



# wwPDB NMR Structure Validation Summary Report ⓘ

Apr 26, 2016 – 02:57 PM BST

PDB ID : 1J6T  
Title : COMPLEX OF ENZYME IIAMTL AND THE HISTIDINE-CONTAINING  
PHOSPHOCARRIER PROTEIN HPR FROM ESCHERICHIA COLI NMR,  
RESTRAINED REGULARIZED MEAN STRUCTURE  
Authors : Clore, G.M.; Cornilescu, G.  
Deposited on : 2002-08-14

This is a wwPDB NMR Structure Validation Summary Report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/NMRValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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

Cyrange : NOT EXECUTED  
NmrClust : NOT EXECUTED  
MolProbity : NOT EXECUTED  
Mogul : 1.7.1 (RC1), CSD as537be (2016)  
Percentile statistics : NOT EXECUTED  
RCI : NOT EXECUTED  
PANAV : NOT EXECUTED  
ShiftChecker : NOT EXECUTED  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : rb-20027457

## 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 percentiles available for this entry.

The sequence quality summary graphics cannot be shown.

## 2 Ensemble composition and analysis ⓘ

This entry contains 3 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.

Cyrange was unable to find well-defined residues.

Error message: Cyrange did not run

NmrClust was unable to cluster the ensemble.

Error message: NmrClust did not run

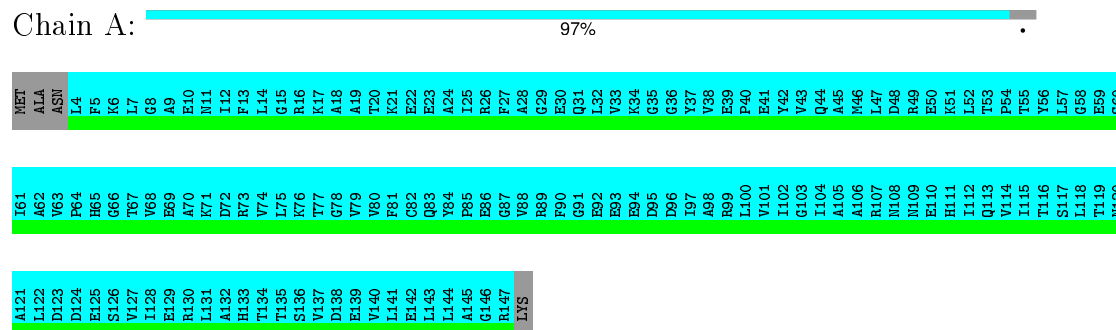
ENTRY-COMPOSITION INFOmissingINFO

## 3 Residue-property plots

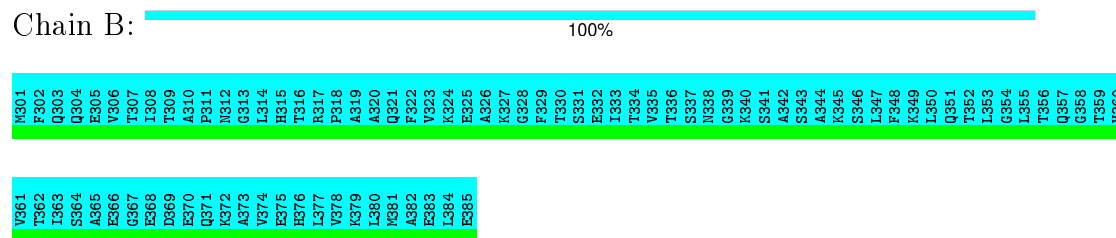
### 3.1 Average score per residue in the NMR ensemble

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: PTS SYSTEM, MANNITOL-SPECIFIC IIABC COMPONENT



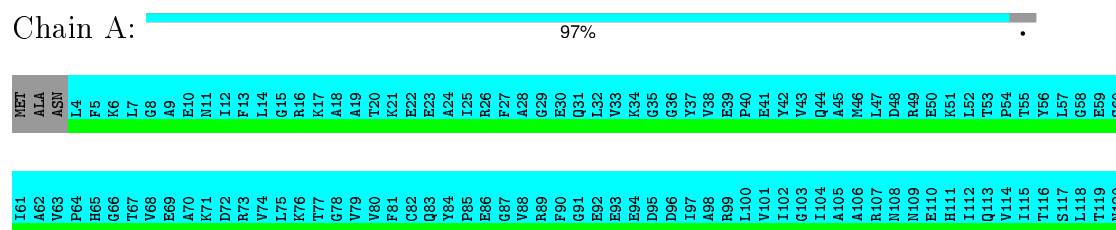
- Molecule 2: Phosphocarrier protein HPr



### 3.2 Residue scores for the first model from the NMR ensemble

No representative models were identified. Colouring as in section 3.1 above.

- Molecule 1: PTS SYSTEM, MANNITOL-SPECIFIC IIABC COMPONENT





## 4 Refinement protocol and experimental data overview

The models were refined using the following method: *CONJOINED RIGID BODY/TORSION ANGLE DYNAMICS*.

Of the 200 calculated structures, 3 were deposited, based on the following criterion: *REGULARIZED MEAN STRUCTURES*.

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

Software name	Classification	Version
X-PLOR NIH (HTTP://NMR.CIT.NIH.GOV/XPLOR NIH)	refinement	

No chemical shift data was provided. No validations of the models with respect to experimental NMR restraints is performed at this time.

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

MolProbity was not executed - this section will have to be empty.

### 5.2 Too-close contacts [i](#)

MolProbity was not executed - this section will have to be empty.

### 5.3 Torsion angles [i](#)

#### 5.3.1 Protein backbone [i](#)

MolProbity was not executed - this section will have to be empty.

#### 5.3.2 Protein sidechains [i](#)

MolProbity was not executed - this section will have to be empty.

#### 5.3.3 RNA [i](#)

MolProbity was not executed - this section will have to be empty.

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

MolProbity was not executed - this section will have to be empty.

### 5.5 Carbohydrates [i](#)

MolProbity was not executed - this section will have to be empty.

### 5.6 Ligand geometry [i](#)

MolProbity was not executed - this section will have to be empty.

### 5.7 Other polymers [i](#)

MolProbity was not executed - this section will have to be empty.

## 5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.



## 6 Chemical shift validation

No chemical shift data were provided