# wwPDB NMR Structure Validation Summary Report (i)

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|---|---|---|
| PDB ID | : | 1V31 |
| Title | : | Solution structure of the SWIB/MDM2 domain of the hypothetical protein At5g14170 from Arabidopsis thaliana |
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| Deposited on | : | 2003-10-21 |

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:

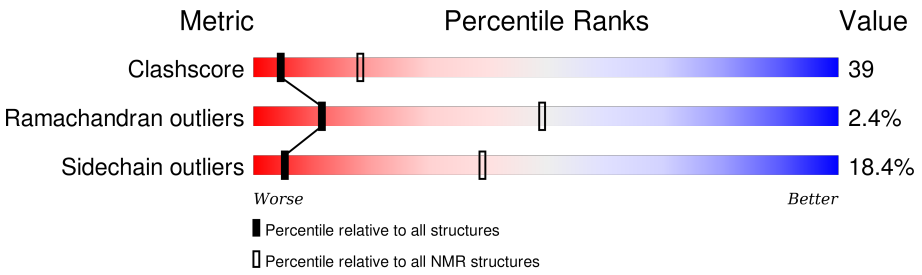
| | | |
|---|---|---|
| Cyrange | : | Kirchner and Güntert (2011) |
| NmrClust | : | Kelley et al. (1996) |
| MolProbity | : | 4.02b-467 |
| Mogul | : | unknown |
| Percentile statistics | : | 20151230.v01 (using entries in the PDB archive December 30th 2015) |
| RCI | : | v_1n_11_5_13_A (Berjanski et 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 is 92%.

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 | 93 | 20% 56% • 19% |

# 2 Ensemble composition and analysis (i)

This entry contains 20 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:11-A:85 (75) | 0.22 | 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 and 3 single-model clusters were found.

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

# 3 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 1426 atoms, of which 716 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called hypothetical protein RAFL11-05-P19.

| Mol | Chain | Residues | Atoms | | | | | | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | H | N | O | S | |
| 1 | A | 93 | 1426 | 453 | 716 | 123 | 131 | 3 | 0 |

There are 13 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|---|---|---|---|---|---|
| A | 1 | GLY | - | CLONING ARTIFACT | UNP Q9FMT4 |
| A | 2 | SER | - | CLONING ARTIFACT | UNP Q9FMT4 |
| A | 3 | SER | - | CLONING ARTIFACT | UNP Q9FMT4 |
| A | 4 | GLY | - | CLONING ARTIFACT | UNP Q9FMT4 |
| A | 5 | SER | - | CLONING ARTIFACT | UNP Q9FMT4 |
| A | 6 | SER | - | CLONING ARTIFACT | UNP Q9FMT4 |
| A | 7 | GLY | - | CLONING ARTIFACT | UNP Q9FMT4 |
| A | 88 | SER | - | CLONING ARTIFACT | UNP Q9FMT4 |
| A | 89 | GLY | - | CLONING ARTIFACT | UNP Q9FMT4 |
| A | 90 | PRO | - | CLONING ARTIFACT | UNP Q9FMT4 |
| A | 91 | SER | - | CLONING ARTIFACT | UNP Q9FMT4 |
| A | 92 | SER | - | CLONING ARTIFACT | UNP Q9FMT4 |
| A | 93 | GLY | - | CLONING ARTIFACT | UNP Q9FMT4 |

# 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: hypothetical protein RAFL11-05-P19

Chain A: 20% 56% • 19%

G1 S2 S3 G4 S5 S6 G7 V8 P9 E10 K11 F12 K13 L14 S15 T16 A17 L18 M19 D20 V21 L22 G23 I24 E25 V26 E27 T28 R29 P30 R31 I32 I33 A34 A35 I36 W37 H38 Y39 V40 K41 A42 R43 K44 L45 Q46 N47 S52 F53 F54 D57 A58 A59 L60 Q61 K62 V63 F64

G65 K68 L69 K70 F71 T72 M73 V74 S75 Q76 K77 I78 S79 H80 H81 L82 S83 P86 P87 S88 G89 P90 S91 S92 G93

## 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: hypothetical protein RAFL11-05-P19

Chain A: 35% 37% 9% 19%

G1 S2 S3 G4 S5 S6 G7 V8 P9 E10 K13 L14 S15 L18 M19 D20 I24 T28 R29 P30 R31 I32 I33 A34 A35 I36 W37 V40 K41 A42 R43 K44 L45 S52 F53 F54 D57 A58 Q61 K62 V63 F64 G65 K68 L69 K70 F71 T72 M73 V74 S75

Q76 K77 I78 S79 L82 P86 P87 S88 G89 P90 S91 S92 G93

# 5 Refinement protocol and experimental data overview (i)

The models were refined using the following method: *torsion angle dynamics*.

Of the 100 calculated structures, 20 were deposited, based on the following criterion: *structures with the least restraint violations, structures with the lowest energy, target function*.

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

| Software name | Classification | Version |
|---|---|---|
| CYANA | structure solution | 1.0.7 |
| CYANA | refinement | 1.0.7 |

The following table shows chemical shift validation statistics as aggregates over all chemical shift files. Detailed validation can be found in section 7 of this report.

| Chemical shift file(s) | BMRB entry 10105 |
|---|---|
| Number of chemical shift lists | 1 |
| Total number of shifts | 1058 |
| Number of shifts mapped to atoms | 1058 |
| Number of unparsed shifts | 0 |
| Number of shifts with mapping errors | 0 |
| Number of shifts with mapping warnings | 0 |
| Assignment completeness (well-defined parts) | 92% |

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)

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 | 604 | 623 | 623 | 48±6 |
| All | All | 12080 | 12460 | 12460 | 961 |

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 39.

5 of 254 unique clashes are listed below, sorted by their clash magnitude.

| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|---|---|---|---|---|---|
| | | | | Worst | Total |
| 1:A:17:ALA:O | 1:A:21:VAL:HG23 | 0.89 | 1.65 | 14 | 14 |
| 1:A:45:LEU:HD11 | 1:A:57:ASP:OD2 | 0.86 | 1.69 | 16 | 3 |
| 1:A:14:LEU:HD23 | 1:A:18:LEU:HD23 | 0.86 | 1.48 | 3 | 3 |
| 1:A:45:LEU:HD21 | 1:A:57:ASP:OD1 | 0.85 | 1.71 | 13 | 12 |
| 1:A:64:PHE:CG | 1:A:69:LEU:HD13 | 0.84 | 2.05 | 18 | 20 |

## 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 | 75/93 (81%) | 54±3 (72±4%) | 19±3 (25±3%) | 2±1 (2±1%) | 12 49 |
| All | All | 1500/1860 (81%) | 1087 (72%) | 377 (25%) | 36 (2%) | 12 49 |

5 of 10 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 | 30 | PRO | 9 |
| 1 | A | 58 | ALA | 9 |
| 1 | A | 28 | THR | 5 |
| 1 | A | 26 | VAL | 4 |
| 1 | A | 57 | ASP | 3 |

### 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 | 67/80 (84%) | 55±3 (82±4%) | 12±3 (18±4%) | 5 39 |
| All | All | 1340/1600 (84%) | 1093 (82%) | 247 (18%) | 5 39 |

5 of 33 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 | 69 | LEU | 20 |
| 1 | A | 14 | LEU | 16 |
| 1 | A | 61 | GLN | 15 |
| 1 | A | 20 | ASP | 14 |
| 1 | A | 68 | LYS | 13 |

### 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)

The completeness of assignment taking into account all chemical shift lists is 92% for the well-defined parts and 85% for the entire structure.

## 7.1 Chemical shift list 1

File name: BMRB entry 10105

Chemical shift list name: *assigned_ chem_ shift_ list_ 1*

### 7.1.1 Bookkeeping (i)

The following table shows the results of parsing the chemical shift list and reports the number of nuclei with statistically unusual chemical shifts.

| | |
|---|---|
| Total number of shifts | 1058 |
| Number of shifts mapped to atoms | 1058 |
| Number of unparsed shifts | 0 |
| Number of shifts with mapping errors | 0 |
| Number of shifts with mapping warnings | 0 |
| Number of shift outliers (ShiftChecker) | 1 |

### 7.1.2 Chemical shift referencing (i)

The following table shows the suggested chemical shift referencing corrections.

| Nucleus | # values | Correction ± precision, *ppm* | Suggested action |
|---|---|---|---|
| $^{13}C_{\alpha}$ | 79 | -0.36 ± 0.15 | None needed (< 0.5 ppm) |
| $^{13}C_{\beta}$ | 77 | 0.03 ± 0.16 | None needed (< 0.5 ppm) |
| $^{13}C'$ | 75 | -0.22 ± 0.12 | None needed (< 0.5 ppm) |
| $^{15}N$ | 71 | 0.91 ± 0.39 | Should be applied |

### 7.1.3 Completeness of resonance assignments (i)

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 92%, i.e. 897 atoms were assigned a chemical shift out of a possible 971. 0 out of 12 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

| | Total | $^{1}H$ | $^{13}C$ | $^{15}N$ |
|---|---|---|---|---|
| Backbone | 357/365 (98%) | 143/145 (99%) | 145/150 (97%) | 69/70 (99%) |
| Sidechain | 468/520 (90%) | 291/308 (94%) | 170/189 (90%) | 7/23 (30%) |

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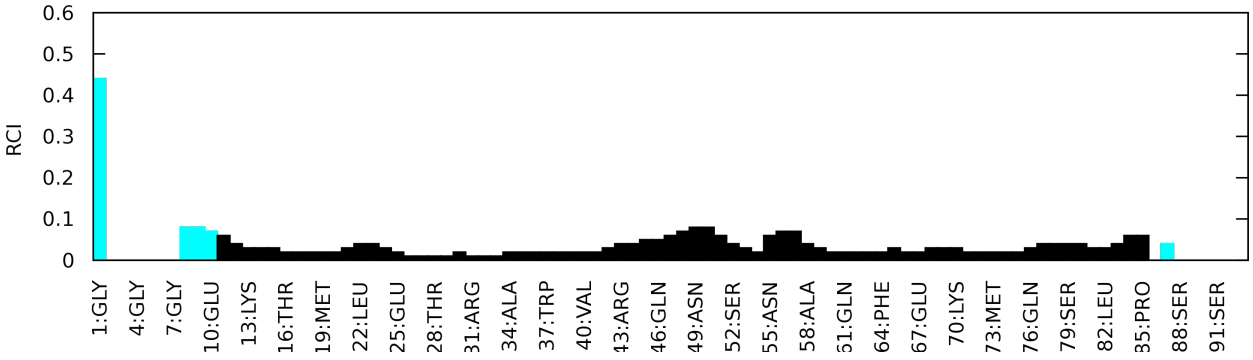
| | Total | $^{1}$H | $^{13}$C | $^{15}$N |
|---|---|---|---|---|
| Aromatic | 72/86 (84%) | 38/47 (81%) | 33/35 (94%) | 1/4 (25%) |
| Overall | 897/971 (92%) | 472/500 (94%) | 348/374 (93%) | 77/97 (79%) |

### 7.1.4 Statistically unusual chemical shifts (i)

The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

| Mol | Chain | Res | Type | Atom | Shift, *ppm* | Expected range, *ppm* | Z-score |
|---|---|---|---|---|---|---|---|
| 1 | A | 31 | ARG | NE | 126.12 | 92.63 – 76.73 | 26.1 |

### 7.1.5 Random Coil Index (RCI) plots (i)

The image below reports *random coil index* values for the protein chains in the structure. The height of each bar gives a probability of a given residue to be disordered, as predicted from the available chemical shifts and the amino acid sequence. A value above 0.2 is an indication of significant predicted disorder. The colour of the bar shows whether the residue is in the well-defined core (black) or in the ill-defined residue ranges (cyan), as described in section 2 on ensemble composition.

Random coil index (RCI) for chain A: