



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 13, 2017 – 02:26 pm GMT

PDB ID : 3IBC  
Title : Crystal Structure of Caspase-7 incomplex with Acetyl-YVAD-CHO  
Authors : Agniswamy, J.  
Deposited on : 2009-07-15  
Resolution : 2.75 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

<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
Xtriage (Phenix)	:	1.9-1692
EDS	:	trunk28620
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
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)	:	recalc28949

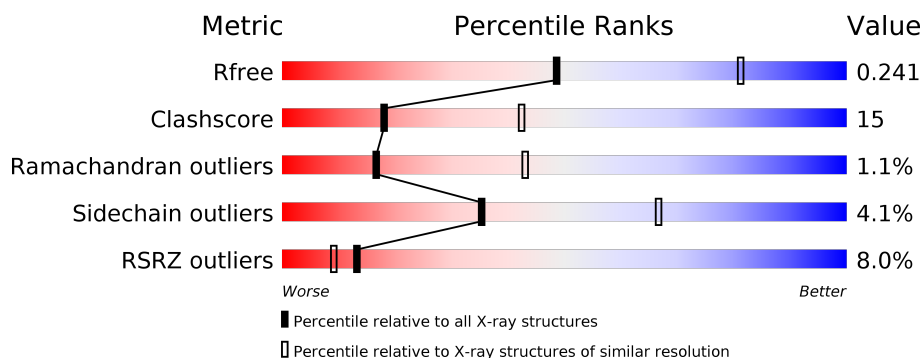
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.75 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))
$R_{free}$	100719	3666 (2.80-2.72)
Clashscore	112137	4174 (2.80-2.72)
Ramachandran outliers	110173	4103 (2.80-2.72)
Sidechain outliers	110143	4106 (2.80-2.72)
RSRZ outliers	101464	3697 (2.80-2.72)

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	173	<div> <div>3%</div> <div> <div>51%</div> <div>28%</div> <div>•</div> <div>19%</div> </div> </div>
1	C	173	<div> <div>2%</div> <div> <div>58%</div> <div>21%</div> <div>•</div> <div>19%</div> </div> </div>
2	B	97	<div> <div>14%</div> <div> <div>54%</div> <div>41%</div> <div>5%</div> </div> </div>
2	D	97	<div> <div>14%</div> <div> <div>63%</div> <div>30%</div> <div>•</div> <div>•</div> </div> </div>
3	E	5	<div> <div>40%</div> <div> <div>20%</div> <div>60%</div> <div>20%</div> </div> </div>
3	F	5	<div> <div>60%</div> <div> <div>20%</div> <div>20%</div> </div> </div>

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 3857 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-7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	140	Total	C	N	O	S	0	0	0
			1100	691	188	210	11			
1	C	140	Total	C	N	O	S	0	0	0
			1100	691	188	210	11			

- Molecule 2 is a protein called Caspase-7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	92	Total	C	N	O	S	0	0	0
			758	487	128	139	4			
2	D	93	Total	C	N	O	S	0	0	0
			770	496	129	141	4			

- Molecule 3 is a protein called Acetyl-YVAD-CHO.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	E	5	Total	C	N	O	0	0	0
			35	23	4	8			
3	F	5	Total	C	N	O	0	0	0
			35	23	4	8			

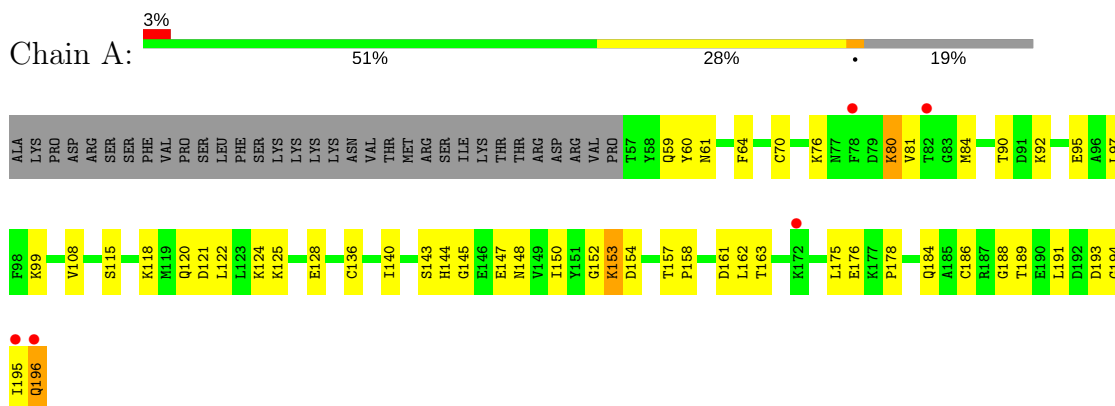
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	15	Total	O	0	0
			15	15		
4	B	8	Total	O	0	0
			8	8		
4	C	24	Total	O	0	0
			24	24		
4	D	12	Total	O	0	0
			12	12		

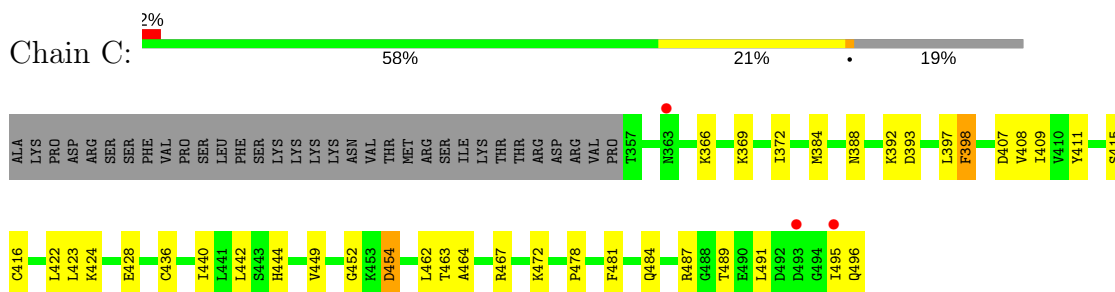
### 3 Residue-property plots

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 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.

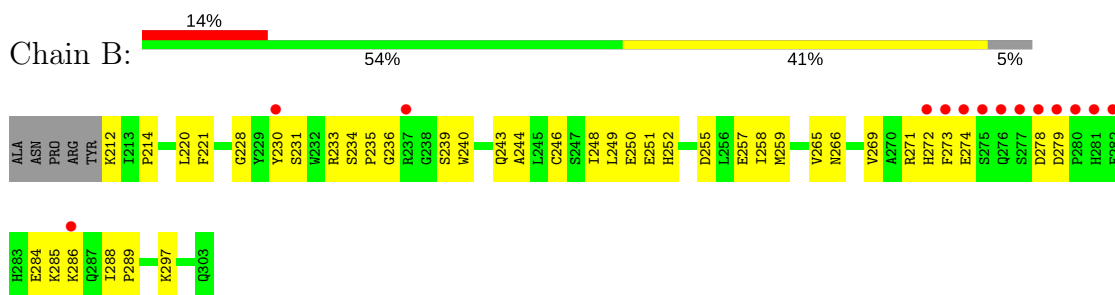
#### • Molecule 1: Caspase-7



#### • Molecule 1: Caspase-7



#### • Molecule 2: Caspase-7



#### • Molecule 2: Caspase-7





● Molecule 3: Acetyl-YVAD-CHO



● Molecule 3: Acetyl-YVAD-CHO



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	88.25Å 88.25Å 188.15Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	50.00 – 2.75 48.48 – 2.75	Depositor EDS
% Data completeness (in resolution range)	83.5 (50.00-2.75) 83.8 (48.48-2.75)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.38 (at 2.77Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, $R_{free}$	0.203 , 0.242 0.203 , 0.241	Depositor DCC
$R_{free}$ test set	915 reflections (4.81%)	DCC
Wilson B-factor (Å <sup>2</sup> )	58.8	Xtriage
Anisotropy	0.615	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 60.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.025 for -h,-k,l	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	3857	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	73.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.27% 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](#)

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

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	0.39	0/1117	0.61	1/1496 (0.1%)
1	C	0.41	0/1117	0.62	1/1496 (0.1%)
2	B	0.39	0/780	0.59	0/1054
2	D	0.40	0/793	0.62	0/1072
3	E	2.01	1/33 (3.0%)	1.07	0/45
3	F	2.10	1/33 (3.0%)	0.99	0/45
All	All	0.48	2/3873 (0.1%)	0.62	2/5208 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	805	ASP	C-O	11.67	1.45	1.23
3	E	705	ASP	C-O	11.14	1.44	1.23

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	452	GLY	N-CA-C	-5.99	98.14	113.10
1	A	152	GLY	N-CA-C	-5.96	98.20	113.10

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	1100	0	1085	45	0
1	C	1100	0	1085	33	0
2	B	758	0	731	29	0
2	D	770	0	740	28	0
3	E	35	0	30	3	0
3	F	35	0	30	2	0
4	A	15	0	0	0	0
4	B	8	0	0	0	0
4	C	24	0	0	0	0
4	D	12	0	0	0	0
All	All	3857	0	3701	113	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 15.

The worst 5 of 113 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:80:LYS:HD2	1:A:80:LYS:H	1.08	1.18
1:A:175:LEU:HD11	1:C:495:ILE:HG21	1.51	0.93
1:A:191:LEU:HD23	2:B:285:LYS:HG3	1.53	0.90
1:A:80:LYS:N	1:A:80:LYS:HD2	1.93	0.76
1:A:195:ILE:HD11	1:C:472:LYS:HE3	1.65	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	138/173 (80%)	131 (95%)	7 (5%)	0	100	100
1	C	138/173 (80%)	130 (94%)	8 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	90/97 (93%)	79 (88%)	9 (10%)	2 (2%)	8	22
2	D	91/97 (94%)	85 (93%)	4 (4%)	2 (2%)	8	22
3	E	3/5 (60%)	2 (67%)	0	1 (33%)	0	0
3	F	3/5 (60%)	3 (100%)	0	0	100	100
All	All	463/550 (84%)	430 (93%)	28 (6%)	5 (1%)	17	43

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	272	HIS
2	D	572	HIS
3	E	702	TYR
2	D	571	ARG
2	B	235	PRO

### 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	120/152 (79%)	113 (94%)	7 (6%)	23	52
1	C	120/152 (79%)	115 (96%)	5 (4%)	34	66
2	B	84/88 (96%)	83 (99%)	1 (1%)	75	92
2	D	85/88 (97%)	82 (96%)	3 (4%)	41	72
3	E	3/3 (100%)	3 (100%)	0	100	100
3	F	3/3 (100%)	2 (67%)	1 (33%)	0	0
All	All	415/486 (85%)	398 (96%)	17 (4%)	35	67

5 of 17 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	255	ASP
1	C	392	LYS

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Mol	Chain	Res	Type
2	D	513	ILE
1	A	196	GLN
2	D	554	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	144	HIS
1	A	184	GLN
2	B	252	HIS
2	B	283	HIS
1	C	448	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 [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	140/173 (80%)	0.29	5 (3%) 43 37	52, 74, 99, 107	0
1	C	140/173 (80%)	0.37	3 (2%) 64 59	49, 63, 91, 121	0
2	B	92/97 (94%)	0.93	14 (15%) 2 2	47, 69, 134, 144	0
2	D	93/97 (95%)	0.69	14 (15%) 3 2	46, 66, 134, 141	0
3	E	4/5 (80%)	2.12	2 (50%) 0 0	95, 100, 103, 112	0
3	F	4/5 (80%)	0.54	0 100 100	80, 82, 87, 98	0
All	All	473/550 (86%)	0.53	38 (8%) 13 9	46, 68, 114, 144	0

The worst 5 of 38 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	278	ASP	5.9
2	B	280	PRO	5.5
2	B	277	SER	5.4
2	B	282	PHE	5.2
2	D	580	PRO	5.1

### 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.