



# Full wwPDB X-ray Structure Validation Report ⓘ

Apr 27, 2026 – 07:35 PM EDT

PDB ID : 2PE8 / pdb\_00002pe8  
Title : Crystal structure of the UHM domain of human SPF45 (free form)  
Authors : Corsini, L.; Basquin, J.; Hothorn, M.; Sattler, M.  
Deposited on : 2007-04-02  
Resolution : 2.00 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

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

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>.

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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)               | : | 2.0                                                              |
| EDS                            | : | <b>FAILED</b>                                                    |
| Percentile statistics          | : | 20250101.v01 (using entries in the PDB archive January 1st 2025) |
| Ideal geometry (proteins)      | : | Engh & Huber (2001)                                              |
| Ideal geometry (DNA, RNA)      | : | Parkinson et al. (1996)                                          |
| Validation Pipeline (wwPDB-VP) | : | 2.49                                                             |

## 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 2.00 Å.

There are no overall percentile quality scores available for this entry.

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 791 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 Splicing factor 45.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 1   | A     | 101      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 761   | 487 | 128 | 140 | 6 |         |         |       |

There are 4 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment          | Reference  |
|-------|---------|----------|--------|------------------|------------|
| A     | 297     | GLY      | -      | cloning artifact | UNP Q96I25 |
| A     | 298     | ALA      | -      | cloning artifact | UNP Q96I25 |
| A     | 299     | MET      | -      | cloning artifact | UNP Q96I25 |
| A     | 300     | GLY      | -      | cloning artifact | UNP Q96I25 |

- Molecule 2 is water.

| Mol | Chain | Residues | Atoms |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 2   | A     | 30       | Total | O  | 0       | 0       |
|     |       |          | 30    | 30 |         |         |

SEQUENCE-PLOTS INFOmissingINFO

### 3 Data and refinement statistics

EDS failed to run properly - this section is therefore incomplete.

| Property                                                 | Value                                                       | Source    |
|----------------------------------------------------------|-------------------------------------------------------------|-----------|
| Space group                                              | F 2 2 2                                                     | Depositor |
| Cell constants<br>a, b, c, $\alpha$ , $\beta$ , $\gamma$ | 63.90Å 90.20Å 99.10Å<br>90.00° 90.00° 90.00°                | Depositor |
| Resolution (Å)                                           | 19.58 – 2.00                                                | Depositor |
| % Data completeness<br>(in resolution range)             | 100.0 (19.58-2.00)                                          | Depositor |
| $R_{merge}$                                              | 0.06                                                        | Depositor |
| $R_{sym}$                                                | 0.05                                                        | Depositor |
| $\langle I/\sigma(I) \rangle$ <sup>1</sup>               | 4.67 (at 2.01Å)                                             | Xtriage   |
| Refinement program                                       | REFMAC 5.2.0019                                             | Depositor |
| R, $R_{free}$                                            | 0.231 , 0.243                                               | Depositor |
| Wilson B-factor (Å <sup>2</sup> )                        | 47.8                                                        | Xtriage   |
| Anisotropy                                               | 0.550                                                       | Xtriage   |
| L-test for twinning <sup>2</sup>                         | $\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$ | Xtriage   |
| Estimated twinning fraction                              | No twinning to report.                                      | Xtriage   |
| Total number of atoms                                    | 791                                                         | wwPDB-VP  |
| Average B, all atoms (Å <sup>2</sup> )                   | 57.0                                                        | wwPDB-VP  |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.74% 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](#)

MolProbity failed to run properly - this section is therefore empty.

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

MolProbity failed to run properly - this section is therefore empty.

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

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

MolProbity failed to run properly - this section is therefore empty.

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

MolProbity failed to run properly - this section is therefore empty.

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

MolProbity failed to run properly - this section is therefore empty.

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

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

### 4.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

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

There are no ligands in this entry.

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

There are no such residues in this entry.

## 4.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

## 5 Fit of model and data

### 5.1 Protein, DNA and RNA chains

EDS failed to run properly - this section is therefore empty.

### 5.2 Non-standard residues in protein, DNA, RNA chains

EDS failed to run properly - this section is therefore empty.

### 5.3 Carbohydrates

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### 5.4 Ligands

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### 5.5 Other polymers

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