Full wwPDB NMR Structure Validation Report (i)

Apr 26, 2016 – 03:44 PM BST

PDB ID	:	1O2F
Title	:	COMPLEX OF ENZYME IIAGLC AND IIBGLC PHOSPHOCARRIER PROTEIN HPR FROM ESCHERICHIA COLI NMR, RESTRAINED REGULARIZED MEAN STRUCTURE
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Deposited on	:	2003-03-11

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
http://wwpdb.org/validation/2016/NMRValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) 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 (i)

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

3 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 3435 atoms, of which 1742 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called PTS system, glucose-specific IIA component.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	150	2305	729	1169	181	224	2	0

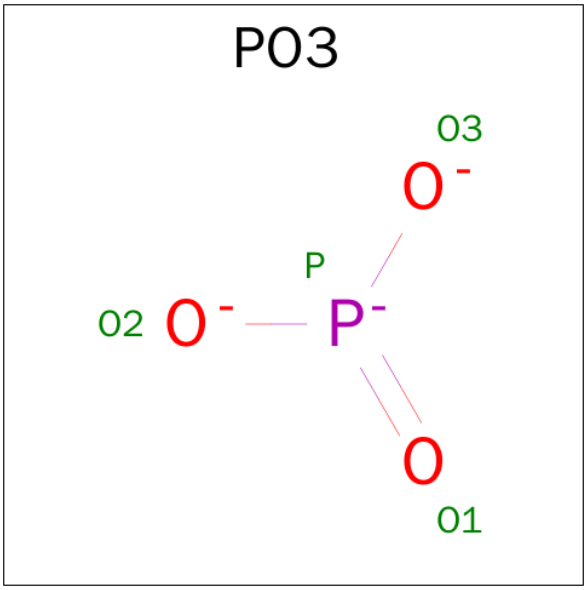
- Molecule 2 is a protein called PTS system, glucose-specific IIBC component.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
2	B	77	1130	345	573	98	111	3	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	317	ALA	PRO	SEE REMARK 999	UNP P69786

- Molecule 3 is PHOSPHITE ION (three-letter code: PO3) (formula: O_3P).



Mol	Chain	Residues	Atoms

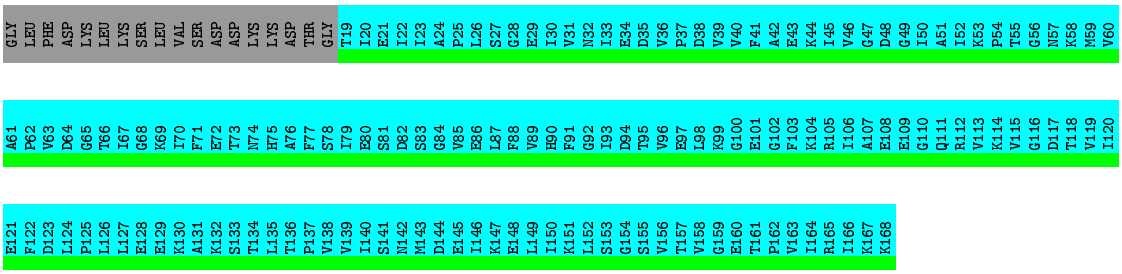
4 Residue-property plots

4.1 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.

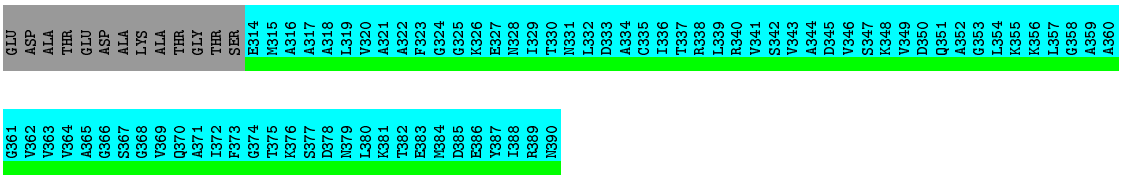
• Molecule 1: PTS system, glucose-specific IIA component

Chain A:



• Molecule 2: PTS system, glucose-specific IIBC component

Chain B:



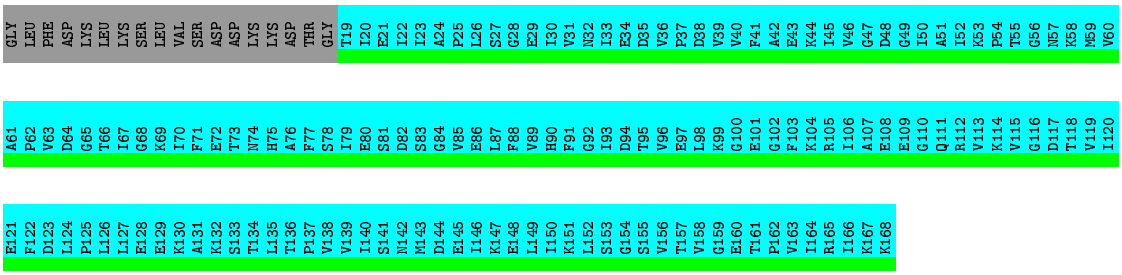
4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

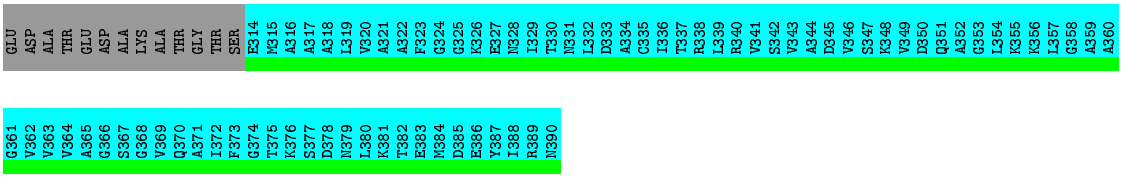
• Molecule 1: PTS system, glucose-specific IIA component

Chain A:



• Molecule 2: PTS system, glucose-specific IIBC component

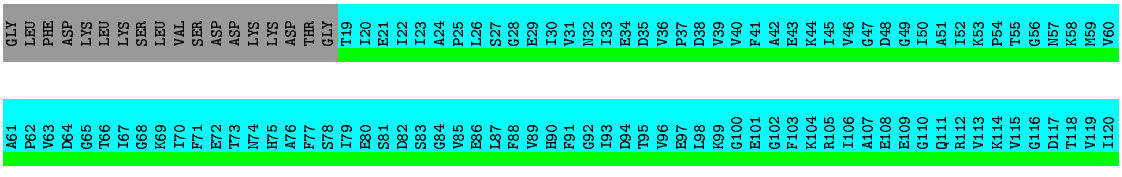
Chain B:



4.2.2 Score per residue for model 2

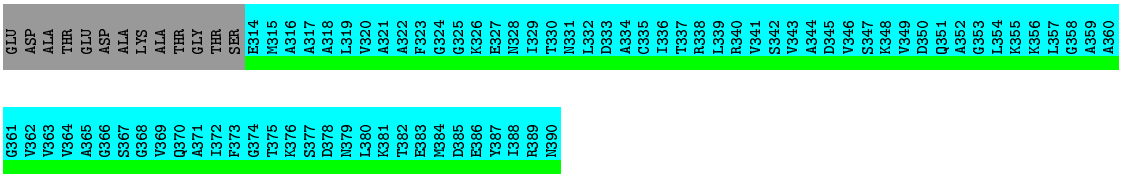
• Molecule 1: PTS system, glucose-specific IIA component

Chain A:



• Molecule 2: PTS system, glucose-specific IIBC component

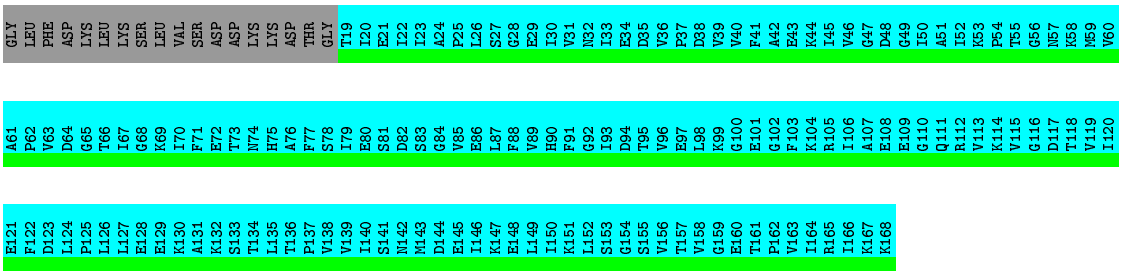
Chain B:



4.2.3 Score per residue for model 3

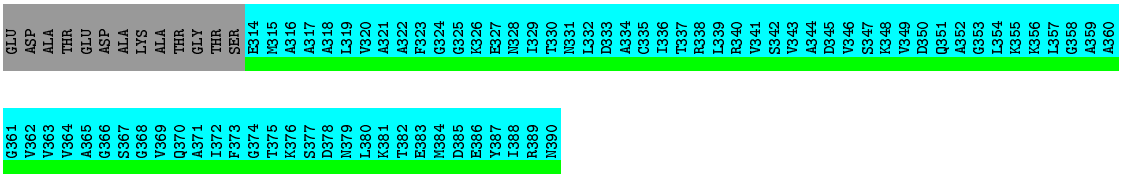
• Molecule 1: PTS system, glucose-specific IIA component

Chain A:



- Molecule 2: PTS system, glucose-specific IIBC component

Chain B:



5 Refinement protocol and experimental data overview

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

Of the 60 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	refinement	(HTTP://NMR.CIT.NIH.GOV/XPLOR_NIH)

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

6 Model quality

6.1 Standard geometry

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

6.2 Too-close contacts

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

6.3 Torsion angles

6.3.1 Protein backbone

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

6.3.2 Protein sidechains

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

6.3.3 RNA

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

6.4 Non-standard residues in protein, DNA, RNA chains

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

6.5 Carbohydrates

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

6.6 Ligand geometry

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

6.7 Other polymers

MolProbity was not executed - 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