



Full wwPDB NMR Structure Validation Report ⓘ

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 REG-
ULARIZED MEAN STRUCTURE
Authors : Clore, G.M.; Cai, M.; Williams, D.C.
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 ⓘ 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 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
1	A	150	Total	C	H	N	O	S	0
			2305	729	1169	181	224	2	

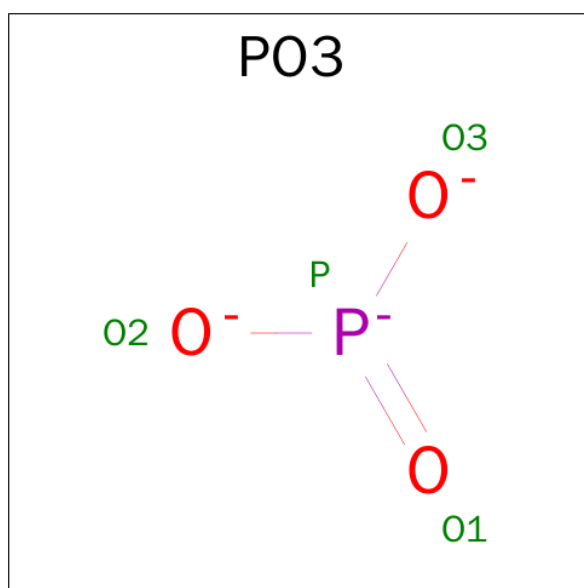
- Molecule 2 is a protein called PTS system, glucose-specific IIBC component.

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

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: O₃P).




Mol	Chain	Residues	Atoms
-----	-------	----------	-------

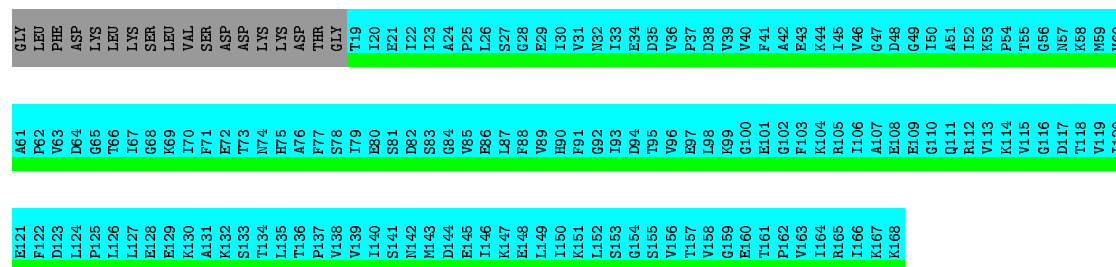
4 Residue-property plots

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.

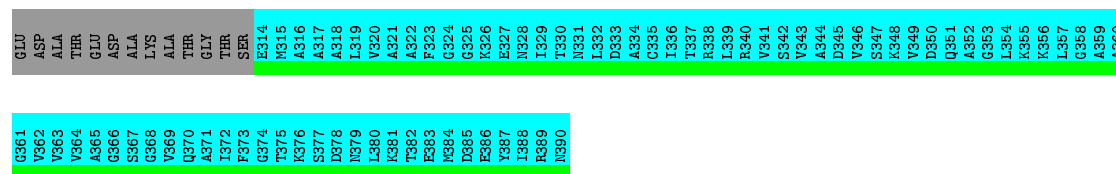
- Molecule 1: PTS system, glucose-specific IIA component

Chain A: 



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

Chain B: 

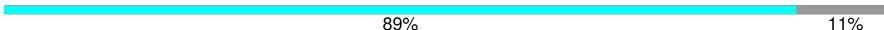


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

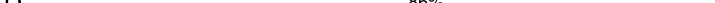
4.2.1 Score per residue for model 1

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

Chain A: 

E121	E122	D123	P124	P125	L126	L127	E128	E129	K130	A131	K132	S133	T134	L135	T136	P137	V138	V139	I140	S141	M142	M143	D144	E145	I146	K147	E148	L149	I150	K151	L152	S153	G154	S155	V156	T157	V158	E160	P160	P162	V163	I164	R165	I166	K167	K168													
A61	P62	P63	D64	G65	L66	I67	G68	K69	I70	F71	E72	T73	H74	H75	A76	F77	S78	I79	E80	S81	D82	S83	G84	H85	E86	L87	F88	V89	H90	F91	G92	I93	D94	T95	V96	E97	L98	K99	G100	E101	G102	F103	K104	R105	I106	A107	E108	E109	G110	Q111	R112	V113	K114	V115	G116	D117	T118	V119	I120
GLY	LEU	PHE	ASP	LYS	LEU	LYS	SER	LEU	VAL	ASP	ASP	LYS	LYS	ASP	THR	GLY	T19	I20	E21	I22	I23	A24	P25	L26	S27	G28	E29	I30	V31	N32	I33	E34	D35	V36	P37	D38	V39	F40	V41	A42	E43	K44	I45	V46	G47	D48	G49	A51	I52	K53	P54	T55	G56	N57	K58	M59	I60		

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

Chain B:  86% 14%

GLU	ASP	ALA	THR	GLU	ASP	ALA	LYS	ALA	THR	GLU	THR	SEN	E314	M315	A316	A317	A318	L319	V320	A321	A322	F323	G324	G325	A326	E327	N328	I329	T330	N331	L332	D333	A334	G335	L336	T337	R338	L339	R340	V341	S342	V343	A344	D345	V346	S347	K348	V349	D350	Q351	A352	G353	L354	K355	L356	L357	G358	A359	A360																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																						
G361	V362	V363	V364	A365	G366	S367	G368	V369	Q370	A371	I372	F373	G374	T375	K376	G377	D378	N379	L380	K381	T382	E383	M384	D385	E386	V387	I388	R389	N390																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																				

4.2.2 Score per residue for model 2

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

Chain A: 89% 11%

A61	GLY	T19	GLY
P62	LEU	120	
V63	PHE	E21	
D64	ASP	E21	
G65	LYS	122	
T66	LEU	123	
L67	LYS	A24	
G68	SER	124	
K69	LEU	P25	
I70	VAL	L26	
F71	SER	G28	
E72	ASP	E29	
T73	ASP	L30	
H74	LYS	V31	
M75	LYS	N32	
A76	ASP	E34	
F77	THR	D35	
S78	GLY	V36	
E79		F37	
B80		D38	
S81		V39	
D82		V40	
S83		F41	
G84		A42	
H85		K44	
B86		E45	
L87		V46	
F88		G47	
L87		D48	
F88		G49	
V89		L50	
H90		A51	
F91		E52	
G92		K53	
I93		P54	
D94		L55	
T95		N57	
V96		K58	
E97		V59	
L98		L60	
K99			
G100			
E101			
G102			
F103			
K104			
R105			
I106			
A107			
E108			
E109			
G110			
I111			
K112			
V113			
K114			
V115			
G116			
D117			
L118			
V119			
L120			

E121	F122	D123	L124	P125	L126	L127	E128	E129	K130	A131	K132	S133	L134	L135	T136	P137	V138	V139	L140	S141	M142	M143	D144	E145	L146	K147	E148	L149	L150	K151	L152	S153	G154	S155	V156	L157	V158	G159	E160	L161	T162	V163	L164	R165	L166	K167	K168
------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------

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

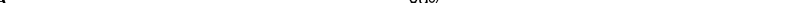
Chain B: 86% 14%

G361	GLU
V362	ASP
V363	ALA
V364	THR
A365	GLU
G366	ASP
S367	ALA
G368	LYS
V369	ALA
Q370	THR
A371	GLY
I372	THR
F373	SEN
G374	E314
T375	M315
S377	A316
D378	A317
N379	A318
L380	L319
K381	V320
T382	A321
E383	A322
M384	F323
D385	G324
E386	G325
F387	K326
I388	E327
R389	N328
N390	I329
	T330
	M331
	L332
	D333
	A334
	K335
	I336
	T337
	R338
	L339
	R340
	V341
	S342
	V343
	A344
	D345
	V346
	S347
	K348
	V349
	R350
	Q351
	A352
	G353
	L354
	K355
	G356
	L357
	G358
	A359
	A360

4.2.2. Stronger models for model 2

4.2.3 Score per residue for model 3

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

Chain A:  89% 11%

GLY	A61	E121
LEU	P62	F122
PHE	V63	D123
ASP	D64	L124
LYS	G65	P125
LEU	T66	L126
LYS	L67	L127
LEU	G68	E128
SER	R69	E129
LEU	I70	K130
VAL	F71	A131
SER	F72	K132
ASP	T73	S133
ASP	N74	T134
LYS	H75	L135
LYS	A76	T136
ASP	F77	P137
THR	S78	V138
GLY	I79	V139
T19	E80	I140
I20	S81	S141
E21	D82	N142
I22	S83	M143
I23	A84	D144
A24	V85	E145
P25	E86	I146
L26	L87	K147
S27	F88	E148
G28	H89	I149
E29	V90	I150
I30	P91	K151
V31	G92	L152
N32	I93	S153
I33	D94	G154
E34	T95	S155
D35	V96	V156
V36	E97	T157
P37	L98	V158
D38	R99	G159
V39	G100	E160
V40	E101	T161
F41	G102	P162
A42	E43	V163
E43	F103	V164
K44	K104	I164
I45	R105	R165
V46	I106	I166
G47	A107	K167
D48	E108	K168
G49	E109	
I50	G110	
A51	Q111	
I52	R112	
K53	V113	
P54	K114	
T55	V115	
G56	G116	
N57	D117	
K58	T118	
M59	V119	
V60	I120	

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

Chain B:

86%

14%

GLU	E314
ASP	M315
ALA	A316
THR	A317
GLU	A318
ASP	A319
ALA	V320
LYS	A321
ALA	A322
THR	F323
GLY	M324
THR	G325
SER	V326
E314	E327
M315	E328
A316	N328
A317	I329
A318	T330
A319	N331
V320	L332
A321	D333
A322	A334
F323	C335
M324	I336
G325	T337
V326	R338
E327	L339
E328	R340
N328	V341
I329	S342
T330	V343
N331	A344
L332	D345
D333	V346
A334	S347
C335	K348
I336	V349
T337	D350
R338	Q351
L339	A352
R340	G353
V341	L354
S342	K355
V343	K356
A344	L357
D345	G358
V346	A359
S347	A360
K348	
V349	
D350	
Q351	
A352	
G353	
L354	
K355	
K356	
L357	
G358	
A359	
A360	

G381
V382
V383
V384
A385
G386
S387
G388
V389
Q370
A371
I372
F373
G374
T375
K376
S377
D378
N379
L380
K381
T382
E383
M384
D385
E386
T387
I388
R389
N390

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 [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