



wwPDB X-ray Structure Validation Summary Report ⓘ

Oct 17, 2021 – 05:11 AM EDT

PDB ID : 1IED
Title : CRYSTAL STRUCTURE OF THE CATALYTIC SITE MUTANT (H157E)
OF THE HUMAN CYTOMEGALOVIRUS PROTEASE
Authors : Khayat, R.; Batra, R.; Massariol, M.J.; Lagace, L.; Tong, L.
Deposited on : 2001-04-09
Resolution : 2.00 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Xtrriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.23.2

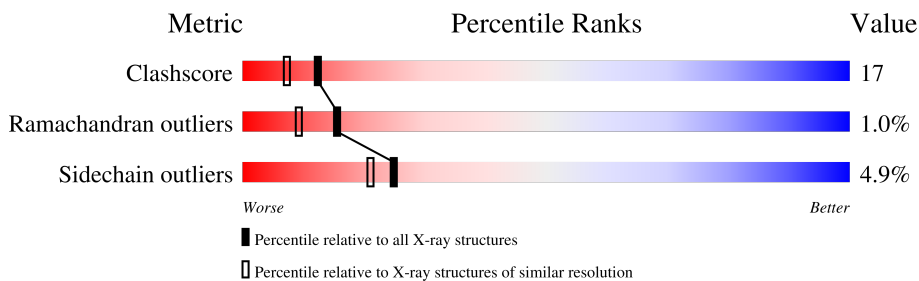
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 Å.

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)	Similar resolution (#Entries, resolution range(Å))
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. 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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	256	
1	B	256	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 3618 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 CAPSID PROTEIN P40: ASSEMBLIN PROTEASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	214	1679	1058	305	312	4	0	0	0
1	B	223	1742	1093	313	332	4	0	0	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	143	GLN	ALA	engineered mutation	UNP P16753
A	157	GLU	HIS	engineered mutation	UNP P16753
B	443	GLN	ALA	engineered mutation	UNP P16753
B	457	GLU	HIS	engineered mutation	UNP P16753

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	92	Total 92	O 92	0	0
2	B	105	Total 105	O 105	0	0

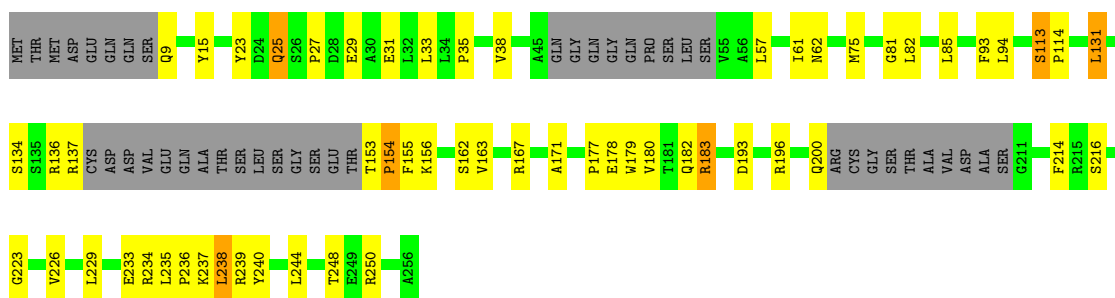
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-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 outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

Note EDS was not executed.

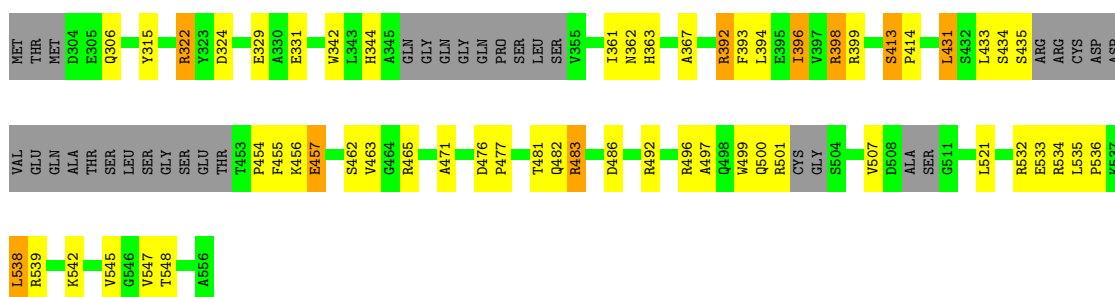
- Molecule 1: CAPSID PROTEIN P40: ASSEMBLIN PROTEASE

Chain A:  61% 20% 16%



- Molecule 1: CAPSID PROTEIN P40: ASSEMBLIN PROTEASE

Chain B:  65% 19% 13%



4 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	76.20Å 76.20Å 170.60Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.23 – 2.00	Depositor
% Data completeness (in resolution range)	87.0 (29.23-2.00)	Depositor
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.226 , 0.269	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	3618	wwPDB-VP
Average B, all atoms (Å ²)	29.0	wwPDB-VP

5 Model quality [i](#)

5.1 Standard geometry [i](#)

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.34	0/1713	0.59	0/2321
1	B	0.35	0/1775	0.59	0/2405
All	All	0.34	0/3488	0.59	0/4726

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 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 the 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 within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1679	0	1665	62	0
1	B	1742	0	1712	54	0
2	A	92	0	0	1	0
2	B	105	0	0	5	0
All	All	3618	0	3377	115	0

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 17.

The worst 5 of 115 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:398:ARG:HH11	1:B:398:ARG:HB3	1.27	0.97

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:248:THR:HG22	1:A:250:ARG:H	1.31	0.96
1:A:156:LYS:HA	1:A:156:LYS:HE2	1.65	0.79
1:B:398:ARG:HH12	1:B:399:ARG:HG3	1.48	0.79
1:A:163:VAL:HG11	1:A:234:ARG:HG3	1.65	0.79

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 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 X-ray entries followed by that with respect to entries of similar resolution.

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	206/256 (80%)	190 (92%)	14 (7%)	2 (1%)	15 9
1	B	213/256 (83%)	202 (95%)	9 (4%)	2 (1%)	17 11
All	All	419/512 (82%)	392 (94%)	23 (6%)	4 (1%)	15 9

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	113	SER
1	B	413	SER
1	A	154	PRO
1	B	344	HIS

5.3.2 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 X-ray entries followed by that with respect to entries of similar resolution.

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	180/215 (84%)	174 (97%)	6 (3%)	38	37
1	B	188/215 (87%)	176 (94%)	12 (6%)	17	13
All	All	368/430 (86%)	350 (95%)	18 (5%)	25	21

5 of 18 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	431	LEU
1	B	538	LEU
1	B	483	ARG
1	B	324	ASP
1	B	398	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 8 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	482	GLN
1	B	362	ASN
1	A	224	ASN
1	A	182	GLN
1	B	306	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.