3.09	15	1
3:A:43:PRO:C	3:A:45:THR:N	0.41	2.74	6	2
3:A:56:ARG:NH1	3:A:56:ARG:HG2	0.41	2.31	4	1
3:A:39:GLN:OE1	3:A:39:GLN:O	0.41	2.38	23	1
3:A:56:ARG:NH1	3:A:56:ARG:CG	0.41	2.81	26	1
3:A:39:GLN:O	3:A:40:VAL:CG1	0.41	2.69	33	1
3:A:7:CYS:SG	3:A:28:CYS:N	0.41	2.93	14	1
1:B:108:DA:H2'	1:B:109:DT:H72	0.40	1.92	33	1
3:A:28:CYS:SG	3:A:47:ARG:NE	0.40	2.95	19	1
3:A:19:ARG:HH21	3:A:29:ASN:CG	0.40	2.20	31	1
2:C:119:DT:C2	2:C:120:DG:C5	0.40	3.09	15	2
3:A:56:ARG:HH11	3:A:56:ARG:CB	0.40	2.29	16	1
3:A:47:ARG:NE	3:A:47:ARG:CA	0.40	2.84	16	1
3:A:11:GLN:CG	3:A:11:GLN:O	0.40	2.69	27	1
2:C:120:DG:H2''	2:C:121:DT:O5'	0.40	2.17	3	1
3:A:34:TYR:CG	3:A:42:ARG:NH1	0.40	2.89	21	1
3:A:20:ARG:HH11	3:A:20:ARG:CG	0.40	2.29	34	1

## 6.3 Torsion angles [i](#)

### 6.3.1 Protein backbone [i](#)

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	A	56/66 (85%)	50±1 (89±3%)	4±2 (6±3%)	2±1 (4±2%)	6	30
All	All	1904/2244 (85%)	1699 (89%)	121 (6%)	84 (4%)	6	30

All 9 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	49	ASP	26
3	A	57	LYS	16
3	A	44	LEU	10
3	A	39	GLN	10
3	A	45	THR	7
3	A	11	GLN	6
3	A	58	VAL	4
3	A	21	SER	4
3	A	5	THR	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	50/59 (85%)	47±1 (93±3%)	3±1 (7±3%)	25	70
All	All	1700/2006 (85%)	1586 (93%)	114 (7%)	25	70

All 18 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	53	THR	33

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Mol	Chain	Res	Type	Models (Total)
3	A	21	SER	24
3	A	42	ARG	12
3	A	47	ARG	9
3	A	54	ARG	7
3	A	20	ARG	5
3	A	46	MET	4
3	A	56	ARG	3
3	A	23	MET	3
3	A	45	THR	3
3	A	57	LYS	2
3	A	13	SER	2
3	A	39	GLN	2
3	A	22	PRO	1
3	A	48	LYS	1
3	A	25	ASP	1
3	A	36	LYS	1
3	A	49	ASP	1

### 6.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 6.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.6 Ligand geometry [i](#)

Of 1 ligands modelled in this entry, 1 is monoatomic - leaving 0 for Mogul analysis.

## 6.7 Other polymers [i](#)

There are no such molecules in this entry.

## 6.8 Polymer linkage issues

There are no chain breaks in this entry.

## 7 Chemical shift validation

No chemical shift data were provided