wwPDB NMR Structure Validation Summary Report

May 7, 2024 – 04:05 pm BST

PDB ID	:	1W4E
Title	:	Peripheral-subunit binding domains from mesophilic, thermophilic, and hyper-thermophilic bacteria fold by ultrafast, apparently two-state transitions
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Deposited on	:	2004-07-23

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 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:

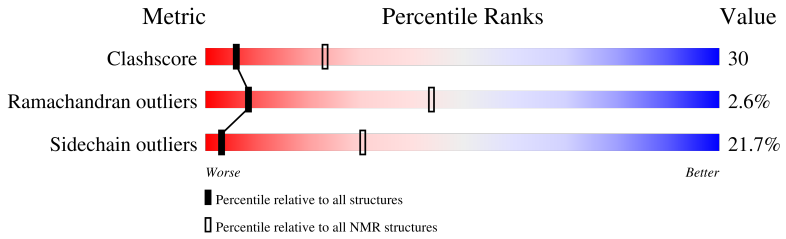
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
wwPDB-RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
wwPDB-ShiftChecker	:	v1.2
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson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

1 Overall quality at a glance

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

Molprobity failed to run

2 Ensemble composition and analysis

This entry contains 20 models. Model 17 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative.

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:130-A:168 (39)	0.17	17

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 5 clusters and 4 single-model clusters were found.

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

3 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 723 atoms, of which 372 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called DIHYDROLIPOYLLYSINE-RESIDUE ACETYLTRANSFERASE.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	45	723	217	372	71	62	1	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	166	TRP	PHE	engineered mutation	UNP P11961

SEQUENCE-PLOTS INFOmissingINFO

4 Refinement protocol and experimental data overview

The models were refined using the following method: *?*.

Of the 20 calculated structures, 20 were deposited, based on the following criterion: *NO VIOLATIONS > 0.25A*.

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

Software name	Classification	Version
CNS	refinement	
ANSIG	structure solution	
Azara	structure solution	
CNS	structure solution	

No chemical shift data was provided.

5 Model quality

5.1 Standard geometry

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.

5.2 Too-close contacts

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	305	323	323	19±2
All	All	6100	6460	6460	371

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 30.

5 of 47 unique clashes are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:139:ALA:HB2	1:A:163:ILE:HD12	0.94	1.40	10	20
1:A:144:VAL:HG22	1:A:166:TRP:CE3	0.74	2.18	7	20
1:A:146:ILE:HG23	1:A:158:VAL:CG2	0.73	2.13	12	11
1:A:142:LYS:O	1:A:167:LEU:HD21	0.73	1.84	8	14
1:A:146:ILE:HG23	1:A:158:VAL:HG21	0.68	1.66	12	11

5.3 Torsion angles

5.3.1 Protein backbone

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	39/47 (83%)	36±0 (92±1%)	2±0 (6±1%)	1±0 (3±0%)	8 44
All	All	780/940 (83%)	717 (92%)	43 (6%)	20 (3%)	8 44

All 1 unique Ramachandran outliers are listed below.

Mol	Chain	Res	Type	Models (Total)
1	A	154	LYS	20

5.3.2 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	31/36 (86%)	13±12 (43±39%)	4±3 (12±11%)	8 51
All	All	341/720 (47%)	267 (78%)	74 (22%)	3 30

5 of 14 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	148	LEU	11
1	A	152	THR	11
1	A	140	ARG	10
1	A	150	GLN	8
1	A	154	LYS	7

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

5.7 Other polymers (i)

There are no such molecules in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Chemical shift validation (i)

No chemical shift data were provided