# wwPDB NMR Structure Validation Summary Report (i)

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| PDB ID | : | 2DLY |
| Title | : | Solution structure of the SH2 domain of murine Fyn-related kinase |
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| Deposited on | : | 2006-04-20 |

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:

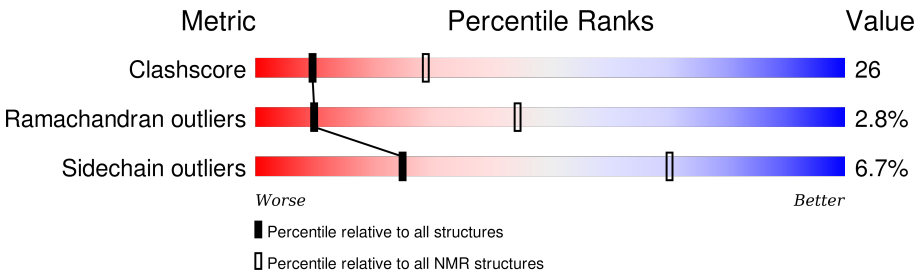
| | | |
|---|---|---|
| Cyrange | : | Kirchner and Güntert (2011) |
| NmrClust | : | Kelley et al. (1996) |
| MolProbity | : | 4.02b-467 |
| Mogul | : | unknown |
| Percentile statistics | : | 20151230.v01 (using entries in the PDB archive December 30th 2015) |
| RCI | : | v_1n_11_5_13_A (Berjanski et 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 | 121 | 39% 33% • 26% |

# 2 Ensemble composition and analysis (i)

This entry contains 20 models. Model 9 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *lowest energy*.

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:13-A:47, A:53-A:72, A:77-A:111 (90) | 0.16 | 9 |

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 2 clusters and 3 single-model clusters were found.

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

# 3 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 1875 atoms, of which 928 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Fyn-related kinase.

| Mol | Chain | Residues | Atoms | | | | | | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | H | N | O | S | |
| 1 | A | 121 | 1875 | 595 | 928 | 164 | 186 | 2 | 0 |

There are 13 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|---|---|---|---|---|---|
| A | 1 | GLY | - | CLONING ARTIFACT | UNP Q8BPC1 |
| A | 2 | SER | - | CLONING ARTIFACT | UNP Q8BPC1 |
| A | 3 | SER | - | CLONING ARTIFACT | UNP Q8BPC1 |
| A | 4 | GLY | - | CLONING ARTIFACT | UNP Q8BPC1 |
| A | 5 | SER | - | CLONING ARTIFACT | UNP Q8BPC1 |
| A | 6 | SER | - | CLONING ARTIFACT | UNP Q8BPC1 |
| A | 7 | GLY | - | CLONING ARTIFACT | UNP Q8BPC1 |
| A | 116 | SER | - | CLONING ARTIFACT | UNP Q8BPC1 |
| A | 117 | GLY | - | CLONING ARTIFACT | UNP Q8BPC1 |
| A | 118 | PRO | - | CLONING ARTIFACT | UNP Q8BPC1 |
| A | 119 | SER | - | CLONING ARTIFACT | UNP Q8BPC1 |
| A | 120 | SER | - | CLONING ARTIFACT | UNP Q8BPC1 |
| A | 121 | GLY | - | CLONING ARTIFACT | UNP Q8BPC1 |

# 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: Fyn-related kinase

Chain A: 39% 33% • 26%

G1 S2 S3 G4 S5 S6 G7 A8 E9 D10 R11 S12 L13 F19 F20 I23 A28 E29 K30 Q31 L32 L33 Y34 N37 F42 L43 E48 S49 Q50 K51 G52 V58 L59 D60 E61 G62 V63 V64 K65 H66 Y67 R70 R71 L72 D73 E74 G75 G76 F77 F78 L79 T80

R81 R82 K83 V84 F85 L88 F91 V92 N93 Y94 Y95 T96 S99 D100 G101 L102 G103 V104 K105 L111 K112 I113 Q114 V115 S116 G117 P118 S119 S120 G121

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

The representative model is number 9. Colouring as in section 4.1 above.

- Molecule 1: Fyn-related kinase

Chain A: 43% 28% • 26%

G1 S2 S3 G4 S5 S6 G7 A8 E9 D10 R11 S12 L13 P17 F20 I23 A28 E29 K30 Q31 L32 L33 Y34 S35 E36 N37 Q38 T39 F42 S47 E48 S49 Q50 K51 G52 D53 F54 V58 L59 D60 E61 G62 V63 V64 K65 H66 Y67 R70 R71 L72 D73 E74

G75 G76 F77 F78 K83 V84 F85 F91 V92 N93 Y94 Y95 T96 D100 V104 K105 K112 I113 Q114 V115 S116 G117 P118 S119 S120 G121

# 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: *target function,structures with the lowest energy,structures with the least restraint violations.*

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

| Software name | Classification | Version |
|---|---|---|
| CYANA | structure solution | 2.0.17 |
| CYANA | refinement | 2.0.17 |

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)

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 | 744 | 746 | 746 | 38±5 |
| All | All | 14880 | 14920 | 14920 | 769 |

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 26.

5 of 199 unique clashes are listed below, sorted by their clash magnitude.

| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|---|---|---|---|---|---|
| | | | | Worst | Total |
| 1:A:34:TYR:CD2 | 1:A:111:LEU:HD21 | 0.97 | 1.93 | 15 | 7 |
| 1:A:13:LEU:HD11 | 1:A:88:LEU:HD12 | 0.94 | 1.32 | 15 | 4 |
| 1:A:42:PHE:CE2 | 1:A:92:VAL:HG11 | 0.91 | 2.00 | 15 | 18 |
| 1:A:60:ASP:O | 1:A:63:VAL:HG12 | 0.88 | 1.68 | 11 | 19 |
| 1:A:23:ILE:HD11 | 1:A:28:ALA:HB2 | 0.81 | 1.50 | 13 | 12 |

## 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 | 90/121 (74%) | 74±3 (82±3%) | 14±3 (15±3%) | 3±1 (3±1%) | 10 44 |
| All | All | 1800/2420 (74%) | 1480 (82%) | 270 (15%) | 50 (3%) | 10 44 |

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 | 34 | TYR | 17 |
| 1 | A | 100 | ASP | 14 |
| 1 | A | 96 | THR | 5 |
| 1 | A | 36 | GLU | 4 |
| 1 | A | 81 | ARG | 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 | 81/103 (79%) | 76±2 (93±2%) | 5±2 (7±2%) | 25 70 |
| All | All | 1620/2060 (79%) | 1511 (93%) | 109 (7%) | 25 70 |

5 of 26 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 | 65 | LYS | 19 |
| 1 | A | 72 | LEU | 16 |
| 1 | A | 60 | ASP | 7 |
| 1 | A | 43 | LEU | 7 |
| 1 | A | 96 | THR | 7 |

### 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