# wwPDB NMR Structure Validation Summary Report (i)

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| PDB ID | : | 1MG8 |
| Title | : | NMR structure of ubiquitin-like domain in murine Parkin |
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| Deposited on | : | 2002-08-15 |

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
http://wwpdb.org/validation/2016/NMRValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (i)) were used in the production of this report:

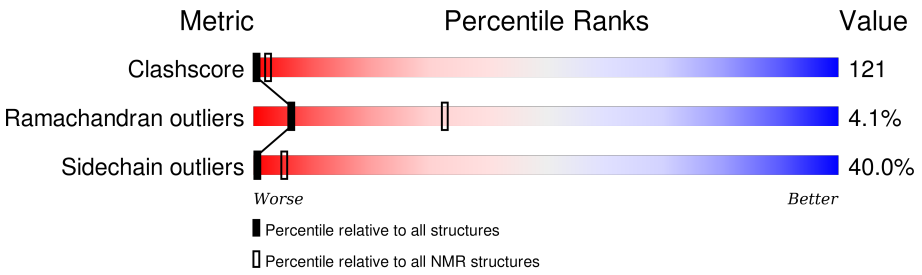
| | | |
|---|---|---|
| Cyrange | : | Kirchner and Güntert (2011) |
| NmrClust | : | Kelley et al. (1996) |
| MolProbity | : | 4.02b-467 |
| Mogul | : | unknown |
| Percentile statistics | : | 20151230.v01 (using entries in the PDB archive December 30th 2015) |
| RCI | : | v_1n_11_5_13_A (Berjanski et al., 2005) |
| PANAV | : | Wang et al. (2010) |
| ShiftChecker | : | rb-20027457 |
| Ideal geometry (proteins) | : | Engh & Huber (2001) |
| Ideal geometry (DNA, RNA) | : | Parkinson et al. (1996) |
| Validation Pipeline (wwPDB-VP) | : | rb-20027457 |

# 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 | 114402 | 11133 |
| Ramachandran outliers | 111179 | 9975 |
| Sidechain outliers | 111093 | 9958 |

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 | 78 | 5% 47% 29% • 15% |

# 2 Ensemble composition and analysis (i)

This entry contains 10 models. Model 1 is the overall representative, medoid model (most similar to other models).

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:9, A:15-A:73 (66) | 0.28 | 1 |

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 4 clusters. No single-model clusters were found.

| Cluster number | Models |
|---|---|
| 1 | 3, 5, 7 |
| 2 | 1, 2, 6 |
| 3 | 4, 8 |
| 4 | 9, 10 |

# 3 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 1268 atoms, of which 642 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Parkin.

| Mol | Chain | Residues | Atoms | | | | | | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | H | N | O | S | |
| 1 | A | 78 | 1268 | 394 | 642 | 116 | 113 | 3 | 0 |

There are 2 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|---|---|---|---|---|---|
| A | 1 | MET | - | INITIATING MET | UNP Q9WVS6 |
| A | 2 | GLY | - | CLONING ARTIFACT | UNP Q9WVS6 |

# 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: Parkin

Chain A: 5% 47% 29% • 15%

M1 G2 M3 I4 V5 F6 V7 R8 F9 N10 S11 S12 Y13 G14 F15 P16 V17 E18 V19 D20 S21 D22 T23 S24 I25 L26 Q27 L28 K29 E30 V31 V32 A33 K34 R35 Q36 G37 V38 P39 A40 D41 Q42 L43 R44 V45 I46 F47 A48 G49 K50 E51 L52 P53 N54 H55 L56 T57 V58 Q59 N60

C61 D62 L63 E64 Q65 Q66 S67 I68 V69 H70 I71 V72 Q73 R74 P75 R76 R77 R78

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

The representative model is number 1. Colouring as in section 4.1 above.

- Molecule 1: Parkin

Chain A: 13% 44% 27% • 15%

M1 G2 M3 I4 V5 F6 V7 R8 F9 N10 S11 S12 Y13 G14 F15 P16 V17 E18 V19 D20 S21 D22 T23 S24 I25 L26 Q27 L28 K29 E30 V31 V32 A33 K34 R35 Q36 G37 V38 P39 A40 D41 Q42 L43 R44 V45 I46 F47 K50 E51 L52 P53 N54 H55 L56 T57 V58 Q59 N60 C61

D62 L63 E64 Q65 Q66 S67 I68 V69 H70 I71 V72 Q73 R74 P75 R76 R77 R78

# 5 Refinement protocol and experimental data overview (i)

The models were refined using the following method: *simulated annealing*.

Of the 50 calculated structures, 10 were deposited, based on the following criterion: *structures with the lowest energy*.

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

| Software name | Classification | Version |
|---|---|---|
| X-PLOR | refinement | |

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

# 6 Model quality (i)

## 6.1 Standard geometry (i)

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 | 1.02±0.00 | 0±0/535 (0.0±0.0%) | 0.98±0.01 | 1±1/727 (0.1±0.1%) |
| All | All | 1.02 | 0/5350 (0.0%) | 0.98 | 8/7270 (0.1%) |

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 | 0.0±0.0 | 2.8±0.6 |
| All | All | 0 | 28 |

There are no bond-length outliers.

All unique angle outliers are listed below. They are sorted according to the Z-score of the worst occurrence in the ensemble.

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) | Models | |
|---|---|---|---|---|---|---|---|---|---|
| | | | | | | | | Worst | Total |
| 1 | A | 9 | PHE | CB-CG-CD2 | -7.21 | 115.75 | 120.80 | 9 | 7 |
| 1 | A | 9 | PHE | CB-CG-CD1 | 5.22 | 124.45 | 120.80 | 9 | 1 |

There are no chirality outliers.

All unique planar outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

| Mol | Chain | Res | Type | Group | Models (Total) |
|---|---|---|---|---|---|
| 1 | A | 8 | ARG | Sidechain | 10 |
| 1 | A | 44 | ARG | Sidechain | 9 |
| 1 | A | 35 | ARG | Sidechain | 9 |

## 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 | 526 | 541 | 541 | 129±9 |
| All | All | 5260 | 5410 | 5410 | 1289 |

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 121.

5 of 443 unique clashes are listed below, sorted by their clash magnitude.

| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|---|---|---|---|---|---|
| | | | | Worst | Total |
| 1:A:28:LEU:HD12 | 1:A:45:VAL:HG21 | 1.10 | 1.15 | 7 | 9 |
| 1:A:32:VAL:HG13 | 1:A:43:LEU:HD23 | 1.08 | 1.08 | 6 | 1 |
| 1:A:32:VAL:HG12 | 1:A:43:LEU:HD21 | 1.06 | 1.15 | 2 | 9 |
| 1:A:23:THR:O | 1:A:58:VAL:HG23 | 0.97 | 1.57 | 6 | 8 |
| 1:A:32:VAL:HG13 | 1:A:43:LEU:CD2 | 0.96 | 1.90 | 6 | 1 |

## 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 | 66/78 (85%) | 55±2 (83±3%) | 9±2 (13±3%) | 3±1 (4±1%) | 6 33 |
| All | All | 660/780 (85%) | 546 (83%) | 87 (13%) | 27 (4%) | 6 33 |

5 of 8 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 | 62 | ASP | 10 |
| 1 | A | 24 | SER | 5 |
| 1 | A | 64 | GLU | 4 |

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| Mol | Chain | Res | Type | Models (Total) |
|---|---|---|---|---|
| 1 | A | 25 | ILE | 3 |
| 1 | A | 51 | GLU | 2 |

### 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 | 61/71 (86%) | 37±2 (60±3%) | 24±2 (40±3%) | 1 5 |
| All | All | 610/710 (86%) | 366 (60%) | 244 (40%) | 1 5 |

5 of 44 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 | 57 | THR | 10 |
| 1 | A | 9 | PHE | 10 |
| 1 | A | 27 | GLN | 10 |
| 1 | A | 67 | SER | 10 |
| 1 | A | 23 | THR | 10 |

### 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 carbohydrates in this entry.

## 6.6 Ligand geometry (i)

There are no ligands in this entry.

## 6.7 Other polymers (i)

There are no such molecules in this entry.

## 6.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

# 7 Chemical shift validation (i)

No chemical shift data were provided