



# Full wwPDB X-ray Structure Validation Report ⓘ

Oct 1, 2017 – 01:53 AM EDT

PDB ID : 1Q4R  
Title : Gene Product of At3g17210 from Arabidopsis Thaliana  
Authors : Phillips Jr., G.N.; Bingman, C.A.; Johnson, K.A.; Smith, D.W.; Center for Eukaryotic Structural Genomics (CESG)  
Deposited on : unknown  
Resolution : 1.90 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

|                                |   |  |
|--------------------------------|---|--|
| MolProbity                     | : | <b>FAILED</b>  |
| Xtriage (Phenix)               | : | 1.9-1692   |
| EDS                            | : | rb-20030345  |
| Percentile statistics          | : | 20161228.v01 (using entries in the PDB archive December 28th 2016) |
| Refmac                         | : | 5.8.0135   |
| CCP4                           | : | 6.5.0  |
| Ideal geometry (proteins)      | : | Engh & Huber (2001)  |
| Ideal geometry (DNA, RNA)      | : | Parkinson et al. (1996)  |
| Validation Pipeline (wwPDB-VP) | : | rb-20030345  |

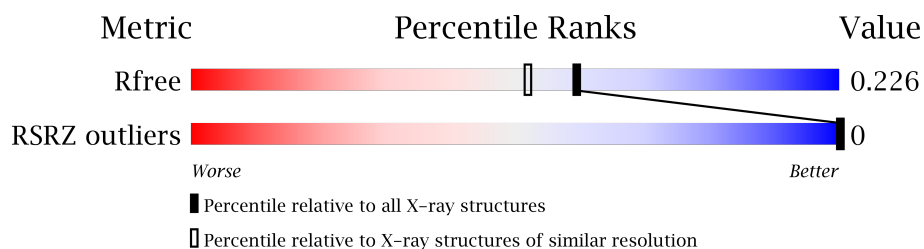
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.90 Å.

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<br>(#Entries) | Similar resolution<br>(#Entries, resolution range(Å)) |
|---------------|-----------------------------|---|
| $R_{free}$    | 100719                      | 5047 (1.90-1.90)                                      |
| RSRZ outliers | 101464                      | 5100 (1.90-1.90)                                      |

MolProbity failed to run properly - the sequence quality summary graphics cannot be shown.

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 937 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called protein At3g17210.

| Mol | Chain | Residues | Atoms |     |     |     |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---------|---------|-------|
| 1   | A     | 103      | Total | C   | N   | O   | Se | 0       | 2       | 0     |
|     |       |          | 827   | 542 | 131 | 153 | 1  |         |         |       |

There are 5 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment          | Reference  |
|-------|---------|----------|--------|------------------|------------|
| A     | 1       | GLY      | -      | CLONING ARTIFACT | UNP Q9LUV2 |
| A     | 2       | SER      | -      | CLONING ARTIFACT | UNP Q9LUV2 |
| A     | 3       | HIS      | -      | CLONING ARTIFACT | UNP Q9LUV2 |
| A     | 4       | MSE      | MET    | MODIFIED RESIDUE | UNP Q9LUV2 |
| A     | 45      | MSE      | MET    | MODIFIED RESIDUE | UNP Q9LUV2 |

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

| Mol | Chain | Residues | Atoms |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 2   | A     | 1        | Total | Mg | 0       | 0       |
|     |       |          | 1     | 1  |         |         |

- Molecule 3 is water.

| Mol | Chain | Residues | Atoms |     | ZeroOcc | AltConf |
|-----|-------|----------|-------|-----|---------|---------|
| 3   | A     | 109      | Total | O   | 0       | 0       |
|     |       |          | 109   | 109 |         |         |

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### 3 Data and refinement statistics

| Property  | Value   | Source           |
|---|---|------------------|
| Space group   | P 62  | Depositor        |
| Cell constants<br>a, b, c, $\alpha$ , $\beta$ , $\gamma$                | 55.47Å 55.47Å 57.67Å<br>90.00° 90.00° 120.00°               | Depositor        |
| Resolution (Å)  | 20.00 – 1.90<br>19.99 – 1.90                                | Depositor<br>EDS |
| % Data completeness<br>(in resolution range)                            | 94.8 (20.00-1.90)<br>94.7 (19.99-1.90)                      | Depositor<br>EDS |
| $R_{merge}$   | 0.04  | Depositor        |
| $R_{sym}$   | (Not available)   | Depositor        |
| $\langle I/\sigma(I) \rangle$ <sup>1</sup>                              | 2.10 (at 1.90Å)   | Xtriage          |
| Refinement program  | REFMAC 5.1.24   | Depositor        |
| R, $R_{free}$   | 0.182 , 0.232<br>0.190 , 0.226                              | Depositor<br>DCC |
| $R_{free}$ test set   | 369 reflections (5.12%)                                     | DCC              |
| Wilson B-factor (Å <sup>2</sup> )                                       | 22.5  | Xtriage          |
| Anisotropy  | 0.016   | Xtriage          |
| Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> ) | 0.31 , 40.9   | EDS              |
| L-test for twinning <sup>2</sup>  | $\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.34$ | Xtriage          |
| Estimated twinning fraction   | 0.076 for h,-h-k,-l   | Xtriage          |
| $F_o, F_c$ correlation  | 0.95  | EDS              |
| Total number of atoms   | 937   | wwPDB-VP         |
| Average B, all atoms (Å <sup>2</sup> )                                  | 25.0  | wwPDB-VP         |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 12.76% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 4 Model quality [i](#)

### 4.1 Standard geometry [i](#)

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### 4.2 Too-close contacts [i](#)

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### 4.3 Torsion angles [i](#)

#### 4.3.1 Protein backbone [i](#)

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#### 4.3.2 Protein sidechains [i](#)

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#### 4.3.3 RNA [i](#)

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### 4.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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### 4.5 Carbohydrates [i](#)

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### 4.6 Ligand geometry [i](#)

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### 4.7 Other polymers [i](#)

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## 4.8 Polymer linkage issues

There are no chain breaks in this entry.

## 5 Fit of model and data [i](#)

### 5.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

| Mol | Chain | Analysed      | <RSRZ> | #RSRZ>2   | OWAB(Å <sup>2</sup> ) | Q<0.9 |
|-----|-------|---------------|--------|-----------|-----------------------|-------|
| 1   | A     | 102/112 (91%) | -0.23  | 0 100 100 | 14, 24, 32, 36        | 0     |

There are no RSRZ outliers to report.

### 5.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

### 5.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

### 5.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists the number of atoms with occupancy less than 0.9.

| Mol | Type | Chain | Res | Atoms | RSCC | RSR  | LLDF  | B-factors(Å <sup>2</sup> ) | Q<0.9 |
|-----|------|-------|-----|-------|------|------|-------|----------------------------|-------|
| 2   | MG   | A     | 901 | 1/1   | 0.96 | 0.10 | -0.08 | 25,25,25,25                | 0     |

### 5.5 Other polymers [i](#)

There are no such residues in this entry.