



Full wwPDB NMR Structure Validation Report ⓘ

Apr 26, 2016 – 05:27 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 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 ⓘ symbol.

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.

3 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 6534 atoms, of which 3284 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called PTS system, mannose-specific IIAB component.

Mol	Chain	Residues	Atoms						Trace
1	A	129	Total	C	H	N	O	S	0
			1975	632	988	160	192	3	
1	B	129	Total	C	H	N	O	S	0
			1975	632	988	160	192	3	

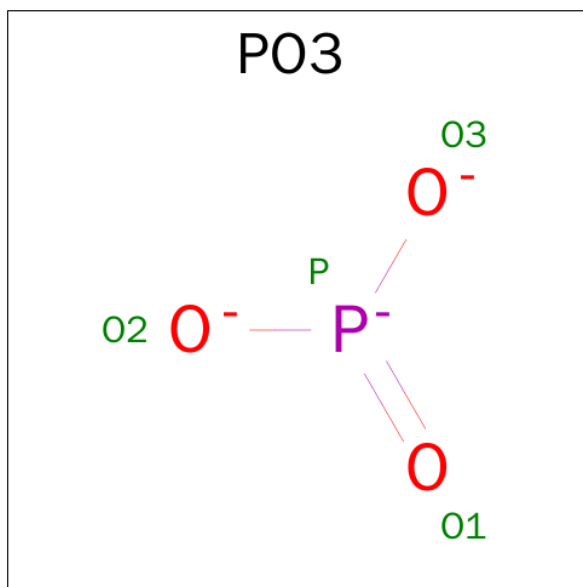
There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	INITIATING METHIONINE	UNP P69797
A	134	PHE	-	CLONING ARTIFACT	UNP P69797
A	135	ALA	-	CLONING ARTIFACT	UNP P69797
A	136	GLY	-	CLONING ARTIFACT	UNP P69797
B	1	MET	-	INITIATING METHIONINE	UNP P69797
B	134	PHE	-	CLONING ARTIFACT	UNP P69797
B	135	ALA	-	CLONING ARTIFACT	UNP P69797
B	136	GLY	-	CLONING ARTIFACT	UNP P69797

- Molecule 2 is a protein called Phosphocarrier protein HPr.

Mol	Chain	Residues	Atoms						Trace
2	C	85	Total	C	H	N	O	S	0
			1292	401	654	107	128	2	
2	D	85	Total	C	H	N	O	S	0
			1292	401	654	107	128	2	

- Molecule 3 is PHOSPHITE ION (three-letter code: PO3) (formula: O₃P).



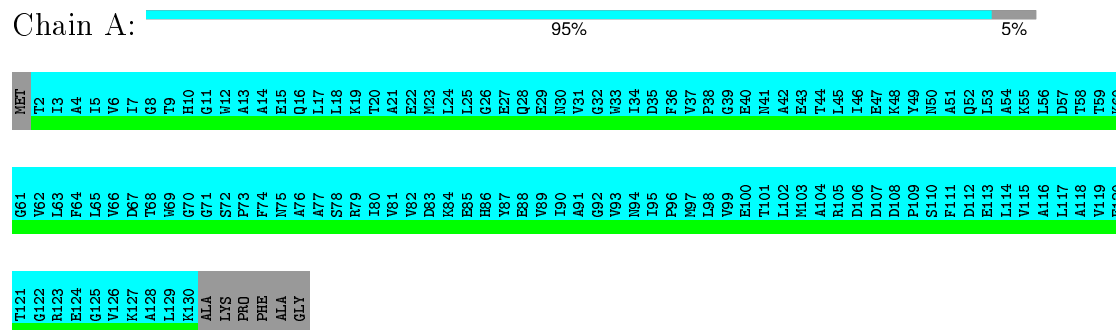
Mol	Chain	Residues	Atoms
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4 Residue-property plots

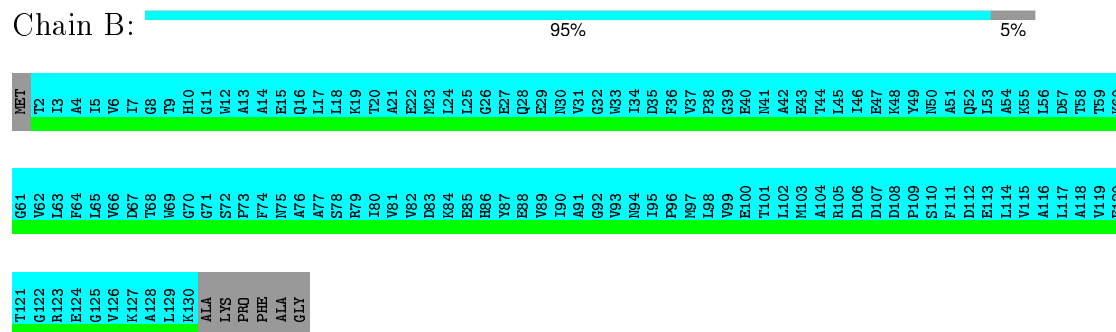
4.1 Average score per residue in the NMR ensemble

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.

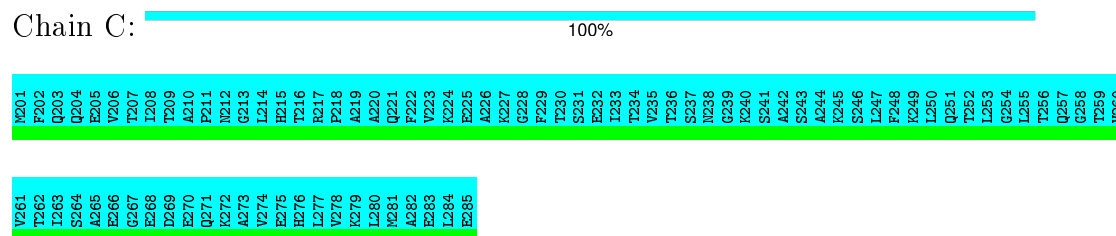
- Molecule 1: PTS system, mannose-specific IIAB component



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

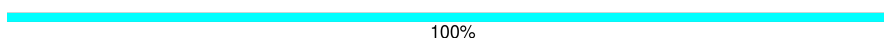


- Molecule 2: Phosphocarrier protein HPr

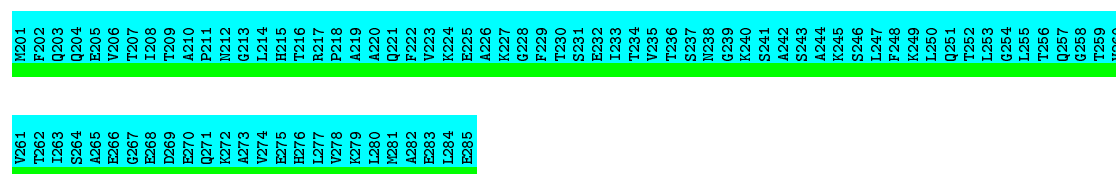


- Molecule 2: Phosphocarrier protein HPr

Chain D:



100%



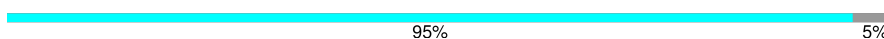
4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

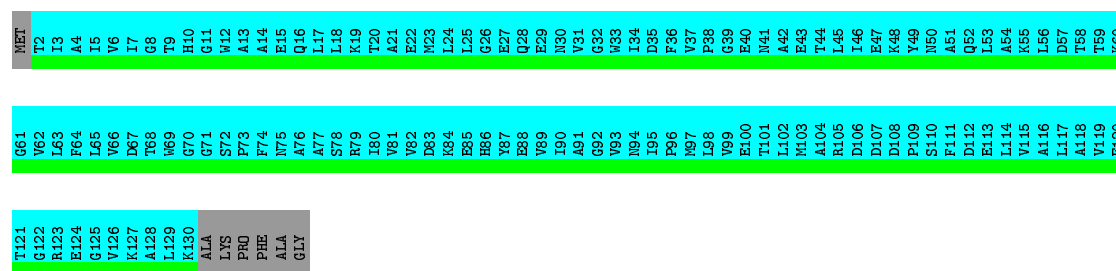
- Molecule 1: PTS system, mannose-specific IIAB component

Chain A:



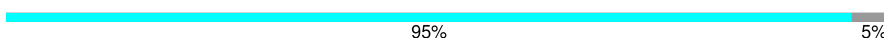
95%

5%



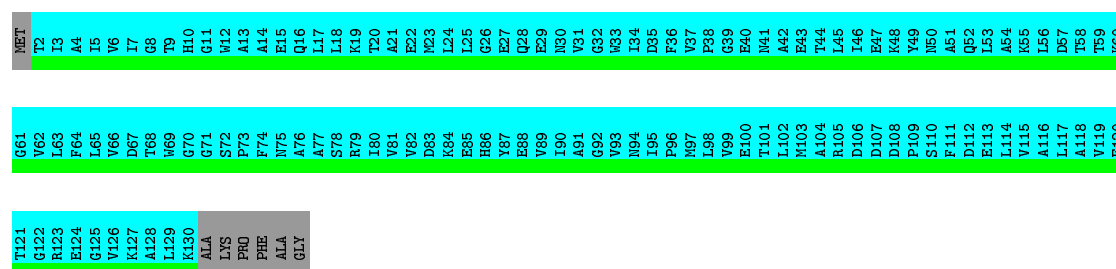
- Molecule 1: PTS system, mannose-specific IIAB component

Chain B:



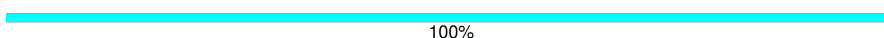
95%

5%

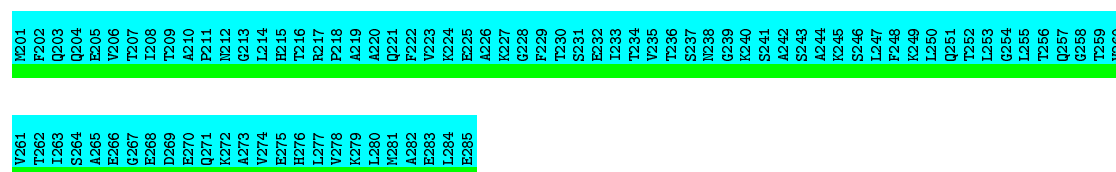


- Molecule 2: Phosphocarrier protein HPr

Chain C:



100%



- Molecule 2: Phosphocarrier protein HPr

Chain D:  100%

V201	F202	Q203	Q204	E205	V206	T207	L208	T209	A210	P211	N212	G213	L214	H215	T216	R217	P218	A219	A220	Q221	F222	V223	K224	E225	A226	K227	G228	F229	T230	S231	E232	L233	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	S263	S264	A265	E266	G267	E268	D269	E270	Q271	K272	A273	V274	E275	H276	L277	V278	K279	L280	N281	A282	E283	L284	E285
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4.2.2 Score per residue for model 2

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

Chain A:  95% 5%

MET	T2	I3	A4	I5	V6	V6	D67	G8	T9	H10	G11	W12	A13	A14	E15	Q16	L17	L18	K19	T20	A21	E22	N23	L24	L25	G26	E27	Q28	E29	N30	V31	G32	N33	I34	D35	P36	V37	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	W69	G70	G71	S72	P73	F74	N75	A76	A77	S78	R79	I80	V81	E82	D83	K84	E85	H86	I87	Q88	V89	I90	A91	G92	V93	N94	I95	P96	N97	L98	V99	E100	T101	A102	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%

MET	T2	I3	A4	I5	V6	V6	D67	G8	T9	H10	G11	W12	A13	A14	E15	Q16	L17	L18	K19	T20	A21	E22	N23	L24	L25	G26	E27	Q28	E29	N30	V31	G32	N33	I34	D35	P36	V37	P38	G39	E40	N41	A42	E43	T44	L45	I46	E47	K48	Y49	N50	A51	Q52	L53	A54	K55	L56	D57	T58	V59	E120
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G61	V62	L63	F64	L65	V66	D67	T68	W69	G70	G71	S72	P73	F74	N75	A76	A77	S78	R79	I80	V81	E82	D83	K84	E85	H86	I87	Q88	V89	I90	A91	G92	V93	N94	I95	P96	N97	L98	V99	E100	T101	A102	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	L208	T209	A210	P211	N212	G213	L214	H215	T216	R217	P218	A219	A220	Q221	F222	V223	K224	E225	A226	K227	G228	F229	T230	S231	E232	L233	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	S263	S264	A265	E266	G267	E268	D269	E270	Q271	K272	A273	V274	E275	H276	L277	V278	K279	L280	N281	A282	E283	L284	E285
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- Molecule 2: Phosphocarrier protein HPr

Chain D:

100%

V261	V262	V263	S264	A265	E266	G267	E268	D269	E270	E271	K272	K273	A274	E275	A282	E283	L284	E285	V281	V282	V283	V284	V285	V286	V287	V288	V289	V290
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5 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.

6 Model quality [i](#)

6.1 Standard geometry [i](#)

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

6.2 Too-close contacts [i](#)

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

6.3 Torsion angles [i](#)

6.3.1 Protein backbone [i](#)

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

6.3.2 Protein sidechains [i](#)

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

6.3.3 RNA [i](#)

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

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

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

6.5 Carbohydrates [i](#)

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

6.6 Ligand geometry [i](#)

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

6.7 Other polymers [i](#)

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