



# wwPDB NMR Structure Validation Summary Report ⓘ

Apr 26, 2016 – 05:26 PM BST

PDB ID : 1VRC  
Title : Complex of enzyme IIAMannose and the histidine-containing phosphocarrier protein HPr from escherichia coli nmr, restrained regularized mean structure  
Authors : Clore, G.M.; Williams, D.C.  
Deposited on : 2005-02-21

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 2 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. Identification of well-defined residues and clustering analysis are not possible.

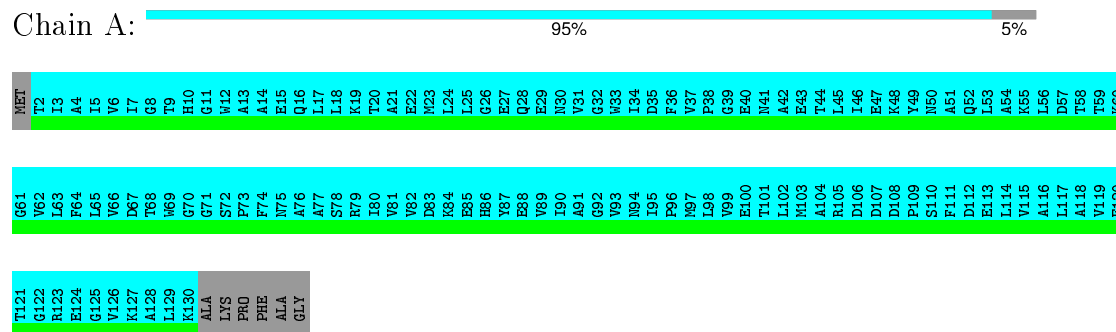
ENTRY-COMPOSITION INFOmissingINFO

## 3 Residue-property plots

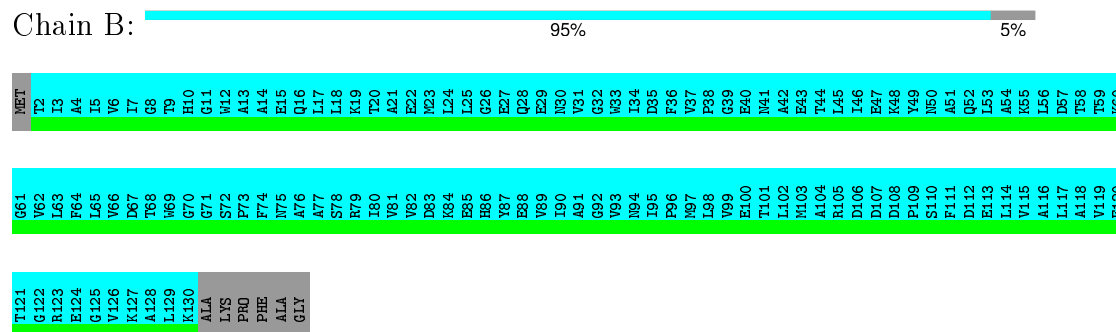
### 3.1 Average score per residue in the NMR ensemble

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.

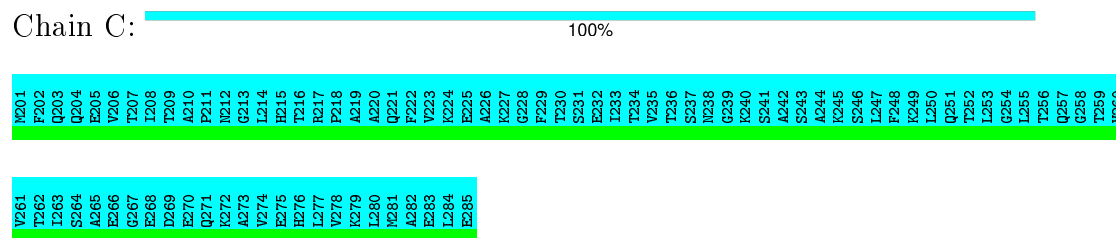
- Molecule 1: PTS system, mannose-specific IIAB component



- Molecule 1: PTS system, mannose-specific IIAB component



- Molecule 2: Phosphocarrier protein HPr



- Molecule 2: Phosphocarrier protein HPr

Chain D:  100%

V201	F202	Q203	Q204	E205	V206	T207	I208	T209	A210	Q211	N212	G213	L214	H215	T216	R217	P218	A219	A220	Q221	F222	V223	K224	E225	A226	K227	G228	F229	T230	S231	E232	I233	T234	V235	T236	S237	N238	G239	K240	S241	A242	S243	A244	K245	S246	L247	F248	K249	L250	Q251	T252	L253	G254	L255	T256	Q257	G258	T259	V260
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V261	T262	I263	S264	A265	E266	G267	E268	D269	E270	Q271	K272	A273	V274	E275	H276	L277	V278	K279	L280	M281	A282	E283	L284	E285
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### 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, mannose-specific IIAB component

Chain A:  95% 5%

ME1	T2	I3	A4	I5	V6	I7	G8	T9	H10	G11	M12	A13	A14	E15	Q16	L17	L18	K19	T20	A21	E22	M23	L24	L25	G26	E27	Q28	E29	N30	V31	G32	G33	I34	D35	F36	N37	P38	G39	E40	N41	A42	E43	T44	L45	I46	E47	K48	Y49	N50	A51	Q52	L53	A54	K55	L56	D57	T58	V59	K60
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G61	V62	L63	F64	L65	V66	D67	T68	N69	G70	G71	S72	P73	F74	N75	A76	A77	S78	R79	I80	V81	W82	D83	K84	E85	H86	I87	B88	V89	I90	A91	G92	V93	N94	I95	P96	N97	L98	V99	E100	T101	L102	M103	A104	R105	D106	D107	D108	P109	S110	F111	D112	E113	L114	V115	A116	L117	A118	V119	E120
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T121	G122	R123	E124	G125	V126	K127	A128	L129	K130	ALA	LYS	PRO	PHE	ALA	GLY
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- Molecule 1: PTS system, mannose-specific IIAB component

Chain B:  95% 5%

ME1	T2	I3	A4	I5	V6	I7	G8	T9	H10	G11	M12	A13	A14	E15	Q16	L17	L18	K19	T20	A21	E22	M23	L24	L25	G26	E27	Q28	E29	N30	V31	G32	G33	I34	D35	F36	N37	P38	G39	E40	N41	A42	E43	T44	L45	I46	E47	K48	Y49	N50	A51	Q52	L53	A54	K55	L56	D57	T58	V59	K60
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G61	V62	L63	F64	L65	V66	D67	T68	N69	G70	G71	S72	P73	F74	N75	A76	A77	S78	R79	I80	V81	W82	D83	K84	E85	H86	I87	B88	V89	I90	A91	G92	V93	N94	I95	P96	N97	L98	V99	E100	T101	L102	M103	A104	R105	D106	D107	D108	P109	S110	F111	D112	E113	L114	V115	A116	L117	A118	V119	E120
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T121	G122	R123	E124	G125	V126	K127	A128	L129	K130	ALA	LYS	PRO	PHE	ALA	GLY
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- Molecule 2: Phosphocarrier protein HPr

Chain C:  100%

V201	F202	Q203	Q204	E205	V206	T207	I208	T209	A210	Q211	N212	G213	L214	H215	T216	R217	P218	A219	A220	Q221	F222	V223	K224	E225	A226	K227	G228	F229	T230	S231	E232	I233	T234	V235	T236	S237	N238	G239	K240	S241	A242	S243	A244	K245	S246	L247	F248	K249	L250	Q251	T252	L253	G254	L255	T256	Q257	G258	T259	V260
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V261	T262	I263	S264	A265	E266	G267	E268	D269	E270	Q271	K272	A273	V274	E275	H276	L277	V278	K279	L280	M281	A282	E283	L284	E285
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- Molecule 2: Phosphocarrier protein HPr

Chain D:

100%

W261	W201
W262	W202
W263	W203
W264	W204
W265	W205
W266	W206
W267	W207
W268	W208
W269	W209
W270	W210
W271	W211
W272	W212
W273	W213
W274	W214
W275	W215
W276	W216
W277	W217
W278	W218
W279	W219
W280	W220
W281	W221
W282	W222
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W284	W224
W285	W225
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	W259
	W260

## 4 Refinement protocol and experimental data overview ⓘ

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

Of the 100 calculated structures, 2 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)
XPLOR-NIH	structure solution	

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