



# Full wwPDB NMR Structure Validation Report ⓘ

Feb 12, 2017 – 06:10 pm GMT

PDB ID : 1GAU  
Title : SOLUTION STRUCTURE OF THE SPECIFIC DNA COMPLEX OF THE ZINC CONTAINING DNA BINDING DOMAIN OF THE ERYTHROID TRANSCRIPTION FACTOR GATA-1 BY MULTIDIMENSIONAL NMR  
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Deposited on : 1993-06-28

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

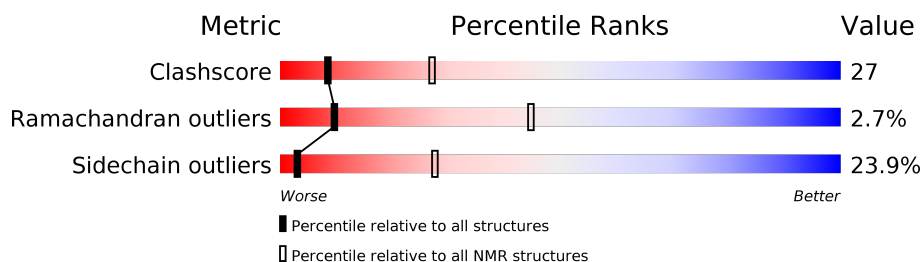
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*SOLUTION NMR*

The overall completeness of chemical shifts assignment was not calculated.

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



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

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

Mol	Chain	Length	Quality of chain
1	B	8	
2	C	8	
3	A	60	

## 2 Ensemble composition and analysis

This entry contains 30 models. Model 30 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:57 (55)	0.45	30

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 4 clusters and 2 single-model clusters were found.

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

### 3 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 1458 atoms, of which 660 are hydrogens and 0 are deuteriums.

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

Mol	Chain	Residues	Atoms						Trace
1	B	8	Total	C	H	N	O	P	0
			255	79	89	35	44	8	

- Molecule 2 is a DNA chain called DNA (5'-D(P\*GP\*TP\*TP\*TP\*AP\*TP\*CP\*T)-3').

Mol	Chain	Residues	Atoms						Trace
2	C	8	Total	C	H	N	O	P	0
			255	79	93	23	52	8	

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

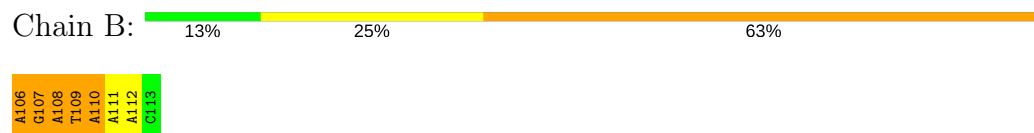
Mol	Chain	Residues	Atoms						Trace
3	A	60	Total	C	H	N	O	S	0
			948	284	478	95	85	6	

## 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.

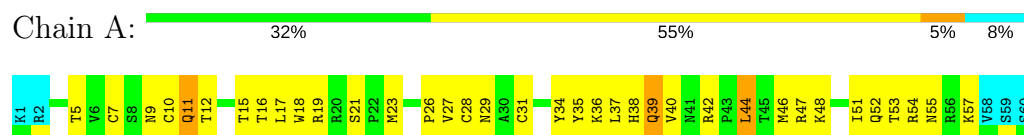
- Molecule 1: DNA (5'-D(P\*AP\*GP\*AP\*TP\*AP\*AP\*AP\*C)-3')



- Molecule 2: DNA (5'-D(P\*GP\*TP\*TP\*TP\*AP\*TP\*CP\*T)-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

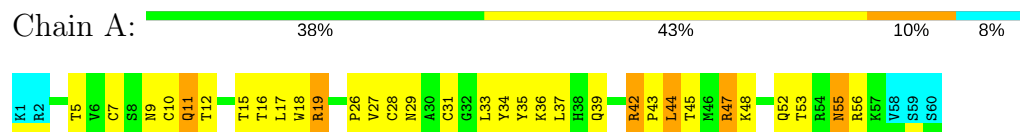
- Molecule 1: DNA (5'-D(P\*AP\*GP\*AP\*TP\*AP\*AP\*AP\*C)-3')



- Molecule 2: DNA (5'-D(P\*GP\*TP\*TP\*TP\*AP\*TP\*CP\*T)-3')



- Molecule 3: ERYTHROID TRANSCRIPTION FACTOR GATA-1



#### 4.2.2 Score per residue for model 2

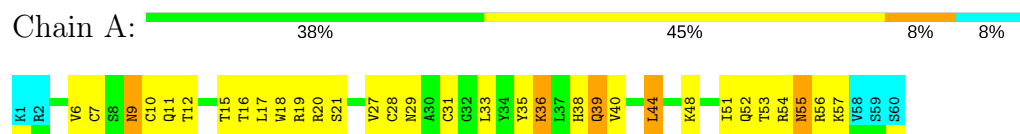
- Molecule 1: DNA (5'-D(P\*AP\*GP\*AP\*TP\*AP\*AP\*AP\*C)-3')



- Molecule 2: DNA (5'-D(P\*GP\*TP\*TP\*TP\*AP\*TP\*CP\*T)-3')

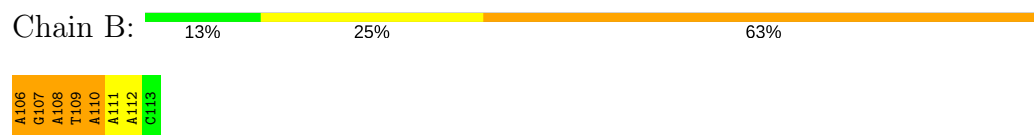


- Molecule 3: ERYTHROID TRANSCRIPTION FACTOR GATA-1



#### 4.2.3 Score per residue for model 3

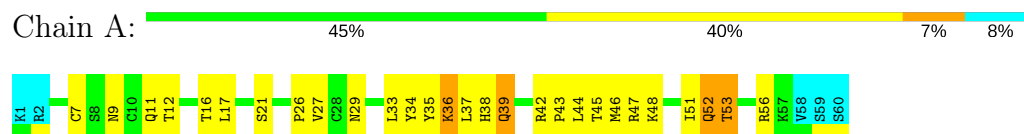
- Molecule 1: DNA (5'-D(P\*AP\*GP\*AP\*TP\*AP\*AP\*AP\*C)-3')



- Molecule 2: DNA (5'-D(P\*GP\*TP\*TP\*TP\*AP\*TP\*CP\*T)-3')



• Molecule 3: ERYTHROID TRANSCRIPTION FACTOR GATA-1



#### 4.2.4 Score per residue for model 4

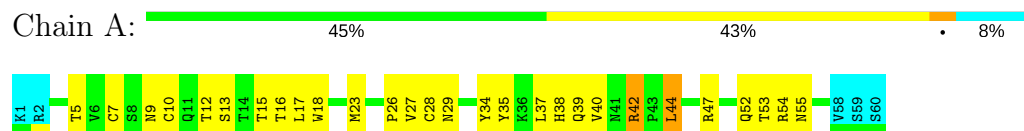
• Molecule 1: DNA (5'-D(P\*AP\*GP\*AP\*TP\*AP\*AP\*AP\*C)-3')



• Molecule 2: DNA (5'-D(P\*GP\*TP\*TP\*TP\*AP\*TP\*CP\*T)-3')



• Molecule 3: ERYTHROID TRANSCRIPTION FACTOR GATA-1



#### 4.2.5 Score per residue for model 5

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



• Molecule 2: DNA (5'-D(P\*GP\*TP\*TP\*TP\*AP\*TP\*CP\*T)-3')





- Molecule 3: ERYTHROID TRANSCRIPTION FACTOR GATA-1

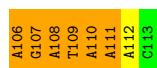
Chain A: 40% 47% 5% 8%



#### 4.2.6 Score per residue for model 6

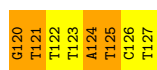
- Molecule 1: DNA (5'-D(P\*AP\*GP\*AP\*TP\*AP\*AP\*AP\*C)-3')

Chain B: 13% 13% 75%



- Molecule 2: DNA (5'-D(P\*GP\*TP\*TP\*TP\*AP\*TP\*CP\*T)-3')

Chain C: 50% 50%



- Molecule 3: ERYTHROID TRANSCRIPTION FACTOR GATA-1

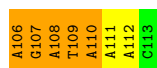
Chain A: 38% 43% 10% 8%



#### 4.2.7 Score per residue for model 7

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

Chain B: 13% 25% 63%



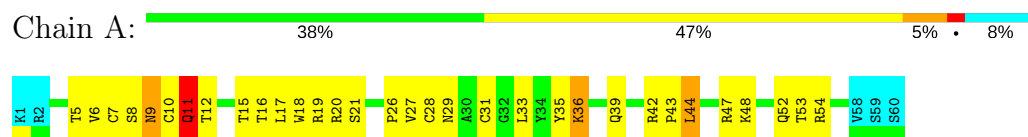
- Molecule 2: DNA (5'-D(P\*GP\*TP\*TP\*TP\*AP\*TP\*CP\*T)-3')

Chain C: 13% 25% 63%





- Molecule 3: ERYTHROID TRANSCRIPTION FACTOR GATA-1



#### 4.2.8 Score per residue for model 8

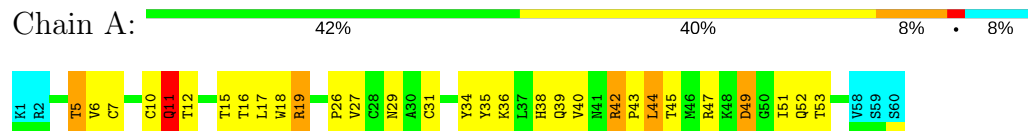
- Molecule 1: DNA (5'-D(P\*AP\*GP\*AP\*TP\*AP\*AP\*AP\*C)-3')



- Molecule 2: DNA (5'-D(P\*GP\*TP\*TP\*TP\*AP\*TP\*CP\*T)-3')



- Molecule 3: ERYTHROID TRANSCRIPTION FACTOR GATA-1



#### 4.2.9 Score per residue for model 9

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



- Molecule 2: DNA (5'-D(P\*GP\*TP\*TP\*TP\*AP\*TP\*CP\*T)-3')



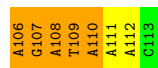
- Molecule 3: ERYTHROID TRANSCRIPTION FACTOR GATA-1



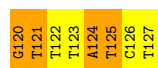


#### 4.2.10 Score per residue for model 10

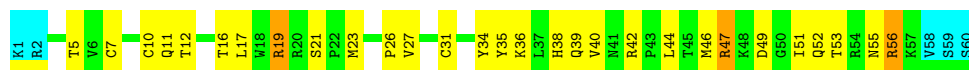
- Molecule 1: DNA (5'-D(P\*AP\*GP\*AP\*TP\*AP\*AP\*AP\*C)-3')



- Molecule 2: DNA (5'-D(P\*GP\*TP\*TP\*TP\*AP\*TP\*CP\*T)-3')

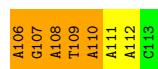


- Molecule 3: ERYTHROID TRANSCRIPTION FACTOR GATA-1



#### 4.2.11 Score per residue for model 11

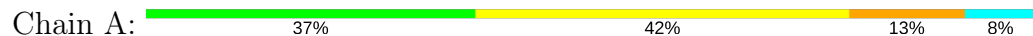
- Molecule 1: DNA (5'-D(P\*AP\*GP\*AP\*TP\*AP\*AP\*AP\*C)-3')



- Molecule 2: DNA (5'-D(P\*GP\*TP\*TP\*TP\*AP\*TP\*CP\*T)-3')



- Molecule 3: ERYTHROID TRANSCRIPTION FACTOR GATA-1



### 4.2.12 Score per residue for model 12

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

Chain B: 




- Molecule 2: DNA (5'-D(P\*GP\*TP\*TP\*TP\*AP\*TP\*CP\*T)-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(P\*AP\*GP\*AP\*TP\*AP\*AP\*AP\*C)-3')

Chain B: 



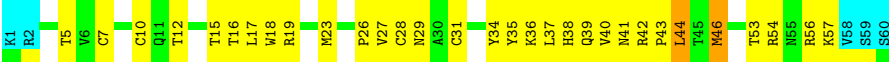
- Molecule 2: DNA (5'-D(P\*GP\*TP\*TP\*TP\*AP\*TP\*CP\*T)-3')

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(P\*AP\*GP\*AP\*TP\*AP\*AP\*AP\*C)-3')

Chain B: 



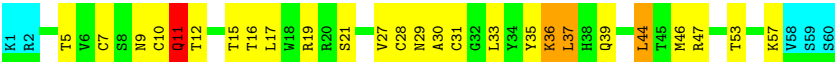
- Molecule 2: DNA (5'-D(P\*GP\*TP\*TP\*TP\*AP\*TP\*CP\*T)-3')

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(P\*AP\*GP\*AP\*TP\*AP\*AP\*AP\*C)-3')

Chain B: 



- Molecule 2: DNA (5'-D(P\*GP\*TP\*TP\*TP\*AP\*TP\*CP\*T)-3')

Chain C: 



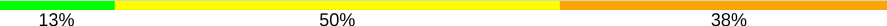
- Molecule 3: ERYTHROID TRANSCRIPTION FACTOR GATA-1

Chain A: 



#### 4.2.16 Score per residue for model 16

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

Chain B: 



- Molecule 2: DNA (5'-D(P\*GP\*TP\*TP\*TP\*AP\*TP\*CP\*T)-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(P\*AP\*GP\*AP\*TP\*AP\*AP\*AP\*C)-3')

Chain B: 

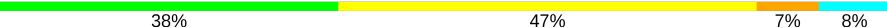


- Molecule 2: DNA (5'-D(P\*GP\*TP\*TP\*TP\*AP\*TP\*CP\*T)-3')

Chain C: 



- Molecule 3: ERYTHROID TRANSCRIPTION FACTOR GATA-1

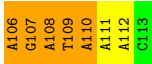
Chain A: 



#### 4.2.18 Score per residue for model 18


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

Chain B: 



- Molecule 2: DNA (5'-D(P\*GP\*TP\*TP\*TP\*AP\*TP\*CP\*T)-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(P\*AP\*GP\*AP\*TP\*AP\*AP\*AP\*C)-3')

Chain B: 



- Molecule 2: DNA (5'-D(P\*GP\*TP\*TP\*TP\*AP\*TP\*CP\*T)-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(P\*AP\*GP\*AP\*TP\*AP\*AP\*AP\*C)-3')

Chain B:  25% 75%

A106  
G107  
A108  
T109  
A110  
A111  
A112  
C113

- Molecule 2: DNA (5'-D(P\*GP\*TP\*TP\*TP\*AP\*TP\*CP\*T)-3')

Chain C:  50% 50%

G120  
T121  
T122  
T123  
A124  
T125  
C126  
T127

- Molecule 3: ERYTHROID TRANSCRIPTION FACTOR GATA-1

Chain A:  40% 40% 12% 8%

K1  
R2  
C7  
C10  
Q11  
T12  
S13  
T14  
T15  
T16  
L17  
W18  
S21  
P22  
M23  
V27  
C28  
N29  
A30  
C31  
G32  
L33  
Y34  
Y35  
K36  
L37  
H38  
Q39  
R42  
P43  
L44  
T45  
M46  
R47  
I51  
Q52  
T53  
R54  
R55  
R56  
R57  
V58  
S59  
S60

#### 4.2.21 Score per residue for model 21

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

Chain B:  13% 25% 63%

A106  
G107  
A108  
T109  
A110  
A111  
A112  
G113

- Molecule 2: DNA (5'-D(P\*GP\*TP\*TP\*TP\*AP\*TP\*CP\*T)-3')

Chain C:  25% 75%

G120  
T121  
T122  
T123  
A124  
T125  
C126  
T127

- Molecule 3: ERYTHROID TRANSCRIPTION FACTOR GATA-1

Chain A:  45% 37% 10% 8%

K1  
R2  
T5  
V6  
C7  
S8  
N9  
C10  
Q11  
T12  
S13  
T14  
T15  
T16  
L17  
W18  
R19  
P26  
V27  
C28  
N29  
A30  
C31  
Y34  
Y35  
K36  
L37  
H38  
Q39  
L44  
T45  
M46  
R47  
T53  
R54  
V58  
S59  
S60

#### 4.2.22 Score per residue for model 22

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

Chain B: 

A106  
G107  
A108  
T109  
A110  
A111  
A112  
G113

- Molecule 2: DNA (5'-D(P\*GP\*TP\*TP\*TP\*AP\*TP\*CP\*T)-3')

Chain C: 

G120  
T121  
T122  
T123  
A124  
T125  
G126  
T127

- Molecule 3: ERYTHROID TRANSCRIPTION FACTOR GATA-1

Chain A: 

K1  
R2  
T5  
V6  
C7  
Q11  
T15  
T16  
L17  
W18  
R19  
R20  
S21  
P22  
M23  
P26  
V27  
Y34  
Y35  
K36  
L37  
H38  
Q39  
V40  
R41  
R42  
R47  
K48  
D49  
G50  
I51  
Q52  
T53  
R54  
N55  
R56  
K57  
V58  
S59  
S60

#### 4.2.23 Score per residue for model 23

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

Chain B: 


A106  
G107  
A108  
T109  
A110  
A111  
A112  
G113

- Molecule 2: DNA (5'-D(P\*GP\*TP\*TP\*TP\*AP\*TP\*CP\*T)-3')

Chain C: 

G120  
T121  
T122  
T123  
A124  
T125  
G126  
T127

- Molecule 3: ERYTHROID TRANSCRIPTION FACTOR GATA-1

Chain A: 

K1  
R2  
T5  
V6  
C7  
S8  
N9  
C10  
Q11  
T12  
S13  
T14  
T15  
T16  
L17  
W18  
R19  
R20  
S21  
P26  
V27  
C28  
M29  
Y34  
Y35  
K36  
L37  
H38  
Q39  
V40  
R41  
R42  
P43  
L44  
T45  
M46  
R47  
K48  
I51  
Q52  
T53  
R54  
N55  
V58  
S59  
S60



#### 4.2.24 Score per residue for model 24

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

Chain B: 

A106  
G107  
A108  
T109  
A110  
A111  
A112  
C113

- Molecule 2: DNA (5'-D(P\*GP\*TP\*TP\*TP\*AP\*TP\*CP\*T)-3')

Chain C: 

G120  
T121  
T122  
T123  
A124  
T125  
C126  
T127

- Molecule 3: ERYTHROID TRANSCRIPTION FACTOR GATA-1

Chain A: 

K1  
R2  
T5  
V6  
C7  
S8  
N9  
C10  
Q11  
T12  
T15  
T16  
L17  
W18  
R19  
R20  
S21  
P22  
M23  
C31  
Y34  
Y35  
H38  
Q39  
V40  
N41  
R42  
P43  
R47  
K48  
Q52  
T53  
R54  
K57  
V58  
S59  
S60

#### 4.2.25 Score per residue for model 25

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

Chain B: 

A106  
G107  
A108  
T109  
A110  
A111  
A112  
G113

- Molecule 2: DNA (5'-D(P\*GP\*TP\*TP\*TP\*AP\*TP\*CP\*T)-3')

Chain C: 

G120  
T121  
T122  
T123  
A124  
T125  
C126  
T127

- Molecule 3: ERYTHROID TRANSCRIPTION FACTOR GATA-1

Chain A: 

K1  
R2  
T5  
V6  
C7  
S8  
N9  
C10  
Q11  
T12  
T15  
T16  
L17  
W18  
R19  
R20  
S21  
P22  
M23  
P26  
V27  
C28  
Y35  
K36  
Q39  
L44  
R47  
K48  
Q52  
T53  
R54  
N55  
R56  
K57  
V58  
S59  
S60

#### 4.2.26 Score per residue for model 26

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

Chain B: 

A106  
G107  
A108  
T109  
A110  
A111  
A112  
G113

- Molecule 2: DNA (5'-D(P\*GP\*TP\*TP\*TP\*AP\*TP\*CP\*T)-3')

Chain C: 

G120  
T121  
T122  
T123  
A124  
T125  
C126  
T127

- Molecule 3: ERYTHROID TRANSCRIPTION FACTOR GATA-1

Chain A: 

K1  
R2  
V6  
C7  
S8  
N9  
Q10  
Q11  
T12  
T15  
T16  
L17  
W18  
R19  
R20  
R21  
V27  
C28  
C31  
K36  
L37  
H38  
Q39  
V40  
L44  
R47  
K48  
T51  
Q52  
T53  
R54  
R55  
R56  
K57  
V58  
S59  
S60

#### 4.2.27 Score per residue for model 27

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

Chain B: 

A106  
G107  
A108  
T109  
A110  
A111  
A112  
G113

- Molecule 2: DNA (5'-D(P\*GP\*TP\*TP\*TP\*AP\*TP\*CP\*T)-3')

Chain C: 

G120  
T121  
T122  
T123  
A124  
T125  
C126  
T127

- Molecule 3: ERYTHROID TRANSCRIPTION FACTOR GATA-1

Chain A: 

K1  
R2  
T5  
V6  
Q10  
Q11  
T12  
T15  
T16  
L17  
W18  
R19  
R20  
M23  
P26  
C31  
Y35  
H38  
Q39  
V40  
L44  
T45  
M46  
R47  
T51  
Q52  
T53  
R54  
K57  
V58  
S59  
S60

#### 4.2.28 Score per residue for model 28

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

Chain B: 

A106  
G107  
A108  
T109  
A110  
A111  
A112  
G113

- Molecule 2: DNA (5'-D(P\*GP\*TP\*TP\*TP\*AP\*TP\*CP\*T)-3')

Chain C: 

G120  
T121  
T122  
T123  
A124  
T125  
C126  
T127

- Molecule 3: ERYTHROID TRANSCRIPTION FACTOR GATA-1

Chain A: 

K1  
R2  
T5  
V6  
C7  
G10  
S13  
T14  
T15  
T16  
L17  
W18  
R19  
R20  
S21  
P22  
M23  
P26  
V27  
C28  
N29  
Y34  
Y35  
K36  
L37  
H38  
Q39  
R42  
P43  
L44  
T45  
M46  
R47  
K48  
D49  
G50  
I51  
Q52  
T53  
R54  
N55  
R56  
K57  
V58  
S59  
S60

#### 4.2.29 Score per residue for model 29

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

Chain B: 

A106  
G107  
A108  
T109  
A110  
A111  
A112  
G113

- Molecule 2: DNA (5'-D(P\*GP\*TP\*TP\*TP\*AP\*TP\*CP\*T)-3')

Chain C: 

G120  
T121  
T122  
T123  
A124  
T125  
C126  
T127

- Molecule 3: ERYTHROID TRANSCRIPTION FACTOR GATA-1

Chain A: 

K1  
R2  
T5  
V6  
C7  
S8  
N9  
C10  
Q11  
T12  
T15  
T16  
L17  
W18  
R19  
R20  
P26  
V27  
C28  
N29  
A30  
C31  
G32  
L33  
Y34  
Y35  
K36  
L37  
H38  
Q39  
N41  
R42  
P43  
L44  
T45  
M46  
R47  
K48  
Q52  
T53  
R54  
V58  
S59  
S60

#### 4.2.30 Score per residue for model 30 (medoid)

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

Chain B: 

A106  
G107  
A108  
T109  
A110  
A111  
A112  
G113

- Molecule 2: DNA (5'-D(P\*GP\*TP\*TP\*TP\*AP\*TP\*CP\*T)-3')

Chain C: 

G120  
T121  
T122  
T123  
A124  
T125  
C126  
T127

- Molecule 3: ERYTHROID TRANSCRIPTION FACTOR GATA-1

Chain A: 

K1  
R2  
V6  
C7  
C10  
Q11  
T12  
S13  
T14  
T15  
T16  
L17  
W18  
R19  
R20  
M23  
V27  
C28  
N29  
A30  
G31  
G32  
L33  
Y34  
Y35  
K36  
L37  
H38  
Q39  
V40  
N41  
R42  
P43  
L44  
T45  
M46  
R47  
Q52  
T53  
R54  
N55  
R56  
K57  
V58  
S59  
S60

## 5 Refinement protocol and experimental data overview ⓘ

The models were refined using the following method: ?.

Of the ? calculated structures, 30 were deposited, based on the following criterion: ?.

The authors did not provide any information on software used for structure solution, optimization or refinement.

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

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	1.48±0.04	2±0/187 (1.1±0.1%)	3.06±0.01	20±1/286 (6.9±0.2%)
2	C	1.46±0.02	4±1/179 (2.4±0.4%)	2.56±0.01	16±1/274 (5.9±0.4%)
3	A	1.05±0.01	0±0/439 (0.0±0.0%)	0.91±0.01	0±0/594 (0.0±0.0%)
All	All	1.26	189/24150 (0.8%)	2.08	1079/34620 (3.1%)

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	106	DA	N9-C8	-6.19	1.32	1.37	18	30
2	C	124	DA	N9-C8	-6.04	1.32	1.37	26	30
2	C	122	DT	C5-C7	5.67	1.53	1.50	19	30
1	B	109	DT	C5-C7	5.66	1.53	1.50	25	30
2	C	127	DT	C5-C7	5.46	1.53	1.50	17	30
2	C	123	DT	C5-C7	5.38	1.53	1.50	18	23
2	C	120	DG	N9-C8	-5.21	1.34	1.37	10	14
1	B	108	DA	C8-N7	-5.07	1.28	1.31	22	2

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	N7-C8-N9	14.53	120.36	113.10	10	30
1	B	107	DG	N7-C8-N9	14.32	120.26	113.10	20	30
1	B	106	DA	N7-C8-N9	13.49	120.55	113.80	12	30
2	C	124	DA	N7-C8-N9	13.45	120.52	113.80	26	30
1	B	111	DA	N7-C8-N9	12.84	120.22	113.80	18	30
1	B	108	DA	N7-C8-N9	12.55	120.08	113.80	25	30
1	B	110	DA	N7-C8-N9	12.51	120.06	113.80	19	30
1	B	112	DA	N7-C8-N9	12.36	119.98	113.80	20	30
1	B	107	DG	C8-N9-C4	-10.10	102.36	106.40	17	30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
2	C	120	DG	C8-N9-C4	-9.87	102.45	106.40	7	30
1	B	110	DA	C8-N9-C4	-8.72	102.31	105.80	9	30
1	B	111	DA	C8-N9-C4	-8.49	102.41	105.80	9	30
1	B	112	DA	C8-N9-C4	-8.30	102.48	105.80	6	30
2	C	120	DG	C5-N7-C8	-8.27	100.17	104.30	20	30
1	B	108	DA	C8-N9-C4	-8.26	102.50	105.80	6	30
2	C	124	DA	C5-N7-C8	-8.23	99.79	103.90	19	30
1	B	107	DG	C5-N7-C8	-8.20	100.20	104.30	7	30
1	B	106	DA	C5-N7-C8	-8.05	99.87	103.90	2	30
1	B	106	DA	C8-N9-C4	-8.03	102.59	105.80	13	30
2	C	124	DA	C8-N9-C4	-8.02	102.59	105.80	5	30
1	B	108	DA	C5-N7-C8	-7.86	99.97	103.90	15	30
1	B	111	DA	C5-N7-C8	-7.72	100.04	103.90	8	30
1	B	112	DA	C5-N7-C8	-7.71	100.05	103.90	26	30
1	B	110	DA	C5-N7-C8	-7.49	100.16	103.90	26	30
2	C	125	DT	O4'-C1'-N1	7.06	112.94	108.00	13	30
2	C	121	DT	C6-C5-C7	-6.56	118.96	122.90	12	29
1	B	107	DG	O4'-C1'-N9	6.54	112.58	108.00	27	18
2	C	122	DT	O4'-C1'-N1	6.21	112.35	108.00	26	6
2	C	121	DT	O4'-C1'-N1	6.12	112.29	108.00	7	30
2	C	123	DT	C6-C5-C7	-6.04	119.28	122.90	9	30
2	C	127	DT	C6-C5-C7	-5.88	119.37	122.90	14	30
2	C	122	DT	C6-C5-C7	-5.84	119.40	122.90	10	30
1	B	109	DT	C6-C5-C7	-5.62	119.53	122.90	8	30
2	C	125	DT	C6-C5-C7	-5.59	119.55	122.90	20	20
2	C	120	DG	O4'-C1'-N9	5.56	111.89	108.00	8	5
2	C	125	DT	C4-C5-C6	5.55	121.33	118.00	3	29
2	C	121	DT	C4-C5-C6	5.35	121.21	118.00	19	30
1	B	112	DA	O4'-C1'-N9	5.30	111.71	108.00	30	3
2	C	123	DT	C4-C5-C6	5.21	121.13	118.00	2	19
2	C	127	DT	C4-C5-C6	5.16	121.10	118.00	26	19
2	C	122	DT	C4-C5-C6	5.00	121.00	118.00	12	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	166	89	90	9±3
2	C	162	93	94	10±3
3	A	431	431	435	25±5
All	All	22770	18390	18570	1110

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 27.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:107:DG:O6	3:A:17:LEU:HD11	0.86	1.69	13	13
2:C:124:DA:OP2	3:A:30:ALA:HB2	0.84	1.73	20	3
3:A:7:CYS:HB2	3:A:12:THR:HG22	0.77	1.55	8	7
2:C:125:DT:H71	3:A:16:THR:HB	0.74	1.57	4	6
3:A:38:HIS:O	3:A:40:VAL:HG22	0.72	1.85	26	3
2:C:120:DG:C8	2:C:121:DT:H71	0.68	2.23	7	2
3:A:11:GLN:HB2	3:A:44:LEU:HD22	0.67	1.67	7	2
2:C:124:DA:H3'	3:A:16:THR:HG21	0.65	1.67	2	16
2:C:125:DT:O4	3:A:17:LEU:HD11	0.64	1.92	28	2
3:A:15:THR:C	3:A:51:ILE:HD11	0.64	2.13	22	6
3:A:9:ASN:HB2	3:A:27:VAL:HG12	0.64	1.69	7	1
3:A:35:TYR:O	3:A:39:GLN:N	0.63	2.31	30	29
2:C:125:DT:C7	3:A:16:THR:HB	0.63	2.24	3	23
3:A:15:THR:HG21	3:A:18:TRP:CH2	0.63	2.29	23	10
1:B:106:DA:N7	3:A:17:LEU:HD22	0.62	2.08	27	8
3:A:34:TYR:HA	3:A:37:LEU:HD22	0.62	1.72	13	6
1:B:107:DG:O6	3:A:17:LEU:HD13	0.62	1.95	11	1
2:C:120:DG:H2''	2:C:121:DT:O5'	0.61	1.95	28	30
1:B:108:DA:H2'	1:B:109:DT:H72	0.61	1.72	6	10
3:A:9:ASN:OD1	3:A:27:VAL:HG11	0.61	1.96	16	7
2:C:120:DG:C4	2:C:121:DT:C6	0.61	2.89	20	13
2:C:120:DG:C2	2:C:121:DT:C2	0.61	2.89	22	17
3:A:5:THR:HG23	3:A:26:PRO:HB2	0.61	1.72	27	11
3:A:17:LEU:HB2	3:A:29:ASN:CB	0.60	2.27	21	8
2:C:124:DA:H62	3:A:33:LEU:HD11	0.59	1.58	14	2
3:A:10:CYS:HA	3:A:44:LEU:HD22	0.58	1.73	2	1
3:A:10:CYS:O	3:A:44:LEU:HD13	0.58	1.98	2	2
3:A:44:LEU:HD12	3:A:47:ARG:HB2	0.57	1.74	18	1
2:C:125:DT:O3'	3:A:56:ARG:HD3	0.57	2.00	9	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:108:DA:H2''	1:B:109:DT:O5'	0.56	2.00	23	18
2:C:125:DT:H2''	2:C:126:DC:O5'	0.56	2.00	6	12
1:B:107:DG:N7	3:A:17:LEU:CD1	0.56	2.68	29	6
3:A:7:CYS:SG	3:A:27:VAL:HA	0.56	2.40	7	23
3:A:16:THR:HG22	3:A:51:ILE:CG2	0.56	2.31	20	5
2:C:120:DG:C5	2:C:121:DT:C4	0.56	2.94	27	13
3:A:10:CYS:SG	3:A:12:THR:HG22	0.56	2.41	2	7
2:C:122:DT:OP2	3:A:37:LEU:HD23	0.55	2.01	15	3
3:A:44:LEU:O	3:A:44:LEU:HD12	0.55	2.00	30	3
3:A:10:CYS:HB2	3:A:44:LEU:CB	0.55	2.32	16	13
1:B:106:DA:C6	1:B:107:DG:C6	0.55	2.95	3	21
1:B:107:DG:O6	3:A:17:LEU:CD1	0.55	2.55	27	15
3:A:10:CYS:SG	3:A:12:THR:CG2	0.55	2.95	2	10
3:A:5:THR:HG22	3:A:18:TRP:CH2	0.55	2.37	7	4
3:A:11:GLN:OE1	3:A:44:LEU:HD13	0.55	2.01	14	1
3:A:15:THR:HG21	3:A:18:TRP:CZ3	0.55	2.37	23	17
3:A:15:THR:HG23	3:A:18:TRP:CZ2	0.54	2.37	29	10
3:A:44:LEU:HD12	3:A:44:LEU:O	0.54	2.02	9	3
3:A:15:THR:O	3:A:51:ILE:HD11	0.54	2.01	16	5
1:B:108:DA:N6	2:C:124:DA:N6	0.54	2.55	24	15
3:A:38:HIS:HB2	3:A:40:VAL:HG22	0.54	1.79	13	6
1:B:108:DA:N6	3:A:17:LEU:CD1	0.54	2.71	26	5
1:B:110:DA:C2	1:B:111:DA:C2	0.54	2.96	20	1
3:A:34:TYR:CE1	3:A:42:ARG:HG3	0.54	2.38	5	4
3:A:34:TYR:CE1	3:A:43:PRO:HD2	0.54	2.38	24	2
3:A:43:PRO:HB2	3:A:45:THR:HG23	0.53	1.80	20	1
3:A:10:CYS:SG	3:A:47:ARG:HD2	0.53	2.43	30	2
3:A:17:LEU:HB2	3:A:29:ASN:HB2	0.53	1.79	6	13
1:B:107:DG:N7	3:A:17:LEU:HD13	0.53	2.19	13	2
3:A:37:LEU:N	3:A:37:LEU:CD1	0.52	2.73	14	1
1:B:106:DA:N6	2:C:126:DC:N4	0.52	2.57	9	11
1:B:106:DA:H2''	1:B:107:DG:O5'	0.52	2.04	28	28
3:A:6:VAL:HG23	3:A:6:VAL:O	0.52	2.05	11	5
3:A:38:HIS:O	3:A:39:GLN:CG	0.52	2.57	19	3
1:B:108:DA:H61	3:A:17:LEU:CD1	0.52	2.17	26	4
3:A:37:LEU:HD12	3:A:37:LEU:N	0.52	2.19	3	1
2:C:122:DT:P	3:A:37:LEU:HD23	0.51	2.45	15	4
3:A:7:CYS:O	3:A:11:GLN:N	0.51	2.43	18	15
2:C:121:DT:H2'	2:C:122:DT:H72	0.51	1.82	30	3
3:A:44:LEU:HD13	3:A:47:ARG:CZ	0.51	2.36	12	1
2:C:124:DA:H62	3:A:33:LEU:CD1	0.51	2.19	17	4

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:A:15:THR:CG2	3:A:28:CYS:CB	0.51	2.88	18	16
3:A:35:TYR:CD2	3:A:40:VAL:O	0.51	2.64	24	6
3:A:7:CYS:CB	3:A:12:THR:HG22	0.51	2.32	8	8
1:B:106:DA:C2	1:B:107:DG:C4	0.51	2.98	27	10
3:A:10:CYS:O	3:A:47:ARG:HD3	0.51	2.05	15	1
1:B:107:DG:O6	3:A:17:LEU:HD22	0.51	2.06	11	1
1:B:106:DA:N7	3:A:17:LEU:HD13	0.50	2.21	8	3
2:C:125:DT:H2''	2:C:126:DC:C6	0.50	2.42	30	18
1:B:106:DA:C2	1:B:107:DG:C2	0.50	2.99	5	15
3:A:5:THR:HG23	3:A:26:PRO:CB	0.50	2.36	27	14
3:A:5:THR:CG2	3:A:26:PRO:HB2	0.50	2.36	16	5
3:A:31:CYS:O	3:A:42:ARG:HD2	0.50	2.06	15	2
3:A:36:LYS:HD3	3:A:37:LEU:HD12	0.50	1.82	20	1
3:A:6:VAL:O	3:A:6:VAL:HG23	0.50	2.06	26	5
3:A:16:THR:HG23	3:A:51:ILE:CG2	0.50	2.36	11	1
3:A:42:ARG:CD	3:A:42:ARG:N	0.50	2.75	30	2
3:A:19:ARG:O	3:A:27:VAL:HG23	0.50	2.07	7	1
3:A:34:TYR:CD1	3:A:42:ARG:HB2	0.50	2.42	22	2
1:B:107:DG:C2	1:B:108:DA:C4	0.49	3.00	16	8
3:A:34:TYR:CD1	3:A:42:ARG:HB3	0.49	2.43	29	2
1:B:109:DT:H2''	1:B:110:DA:O5'	0.49	2.08	8	20
1:B:108:DA:C2	1:B:109:DT:C2	0.49	3.00	12	3
3:A:15:THR:CG2	3:A:18:TRP:CZ2	0.49	2.95	29	4
2:C:123:DT:H2''	2:C:124:DA:C8	0.49	2.43	1	14
2:C:120:DG:N7	2:C:121:DT:H72	0.49	2.23	3	5
1:B:106:DA:N7	3:A:17:LEU:CD2	0.49	2.76	22	9
3:A:34:TYR:CE1	3:A:42:ARG:HB3	0.49	2.43	6	1
3:A:10:CYS:O	3:A:47:ARG:CD	0.49	2.61	17	2
3:A:10:CYS:O	3:A:44:LEU:HB3	0.49	2.07	27	4
3:A:35:TYR:CD1	3:A:39:GLN:HA	0.49	2.43	27	5
1:B:107:DG:O6	3:A:17:LEU:HD21	0.49	2.07	3	3
3:A:16:THR:HG22	3:A:51:ILE:HG21	0.48	1.84	2	9
2:C:124:DA:H2'	3:A:16:THR:HG21	0.48	1.85	26	8
3:A:10:CYS:SG	3:A:47:ARG:CZ	0.48	3.02	5	1
3:A:9:ASN:HB3	3:A:31:CYS:SG	0.48	2.49	2	5
1:B:106:DA:N6	3:A:17:LEU:HD11	0.48	2.23	27	3
1:B:107:DG:C6	1:B:108:DA:C6	0.48	3.02	1	3
3:A:19:ARG:HG3	3:A:27:VAL:O	0.48	2.08	1	1
3:A:35:TYR:O	3:A:39:GLN:CA	0.48	2.62	20	10
3:A:10:CYS:HB2	3:A:44:LEU:HB3	0.48	1.86	26	6
3:A:33:LEU:O	3:A:36:LYS:HG3	0.47	2.08	2	4

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:A:38:HIS:CB	3:A:40:VAL:HG22	0.47	2.39	29	9
2:C:125:DT:H73	3:A:16:THR:HB	0.47	1.85	3	5
3:A:36:LYS:HD3	3:A:37:LEU:CD1	0.47	2.39	20	1
2:C:125:DT:H72	3:A:16:THR:HB	0.47	1.86	15	4
3:A:35:TYR:CE1	3:A:39:GLN:HG3	0.47	2.45	7	2
3:A:10:CYS:SG	3:A:12:THR:HB	0.47	2.49	13	2
2:C:120:DG:C8	2:C:121:DT:H72	0.47	2.43	9	2
3:A:44:LEU:HD23	3:A:44:LEU:H	0.47	1.70	1	1
3:A:39:GLN:O	3:A:39:GLN:CG	0.47	2.63	12	7
3:A:10:CYS:O	3:A:44:LEU:CB	0.47	2.62	5	3
3:A:54:ARG:HG3	3:A:54:ARG:NH1	0.47	2.23	28	3
3:A:9:ASN:CB	3:A:31:CYS:SG	0.47	3.03	29	5
3:A:33:LEU:O	3:A:36:LYS:HD3	0.47	2.10	17	1
3:A:34:TYR:CE2	3:A:42:ARG:HB2	0.47	2.44	20	1
3:A:34:TYR:OH	3:A:42:ARG:HD2	0.47	2.09	28	1
2:C:120:DG:N3	2:C:121:DT:C6	0.47	2.83	20	2
3:A:36:LYS:CD	3:A:37:LEU:CD1	0.47	2.93	20	1
3:A:35:TYR:O	3:A:39:GLN:HA	0.47	2.08	17	3
3:A:31:CYS:O	3:A:35:TYR:HB2	0.47	2.09	8	8
2:C:121:DT:N3	2:C:122:DT:C4	0.47	2.83	26	3
3:A:5:THR:O	3:A:5:THR:HG22	0.47	2.08	24	3
3:A:10:CYS:HA	3:A:44:LEU:HB3	0.47	1.85	13	1
2:C:122:DT:O3'	3:A:46:MET:HE1	0.47	2.10	13	1
1:B:106:DA:H61	2:C:126:DC:N4	0.46	2.09	9	4
2:C:121:DT:H2'	2:C:122:DT:H71	0.46	1.86	21	5
3:A:47:ARG:NH1	3:A:47:ARG:HG3	0.46	2.26	1	1
3:A:12:THR:HG23	3:A:12:THR:O	0.46	2.11	4	1
3:A:35:TYR:HB2	3:A:42:ARG:NE	0.46	2.25	9	1
3:A:42:ARG:N	3:A:42:ARG:CD	0.46	2.78	4	2
3:A:52:GLN:HG3	3:A:53:THR:N	0.46	2.26	3	2
3:A:52:GLN:CG	3:A:53:THR:N	0.46	2.79	23	2
2:C:122:DT:H2''	2:C:123:DT:O5'	0.46	2.11	4	6
3:A:15:THR:CG2	3:A:18:TRP:CH2	0.46	2.98	23	5
3:A:20:ARG:CB	3:A:26:PRO:HA	0.45	2.41	27	1
3:A:17:LEU:O	3:A:29:ASN:CB	0.45	2.64	17	1
3:A:15:THR:HG22	3:A:28:CYS:CB	0.45	2.41	18	2
3:A:15:THR:CG2	3:A:28:CYS:HB3	0.45	2.41	29	1
3:A:38:HIS:O	3:A:39:GLN:HG2	0.45	2.11	2	6
3:A:31:CYS:O	3:A:42:ARG:HG2	0.45	2.11	9	1
2:C:126:DC:H2'	2:C:127:DT:C5	0.45	2.46	16	2
3:A:35:TYR:CD2	3:A:42:ARG:CZ	0.45	2.99	4	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:A:34:TYR:CE2	3:A:42:ARG:HG3	0.45	2.46	23	1
3:A:10:CYS:SG	3:A:47:ARG:HD3	0.45	2.51	11	5
1:B:108:DA:N1	2:C:125:DT:O4	0.45	2.48	30	3
2:C:121:DT:C2	2:C:122:DT:C5	0.45	3.05	3	4
2:C:120:DG:C5	2:C:121:DT:H72	0.45	2.47	9	1
3:A:5:THR:O	3:A:18:TRP:CH2	0.45	2.70	11	6
3:A:44:LEU:HB2	3:A:47:ARG:HD3	0.45	1.88	12	1
2:C:123:DT:H73	3:A:33:LEU:HB3	0.45	1.89	29	1
1:B:107:DG:O6	3:A:17:LEU:HD12	0.45	2.12	5	2
1:B:110:DA:H2''	1:B:111:DA:C8	0.45	2.47	1	2
3:A:9:ASN:OD1	3:A:42:ARG:HD2	0.45	2.12	24	1
3:A:19:ARG:HD3	3:A:29:ASN:HA	0.45	1.87	29	1
3:A:7:CYS:SG	3:A:28:CYS:N	0.45	2.90	7	1
1:B:106:DA:N7	3:A:17:LEU:CD1	0.45	2.80	22	9
3:A:39:GLN:CG	3:A:39:GLN:O	0.45	2.64	7	5
3:A:29:ASN:OD1	3:A:33:LEU:HD12	0.45	2.12	7	1
3:A:19:ARG:HD2	3:A:29:ASN:HA	0.45	1.89	8	1
3:A:7:CYS:HA	3:A:26:PRO:O	0.45	2.11	3	6
3:A:33:LEU:HD23	3:A:36:LYS:CE	0.45	2.42	3	1
1:B:108:DA:H2'	1:B:109:DT:H71	0.45	1.88	1	2
3:A:12:THR:HG23	3:A:15:THR:HG22	0.45	1.87	14	1
3:A:17:LEU:O	3:A:29:ASN:HB2	0.44	2.12	17	2
2:C:125:DT:H2''	2:C:126:DC:C5	0.44	2.47	26	1
1:B:112:DA:C6	1:B:113:DC:N4	0.44	2.85	24	1
1:B:108:DA:C2	2:C:126:DC:N3	0.44	2.86	26	1
3:A:16:THR:CG2	3:A:51:ILE:HG21	0.44	2.42	11	1
1:B:107:DG:O6	3:A:17:LEU:CD2	0.44	2.65	30	2
3:A:19:ARG:HG3	3:A:19:ARG:O	0.44	2.13	15	1
2:C:124:DA:H3'	3:A:16:THR:CG2	0.44	2.43	28	4
3:A:34:TYR:CZ	3:A:42:ARG:HG3	0.44	2.48	3	1
2:C:125:DT:O4	3:A:17:LEU:CD1	0.44	2.65	11	1
3:A:34:TYR:C	3:A:34:TYR:CD1	0.44	2.91	24	4
3:A:19:ARG:HB2	3:A:27:VAL:O	0.44	2.13	10	1
3:A:16:THR:CG2	3:A:51:ILE:CG2	0.44	2.95	28	1
3:A:10:CYS:SG	3:A:47:ARG:CD	0.44	3.06	9	3
2:C:124:DA:OP1	3:A:51:ILE:HG23	0.44	2.12	9	1
3:A:35:TYR:CE1	3:A:39:GLN:CG	0.44	3.01	20	1
3:A:36:LYS:HD2	3:A:37:LEU:CD1	0.44	2.43	14	1
3:A:33:LEU:O	3:A:37:LEU:HD13	0.44	2.13	30	3
3:A:7:CYS:HB3	3:A:12:THR:HG22	0.44	1.90	18	1
2:C:124:DA:C4	2:C:125:DT:C4	0.43	3.06	11	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:111:DA:C2	1:B:112:DA:C2	0.43	3.06	8	1
3:A:38:HIS:HB2	3:A:40:VAL:CG2	0.43	2.43	13	3
2:C:124:DA:C3'	3:A:16:THR:HG21	0.43	2.41	26	6
3:A:38:HIS:O	3:A:39:GLN:HG3	0.43	2.14	4	1
3:A:9:ASN:ND2	3:A:27:VAL:HG11	0.43	2.28	2	2
3:A:33:LEU:HA	3:A:36:LYS:HD3	0.43	1.90	17	1
3:A:19:ARG:CB	3:A:27:VAL:O	0.43	2.66	19	1
2:C:122:DT:OP2	3:A:37:LEU:CD2	0.43	2.66	21	1
1:B:106:DA:H2''	1:B:107:DG:C5'	0.43	2.43	12	1
3:A:31:CYS:HB3	3:A:42:ARG:HD3	0.43	1.90	13	1
3:A:28:CYS:SG	3:A:30:ALA:HB3	0.43	2.54	17	1
2:C:126:DC:P	3:A:56:ARG:HD3	0.43	2.53	9	1
1:B:112:DA:C5	1:B:113:DC:N4	0.43	2.87	13	2
3:A:10:CYS:O	3:A:11:GLN:HG2	0.43	2.13	30	4
3:A:35:TYR:C	3:A:35:TYR:CD1	0.43	2.91	24	1
3:A:8:SER:OG	3:A:26:PRO:HD2	0.42	2.14	7	1
3:A:10:CYS:HB2	3:A:44:LEU:HB2	0.42	1.91	16	1
1:B:106:DA:C2	1:B:107:DG:N3	0.42	2.87	27	3
3:A:10:CYS:O	3:A:12:THR:N	0.42	2.53	24	2
3:A:33:LEU:O	3:A:37:LEU:CD1	0.42	2.67	3	1
3:A:15:THR:HB	3:A:28:CYS:HB2	0.42	1.91	1	2
2:C:126:DC:H2'	2:C:127:DT:C6	0.42	2.49	19	4
3:A:31:CYS:O	3:A:42:ARG:NE	0.42	2.51	17	1
2:C:124:DA:C5'	3:A:52:GLN:O	0.42	2.67	28	1
2:C:124:DA:C2'	3:A:16:THR:HG21	0.42	2.45	26	1
3:A:9:ASN:OD1	3:A:42:ARG:HD3	0.42	2.15	19	1
2:C:125:DT:C7	3:A:16:THR:OG1	0.42	2.67	1	1
2:C:124:DA:N6	3:A:33:LEU:HD11	0.42	2.29	14	1
3:A:12:THR:HB	3:A:47:ARG:HD3	0.42	1.92	10	1
3:A:9:ASN:HB2	3:A:31:CYS:SG	0.42	2.55	29	1
3:A:5:THR:HG22	3:A:5:THR:O	0.42	2.14	1	2
1:B:106:DA:N7	3:A:17:LEU:HD21	0.42	2.28	17	1
3:A:44:LEU:O	3:A:47:ARG:HG2	0.42	2.14	30	1
3:A:54:ARG:CG	3:A:54:ARG:NH1	0.42	2.81	29	1
3:A:28:CYS:O	3:A:29:ASN:C	0.42	2.58	14	3
3:A:54:ARG:HG3	3:A:55:ASN:N	0.42	2.29	28	1
3:A:47:ARG:HG3	3:A:47:ARG:NH1	0.42	2.30	24	1
2:C:124:DA:C5'	3:A:52:GLN:HG2	0.42	2.45	26	3
3:A:19:ARG:HB3	3:A:27:VAL:O	0.42	2.14	19	2
2:C:124:DA:C2	2:C:125:DT:N3	0.42	2.88	30	3
3:A:34:TYR:CZ	3:A:43:PRO:HD2	0.42	2.50	1	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:A:42:ARG:CG	3:A:43:PRO:HD2	0.41	2.44	8	2
1:B:111:DA:N6	2:C:121:DT:O4	0.41	2.53	9	1
3:A:5:THR:O	3:A:18:TRP:CZ2	0.41	2.73	5	2
3:A:38:HIS:O	3:A:39:GLN:CB	0.41	2.68	19	1
3:A:47:ARG:HG2	3:A:48:LYS:N	0.41	2.29	28	1
3:A:15:THR:CG2	3:A:28:CYS:HB2	0.41	2.45	1	3
3:A:44:LEU:HB2	3:A:47:ARG:HG2	0.41	1.92	8	1
3:A:44:LEU:O	3:A:47:ARG:HB3	0.41	2.16	17	1
3:A:35:TYR:CE1	3:A:39:GLN:HG2	0.41	2.50	20	1
3:A:28:CYS:SG	3:A:47:ARG:NH2	0.41	2.94	5	1
3:A:11:GLN:HG2	3:A:47:ARG:NH1	0.41	2.30	15	1
3:A:34:TYR:CD1	3:A:34:TYR:C	0.41	2.93	10	1
1:B:113:DC:N3	2:C:120:DG:N2	0.41	2.68	20	1
2:C:126:DC:OP1	3:A:56:ARG:HD3	0.41	2.15	26	1
1:B:107:DG:H2''	1:B:108:DA:O5'	0.41	2.15	14	1
3:A:34:TYR:CE1	3:A:38:HIS:CD2	0.41	3.09	21	1
3:A:16:THR:HG23	3:A:51:ILE:HG21	0.41	1.91	11	1
2:C:122:DT:O5'	3:A:37:LEU:HD23	0.41	2.15	15	1
3:A:16:THR:CG2	3:A:51:ILE:HG23	0.41	2.45	3	1
3:A:28:CYS:O	3:A:28:CYS:SG	0.41	2.79	21	1
3:A:4:GLY:O	3:A:6:VAL:HG13	0.41	2.16	6	1
3:A:10:CYS:SG	3:A:47:ARG:HG3	0.41	2.56	25	1
2:C:125:DT:O3'	3:A:56:ARG:HD2	0.41	2.16	10	2
2:C:126:DC:C4	2:C:127:DT:O4	0.41	2.74	14	1
2:C:123:DT:OP2	3:A:34:TYR:HB2	0.40	2.16	8	1
3:A:36:LYS:HG2	3:A:37:LEU:N	0.40	2.30	17	1
1:B:107:DG:N2	1:B:108:DA:N3	0.40	2.69	12	2
3:A:12:THR:HB	3:A:47:ARG:HD2	0.40	1.93	12	1
1:B:106:DA:C6	1:B:107:DG:O6	0.40	2.75	26	1
2:C:125:DT:C2'	2:C:126:DC:C5	0.40	3.04	26	1
2:C:125:DT:H71	3:A:16:THR:CB	0.40	2.46	30	1
1:B:109:DT:O2	3:A:57:LYS:NZ	0.40	2.54	17	1
2:C:122:DT:OP2	3:A:37:LEU:HD22	0.40	2.16	21	1
2:C:123:DT:H71	3:A:33:LEU:HB3	0.40	1.94	11	1

## 6.3 Torsion angles

### 6.3.1 Protein backbone

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	55/60 (92%)	43±2 (78±4%)	11±2 (19±4%)	2±1 (3±2%)	10	45
All	All	1650/1800 (92%)	1287 (78%)	318 (19%)	45 (3%)	10	45

All 10 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	11	GLN	15
3	A	5	THR	8
3	A	49	ASP	6
3	A	55	ASN	5
3	A	18	TRP	3
3	A	51	ILE	2
3	A	20	ARG	2
3	A	41	ASN	2
3	A	39	GLN	1
3	A	52	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	
3	A	49/54 (91%)	37±2 (76±4%)	12±2 (24±4%)	3	27
All	All	1470/1620 (91%)	1118 (76%)	352 (24%)	3	27

All 26 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	30
3	A	44	LEU	24
3	A	47	ARG	23
3	A	54	ARG	21
3	A	36	LYS	20
3	A	19	ARG	20

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Mol	Chain	Res	Type	Models (Total)
3	A	52	GLN	18
3	A	21	SER	18
3	A	23	MET	17
3	A	46	MET	16
3	A	39	GLN	16
3	A	48	LYS	16
3	A	42	ARG	15
3	A	57	LYS	14
3	A	20	ARG	12
3	A	11	GLN	12
3	A	56	ARG	10
3	A	55	ASN	10
3	A	49	ASP	9
3	A	13	SER	8
3	A	45	THR	7
3	A	9	ASN	6
3	A	37	LEU	4
3	A	41	ASN	3
3	A	43	PRO	2
3	A	6	VAL	1

### 6.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

### 6.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

### 6.6 Ligand geometry ⓘ

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