wwPDB NMR Structure Validation Summary Report

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PDB ID	:	1NIL
Title	:	A COMPARISON OF NMR SOLUTION STRUCTURES OF THE RECEPTOR BINDING DOMAINS OF PSEUDOMONAS AERUGINOSA PILI STRAINS PAO, KB7, AND PAK: IMPLICATIONS FOR RECEPTOR BINDING AND SYNTHETIC VACCINE DESIGN
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Deposited on	:	1995-10-05

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

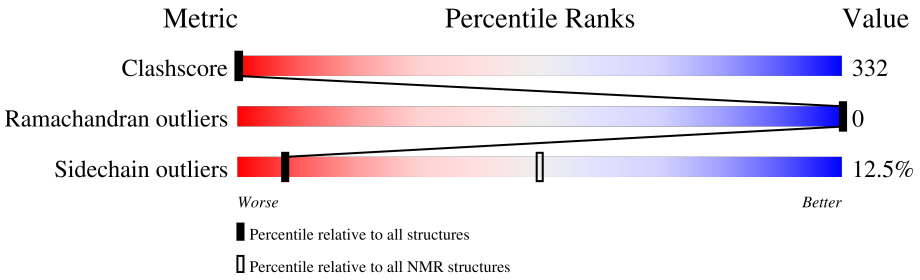
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
wwPDB-RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
wwPDB-ShiftChecker	:	v1.2
Ideal geometry (proteins)	:	Engh & Huber (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	18	11% 17% 67% 6%

2 Ensemble composition and analysis (i)

This entry contains 1 models. Identification of well-defined residues and clustering analysis are not possible.

3 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 263 atoms, of which 128 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called PAK PILIN, TRANS.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	18	263	81	128	22	30	2	0

4 Residue-property plots

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: PAK PILIN, TRANS

Chain A:

5 Refinement protocol and experimental data overview

Of the ? calculated structures, 1 were deposited, based on the following criterion: *?*.

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

Software name	Classification	Version
PEPFLEX II	refinement	

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: ACE

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	19.14	80/134 (59.7%)	17.31	44/176 (25.0%)
All	All	19.14	80/134 (59.7%)	17.31	44/176 (25.0%)

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	1	0
All	All	1	0

5 of 80 bond outliers are listed below. They are sorted according to the Z-score.

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	131	SER	CB-OG	-89.99	0.25	1.42
1	A	143	SER	CB-OG	-68.75	0.52	1.42
1	A	137	PHE	CG-CD1	-46.89	0.68	1.38
1	A	135	GLU	CD-OE1	-45.62	0.75	1.25
1	A	137	PHE	CG-CD2	-44.13	0.72	1.38

5 of 44 angle outliers are listed below. They are sorted according to the Z-score.

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	137	PHE	CD1-CG-CD2	-84.26	8.76	118.30
1	A	137	PHE	CB-CG-CD1	76.69	174.48	120.80
1	A	137	PHE	CB-CG-CD2	74.83	173.18	120.80
1	A	137	PHE	CE1-CZ-CE2	-61.71	8.92	120.00
1	A	137	PHE	CG-CD2-CE2	50.14	175.95	120.80

All chiral outliers are listed below.

Mol	Chain	Res	Type	Atoms
1	A	130	THR	CB

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	135	128	121	85
All	All	135	128	121	85

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 332.

5 of 85 clashes are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Clash(Å)	Distance(Å)
1:A:144:LYS:CG	1:A:144:LYS:CE	1.56	1.77
1:A:144:LYS:CD	1:A:144:LYS:CB	1.54	1.75
1:A:136:GLN:NE2	1:A:136:GLN:CG	1.44	1.79
1:A:137:PHE:CG	1:A:137:PHE:CE1	1.43	2.05
1:A:140:LYS:NZ	1:A:140:LYS:CD	1.43	1.80

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	16/18 (89%)	12 (75%)	4 (25%)	0 (0%)	100	100
All	All	16/18 (89%)	12 (75%)	4 (25%)	0 (0%)	100	100

There are no Ramachandran outliers.

6.3.2 Protein sidechains

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	16/16 (100%)	14 (88%)	2 (12%)	8 50
All	All	16/16 (100%)	14 (88%)	2 (12%)	8 50

All 2 residues with a non-rotameric sidechain are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type
1	A	131	SER
1	A	132	ASP

6.3.3 RNA

There are no RNA molecules in this entry.

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

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

6.5 Carbohydrates

There are no monosaccharides in this entry.

6.6 Ligand geometry

There are no ligands in this entry.

6.7 Other polymers

There are no such molecules in this entry.

6.8 Polymer linkage issues

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	6

The worst 5 of 6 chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	129:CYS	C	130:THR	N	1.17
1	A	142:CYS	C	143:SER	N	1.17
1	A	143:SER	C	144:LYS	N	1.10
1	A	128:LYS	C	129:CYS	N	1.08
1	A	131:SER	C	132:ASP	N	1.04

7 Chemical shift validation (i)

No chemical shift data were provided