



wwPDB NMR Structure Validation Summary Report ⓘ

Apr 15, 2026 – 11:51 AM UTC

PDB ID : 1WJF / pdb_00001wjf
Title : SOLUTION STRUCTURE OF H12C MUTANT OF THE N-TERMINAL
ZN BINDING DOMAIN OF HIV-1 INTEGRASE COMPLEXED TO CAD-
MIUM, NMR, 40 STRUCTURES
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This is a wwPDB NMR Structure Validation Summary 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 40 models. Model 34 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:1-A:45, B:1-B:45 (90)	0.46	34

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 10 clusters and 4 single-model clusters were found.

Cluster number	Models
1	3, 5, 12, 16, 32, 33, 34
2	7, 14, 19, 21, 30, 35
3	2, 10, 13, 15, 37
4	20, 23, 27, 31
5	18, 22, 29
6	6, 17, 38
7	28, 36
8	1, 11
9	9, 39
10	8, 25
Single-model clusters	4; 24; 26; 40

3 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 1676 atoms, of which 816 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called HIV-1 INTEGRASE.

Mol	Chain	Residues	Atoms						Trace
1	A	55	Total	C	H	N	O	S	0
			837	266	408	73	85	5	
1	B	55	Total	C	H	N	O	S	0
			837	266	408	73	85	5	

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	12	CYS	HIS	engineered mutation	UNP P04587
B	12	CYS	HIS	engineered mutation	UNP P04587

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

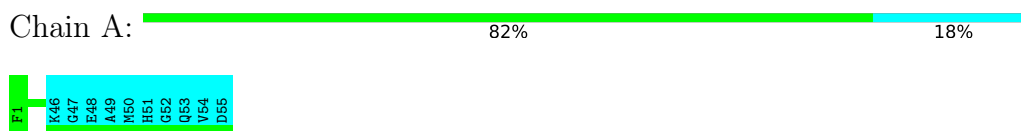
Mol	Chain	Residues	Atoms	
2	A	1	Total	Cd
			1	1
2	B	1	Total	Cd
			1	1

4 Residue-property plots

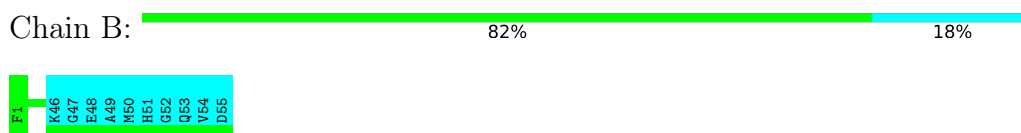
4.1 Average score per residue in the NMR ensemble

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: HIV-1 INTEGRASE



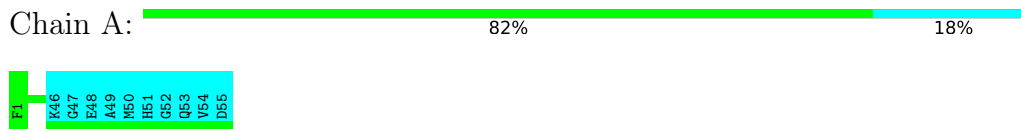
- Molecule 1: HIV-1 INTEGRASE



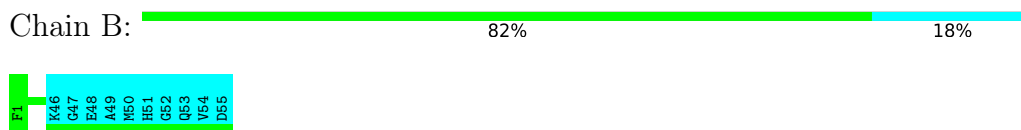
4.2 Residue scores for the representative (medoid) model from the NMR ensemble

The representative model is number 34. Colouring as in section 4.1 above.

- Molecule 1: HIV-1 INTEGRASE



- Molecule 1: HIV-1 INTEGRASE



5 Refinement protocol and experimental data overview ⓘ

The models were refined using the following method: *simulated annealing*.

Of the 40 calculated structures, 40 were deposited, based on the following criterion: ?.

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

Software name	Classification	Version
CNS	refinement	
CNS MODIFIED	structure solution	MODIFIED

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](#)

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6.3 Torsion angles [i](#)

6.3.1 Protein backbone [i](#)

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6.3.2 Protein sidechains [i](#)

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6.3.3 RNA [i](#)

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

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6.5 Carbohydrates [i](#)

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6.6 Ligand geometry [i](#)

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6.7 Other polymers [i](#)

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6.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

7 Chemical shift validation

No chemical shift data were provided