Full wwPDB NMR Structure Validation Report (i)

Jun 3, 2020 – 08:37 am BST

PDB ID	:	2KY8
Title	:	Solution structure and dynamic analysis of chicken MBD2 methyl binding domain bound to a target methylated DNA sequence
Authors	:	Williams Jr., D.C.; Scarsdale Jr., J.N.
Deposited on	:	2010-05-18

This is a Full wwPDB NMR Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/NMRValidationReportHelp
with specific help available everywhere you see the (i) symbol.

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

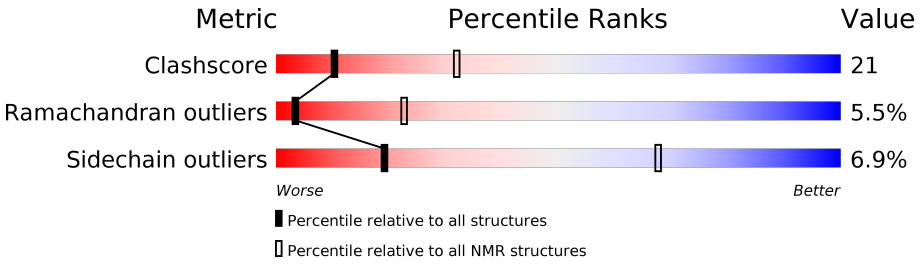
Cyrange	:	Kirchner and Güntert (2011)
NmrClust	:	Kelley et al. (1996)
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
ShiftChecker	:	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 (i)

The following experimental techniques were used to determine the structure:
SOLUTION NMR

The overall completeness of chemical shifts assignment is 62%.

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



Metric	Whole archive (#Entries)	NMR archive (#Entries)
Clashscore	158937	12864
Ramachandran outliers	154571	11451
Sidechain outliers	154315	11428

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

Mol	Chain	Length	Quality of chain
1	A	72	64% 25% • 6% •
2	B	11	9% 64% 27%
3	C	11	9% 45% 45%

2 Ensemble composition and analysis

This entry contains 20 models. Model 13 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *lowest energy*.

The following residues are included in the computation of the global validation metrics.

Well-defined (core) protein residues			
Well-defined core	**Residue range (total)**	**Backbone RMSD (Å)**	**Medoid model**
1	A:6-A:71 (66)	0.47	13

Ill-defined regions of proteins are excluded from the global statistics.

Ligands and non-protein polymers are included in the analysis.

The models can be grouped into 3 clusters and 2 single-model clusters were found.

Cluster number	Models
1	1, 2, 7, 9, 11, 13, 14, 16, 17
2	3, 4, 5, 6, 15, 19
3	12, 18, 20
Single-model clusters	8; 10

3 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 2081 atoms, of which 923 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Methyl-CpG-binding domain protein 2.

Mol	Chain	Residues	Atoms						Trace
1	A	70	Total	C	H	N	O	S	0
			1104	349	555	98	98	4	

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	GLY	-	expression tag	UNP Q5EFL0
A	2	SER	-	expression tag	UNP Q5EFL0

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

Mol	Chain	Residues	Atoms						Trace
2	B	11	Total	C	H	N	O	P	0
			487	150	184	55	88	10	

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

Mol	Chain	Residues	Atoms						Trace
3	C	11	Total	C	H	N	O	P	0
			484	149	184	53	88	10	

- Molecule 4 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

Mol	Chain	Residues	Atoms	
4	B	1	Total	Mn
			3	3
4	C	1	Total	Mn
			3	3

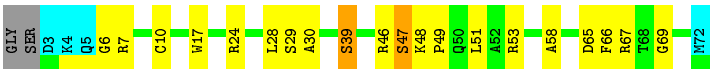
4 Residue-property plots

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: Methyl-CpG-binding domain protein 2

Chain A:



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

Chain B:

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

Chain C:

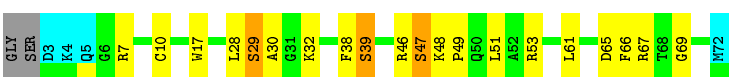
4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

• Molecule 1: Methyl-CpG-binding domain protein 2

Chain A:



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

Chain B:

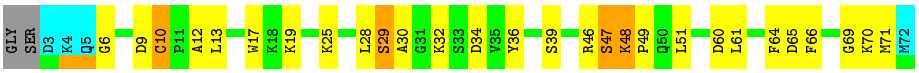
• Molecule 3: DNA (5'-D(*GP*AP*GP*CP*(5CM)P*GP*AP*TP*(TED)P*CP*C)-3')

Chain C:

4.2.2 Score per residue for model 2

• Molecule 1: Methyl-CpG-binding domain protein 2

Chain A:

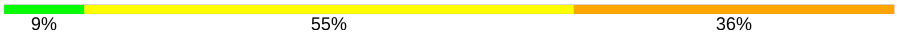


• Molecule 2: DNA (5'-D(*GP*GP*AP*AP*TP*(5CM)P*GP*GP*CP*(TED)P*C)-3')

Chain B:

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

Chain C:



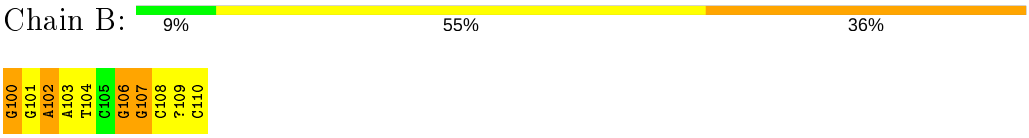
4.2.3 Score per residue for model 3

• Molecule 1: Methyl-CpG-binding domain protein 2

Chain A:

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

Chain B:



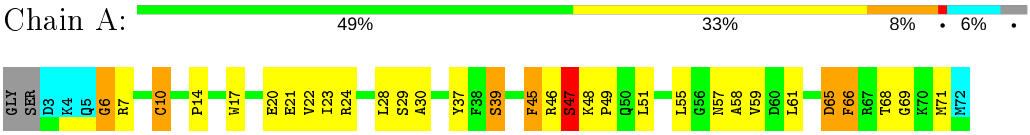
• Molecule 3: DNA (5'-D(*GP*AP*GP*CP*(5CM)P*GP*AP*TP*(TED)P*CP*C)-3')

Chain C:

4.2.4 Score per residue for model 4

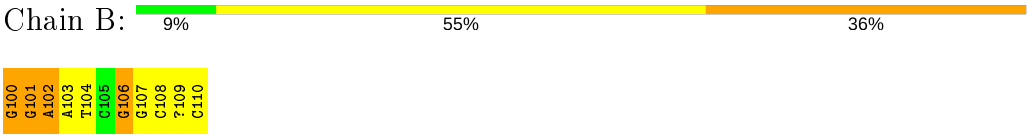
• Molecule 1: Methyl-CpG-binding domain protein 2

Chain A:



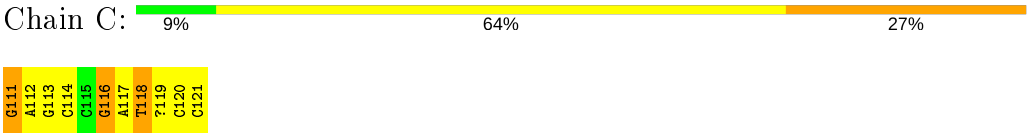
• Molecule 2: DNA (5'-D(*GP*GP*AP*AP*TP*(5CM)P*GP*GP*CP*(TED)P*C)-3')

Chain B:



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

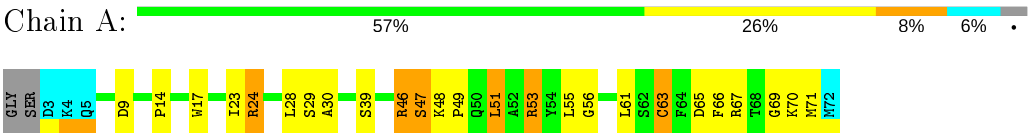
Chain C:



4.2.5 Score per residue for model 5

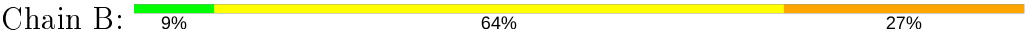
• Molecule 1: Methyl-CpG-binding domain protein 2

Chain A:



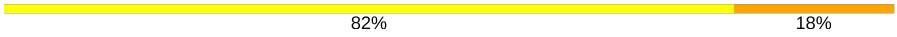
• Molecule 2: DNA (5'-D(*GP*GP*AP*AP*TP*(5CM)P*GP*GP*CP*(TED)P*C)-3')

Chain B:



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

Chain C:



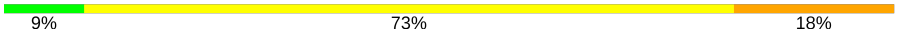
4.2.6 Score per residue for model 6

• Molecule 1: Methyl-CpG-binding domain protein 2

Chain A:

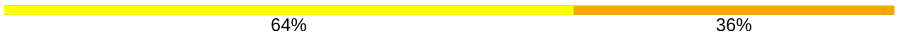
• Molecule 2: DNA (5'-D(*GP*GP*AP*AP*TP*(5CM)P*GP*GP*CP*(TED)P*C)-3')

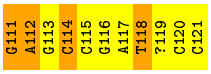
Chain B:



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

Chain C:

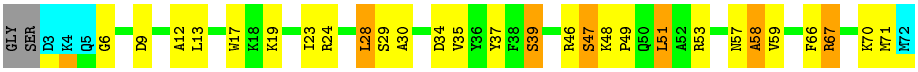




4.2.7 Score per residue for model 7

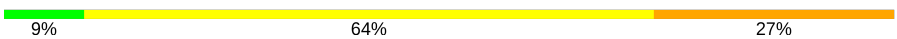
• Molecule 1: Methyl-CpG-binding domain protein 2

Chain A:



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

Chain B:



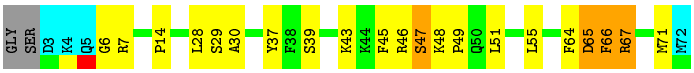
• Molecule 3: DNA (5'-D(*GP*AP*GP*CP*(5CM)P*GP*AP*TP*(TED)P*CP*C)-3')

Chain C: 

4.2.8 Score per residue for model 8

• Molecule 1: Methyl-CpG-binding domain protein 2

Chain A: 



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

Chain B: 

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

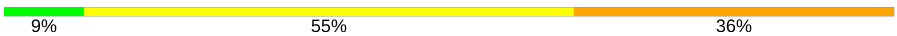
Chain C: 

4.2.9 Score per residue for model 9

• Molecule 1: Methyl-CpG-binding domain protein 2

Chain A: 

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

Chain B: 

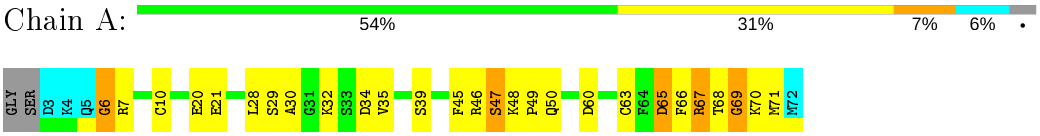
• Molecule 3: DNA (5'-D(*GP*AP*GP*CP*(5CM)P*GP*AP*TP*(TED)P*CP*C)-3')

Chain C:

4.2.10 Score per residue for model 10

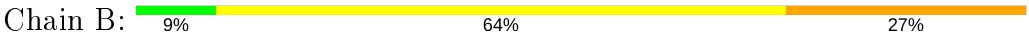
- Molecule 1: Methyl-CpG-binding domain protein 2

Chain A:



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

Chain B:



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

Chain C:

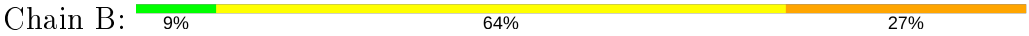
4.2.11 Score per residue for model 11

- Molecule 1: Methyl-CpG-binding domain protein 2

Chain A:

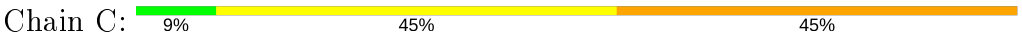
- Molecule 2: DNA (5'-D(*GP*GP*AP*AP*TP*(5CM)P*GP*GP*CP*(TED)P*C)-3')

Chain B:



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

Chain C:



4.2.12 Score per residue for model 12

• Molecule 1: Methyl-CpG-binding domain protein 2

Chain A:

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

Chain B:

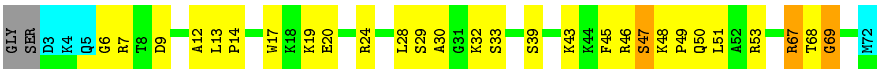
• Molecule 3: DNA (5'-D(*GP*AP*GP*CP*(5CM)P*GP*AP*TP*(TED)P*CP*C)-3')

Chain C:

4.2.13 Score per residue for model 13 (medoid)

• Molecule 1: Methyl-CpG-binding domain protein 2

Chain A:

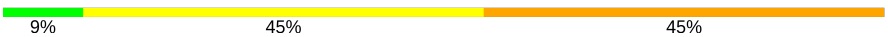


• Molecule 2: DNA (5'-D(*GP*GP*AP*AP*TP*(5CM)P*GP*GP*CP*(TED)P*C)-3')

Chain B:

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

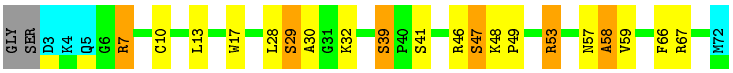
Chain C:



4.2.14 Score per residue for model 14

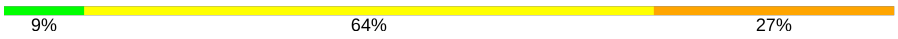
• Molecule 1: Methyl-CpG-binding domain protein 2

Chain A:



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

Chain B:



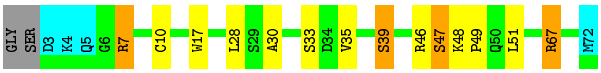
• Molecule 3: DNA (5'-D(*GP*AP*GP*CP*(5CM)P*GP*AP*TP*(TED)P*CP*C)-3')

Chain C:

4.2.15 Score per residue for model 15

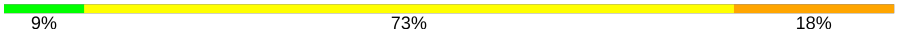
• Molecule 1: Methyl-CpG-binding domain protein 2

Chain A:



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

Chain B:



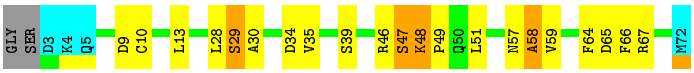
• Molecule 3: DNA (5'-D(*GP*AP*GP*CP*(5CM)P*GP*AP*TP*(TED)P*CP*C)-3')

Chain C:

4.2.16 Score per residue for model 16

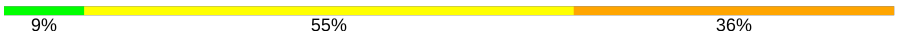
• Molecule 1: Methyl-CpG-binding domain protein 2

Chain A:



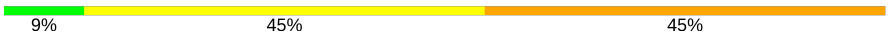
• Molecule 2: DNA (5'-D(*GP*GP*AP*AP*TP*(5CM)P*GP*GP*CP*(TED)P*C)-3')

Chain B:



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

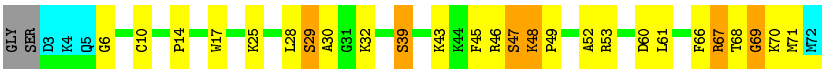
Chain C:



4.2.17 Score per residue for model 17

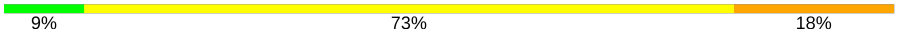
• Molecule 1: Methyl-CpG-binding domain protein 2

Chain A:



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

Chain B:



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

Chain C:

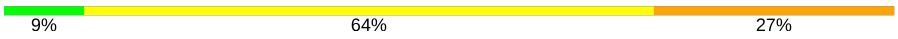
4.2.18 Score per residue for model 18

• Molecule 1: Methyl-CpG-binding domain protein 2

Chain A:

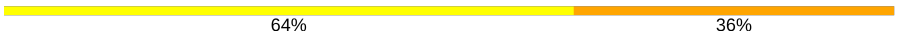
• Molecule 2: DNA (5'-D(*GP*GP*AP*AP*TP*(5CM)P*GP*GP*CP*(TED)P*C)-3')

Chain B:



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

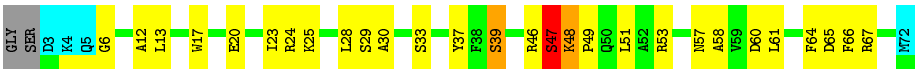
Chain C:



4.2.19 Score per residue for model 19

• Molecule 1: Methyl-CpG-binding domain protein 2

Chain A:

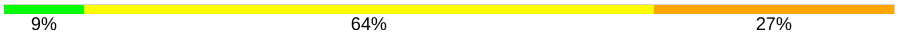


• Molecule 2: DNA (5'-D(*GP*GP*AP*AP*TP*(5CM)P*GP*GP*CP*(TED)P*C)-3')

Chain B:

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

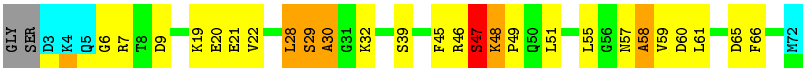
Chain C:



4.2.20 Score per residue for model 20

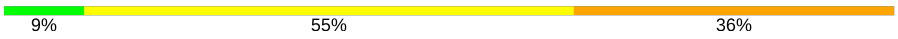
- Molecule 1: Methyl-CpG-binding domain protein 2

Chain A:



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

Chain B:



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

Chain C:

5 Refinement protocol and experimental data overview

The models were refined using the following method: *torsion angle dynamics*.

Of the 20 calculated structures, 20 were deposited, based on the following criterion: *all calculated structures submitted*.

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

Software name	Classification	Version
X-PLOR NIH	refinement	

The following table shows chemical shift validation statistics as aggregates over all chemical shift files. Detailed validation can be found in section 6 of this report.

Chemical shift file(s)	input_cs.cif
Number of chemical shift lists	1
Total number of shifts	959
Number of shifts mapped to atoms	858
Number of unparsed shifts	0
Number of shifts with mapping errors	101
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	62%

No validations of the models with respect to experimental NMR restraints is performed at this time.

COVALENT-GEOMETRY INFOmissingINFO

5.1 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	A	516	521	521	27±5
2	B	303	184	175	9±3
3	C	300	184	175	10±3
All	All	22500	17780	17420	849

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 21.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:C:111:DG:H8	3:C:111:DG:HO5'	0.96	0.99	18	9
2:B:100:DG:H8	2:B:100:DG:HO5'	0.95	0.95	11	9
3:C:111:DG:HO5'	3:C:111:DG:H8	0.95	0.96	6	11
2:B:100:DG:HO5'	2:B:100:DG:H8	0.90	1.08	8	11
1:A:28:LEU:HD13	1:A:28:LEU:O	0.83	1.73	7	2
1:A:26:SER:O	1:A:27:GLY:O	0.81	1.99	18	2
1:A:48:LYS:N	1:A:49:PRO:HD2	0.80	1.92	8	20
1:A:13:LEU:HD23	1:A:17:TRP:CD2	0.79	2.11	19	3
1:A:17:TRP:CH2	1:A:51:LEU:HD11	0.79	2.12	5	1
1:A:65:ASP:O	1:A:69:GLY:N	0.78	2.17	5	5
1:A:46:ARG:O	1:A:47:SER:CB	0.78	2.32	9	19
1:A:61:LEU:N	1:A:61:LEU:HD12	0.77	1.94	4	4
1:A:28:LEU:C	1:A:28:LEU:HD13	0.77	2.00	13	2
1:A:46:ARG:O	1:A:47:SER:OG	0.73	2.06	9	13
1:A:28:LEU:O	1:A:28:LEU:HD13	0.73	1.83	20	1
1:A:26:SER:O	1:A:27:GLY:C	0.73	2.25	18	2
1:A:66:PHE:CG	1:A:67:ARG:N	0.73	2.57	16	6
1:A:51:LEU:C	1:A:51:LEU:HD23	0.72	2.03	16	2
2:B:100:DG:O5'	2:B:100:DG:H8	0.72	1.68	13	8
2:B:100:DG:H8	2:B:100:DG:O5'	0.71	1.67	11	11
1:A:51:LEU:HD23	1:A:51:LEU:C	0.71	2.05	8	1
1:A:13:LEU:HD23	1:A:17:TRP:CE3	0.71	2.20	19	1
3:C:111:DG:O5'	3:C:111:DG:H8	0.71	1.68	6	8
3:C:111:DG:H8	3:C:111:DG:O5'	0.71	1.69	17	12
1:A:13:LEU:HD21	1:A:51:LEU:HD21	0.71	1.60	11	2
1:A:45:PHE:CD1	1:A:51:LEU:HD21	0.69	2.21	4	1
1:A:19:LYS:HZ3	1:A:35:VAL:HG13	0.68	1.45	6	1
1:A:64:PHE:CD1	1:A:65:ASP:N	0.68	2.61	2	1
1:A:66:PHE:CZ	1:A:67:ARG:NH1	0.68	2.61	14	1
1:A:48:LYS:N	1:A:49:PRO:CD	0.67	2.57	11	20
1:A:7:ARG:HH11	1:A:7:ARG:CG	0.67	2.03	15	1
1:A:32:LYS:NZ	3:C:114:DC:N4	0.66	2.44	14	6
1:A:50:GLN:NE2	1:A:53:ARG:HH21	0.66	1.88	9	1
1:A:7:ARG:NH2	1:A:9:ASP:N	0.65	2.44	12	1
1:A:64:PHE:CE1	1:A:70:LYS:O	0.65	2.49	2	1
2:B:109[B]:TED:CY6	2:B:109[B]:TED:CY7	0.65	2.73	15	4
1:A:17:TRP:CH2	1:A:39:SER:OG	0.65	2.48	1	4
1:A:51:LEU:O	1:A:51:LEU:HD23	0.65	1.90	9	4
1:A:45:PHE:CD1	1:A:50:GLN:OE1	0.65	2.50	10	2
2:B:109[C]:TED:CY6	2:B:109[C]:TED:CY7	0.64	2.75	12	7
2:B:109[C]:TED:CY8	2:B:109[C]:TED:CY5	0.64	2.75	20	5
1:A:66:PHE:CD2	1:A:67:ARG:N	0.64	2.65	16	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:109[A]:TED:CY7	2:B:109[A]:TED:CY6	0.64	2.75	7	4
1:A:53:ARG:CG	1:A:53:ARG:HH11	0.64	2.05	5	3
1:A:37:TYR:CD1	1:A:66:PHE:CE2	0.64	2.86	12	1
1:A:28:LEU:O	1:A:30:ALA:N	0.64	2.30	6	17
1:A:32:LYS:NZ	3:C:114:DC:H41	0.64	1.90	1	4
1:A:48:LYS:NZ	1:A:61:LEU:HD12	0.64	2.07	2	1
1:A:13:LEU:HD22	1:A:13:LEU:N	0.64	2.08	14	2
2:B:109[B]:TED:CY8	2:B:109[B]:TED:CY5	0.63	2.75	10	4
2:B:109[A]:TED:CY6	2:B:109[A]:TED:CY7	0.63	2.76	2	2
1:A:67:ARG:HH11	1:A:67:ARG:CG	0.63	2.05	17	6
2:B:109[A]:TED:CY8	2:B:109[A]:TED:CY5	0.63	2.77	9	3
1:A:65:ASP:OD1	1:A:70:LYS:N	0.63	2.31	9	1
1:A:17:TRP:CZ2	1:A:39:SER:OG	0.63	2.51	19	4
1:A:50:GLN:NE2	1:A:53:ARG:NH2	0.63	2.45	13	2
3:C:119[B]:TED:CY6	3:C:119[B]:TED:CY7	0.63	2.77	19	2
3:C:119[C]:TED:CY8	3:C:119[C]:TED:CY5	0.63	2.76	18	2
2:B:109[A]:TED:CY5	2:B:109[A]:TED:CY8	0.63	2.77	13	3
1:A:13:LEU:CD2	1:A:13:LEU:N	0.63	2.62	14	2
3:C:119[C]:TED:CY7	3:C:119[C]:TED:CY6	0.62	2.77	19	8
1:A:19:LYS:NZ	1:A:35:VAL:HG13	0.62	2.09	6	1
3:C:119[B]:TED:CY7	3:C:119[B]:TED:CY6	0.62	2.78	16	3
1:A:64:PHE:CZ	1:A:70:LYS:O	0.62	2.52	2	1
3:C:119[A]:TED:CY8	3:C:119[A]:TED:CY5	0.62	2.78	13	5
1:A:61:LEU:CD1	1:A:61:LEU:N	0.61	2.63	4	2
1:A:68:THR:O	1:A:70:LYS:N	0.61	2.34	9	3
3:C:119[C]:TED:CY6	3:C:119[C]:TED:CY7	0.61	2.78	14	4
3:C:119[B]:TED:CY5	3:C:119[B]:TED:CY8	0.61	2.79	12	7
1:A:37:TYR:CE1	1:A:66:PHE:CD2	0.61	2.88	12	1
1:A:49:PRO:O	1:A:53:ARG:NH1	0.61	2.33	13	3
2:B:109[B]:TED:CY5	2:B:109[B]:TED:CY8	0.61	2.78	14	2
3:C:119[A]:TED:CY5	3:C:119[A]:TED:CY8	0.61	2.78	8	6
1:A:9:ASP:OD1	1:A:10:CYS:N	0.61	2.33	9	2
1:A:67:ARG:HH11	1:A:67:ARG:HG2	0.61	1.55	14	2
3:C:119[A]:TED:CY6	3:C:119[A]:TED:CY7	0.61	2.79	14	3
1:A:20:GLU:OE1	1:A:21:GLU:N	0.61	2.32	10	2
3:C:119[B]:TED:CY8	3:C:119[B]:TED:CY5	0.61	2.79	10	3
1:A:28:LEU:C	1:A:30:ALA:H	0.60	1.99	6	19
1:A:68:THR:O	1:A:69:GLY:C	0.60	2.39	18	6
3:C:119[C]:TED:CY5	3:C:119[C]:TED:CY8	0.60	2.79	13	5
1:A:67:ARG:NH1	1:A:67:ARG:CG	0.60	2.64	18	6
1:A:7:ARG:NH1	1:A:7:ARG:CG	0.60	2.62	15	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:34:ASP:OD1	1:A:35:VAL:N	0.60	2.34	10	5
1:A:7:ARG:CG	1:A:7:ARG:HH11	0.59	2.11	13	1
1:A:12:ALA:C	1:A:13:LEU:HD12	0.59	2.18	13	4
1:A:53:ARG:CG	1:A:53:ARG:NH1	0.59	2.65	18	4
1:A:7:ARG:NH2	1:A:9:ASP:OD1	0.59	2.36	20	1
3:C:111:DG:C8	3:C:111:DG:O5'	0.58	2.56	3	9
1:A:65:ASP:OD1	1:A:69:GLY:N	0.58	2.36	9	1
2:B:109[C]:TED:CY7	2:B:109[C]:TED:CY6	0.58	2.81	20	3
1:A:48:LYS:NZ	1:A:61:LEU:O	0.58	2.36	1	2
1:A:65:ASP:CB	1:A:68:THR:OG1	0.58	2.51	10	1
1:A:20:GLU:CD	1:A:21:GLU:N	0.58	2.57	20	2
1:A:17:TRP:CH2	1:A:51:LEU:CD1	0.58	2.87	1	4
1:A:66:PHE:O	1:A:67:ARG:C	0.57	2.43	10	6
1:A:66:PHE:O	1:A:68:THR:N	0.57	2.38	10	1
2:B:106:DG:C2	3:C:116:DG:N2	0.57	2.73	8	5
1:A:45:PHE:CG	1:A:50:GLN:OE1	0.57	2.58	11	2
2:B:109[B]:TED:CY7	2:B:109[B]:TED:CY6	0.57	2.83	12	1
1:A:34:ASP:OD2	1:A:36:TYR:CZ	0.57	2.58	2	1
1:A:12:ALA:CB	1:A:64:PHE:CD1	0.57	2.88	12	2
2:B:106:DG:N2	3:C:116:DG:C2	0.56	2.73	16	8
2:B:100:DG:H2'	2:B:101:DG:N7	0.56	2.16	11	4
1:A:19:LYS:NZ	1:A:69:GLY:O	0.56	2.37	2	1
1:A:34:ASP:OD2	1:A:36:TYR:CE2	0.56	2.58	2	1
1:A:32:LYS:HZ3	3:C:114:DC:N4	0.56	1.98	14	3
2:B:100:DG:C8	2:B:100:DG:O5'	0.55	2.54	20	4
1:A:12:ALA:CB	1:A:71:MET:SD	0.55	2.94	2	2
1:A:28:LEU:C	1:A:28:LEU:CD1	0.55	2.74	13	2
1:A:24:ARG:HG2	1:A:24:ARG:HH11	0.55	1.61	5	3
1:A:17:TRP:CH2	1:A:51:LEU:CD2	0.55	2.89	18	1
1:A:33:SER:O	1:A:67:ARG:NH1	0.55	2.39	15	2
1:A:9:ASP:OD1	1:A:17:TRP:O	0.55	2.25	3	1
2:B:102:DA:N6	3:C:118:DT:O4	0.55	2.40	9	17
1:A:53:ARG:HH11	1:A:53:ARG:HG2	0.55	1.61	19	3
1:A:66:PHE:N	1:A:66:PHE:CD1	0.55	2.75	19	2
1:A:63:CYS:O	1:A:70:LYS:O	0.55	2.25	5	2
1:A:47:SER:OG	3:C:115:5CM:P	0.55	2.65	18	2
1:A:28:LEU:C	1:A:30:ALA:N	0.54	2.61	18	16
1:A:52:ALA:O	1:A:56:GLY:N	0.54	2.40	9	1
1:A:57:ASN:O	1:A:59:VAL:N	0.54	2.41	16	5
1:A:53:ARG:HH11	1:A:53:ARG:CG	0.54	2.16	19	3
1:A:37:TYR:OH	1:A:66:PHE:O	0.54	2.26	4	5

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:67:ARG:HH11	1:A:67:ARG:CB	0.54	2.15	8	1
1:A:55:LEU:HD12	1:A:56:GLY:O	0.54	2.02	5	1
1:A:65:ASP:OD1	1:A:69:GLY:CA	0.54	2.55	9	1
1:A:37:TYR:CD1	1:A:66:PHE:CD2	0.54	2.96	12	1
1:A:10:CYS:SG	1:A:17:TRP:O	0.54	2.66	4	1
3:C:111:DG:O5'	3:C:111:DG:C8	0.53	2.60	7	6
1:A:65:ASP:C	1:A:68:THR:HG1	0.53	2.05	10	1
1:A:7:ARG:CG	1:A:7:ARG:NH1	0.53	2.67	13	1
1:A:46:ARG:O	1:A:47:SER:HB3	0.53	2.03	8	4
1:A:9:ASP:O	1:A:19:LYS:NZ	0.53	2.42	13	1
1:A:64:PHE:CE2	1:A:65:ASP:O	0.53	2.62	6	2
1:A:67:ARG:CZ	3:C:114:DC:OP2	0.53	2.57	18	1
1:A:51:LEU:C	1:A:51:LEU:CD2	0.52	2.77	16	1
1:A:60:ASP:OD1	1:A:60:ASP:O	0.52	2.27	20	4
1:A:67:ARG:NE	3:C:114:DC:OP2	0.52	2.42	18	1
1:A:51:LEU:O	1:A:51:LEU:HD13	0.52	2.05	7	1
1:A:67:ARG:CA	1:A:67:ARG:HE	0.52	2.17	7	1
1:A:50:GLN:OE1	1:A:50:GLN:C	0.52	2.48	11	1
1:A:50:GLN:C	1:A:50:GLN:OE1	0.52	2.47	10	1
1:A:17:TRP:CH2	1:A:39:SER:CB	0.52	2.93	7	6
1:A:33:SER:C	1:A:67:ARG:NH2	0.52	2.62	13	1
1:A:53:ARG:HG2	1:A:53:ARG:HH11	0.52	1.64	18	3
1:A:7:ARG:HH11	1:A:7:ARG:HG2	0.52	1.65	15	2
1:A:45:PHE:CG	1:A:51:LEU:HD21	0.52	2.40	20	1
1:A:66:PHE:CD1	1:A:66:PHE:N	0.52	2.78	14	2
1:A:24:ARG:HH11	1:A:24:ARG:CG	0.52	2.17	3	3
2:B:100:DG:H2"	2:B:101:DG:C8	0.51	2.40	9	11
1:A:32:LYS:NZ	3:C:113:DG:C8	0.51	2.78	13	1
1:A:47:SER:OG	3:C:115:5CM:OP1	0.51	2.25	5	4
1:A:29:SER:O	1:A:30:ALA:O	0.51	2.27	20	1
1:A:6:GLY:O	1:A:20:GLU:OE1	0.51	2.29	19	1
2:B:109[B]:TED:CY8	2:B:109[B]:TED:CYB	0.51	2.88	8	1
1:A:45:PHE:CD1	1:A:50:GLN:CD	0.51	2.84	11	2
1:A:67:ARG:NH2	3:C:114:DC:OP2	0.51	2.44	18	1
1:A:17:TRP:CE2	1:A:39:SER:OG	0.51	2.64	17	1
1:A:24:ARG:NH1	1:A:24:ARG:CG	0.51	2.72	3	2
1:A:65:ASP:OD2	1:A:68:THR:OG1	0.51	2.29	9	1
1:A:28:LEU:HD13	1:A:28:LEU:C	0.51	2.25	7	1
1:A:33:SER:O	1:A:67:ARG:NH2	0.51	2.44	12	1
1:A:30:ALA:C	1:A:32:LYS:H	0.50	2.10	18	1
1:A:32:LYS:HZ3	3:C:114:DC:H41	0.50	1.48	1	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:65:ASP:O	1:A:66:PHE:CB	0.50	2.57	4	1
1:A:35:VAL:CG2	1:A:67:ARG:NH2	0.50	2.74	15	1
1:A:17:TRP:CE3	1:A:38:PHE:O	0.50	2.63	1	1
1:A:46:ARG:C	1:A:47:SER:OG	0.50	2.49	5	6
2:B:100:DG:C2'	2:B:101:DG:C8	0.50	2.94	9	8
2:B:109[B]:TED:CY6	2:B:109[B]:TED:CYA	0.50	2.88	8	5
1:A:19:LYS:HZ1	1:A:35:VAL:CG2	0.50	2.18	6	1
1:A:20:GLU:OE2	1:A:21:GLU:O	0.50	2.29	4	1
1:A:60:ASP:O	1:A:60:ASP:OD1	0.50	2.30	6	2
1:A:64:PHE:CD1	1:A:70:LYS:O	0.50	2.65	2	1
1:A:68:THR:C	1:A:70:LYS:N	0.50	2.65	9	2
1:A:51:LEU:N	1:A:51:LEU:HD12	0.50	2.22	19	1
1:A:32:LYS:NZ	3:C:113:DG:N7	0.50	2.60	13	1
1:A:6:GLY:O	1:A:20:GLU:OE2	0.49	2.30	10	1
1:A:67:ARG:HG2	1:A:67:ARG:HH11	0.49	1.67	18	2
1:A:53:ARG:NH1	1:A:53:ARG:CG	0.49	2.72	1	3
1:A:65:ASP:OD1	1:A:66:PHE:N	0.49	2.45	20	1
1:A:29:SER:O	1:A:30:ALA:C	0.49	2.51	16	8
1:A:50:GLN:CD	1:A:53:ARG:HH22	0.49	2.10	13	1
1:A:28:LEU:CD1	1:A:28:LEU:O	0.49	2.55	7	1
2:B:109[C]:TED:CYA	2:B:109[C]:TED:CY6	0.49	2.91	1	3
1:A:64:PHE:CG	1:A:65:ASP:N	0.48	2.81	8	2
1:A:19:LYS:HZ1	1:A:35:VAL:HG22	0.48	1.69	6	1
2:B:109[A]:TED:CY6	2:B:109[A]:TED:CYA	0.48	2.91	13	2
1:A:57:ASN:OD1	1:A:58:ALA:N	0.48	2.47	20	1
1:A:6:GLY:C	1:A:20:GLU:OE1	0.48	2.52	19	1
1:A:43:LYS:CG	1:A:45:PHE:CZ	0.48	2.97	8	1
1:A:66:PHE:O	1:A:69:GLY:N	0.48	2.46	10	1
1:A:19:LYS:NZ	1:A:35:VAL:CG1	0.48	2.77	6	1
2:B:109[A]:TED:CYA	2:B:109[A]:TED:CY6	0.48	2.92	12	3
1:A:33:SER:CB	1:A:67:ARG:HH22	0.48	2.21	13	1
1:A:12:ALA:HB1	1:A:71:MET:SD	0.48	2.48	9	1
1:A:61:LEU:N	1:A:61:LEU:CD1	0.48	2.76	3	1
1:A:65:ASP:OD2	1:A:70:LYS:NZ	0.47	2.47	5	1
1:A:20:GLU:OE1	1:A:22:VAL:HG23	0.47	2.08	4	2
1:A:48:LYS:HZ2	1:A:61:LEU:HD12	0.47	1.68	2	1
1:A:60:ASP:C	1:A:61:LEU:HD22	0.47	2.30	2	1
2:B:109[B]:TED:CYA	2:B:109[B]:TED:CY6	0.47	2.92	6	1
1:A:65:ASP:CG	1:A:66:PHE:H	0.47	2.12	16	1
1:A:57:ASN:C	1:A:59:VAL:N	0.47	2.68	14	4
1:A:9:ASP:OD1	1:A:9:ASP:O	0.47	2.32	16	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:C:112:DA:H2"	3:C:113:DG:C8	0.47	2.45	20	9
1:A:17:TRP:CZ3	1:A:51:LEU:HD13	0.47	2.44	11	1
1:A:50:GLN:CD	1:A:50:GLN:C	0.47	2.73	11	1
2:B:101:DG:H2'	2:B:102:DA:N7	0.47	2.25	9	3
1:A:28:LEU:CD1	1:A:28:LEU:C	0.47	2.83	7	1
2:B:101:DG:H2"	2:B:102:DA:C8	0.47	2.45	8	14
1:A:46:ARG:O	1:A:47:SER:HB2	0.47	2.08	5	3
1:A:67:ARG:HG3	1:A:67:ARG:NH1	0.46	2.25	9	2
1:A:32:LYS:NZ	2:B:107:DG:O6	0.46	2.48	3	1
1:A:48:LYS:NZ	1:A:64:PHE:O	0.46	2.48	19	1
1:A:53:ARG:HH11	1:A:53:ARG:HG3	0.46	1.70	3	1
3:C:111:DG:C2'	3:C:112:DA:C8	0.46	2.98	14	5
1:A:57:ASN:O	1:A:58:ALA:C	0.46	2.53	16	6
1:A:65:ASP:CB	1:A:68:THR:HG1	0.46	2.24	10	1
1:A:61:LEU:O	1:A:64:PHE:O	0.46	2.33	2	1
2:B:109[C]:TED:C12	2:B:109[C]:TED:O9	0.46	2.64	4	1
1:A:61:LEU:N	1:A:61:LEU:CD2	0.46	2.79	2	1
2:B:101:DG:C2'	2:B:102:DA:C8	0.46	2.99	13	4
1:A:17:TRP:CH2	1:A:51:LEU:HD13	0.46	2.45	1	2
1:A:55:LEU:HD12	1:A:61:LEU:HD11	0.45	1.88	11	2
1:A:65:ASP:O	1:A:66:PHE:HB2	0.45	2.09	4	1
3:C:119[A]:TED:C12	3:C:119[A]:TED:O9	0.45	2.64	2	1
1:A:7:ARG:HD3	1:A:7:ARG:N	0.45	2.27	14	1
3:C:111:DG:H2'	3:C:112:DA:N7	0.45	2.27	20	3
1:A:21:GLU:OE1	1:A:21:GLU:C	0.45	2.54	12	1
1:A:24:ARG:CG	1:A:24:ARG:HH11	0.45	2.24	6	1
3:C:113:DG:H2"	3:C:114:DC:C6	0.45	2.46	20	6
1:A:48:LYS:HB3	1:A:49:PRO:HD3	0.45	1.89	2	1
1:A:23:ILE:O	1:A:24:ARG:C	0.45	2.54	4	5
1:A:66:PHE:CD2	3:C:114:DC:OP1	0.45	2.70	5	1
1:A:21:GLU:CB	1:A:67:ARG:HH21	0.45	2.25	10	1
1:A:9:ASP:O	1:A:9:ASP:OD1	0.45	2.35	5	1
1:A:10:CYS:SG	1:A:13:LEU:CD1	0.45	3.05	16	1
1:A:50:GLN:C	1:A:50:GLN:CD	0.45	2.75	10	1
1:A:24:ARG:HB2	1:A:30:ALA:HB1	0.45	1.87	12	1
1:A:67:ARG:HH11	1:A:67:ARG:HG3	0.45	1.72	1	1
1:A:51:LEU:HD21	1:A:55:LEU:CD1	0.44	2.42	8	1
1:A:9:ASP:C	1:A:9:ASP:OD1	0.44	2.56	16	1
1:A:32:LYS:HZ1	3:C:114:DC:H41	0.44	1.56	6	1
1:A:64:PHE:CE2	1:A:70:LYS:O	0.44	2.71	2	1
1:A:19:LYS:NZ	1:A:68:THR:O	0.44	2.50	18	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:13:LEU:N	1:A:13:LEU:HD12	0.44	2.27	2	1
1:A:53:ARG:HG3	1:A:53:ARG:NH1	0.44	2.28	17	1
2:B:100:DG:O5'	2:B:100:DG:C8	0.44	2.56	7	3
1:A:24:ARG:CG	1:A:24:ARG:NH1	0.44	2.78	6	1
1:A:17:TRP:CZ2	1:A:39:SER:HB2	0.44	2.48	12	1
1:A:17:TRP:CZ3	1:A:51:LEU:HD21	0.44	2.47	7	2
1:A:55:LEU:HD12	1:A:55:LEU:N	0.44	2.27	20	1
1:A:19:LYS:NZ	1:A:69:GLY:C	0.44	2.71	2	1
1:A:13:LEU:N	1:A:13:LEU:CD1	0.44	2.81	2	1
3:C:111:DG:H2"	3:C:112:DA:C8	0.43	2.49	14	8
1:A:64:PHE:CD2	1:A:65:ASP:O	0.43	2.71	16	2
1:A:53:ARG:NH1	1:A:53:ARG:HG2	0.43	2.28	14	1
1:A:60:ASP:OD1	1:A:60:ASP:N	0.43	2.51	10	1
1:A:17:TRP:CH2	1:A:39:SER:HB2	0.43	2.48	18	2
1:A:50:GLN:OE1	1:A:50:GLN:O	0.43	2.36	11	1
1:A:10:CYS:SG	1:A:64:PHE:CZ	0.43	3.12	16	1
1:A:17:TRP:CZ3	1:A:51:LEU:CD2	0.43	3.01	18	1
1:A:43:LYS:CG	1:A:45:PHE:CE1	0.43	3.02	8	1
1:A:60:ASP:C	1:A:61:LEU:HD12	0.43	2.34	17	1
1:A:34:ASP:OD2	1:A:36:TYR:OH	0.43	2.30	2	1
1:A:12:ALA:C	1:A:13:LEU:HD22	0.43	2.35	6	1
1:A:67:ARG:HE	1:A:67:ARG:CA	0.43	2.27	15	1
1:A:10:CYS:SG	1:A:13:LEU:HD13	0.43	2.54	16	1
1:A:66:PHE:CD1	1:A:67:ARG:N	0.43	2.87	3	1
3:C:119[C]:TED:CY8	3:C:119[C]:TED:CYB	0.42	2.97	11	1
1:A:61:LEU:N	1:A:61:LEU:HD22	0.42	2.29	2	1
1:A:43:LYS:O	1:A:45:PHE:CE1	0.42	2.73	13	2
1:A:7:ARG:N	1:A:7:ARG:CD	0.42	2.81	14	1
1:A:10:CYS:SG	1:A:17:TRP:CB	0.42	3.08	2	1
1:A:34:ASP:OD1	1:A:34:ASP:N	0.42	2.53	2	1
1:A:13:LEU:CD2	1:A:17:TRP:CE3	0.42	2.98	19	1
1:A:65:ASP:O	1:A:69:GLY:CA	0.42	2.67	5	1
1:A:47:SER:O	1:A:48:LYS:C	0.42	2.59	6	2
1:A:17:TRP:CZ3	1:A:39:SER:CB	0.41	3.03	17	1
1:A:30:ALA:C	1:A:32:LYS:N	0.41	2.73	18	1
1:A:51:LEU:N	1:A:51:LEU:CD1	0.41	2.83	19	1
1:A:61:LEU:HD12	1:A:61:LEU:N	0.41	2.30	5	1
1:A:13:LEU:HD12	1:A:13:LEU:N	0.41	2.31	19	2
1:A:46:ARG:NH2	3:C:115:5CM:C6	0.41	2.83	6	1
1:A:48:LYS:HZ1	1:A:51:LEU:HD22	0.41	1.74	16	1
1:A:67:ARG:NH1	1:A:67:ARG:HG3	0.41	2.31	5	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:48:LYS:CB	1:A:49:PRO:CD	0.41	2.99	18	1
1:A:47:SER:OG	3:C:115:5CM:OP2	0.41	2.39	18	1
1:A:32:LYS:HZ1	3:C:114:DC:N4	0.41	2.13	1	1
1:A:48:LYS:O	1:A:52:ALA:N	0.41	2.52	17	1
1:A:60:ASP:N	1:A:60:ASP:OD1	0.41	2.52	12	1
1:A:45:PHE:CD1	1:A:45:PHE:N	0.41	2.87	4	2
1:A:48:LYS:NZ	1:A:48:LYS:CB	0.41	2.84	11	1
1:A:39:SER:OG	1:A:45:PHE:CE1	0.40	2.73	6	1
1:A:66:PHE:C	1:A:68:THR:N	0.40	2.74	10	1
1:A:50:GLN:CD	1:A:50:GLN:O	0.40	2.60	11	1
1:A:68:THR:O	1:A:69:GLY:O	0.40	2.39	10	1
1:A:17:TRP:CH2	1:A:55:LEU:HD21	0.40	2.51	4	1
1:A:20:GLU:OE1	1:A:20:GLU:C	0.40	2.59	20	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	
1	A	66/72 (92%)	58±2 (88±2%)	4±2 (7±3%)	4±1 (5±2%)	3	23
All	All	1320/1440 (92%)	1161 (88%)	87 (7%)	72 (5%)	3	23

All 12 unique Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	A	47	SER	19
1	A	29	SER	18
1	A	6	GLY	9
1	A	14	PRO	5
1	A	69	GLY	4
1	A	58	ALA	4
1	A	66	PHE	3
1	A	65	ASP	3
1	A	30	ALA	3

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Mol	Chain	Res	Type	Models (Total)
1	A	27	GLY	2
1	A	67	ARG	1
1	A	71	MET	1

5.2.2 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	
1	A	55/60 (92%)	51±1 (93±2%)	4±1 (7±2%)	19	68
All	All	1100/1200 (92%)	1024 (93%)	76 (7%)	19	68

All 19 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)
1	A	39	SER	17
1	A	10	CYS	9
1	A	67	ARG	7
1	A	47	SER	7
1	A	48	LYS	6
1	A	24	ARG	5
1	A	25	LYS	4
1	A	7	ARG	3
1	A	53	ARG	2
1	A	51	LEU	2
1	A	19	LYS	2
1	A	28	LEU	2
1	A	71	MET	2
1	A	41	SER	2
1	A	32	LYS	2
1	A	45	PHE	1
1	A	65	ASP	1
1	A	46	ARG	1
1	A	63	CYS	1

5.2.3 RNA

There are no RNA molecules in this entry.

MODRES-GEOMETRY INFOmissingINFO

5.3 Carbohydrates

There are no carbohydrates in this entry.

5.4 Ligand geometry

Of 6 ligands modelled in this entry, 6 are monoatomic - leaving 0 for Mogul analysis.

5.5 Other polymers

There are no such molecules in this entry.

5.6 Polymer linkage issues

The following chains have linkage breaks:

Mol	Chain	Number of breaks
2	19-B	3
3	7-C	3
3	18-C	3
2	1-B	3
3	6-C	3
2	2-B	3
2	15-B	3
3	14-C	3
3	11-C	3
2	7-B	3
2	16-B	3
2	10-B	3
3	3-C	3
3	2-C	3
3	17-C	3
3	9-C	3
3	20-C	3
2	11-B	3
2	8-B	3

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Mol	Chain	Number of breaks
3	16-C	3
3	10-C	3
2	3-B	3
2	12-B	3
3	5-C	3
2	4-B	3
2	17-B	3
2	9-B	3
2	20-B	3
3	13-C	3
3	8-C	3
3	12-C	3
3	19-C	3
2	5-B	3
2	18-B	3
3	4-C	3
3	1-C	3
2	6-B	3
2	13-B	3
3	15-C	3
2	14-B	3

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
10	C	119[C]:TED	OY6	120:DC	P	20.80
8	C	119[B]:TED	OY4	120:DC	P	19.91
13	C	119[C]:TED	OY6	120:DC	P	19.06
17	C	119[B]:TED	OY6	120:DC	P	18.52
11	C	119[C]:TED	OY6	120:DC	P	18.51
6	C	119[C]:TED	OY4	120:DC	P	18.49
14	C	119[C]:TED	OY6	120:DC	P	18.44
18	C	119[C]:TED	OY6	120:DC	P	18.43
16	C	119[B]:TED	OY4	120:DC	P	17.88
4	C	119[C]:TED	OY6	120:DC	P	17.71
14	C	119[B]:TED	OY6	120:DC	P	17.53
6	C	119[A]:TED	OY4	120:DC	P	17.33
8	C	119[C]:TED	OY4	120:DC	P	17.15
15	C	119[C]:TED	OY4	120:DC	P	16.83
12	C	119[B]:TED	OY4	120:DC	P	16.78
17	C	119[C]:TED	OY6	120:DC	P	16.73
11	C	119[B]:TED	OY6	120:DC	P	16.50
17	B	109[B]:TED	OY6	110:DC	P	16.42

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
4	C	119[A]:TED	OY6	120:DC	P	16.40
12	C	119[A]:TED	OY4	120:DC	P	16.29
13	B	109[C]:TED	OY7	110:DC	P	16.28
7	C	119[A]:TED	OY6	120:DC	P	16.27
5	C	119[C]:TED	OY4	120:DC	P	16.23
3	C	119[B]:TED	OY4	120:DC	P	16.21
3	B	109[B]:TED	OY6	110:DC	P	16.20
2	B	109[B]:TED	OY6	110:DC	P	16.16
2	B	109[C]:TED	OY6	110:DC	P	16.15
20	C	119[C]:TED	OY4	120:DC	P	16.14
1	C	119[B]:TED	OY4	120:DC	P	16.13
13	B	109[B]:TED	OY7	110:DC	P	15.93
16	C	119[C]:TED	OY4	120:DC	P	15.92
8	B	109[A]:TED	OY4	110:DC	P	15.69
18	C	119[B]:TED	OY6	120:DC	P	15.65
19	C	119[A]:TED	OY4	120:DC	P	15.60
2	C	119[C]:TED	OY4	120:DC	P	15.56
10	C	119[A]:TED	OY6	120:DC	P	15.48
18	B	109[B]:TED	OY6	110:DC	P	15.33
10	B	109[A]:TED	OY6	110:DC	P	15.31
18	B	109[C]:TED	OY6	110:DC	P	15.29
9	B	109[C]:TED	OY4	110:DC	P	15.13
11	B	109[C]:TED	OY4	110:DC	P	15.10
13	C	119[A]:TED	OY6	120:DC	P	14.85
1	B	109[C]:TED	OY6	110:DC	P	14.78
6	B	109[A]:TED	OY6	110:DC	P	14.73
17	B	109[C]:TED	OY6	110:DC	P	14.60
2	C	119[A]:TED	OY4	120:DC	P	14.55
3	C	119[A]:TED	OY4	120:DC	P	14.43
17	C	119[A]:TED	OY6	120:DC	P	14.41
5	C	119[B]:TED	OY4	120:DC	P	14.39
9	C	119[C]:TED	OY4	120:DC	P	14.32
4	B	109[A]:TED	OY4	110:DC	P	14.15
19	B	109[C]:TED	OY6	110:DC	P	14.08
15	C	119[B]:TED	OY4	120:DC	P	14.02
7	C	119[C]:TED	OY6	120:DC	P	13.98
7	B	109[C]:TED	OY6	110:DC	P	13.95
20	C	119[B]:TED	OY4	120:DC	P	13.81
20	C	119[A]:TED	OY4	120:DC	P	13.78
5	B	109[C]:TED	OY6	110:DC	P	13.69
10	B	109[B]:TED	OY6	110:DC	P	13.68
6	C	119[B]:TED	OY4	120:DC	P	13.53

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
20	B	109[B]:TED	OY4	110:DC	P	13.38
19	C	119[B]:TED	OY4	120:DC	P	13.30
9	B	109[A]:TED	OY4	110:DC	P	13.27
2	C	119[B]:TED	OY4	120:DC	P	13.26
20	B	109[A]:TED	OY4	110:DC	P	13.24
19	B	109[B]:TED	OY6	110:DC	P	13.23
12	B	109[B]:TED	OY6	110:DC	P	13.21
16	C	119[A]:TED	OY4	120:DC	P	13.19
5	C	119[A]:TED	OY4	120:DC	P	13.18
3	C	119[C]:TED	OY4	120:DC	P	13.15
9	C	119[B]:TED	OY4	120:DC	P	13.14
5	B	109[A]:TED	OY6	110:DC	P	13.10
16	B	109[A]:TED	OY4	110:DC	P	13.07
1	C	119[A]:TED	OY4	120:DC	P	13.00
7	C	119[B]:TED	OY6	120:DC	P	12.95
1	C	119[C]:TED	OY4	120:DC	P	12.86
1	B	109[A]:TED	OY6	110:DC	P	12.70
14	B	109[A]:TED	OY4	110:DC	P	12.68
4	B	109[B]:TED	OY4	110:DC	P	12.66
16	B	109[B]:TED	OY4	110:DC	P	12.56
9	C	119[A]:TED	OY4	120:DC	P	12.54
8	C	119[A]:TED	OY4	120:DC	P	12.40
11	B	109[B]:TED	OY4	110:DC	P	12.18
8	B	109[B]:TED	OY4	110:DC	P	11.99
15	B	109[A]:TED	OY6	110:DC	P	11.98
8	B	109[C]:TED	OY4	110:DC	P	11.95
14	C	119[A]:TED	OY6	120:DC	P	11.94
19	C	119[C]:TED	OY4	120:DC	P	11.88
11	C	119[A]:TED	OY6	120:DC	P	11.84
14	B	109[B]:TED	OY4	110:DC	P	11.73
12	C	119[C]:TED	OY4	120:DC	P	11.72
15	B	109[B]:TED	OY6	110:DC	P	11.72
15	C	119[A]:TED	OY4	120:DC	P	11.54
16	B	109[C]:TED	OY4	110:DC	P	11.50
11	B	109[A]:TED	OY4	110:DC	P	11.49
1	B	109[B]:TED	OY6	110:DC	P	11.36
4	C	119[B]:TED	OY6	120:DC	P	11.24
2	B	109[A]:TED	OY6	110:DC	P	11.02
18	B	109[A]:TED	OY6	110:DC	P	11.01
13	C	119[B]:TED	OY6	120:DC	P	10.99
10	C	119[B]:TED	OY6	120:DC	P	10.97
14	B	109[C]:TED	OY4	110:DC	P	10.96

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
15	B	109[C]:TED	OY6	110:DC	P	10.96
7	B	109[A]:TED	OY6	110:DC	P	10.20
20	B	109[C]:TED	OY4	110:DC	P	9.97
9	B	109[B]:TED	OY4	110:DC	P	9.92
10	B	109[C]:TED	OY6	110:DC	P	9.80
3	B	109[C]:TED	OY6	110:DC	P	9.45
4	B	109[C]:TED	OY4	110:DC	P	9.43
7	B	109[B]:TED	OY6	110:DC	P	9.29
17	B	109[A]:TED	OY6	110:DC	P	9.25
12	B	109[C]:TED	OY6	110:DC	P	9.23
6	B	109[B]:TED	OY6	110:DC	P	8.80
12	B	109[A]:TED	OY6	110:DC	P	8.02
18	C	119[A]:TED	OY6	120:DC	P	8.00
19	B	109[A]:TED	OY6	110:DC	P	7.80
3	B	109[A]:TED	OY6	110:DC	P	7.65
6	B	109[C]:TED	OY6	110:DC	P	6.97
13	B	109[A]:TED	OY7	110:DC	P	6.79
5	B	109[B]:TED	OY6	110:DC	P	5.26

6 Chemical shift validation

The completeness of assignment taking into account all chemical shift lists is 62% for the well-defined parts and 64% for the entire structure.

6.1 Chemical shift list 1

File name: input_cs.cif

Chemical shift list name: *assigned_chem_shift_list_1*

6.1.1 Bookkeeping

The following table shows the results of parsing the chemical shift list and reports the number of nuclei with statistically unusual chemical shifts.

Total number of shifts	959
Number of shifts mapped to atoms	858
Number of unparsed shifts	0
Number of shifts with mapping errors	101
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	2

The following assigned chemical shifts were not mapped to the molecules present in the coordinate file.

- Chain not found in structure. All 101 occurences are reported below.

Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
UNMAPPED	4	DC	H5’	4.094	-1.0	2
UNMAPPED	3	DG	H1’	5.938	-1.0	1
UNMAPPED	11	DC	H5	5.889	-1.0	1
UNMAPPED	9	DC	H41	7.888	-1.0	2
UNMAPPED	4	DA	H2”	2.555	-1.0	2
UNMAPPED	6	DG	H2”	2.668	-1.0	2
UNMAPPED	5	DT	H5”	4.196	-1.0	2
UNMAPPED	5	5CM	H5A1	1.637	-1.0	1
UNMAPPED	4	DC	H2”	2.478	-1.0	2
UNMAPPED	5	5CM	H5A2	1.637	-1.0	1
UNMAPPED	3	DG	H5’	3.66	-1.0	1
UNMAPPED	9	DC	H2’	2.528	-1.0	2
UNMAPPED	6	5CM	H5A2	1.585	-1.0	1
UNMAPPED	5	DT	H6	7.264	-1.0	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
UNMAPPED	4	DC	H42	8.171	-1.0	2
UNMAPPED	11	DC	H5'	4.181	-1.0	2
UNMAPPED	3	DG	H8	7.844	-1.0	1
UNMAPPED	9	THY	H2"	2.468	-1.0	2
UNMAPPED	10	THY	H73	1.755	-1.0	1
UNMAPPED	9	THY	H73	1.248	-1.0	1
UNMAPPED	11	DC	H6	7.692	-1.0	1
UNMAPPED	5	5CM	H5A3	1.637	-1.0	1
UNMAPPED	5	DT	H2"	2.536	-1.0	2
UNMAPPED	3	DG	H2'	2.457	-1.0	1
UNMAPPED	6	5CM	H5A1	1.585	-1.0	1
UNMAPPED	3	DG	H1	12.901	-1.0	1
UNMAPPED	6	DG	H1	12.681	-1.0	1
UNMAPPED	4	DC	H41	6.957	-1.0	2
UNMAPPED	5	5CM	H1'	5.586	-1.0	1
UNMAPPED	5	5CM	H41	6.814	-1.0	2
UNMAPPED	10	THY	H2"	2.528	-1.0	2
UNMAPPED	2	DA	H2	7.875	-1.0	1
UNMAPPED	10	THY	H71	1.755	-1.0	1
UNMAPPED	9	THY	H71	1.248	-1.0	1
UNMAPPED	5	DT	H1'	5.913	-1.0	1
UNMAPPED	6	DG	H1'	5.83	-1.0	1
UNMAPPED	9	THY	H3	13.445	-1.0	1
UNMAPPED	4	DC	H6	7.367	-1.0	1
UNMAPPED	10	THY	H3'	4.888	-1.0	1
UNMAPPED	2	DA	H1'	5.565	-1.0	1
UNMAPPED	10	THY	H3	13.883	-1.0	1
UNMAPPED	7	DA	H8	8.255	-1.0	1
UNMAPPED	5	5CM	H3'	4.86	-1.0	1
UNMAPPED	4	DC	H2'	2.772	-1.0	2
UNMAPPED	7	DA	H2	7.897	-1.0	1
UNMAPPED	10	THY	H2'	2.226	-1.0	2
UNMAPPED	2	DA	H8	8.228	-1.0	1
UNMAPPED	4	DC	H5"	4.094	-1.0	2
UNMAPPED	9	THY	H72	1.248	-1.0	1
UNMAPPED	6	5CM	H5A3	1.585	-1.0	1
UNMAPPED	8	DG	H2'	2.612	-1.0	2
UNMAPPED	10	THY	H72	1.755	-1.0	1
UNMAPPED	5	5CM	H6	7.382	-1.0	1
UNMAPPED	7	DA	H62	7.902	-1.0	2
UNMAPPED	6	5CM	H2"	2.602	-1.0	2

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
UNMAPPED	6	DG	H2'	2.464	-1.0	2
UNMAPPED	7	DA	H2'	2.625	-1.0	2
UNMAPPED	9	THY	H6	7.248	-1.0	1
UNMAPPED	4	DC	H3'	4.792	-1.0	1
UNMAPPED	6	DG	H8	7.855	-1.0	1
UNMAPPED	10	THY	H6	7.542	-1.0	1
UNMAPPED	6	5CM	H6	7.208	-1.0	1
UNMAPPED	9	THY	H2'	2.115	-1.0	2
UNMAPPED	5	5CM	H5"	4.094	-1.0	2
UNMAPPED	5	DT	H3	13.984	-1.0	1
UNMAPPED	1	DG	H1'	5.966	-1.0	1
UNMAPPED	8	DG	H1	12.694	-1.0	1
UNMAPPED	6	5CM	H2'	2.09	-1.0	2
UNMAPPED	7	DA	H1'	6.229	-1.0	1
UNMAPPED	2	DA	H2"	2.459	-1.0	2
UNMAPPED	11	DC	H2"	2.623	-1.0	2
UNMAPPED	9	DC	H42	6.456	-1.0	2
UNMAPPED	5	5CM	H2'	2.342	-1.0	2
UNMAPPED	4	DA	H62	6.472	-1.0	2
UNMAPPED	5	5CM	H2"	2.611	-1.0	2
UNMAPPED	5	5CM	H42	8.686	-1.0	2
UNMAPPED	5	DT	H2'	2.054	-1.0	2
UNMAPPED	2	DA	H2'	2.79	-1.0	2
UNMAPPED	7	DG	H8	7.82	-1.0	1
UNMAPPED	4	DC	H1'	5.428	-1.0	1
UNMAPPED	7	DA	H3'	5.056	-1.0	1
UNMAPPED	5	DT	H72	1.206	-1.0	1
UNMAPPED	5	DT	H73	1.206	-1.0	1
UNMAPPED	6	5CM	HN42	9.212	-1.0	2
UNMAPPED	10	THY	H1'	6.152	-1.0	1
UNMAPPED	8	DG	H2"	2.531	-1.0	2
UNMAPPED	5	5CM	H5'	4.094	-1.0	2
UNMAPPED	6	5CM	HN41	6.759	-1.0	2
UNMAPPED	7	DA	H2"	2.928	-1.0	2
UNMAPPED	4	DC	H5	5.412	-1.0	1
UNMAPPED	5	DT	H5'	4.196	-1.0	2
UNMAPPED	9	DC	H6	7.562	-1.0	1
UNMAPPED	9	DC	H5	5.425	-1.0	1
UNMAPPED	11	DC	H5"	4.054	-1.0	2
UNMAPPED	4	DA	H8	7.883	-1.0	1
UNMAPPED	9	DC	H2"	2.226	-1.0	2

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
UNMAPPED	5	DT	H71	1.206	-1.0	1
UNMAPPED	7	DG	H1	13.024	-1.0	1
UNMAPPED	11	DC	H2'	2.287	-1.0	2
UNMAPPED	4	DA	H2	7.826	-1.0	1
UNMAPPED	4	DA	H2'	2.887	-1.0	2

6.1.2 Chemical shift referencing

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction ± precision, *ppm*	Suggested action
$^{13}C_{\alpha}$	71	-0.28 ± 0.20	None needed (< 0.5 ppm)
$^{13}C_{\beta}$	62	-0.43 ± 0.37	None needed (< 0.5 ppm)
$^{13}C'$	61	-0.12 ± 0.29	None needed (< 0.5 ppm)
^{15}N	61	-0.40 ± 0.35	None needed (< 0.5 ppm)

6.1.3 Completeness of resonance assignments

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 62%, i.e. 739 atoms were assigned a chemical shift out of a possible 1188. 0 out of 8 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	302/320 (94%)	122/127 (96%)	123/132 (93%)	57/61 (93%)
Sidechain	372/433 (86%)	233/261 (89%)	130/147 (88%)	9/25 (36%)
Aromatic	65/72 (90%)	33/38 (87%)	31/33 (94%)	1/1 (100%)
Overall	739/1188 (62%)	388/645 (60%)	284/431 (66%)	67/112 (60%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 64%, i.e. 790 atoms were assigned a chemical shift out of a possible 1243. 0 out of 8 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	321/340 (94%)	130/135 (96%)	130/140 (93%)	61/65 (94%)
Sidechain	404/468 (86%)	254/282 (90%)	140/159 (88%)	10/27 (37%)
Aromatic	65/72 (90%)	33/38 (87%)	31/33 (94%)	1/1 (100%)
Overall	790/1243 (64%)	417/674 (62%)	301/451 (67%)	72/118 (61%)

6.1.4 Statistically unusual chemical shifts (i)

The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

Mol	Chain	Res	Type	Atom	Shift, *ppm*	Expected range, *ppm*	Z-score
1	A	39	SER	HA	2.00	6.53 – 2.43	-6.0
1	A	40	PRO	HD2	1.63	5.45 – 1.85	-5.6

6.1.5 Random Coil Index (RCI) plots (i)

The image below reports *random coil index* values for the protein chains in the structure. The height of each bar gives a probability of a given residue to be disordered, as predicted from the available chemical shifts and the amino acid sequence. A value above 0.2 is an indication of significant predicted disorder. The colour of the bar shows whether the residue is in the well-defined core (black) or in the ill-defined residue ranges (cyan), as described in section 2 on ensemble composition.

Random coil index (RCI) for chain A: