wwPDB NMR Structure Validation Summary Report

May 29, 2020 – 05:08 am BST

PDB ID	:	4A52
Title	:	NMR structure of the imipenem-acylated L,D-transpeptidase from Bacillus subtilis
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Deposited on	:	2011-10-24

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

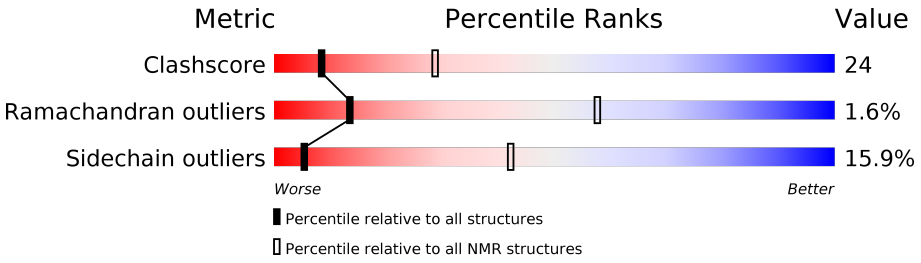
Cyrange	:	Kirchner and Güntert (2011)
NmrClust	:	Kelley et al. (1996)
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
ShiftChecker	:	2.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

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

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	175	38% 35% 5% 18% ·

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA and RNA chains that are outliers for geometric criteria:

Mol	Chain	Compound	Res	Total models with violations	
				Chirality	Geometry
2	A	IM2	1142	20	-

2 Ensemble composition and analysis

This entry contains 20 models. Model 13 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:3-A:85, A:98-A:119, A:125-A:134, A:145-A:166 (137)	0.27	13

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 3 clusters and 4 single-model clusters were found.

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

3 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 2498 atoms, of which 1202 are hydrogens and 0 are deuteriums.

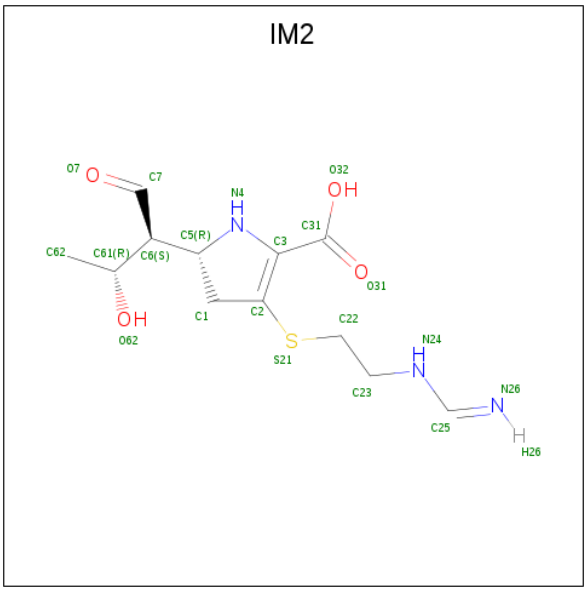
- Molecule 1 is a protein called PUTATIVE L, D-TRANSPEPTIDASE YKUD.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	169	2460	810	1184	230	233	3	0

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	GLY	-	expression tag	UNP O34816
A	2	ARG	-	expression tag	UNP O34816
A	3	LYS	-	expression tag	UNP O34816
A	4	LEU	-	expression tag	UNP O34816
A	168	GLY	-	expression tag	UNP O34816
A	169	SER	-	expression tag	UNP O34816
A	170	HIS	-	expression tag	UNP O34816
A	171	HIS	-	expression tag	UNP O34816
A	172	HIS	-	expression tag	UNP O34816
A	173	HIS	-	expression tag	UNP O34816
A	174	HIS	-	expression tag	UNP O34816
A	175	HIS	-	expression tag	UNP O34816

- Molecule 2 is (5R)-5-[(1S,2R)-1-formyl-2-hydroxypropyl]-3-[(2-{[(E)-iminomethyl]amino}ethyl)sulfanyl]-4,5-dihydro-1H-pyrrole-2-carboxylic acid (three-letter code: IM2) (formula: $C_{12}H_{19}N_3O_4S$).



Mol	Chain	Residues	Atoms					
			Total	C	H	N	O	S
2	A	1	38	12	18	3	4	1

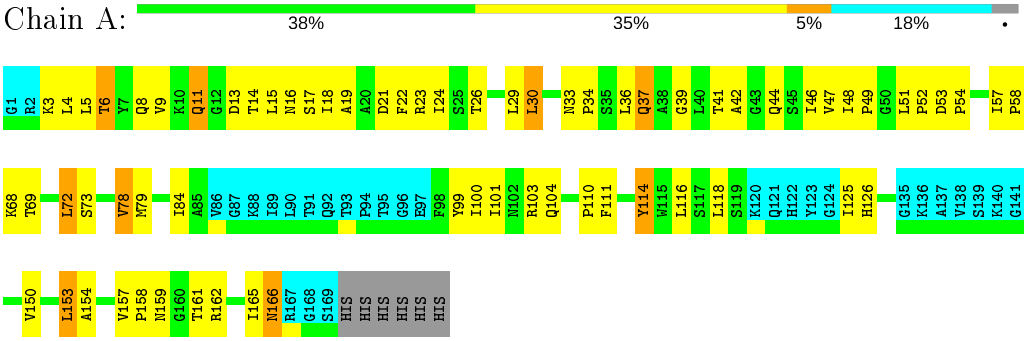
4 Residue-property plots (i)

4.1 Average score per residue in the NMR ensemble

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: PUTATIVE L, D-TRANSPEPTIDASE YKUD

Chain A:

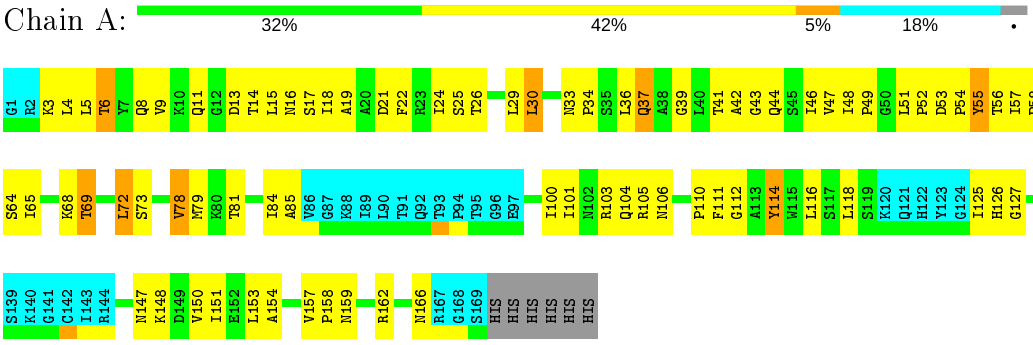


4.2 Residue scores for the representative (medoid) model from the NMR ensemble

The representative model is number 13. Colouring as in section 4.1 above.

- Molecule 1: PUTATIVE L, D-TRANSPEPTIDASE YKUD

Chain A:



5 Refinement protocol and experimental data overview

The models were refined using the following method: *ITERATIVE STRUCTURE CALCULATION WITH ARIA2.3.*

Of the 20 calculated structures, 20 were deposited, based on the following criterion: *STRUCTURE WITH THE LOWEST ENERGY.*

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

Software name	Classification	Version
CNS1.2	refinement	
CNS	structure solution	1.2
TALOS ANY	structure solution	ANY
UNIO	structure solution	10
NMRDRAW ANY	structure solution	ANY
NMRPIPE ANY	structure solution	ANY
CCPNMR ANALYSIS	structure solution	2.2

No chemical shift data was provided. No validations of the models with respect to experimental NMR restraints is performed at this time.

COVALENT-GEOMETRY INFOmissingINFO

5.1 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	1041	955	1070	50±4
2	A	20	18	16	2±1
All	All	21220	19460	21720	1036

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 24.

5 of 170 unique clashes are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:44:GLN:OE1	1:A:46:ILE:HG23	0.79	1.76	6	1
1:A:11:GLN:HA	1:A:42:ALA:HB2	0.76	1.58	5	20
1:A:98:PHE:CE1	1:A:163:VAL:HG11	0.74	2.18	14	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:17:SER:O	1:A:21:ASP:HB2	0.72	1.84	1	12
1:A:59:TYR:HA	1:A:73:SER:O	0.70	1.86	2	5

5.2 Torsion angles (i)

5.2.1 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	137/175 (78%)	121±2 (89±1%)	13±2 (10±1%)	2±1 (2±0%)	13	57
All	All	2740/3500 (78%)	2429 (89%)	268 (10%)	43 (2%)	13	57

All 5 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	58	PRO	20
1	A	110	PRO	16
1	A	23	ARG	3
1	A	119	SER	3
1	A	113	ALA	1

5.2.2 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	114/144 (79%)	96±2 (84±2%)	18±2 (16±2%)	5	42
All	All	2280/2880 (79%)	1917 (84%)	363 (16%)	5	42

5 of 41 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	114	TYR	20
1	A	69	THR	20
1	A	6	THR	20
1	A	37	GLN	20
1	A	166	ASN	20

5.2.3 RNA

There are no RNA molecules in this entry.

5.3 Non-standard residues in protein, DNA, RNA chains

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

5.4 Carbohydrates

There are no carbohydrates in this entry.

LIGAND-GEOMETRY INFOmissingINFO

5.5 Other polymers

There are no such molecules in this entry.

5.6 Polymer linkage issues

There are no chain breaks in this entry.

6 Chemical shift validation

No chemical shift data were provided