



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 13, 2025 – 04:05 PM EDT

PDB ID : 9E0V / pdb_00009e0v
Title : GSDMD bound to a peptide
Authors : Wang, R.
Deposited on : 2024-10-19
Resolution : 1.64 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
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.46

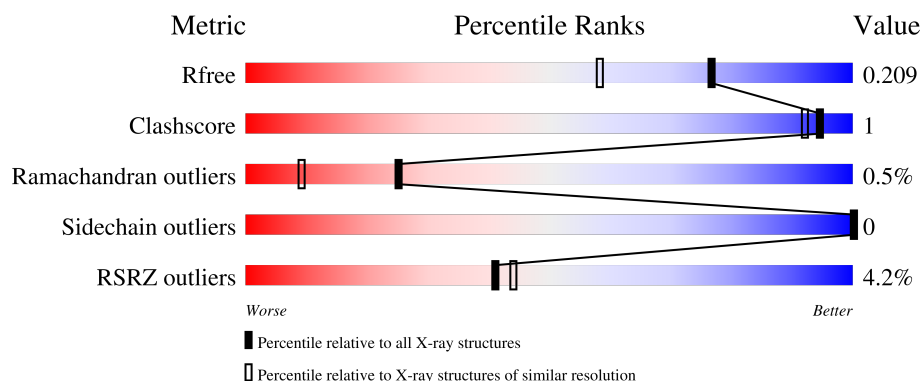
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.64 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	1015 (1.64-1.64)
Clashscore	180529	1093 (1.64-1.64)
Ramachandran outliers	177936	1077 (1.64-1.64)
Sidechain outliers	177891	1077 (1.64-1.64)
RSRZ outliers	164620	1015 (1.64-1.64)

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	590	
2	B	11	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 1759 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 Maltose/maltodextrin-binding periplasmic protein, Gasdermin-D, C-terminal chimera.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	204	Total	C	N	O	S	0	1	0
			1529	970	245	304	10			

There are 29 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-105	MET	-	expression tag	UNP P0AEX9
A	-104	ALA	-	expression tag	UNP P0AEX9
A	-103	HIS	-	expression tag	UNP P0AEX9
A	-102	HIS	-	expression tag	UNP P0AEX9
A	-101	HIS	-	expression tag	UNP P0AEX9
A	-100	HIS	-	expression tag	UNP P0AEX9
A	-99	HIS	-	expression tag	UNP P0AEX9
A	-98	HIS	-	expression tag	UNP P0AEX9
A	-97	LYS	-	expression tag	UNP P0AEX9
A	-96	THR	-	expression tag	UNP P0AEX9
A	-16	ALA	ASP	conflict	UNP P0AEX9
A	-15	ALA	LYS	conflict	UNP P0AEX9
A	74	ALA	GLU	conflict	UNP P0AEX9
A	75	ALA	ASN	conflict	UNP P0AEX9
A	117	HIS	ALA	conflict	UNP P0AEX9
A	121	HIS	LYS	conflict	UNP P0AEX9
A	141	ALA	LYS	conflict	UNP P0AEX9
A	214	VAL	ALA	conflict	UNP P0AEX9
A	219	VAL	ILE	conflict	UNP P0AEX9
A	261	ALA	GLU	conflict	UNP P0AEX9
A	264	ALA	LYS	conflict	UNP P0AEX9
A	265	ALA	ASP	conflict	UNP P0AEX9
A	269	GLU	-	linker	UNP P0AEX9
A	270	ASN	-	linker	UNP P0AEX9
A	271	LEU	-	linker	UNP P0AEX9
A	272	TYR	-	linker	UNP P0AEX9

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Chain	Residue	Modelled	Actual	Comment	Reference
A	273	PHE	-	linker	UNP P0AEX9
A	274	GLN	-	linker	UNP P0AEX9
A	275	GLY	-	linker	UNP P0AEX9

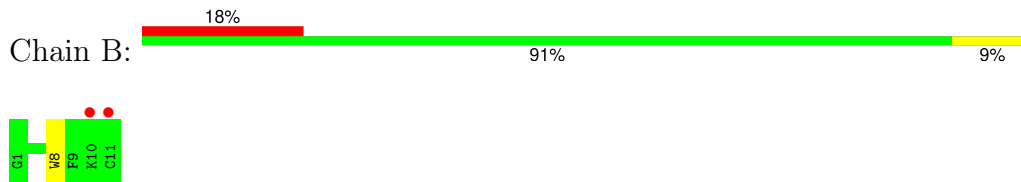
- Molecule 2 is a protein called GLY-CYS-ILE-LYS-LYS-ALA-VAL-6CW-PHE-LYS-CYS.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	B	11	Total	C	Cl	N	O	S	0	0	0
			89	60	1	15	11	2			

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	133	Total	O	0	0
			133	133		
3	B	8	Total	O	0	0
			8	8		

- Molecule 1: Maltose/maltodextrin-binding periplasmic protein, Gasdermin-D, C-terminal chimera



4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α , β , γ	47.58Å 47.58Å 194.72Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.19 – 1.64 19.19 – 1.64	Depositor EDS
% Data completeness (in resolution range)	89.6 (19.19-1.64) 89.5 (19.19-1.64)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.06 (at 1.64Å)	Xtriage
Refinement program	BUSTER 2.11.8 (10-JUL-2024)	Depositor
R, R_{free}	0.200 , 0.212 0.192 , 0.209	Depositor DCC
R_{free} test set	1268 reflections (4.40%)	wwPDB-VP
Wilson B-factor (Å ²)	22.0	Xtriage
Anisotropy	0.049	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.44 , 43.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	1759	wwPDB-VP
Average B, all atoms (Å ²)	25.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.45% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 6CW

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	0.78	0/1558	0.90	0/2122
2	B	0.49	0/73	0.69	0/92
All	All	0.77	0/1631	0.89	0/2214

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

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	1529	0	1534	4	0
2	B	89	0	97	0	0
3	A	133	0	0	0	0
3	B	8	0	0	0	0
All	All	1759	0	1631	4	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 (4) 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:420:THR:HG22	1:A:457[A]:CYS:SG	2.41	0.61
1:A:424:PRO:HG2	1:A:427:LEU:HD12	1.89	0.54
1:A:383:GLU:HG2	1:A:387:LYS:HE2	1.92	0.52
1:A:340:GLY:H	1:A:362:MET:HE1	1.85	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	203/590 (34%)	201 (99%)	1 (0%)	1 (0%)	25	9
2	B	8/11 (73%)	8 (100%)	0	0	100	100
All	All	211/601 (35%)	209 (99%)	1 (0%)	1 (0%)	25	9

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	424	PRO

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	166/469 (35%)	166 (100%)	0	100	100
2	B	8/8 (100%)	8 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
All	All	174/477 (36%)	174 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	323	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

1 non-standard protein/DNA/RNA residue is modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	6CW	B	8	2	14,16,17	2.24	5 (35%)	13,22,24	1.31	3 (23%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	6CW	B	8	2	-	0/4/6/8	0/2/2/2

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	8	6CW	CZ3-CH2	3.84	1.45	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	8	6CW	CD1-CG	3.78	1.47	1.37
2	B	8	6CW	CZ2-CH2	3.59	1.43	1.36
2	B	8	6CW	CH2-CLL	-3.06	1.67	1.74
2	B	8	6CW	CE3-CZ3	2.25	1.41	1.36

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	8	6CW	CZ2-CH2-CLL	-2.53	116.60	119.65
2	B	8	6CW	CZ3-CH2-CLL	2.08	122.42	119.36
2	B	8	6CW	CE3-CD2-CE2	2.00	120.83	118.17

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides 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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	204/590 (34%)	0.03	7 (3%) 48 51	13, 22, 37, 49	1 (0%)
2	B	10/11 (90%)	0.62	2 (20%) 3 4	23, 29, 38, 39	0
All	All	214/601 (35%)	0.06	9 (4%) 41 44	13, 22, 37, 49	1 (0%)

All (9) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	339	LEU	5.2
1	A	278	PRO	3.5
1	A	340	GLY	2.7
1	A	280	GLU	2.6
1	A	279	ALA	2.5
1	A	344	PRO	2.2
2	B	11	CYS	2.2
1	A	306	ARG	2.1
2	B	10	LYS	2.1

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q < 0.9’ lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	6CW	B	8	15/16	0.93	0.07	20,21,24,28	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands

There are no ligands in this entry.

6.5 Other polymers

There are no such residues in this entry.