



wwPDB X-ray Structure Validation Summary Report ⓘ

Apr 15, 2026 – 10:35 AM UTC

PDB ID : 1CMV / pdb_00001cmv
Title : HUMAN CYTOMEGALOVIRUS PROTEASE
Authors : Shieh, H.-S.; Kurumbail, R.G.; Stevens, A.M.; Stegeman, R.A.; Sturman, E.J.;
Pak, J.Y.; Wittwer, A.J.; Palmier, M.O.; Wiegand, R.C.; Holwerda, B.C.;
Stallings, W.C.
Deposited on : 1996-08-26
Resolution : 2.27 Å(reported)

This is a wwPDB X-ray 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

<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>.

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

MolProbity : **FAILED**
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
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 2.27 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

There are 2 unique types of molecules in this entry. The entry contains 3914 atoms, of which 748 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 HUMAN CYTOMEGALOVIRUS PROTEASE.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	197	Total	C	H	N	O	S	0	0	0
			1887	972	349	280	282	4			
1	B	206	Total	C	H	N	O	S	0	0	0
			1973	1015	363	292	299	4			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	141	ALA	VAL	conflict	UNP P16753
A	144	PRO	ALA	conflict	UNP P16753
B	141	ALA	VAL	conflict	UNP P16753
B	144	PRO	ALA	conflict	UNP P16753

- Molecule 2 is water.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	7	Total	H	O	0	0
			21	14	7		
2	B	11	Total	H	O	0	0
			33	22	11		

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

3 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α , β , γ	76.80Å 76.80Å 172.60Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	8.00 – 2.27	Depositor
% Data completeness (in resolution range)	(Not available) (8.00-2.27)	Depositor
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR 3.1	Depositor
R, R_{free}	0.241 , 0.310	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	3914	wwPDB-VP
Average B, all atoms (Å ²)	24.0	wwPDB-VP

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 was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

5.3 Carbohydrates ⓘ

EDS was not executed - this section is therefore empty.

5.4 Ligands ⓘ

EDS was not executed - this section is therefore empty.

5.5 Other polymers ⓘ

EDS was not executed - this section is therefore empty.