

# Full wwPDB X-ray Structure Validation Report (i)

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PDB ID : 6NS7

Title: Crystal structure of murine caspase-11

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Deposited on : 2019-01-24

Resolution : 2.40 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 (i) 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 (i)) were used in the production of this report:

MolProbity : FAILED

Mogul : 1.8.5 (274361), CSD as541be (2020)

Xtriage (Phenix) : 1.13 EDS : FAILED

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) : 2.35.1

## 1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure: X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 Å.

There are no overall percentile quality scores available for this entry.

MolProbity and EDS failed to run properly - the sequence quality summary graphics cannot be shown.



## 2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 7887 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-11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	244	Total	С	N	О	S	0	0	0
1			1952	1237	336	364	15	0		
1	1 B	242	Total	С	N	О	S	0	0	0
1	Б	242	1940	1231	334	360	15	U		
1	С	242	Total	С	N	О	S	0	0	0
1		242	1940	1231	334	360	15	0	0	U
1	D	D 241	Total	С	N	О	S	0	0	0
		D	241	1932	1227	332	358	15	U	U

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference	
A	90	GLY	-	expression tag	UNP P70343	
A	91	SER	-	expression tag	UNP P70343	
A	254	ALA	CYS	conflict	UNP P70343	
В	90	GLY	-	expression tag	UNP P70343	
В	91	SER	-	expression tag	UNP P70343	
В	254	ALA	CYS	conflict	UNP P70343	
С	90	GLY	-	expression tag	UNP P70343	
С	91	SER	-	expression tag	UNP P70343	
С	254	ALA	CYS	conflict	UNP P70343	
D	90	GLY	-	expression tag	UNP P70343	
D	91	SER	-	expression tag	UNP P70343	
D	254	ALA	CYS	conflict	UNP P70343	

• Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).





Mol	Chain	Residues	Atoms	ZeroOcc	AltConf			
2	Λ	1	Total O S	0	0			
	A		5   4   1	0				
2	В	1	Total O S	0	0			
	Б	1	5   4   1	0				
2	C	1	Total O S	0	n			
	C	C	C	1	5   4   1	0	U	
2	D	1	Total O S	0	0			
		1	5 4 1		U			

#### • Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	
3	A	32	Total O 32 32	0	0	
3	В	39	Total O 39 39	0	0	
3	С	18	Total O 18 18	0	0	
3	D	14	Total O 14 14	0	0	

MolProbity and EDS failed to run properly - this section is therefore empty.



## 3 Data and refinement statistics (i)

EDS failed to run properly - this section is therefore incomplete.

Property	Value	Source	
Space group	P 21 21 2	Depositor	
Cell constants	120.71Å 121.09Å 78.43Å	Depositor	
a, b, c, $\alpha$ , $\beta$ , $\gamma$	$90.00^{\circ}$ $90.00^{\circ}$ $90.00^{\circ}$	Depositor	
Resolution (Å)	47.93 - 2.40	Depositor	
% Data completeness	99.9 (47.93-2.40)	Depositor	
(in resolution range)	, ,	-	
$R_{merge}$	(Not available)	Depositor	
$R_{sym}$	(Not available)	Depositor	
$< I/\sigma(I) > 1$	2.14  (at  2.39Å)	Xtriage	
Refinement program	PHENIX (1.12_2829: ???)	Depositor	
$R, R_{free}$	0.194 , $0.242$	Depositor	
Wilson B-factor $(Å^2)$	52.0	Xtriage	
Anisotropy	0.413	Xtriage	
L-test for twinning <sup>2</sup>	$< L > = 0.49, < L^2> = 0.32$	Xtriage	
Estimated twinning fraction	0.014 for k,h,-l	Xtriage	
Total number of atoms	7887	wwPDB-VP	
Average B, all atoms $(\mathring{A}^2)$	70.0	wwPDB-VP	

Xtriage's analysis on translational NCS is as follows: The analyses of the Patterson function reveals a significant off-origin peak that is 32.51 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 9.2864e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.

<sup>&</sup>lt;sup>2</sup>Theoretical values of <|L|>,  $<L^2>$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.



<sup>&</sup>lt;sup>1</sup>Intensities estimated from amplitudes.

## 4 Model quality (i)

#### 4.1 Standard geometry (i)

MolProbity failed to run properly - this section is therefore empty.

#### 4.2 Too-close contacts (i)

MolProbity failed to run properly - this section is therefore empty.

#### 4.3 Torsion angles (i)

#### 4.3.1 Protein backbone (i)

MolProbity failed to run properly - this section is therefore empty.

#### 4.3.2 Protein sidechains (i)

MolProbity failed to run properly - this section is therefore empty.

#### 4.3.3 RNA (i)

MolProbity failed to run properly - this section is therefore empty.

### 4.4 Non-standard residues in protein, DNA, RNA chains (i)

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

### 4.5 Carbohydrates (i)

There are no monosaccharides in this entry.

### 4.6 Ligand geometry (i)

4 ligands are 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		
MIOI	туре	Chain	nes	LIIIK	Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	SO4	A	401	-	4,4,4	0.23	0	6,6,6	0.51	0
2	SO4	D	401	-	4,4,4	0.19	0	6,6,6	0.37	0
2	SO4	С	401	-	4,4,4	0.14	0	6,6,6	0.29	0
2	SO4	В	401	-	4,4,4	0.19	0	6,6,6	0.24	0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

#### 4.7 Other polymers (i)

There are no such residues in this entry.

### 4.8 Polymer linkage issues (i)

There are no chain breaks in this entry.



## 5 Fit of model and data (i)

#### 5.1 Protein, DNA and RNA chains (i)

EDS failed to run properly - this section is therefore empty.

#### 5.2 Non-standard residues in protein, DNA, RNA chains (i)

EDS failed to run properly - this section is therefore empty.

#### 5.3 Carbohydrates (i)

EDS failed to run properly - this section is therefore empty.

#### 5.4 Ligands (i)

EDS failed to run properly - this section is therefore empty.

### 5.5 Other polymers (i)

EDS failed to run properly - this section is therefore empty.

