



# Full wwPDB Geometry-Only Validation Report ⓘ

Apr 15, 2026 – 10:25 AM UTC

PDB ID : 2VS2 / pdb\_00002vs2  
Title : Neutron diffraction structure of endothiapepsin in complex with a gem- diol inhibitor.  
Authors : Coates, L.; Tuan, H.-F.; Tomanicek, S.; Kovalevsky, A.; Mustyakimov, M.; Erskine, P.; Cooper, J.  
Deposited on : 2008-04-17  
Resolution : 2.00 Å(reported)

This is a Full wwPDB Geometry-Only 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 : **FAILED**  
Mogul : 2022.3.0, CSD as543be (2022)  
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:

*NEUTRON DIFFRACTION*

The reported resolution of this entry is 2.00 Å.

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

MolProbity failed to run properly; EDS was not executed - the sequence quality summary graphics cannot be shown.

## 2 Entry composition [i](#)

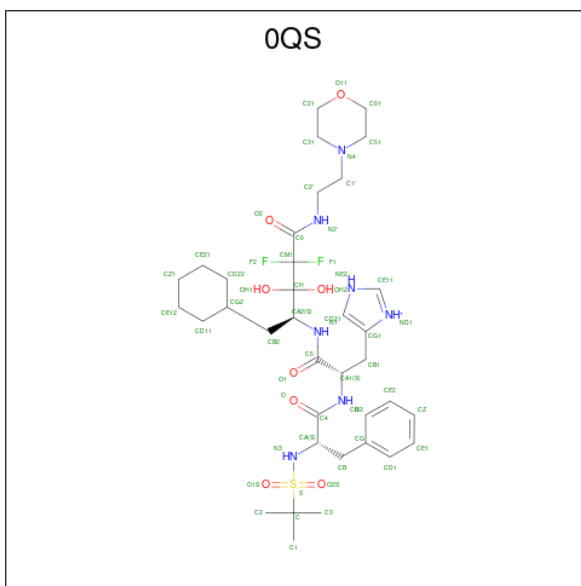
There are 3 unique types of molecules in this entry. The entry contains 5876 atoms, of which 2303 are hydrogens and 911 are deuteriums.

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 ENDOTHIAPEPSIN.

Mol	Chain	Residues	Atoms								ZeroOcc	AltConf	Trace
			Total	C	D	H	N	O	S				
1	A	329	5107	1514	468	2251	366	506	2	0	299	0	

- Molecule 2 is N 2 -[(2R)-2-benzyl-3-(tert-butylsulfonyl)propanoyl]-N-{(1R)-1-(cyclohexylmethyl)-3,3-difluoro-2,2-dihydroxy-4-[(2-morpholin-4-ylethyl)amino]-4-oxobutyl}-3-(1H-imidazol-3-ium-4-yl)-L-alaninamide (CCD ID: 0QS) (formula: C<sub>36</sub>H<sub>56</sub>F<sub>2</sub>N<sub>7</sub>O<sub>8</sub>S).



Mol	Chain	Residues	Atoms								ZeroOcc	AltConf
			Total	C	D	F	H	N	O	S		
2	A	1	109	36	3	2	52	7	8	1	0	1

- Molecule 3 is water.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	D	O		
3	A	220	660	440	220	0	0

MolProbity failed to run properly; EDS was not executed - this section is therefore empty.

### 3 Model quality [i](#)

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

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

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

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

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

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

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

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

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

##### 3.3.3 RNA [i](#)

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

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

2 non-standard protein/DNA/RNA residues are modelled in this entry.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

#### 3.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

### 3.6 Ligand geometry

2 ligands are modelled in this entry.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

### 3.7 Other polymers

There are no such residues in this entry.

### 3.8 Polymer linkage issues

There are no chain breaks in this entry.