Full wwPDB NMR Structure Validation Report (i)

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PDB ID	:	2JZN
Title	:	Solution NMR structure of the productive complex between IIAMannose and IIBMannose of the mannose transporter of the E. coli phosphotransferase system
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Deposited on	:	2008-01-10

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 (i)) were used in the production of this report:

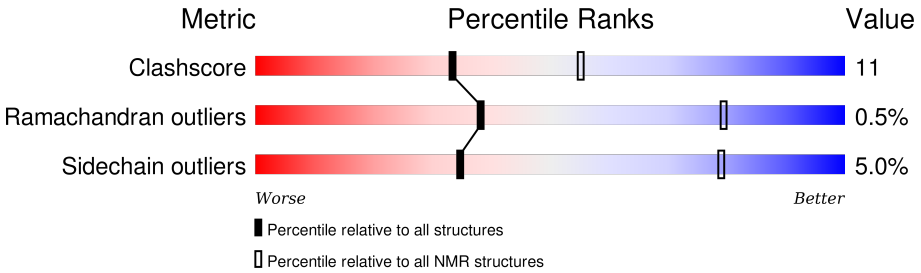
Cyrange	:	Kirchner and Güntert (2011)
NmrClust	:	Kelley et al. (1996)
MolProbity	:	4.02b-467
Mogul	:	unknown
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
ShiftChecker	:	rb-20027457
Ideal 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.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	NMR archive (#Entries)
Clashscore	114402	11133
Ramachandran outliers	111179	9975
Sidechain outliers	111093	9958

The table below summarises the geometric issues observed across the polymeric chains and their fit to the experimental data. The red, orange, yellow and green segments indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. A cyan segment indicates the fraction of residues that are not part of the well-defined cores, and a grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5%

Mol	Chain	Length	Quality of chain
1	A	133	86% 11% • •
1	B	133	86% 11% •
2	C	165	73% 24% • •

2 Ensemble composition and analysis (i)

This entry contains 1 models. Identification of well-defined residues and clustering analysis are not possible.

3 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 6705 atoms, of which 3390 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Mannose-specific phosphotransferase enzyme IIA component.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	133	2039	650	1023	163	200	3	0
1	B	133	2039	650	1023	163	200	3	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	10	GLU	HIS	ENGINEERED	UNP P69797
B	10	GLU	HIS	ENGINEERED	UNP P69797

- Molecule 2 is a protein called Mannose-specific phosphotransferase enzyme IIB component.

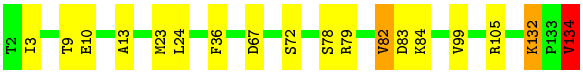
Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
2	C	165	2627	805	1344	230	242	6	0

4 Residue-property plots (i)

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.

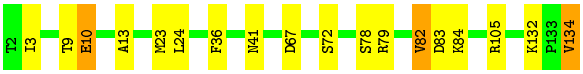
- Molecule 1: Mannose-specific phosphotransferase enzyme IIA component

Chain A:



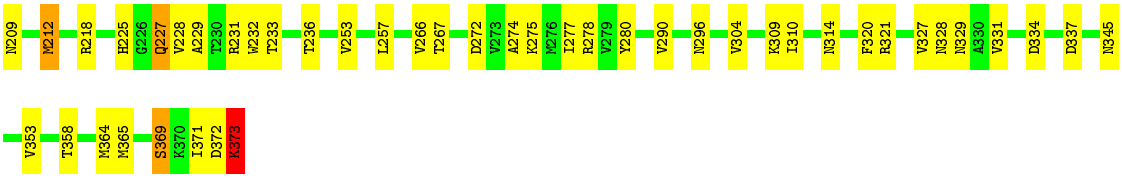
- Molecule 1: Mannose-specific phosphotransferase enzyme IIA component

Chain B:



- Molecule 2: Mannose-specific phosphotransferase enzyme IIB component

Chain C:



5 Refinement protocol and experimental data overview (i)

The models were refined using the following method: *conjoined rigid body/torsion angle simulated annealing.*

Of the 120 calculated structures, 1 were deposited, based on the following criterion: *restrained regularized mean.*

The following table shows the software used for structure solution, optimisation and refinement.

Software name	Classification	Version
X-PLOR NIH	structure solution	2.18.1
X-PLOR NIH	refinement	2.18.1

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)

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the (average) root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#Z>5	RMSZ	#Z>5
1	A	0.76	1/1033 (0.1%)	0.83	0/1404 (0.0%)
1	B	0.91	2/1033 (0.2%)	0.85	1/1404 (0.1%)
2	C	1.19	2/1297 (0.2%)	0.91	0/1751 (0.0%)
All	All	0.99	5/3363 (0.1%)	0.86	1/4559 (0.0%)

All bond outliers are listed below. They are sorted according to the Z-score.

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	10	GLU	CB-CG	16.18	1.82	1.52
2	C	373	LYS	C-O	15.54	1.52	1.23
2	C	373	LYS	C-OXT	13.51	1.49	1.23
1	B	134	VAL	C-OXT	9.06	1.40	1.23
1	A	134	VAL	C-OXT	9.00	1.40	1.23

All angle outliers are listed below.

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	10	GLU	CA-CB-CG	-6.73	98.60	113.40

There are no chirality outliers.

There are no planarity outliers.

6.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in each chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes averaged over the ensemble.

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	A	1016	1023	1019	19

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Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	B	1016	1023	1019	18
2	C	1283	1344	1341	49
All	All	3315	3390	3379	73

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 11.

All clashes are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Clash(Å)	Distance(Å)
1:B:10:GLU:CG	1:B:10:GLU:CB	1.52	1.82
2:C:373:LYS:HA	2:C:373:LYS:NZ	1.16	1.54
1:A:10:GLU:OE1	1:B:24:LEU:HD21	0.90	1.67
2:C:373:LYS:HZ3	2:C:373:LYS:HA	0.90	1.23
1:A:24:LEU:HD21	1:B:10:GLU:OE1	0.86	1.69
2:C:218:ARG:NH1	2:C:228:VAL:HG12	0.85	1.87
1:B:10:GLU:CG	1:B:10:GLU:CA	0.83	2.56
2:C:274:ALA:O	2:C:277:ILE:HG22	0.75	1.82
2:C:373:LYS:CE	2:C:373:LYS:HA	0.72	2.14
2:C:209:ASN:ND2	2:C:309:LYS:NZ	0.71	2.39
1:A:10:GLU:OE1	1:B:24:LEU:CD2	0.71	2.37
1:A:24:LEU:CD2	1:B:10:GLU:OE1	0.70	2.38
2:C:227:GLN:NE2	2:C:227:GLN:H	0.68	1.86
2:C:272:ASP:OD1	2:C:275:LYS:N	0.62	2.23
2:C:353:VAL:CG2	2:C:364:MET:SD	0.61	2.88
2:C:233:THR:HG21	2:C:266:VAL:HG21	0.61	1.71
2:C:373:LYS:NZ	2:C:373:LYS:CA	0.58	2.50
2:C:209:ASN:HD21	2:C:309:LYS:NZ	0.57	1.96
2:C:334:ASP:OD1	2:C:337:ASP:N	0.57	2.32
2:C:227:GLN:CD	2:C:227:GLN:N	0.57	2.58
1:B:78:SER:O	1:B:82:VAL:HG13	0.57	2.00
2:C:373:LYS:HA	2:C:373:LYS:HZ2	0.57	1.51
1:A:78:SER:O	1:A:82:VAL:HG13	0.57	2.00
2:C:225:HIS:CE1	2:C:228:VAL:HG21	0.56	2.35
2:C:218:ARG:HH12	2:C:228:VAL:HG12	0.56	1.60
2:C:212:MET:SD	2:C:290:VAL:CG2	0.56	2.94
1:A:132:LYS:HD3	2:C:257:LEU:HD11	0.55	1.76
1:B:79:ARG:O	1:B:82:VAL:HG22	0.55	2.02
1:A:99:VAL:HG11	2:C:227:GLN:CG	0.54	2.32
2:C:212:MET:SD	2:C:290:VAL:HG21	0.54	2.42
2:C:231:ARG:NH2	2:C:358:THR:CG2	0.54	2.71
1:B:9:THR:HG21	1:B:13:ALA:HB3	0.54	1.78
1:A:79:ARG:O	1:A:82:VAL:HG22	0.54	2.02

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Atom-1	Atom-2	Clash(Å)	Distance(Å)
2:C:320:PHE:CG	2:C:321:ARG:N	0.54	2.76
2:C:209:ASN:ND2	2:C:309:LYS:HZ2	0.54	2.01
1:B:10:GLU:CD	1:B:10:GLU:CB	0.53	2.73
1:A:24:LEU:HD21	1:B:10:GLU:CD	0.52	2.25
1:B:3:ILE:O	1:B:105:ARG:HD2	0.52	2.05
1:A:10:GLU:CD	1:B:24:LEU:HD21	0.50	2.26
2:C:227:GLN:N	2:C:227:GLN:NE2	0.50	2.58
1:A:9:THR:HG21	1:A:13:ALA:HB3	0.50	1.84
1:A:3:ILE:O	1:A:105:ARG:HD2	0.50	2.05
2:C:345:ASN:OD1	2:C:345:ASN:O	0.49	2.29
1:A:67:ASP:OD1	1:A:67:ASP:N	0.49	2.43
1:A:134:VAL:HG12	2:C:253:VAL:HG22	0.49	1.84
1:B:67:ASP:N	1:B:67:ASP:OD1	0.48	2.43
2:C:272:ASP:OD1	2:C:275:LYS:CB	0.48	2.62
2:C:369:SER:O	2:C:373:LYS:C	0.47	2.52
1:A:24:LEU:CG	1:B:10:GLU:OE1	0.47	2.62
2:C:232:TRP:O	2:C:236:THR:HG23	0.47	2.08
2:C:232:TRP:CH2	2:C:314:ASN:ND2	0.47	2.82
2:C:345:ASN:OD1	2:C:345:ASN:C	0.47	2.52
2:C:320:PHE:CD1	2:C:321:ARG:N	0.46	2.84
2:C:304:VAL:CG2	2:C:310:ILE:HD12	0.46	2.40
2:C:218:ARG:HH11	2:C:228:VAL:HG12	0.45	1.68
2:C:209:ASN:HD21	2:C:309:LYS:HZ3	0.45	1.55
2:C:328:ASN:OD1	2:C:329:ASN:N	0.45	2.44
2:C:296:ASN:OD1	2:C:296:ASN:O	0.44	2.34
2:C:229:ALA:O	2:C:233:THR:OG1	0.44	2.30
2:C:218:ARG:NH1	2:C:228:VAL:CG1	0.44	2.73
2:C:345:ASN:HD22	2:C:365:MET:HG3	0.43	1.73
1:A:10:GLU:OE1	1:B:24:LEU:CG	0.43	2.67
1:A:132:LYS:CD	2:C:257:LEU:HD11	0.43	2.44
1:B:41:ASN:OD1	1:B:41:ASN:C	0.42	2.58
2:C:228:VAL:O	2:C:232:TRP:CD1	0.42	2.72
2:C:372:ASP:O	2:C:373:LYS:C	0.42	2.54
2:C:373:LYS:HZ3	2:C:373:LYS:CA	0.41	2.12
2:C:280:TYR:C	2:C:280:TYR:CD1	0.41	2.94
1:A:36:PHE:C	1:A:36:PHE:CD1	0.41	2.94
2:C:327:VAL:HG22	2:C:331:VAL:O	0.41	2.15
1:B:36:PHE:C	1:B:36:PHE:CD1	0.41	2.93
1:A:99:VAL:HG11	2:C:227:GLN:HG2	0.41	1.92
2:C:327:VAL:HG12	2:C:371:ILE:CD1	0.40	2.47

6.3 Torsion angles (i)

6.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all NMR entries. The Analysed column shows the number of residues for which the backbone conformation was analysed and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	131/133 (98%)	129 (98%)	1 (1%)	1 (1%)	29	74
1	B	131/133 (98%)	129 (98%)	1 (1%)	1 (1%)	29	74
2	C	163/165 (99%)	155 (95%)	8 (5%)	0 (0%)	100	100
All	All	425/431 (99%)	413 (97%)	10 (2%)	2 (0%)	38	79

All 2 Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type
1	B	82	VAL
1	A	82	VAL

6.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all NMR entries. The Analysed column shows the number of residues for which the sidechain conformation was analysed and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	107/107 (100%)	101 (94%)	6 (6%)	31	76
1	B	107/107 (100%)	101 (94%)	6 (6%)	31	76
2	C	143/143 (100%)	137 (96%)	6 (4%)	41	84
All	All	357/357 (100%)	339 (95%)	18 (5%)	35	79

All 18 residues with a non-rotameric sidechain are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type
1	B	84	LYS
1	A	132	LYS
2	C	369	SER

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Mol	Chain	Res	Type
1	B	72	SER
1	A	83	ASP
1	B	83	ASP
1	B	132	LYS
2	C	212	MET
2	C	278	ARG
1	B	134	VAL
2	C	373	LYS
1	A	23	MET
1	A	84	LYS
1	A	134	VAL
1	B	23	MET
2	C	267	THR
2	C	227	GLN
1	A	72	SER

6.3.3 RNA (i)

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

6.5 Carbohydrates (i)

There are no carbohydrates in this entry.

6.6 Ligand geometry (i)

There are no ligands in this entry.

6.7 Other polymers (i)

There are no such molecules in this entry.

6.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

7 Chemical shift validation (i)

No chemical shift data were provided