wwPDB NMR Structure Validation Summary Report (i)

Oct 16, 2021 – 09:47 PM EDT

PDB ID	:	1T3K
Title	:	NMR structure of a CDC25-like dual-specificity tyrosine phosphatase of Arabidopsis thaliana
Authors	:	Landrieu, I.; da Costa, M.; De Veylder, L.; Dewitte, F.; Vandepoele, K.; Hassan, S.; Wieruszeski, J.M.; Faure, J.D.; Inze, D.; Lippens, G.
Deposited on	:	2004-04-27

This is a wwPDB NMR Structure Validation Summary 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 following versions of software and data (see references (i)) were used in the production of this report:

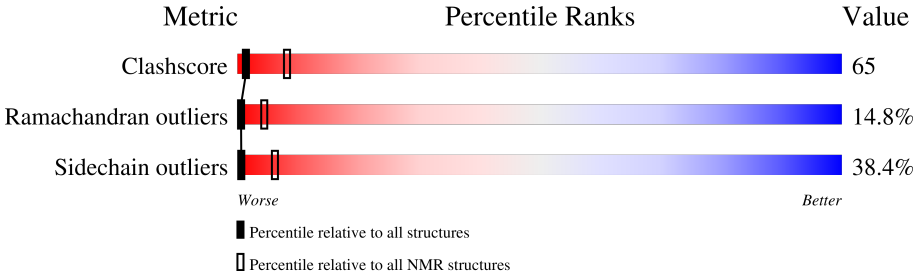
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
ShiftChecker	:	2.23.2
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.23.2

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	152	8% 61% 16% • 13%

2 Ensemble composition and analysis (i)

This entry contains 20 models. Model 20 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:1-A:129 (129)	1.43	20

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

3 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 2059 atoms, of which 1026 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Dual-specificity tyrosine phosphatase.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	132	2058	639	1026	190	195	8	0

There are 21 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	cloning artifact	UNP Q8GY31
A	-18	GLY	-	cloning artifact	UNP Q8GY31
A	-17	SER	-	cloning artifact	UNP Q8GY31
A	-16	SER	-	cloning artifact	UNP Q8GY31
A	-15	HIS	-	cloning artifact	UNP Q8GY31
A	-14	HIS	-	cloning artifact	UNP Q8GY31
A	-13	HIS	-	cloning artifact	UNP Q8GY31
A	-12	HIS	-	cloning artifact	UNP Q8GY31
A	-11	HIS	-	cloning artifact	UNP Q8GY31
A	-10	HIS	-	cloning artifact	UNP Q8GY31
A	-9	SER	-	cloning artifact	UNP Q8GY31
A	-8	SER	-	cloning artifact	UNP Q8GY31
A	-7	GLY	-	cloning artifact	UNP Q8GY31
A	-6	LEU	-	cloning artifact	UNP Q8GY31
A	-5	VAL	-	cloning artifact	UNP Q8GY31
A	-4	PRO	-	cloning artifact	UNP Q8GY31
A	-3	ARG	-	cloning artifact	UNP Q8GY31
A	-2	GLY	-	cloning artifact	UNP Q8GY31
A	-1	SER	-	cloning artifact	UNP Q8GY31
A	0	HIS	-	cloning artifact	UNP Q8GY31
A	72	SER	CYS	engineered mutation	UNP Q8GY31

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	
			Total	Zn
2	A	1	1	1

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: Dual-specificity tyrosine phosphatase

Chain A: 8% 61% 16% • 13%

MET GLY SER SER HIS HIS HIS HIS HIS HIS HIS HIS SER SER GLY LEU VAL PRO ARG GLY SER HIS M1 A2 M3 A4 R5 S6 I7 S8 Y9 I10 T11 S12 T13 Q14 L15 L16 P17 L18 H19 R20 R21 P22 N23 I24 A25 I26 I27 D28 V29 R30 D31 E32 N35 Y36 D37 G38 H39 I40 A41

G42 S43 L44 H45 Y46 A47 S48 G49 S50 F51 D52 D53 K54 I55 S56 H57 L58 V59 Q60 N61 V62 K63 D64 K65 D66 T67 L68 V69 F70 H71 S72 A73 L74 S75 Q76 V77 R78 G79 P80 T81 C82 A83 R84 R85 L86 V87 N88 Y89 L90 D91 E92 K93 K94 E95 D96 T97 G98 I99 K100 N101

I102 M103 I104 L105 E106 R107 G108 F109 N110 G111 W112 E113 A114 S115 G116 K117 P118 V119 C120 R121 C122 A123 E124 V125 P126 C127 K128 G129 D130 C131 A132

4.2 Residue scores for the representative (medoid) model from the NMR ensemble

The representative model is number 20. Colouring as in section 4.1 above.

• Molecule 1: Dual-specificity tyrosine phosphatase

Chain A: 20% 38% 23% • • 13%

MET GLY SER SER HIS HIS HIS HIS HIS HIS HIS HIS SER SER GLY LEU VAL PRO ARG GLY SER HIS M1 A4 R5 S6 I7 S8 Y9 I10 T11 S12 T13 Q14 L15 L16 P17 L18 H19 R20 R21 P22 N23 I24 A25 I26 I27 R30 D31 E32 E33 R34 N35 Y36 D37 G38 H39 I40 A41 G42

S43 Y46 A47 F51 D52 I55 S56 V59 Q60 N61 V62 K63 D64 K65 D66 T67 L68 V69 F70 H71 S72 A73 L74 S75 Q76 V77 R78 G79 P80 T81 C82 A83 R84 R85 N88 Y89 L90 D91 E92 K93 K94 E95 I99 K100 M103 I104 L105 E106 R107 G108 F109 N110 G111

W112 E113 A114 S115 G116 K117 P118 V119 C120 R121 C122 A123 E124 V125 P126 C127 K128 G129 D130 C131 A132

5 Refinement protocol and experimental data overview (i)

The models were refined using the following method: *distance geometry simulated annealing*.

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	structure solution	1.1
CNS	refinement	1.1

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: ZN

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

There are no bond-length outliers.

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	1012	1012	1010	132±13
All	All	20260	20240	20199	2633

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 65.

5 of 1573 unique clashes are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:69:VAL:HG22	1:A:105:LEU:HD22	1.10	1.12	2	1
1:A:23:ASN:O	1:A:67:THR:OG1	1.08	1.69	7	2
1:A:7:ILE:HD12	1:A:104:ILE:HG21	1.04	1.26	3	1
1:A:10:ILE:HB	1:A:14:GLN:HG2	1.01	1.32	13	3
1:A:10:ILE:HD13	1:A:18:LEU:HD13	1.00	1.31	20	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	128/152 (84%)	84±4 (65±3%)	26±5 (20±4%)	19±2 (15±2%)	0 4
All	All	2560/3040 (84%)	1670 (65%)	512 (20%)	378 (15%)	0 4

5 of 65 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	71	HIS	17
1	A	77	VAL	17
1	A	120	CYS	17
1	A	123	ALA	16
1	A	31	ASP	15

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	111/130 (85%)	68±5 (62±4%)	43±5 (38±4%)	0 6
All	All	2220/2600 (85%)	1368 (62%)	852 (38%)	0 6

5 of 103 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	88	ASN	20
1	A	99	ILE	18
1	A	97	THR	16
1	A	104	ILE	16
1	A	46	TYR	16

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)

Of 1 ligands modelled in this entry, 1 is monoatomic - leaving 0 for Mogul analysis.

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