



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 5, 2025 – 02:09 PM EDT

PDB ID : 9N3E / pdb_00009n3e
Title : Crystal structure of Arabidopsis metacaspase 9 C147G at pH 5.5
Authors : Liu, H.; Liu, Q.
Deposited on : 2025-01-30
Resolution : 1.55 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 Phenix2.0rc1
Xtriage (Phenix) : 2.0rc1
EDS : 3.0
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4 : 9.0.006 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.43.1

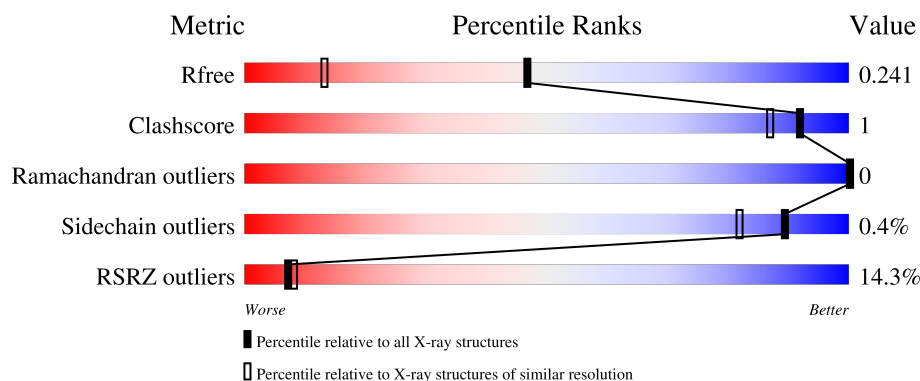
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.55 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))
R_{free}	164625	1935 (1.56-1.56)
Clashscore	180529	2073 (1.56-1.56)
Ramachandran outliers	177936	2037 (1.56-1.56)
Sidechain outliers	177891	2034 (1.56-1.56)
RSRZ outliers	164620	1935 (1.56-1.56)

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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	325	<div> <div>17%</div> <div>92%</div> <div>5%</div> </div>
1	B	325	<div> <div>11%</div> <div>94%</div> <div>.</div> </div>

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 5220 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 Metacaspase-9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	314	Total	C	N	O	S	0	0	0
			2402	1498	421	466	17			
1	B	317	Total	C	N	O	S	0	0	0
			2419	1508	424	470	17			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	147	GLY	CYS	engineered mutation	UNP Q9FYE1
B	147	GLY	CYS	engineered mutation	UNP Q9FYE1

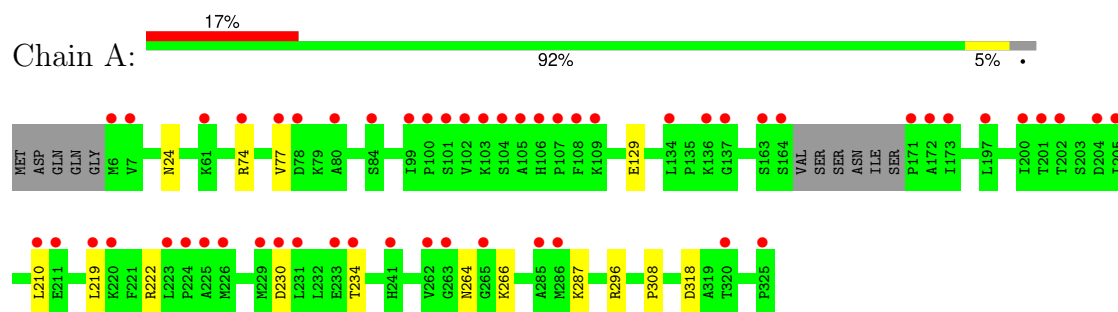
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	203	Total	O	0	0
			203	203		
2	B	196	Total	O	0	0
			196	196		

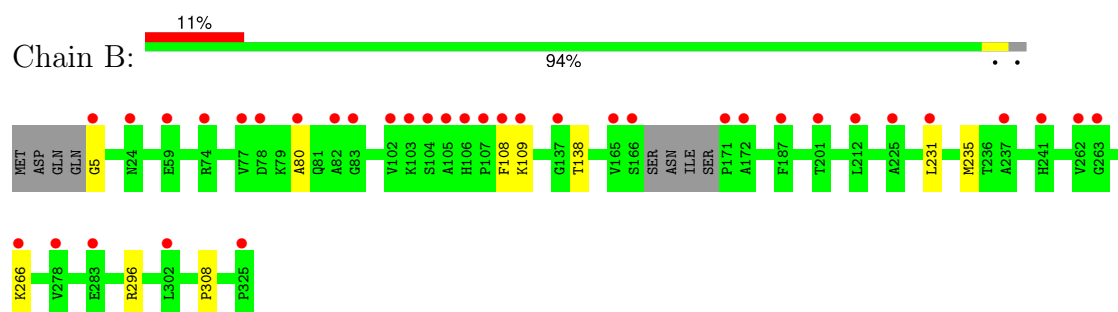
3 Residue-property plots [i](#)

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 and electron density. 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. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). 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.

• Molecule 1: Metacaspase-9



• Molecule 1: Metacaspase-9



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	58.63Å 89.05Å 64.69Å 90.00° 97.87° 90.00°	Depositor
Resolution (Å)	29.84 – 1.55 29.84 – 1.55	Depositor EDS
% Data completeness (in resolution range)	97.8 (29.84-1.55) 97.9 (29.84-1.55)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.37 (at 1.55Å)	Xtriage
Refinement program	PHENIX 1.18.2	Depositor
R, R_{free}	0.233 , 0.240 0.233 , 0.241	Depositor DCC
R_{free} test set	4762 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	17.6	Xtriage
Anisotropy	0.463	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 27.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	5220	wwPDB-VP
Average B, all atoms (Å ²)	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.70% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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.

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	0.09	0/2441	0.28	0/3289
1	B	0.08	0/2458	0.27	0/3312
All	All	0.09	0/4899	0.27	0/6601

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	2402	0	2394	8	0
1	B	2419	0	2411	6	0
2	A	203	0	0	0	0
2	B	196	0	0	1	0
All	All	5220	0	4805	14	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 1.

All (14) 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:108:PHE:HD2	1:B:109:LYS:HG3	1.59	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:74:ARG:O	1:A:77:VAL:HG22	1.99	0.61
1:B:108:PHE:CD2	1:B:109:LYS:HG3	2.42	0.53
1:A:210:LEU:HD21	1:A:222:ARG:HA	1.92	0.52
1:A:74:ARG:HA	1:A:77:VAL:HG22	1.92	0.52
1:B:5:GLY:N	2:B:403:HOH:O	2.43	0.51
1:B:296:ARG:HG2	1:B:308:PRO:HD2	1.96	0.47
1:A:129:GLU:CD	1:A:219:LEU:HD11	2.40	0.46
1:A:230:ASP:O	1:A:234:THR:HG23	2.14	0.46
1:A:264:ASN:HD21	1:A:266:LYS:HE3	1.83	0.44
1:B:231:LEU:HG	1:B:235:MET:HE3	2.00	0.43
1:A:287:LYS:HD3	1:A:318:ASP:HA	2.01	0.42
1:B:80:ALA:HB1	1:B:138:THR:HG21	1.99	0.42
1:A:296:ARG:HG2	1:A:308:PRO:HD2	2.01	0.42

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	310/325 (95%)	307 (99%)	3 (1%)	0	100	100
1	B	313/325 (96%)	309 (99%)	4 (1%)	0	100	100
All	All	623/650 (96%)	616 (99%)	7 (1%)	0	100	100

There are no Ramachandran outliers to report.

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	265/275 (96%)	264 (100%)	1 (0%)	89	82
1	B	267/275 (97%)	266 (100%)	1 (0%)	89	82
All	All	532/550 (97%)	530 (100%)	2 (0%)	89	82

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	24	ASN
1	B	266	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	282	ASN
1	B	24	ASN
1	B	110	GLN
1	B	276	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

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 ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	314/325 (96%)	1.14	54 (17%) 5 5	15, 25, 46, 70	0
1	B	317/325 (97%)	0.93	36 (11%) 11 13	15, 24, 43, 92	0
All	All	631/650 (97%)	1.04	90 (14%) 7 8	15, 25, 45, 92	0

All (90) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	108	PHE	10.4
1	A	105	ALA	7.6
1	B	137	GLY	6.9
1	A	325	PRO	6.3
1	B	105	ALA	6.3
1	A	7	VAL	5.9
1	A	102	VAL	5.6
1	A	226	MET	5.1
1	A	77	VAL	5.0
1	A	108	PHE	5.0
1	B	107	PRO	4.9
1	A	265	GLY	4.6
1	B	104	SER	4.6
1	A	171	PRO	4.5
1	B	171	PRO	4.5
1	A	103	LYS	4.4
1	A	106	HIS	4.3
1	A	137	GLY	4.2
1	A	107	PRO	4.2
1	B	106	HIS	4.0
1	B	109	LYS	4.0
1	A	104	SER	3.7
1	A	234	THR	3.6
1	A	201	THR	3.6

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Mol	Chain	Res	Type	RSRZ
1	A	78	ASP	3.6
1	B	5	GLY	3.6
1	A	220	LYS	3.5
1	A	229	MET	3.5
1	A	100	PRO	3.4
1	A	163	SER	3.4
1	A	230	ASP	3.4
1	B	201	THR	3.3
1	A	262	VAL	3.3
1	A	200	ILE	3.2
1	B	172	ALA	3.2
1	B	103	LYS	3.1
1	A	99	ILE	3.1
1	B	237	ALA	3.0
1	B	263	GLY	3.0
1	A	219	LEU	3.0
1	B	59	GLU	3.0
1	B	77	VAL	2.9
1	B	102	VAL	2.9
1	A	223	LEU	2.9
1	A	172	ALA	2.8
1	A	74	ARG	2.8
1	A	101	SER	2.8
1	A	205	ILE	2.8
1	A	204	ASP	2.8
1	B	325	PRO	2.8
1	A	80	ALA	2.8
1	B	166	SER	2.7
1	A	61	LYS	2.7
1	A	263	GLY	2.7
1	A	225	ALA	2.7
1	B	78	ASP	2.6
1	B	165	VAL	2.6
1	B	262	VAL	2.6
1	A	231	LEU	2.6
1	B	241	HIS	2.6
1	A	285	ALA	2.5
1	A	164	SER	2.5
1	A	109	LYS	2.4
1	A	136	LYS	2.3
1	A	224	PRO	2.3
1	A	233	GLU	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	266	LYS	2.3
1	B	278	VAL	2.3
1	A	202	THR	2.3
1	B	74	ARG	2.3
1	B	283	GLU	2.2
1	B	80	ALA	2.2
1	B	302	LEU	2.2
1	A	211	GLU	2.2
1	A	320	THR	2.2
1	B	82	ALA	2.2
1	A	241	HIS	2.2
1	A	6	MET	2.2
1	A	134	LEU	2.2
1	A	173	ILE	2.2
1	A	197	LEU	2.1
1	B	231	LEU	2.1
1	A	286	MET	2.1
1	A	84	SER	2.1
1	B	187	PHE	2.1
1	B	225	ALA	2.1
1	A	210	LEU	2.1
1	B	212	LEU	2.1
1	B	83	GLY	2.1
1	B	24	ASN	2.0

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

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

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.