



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 02:26 AM GMT

PDB ID : 2H4W  
Title : Crystal structure of human caspase-1 (Glu390->Asp) in complex with 3-[2-(2-benzyloxycarbonylamino-3-methyl-butyrylamino)-propionylamino]-4-oxo-pentanoic acid (z-VAD-FMK)  
Authors : Scheer, J.M.; Wells, J.A.; Romanowski, M.J.  
Deposited on : 2006-05-25  
Resolution : 2.00 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](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/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  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

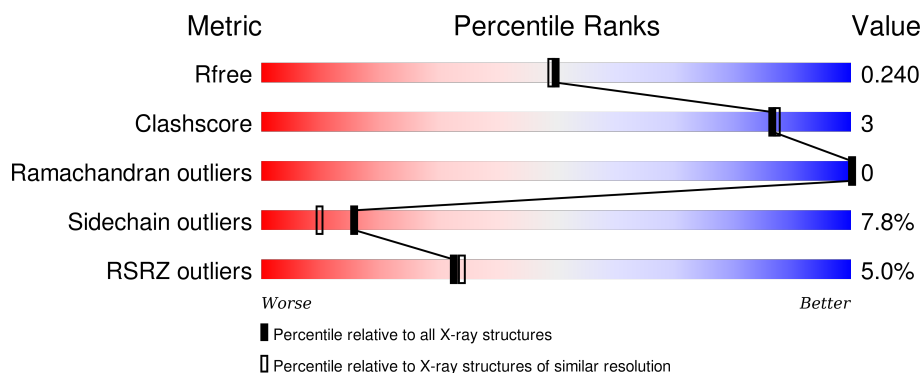
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.00 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))
$R_{free}$	91344	6249 (2.00-2.00)
Clashscore	102246	7340 (2.00-2.00)
Ramachandran outliers	100387	7248 (2.00-2.00)
Sidechain outliers	100360	7247 (2.00-2.00)
RSRZ outliers	91569	6262 (2.00-2.00)

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. 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	178	<div> <div>7%</div> <div> <div></div> <div>79%</div> <div>15%</div> <div>6%</div> </div> </div>
2	B	88	<div> <div></div> <div> <div>86%</div> <div>13%</div> <div></div> </div> </div>
3	C	5	<div> <div></div> <div> <div>80%</div> <div>20%</div> </div> </div>

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 2243 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.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	168	Total	C	N	O	S	0	3	0
			1310	816	226	257	11			

- Molecule 2 is a protein called Caspase-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	88	Total	C	N	O	S	0	2	0
			723	459	126	131	7			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	390	ASP	GLU	ENGINEERED	UNP P29466

- Molecule 3 is a protein called N-[(benzyloxy)carbonyl]-L-valyl-N-[(2S)-1-carboxy-4-fluoro-3-oxobutan-2-yl]-L-alaninamide.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	C	5	Total	C	N	O	0	0	1
			31	21	3	7			

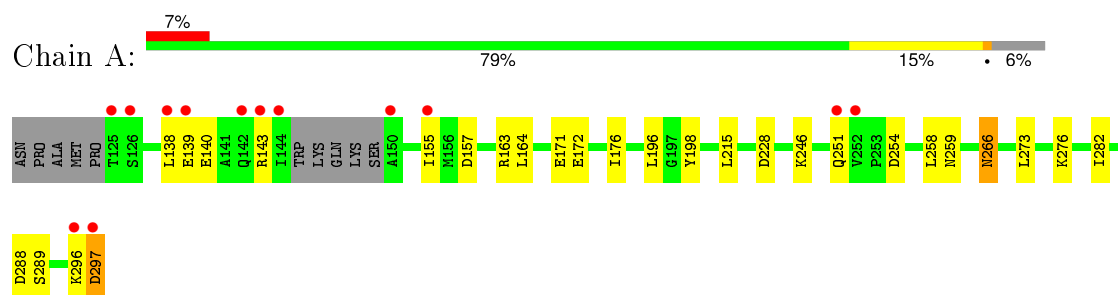
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	120	Total	O	0	0
			120	120		
4	B	58	Total	O	0	0
			58	58		
4	C	1	Total	O	0	0
			1	1		

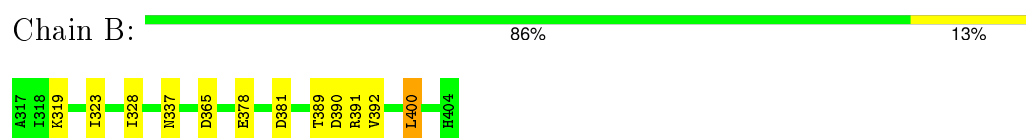
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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 ( $\text{RSRZ} > 2$ ). 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.

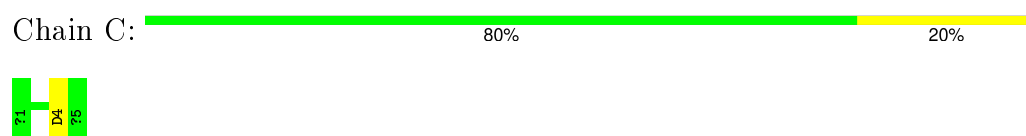
#### • Molecule 1: Caspase-1



#### • Molecule 2: Caspase-1



#### • Molecule 3: N-[(benzyloxy)carbonyl]-L-valyl-N-[(2S)-1-carboxy-4-fluoro-3-oxobutan-2-yl]-L-alaninamide



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	63.21Å 63.21Å 161.33Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.00 19.99 – 2.00	Depositor EDS
% Data completeness (in resolution range)	91.8 (20.00-2.00) 91.8 (19.99-2.00)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.44 (at 2.01Å)	Xtriage
Refinement program	REFMAC 5.1.19	Depositor
R, $R_{free}$	0.210 , 0.247 0.205 , 0.240	Depositor DCC
$R_{free}$ test set	1081 reflections (5.41%)	DCC
Wilson B-factor (Å <sup>2</sup> )	29.6	Xtriage
Anisotropy	0.340	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 42.5	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.45$ , $\langle L^2 \rangle = 0.28$	Xtriage
Outliers	1 of 21109 reflections (0.005%)	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	2243	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	26.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.30% 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, 0.375 respectively for untwinned datasets, and 0.333, 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: PHQ, CF0

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	0.32	0/1345	0.66	5/1810 (0.3%)
2	B	0.36	0/752	0.70	4/1015 (0.4%)
3	C	2.28	1/19 (5.3%)	1.43	0/25
All	All	0.40	1/2116 (0.0%)	0.68	9/2850 (0.3%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	4	ASP	C-O	9.85	1.42	1.23

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	228	ASP	CB-CG-OD2	5.80	123.52	118.30
2	B	365	ASP	CB-CG-OD2	5.72	123.45	118.30
1	A	254	ASP	CB-CG-OD2	5.70	123.43	118.30
1	A	288	ASP	CB-CG-OD2	5.36	123.13	118.30
2	B	381	ASP	CB-CG-OD2	5.31	123.08	118.30
2	B	390[A]	ASP	CB-CG-OD2	5.29	123.06	118.30
2	B	390[B]	ASP	CB-CG-OD2	5.29	123.06	118.30
1	A	297	ASP	CB-CG-OD2	5.26	123.03	118.30
1	A	157	ASP	CB-CG-OD2	5.04	122.83	118.30

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	1310	0	1311	9	0
2	B	723	0	694	7	0
3	C	31	0	24	0	0
4	A	120	0	0	0	0
4	B	58	0	0	0	0
4	C	1	0	0	0	0
All	All	2243	0	2029	11	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 3.

All (11) 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:259:ASN:HD22	2:B:391:ARG:HH12	1.46	0.64
1:A:266:ASN:HB2	2:B:323:ILE:O	2.00	0.61
1:A:266:ASN:HD22	1:A:266:ASN:C	2.07	0.58
1:A:258:LEU:HD13	1:A:282:ILE:HD11	1.89	0.56
1:A:196:LEU:HD22	2:B:400:LEU:HG	1.91	0.52
1:A:289:SER:HB2	2:B:337:ASN:HD22	1.74	0.51
2:B:389[B]:THR:HG22	2:B:392:VAL:CG2	2.45	0.47
1:A:163:ARG:HB3	1:A:198:TYR:CD2	2.49	0.47
1:A:259:ASN:ND2	2:B:391:ARG:HH12	2.13	0.46
1:A:273:LEU:HA	1:A:276:LYS:HD2	1.99	0.45
2:B:328:ILE:HD11	2:B:389[B]:THR:HG21	2.03	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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	167/178 (94%)	164 (98%)	3 (2%)	0	100	100
2	B	88/88 (100%)	85 (97%)	3 (3%)	0	100	100
3	C	1/5 (20%)	1 (100%)	0	0	100	100
All	All	256/271 (94%)	250 (98%)	6 (2%)	0	100	100

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains ⓘ

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	152/158 (96%)	137 (90%)	15 (10%)	10	5
2	B	81/79 (102%)	78 (96%)	3 (4%)	41	38
3	C	2/2 (100%)	2 (100%)	0	100	100
All	All	235/239 (98%)	217 (92%)	18 (8%)	16	10

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	138	LEU
1	A	139	GLU
1	A	140	GLU
1	A	143	ARG
1	A	155	ILE
1	A	164	LEU
1	A	171	GLU
1	A	172	GLU
1	A	176	ILE
1	A	215	LEU
1	A	246	LYS
1	A	251	GLN
1	A	266	ASN

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Mol	Chain	Res	Type
1	A	296	LYS
1	A	297	ASP
2	B	319	LYS
2	B	378	GLU
2	B	400	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	170	ASN
1	A	259	ASN
1	A	263	ASN
1	A	266	ASN
1	A	269	ASN
2	B	337	ASN
2	B	358	GLN

### 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 ⓘ

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	168/178 (94%)	0.18	13 (7%) 16 17	13, 23, 49, 80	0
2	B	88/88 (100%)	-0.14	0 100 100	13, 19, 35, 45	0
3	C	3/5 (60%)	-0.30	0 100 100	31, 31, 33, 34	0
All	All	259/271 (95%)	0.07	13 (5%) 32 34	13, 22, 47, 80	0

All (13) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	143	ARG	5.1
1	A	297	ASP	4.2
1	A	142	GLN	4.0
1	A	125	THR	3.5
1	A	138	LEU	3.5
1	A	252	VAL	3.4
1	A	251	GLN	3.1
1	A	139	GLU	3.0
1	A	144	ILE	3.0
1	A	150	ALA	2.6
1	A	155	ILE	2.3
1	A	126	SER	2.3
1	A	296	LYS	2.1

### 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 carbohydrates 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.