Full wwPDB NMR Structure Validation Report (i)

Dec 18, 2023 – 09:36 AM EST

PDB ID	:	1VSQ
Title	:	Solution NMR structure of the productive complex between IIAMannose and IIBMannose of the mannose transporter of the E. coli phosphotransferase system
Authors	:	Clore, G.M.; Hu, J.; Hu, K.
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
https://www.wwpdb.org/validation/2017/NMRValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

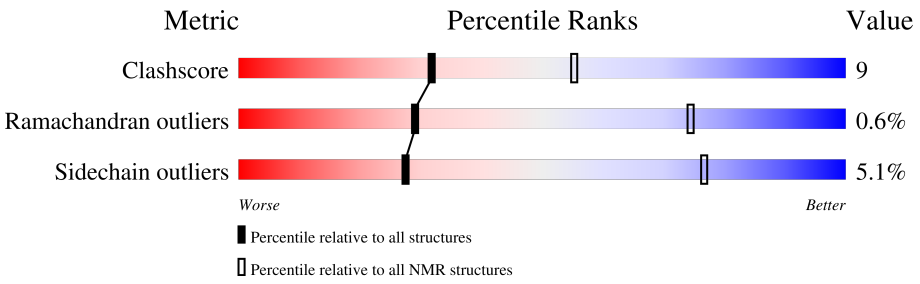
SOFTWARE-VERSIONS INFOmissingINFO

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	158937	12864
Ramachandran outliers	154571	11451
Sidechain outliers	154315	11428

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	89% 9% • •
1	B	133	89% 9% •
2	C	165	73% 24% • •

2 Ensemble composition and analysis (i)

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 (i)

There are 2 unique types of molecules in this entry. The entry contains 6713 atoms, of which 3392 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	P	S	
1	A	133	2041	651	1024	165	198		3	0
1	B	133	2045	651	1024	165	201	1	3	0

- 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

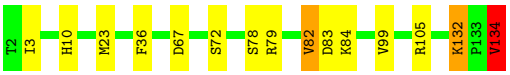
4 Residue-property plots (i)

4.1 Average score per residue in the NMR ensemble

These plots are provided for all protein, RNA, DNA and oligosaccharide 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.

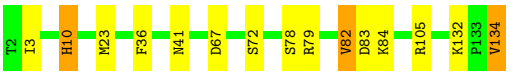
• Molecule 1: Mannose-specific phosphotransferase enzyme IIA component

Chain A:



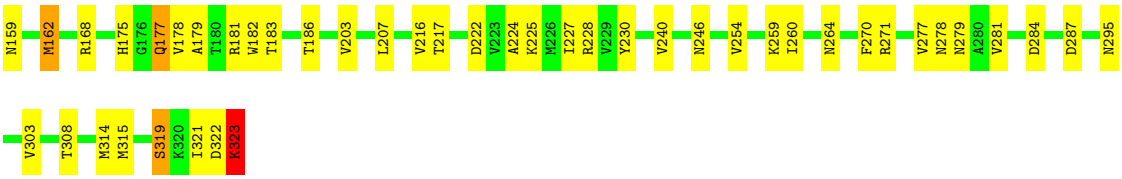
• Molecule 1: Mannose-specific phosphotransferase enzyme IIA component

Chain B:



• Molecule 2: Mannose-specific phosphotransferase enzyme IIB component

Chain C:



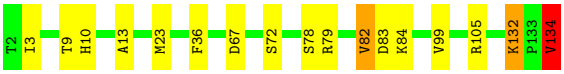
4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

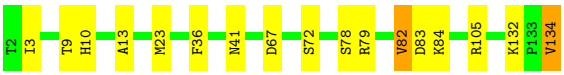
• Molecule 1: Mannose-specific phosphotransferase enzyme IIA component

Chain A:



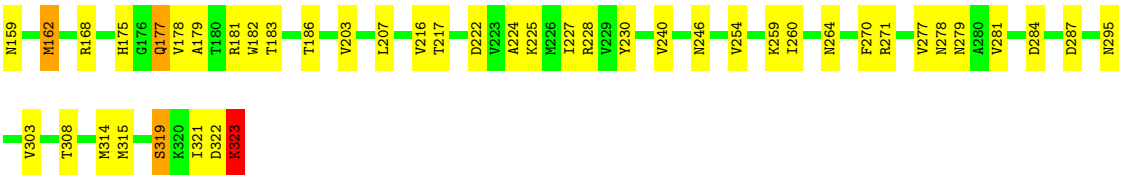
• Molecule 1: Mannose-specific phosphotransferase enzyme IIA component

Chain B:



• Molecule 2: Mannose-specific phosphotransferase enzyme IIB component

Chain C:



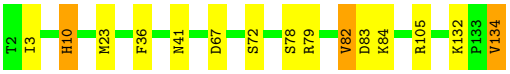
4.2.2 Score per residue for model 2

• 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, 2 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.

6 Model quality (i)

6.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: NEP

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	0.77±0.01	1±0/1023 (0.1± 0.0%)	0.82±0.00	0±0/1389 (0.0± 0.0%)
1	B	0.77±0.01	1±0/1023 (0.1± 0.0%)	0.82±0.00	0±0/1389 (0.0± 0.0%)
2	C	1.19±0.00	2±0/1297 (0.2± 0.0%)	0.91±0.00	0±0/1751 (0.0± 0.0%)
All	All	0.95	8/6686 (0.1%)	0.85	0/9058 (0.0%)

All unique bond outliers are listed below. They are sorted according to the Z-score of the worst occurrence in the ensemble.

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
2	C	323	LYS	C-O	15.54	1.52	1.23	1	2
2	C	323	LYS	C-OXT	13.51	1.49	1.23	1	2
1	B	134	VAL	C-OXT	9.06	1.40	1.23	1	2
1	A	134	VAL	C-OXT	9.00	1.40	1.23	1	2

There are no bond-angle outliers.

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	1017	1024	1018	11±1
1	B	1021	1024	1018	8±0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes
2	C	1283	1345	1341	50±1
All	All	6642	6785	6754	127

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 9.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:C:323:LYS:HA	2:C:323:LYS:NZ	1.16	1.54	1	2
2:C:323:LYS:HA	2:C:323:LYS:HZ3	0.90	1.23	1	2
2:C:168:ARG:NH1	2:C:178:VAL:HG12	0.85	1.87	1	2
1:B:10:NEP:P	1:B:10:NEP:NE2	0.75	2.60	2	1
2:C:224:ALA:O	2:C:227:ILE:HG22	0.75	1.82	1	2
1:B:10:NEP:P	2:C:175:HIS:ND1	0.74	2.60	2	1
2:C:323:LYS:HA	2:C:323:LYS:CE	0.72	2.14	1	2
2:C:159:ASN:ND2	2:C:259:LYS:NZ	0.71	2.39	1	2
2:C:177:GLN:NE2	2:C:177:GLN:H	0.68	1.86	1	2
2:C:222:ASP:OD1	2:C:225:LYS:N	0.62	2.23	1	2
2:C:303:VAL:CG2	2:C:314:MET:SD	0.61	2.88	1	2
2:C:183:THR:HG21	2:C:216:VAL:HG21	0.61	1.71	1	2
1:A:10:NEP:ND1	1:A:67:ASP:OD2	0.59	2.36	1	2
2:C:323:LYS:NZ	2:C:323:LYS:CA	0.58	2.50	1	2
1:A:132:LYS:HD3	2:C:207:LEU:HD11	0.57	1.76	2	2
2:C:159:ASN:HD21	2:C:259:LYS:NZ	0.57	1.96	1	2
2:C:284:ASP:OD1	2:C:287:ASP:N	0.57	2.32	1	2
2:C:177:GLN:N	2:C:177:GLN:CD	0.57	2.58	1	2
1:B:78:SER:O	1:B:82:VAL:HG13	0.57	2.00	1	2
1:A:78:SER:O	1:A:82:VAL:HG13	0.57	2.00	1	2
2:C:323:LYS:HA	2:C:323:LYS:HZ2	0.57	1.51	1	2
2:C:175:HIS:CE1	2:C:178:VAL:HG21	0.56	2.35	1	2
2:C:168:ARG:HH12	2:C:178:VAL:HG12	0.56	1.60	1	2
2:C:162:MET:SD	2:C:240:VAL:CG2	0.56	2.94	1	2
1:B:79:ARG:O	1:B:82:VAL:HG22	0.55	2.02	1	2
1:A:99:VAL:HG11	2:C:177:GLN:CG	0.54	2.32	1	2
2:C:162:MET:SD	2:C:240:VAL:HG21	0.54	2.42	1	2
2:C:181:ARG:NH2	2:C:308:THR:CG2	0.54	2.71	1	2
1:B:9:THR:HG21	1:B:13:ALA:HB3	0.54	1.78	1	1
1:A:79:ARG:O	1:A:82:VAL:HG22	0.54	2.02	1	2
2:C:270:PHE:CG	2:C:271:ARG:N	0.54	2.76	1	2
2:C:159:ASN:ND2	2:C:259:LYS:HZ2	0.54	2.01	1	2
1:B:3:ILE:O	1:B:105:ARG:HD2	0.52	2.05	1	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:9:THR:HG21	1:A:13:ALA:HB3	0.50	1.84	1	1
2:C:177:GLN:NE2	2:C:177:GLN:N	0.50	2.58	1	2
1:A:3:ILE:O	1:A:105:ARG:HD2	0.50	2.05	1	2
2:C:295:ASN:O	2:C:295:ASN:OD1	0.49	2.29	1	2
1:A:67:ASP:N	1:A:67:ASP:OD1	0.49	2.43	1	2
1:A:134:VAL:HG12	2:C:203:VAL:HG22	0.49	1.84	1	2
1:B:67:ASP:OD1	1:B:67:ASP:N	0.48	2.43	1	2
2:C:222:ASP:OD1	2:C:225:LYS:CB	0.48	2.62	1	2
2:C:319:SER:O	2:C:323:LYS:C	0.47	2.52	1	2
2:C:182:TRP:O	2:C:186:THR:HG23	0.47	2.08	1	2
2:C:182:TRP:CH2	2:C:264:ASN:ND2	0.47	2.82	1	2
2:C:295:ASN:OD1	2:C:295:ASN:C	0.47	2.52	1	2
2:C:175:HIS:O	2:C:175:HIS:CG	0.47	2.68	2	1
2:C:270:PHE:CD1	2:C:271:ARG:N	0.46	2.84	1	2
2:C:254:VAL:CG2	2:C:260:ILE:HD12	0.46	2.40	1	2
2:C:168:ARG:HH11	2:C:178:VAL:HG12	0.45	1.68	1	2
2:C:159:ASN:HD21	2:C:259:LYS:HZ3	0.45	1.55	1	2
2:C:278:ASN:OD1	2:C:279:ASN:N	0.45	2.44	1	2
2:C:246:ASN:O	2:C:246:ASN:OD1	0.44	2.34	1	2
2:C:179:ALA:O	2:C:183:THR:OG1	0.44	2.30	1	2
2:C:168:ARG:NH1	2:C:178:VAL:CG1	0.44	2.73	1	2
2:C:295:ASN:HD22	2:C:315:MET:HG3	0.43	1.73	1	2
2:C:172:ARG:O	2:C:174:ILE:N	0.43	2.51	2	1
1:A:132:LYS:CD	2:C:207:LEU:HD11	0.43	2.44	1	1
1:B:41:ASN:OD1	1:B:41:ASN:C	0.42	2.58	1	2
2:C:178:VAL:O	2:C:182:TRP:CD1	0.42	2.72	1	2
2:C:322:ASP:O	2:C:323:LYS:C	0.42	2.54	1	2
2:C:230:TYR:CD1	2:C:230:TYR:C	0.41	2.94	1	2
2:C:323:LYS:HZ3	2:C:323:LYS:CA	0.41	2.12	1	2
1:A:36:PHE:CD1	1:A:36:PHE:C	0.41	2.94	1	2
1:B:36:PHE:CD1	1:B:36:PHE:C	0.41	2.93	1	2
2:C:277:VAL:HG22	2:C:281:VAL:O	0.41	2.15	1	2
1:A:99:VAL:HG11	2:C:177:GLN:HG2	0.41	1.92	1	2
2:C:277:VAL:HG12	2:C:321:ILE:CD1	0.40	2.47	1	2

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	130/133 (98%)	128±0 (98±0%)	1±0 (1±0%)	1±0 (1±0%)	24	71
1	B	130/133 (98%)	128±0 (98±0%)	1±0 (1±0%)	1±0 (1±0%)	24	71
2	C	163/165 (99%)	155±0 (95±0%)	8±0 (5±0%)	0±0 (0±0%)	44	80
All	All	846/862 (98%)	822 (97%)	19 (2%)	5 (1%)	29	74

All 3 unique Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	A	82	VAL	2
1	B	82	VAL	2
2	C	173	LEU	1

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	106/106 (100%)	100±0 (94±0%)	6±0 (6±0%)	24	73
1	B	106/106 (100%)	100±0 (94±0%)	6±0 (6±0%)	24	73
2	C	143/143 (100%)	137±0 (96±0%)	6±0 (4±0%)	33	82
All	All	710/710 (100%)	674 (95%)	36 (5%)	27	77

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

Mol	Chain	Res	Type	Models (Total)
1	A	23	MET	2
1	A	72	SER	2
1	A	83	ASP	2
1	A	84	LYS	2
1	A	132	LYS	2
1	A	134	VAL	2
1	B	23	MET	2

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Mol	Chain	Res	Type	Models (Total)
1	B	72	SER	2
1	B	83	ASP	2
1	B	84	LYS	2
1	B	132	LYS	2
1	B	134	VAL	2
2	C	162	MET	2
2	C	177	GLN	2
2	C	217	THR	2
2	C	228	ARG	2
2	C	319	SER	2
2	C	323	LYS	2

6.3.3 RNA (i)

There are no RNA molecules in this entry.

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

2 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds for which Mogul statistics could be retrieved, the number of bonds that are observed in the model and the number of bonds that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length is the number of standard deviations the observed value is removed from the expected value. A bond length with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the average root-mean-square of all Z scores of the bond lengths.

Mol	Type	Chain	Res	Link	Bond lengths		
					Counts	RMSZ	#Z>2
1	NEP	B	10	1	10,14,15	1.58±0.04	2±0 (20±0%)
1	NEP	A	10	1	5,10,15	0.66±0.03	0±0 (0±0%)

In the following table, the Counts columns list the number of angles for which Mogul statistics could be retrieved, the number of angles that are observed in the model and the number of angles that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond angle is the number of standard deviations the observed value is removed from the expected value. A bond angle with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the average root-mean-square of all Z scores of the bond angles.

Mol	Type	Chain	Res	Link	Bond angles		
					Counts	RMSZ	#Z>2
1	NEP	B	10	1	5,20,22	2.33±0.48	2±2 (50±30%)
1	NEP	A	10	1	3,12,22	0.46±0.14	0±0 (0±0%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	NEP	A	10	1	-	0±0,5,6,14	0±0,1,1,1
1	NEP	B	10	1	-	0±0,5,12,14	0±0,1,1,1

All unique bond outliers are listed below. They are sorted according to the Z-score of the worst occurrence in the ensemble.

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
1	B	10	NEP	P-O1P	3.13	1.48	1.54	1	2
1	B	10	NEP	P-O2P	3.10	1.48	1.54	1	2

All unique angle outliers are listed below. They are sorted according to the Z-score of the worst occurrence in the ensemble.

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
1	B	10	NEP	O1P-P-O2P	3.41	119.98	106.57	2	1
1	B	10	NEP	O1P-P-O3P	3.04	120.01	113.44	2	1
1	B	10	NEP	O2P-P-O3P	3.03	120.00	113.44	2	1
1	B	10	NEP	CB-CA-C	2.83	106.17	111.47	2	2

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

6.5 Carbohydrates (i)

There are no monosaccharides 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