Full wwPDB NMR Structure Validation Report (i)

Apr 21, 2024 – 03:32 PM EDT

PDB ID	:	2KNO
Title	:	NMR Solution Structure of SH2 Domain of the Human Tensin Like C1 Domain Containing Phosphatase (TENC1)
Authors	:	Chen, L.; Feng, R.; Liu, C.; Zhu, G.
Deposited on	:	2009-08-27

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.

The following versions of software and data (see references (i)) were used in the production of this report:

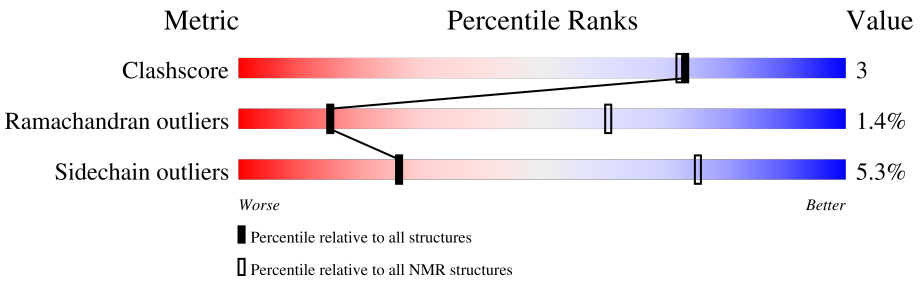
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
wwPDB-RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
wwPDB-ShiftChecker	:	v1.2
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

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	131	79% 6% 15%

2 Ensemble composition and analysis (i)

This entry contains 20 models. Model 7 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *lowest energy*.

The following residues are included in the computation of the global validation metrics.

Well-defined (core) protein residues			
Well-defined core	**Residue range (total)**	**Backbone RMSD (Å)**	**Medoid model**
1	A:18-A:128 (111)	1.04	7

Ill-defined regions of proteins are excluded from the global statistics.

Ligands and non-protein polymers are included in the analysis.

The models can be grouped into 2 clusters and 4 single-model clusters were found.

Cluster number	Models
1	3, 5, 6, 7, 8, 9, 10, 11, 13, 14, 15, 16, 17, 19
2	2, 12
Single-model clusters	1; 4; 18; 20

3 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 2028 atoms, of which 1012 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Tensin-like C1 domain-containing phosphatase.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	131	2028	650	1012	183	179	4	0

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	expression tag	UNP Q63HR2
A	2	HIS	-	expression tag	UNP Q63HR2
A	3	HIS	-	expression tag	UNP Q63HR2
A	4	HIS	-	expression tag	UNP Q63HR2
A	5	HIS	-	expression tag	UNP Q63HR2
A	6	HIS	-	expression tag	UNP Q63HR2
A	7	HIS	-	expression tag	UNP Q63HR2
A	8	SER	-	expression tag	UNP Q63HR2
A	9	SER	-	expression tag	UNP Q63HR2
A	10	GLY	-	expression tag	UNP Q63HR2
A	11	LEU	-	expression tag	UNP Q63HR2
A	12	VAL	-	expression tag	UNP Q63HR2
A	13	PRO	-	expression tag	UNP Q63HR2
A	14	ARG	-	expression tag	UNP Q63HR2
A	15	GLY	-	expression tag	UNP Q63HR2
A	16	SER	-	expression tag	UNP Q63HR2

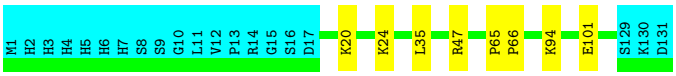
4 Residue-property plots (i)

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: Tensin-like C1 domain-containing phosphatase

Chain A: 79% 6% 15%



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

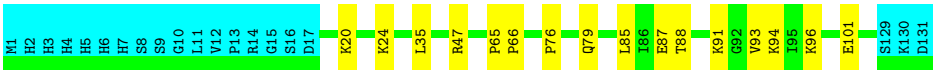
• Molecule 1: Tensin-like C1 domain-containing phosphatase

Chain A: 70% 13% • 15%

4.2.2 Score per residue for model 2

• Molecule 1: Tensin-like C1 domain-containing phosphatase

Chain A: 73% 12% 15%



4.2.3 Score per residue for model 3

- Molecule 1: Tensin-like C1 domain-containing phosphatase

Chain A: 73% 11% • 15%

M1 H2 H3 H4 H5 H6 H7 S8 S9 G10 L11 V12 P13 R14 G15 S16 D17 W22 Y23 K24 S28 Q31 K39 I46 R47 P65 P66 A69 G74 Q79 K94 E101 Q113 R126 S129 K130 D131

4.2.4 Score per residue for model 4

- Molecule 1: Tensin-like C1 domain-containing phosphatase

Chain A: 72% 11% • 15%

M1 H2 H3 H4 H5 H6 H7 S8 S9 G10 L11 V12 P13 R14 G15 S16 D17 F21 K24 L27 L35 K39 R47 P65 P66 G74 R82 L85 K94 S100 E101 P102 A109 Q113 S129 K130 D131

4.2.5 Score per residue for model 5

- Molecule 1: Tensin-like C1 domain-containing phosphatase

Chain A: 77% 7% • 15%

M1 H2 H3 H4 H5 H6 H7 S8 S9 G10 L11 V12 P13 R14 G15 S16 D17 K20 K24 P65 P66 E87 K94 I95 K96 Y103 H114 P118 S129 K130 D131

4.2.6 Score per residue for model 6

- Molecule 1: Tensin-like C1 domain-containing phosphatase

Chain A: 76% 8% 15%

M1 H2 H3 H4 H5 H6 H7 S8 S9 G10 L11 V12 P13 R14 G15 S16 D17 K20 F21 W22 L35 I46 P65 P66 A69 Q79 K94 E101 I119 S129 K130 D131

4.2.7 Score per residue for model 7 (medoid)

- Molecule 1: Tensin-like C1 domain-containing phosphatase

Chain A: 75% 8% • 15%

M1 H2 H3 H4 H5 H6 H7 S8 S9 G10 L11 V12 P13 R14 G15 S16 D17 K20 K24 P65 P66 E87 K91 K94 I95 K96 E101 L110 R126 I127 P128 S129 K130 D131

4.2.8 Score per residue for model 8

- Molecule 1: Tensin-like C1 domain-containing phosphatase

Chain A: 72% 13% 15%

4.2.9 Score per residue for model 9

- Molecule 1: Tensin-like C1 domain-containing phosphatase

Chain A: 73% 11% 15%

4.2.10 Score per residue for model 10

- Molecule 1: Tensin-like C1 domain-containing phosphatase

Chain A: 76% 9% 15%

4.2.11 Score per residue for model 11

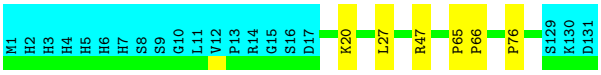
- Molecule 1: Tensin-like C1 domain-containing phosphatase

Chain A: 75% 10% 15%

4.2.12 Score per residue for model 12

- Molecule 1: Tensin-like C1 domain-containing phosphatase

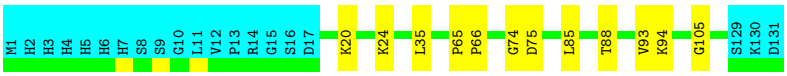
Chain A: 80% 5% 15%



4.2.13 Score per residue for model 13

• Molecule 1: Tensin-like C1 domain-containing phosphatase

Chain A: 76% 9% 15%



4.2.14 Score per residue for model 14

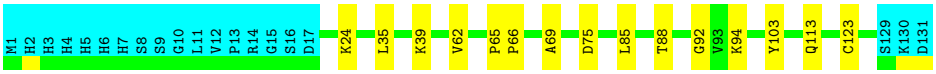
• Molecule 1: Tensin-like C1 domain-containing phosphatase

Chain A: 75% 9% • 15%

4.2.15 Score per residue for model 15

• Molecule 1: Tensin-like C1 domain-containing phosphatase

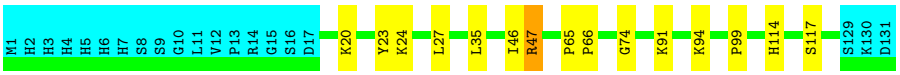
Chain A: 73% 11% 15%



4.2.16 Score per residue for model 16

• Molecule 1: Tensin-like C1 domain-containing phosphatase

Chain A: 73% 11% • 15%



4.2.17 Score per residue for model 17

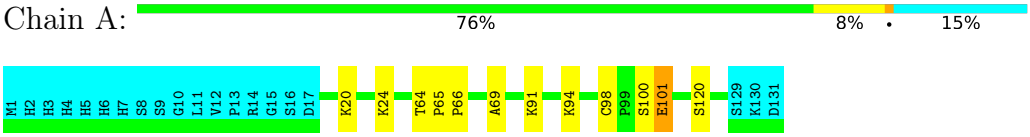
• Molecule 1: Tensin-like C1 domain-containing phosphatase

Chain A: 76% 9% 15%

4.2.18 Score per residue for model 18

- Molecule 1: Tensin-like C1 domain-containing phosphatase

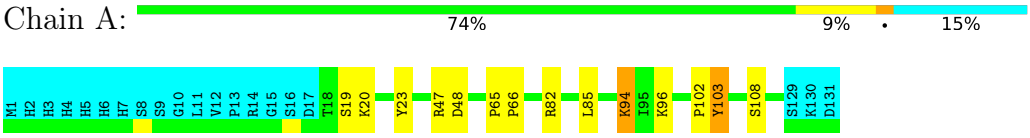
Chain A:



4.2.19 Score per residue for model 19

- Molecule 1: Tensin-like C1 domain-containing phosphatase

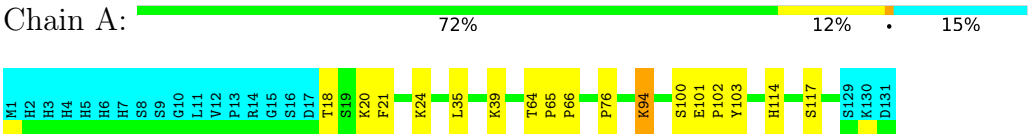
Chain A:



4.2.20 Score per residue for model 20

- Molecule 1: Tensin-like C1 domain-containing phosphatase

Chain A:



5 Refinement protocol and experimental data overview (i)

The models were refined using the following method: *water refine*.

Of the 200 calculated structures, 20 were deposited, based on the following criterion: *structures with the least restraint violations*.

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

Software name	Classification	Version
CNS	refinement	
CNS	structure solution	
CYANA	structure solution	

No chemical shift data was provided.

6 Model quality (i)

6.1 Standard geometry (i)

There are no covalent bond-length or bond-angle outliers.

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	Chirality	Planarity
1	A	0.0±0.0	0.1±0.5
All	All	0	3

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

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

Mol	Chain	Res	Type	Group	Models (Total)
1	A	126	ARG	Sidechain	2
1	A	82	ARG	Sidechain	1

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	857	872	872	6±2
All	All	17140	17440	17440	113

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 3.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:94:LYS:HG2	1:A:103:TYR:CD2	0.60	2.31	19	2
1:A:66:PRO:HG2	1:A:69:ALA:HB2	0.56	1.76	14	4
1:A:88:THR:HB	1:A:93:VAL:HG12	0.56	1.78	1	4
1:A:95:ILE:O	1:A:101:GLU:HG3	0.55	2.02	7	1
1:A:98:CYS:SG	1:A:101:GLU:HB2	0.53	2.44	9	1
1:A:65:PRO:HD2	1:A:66:PRO:HD2	0.53	1.81	15	18
1:A:65:PRO:N	1:A:66:PRO:HD3	0.52	2.18	1	1
1:A:94:LYS:HG2	1:A:103:TYR:CE2	0.52	2.38	19	1
1:A:65:PRO:CD	1:A:66:PRO:HD2	0.51	2.36	3	18
1:A:98:CYS:SG	1:A:119:ILE:HG22	0.50	2.47	1	1
1:A:87:GLU:O	1:A:93:VAL:HA	0.50	2.07	9	2
1:A:109:ALA:O	1:A:113:GLN:HG2	0.49	2.07	4	1
1:A:98:CYS:SG	1:A:100:SER:HB3	0.49	2.48	18	1
1:A:101:GLU:OE2	1:A:119:ILE:HB	0.48	2.08	6	1
1:A:88:THR:HA	1:A:92:GLY:O	0.48	2.08	9	2
1:A:93:VAL:HG12	1:A:105:GLY:H	0.48	1.69	13	1
1:A:101:GLU:HB2	1:A:102:PRO:HD3	0.48	1.86	4	1
1:A:86:ILE:CG2	1:A:93:VAL:HB	0.48	2.38	1	1
1:A:39:LYS:HE2	1:A:39:LYS:HA	0.48	1.85	4	1
1:A:114:HIS:CD2	1:A:118:PRO:HA	0.47	2.44	5	1
1:A:65:PRO:N	1:A:66:PRO:HD2	0.47	2.25	9	8
1:A:98:CYS:SG	1:A:120:SER:HB3	0.46	2.50	9	2
1:A:28:SER:HB2	1:A:31:GLN:OE1	0.46	2.10	3	1
1:A:79:GLN:HE21	1:A:79:GLN:HA	0.46	1.69	3	1
1:A:94:LYS:HB2	1:A:100:SER:OG	0.46	2.11	20	1
1:A:23:TYR:HA	1:A:46:ILE:O	0.45	2.11	16	1
1:A:27:LEU:O	1:A:47:ARG:HD2	0.45	2.12	12	4
1:A:91:LYS:N	1:A:91:LYS:HD3	0.45	2.26	7	1
1:A:87:GLU:OE1	1:A:96:LYS:HE2	0.45	2.12	7	1
1:A:35:LEU:O	1:A:39:LYS:HG2	0.44	2.12	15	1
1:A:65:PRO:HD2	1:A:66:PRO:CD	0.44	2.42	10	1
1:A:76:PRO:O	1:A:80:LEU:HG	0.44	2.12	1	1
1:A:104:PHE:CD2	1:A:110:LEU:HB3	0.44	2.48	17	1
1:A:18:THR:HA	1:A:21:PHE:CD2	0.44	2.47	20	1
1:A:44:PHE:CD1	1:A:125:LEU:HD11	0.44	2.48	8	1
1:A:82:ARG:HA	1:A:82:ARG:NE	0.44	2.28	19	2
1:A:126:ARG:O	1:A:128:PRO:HD3	0.43	2.13	7	1
1:A:101:GLU:N	1:A:102:PRO:HD2	0.43	2.29	20	1
1:A:87:GLU:CD	1:A:96:LYS:HE2	0.43	2.34	2	1
1:A:22:TRP:CZ3	1:A:46:ILE:HD12	0.43	2.49	3	2
1:A:95:ILE:HB	1:A:101:GLU:OE2	0.43	2.13	8	1
1:A:88:THR:HB	1:A:93:VAL:HG23	0.43	1.90	13	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:27:LEU:O	1:A:47:ARG:HG3	0.43	2.13	16	1
1:A:113:GLN:HG2	1:A:114:HIS:H	0.42	1.73	8	1
1:A:62:VAL:HG22	1:A:80:LEU:O	0.42	2.14	8	1
1:A:87:GLU:OE2	1:A:96:LYS:HE2	0.42	2.15	5	1
1:A:62:VAL:HB	1:A:123:CYS:SG	0.42	2.55	15	1
1:A:114:HIS:HA	1:A:117:SER:O	0.41	2.15	16	2
1:A:47:ARG:HG3	1:A:48:ASP:O	0.41	2.14	19	1
1:A:86:ILE:HA	1:A:94:LYS:O	0.41	2.16	8	1
1:A:19:SER:O	1:A:23:TYR:HB3	0.41	2.16	19	1
1:A:65:PRO:HA	1:A:82:ARG:NH2	0.41	2.31	11	1
1:A:113:GLN:HA	1:A:113:GLN:OE1	0.41	2.16	15	1
1:A:91:LYS:N	1:A:91:LYS:HD2	0.40	2.31	2	1
1:A:79:GLN:OE1	1:A:79:GLN:HA	0.40	2.16	1	1
1:A:97:GLY:O	1:A:99:PRO:HD3	0.40	2.16	10	1

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	111/131 (85%)	101±3 (91±3%)	8±3 (8±2%)	2±1 (1±1%)	15	61
All	All	2220/2620 (85%)	2021 (91%)	168 (8%)	31 (1%)	15	61

All 11 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	101	GLU	7
1	A	74	GLY	6
1	A	76	PRO	4
1	A	102	PRO	3
1	A	103	TYR	3
1	A	100	SER	2
1	A	75	ASP	2
1	A	51	SER	1

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Mol	Chain	Res	Type	Models (Total)
1	A	118	PRO	1
1	A	99	PRO	1
1	A	69	ALA	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	95/113 (84%)	90±2 (95±2%)	5±2 (5±2%)	26 75
All	All	1900/2260 (84%)	1800 (95%)	100 (5%)	26 75

All 19 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	94	LYS	18
1	A	20	LYS	17
1	A	24	LYS	15
1	A	35	LEU	11
1	A	85	LEU	7
1	A	47	ARG	6
1	A	64	THR	5
1	A	91	LYS	4
1	A	79	GLN	3
1	A	39	LYS	3
1	A	110	LEU	3
1	A	121	LEU	1
1	A	113	GLN	1
1	A	61	LYS	1
1	A	18	THR	1
1	A	73	LYS	1
1	A	83	HIS	1
1	A	101	GLU	1
1	A	96	LYS	1

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 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