



# wwPDB X-ray Structure Validation Summary Report ⓘ

May 13, 2020 – 02:55 am BST

PDB ID : 2FUN  
Title : alternative p35-caspase-8 complex  
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Deposited on : 2006-01-27  
Resolution : 3.00 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) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
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) : 2.11

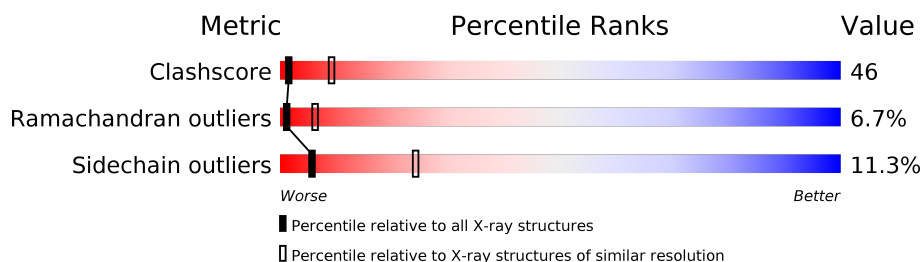
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.00 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	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)

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 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  $\leq 5\%$ .

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	298	<div> <div>36%</div> <div>49%</div> <div>12%</div> <div>••</div> </div>
1	C	298	<div> <div>35%</div> <div>51%</div> <div>11%</div> <div>••</div> </div>
2	B	258	<div> <div>35%</div> <div>51%</div> <div>8%</div> <div>6%</div> </div>
2	D	258	<div> <div>28%</div> <div>51%</div> <div>14%</div> <div>7%</div> </div>

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 8713 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 Early 35 kDa protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	293	Total	C	N	O	S	0	0	0
			2406	1541	393	461	11			
1	C	293	Total	C	N	O	S	0	0	0
			2406	1541	393	461	11			

- Molecule 2 is a protein called caspase-8.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	243	Total	C	N	O	S	0	0	0
			1945	1228	333	368	16			
2	D	241	Total	C	N	O	S	0	0	0
			1930	1221	331	362	16			

- Molecule 3 is water.

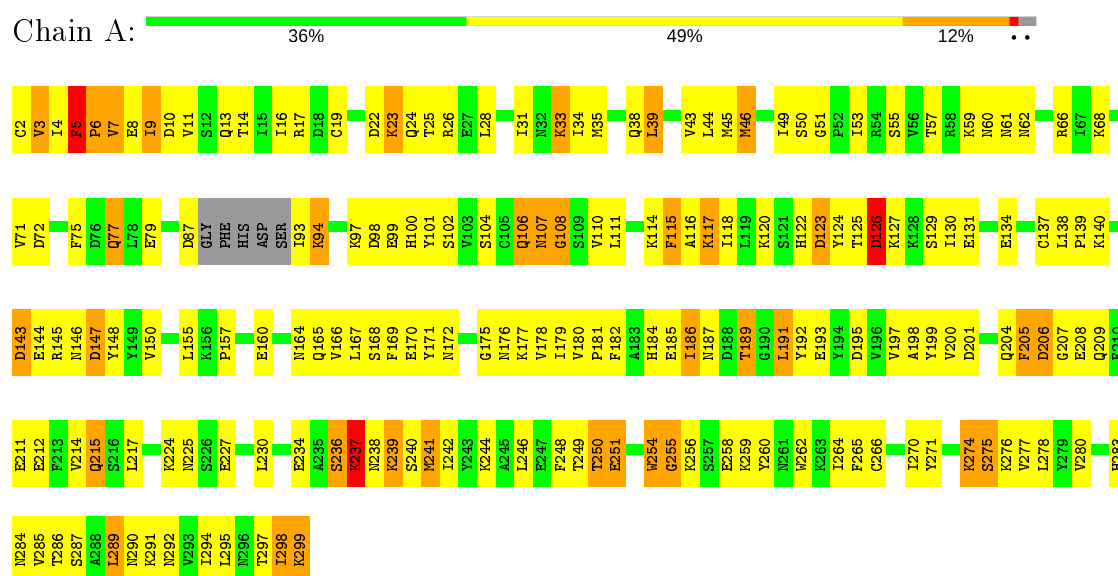
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	10	Total	O	0	0
			10	10		
3	B	4	Total	O	0	0
			4	4		
3	C	9	Total	O	0	0
			9	9		
3	D	3	Total	O	0	0
			3	3		

### 3 Residue-property plots

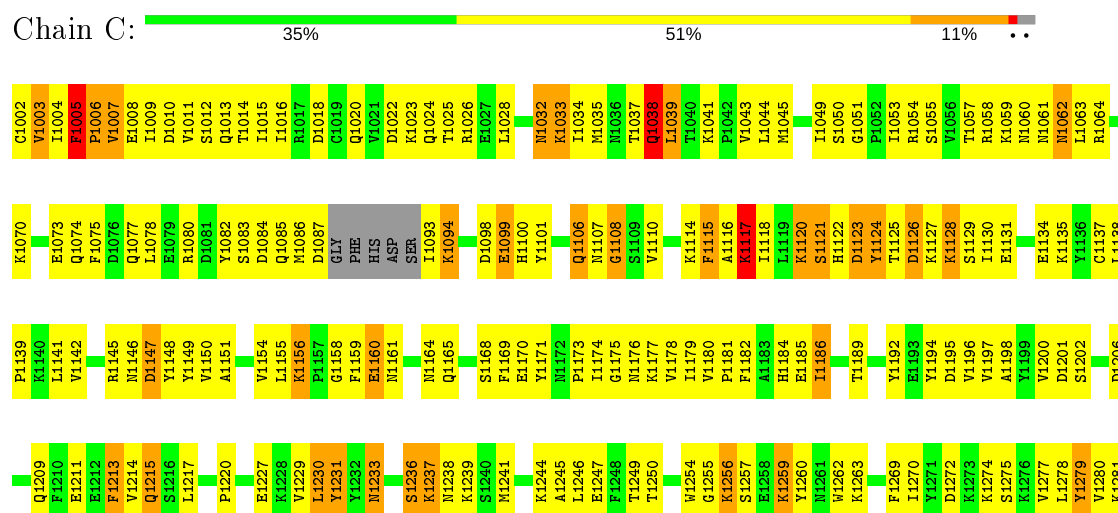
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according 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. 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.

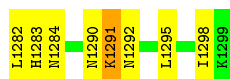
Note EDS was not executed.

#### • Molecule 1: Early 35 kDa protein



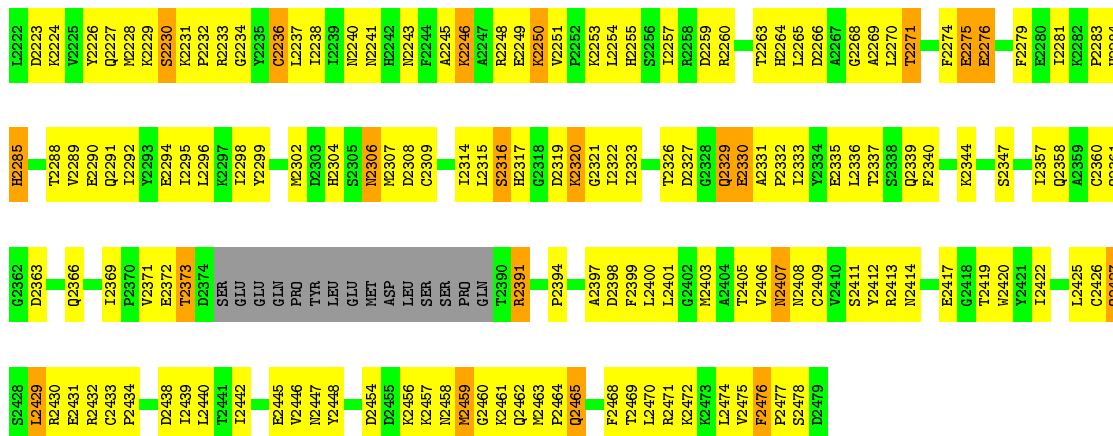
#### • Molecule 1: Early 35 kDa protein





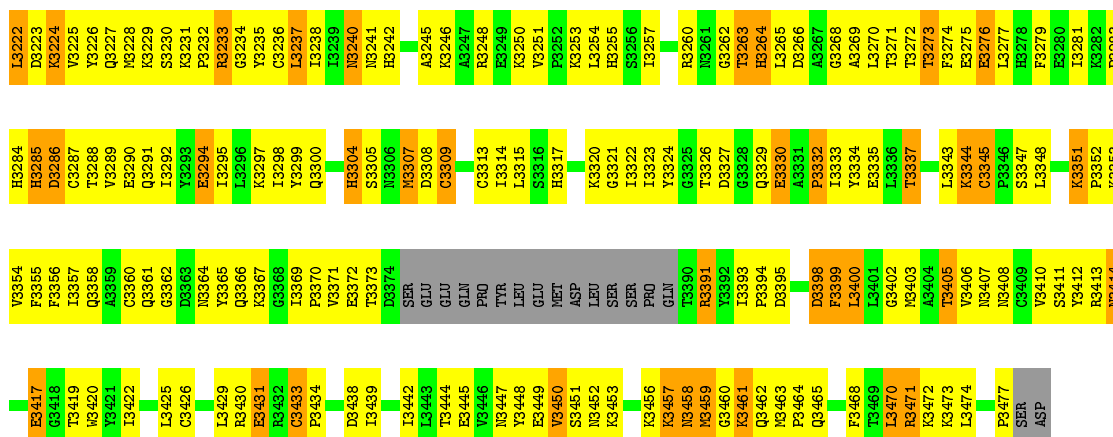
• Molecule 2: caspase-8

Chain B: 35% 51% 8% 6%



• Molecule 2: caspase-8

Chain D: 28% 51% 14% 7%



## 4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	99.97Å 117.34Å 346.45Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	24.00 – 3.00	Depositor
% Data completeness (in resolution range)	(Not available) (24.00-3.00)	Depositor
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.229 , 0.260	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	8713	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	87.0	wwPDB-VP

## 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	0.40	0/2454	0.65	0/3307
1	C	0.40	0/2454	0.66	0/3307
2	B	0.37	0/1987	0.60	0/2682
2	D	0.34	0/1972	0.56	0/2663
All	All	0.38	0/8867	0.62	0/11959

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	2406	0	2389	219	0
1	C	2406	0	2389	210	0
2	B	1945	0	1915	168	0
2	D	1930	0	1906	211	0
3	A	10	0	0	3	0
3	B	4	0	0	2	0
3	C	9	0	0	3	0
3	D	3	0	0	1	0
All	All	8713	0	8599	796	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 46.

The worst 5 of 796 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:C:1039:LEU:HD12	1:C:1043:VAL:HG21	1.33	1.10
2:D:3273:THR:HG23	2:D:3430:ARG:HB3	1.32	1.10
2:B:2231:LYS:HB2	2:B:2232:PRO:HD3	1.34	1.08
2:D:3393:ILE:HG12	2:D:3471:ARG:HH22	1.13	1.07
1:A:104:SER:HB2	1:A:120:LYS:HD2	1.36	1.07

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	289/298 (97%)	218 (75%)	44 (15%)	27 (9%)	0	3
1	C	289/298 (97%)	221 (76%)	45 (16%)	23 (8%)	1	4
2	B	239/258 (93%)	193 (81%)	36 (15%)	10 (4%)	3	16
2	D	237/258 (92%)	181 (76%)	45 (19%)	11 (5%)	2	14
All	All	1054/1112 (95%)	813 (77%)	170 (16%)	71 (7%)	1	6

5 of 71 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	3	VAL
1	A	94	LYS
1	A	108	GLY
1	A	115	PHE
1	A	126	ASP



### 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	276/280 (99%)	252 (91%)	24 (9%)	10	37
1	C	276/280 (99%)	245 (89%)	31 (11%)	6	24
2	B	218/233 (94%)	198 (91%)	20 (9%)	9	34
2	D	216/233 (93%)	180 (83%)	36 (17%)	2	11
All	All	986/1026 (96%)	875 (89%)	111 (11%)	6	24

5 of 111 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	1057	THR
1	C	1160	GLU
2	D	3417	GLU
1	C	1062	ASN
1	C	1120	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 46 such sidechains are listed below:

Mol	Chain	Res	Type
2	B	2407	ASN
2	B	2465	GLN
2	D	3361	GLN
2	B	2414	ASN
2	B	2447	ASN

### 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 carbohydrates 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 ⓘ

### 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.