



wwPDB NMR Structure Validation Summary Report ⓘ

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PDB ID : 1SF0
Title : BACKBONE SOLUTION STRUCTURE OF MIXED ALPHA/BETA PROTEIN PF1061
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Deposited on : 2004-02-19

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 ⓘ 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 ⓘ](#)) 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 |

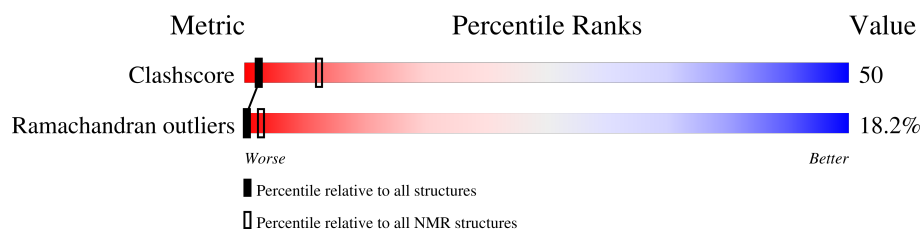
1 Overall quality at a glance

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 |

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 $\leq 5\%$

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|--|
| 1 | A | 77 |  |

2 Ensemble composition and analysis ⓘ

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

3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 475 atoms, of which 142 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called hypothetical protein PF1061.

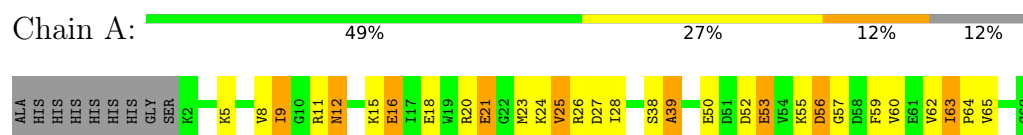
| Mol | Chain | Residues | Atoms | | | | | Trace |
|-----|-------|----------|-------|-----|-----|----|----|-------|
| 1 | A | 68 | Total | C | H | N | O | 0 |
| | | | 475 | 197 | 142 | 68 | 68 | |

There are 9 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|-------|---------|----------|--------|------------------|------------|
| A | -7 | ALA | - | cloning artifact | UNP Q8U1Z3 |
| A | -6 | HIS | - | expression tag | UNP Q8U1Z3 |
| A | -5 | HIS | - | expression tag | UNP Q8U1Z3 |
| A | -4 | HIS | - | expression tag | UNP Q8U1Z3 |
| A | -3 | HIS | - | expression tag | UNP Q8U1Z3 |
| A | -2 | HIS | - | expression tag | UNP Q8U1Z3 |
| A | -1 | HIS | - | expression tag | UNP Q8U1Z3 |
| A | 0 | GLY | - | cloning artifact | UNP Q8U1Z3 |
| A | 1 | SER | - | cloning artifact | UNP Q8U1Z3 |

i

- Molecule 1: hypothetical protein PF1061



5 Refinement protocol and experimental data overview

The models were refined using the following method: *RDC DIRECTED FRAGMENT ASSEMBLY*.

Of the 1 calculated structures, 1 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 |
|---------------|--------------------|---------|
| XPLOR-NIH | refinement | 2.9.1 |
| NMRPipe | structure solution | 5.0.4 |
| REDcRAFT | structure solution | 1.0 |
| REDCAT | structure solution | 1.0 |

No chemical shift data was provided.

6 Model quality [i](#)

6.1 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.

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 | 333 | 142 | 150 | 24 |
| All | All | 333 | 142 | 150 | 24 |

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 50.

5 of 24 clashes are listed below, sorted by their clash magnitude.

| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) |
|--------------|----------------|----------|-------------|
| 1:A:38:SER:O | 1:A:39:ALA:HB2 | 0.75 | 1.79 |
| 1:A:5:LYS:O | 1:A:60:VAL:N | 0.72 | 2.22 |
| 1:A:55:LYS:O | 1:A:57:GLY:N | 0.68 | 2.26 |
| 1:A:62:VAL:O | 1:A:63:ILE:CB | 0.66 | 2.44 |
| 1:A:38:SER:O | 1:A:39:ALA:CB | 0.63 | 2.44 |

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 | 66/77 (86%) | 36 (55%) | 18 (27%) | 12 (18%) | 0 | 3 |
| All | All | 66/77 (86%) | 36 (55%) | 18 (27%) | 12 (18%) | 0 | 3 |

5 of 12 Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | A | 9 | ILE |
| 1 | A | 12 | ASN |
| 1 | A | 16 | GLU |
| 1 | A | 18 | GLU |
| 1 | A | 21 | GLU |

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 | 0 | - | - | - |
| All | All | 0 | - | - | - |

There are no protein residues with a non-rotameric sidechain to report.

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

There are no ligands in this entry.

6.7 Other polymers

There are no such molecules in this entry.

6.8 Polymer linkage issues

There are no chain breaks in this entry.

7 Chemical shift validation

No chemical shift data were provided