



Full wwPDB NMR Structure Validation Report ⓘ

Apr 15, 2026 – 10:33 AM UTC

PDB ID : 2JSC / pdb_00002jsc
Title : NMR structure of the cadmium metal-sensor CMTR from Mycobacterium tuberculosis
Authors : Banci, L.; Bertini, I.; Cantini, F.; Ciofi-Baffoni, S.; Cavet, J.S.; Dennison, C.; Graham, A.I.; Harvie, D.R.; Robinson, N.J.; Structural Proteomics in Europe (SPINE)
Deposited on : 2007-07-02

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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	FAILED
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
wwPDB-RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
wwPDB-ShiftChecker	:	v1.2
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

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.

There are no overall percentile quality scores available for this entry.

The sequence quality summary graphics cannot be shown.

2 Ensemble composition and analysis ⓘ

This entry contains 30 models. The atoms present in the NMR models are not consistent. Some calculations may have failed as a result. All residues are included in the validation scores. Model 3 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *fewest violations*.

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:11-A:102, B:11-B:95 (177)	1.56	3

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

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

NmrClust was unable to cluster the ensemble.

Error message: Inconsistent models in file

3 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 2920 atoms, of which 1481 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Transcriptional regulator Rv1994c/MT2050.

Mol	Chain	Residues	Atoms						Trace
1	A	96	Total	C	H	N	O	S	0
			1454	444	738	138	129	5	
1	B	97	Total	C	H	N	O	S	0
			1464	447	743	139	130	5	

- Molecule 2 is CADMIUM ION (CCD ID: CD) (formula: Cd).

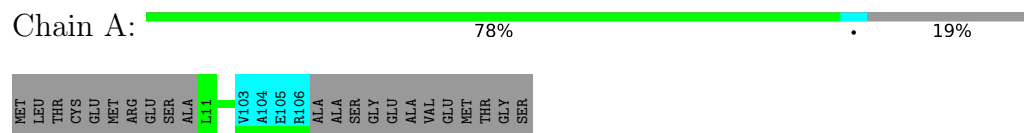
Mol	Chain	Residues	Atoms	
2	A	1	Total	Cd
			1	1
2	B	1	Total	Cd
			1	1

4 Residue-property plots [i](#)

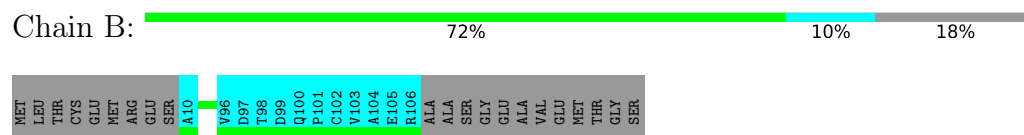
4.1 Average score per residue in the NMR ensemble

These plots are provided for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic is the same as shown in the summary in section 1 of this report. The second graphic shows the sequence where residues are colour-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outliers are shown as green connectors. Residues which are classified as ill-defined in the NMR ensemble, are shown in cyan with an underline colour-coded according to the previous scheme. Residues which were present in the experimental sample, but not modelled in the final structure are shown in grey.

- Molecule 1: Transcriptional regulator Rv1994c/MT2050



- Molecule 1: Transcriptional regulator Rv1994c/MT2050

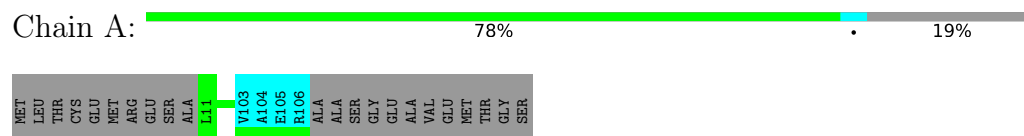


4.2 Scores per residue for each member of the ensemble

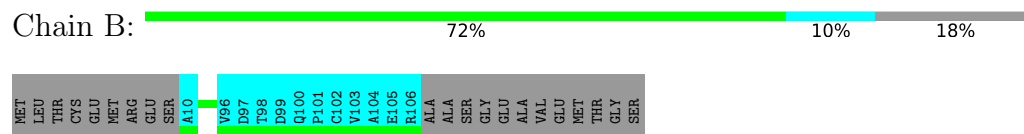
Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

- Molecule 1: Transcriptional regulator Rv1994c/MT2050



- Molecule 1: Transcriptional regulator Rv1994c/MT2050



4.2.5 Score per residue for model 5

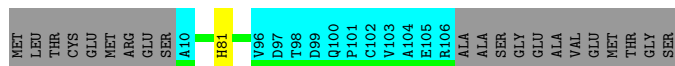
- Molecule 1: Transcriptional regulator Rv1994c/MT2050

Chain A:  77% 19%



- Molecule 1: Transcriptional regulator Rv1994c/MT2050

Chain B:  71% 10% 18%



4.2.6 Score per residue for model 6

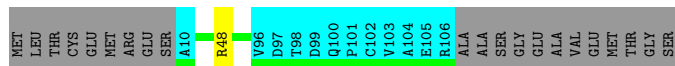
- Molecule 1: Transcriptional regulator Rv1994c/MT2050

Chain A:  78% 19%



- Molecule 1: Transcriptional regulator Rv1994c/MT2050

Chain B:  71% 10% 18%



4.2.7 Score per residue for model 7

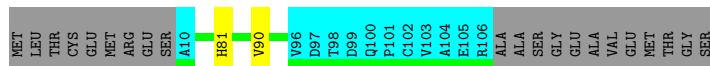
- Molecule 1: Transcriptional regulator Rv1994c/MT2050

Chain A:  76% 19%



- Molecule 1: Transcriptional regulator Rv1994c/MT2050

Chain B:  70% 10% 18%



4.2.8 Score per residue for model 8

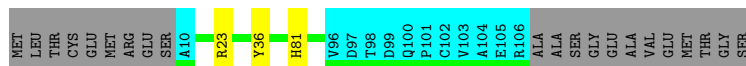
- Molecule 1: Transcriptional regulator Rv1994c/MT2050

Chain A:  75% 19%



- Molecule 1: Transcriptional regulator Rv1994c/MT2050

Chain B:  69% 10% 18%



4.2.9 Score per residue for model 9

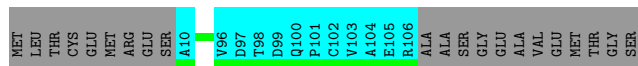
- Molecule 1: Transcriptional regulator Rv1994c/MT2050

Chain A:  75% 19%



- Molecule 1: Transcriptional regulator Rv1994c/MT2050

Chain B:  72% 10% 18%



4.2.10 Score per residue for model 10

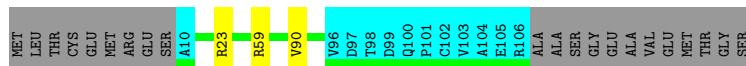
- Molecule 1: Transcriptional regulator Rv1994c/MT2050

Chain A:  76% 19%



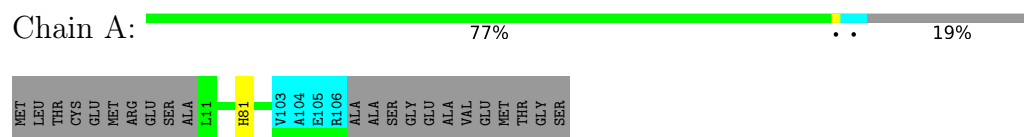
- Molecule 1: Transcriptional regulator Rv1994c/MT2050

Chain B:  69% 10% 18%

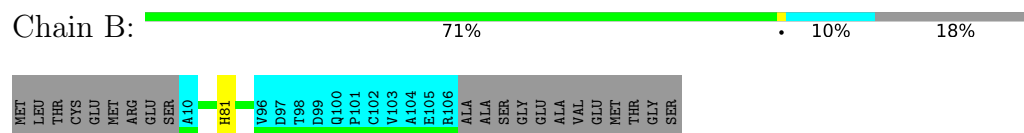


4.2.11 Score per residue for model 11

- Molecule 1: Transcriptional regulator Rv1994c/MT2050

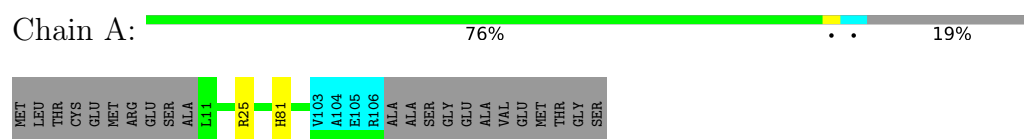


- Molecule 1: Transcriptional regulator Rv1994c/MT2050

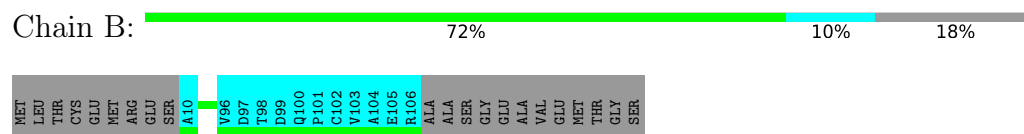


4.2.12 Score per residue for model 12

- Molecule 1: Transcriptional regulator Rv1994c/MT2050

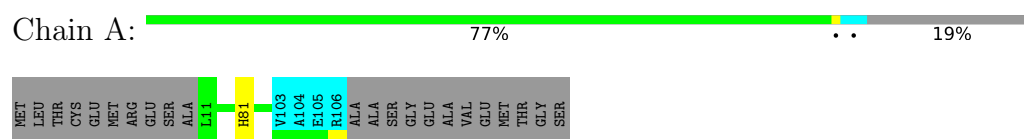


- Molecule 1: Transcriptional regulator Rv1994c/MT2050

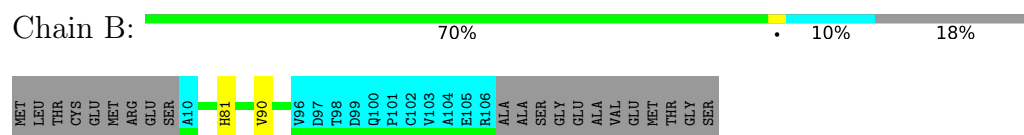


4.2.13 Score per residue for model 13

- Molecule 1: Transcriptional regulator Rv1994c/MT2050



- Molecule 1: Transcriptional regulator Rv1994c/MT2050



4.2.14 Score per residue for model 14

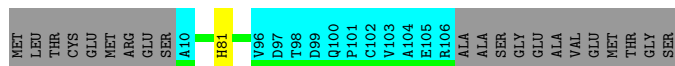
- Molecule 1: Transcriptional regulator Rv1994c/MT2050

Chain A:  77% 19%



- Molecule 1: Transcriptional regulator Rv1994c/MT2050

Chain B:  71% 10% 18%



4.2.15 Score per residue for model 15

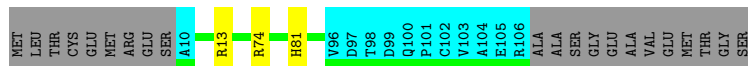
- Molecule 1: Transcriptional regulator Rv1994c/MT2050

Chain A:  77% 19%



- Molecule 1: Transcriptional regulator Rv1994c/MT2050

Chain B:  69% 10% 18%



4.2.16 Score per residue for model 16

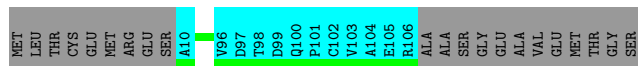
- Molecule 1: Transcriptional regulator Rv1994c/MT2050

Chain A:  77% 19%



- Molecule 1: Transcriptional regulator Rv1994c/MT2050

Chain B:  72% 10% 18%



4.2.17 Score per residue for model 17

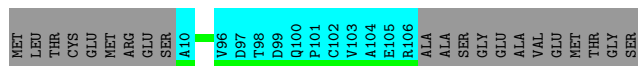
- Molecule 1: Transcriptional regulator Rv1994c/MT2050

Chain A:  78% 19%



- Molecule 1: Transcriptional regulator Rv1994c/MT2050

Chain B:  72% 10% 18%



4.2.18 Score per residue for model 18

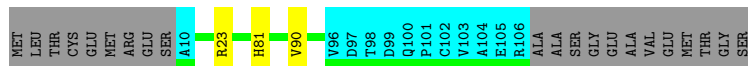
- Molecule 1: Transcriptional regulator Rv1994c/MT2050

Chain A:  76% 19%



- Molecule 1: Transcriptional regulator Rv1994c/MT2050

Chain B:  69% 10% 18%



4.2.19 Score per residue for model 19

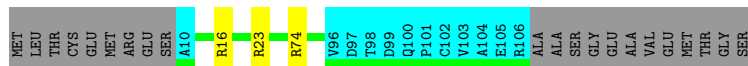
- Molecule 1: Transcriptional regulator Rv1994c/MT2050

Chain A:  76% 19%



- Molecule 1: Transcriptional regulator Rv1994c/MT2050

Chain B:  69% 10% 18%



4.2.20 Score per residue for model 20

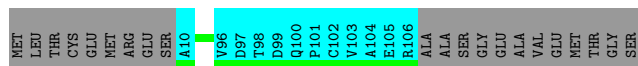
- Molecule 1: Transcriptional regulator Rv1994c/MT2050

Chain A:  77% 19%



- Molecule 1: Transcriptional regulator Rv1994c/MT2050

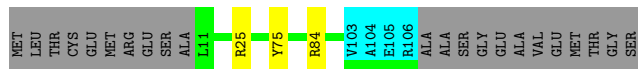
Chain B:  72% 10% 18%



4.2.21 Score per residue for model 21

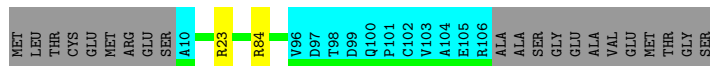
- Molecule 1: Transcriptional regulator Rv1994c/MT2050

Chain A:  75% 19%



- Molecule 1: Transcriptional regulator Rv1994c/MT2050

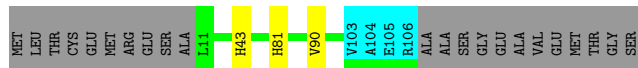
Chain B:  70% 10% 18%



4.2.22 Score per residue for model 22

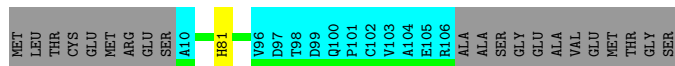
- Molecule 1: Transcriptional regulator Rv1994c/MT2050

Chain A:  75% 19%



- Molecule 1: Transcriptional regulator Rv1994c/MT2050

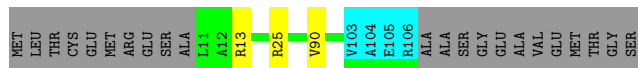
Chain B:  71% 10% 18%



4.2.23 Score per residue for model 23

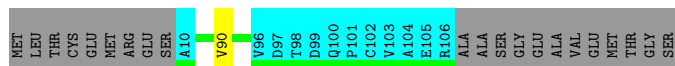
- Molecule 1: Transcriptional regulator Rv1994c/MT2050

Chain A:  75% 19%



- Molecule 1: Transcriptional regulator Rv1994c/MT2050

Chain B:  71% 18% 10%



4.2.24 Score per residue for model 24

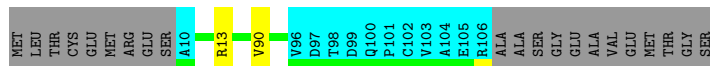
- Molecule 1: Transcriptional regulator Rv1994c/MT2050

Chain A:  78% 19%



- Molecule 1: Transcriptional regulator Rv1994c/MT2050

Chain B:  70% 18% 10%



4.2.25 Score per residue for model 25

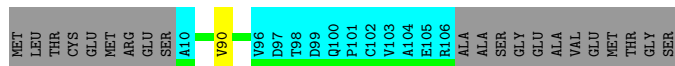
- Molecule 1: Transcriptional regulator Rv1994c/MT2050

Chain A:  77% 19%



- Molecule 1: Transcriptional regulator Rv1994c/MT2050

Chain B:  71% 18% 10%



4.2.26 Score per residue for model 26

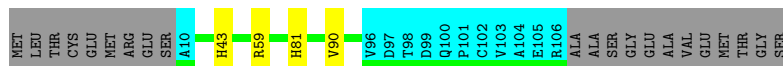
- Molecule 1: Transcriptional regulator Rv1994c/MT2050

Chain A:  77% 19%



- Molecule 1: Transcriptional regulator Rv1994c/MT2050

Chain B:  69% 10% 18%



4.2.27 Score per residue for model 27

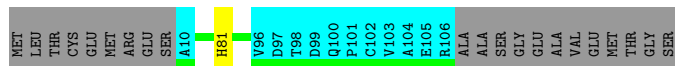
- Molecule 1: Transcriptional regulator Rv1994c/MT2050

Chain A:  76% 19%



- Molecule 1: Transcriptional regulator Rv1994c/MT2050

Chain B:  71% 10% 18%



4.2.28 Score per residue for model 28

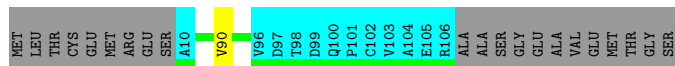
- Molecule 1: Transcriptional regulator Rv1994c/MT2050

Chain A:  76% 19%



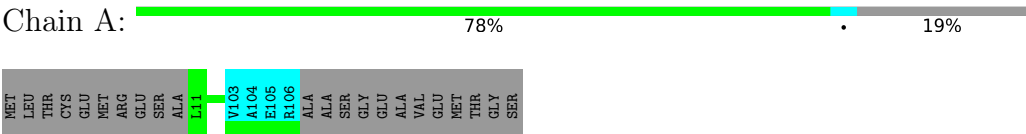
- Molecule 1: Transcriptional regulator Rv1994c/MT2050

Chain B:  71% 10% 18%

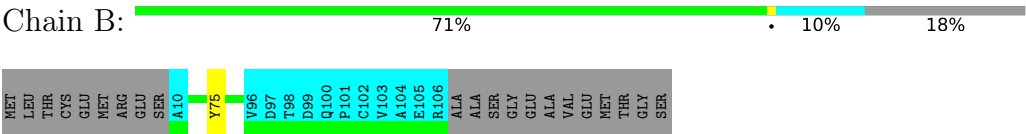


4.2.29 Score per residue for model 29

- Molecule 1: Transcriptional regulator Rv1994c/MT2050

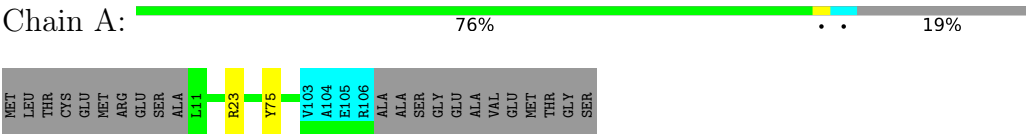


- Molecule 1: Transcriptional regulator Rv1994c/MT2050

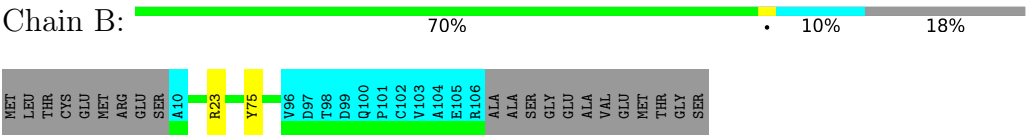


4.2.30 Score per residue for model 30

- Molecule 1: Transcriptional regulator Rv1994c/MT2050



- Molecule 1: Transcriptional regulator Rv1994c/MT2050



5 Refinement protocol and experimental data overview

The models were refined using the following method: *TORSION ANGLE DYNAMICS COUPLED WITH SIMULATED ANNEALING FOLLOWED BY RESTRAINED ENERGY MINIMIZATION*.

Of the 300 calculated structures, 30 were deposited, based on the following criterion: *target function*.

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

Software name	Classification	Version
Amber	refinement	8.0
CYANA	structure solution	1.1

No chemical shift data was provided.

6 Model quality [i](#)

6.1 Standard geometry [i](#)

MolProbity failed to run properly - this section will have to be empty.

6.2 Too-close contacts [i](#)

MolProbity failed to run properly - this section will have to be empty.

6.3 Torsion angles [i](#)

6.3.1 Protein backbone [i](#)

MolProbity failed to run properly - this section will have to be empty.

6.3.2 Protein sidechains [i](#)

MolProbity failed to run properly - this section will have to be empty.

6.3.3 RNA [i](#)

MolProbity failed to run properly - this section will have to be empty.

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

MolProbity failed to run properly - this section will have to be empty.

6.5 Carbohydrates [i](#)

MolProbity failed to run properly - this section will have to be empty.

6.6 Ligand geometry [i](#)

MolProbity failed to run properly - this section will have to be empty.

6.7 Other polymers [i](#)

MolProbity failed to run properly - this section will have to be empty.

6.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

7 Chemical shift validation

No chemical shift data were provided