



wwPDB NMR Structure Validation Summary Report ⓘ

Apr 15, 2026 – 10:56 AM UTC

PDB ID : 2LJY / pdb_00002ljy
BMRB ID : 17968
Title : Haddock model structure of the N-terminal domain dimer of HPV16 E6
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Deposited on : 2011-09-30

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

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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 38%.

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 20 models. Model 17 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:9-A:67 (59)	0.58	20
2	B:8-B:70 (63)	0.69	17

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 1 single-model cluster was found.

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

3 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 2358 atoms, of which 1170 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Protein E6.

Mol	Chain	Residues	Atoms						Trace
1	A	70	Total	C	H	N	O	S	0
			1178	380	585	101	105	7	
1	B	70	Total	C	H	N	O	S	0
			1178	380	585	101	105	7	

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	GLY	-	expression tag	UNP P03126
A	80	SER	CYS	engineered mutation	UNP P03126
B	-1	GLY	-	expression tag	UNP P03126
B	80	SER	CYS	engineered mutation	UNP P03126

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

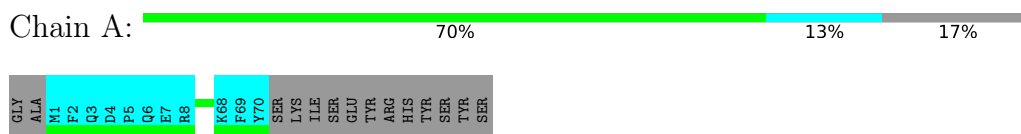
Mol	Chain	Residues	Atoms	
2	A	1	Total	Zn
			1	1
2	B	1	Total	Zn
			1	1

4 Residue-property plots [i](#)

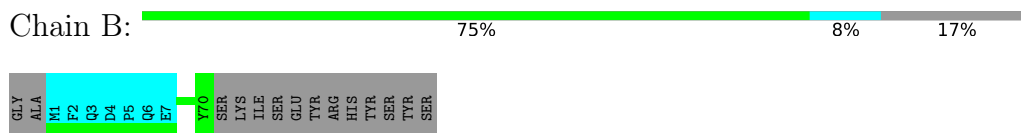
4.1 Average score per residue in the NMR ensemble

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: Protein E6



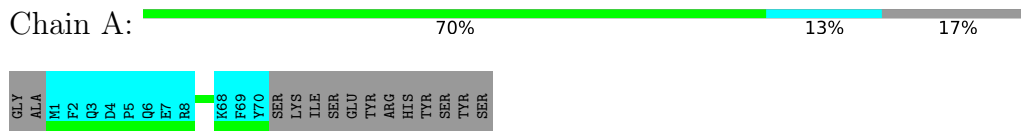
- Molecule 1: Protein E6



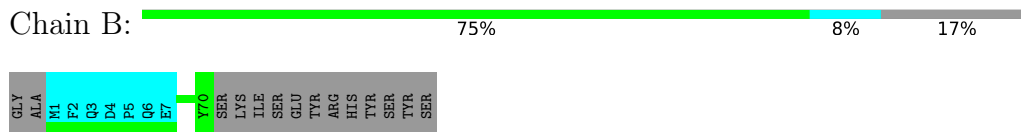
4.2 Residue scores for the representative (medoid) model from the NMR ensemble

The representative model is number 17. Colouring as in section 4.1 above.

- Molecule 1: Protein E6



- Molecule 1: Protein E6



5 Refinement protocol and experimental data overview

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

Of the 200 calculated structures, 20 were deposited, based on the following criterion: *structures with the lowest energy*.

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

Software name	Classification	Version
HADDOCK webserver	structure calculation	
HADDOCK webserver	refinement	

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	891
Number of shifts mapped to atoms	794
Number of unparsed shifts	0
Number of shifts with mapping errors	97
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	38%

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

The completeness of assignment taking into account all chemical shift lists is 38% for the well-defined parts and 39% for the entire structure.

7.1 Chemical shift list 1

File name: working_cs.cif

Chemical shift list name: *E6Ndimer*

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	891
Number of shifts mapped to atoms	794
Number of unparsed shifts	0
Number of shifts with mapping errors	97
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 97) occurrences are reported below.

List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	71	SER	H	7.88	0.02	1
1	A	71	SER	HA	4.32	0.02	1
1	A	71	SER	HB2	3.94	0.02	1
1	A	71	SER	CA	60.13	0.30	1
1	A	71	SER	CB	63.63	0.30	1
1	A	71	SER	N	117.21	0.30	1
1	A	72	LYS	H	7.8	0.02	1
1	A	72	LYS	HA	4.26	0.02	1
1	A	72	LYS	HB2	1.86	0.02	2
1	A	72	LYS	HB3	1.75	0.02	2
1	A	72	LYS	HD2	1.61	0.02	1
1	A	72	LYS	HE2	2.92	0.02	1
1	A	72	LYS	HG2	1.42	0.02	2
1	A	72	LYS	HG3	1.36	0.02	2

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	72	LYS	CA	56.93	0.30	1
1	A	72	LYS	CB	32.63	0.30	1
1	A	72	LYS	CD	29.13	0.30	1
1	A	72	LYS	CE	42.33	0.30	1
1	A	72	LYS	CG	24.93	0.30	1
1	A	72	LYS	N	122.81	0.30	1
1	A	73	ILE	H	7.76	0.02	1
1	A	73	ILE	HA	4.1	0.02	1
1	A	73	ILE	HB	1.88	0.02	1
1	A	73	ILE	HD11	0.77	0.02	1
1	A	73	ILE	HD12	0.77	0.02	1
1	A	73	ILE	HD13	0.77	0.02	1
1	A	73	ILE	HG12	1.4	0.02	2
1	A	73	ILE	HG13	1.12	0.02	2
1	A	73	ILE	HG21	0.85	0.02	1
1	A	73	ILE	HG22	0.85	0.02	1
1	A	73	ILE	HG23	0.85	0.02	1
1	A	73	ILE	CA	61.93	0.30	1
1	A	73	ILE	CB	38.63	0.30	1
1	A	73	ILE	CD1	13.43	0.30	1
1	A	73	ILE	CG1	27.63	0.30	1
1	A	73	ILE	CG2	17.83	0.30	1
1	A	73	ILE	N	121.61	0.30	1
1	A	74	SER	H	8.16	0.02	1
1	A	74	SER	HA	4.3	0.02	1
1	A	74	SER	HB2	3.85	0.02	2
1	A	74	SER	HB3	3.77	0.02	2
1	A	74	SER	CA	59.33	0.30	1
1	A	74	SER	CB	63.93	0.30	1
1	A	74	SER	N	120.31	0.30	1
1	A	75	GLU	H	8.25	0.02	1
1	A	75	GLU	HA	4.18	0.02	1
1	A	75	GLU	HB2	1.94	0.02	2
1	A	75	GLU	HB3	1.87	0.02	2
1	A	75	GLU	HG2	2.13	0.02	2
1	A	75	GLU	HG3	2.16	0.02	2
1	A	75	GLU	CA	57.33	0.30	1
1	A	75	GLU	CB	30.13	0.30	1
1	A	75	GLU	CG	36.43	0.30	1
1	A	75	GLU	N	123.81	0.30	1
1	A	76	TYR	H	8.0	0.02	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	76	TYR	HA	4.46	0.02	1
1	A	76	TYR	HB2	2.95	0.02	2
1	A	76	TYR	HB3	2.92	0.02	2
1	A	76	TYR	HD1	7.0	0.02	1
1	A	76	TYR	HE1	6.74	0.02	1
1	A	76	TYR	CA	58.13	0.30	1
1	A	76	TYR	CB	38.73	0.30	1
1	A	76	TYR	N	122.31	0.30	1
1	A	77	ARG	H	7.9	0.02	1
1	A	77	ARG	HA	4.19	0.02	1
1	A	77	ARG	HB3	1.59	0.02	1
1	A	77	ARG	HD2	3.07	0.02	1
1	A	77	ARG	HG2	1.39	0.02	1
1	A	77	ARG	CA	56.03	0.30	1
1	A	77	ARG	CB	31.03	0.30	1
1	A	77	ARG	CD	43.43	0.30	1
1	A	77	ARG	CG	27.03	0.30	1
1	A	77	ARG	N	124.51	0.30	1
1	A	78	HIS	H	8.13	0.02	1
1	A	78	HIS	HA	4.51	0.02	1
1	A	78	HIS	HB2	3.01	0.02	2
1	A	78	HIS	HB3	2.94	0.02	2
1	A	78	HIS	HD2	6.95	0.02	1
1	A	78	HIS	HE1	7.91	0.02	1
1	A	78	HIS	CA	56.33	0.30	1
1	A	78	HIS	CB	30.73	0.30	1
1	A	78	HIS	N	122.11	0.30	1
1	A	79	TYR	H	8.01	0.02	1
1	A	79	TYR	HA	4.58	0.02	1
1	A	79	TYR	HB2	3.07	0.02	2
1	A	79	TYR	HB3	2.87	0.02	2
1	A	79	TYR	HD1	7.06	0.02	1
1	A	79	TYR	HE1	6.77	0.02	1
1	A	79	TYR	CA	57.93	0.30	1
1	A	79	TYR	CB	39.13	0.30	1
1	A	79	TYR	N	123.61	0.30	1
1	A	80	SER	H	7.84	0.02	1
1	A	80	SER	HA	4.19	0.02	1
1	A	80	SER	HB2	3.8	0.02	1
1	A	80	SER	CA	60.23	0.30	1
1	A	80	SER	CB	65.13	0.30	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	80	SER	N	124.41	0.30	1

7.1.2 Chemical shift referencing [i](#)

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction $\pm$ precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	80	-0.43 ± 0.28	None needed (< 0.5 ppm)
$^{13}\text{C}_\beta$	79	0.04 ± 0.29	None needed (< 0.5 ppm)
$^{13}\text{C}'$	0	—	None (insufficient data)
^{15}N	76	-1.25 ± 0.52	Should be applied

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 38%, i.e. 675 atoms were assigned a chemical shift out of a possible 1792. 0 out of 24 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	231/600 (38%)	116/240 (48%)	59/244 (24%)	56/116 (48%)
Sidechain	428/1047 (41%)	286/677 (42%)	137/320 (43%)	5/50 (10%)
Aromatic	16/145 (11%)	16/69 (23%)	0/74 (0%)	0/2 (0%)
Overall	675/1792 (38%)	418/986 (42%)	196/638 (31%)	61/168 (36%)

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	37	LEU	CG	32.63	21.37 – 32.19	5.4
1	A	61	ALA	HB1	0.12	0.14 – 2.58	-5.1
1	A	61	ALA	HB2	0.12	0.14 – 2.58	-5.1
1	A	61	ALA	HB3	0.12	0.14 – 2.58	-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:

