



# wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 9, 2020 – 09:21 AM BST

PDB ID : 6VIE  
Title : Structure of caspase-1 in complex with gasdermin D  
Authors : Liu, Z.; Xiao, T.S.  
Deposited on : 2020-01-13  
Resolution : 3.40 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](mailto: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.

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

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.13.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.13.1

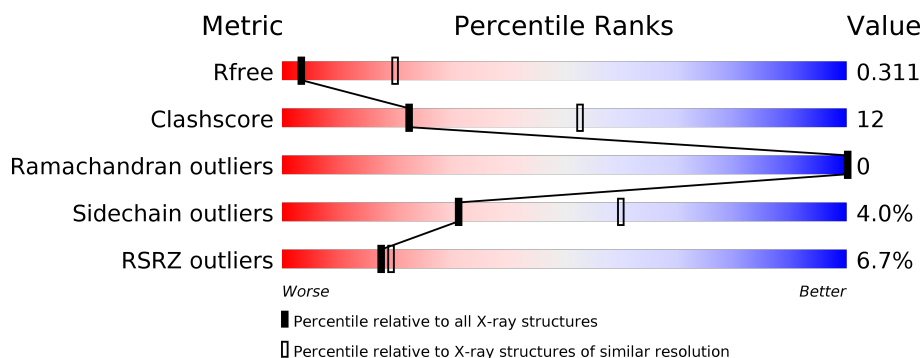
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 3.40 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))
$R_{free}$	130704	1026 (3.48-3.32)
Clashscore	141614	1055 (3.48-3.32)
Ramachandran outliers	138981	1038 (3.48-3.32)
Sidechain outliers	138945	1038 (3.48-3.32)
RSRZ outliers	127900	2173 (3.50-3.30)

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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	198	<div> <div>3%</div> <div> <div></div> <div>73%</div> <div>18%</div> <div>• 8%</div> </div> </div>
2	B	90	<div> <div>%</div> <div> <div></div> <div>80%</div> <div>18%</div> <div>•</div> </div> </div>
3	C	464	<div> <div>6%</div> <div> <div></div> <div>57%</div> <div>26%</div> <div>• 16%</div> </div> </div>
3	D	464	<div> <div>7%</div> <div> <div></div> <div>56%</div> <div>23%</div> <div>• 20%</div> </div> </div>

## 2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 8039 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 Caspase-1 subunit p20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	182	Total	C	N	O	S	0	1	0
			1390	871	244	265	10			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	119	MET	-	initiating methionine	UNP P29466
A	285	ALA	CYS	engineered mutation	UNP P29466

- Molecule 2 is a protein called Caspase-1 subunit p10.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	88	Total	C	N	O	S	0	0	0
			719	457	126	129	7			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	315	GLY	-	expression tag	UNP P29466
B	316	SER	-	expression tag	UNP P29466

- Molecule 3 is a protein called Gasdermin-D.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	389	Total	C	N	O	S	0	0	0
			3020	1909	502	594	15			
3	D	373	Total	C	N	O	S	0	0	0
			2910	1847	487	562	14			

There are 50 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	0	SER	-	expression tag	UNP Q9D8T2
C	?	-	ARG	deletion	UNP Q9D8T2
C	?	-	LYS	deletion	UNP Q9D8T2
C	?	-	ALA	deletion	UNP Q9D8T2
C	?	-	VAL	deletion	UNP Q9D8T2
C	?	-	GLY	deletion	UNP Q9D8T2
C	?	-	GLN	deletion	UNP Q9D8T2
C	?	-	ARG	deletion	UNP Q9D8T2
C	?	-	HIS	deletion	UNP Q9D8T2
C	?	-	HIS	deletion	UNP Q9D8T2
C	?	-	GLY	deletion	UNP Q9D8T2
C	?	-	LEU	deletion	UNP Q9D8T2
C	?	-	ASN	deletion	UNP Q9D8T2
C	?	-	VAL	deletion	UNP Q9D8T2
C	?	-	LEU	deletion	UNP Q9D8T2
C	?	-	ALA	deletion	UNP Q9D8T2
C	?	-	ALA	deletion	UNP Q9D8T2
C	?	-	LEU	deletion	UNP Q9D8T2
C	?	-	CYS	deletion	UNP Q9D8T2
C	?	-	SER	deletion	UNP Q9D8T2
C	?	-	ILE	deletion	UNP Q9D8T2
C	?	-	GLY	deletion	UNP Q9D8T2
C	?	-	LYS	deletion	UNP Q9D8T2
C	?	-	GLN	deletion	UNP Q9D8T2
C	?	-	LEU	deletion	UNP Q9D8T2
D	0	SER	-	expression tag	UNP Q9D8T2
D	?	-	ARG	deletion	UNP Q9D8T2
D	?	-	LYS	deletion	UNP Q9D8T2
D	?	-	ALA	deletion	UNP Q9D8T2
D	?	-	VAL	deletion	UNP Q9D8T2
D	?	-	GLY	deletion	UNP Q9D8T2
D	?	-	GLN	deletion	UNP Q9D8T2
D	?	-	ARG	deletion	UNP Q9D8T2
D	?	-	HIS	deletion	UNP Q9D8T2
D	?	-	HIS	deletion	UNP Q9D8T2
D	?	-	GLY	deletion	UNP Q9D8T2
D	?	-	LEU	deletion	UNP Q9D8T2
D	?	-	ASN	deletion	UNP Q9D8T2
D	?	-	VAL	deletion	UNP Q9D8T2
D	?	-	LEU	deletion	UNP Q9D8T2
D	?	-	ALA	deletion	UNP Q9D8T2
D	?	-	ALA	deletion	UNP Q9D8T2
D	?	-	LEU	deletion	UNP Q9D8T2

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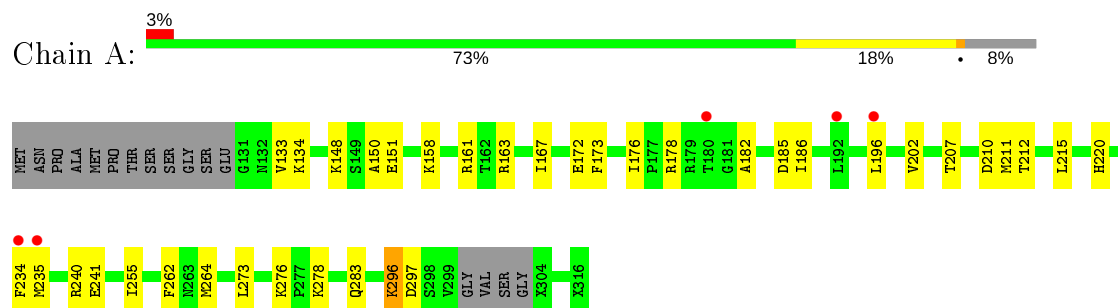
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Chain	Residue	Modelled	Actual	Comment	Reference
D	?	-	CYS	deletion	UNP Q9D8T2
D	?	-	SER	deletion	UNP Q9D8T2
D	?	-	ILE	deletion	UNP Q9D8T2
D	?	-	GLY	deletion	UNP Q9D8T2
D	?	-	LYS	deletion	UNP Q9D8T2
D	?	-	GLN	deletion	UNP Q9D8T2
D	?	-	LEU	deletion	UNP Q9D8T2

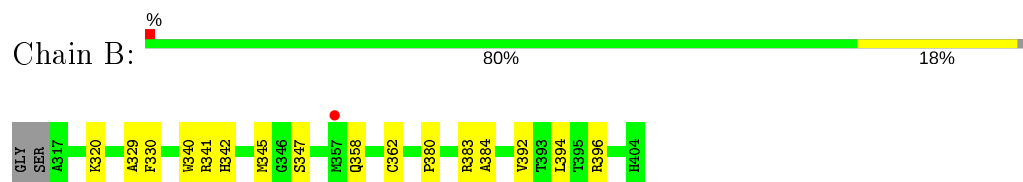
### 3 Residue-property plots [i](#)

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.

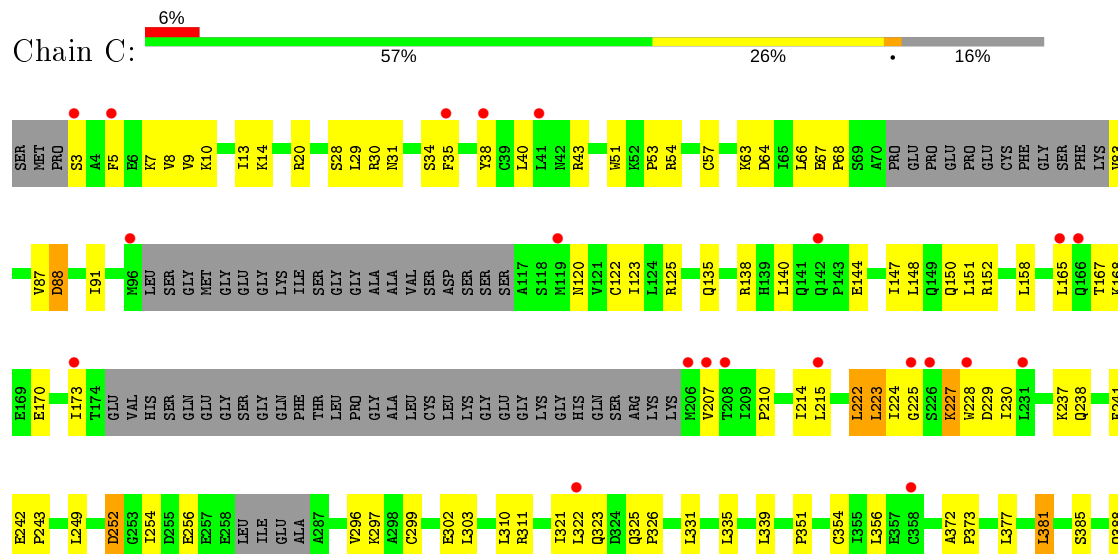
- Molecule 1: Caspase-1 subunit p20



- Molecule 2: Caspase-1 subunit p10



- Molecule 3: Gasdermin-D





## 4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	138.50Å 202.61Å 124.27Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	78.52 – 3.40 84.14 – 3.40	Depositor EDS
% Data completeness (in resolution range)	99.8 (78.52-3.40) 92.1 (84.14-3.40)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	0.91 (at 3.41Å)	Xtriage
Refinement program	PHENIX 1.17.1_3660	Depositor
R, $R_{free}$	0.288 , 0.314 0.288 , 0.311	Depositor DCC
$R_{free}$ test set	1222 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	139.5	Xtriage
Anisotropy	0.247	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.28 , 141.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	8039	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	190.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.98% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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	0.24	0/1352	0.43	0/1822
2	B	0.25	0/739	0.41	0/995
3	C	0.26	0/3065	0.51	0/4153
3	D	0.25	0/2956	0.54	0/4007
All	All	0.25	0/8112	0.50	0/10977

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	1390	0	1361	23	0
2	B	719	0	693	11	0
3	C	3020	0	3043	80	0
3	D	2910	0	2954	82	0
All	All	8039	0	8051	187	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 12.

The worst 5 of 187 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)
3:C:385:SER:HB3	3:C:388:GLN:HE21	1.36	0.91
3:C:385:SER:HB3	3:C:388:GLN:NE2	1.99	0.78
3:D:123:ILE:HG22	3:D:165:LEU:HG	1.67	0.77
3:C:123:ILE:HG22	3:C:165:LEU:HG	1.65	0.76
3:C:91:ILE:HD11	3:C:120:ASN:HB2	1.68	0.76

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	168/198 (85%)	160 (95%)	8 (5%)	0	100	100
2	B	86/90 (96%)	83 (96%)	3 (4%)	0	100	100
3	C	377/464 (81%)	334 (89%)	43 (11%)	0	100	100
3	D	363/464 (78%)	326 (90%)	37 (10%)	0	100	100
All	All	994/1216 (82%)	903 (91%)	91 (9%)	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	151/162 (93%)	146 (97%)	5 (3%)	38	66
2	B	79/80 (99%)	77 (98%)	2 (2%)	47	72

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	C	347/406 (86%)	330 (95%)	17 (5%)	25	55
3	D	334/406 (82%)	322 (96%)	12 (4%)	35	63
All	All	911/1054 (86%)	875 (96%)	36 (4%)	31	60

5 of 36 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	C	297	LYS
3	C	430	LEU
3	D	426	LEU
3	C	323	GLN
3	C	438	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
3	C	388	GLN
3	D	90	ASN

### 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 monosaccharides 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 [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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	169/198 (85%)	0.23	5 (2%) 50 49	91, 150, 197, 249	0
2	B	88/90 (97%)	0.31	1 (1%) 80 79	96, 125, 162, 178	0
3	C	389/464 (83%)	0.41	28 (7%) 15 17	111, 186, 267, 306	0
3	D	373/464 (80%)	0.53	34 (9%) 9 10	133, 221, 292, 325	0
All	All	1019/1216 (83%)	0.42	68 (6%) 17 19	91, 184, 282, 325	0

The worst 5 of 68 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	C	173	ILE	6.3
3	D	423	SER	5.9
3	D	145	ASN	5.8
3	C	418	TRP	5.5
3	D	305	SER	5.5

### 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.