



wwPDB NMR Structure Validation Summary Report ⓘ

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PDB ID : 1E0E / pdb_00001e0e
BMRB ID : 4619
Title : N-terminal zinc-binding HHCC domain of HIV-2 integrase
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Boelens, R.
Deposited on : 2000-03-25

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 is 42%.

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 32 models. Model 27 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *closest to the average*.

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:44 (39)	0.27	27
2	B:6-B:44 (39)	0.27	27

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 6 clusters and 1 single-model cluster was found.

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

3 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 1494 atoms, of which 740 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called HUMAN IMMUNODEFICIENCY VIRUS TYPE 2 INTEGRASE.

Mol	Chain	Residues	Atoms						Trace
1	A	47	Total	C	H	N	O	S	1
			746	235	370	69	70	2	
1	B	47	Total	C	H	N	O	S	1
			746	235	370	69	70	2	

- Molecule 2 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

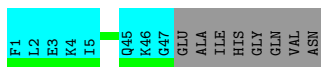
4 Residue-property plots [i](#)

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.

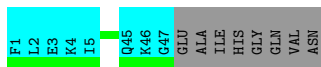
- Molecule 1: HUMAN IMMUNODEFICIENCY VIRUS TYPE 2 INTEGRASE

Chain A: 



- Molecule 1: HUMAN IMMUNODEFICIENCY VIRUS TYPE 2 INTEGRASE

Chain B: 



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

The representative model is number 27. Colouring as in section 4.1 above.

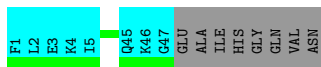
- Molecule 1: HUMAN IMMUNODEFICIENCY VIRUS TYPE 2 INTEGRASE

Chain A: 



- Molecule 1: HUMAN IMMUNODEFICIENCY VIRUS TYPE 2 INTEGRASE

Chain B: 



5 Refinement protocol and experimental data overview

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

Of the 50 calculated structures, 32 were deposited, based on the following criterion: *LOW OVER-ALL ENERGY*.

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

Software name	Classification	Version
X-PLOR	refinement	3.851
X-PLOR	structure solution	3.851

The following table shows chemical shift validation statistics as aggregates over all chemical shift files. Detailed validation can be found in section 7 of this report.

Chemical shift file(s)	working_cs.cif
Number of chemical shift lists	1
Total number of shifts	644
Number of shifts mapped to atoms	552
Number of unparsed shifts	0
Number of shifts with mapping errors	92
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	42%

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](#)

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

The completeness of assignment taking into account all chemical shift lists is 42% for the well-defined parts and 43% for the entire structure.

7.1 Chemical shift list 1

File name: working_cs.cif

Chemical shift list name: *assigned_chem_shift_list_1*

7.1.1 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	644
Number of shifts mapped to atoms	552
Number of unparsed shifts	0
Number of shifts with mapping errors	92
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	4

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

- No matching atom found in the structure. First 5 (of 92) occurrences are reported below.

List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	1	PHE	H	8.3	?	1
1	A	47	GLY	H	8.202	?	1
1	A	47	GLY	HA2	3.981	?	.
1	A	47	GLY	HA3	3.981	?	.
1	A	47	GLY	CA	43.306	?	1
1	A	48	GLU	H	8.224	?	1
1	A	48	GLU	HA	4.28	?	1
1	A	48	GLU	HB2	1.948	?	.
1	A	48	GLU	HB3	2.064	?	.
1	A	48	GLU	HG2	2.277	?	.
1	A	48	GLU	HG3	2.315	?	.
1	A	48	GLU	CA	54.387	?	1
1	A	48	GLU	CB	28.31	?	1
1	A	48	GLU	CG	34.136	?	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	48	GLU	N	121.446	?	1
1	A	49	ALA	H	8.264	?	1
1	A	49	ALA	HA	4.314	?	1
1	A	49	ALA	HB1	1.367	?	1
1	A	49	ALA	HB2	1.367	?	1
1	A	49	ALA	HB3	1.367	?	1
1	A	49	ALA	CA	50.412	?	1
1	A	49	ALA	CB	17.156	?	1
1	A	49	ALA	N	125.657	?	1
1	A	50	ILE	H	7.963	?	1
1	A	50	ILE	HA	4.093	?	1
1	A	50	ILE	HB	1.797	?	1
1	A	50	ILE	HD11	0.805	?	1
1	A	50	ILE	HD12	0.805	?	1
1	A	50	ILE	HD13	0.805	?	1
1	A	50	ILE	HG12	1.134	?	.
1	A	50	ILE	HG13	1.366	?	.
1	A	50	ILE	HG21	0.805	?	1
1	A	50	ILE	HG22	0.805	?	1
1	A	50	ILE	HG23	0.805	?	1
1	A	50	ILE	CA	59.071	?	1
1	A	50	ILE	CB	36.52	?	1
1	A	50	ILE	CD1	10.99	?	1
1	A	50	ILE	CG1	25.196	?	1
1	A	50	ILE	CG2	15.545	?	1
1	A	50	ILE	N	120.168	?	1
1	A	51	HIS	H	8.354	?	1
1	A	51	HIS	HA	4.71	?	1
1	A	51	HIS	HB2	3.137	?	.
1	A	51	HIS	HB3	3.234	?	.
1	A	51	HIS	HD2	7.172	?	1
1	A	51	HIS	HE1	8.19	?	1
1	A	51	HIS	CA	53.47	?	1
1	A	51	HIS	CB	27.625	?	1
1	A	51	HIS	CD2	134.871	?	1
1	A	51	HIS	N	123.39	?	1
1	A	52	GLY	H	8.34	?	1
1	A	52	GLY	HA2	3.957	?	.
1	A	52	GLY	HA3	3.957	?	.
1	A	52	GLY	CA	43.095	?	1
1	A	52	GLY	N	110.96	?	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	53	GLN	H	8.248	?	1
1	A	53	GLN	HA	4.394	?	1
1	A	53	GLN	HB2	1.995	?	.
1	A	53	GLN	HB3	2.108	?	.
1	A	53	GLN	HE21	7.584	?	.
1	A	53	GLN	HE22	6.851	?	.
1	A	53	GLN	HG2	2.335	?	.
1	A	53	GLN	HG3	2.36	?	.
1	A	53	GLN	CA	53.66	?	1
1	A	53	GLN	CB	27.567	?	1
1	A	53	GLN	CG	31.7	?	1
1	A	53	GLN	N	121.184	?	1
1	A	53	GLN	NE2	113.586	?	1
1	A	54	VAL	H	8.248	?	1
1	A	54	VAL	HA	4.165	?	1
1	A	54	VAL	HB	2.096	?	1
1	A	54	VAL	HG11	0.931	?	.
1	A	54	VAL	HG12	0.931	?	.
1	A	54	VAL	HG13	0.931	?	.
1	A	54	VAL	HG21	0.911	?	.
1	A	54	VAL	HG22	0.911	?	.
1	A	54	VAL	HG23	0.911	?	.
1	A	54	VAL	CA	60.109	?	1
1	A	54	VAL	CB	30.81	?	1
1	A	54	VAL	CG1	19.385	?	.
1	A	54	VAL	CG2	18.363	?	.
1	A	54	VAL	N	122.516	?	1
1	A	55	ASN	H	8.073	?	1
1	A	55	ASN	HA	4.488	?	1
1	A	55	ASN	HB2	2.669	?	.
1	A	55	ASN	HB3	2.774	?	.
1	A	55	ASN	HD21	7.5	?	.
1	A	55	ASN	HD22	6.802	?	.
1	A	55	ASN	CA	52.658	?	1
1	A	55	ASN	CB	38.427	?	1
1	A	55	ASN	N	128.509	?	1
1	A	55	ASN	ND2	113.752	?	1

7.1.2 Chemical shift referencing ⓘ

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction $\pm$ precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	55	1.56 ± 0.22	Should be applied
$^{13}\text{C}_\beta$	52	2.06 ± 0.12	Should be applied
$^{13}\text{C}'$	0	—	None (insufficient data)
^{15}N	52	-0.42 ± 0.43	None needed (< 0.5 ppm)

7.1.3 Completeness of resonance assignments [i](#)

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 42%, i.e. 447 atoms were assigned a chemical shift out of a possible 1054. 0 out of 10 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	151/384 (39%)	76/154 (49%)	39/156 (25%)	36/74 (49%)
Sidechain	271/590 (46%)	184/378 (49%)	80/186 (43%)	7/26 (27%)
Aromatic	25/80 (31%)	16/42 (38%)	9/32 (28%)	0/6 (0%)
Overall	447/1054 (42%)	276/574 (48%)	128/374 (34%)	43/106 (41%)

7.1.4 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.

List Id	Chain	Res	Type	Atom	Shift, ppm	Expected range, ppm	Z-score
1	A	16	HIS	HA	1.95	2.49 – 6.71	-6.3
1	A	12	HIS	CD2	138.85	103.95 – 136.66	5.7
1	A	25	LYS	HG2	0.08	0.13 – 2.61	-5.2
1	A	16	HIS	CD2	136.86	103.95 – 136.66	5.1

7.1.5 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. If well-defined core and ill-defined regions are not identified then it is shown as gray bars.

Random coil index (RCI) for chain A:

