



Full wwPDB NMR Structure Validation Report ⓘ

May 28, 2020 – 07:39 pm BST

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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 : 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 : 2.11
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

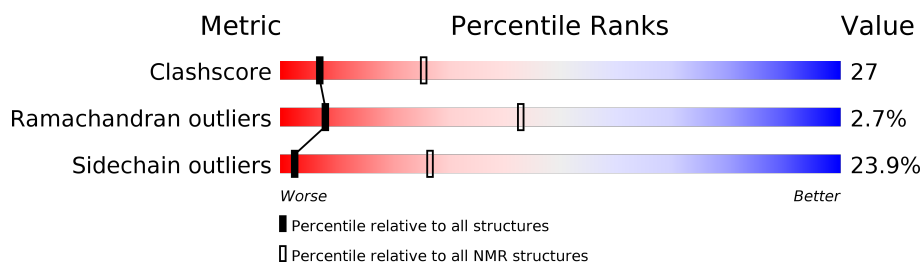
1 Overall quality at a glance

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	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 $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	B	8	<div> <div>13%</div> <div>25%</div> <div>63%</div> </div>
2	C	8	<div> <div>25%</div> <div>75%</div> </div>
3	A	60	<div> <div>32%</div> <div>55%</div> <div>5%</div> <div>8%</div> </div>

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 5 clusters. No single-model clusters were found.

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

3 Entry composition

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.

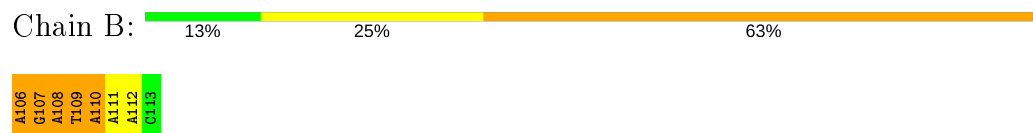
Mol	Chain	Residues	Atoms						Trace
3	A	60	Total	C	H	N	O	S	0
			948	284	478	95	85	6	

4 Residue-property plots

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.

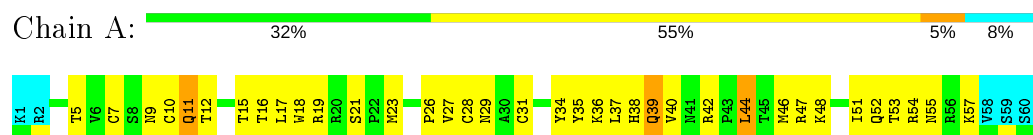
- Molecule 1: DNA (5'-D(P*AP*GP*AP*TP*AP*AP*AP*C)-3')



- 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

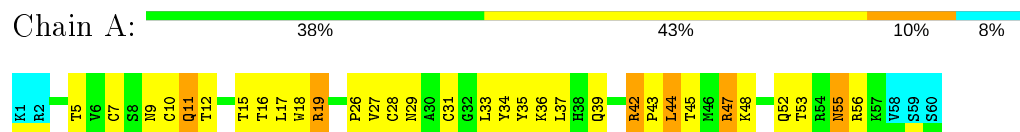
- Molecule 1: DNA (5'-D(P*AP*GP*AP*TP*AP*AP*AP*C)-3')



- 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

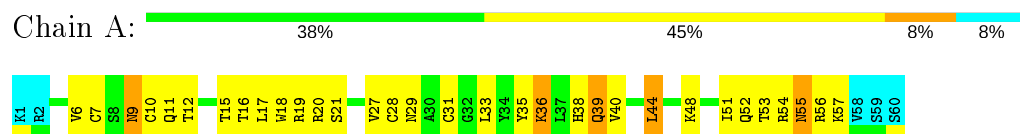
- Molecule 1: DNA (5'-D(P*AP*GP*AP*TP*AP*AP*AP*C)-3')



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

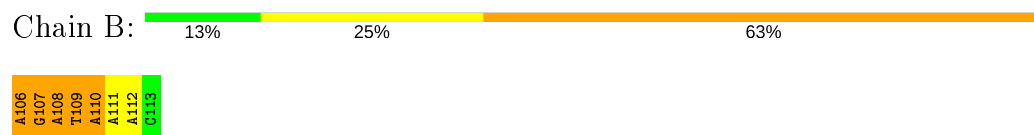


- Molecule 3: ERYTHROID TRANSCRIPTION FACTOR GATA-1



4.2.3 Score per residue for model 3

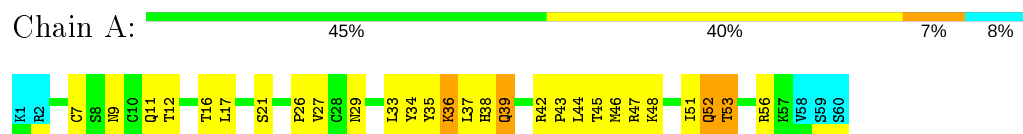
- Molecule 1: DNA (5'-D(P*AP*GP*AP*TP*AP*AP*AP*C)-3')



- 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

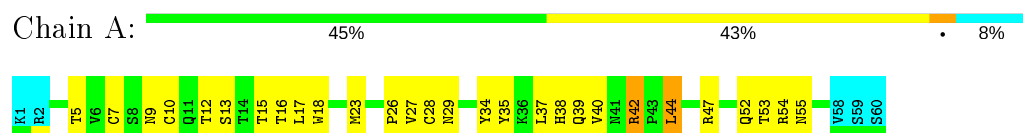
- Molecule 1: DNA (5'-D(P*AP*GP*AP*TP*AP*AP*AP*C)-3')



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



- Molecule 3: ERYTHROID TRANSCRIPTION FACTOR GATA-1



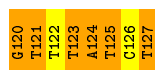
4.2.5 Score per residue for model 5

- 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

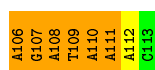
Chain A: 40% 47% 5% 8%



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%

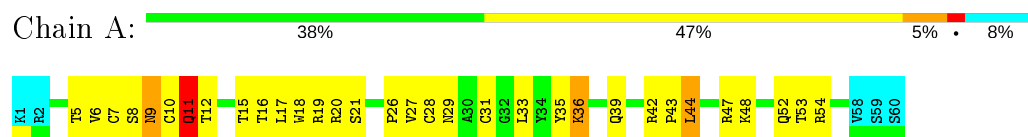


- Molecule 2: DNA (5'-D(P*GP*TP*TP*TP*AP*TP*CP*T)-3')

Chain C: 13% 25% 63%



- Molecule 3: ERYTHROID TRANSCRIPTION FACTOR GATA-1



4.2.8 Score per residue for model 8

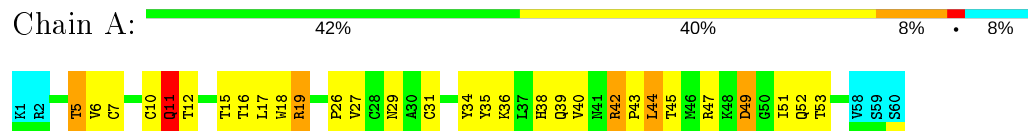
- Molecule 1: DNA (5'-D(P*AP*GP*AP*TP*AP*AP*AP*C)-3')



- 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



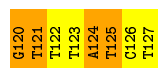


4.2.10 Score per residue for model 10

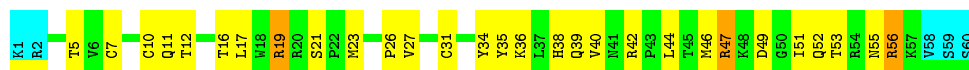
- Molecule 1: DNA (5'-D(P*AP*GP*AP*TP*AP*AP*AP*C)-3')



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



- Molecule 3: ERYTHROID TRANSCRIPTION FACTOR GATA-1

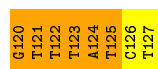


4.2.11 Score per residue for model 11

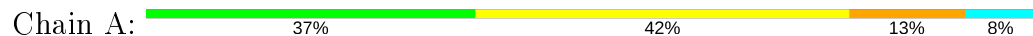
- Molecule 1: DNA (5'-D(P*AP*GP*AP*TP*AP*AP*AP*C)-3')



- 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

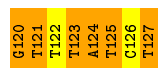
- Molecule 1: DNA (5'-D(P*AP*GP*AP*TP*AP*AP*AP*C)-3')

Chain B: 



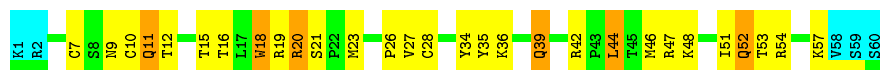
- Molecule 2: DNA (5'-D(P*GP*TP*TP*TP*AP*TP*CP*T)-3')

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: 



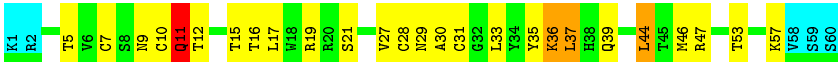
- Molecule 2: DNA (5'-D(P*GP*TP*TP*TP*AP*TP*CP*T)-3')

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: 

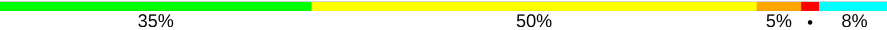


- Molecule 2: DNA (5'-D(P*GP*TP*TP*TP*AP*TP*CP*T)-3')

Chain C: 




- Molecule 3: ERYTHROID TRANSCRIPTION FACTOR GATA-1

Chain A: 



4.2.16 Score per residue for model 16

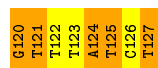
- Molecule 1: DNA (5'-D(P*AP*GP*AP*TP*AP*AP*AP*C)-3')

Chain B: 



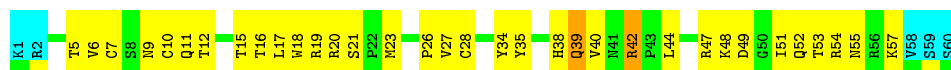
- Molecule 2: DNA (5'-D(P*GP*TP*TP*TP*AP*TP*CP*T)-3')

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: 

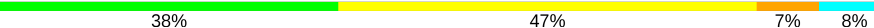


- Molecule 2: DNA (5'-D(P*GP*TP*TP*TP*AP*TP*CP*T)-3')

Chain C: 



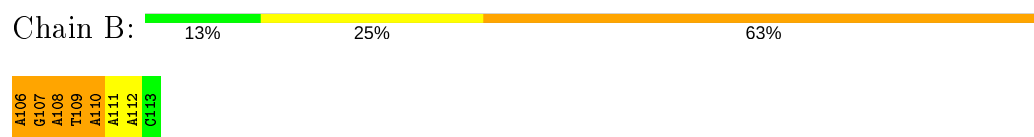
- Molecule 3: ERYTHROID TRANSCRIPTION FACTOR GATA-1

Chain A: 

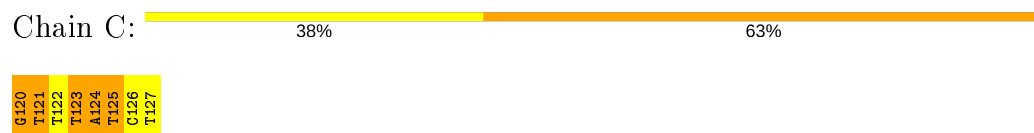


4.2.18 Score per residue for model 18

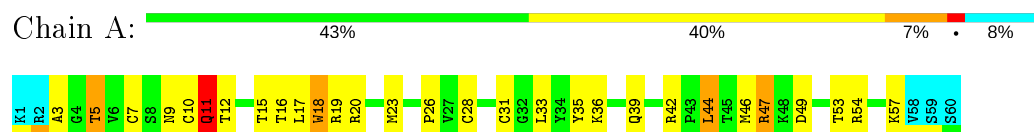
- Molecule 1: DNA (5'-D(P*AP*GP*AP*TP*AP*AP*AP*C)-3')



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



- Molecule 3: ERYTHROID TRANSCRIPTION FACTOR GATA-1



4.2.19 Score per residue for model 19

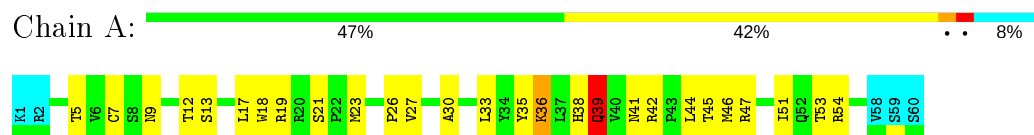
- Molecule 1: DNA (5'-D(P*AP*GP*AP*TP*AP*AP*AP*C)-3')



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



- Molecule 3: ERYTHROID TRANSCRIPTION FACTOR GATA-1



4.2.20 Score per residue for model 20

- 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
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: 

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
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

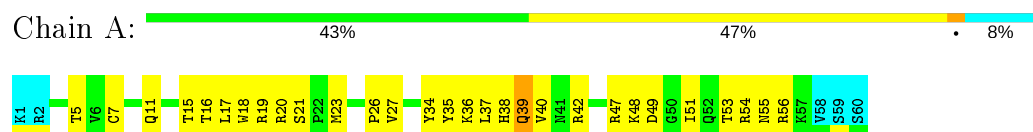
- Molecule 1: DNA (5'-D(P*AP*GP*AP*TP*AP*AP*AP*C)-3')



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



- Molecule 3: ERYTHROID TRANSCRIPTION FACTOR GATA-1



4.2.23 Score per residue for model 23

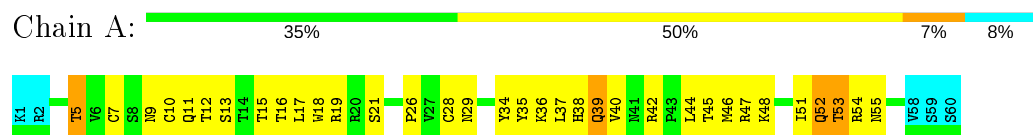
- Molecule 1: DNA (5'-D(P*AP*GP*AP*TP*AP*AP*AP*C)-3')



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



- Molecule 3: ERYTHROID TRANSCRIPTION FACTOR GATA-1



4.2.24 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

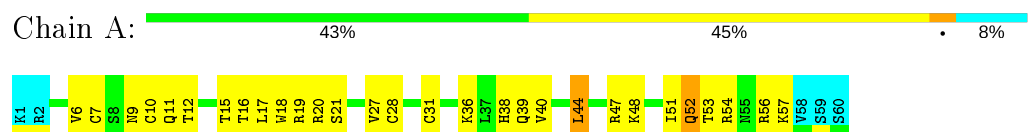
- Molecule 1: DNA (5'-D(P*AP*GP*AP*TP*AP*AP*AP*C)-3')



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

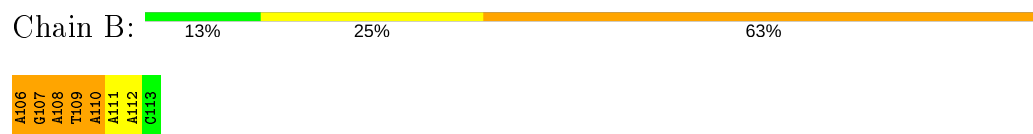


- Molecule 3: ERYTHROID TRANSCRIPTION FACTOR GATA-1

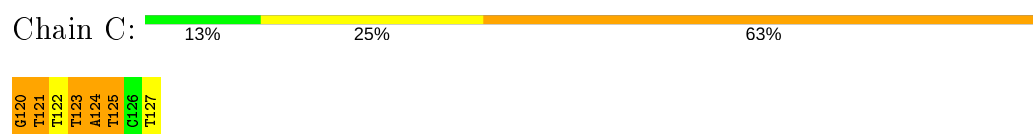


4.2.27 Score per residue for model 27

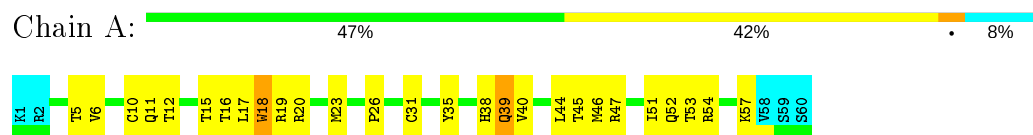
- Molecule 1: DNA (5'-D(P*AP*GP*AP*TP*AP*AP*AP*C)-3')



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

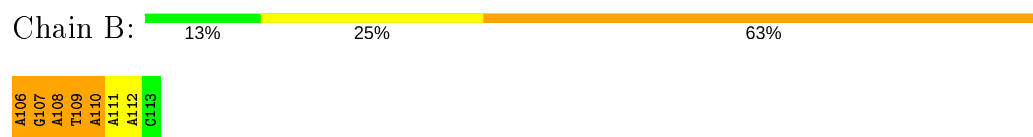


- Molecule 3: ERYTHROID TRANSCRIPTION FACTOR GATA-1

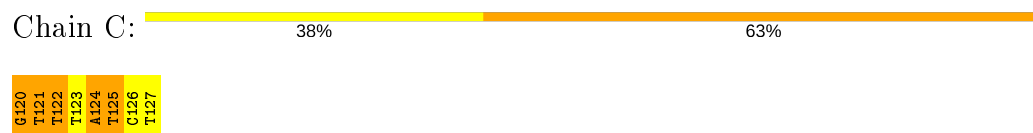


4.2.28 Score per residue for model 28

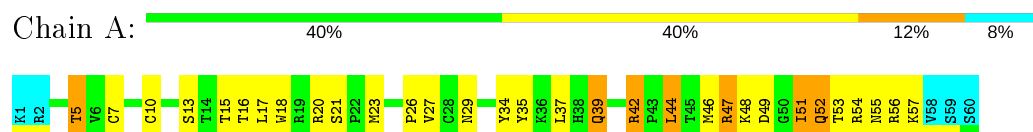
- Molecule 1: DNA (5'-D(P*AP*GP*AP*TP*AP*AP*AP*C)-3')



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

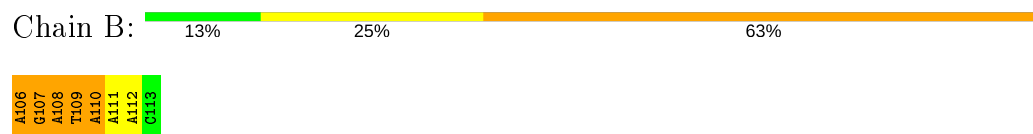


- Molecule 3: ERYTHROID TRANSCRIPTION FACTOR GATA-1

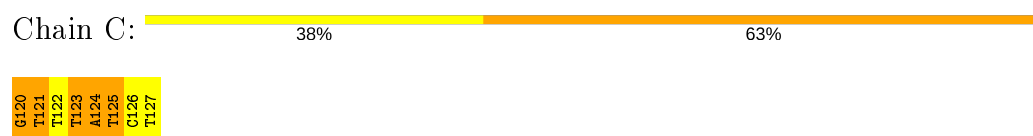


4.2.29 Score per residue for model 29

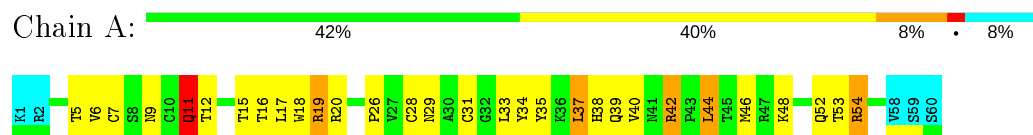
- Molecule 1: DNA (5'-D(P*AP*GP*AP*TP*AP*AP*AP*C)-3')



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



- Molecule 3: ERYTHROID TRANSCRIPTION FACTOR GATA-1



4.2.30 Score per residue for model 30 (medoid)

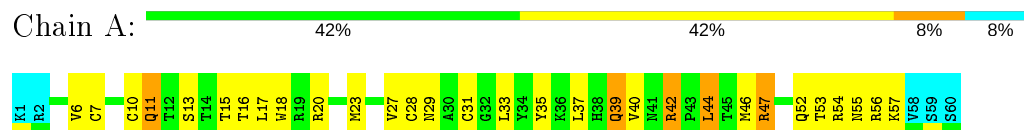
- Molecule 1: DNA (5'-D(P*AP*GP*AP*TP*AP*AP*AP*C)-3')



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



- Molecule 3: ERYTHROID TRANSCRIPTION FACTOR GATA-1



5 Refinement protocol and experimental data overview i

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.

COVALENT-GEOMETRY INFOmissingINFO

5.1 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

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
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
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
2:C:120:DG:C5	2:C:121:DT:C4	0.56	2.94	27	13
3:A:16:THR:HG22	3:A:51:ILE:CG2	0.56	2.31	20	5
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
1:B:106:DA:C6	1:B:107:DG:C6	0.55	2.95	3	21
3:A:10:CYS:HB2	3:A:44:LEU:CB	0.55	2.32	16	13
1:B:107:DG:O6	3:A:17:LEU:CD1	0.55	2.55	27	15
3:A:5:THR:HG22	3:A:18:TRP:CH2	0.55	2.37	7	4
3:A:10:CYS:SG	3:A:12:THR:CG2	0.55	2.95	2	10
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
1:B:108:DA:N6	2:C:124:DA:N6	0.54	2.55	24	15
3:A:15:THR:O	3:A:51:ILE:HD11	0.54	2.01	16	5
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

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
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:H2''	1:B:107:DG:O5'	0.52	2.04	28	28
1:B:106:DA:N6	2:C:126:DC:N4	0.52	2.57	9	11
1:B:108:DA:H61	3:A:17:LEU:CD1	0.52	2.17	26	4
3:A:38:HIS:O	3:A:39:GLN:CG	0.52	2.57	19	3
3:A:6:VAL:HG23	3:A:6:VAL:O	0.52	2.05	11	5
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
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
1:B:107:DG:O6	3:A:17:LEU:HD22	0.51	2.06	11	1
3:A:10:CYS:O	3:A:47:ARG:HD3	0.51	2.05	15	1
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	21	14
1:B:106:DA:N7	3:A:17:LEU:HD13	0.50	2.21	8	3
3:A:31:CYS:O	3:A:42:ARG:HD2	0.50	2.06	15	2
3:A:5:THR:CG2	3:A:26:PRO:HB2	0.50	2.36	16	5
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
3:A:15:THR:CG2	3:A:18:TRP:CZ2	0.49	2.95	29	4
1:B:108:DA:C2	1:B:109:DT:C2	0.49	3.00	12	3
2:C:123:DT:H2''	2:C:124:DA:C8	0.49	2.43	1	14

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
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
1:B:107:DG:O6	3:A:17:LEU:HD21	0.49	2.07	3	3
3:A:35:TYR:CD1	3:A:39:GLN:HA	0.49	2.43	27	5
3:A:10:CYS:O	3:A:44:LEU:HB3	0.49	2.07	27	4
3:A:10:CYS:O	3:A:47:ARG:CD	0.49	2.61	17	2
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
3:A:19:ARG:HG3	3:A:27:VAL:O	0.48	2.08	1	1
1:B:107:DG:C6	1:B:108:DA:C6	0.48	3.02	1	3
1:B:106:DA:N6	3:A:17:LEU:HD11	0.48	2.23	27	3
3:A:10:CYS:HB2	3:A:44:LEU:HB3	0.48	1.86	26	6
3:A:35:TYR:O	3:A:39:GLN:CA	0.48	2.62	20	10
3:A:33:LEU:O	3:A:36:LYS:HG3	0.47	2.08	2	4
2:C:125:DT:H73	3:A:16:THR:HB	0.47	1.85	3	5
3:A:38:HIS:CB	3:A:40:VAL:HG22	0.47	2.39	29	9
3:A:36:LYS:HD3	3:A:37:LEU:CD1	0.47	2.39	20	1
3:A:35:TYR:CE1	3:A:39:GLN:HG3	0.47	2.45	7	2
2:C:125:DT:H72	3:A:16:THR:HB	0.47	1.86	15	4
3:A:44:LEU:HD23	3:A:44:LEU:H	0.47	1.70	1	1
2:C:120:DG:C8	2:C:121:DT:H72	0.47	2.43	9	2
3:A:10:CYS:SG	3:A:12:THR:HB	0.47	2.49	13	2
3:A:10:CYS:O	3:A:44:LEU:CB	0.47	2.62	5	3
3:A:39:GLN:O	3:A:39:GLN:CG	0.47	2.63	12	7
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: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
3:A:33:LEU:O	3:A:36:LYS:HD3	0.47	2.10	17	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: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
3:A:5:THR:O	3:A:5:THR:HG22	0.47	2.08	24	3
3:A:47:ARG:NH1	3:A:47:ARG:HG3	0.46	2.26	1	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:C:121:DT:H2'	2:C:122:DT:H71	0.46	1.86	21	5
3:A:12:THR:HG23	3:A:12:THR:O	0.46	2.11	4	1
1:B:106:DA:H61	2:C:126:DC:N4	0.46	2.09	9	4
3:A:52:GLN:HG3	3:A:53:THR:N	0.46	2.26	3	2
3:A:42:ARG:N	3:A:42:ARG:CD	0.46	2.78	4	2
3:A:35:TYR:HB2	3:A:42:ARG:NE	0.46	2.25	9	1
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:15:THR:HG22	3:A:28:CYS:CB	0.45	2.41	18	2
3:A:20:ARG:CB	3:A:26:PRO:HA	0.45	2.41	27	1
3:A:15:THR:CG2	3:A:28:CYS:HB3	0.45	2.41	29	1
3:A:17:LEU:O	3:A:29:ASN:CB	0.45	2.64	17	1
3:A:38:HIS:O	3:A:39:GLN:HG2	0.45	2.11	2	6
3:A:35:TYR:CD2	3:A:42:ARG:CZ	0.45	2.99	4	1
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:34:TYR:CE2	3:A:42:ARG:HG3	0.45	2.46	23	1
2:C:121:DT:C2	2:C:122:DT:C5	0.45	3.05	3	4
1:B:108:DA:N1	2:C:125:DT:O4	0.45	2.48	30	3
3:A:10:CYS:SG	3:A:47:ARG:HD3	0.45	2.51	11	5
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:110:DA:H2''	1:B:111:DA:C8	0.45	2.47	1	2
1:B:107:DG:O6	3:A:17:LEU:HD12	0.45	2.12	5	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
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
1:B:106:DA:N7	3:A:17:LEU:CD1	0.45	2.80	22	9
3:A:33:LEU:HD23	3:A:36:LYS:CE	0.45	2.42	3	1
3:A:7:CYS:HA	3:A:26:PRO:O	0.45	2.11	3	6
3:A:19:ARG:HD2	3:A:29:ASN:HA	0.45	1.89	8	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
1:B:112:DA:C6	1:B:113:DC:N4	0.44	2.85	24	1
2:C:125:DT:H2''	2:C:126:DC:C5	0.44	2.47	26	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
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
1:B:108:DA:C2	2:C:126:DC:N3	0.44	2.86	26	1
2:C:124:DA:H3'	3:A:16:THR:CG2	0.44	2.43	28	4
3:A:19:ARG:HG3	3:A:19:ARG:O	0.44	2.13	15	1
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:36:LYS:HD2	3:A:37:LEU:CD1	0.44	2.43	14	1
3:A:35:TYR:CE1	3:A:39:GLN:CG	0.44	3.01	20	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
2:C:124:DA:C3'	3:A:16:THR:HG21	0.43	2.41	26	6
3:A:9:ASN:ND2	3:A:27:VAL:HG11	0.43	2.28	2	2
3:A:38:HIS:O	3:A:39:GLN:HG3	0.43	2.14	4	1
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
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
3:A:33:LEU:HA	3:A:36:LYS:HD3	0.43	1.90	17	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
3:A:15:THR:HB	3:A:28:CYS:HB2	0.42	1.91	1	2
3:A:33:LEU:O	3:A:37:LEU:CD1	0.42	2.67	3	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
2:C:126:DC:H2'	2:C:127:DT:C6	0.42	2.49	19	4
2:C:124:DA:C2'	3:A:16:THR:HG21	0.42	2.45	26	1
2:C:124:DA:C5'	3:A:52:GLN:O	0.42	2.67	28	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:A:31:CYS:O	3:A:42:ARG:NE	0.42	2.51	17	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:9:ASN:OD1	3:A:42:ARG:HD3	0.42	2.15	19	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
3:A:54:ARG:CG	3:A:54:ARG:NH1	0.42	2.81	29	1
3:A:44:LEU:O	3:A:47:ARG:HG2	0.42	2.14	30	1
1:B:106:DA:N7	3:A:17:LEU:HD21	0.42	2.28	17	1
3:A:28:CYS:O	3:A:29:ASN:C	0.42	2.58	14	3
3:A:47:ARG:HG3	3:A:47:ARG:NH1	0.42	2.30	24	1
3:A:54:ARG:HG3	3:A:55:ASN:N	0.42	2.29	28	1
2:C:124:DA:C5'	3:A:52:GLN:HG2	0.42	2.45	26	3
3:A:34:TYR:CZ	3:A:43:PRO:HD2	0.42	2.50	1	1
2:C:124:DA:C2	2:C:125:DT:N3	0.42	2.88	30	3
3:A:19:ARG:HB3	3:A:27:VAL:O	0.42	2.14	19	2
3:A:5:THR:O	3:A:18:TRP:CZ2	0.41	2.73	5	2
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:38:HIS:O	3:A:39:GLN:CB	0.41	2.68	19	1
3:A:15:THR:CG2	3:A:28:CYS:HB2	0.41	2.45	1	3
3:A:47:ARG:HG2	3:A:48:LYS:N	0.41	2.29	28	1
3:A:28:CYS:SG	3:A:47:ARG:NH2	0.41	2.94	5	1
3:A:44:LEU:HB2	3:A:47:ARG:HG2	0.41	1.92	8	1
3:A:35:TYR:CE1	3:A:39:GLN:HG2	0.41	2.50	20	1
3:A:44:LEU:O	3:A:47:ARG:HB3	0.41	2.16	17	1
3:A:34:TYR:CD1	3:A:34:TYR:C	0.41	2.93	10	1
3:A:11:GLN:HG2	3:A:47:ARG:NH1	0.41	2.30	15	1
1:B:107:DG:H2''	1:B:108:DA:O5'	0.41	2.15	14	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
3:A:16:THR:HG23	3:A:51:ILE:HG21	0.41	1.91	11	1
3:A:34:TYR:CE1	3:A:38:HIS:CD2	0.41	3.09	21	1
3:A:16:THR:CG2	3:A:51:ILE:HG23	0.41	2.45	3	1
3:A:4:GLY:O	3:A:6:VAL:HG13	0.41	2.16	6	1
2:C:122:DT:O5'	3:A:37:LEU:HD23	0.41	2.15	15	1
3:A:28:CYS:O	3:A:28:CYS:SG	0.41	2.79	21	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

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:C:123:DT:OP2	3:A:34:TYR:HB2	0.40	2.16	8	1
1:B:107:DG:N2	1:B:108:DA:N3	0.40	2.69	12	2
3:A:36:LYS:HG2	3:A:37:LEU:N	0.40	2.30	17	1
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
2:C:123:DT:H71	3:A:33:LEU:HB3	0.40	1.94	11	1
2:C:122:DT:OP2	3:A:37:LEU:HD22	0.40	2.16	21	1
1:B:109:DT:O2	3:A:57:LYS:NZ	0.40	2.54	17	1

5.2 Torsion angles [i](#)

5.2.1 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	55/60 (92%)	43±2 (78±4%)	11±2 (19±4%)	2±1 (3±2%)	8	43
All	All	1650/1800 (92%)	1287 (78%)	318 (19%)	45 (3%)	8	43

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

5.2.2 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%)	2	27
All	All	1470/1620 (91%)	1118 (76%)	352 (24%)	2	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
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

5.2.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.4 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.5 Ligand geometry [i](#)

There are no ligands in this entry.

5.6 Other polymers [i](#)

There are no such molecules in this entry.

5.7 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Chemical shift validation

No chemical shift data were provided