



Full wwPDB NMR Structure Validation Report ⓘ

Apr 26, 2016 – 02:58 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
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Deposited on : 2002-08-14

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 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 [i](#)

There are 3 unique types of molecules in this entry. The entry contains 3555 atoms, of which 1785 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called PTS SYSTEM, MANNITOL-SPECIFIC IIABC COMPONENT.

Mol	Chain	Residues	Atoms						Trace
1	A	144	Total	C	H	N	O	S	0
			2266	714	1134	196	220	2	

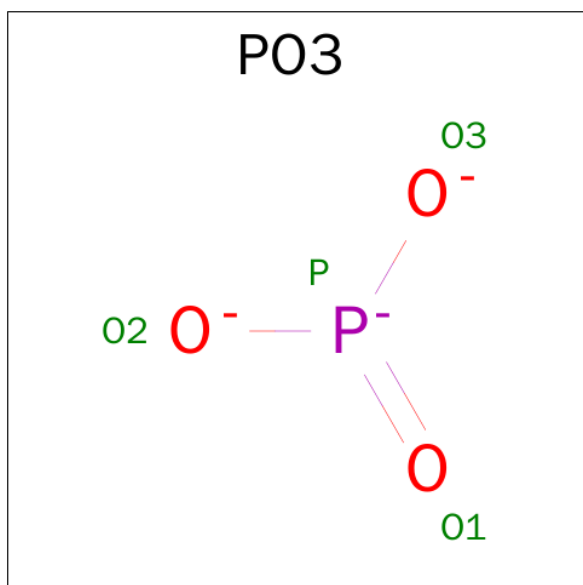
There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	INITIATING MET	UNP P00550

- Molecule 2 is a protein called Phosphocarrier protein HPr.

Mol	Chain	Residues	Atoms						Trace
2	B	85	Total	C	H	N	O	S	0
			1289	401	651	107	128	2	

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



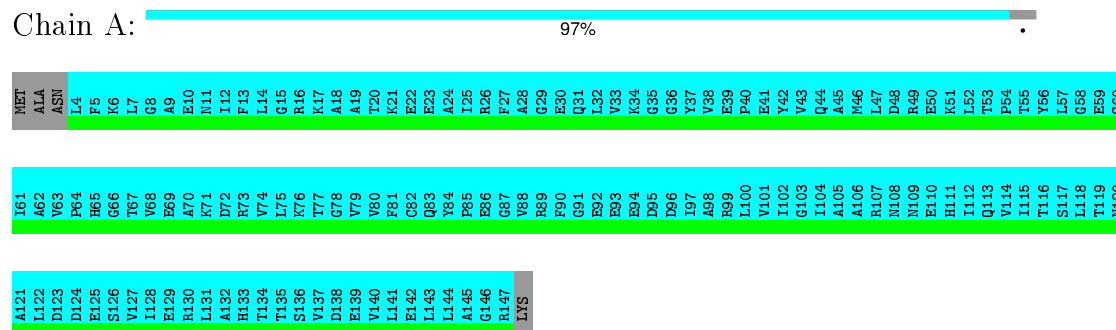
Mol	Chain	Residues	Atoms
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4 Residue-property plots

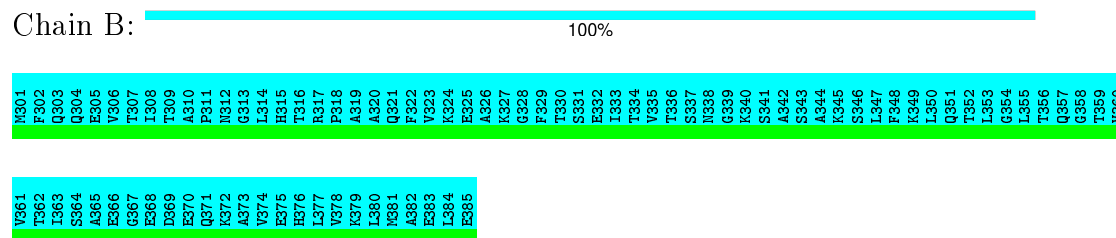
4.1 Average score per residue in the NMR ensemble

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, MANNITOL-SPECIFIC IIABC COMPONENT



- Molecule 2: Phosphocarrier protein HPr



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, MANNITOL-SPECIFIC IIABC COMPONENT



- Molecule 2: Phosphocarrier protein HPr

Chain B:  100%

F361	F362	F363	F364	F365	F366	F367	F368	F369	F370	F371	F372	F373	F374	F375	F376	F377	F378	F379	F380	F381	F382	F383	F384	F385	F386	F387	F388	F389	F390	F391	F392	F393	F394	F395	F396	F397	F398	F399	F400	F401	F402	F403	F404	F405	F406	F407	F408	F409	F410	F411	F412	F413	F414	F415	F416	F417	F418	F419	F420	F421	F422	F423	F424	F425	F426	F427	F428	F429	F430	F431	F432	F433	F434	F435	F436	F437	F438	F439	F440	F441	F442	F443	F444	F445	F446	F447	F448	F449	F450	F451	F452	F453	F454	F455	F456	F457	F458	F459	F460	F461	F462	F463	F464	F465	F466	F467	F468	F469	F470	F471	F472	F473	F474	F475	F476	F477	F478	F479	F480	F481	F482	F483	F484	F485	F486	F487	F488	F489	F490	F491	F492	F493	F494	F495	F496	F497	F498	F499	F500	F501	F502	F503	F504	F505	F506	F507	F508	F509	F510	F511	F512	F513	F514	F515	F516	F517	F518	F519	F520	F521	F522	F523	F524	F525	F526	F527	F528	F529	F530	F531	F532	F533	F534	F535	F536	F537	F538	F539	F540	F541	F542	F543	F544	F545	F546	F547	F548	F549	F550	F551	F552	F553	F554	F555	F556	F557	F558	F559	F560	F561	F562	F563	F564	F565	F566	F567	F568	F569	F570	F571	F572	F573	F574	F575	F576	F577	F578	F579	F580	F581	F582	F583	F584	F585	F586	F587	F588	F589	F590	F591	F592	F593	F594	F595	F596	F597	F598	F599	F600	F601	F602	F603	F604	F605	F606	F607	F608	F609	F610	F611	F612	F613	F614	F615	F616	F617	F618	F619	F620	F621	F622	F623	F624	F625	F626	F627	F628	F629	F630	F631	F632	F633	F634	F635	F636	F637	F638	F639	F640	F641	F642	F643	F644	F645	F646	F647	F648	F649	F650	F651	F652	F653	F654	F655	F656	F657	F658	F659	F660	F661	F662	F663	F664	F665	F666	F667	F668	F669	F670	F671	F672	F673	F674	F675	F676	F677	F678	F679	F680	F681	F682	F683	F684	F685	F686	F687	F688	F689	F690	F691	F692	F693	F694	F695	F696	F697	F698	F699	F700	F701	F702	F703	F704	F705	F706	F707	F708	F709	F710	F711	F712	F713	F714	F715	F716	F717	F718	F719	F720	F721	F722	F723	F724	F725	F726	F727	F728	F729	F730	F731	F732	F733	F734	F735	F736	F737	F738	F739	F740	F741	F742	F743	F744	F745	F746	F747	F748	F749	F750	F751	F752	F753	F754	F755	F756	F757	F758	F759	F760	F761	F762	F763	F764	F765	F766	F767	F768	F769	F770	F771	F772	F773	F774	F775	F776	F777	F778	F779	F780	F781	F782	F783	F784	F785	F786	F787	F788	F789	F790	F791	F792	F793	F794	F795	F796	F797	F798	F799	F800	F801	F802	F803	F804	F805	F806	F807	F808	F809	F810	F811	F812	F813	F814	F815	F816	F817	F818	F819	F820	F821	F822	F823	F824	F825	F826	F827	F828	F829	F830	F831	F832	F833	F834	F835	F836	F837	F838	F839	F840	F841	F842	F843	F844	F845	F846	F847	F848	F849	F850	F851	F852	F853	F854	F855	F856	F857	F858	F859	F860	F861	F862	F863	F864	F865	F866	F867	F868	F869	F870	F871	F872	F873	F874	F875	F876	F877	F878	F879	F880	F881	F882	F883	F884	F885	F886	F887	F888	F889	F890	F891	F892	F893	F894	F895	F896	F897	F898	F899	F900	F901	F902	F903	F904	F905	F906	F907	F908	F909	F910	F911	F912	F913	F914	F915	F916	F917	F918	F919	F920	F921	F922	F923	F924	F925	F926	F927	F928	F929	F930	F931	F932	F933	F934	F935	F936	F937	F938	F939	F940	F941	F942	F943	F944	F945	F946	F947	F948	F949	F950	F951	F952	F953	F954	F955	F956	F957	F958	F959	F960	F961	F962	F963	F964	F965	F966	F967	F968	F969	F970	F971	F972	F973	F974	F975	F976	F977	F978	F979	F980	F981	F982	F983	F984	F985	F986	F987	F988	F989	F990	F991	F992	F993	F994	F995	F996	F997	F998	F999	F1000
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4.2.2 Score per residue for model 2

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

Chain A: 97%

[illegible]

- Molecule 2: Phosphocarrier protein HPr

Chain B: 100%

[illegible]

4.2.3 Score per residue for model 3

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

Chain A: 97%

MET	ALA	ASN
L4	F5	K6
L7	G8	A9
E10	N11	I12
F13	L14	G15
R16	K17	A18
A19	T20	K21
E22	E23	A24
I25	R26	F27
A28	G29	E30
Q31	L32	V33
K34	G35	G36
Y37	V38	E39
P40	E41	Y42
V43	Q44	A45
M46	L47	D48
R49	E50	K51
L52	T53	P54
T55	Y56	L57
G58	E59	S60

I61	A62	V63
P64	H65	G66
T67	V68	E69
A70	K71	D72
R73	L74	L75
V76	E77	G78
V79	V80	F81
C82	Q83	W84
P85	E86	G87
W88	R89	F90
G91	E92	E93
E94	D95	D96
I97	A98	R99
L100	V101	I102
G103	I104	A105
A106	R107	M108
N109	E110	H111
I112	Q113	V114
T115	T116	S117
L118	T119	N120

A121	L122	D123
D124	E125	S126
V127	I128	E129
R130	L131	A132
H133	L134	T135
S136	V137	D138
G139	V140	F141
E142	L143	L144
A145	G146	R147
L148	L149	L150
L151	L152	L153
L154	L155	L156
L157	L158	L159
L160	L161	L162
L163	L164	L165
L166	L167	L168
L169	L170	L171
L172	L173	L174
L175	L176	L177
L178	L179	L180
L181	L182	L183
L184	L185	L186
L187	L188	L189
L190	L191	L192
L193	L194	L195
L196	L197	L198
L199	L200	L201
L202	L203	L204
L205	L206	L207
L208	L209	L210
L211	L212	L213
L214	L215	L216
L217	L218	L219
L220	L221	L222
L223	L224	L225
L226	L227	L228
L229	L230	L231
L232	L233	L234
L235	L236	L237
L238	L239	L240
L241	L242	L243
L244	L245	L246
L247	L248	L249
L250	L251	L252
L253	L254	L255
L256	L257	L258
L259	L260	L261
L262	L263	L264
L265	L266	L267
L268	L269	L270
L271	L272	L273
L274	L275	L276
L277	L278	L279
L280	L281	L282
L283	L284	L285
L286	L287	L288
L289	L290	L291
L292	L293	L294
L295	L296	L297
L298	L299	L300
L301	L302	L303
L304	L305	L306
L307	L308	L309
L310	L311	L312
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L325	L326	L327
L328	L329	L330
L331	L332	L333
L334	L335	L336
L337	L338	L339
L340	L341	L342
L343	L344	L345
L346	L347	L348
L349	L350	L351
L352	L353	L354
L355	L356	L357
L358	L359	L360

V361	T362	I363
S364	A365	E366
G367	E368	D369
E370	Q371	K372
A373	V374	E375
H376	L377	V378
K379	L380	M381
A382	E383	L384
F385		

● Molecule 2: Phosphocarrier protein HPr

Chain B: 100%

M301	F302	Q303
E305	V306	T307
I308	T309	A310
P311	N312	G313
L314	H315	T316
R317	P318	E319
A320	Q321	F322
V323	K324	E325
A326	K327	G328
F329	T330	S331
E332	I333	T334
V335	T336	S337
N338	G339	K340
S341	A342	S343
A344	K345	L347
S346	F348	K349
L350	Q351	T352
L353	G354	L355
T356	Q357	G358
T359	V360	

V361	T362	I363
S364	A365	E366
G367	E368	D369
E370	Q371	K372
A373	V374	E375
H376	L377	V378
K379	L380	M381
A382	E383	L384
F385		

5 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.

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