



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 04:01 AM UTC

PDB ID : 1IEG / pdb_00001ieg
Title : CRYSTAL STRUCTURE OF THE CATALYTIC SITE MUTANT
S134A/H157A OF THE HUMAN CYTOMEGALOVIRUS PROTEASE
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Deposited on : 2001-04-09
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

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	:	4-5-2 with Phenix2.0
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

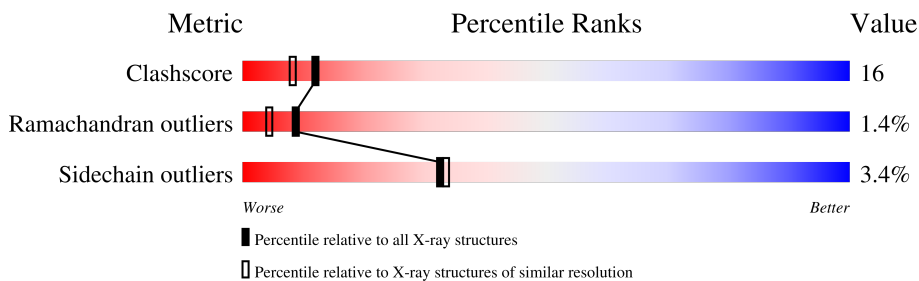
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (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 3576 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
1	A	207	Total	C	N	O	S	0	3	0
			1650	1041	302	303	4			
1	B	223	Total	C	N	O	S	0	2	0
			1743	1093	313	332	5			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	134	ALA	SER	engineered mutation	UNP P16753
A	143	GLN	ALA	engineered mutation	UNP P16753
A	157	ALA	HIS	engineered mutation	UNP P16753
B	434	ALA	SER	engineered mutation	UNP P16753
B	443	GLN	ALA	engineered mutation	UNP P16753
B	457	ALA	HIS	engineered mutation	UNP P16753

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	89	Total	O	0	0
			89	89		
2	B	94	Total	O	0	0
			94	94		

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	76.00Å 76.00Å 167.60Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.72 – 2.00	Depositor
% Data completeness (in resolution range)	96.4 (19.72-2.00)	Depositor
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.226 , 0.259	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	3576	wwPDB-VP
Average B, all atoms (Å ²)	26.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

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	0.37	0/1683	0.89	5/2278 (0.2%)
1	B	0.36	0/1776	0.87	6/2408 (0.2%)
All	All	0.36	0/3459	0.88	11/4686 (0.2%)

There are no bond length outliers.

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	66	THR	N-CA-C	-7.75	103.89	112.72
1	B	413	SER	N-CA-C	6.72	124.67	109.81
1	A	113	SER	N-CA-C	6.00	123.07	109.81
1	B	484	PHE	CA-C-N	5.83	125.69	119.28
1	B	484	PHE	C-N-CA	5.83	125.69	119.28
1	A	160	LEU	N-CA-C	-5.79	99.85	109.46
1	B	320	LEU	N-CA-C	-5.53	106.38	113.23
1	A	20	LEU	N-CA-C	-5.29	106.67	113.23
1	B	500	GLN	N-CA-C	-5.27	106.36	112.89
1	A	119	LYS	N-CA-C	5.19	117.34	111.11
1	B	460	LEU	N-CA-C	-5.11	100.98	109.46

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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	1650	0	1642	64	0
1	B	1743	0	1716	45	0
2	A	89	0	0	2	0
2	B	94	0	0	8	0
All	All	3576	0	3358	106	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 16.

All (106) 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:A:248:THR:HG22	1:A:250:ARG:H	1.24	1.00
1:A:167[B]:ARG:H	1:A:167[B]:ARG:NE	1.65	0.93
1:A:167[B]:ARG:HE	1:A:167[B]:ARG:N	1.71	0.87
1:A:167[B]:ARG:H	1:A:167[B]:ARG:HE	0.86	0.85
1:B:398:ARG:HH11	1:B:398:ARG:HB3	1.42	0.84
1:B:431:LEU:HD13	1:B:471:ALA:HB2	1.62	0.79
1:B:319:PHE:HD1	2:B:1:HOH:O	1.64	0.79
1:A:15:TYR:HD2	1:A:85:LEU:HD11	1.53	0.74
1:A:131:LEU:HD21	1:A:171:ALA:HA	1.71	0.72
1:A:30:ALA:HA	1:A:33:LEU:HD23	1.73	0.71
1:B:398:ARG:HH12	1:B:399:ARG:HG3	1.58	0.69
1:B:319:PHE:CD1	2:B:1:HOH:O	2.44	0.66
1:A:196:ARG:O	1:A:200:GLN:HG3	1.95	0.66
1:B:545:VAL:HG11	2:B:1:HOH:O	1.96	0.65
1:B:523:GLY:O	1:B:526:VAL:HG12	1.98	0.64
1:B:465:ARG:HD2	2:B:42:HOH:O	1.99	0.63
1:A:223:GLY:O	1:A:226:VAL:HG12	1.99	0.62
1:A:229:LEU:HD23	1:B:529:LEU:HD23	1.81	0.62
1:A:134:ALA:O	1:A:156:LYS:HB3	2.00	0.62
1:B:339:VAL:O	1:B:343:LEU:HB2	2.01	0.60
1:A:75:MET:HE3	1:A:82:LEU:HD21	1.84	0.60
1:B:462:SER:HB2	1:B:534[B]:ARG:HE	1.68	0.59
1:A:163:VAL:HG23	1:A:238:LEU:HD13	1.85	0.58
1:A:183:ARG:HD2	1:A:183:ARG:N	2.19	0.58
1:A:232:ARG:NE	1:B:539:ARG:HH22	2.02	0.57
1:A:162:SER:HB2	1:A:234[A]:ARG:HE	1.67	0.57
1:A:15:TYR:CD2	1:A:85:LEU:HD11	2.37	0.57
1:A:23:TYR:CE2	1:A:81:GLY:HA2	2.40	0.57
1:A:196:ARG:HA	1:A:199:TRP:CE2	2.39	0.56
1:B:315:TYR:CD2	1:B:477:PRO:HG3	2.41	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:25:GLN:NE2	1:A:244:LEU:HD22	2.21	0.56
1:A:39:VAL:O	1:A:43:LEU:HB2	2.06	0.55
1:B:545:VAL:HG23	1:B:547:VAL:HG23	1.87	0.55
1:A:57:LEU:HD21	1:A:155:PHE:HB2	1.88	0.55
1:A:25:GLN:HG2	1:A:167[B]:ARG:HB2	1.90	0.54
1:B:545:VAL:CG1	2:B:1:HOH:O	2.54	0.54
1:A:23:TYR:CD2	1:A:81:GLY:HA2	2.43	0.54
1:A:30:ALA:HA	1:A:33:LEU:CD2	2.36	0.53
1:A:131:LEU:HD21	1:A:171:ALA:CA	2.39	0.53
1:A:28:ASP:OD2	1:A:28:ASP:N	2.42	0.53
1:B:532:ARG:HG3	1:B:532:ARG:HH11	1.73	0.53
1:B:479:TRP:O	1:B:483:ARG:HD2	2.08	0.52
1:B:431:LEU:HD13	1:B:471:ALA:CB	2.38	0.52
1:A:244:LEU:HD11	2:A:319:HOH:O	2.08	0.52
1:A:58:PRO:HG2	1:A:157:ALA:HB2	1.90	0.52
1:A:189:ALA:HA	1:A:192[B]:ARG:NH1	2.24	0.52
1:B:510:SER:HA	2:B:163:HOH:O	2.10	0.52
1:B:406:LEU:HA	1:B:409:ARG:HH21	1.75	0.52
1:B:453:THR:N	1:B:454:PRO:HD2	2.25	0.52
1:B:336:ARG:O	1:B:340:GLU:HG3	2.10	0.51
1:A:196:ARG:HA	1:A:199:TRP:NE1	2.25	0.51
1:B:357:LEU:HD11	1:B:455:PHE:HB3	1.93	0.50
1:A:233:GLU:C	1:A:236:PRO:HD2	2.37	0.50
1:A:232:ARG:HH11	1:A:233:GLU:H	1.60	0.50
1:B:398:ARG:HB3	1:B:398:ARG:NH1	2.21	0.50
1:A:248:THR:HG21	1:A:250:ARG:CZ	2.42	0.50
1:A:179:TRP:O	1:A:183:ARG:CD	2.60	0.49
1:B:535:LEU:O	1:B:539:ARG:HG3	2.12	0.49
1:A:113:SER:OG	1:A:114:PRO:HD3	2.12	0.49
1:B:532:ARG:HG3	1:B:533:GLU:HG2	1.95	0.49
1:A:85:LEU:HD13	1:A:86:GLY:N	2.29	0.48
1:B:463:VAL:HG23	1:B:538:LEU:HD13	1.95	0.48
1:B:366:THR:HG22	1:B:515:ARG:NH2	2.29	0.48
1:A:112:VAL:HG12	1:A:113:SER:OG	2.13	0.48
1:B:514:PHE:CZ	1:B:516:SER:HB3	2.49	0.48
1:A:235:LEU:O	1:A:239:ARG:HG3	2.15	0.47
1:B:362:ASN:ND2	2:B:22:HOH:O	2.47	0.47
1:B:398:ARG:NH1	1:B:399:ARG:HG3	2.29	0.47
1:A:232:ARG:NH1	1:A:233:GLU:H	2.12	0.46
1:A:9:GLN:CD	1:A:11:VAL:HG22	2.41	0.46
1:B:542:LYS:HG2	1:B:548:THR:HG23	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:214:PHE:CZ	1:A:216:SER:HB3	2.51	0.46
1:A:131:LEU:HD22	1:A:131:LEU:N	2.31	0.46
1:B:322:ARG:NH2	1:B:486:ASP:OD2	2.43	0.46
1:B:535:LEU:HB2	1:B:536:PRO:HD3	1.97	0.45
1:A:36:ARG:HG2	1:A:40:GLU:OE2	2.17	0.45
1:A:113:SER:CB	1:A:114:PRO:HD3	2.47	0.45
1:B:532:ARG:HH11	1:B:533:GLU:HG2	1.82	0.45
1:A:249:GLU:HG2	1:A:254:VAL:O	2.17	0.44
1:A:15:TYR:HD2	1:A:85:LEU:CD1	2.26	0.44
1:A:131:LEU:HD22	1:A:171:ALA:HB2	1.99	0.44
1:A:25:GLN:HE21	1:A:240:TYR:HE2	1.66	0.44
1:B:496:ARG:HA	1:B:499:TRP:NE1	2.33	0.44
1:B:315:TYR:CE2	1:B:477:PRO:HG3	2.52	0.43
1:A:183:ARG:HH21	1:A:251:GLU:HB2	1.84	0.43
1:A:63:HIS:CE1	1:A:134:ALA:HB2	2.53	0.43
1:B:413:SER:CB	1:B:414:PRO:CD	2.96	0.43
1:A:58:PRO:HG2	1:A:157:ALA:CB	2.49	0.43
1:A:30:ALA:O	1:A:33:LEU:HD23	2.18	0.43
1:A:248:THR:HG22	1:A:250:ARG:N	2.09	0.43
1:A:66:THR:C	2:A:345:HOH:O	2.62	0.43
1:B:342:TRP:HB3	1:B:454:PRO:HG3	2.00	0.43
1:A:27:PRO:HG2	1:A:33:LEU:HD22	2.00	0.42
1:A:113:SER:OG	1:A:114:PRO:CD	2.67	0.42
1:A:232:ARG:NE	1:B:539:ARG:NH2	2.67	0.42
1:A:30:ALA:CA	1:A:33:LEU:HD23	2.44	0.42
1:A:179:TRP:O	1:A:183:ARG:HD2	2.19	0.42
1:A:167[A]:ARG:NE	1:A:167[A]:ARG:HA	2.34	0.42
1:B:506:ALA:O	1:B:509:ALA:HB2	2.19	0.42
1:B:534[A]:ARG:HH11	1:B:534[A]:ARG:HB2	1.85	0.42
1:A:75:MET:CE	1:A:82:LEU:HD21	2.49	0.42
1:A:178:GLU:O	1:A:182:GLN:HG2	2.20	0.41
1:B:483:ARG:O	1:B:485:PRO:HD3	2.20	0.41
1:B:467:ARG:NE	1:B:467:ARG:HA	2.35	0.41
1:B:327:PRO:N	2:B:4:HOH:O	2.54	0.40
1:A:27:PRO:N	1:A:167[B]:ARG:NH1	2.69	0.40

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	202/256 (79%)	188 (93%)	10 (5%)	4 (2%)	6	2
1	B	217/256 (85%)	205 (94%)	10 (5%)	2 (1%)	14	9
All	All	419/512 (82%)	393 (94%)	20 (5%)	6 (1%)	9	4

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	113	SER
1	B	413	SER
1	B	509	ALA
1	A	156	LYS
1	A	114	PRO
1	A	155	PHE

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	175/213 (82%)	171 (98%)	4 (2%)	44	49
1	B	187/213 (88%)	179 (96%)	8 (4%)	26	25
All	All	362/426 (85%)	350 (97%)	12 (3%)	32	34

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	25	GLN
1	A	62	ASN
1	A	85	LEU
1	A	238	LEU
1	B	306	GLN
1	B	322	ARG
1	B	362	ASN
1	B	394	LEU
1	B	398	ARG
1	B	431	LEU
1	B	483	ARG
1	B	538	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	25	GLN
1	A	62	ASN
1	A	76	GLN
1	A	116	GLN
1	A	182	GLN
1	A	224	ASN
1	A	243	GLN
1	B	362	ASN
1	B	482	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 oligosaccharides in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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.