# Full wwPDB NMR Structure Validation Report (i)

Apr 16, 2024 – 08:17 am BST

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|---|---|---|
| PDB ID | : | 2XKM |
| Title | : | Consensus structure of Pf1 filamentous bacteriophage from X-ray fibre diffraction and solid-state NMR |
| Authors | : | Straus, S.K.; P Scott, W.R.; Schwieters, C.D.; Marvin, D.A. |
| Deposited on | : | 2010-07-09 |

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.

SOFTWARE-VERSIONS INFOmissingINFO

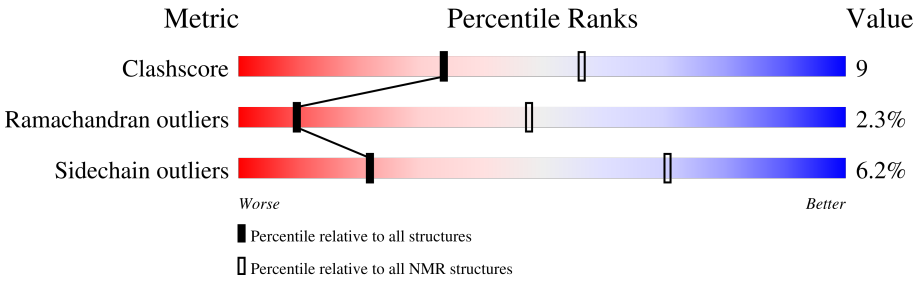
# 1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
*FIBER DIFFRACTION, SOLID-STATE NMR*

The reported resolution of this entry is 3.30 Å.

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 (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 665 atoms, of which 343 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called CAPSID PROTEIN G8P.

| Mol | Chain | Residues | Atoms | | | | | | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | H | N | O | S | |
| 1 | A | 46 | 665 | 205 | 343 | 52 | 63 | 2 | 0 |

SEQUENCE-PLOTS INFOmissingINFO

# 4 Refinement protocol and experimental data overview (i)

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

The authors did not provide any information on software used for structure solution, optimization or refinement.

No chemical shift data was provided. Note: This is a solid-state NMR structure, where hydrogen atoms are typically not assigned a chemical shift value, which may lead to lower completeness of assignment measure.

# 5 Model quality (i)

## 5.1 Standard geometry (i)

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 (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 | 322 | 343 | 343 | 6 |
| All | All | 322 | 343 | 343 | 6 |

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 9.

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

| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) |
|---|---|---|---|
| 1:A:22:ILE:O | 1:A:26:ILE:HG13 | 0.52 | 2.03 |
| 1:A:40:TYR:C | 1:A:40:TYR:CD1 | 0.51 | 2.83 |
| 1:A:3:ILE:HG22 | 1:A:4:ASP:N | 0.50 | 2.22 |
| 1:A:16:GLN:O | 1:A:20:LYS:HG2 | 0.43 | 2.13 |
| 1:A:3:ILE:HG22 | 1:A:4:ASP:H | 0.42 | 1.73 |
| 1:A:17:GLY:O | 1:A:20:LYS:HB2 | 0.41 | 2.15 |

## 5.3 Torsion angles (i)

### 5.3.1 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 | 44/46 (96%) | 42 (95%) | 1 (2%) | 1 (2%) | 9 | 48 |
| All | All | 44/46 (96%) | 42 (95%) | 1 (2%) | 1 (2%) | 9 | 48 |

All 1 Ramachandran outliers are listed below.

| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | A | 2 | VAL |

### 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 | 32/32 (100%) | 30 (94%) | 2 (6%) | 21 | 70 |
| All | All | 32/32 (100%) | 30 (94%) | 2 (6%) | 21 | 70 |

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 | 33 | LEU |
| 1 | A | 40 | TYR |

### 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