



# wwPDB X-ray Structure Validation Summary Report i

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PDB ID : 4HQ0  
Title : Crystal Structure of mutant form of Caspase-7  
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Deposited on : 2012-10-25  
Resolution : 3.00 Å(reported)

This is a wwPDB 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/ValidationPDFNotes.html>

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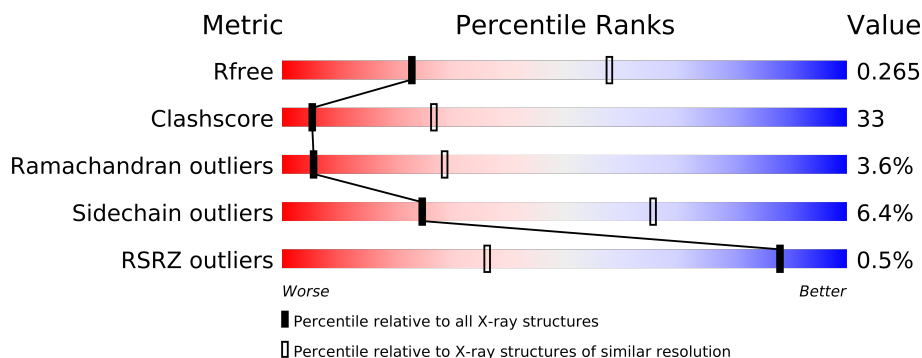
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.15 2013
Xtriage (Phenix)	:	dev-1323
EDS	:	stable22639
Percentile statistics	:	21963
Refmac	:	5.8.0049
CCP4	:	6.3.0 (Settle)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	stable22683

# 1 Overall quality at a glance

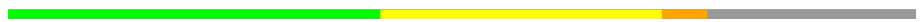

The reported resolution of this entry is 3.00 Å.

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))
$R_{free}$	66092	1216 (3.00-3.00)
Clashscore	79885	1594 (3.00-3.00)
Ramachandran outliers	78287	1537 (3.00-3.00)
Sidechain outliers	78261	1540 (3.00-3.00)
RSRZ outliers	66119	1217 (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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	272	
1	B	272	

## 2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 3424 atoms, of which 0 are hydrogen and 0 are deuterium.

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	210	Total	C	N	O	S	0	0	0
			1681	1072	286	308	15			
1	B	217	Total	C	N	O	S	0	0	0
			1743	1110	302	316	15			

There are 32 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	46	MET	-	EXPRESSION TAG	UNP P55210
A	198	ALA	ASP	ENGINEERED MUTATION	UNP P55210
A	204A	LEU	-	INSERTION	UNP P55210
A	204B	VAL	-	INSERTION	UNP P55210
A	204C	PRO	-	INSERTION	UNP P55210
A	204D	ARG	-	INSERTION	UNP P55210
A	204E	GLY	-	INSERTION	UNP P55210
A	204F	SER	-	INSERTION	UNP P55210
A	304	LEU	-	EXPRESSION TAG	UNP P55210
A	305	GLU	-	EXPRESSION TAG	UNP P55210
A	306	HIS	-	EXPRESSION TAG	UNP P55210
A	307	HIS	-	EXPRESSION TAG	UNP P55210
A	308	HIS	-	EXPRESSION TAG	UNP P55210
A	309	HIS	-	EXPRESSION TAG	UNP P55210
A	310	HIS	-	EXPRESSION TAG	UNP P55210
A	311	HIS	-	EXPRESSION TAG	UNP P55210
B	46	MET	-	EXPRESSION TAG	UNP P55210
B	198	ALA	ASP	ENGINEERED MUTATION	UNP P55210
B	204A	LEU	-	INSERTION	UNP P55210
B	204B	VAL	-	INSERTION	UNP P55210
B	204C	PRO	-	INSERTION	UNP P55210
B	204D	ARG	-	INSERTION	UNP P55210
B	204E	GLY	-	INSERTION	UNP P55210
B	204F	SER	-	INSERTION	UNP P55210
B	304	LEU	-	EXPRESSION TAG	UNP P55210

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Chain	Residue	Modelled	Actual	Comment	Reference
B	305	GLU	-	EXPRESSION TAG	UNP P55210
B	306	HIS	-	EXPRESSION TAG	UNP P55210
B	307	HIS	-	EXPRESSION TAG	UNP P55210
B	308	HIS	-	EXPRESSION TAG	UNP P55210
B	309	HIS	-	EXPRESSION TAG	UNP P55210
B	310	HIS	-	EXPRESSION TAG	UNP P55210
B	311	HIS	-	EXPRESSION TAG	UNP P55210



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	89.60Å 89.60Å 182.84Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	40.00 – 3.00 71.43 – 3.00	Depositor EDS
% Data completeness (in resolution range)	(Not available) (40.00-3.00) 100.0 (71.43-3.00)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.75 (at 3.01Å)	Xtriage
Refinement program	CNS 1.21	Depositor
R, $R_{free}$	0.222 , 0.267 0.221 , 0.265	Depositor DCC
$R_{free}$ test set	846 reflections (4.80%)	DCC
Wilson B-factor (Å <sup>2</sup> )	66.9	Xtriage
Anisotropy	0.486	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 47.7	EDS
Estimated twinning fraction	0.013 for -h,-k,l	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.34$	Xtriage
Outliers	0 of 17650 reflections	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	3424	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	66.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.85% of the height of the origin peak. No significant pseudotranslation is detected.*

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

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

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	0.70	1/1715 (0.1%)	0.63	1/2305 (0.0%)
1	B	0.71	1/1779 (0.1%)	0.69	1/2393 (0.0%)
All	All	0.71	2/3494 (0.1%)	0.66	2/4698 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	186	CYS	CB-SG	-23.68	1.42	1.82
1	B	186	CYS	CB-SG	-23.10	1.43	1.82

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	152	GLY	N-CA-C	-6.06	97.95	113.10
1	A	152	GLY	N-CA-C	-5.01	100.57	113.10

There are no chirality outliers.

There are no planarity outliers.

### 5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1681	0	1661	112	0
1	B	1743	0	1732	129	0
All	All	3424	0	3393	223	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 33.

The worst 5 of 223 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:80:LYS:HD3	1:A:80:LYS:H	1.15	1.11
1:A:186:CYS:SG	1:A:231:SER:HB3	1.90	1.10
1:B:225:THR:HB	1:B:231:SER:HB3	1.29	1.08
1:A:215:VAL:HB	1:B:226:VAL:HG13	1.36	1.05
1:B:210:ARG:HH22	1:B:215:VAL:HA	1.25	1.00

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	204/272 (75%)	178 (87%)	19 (9%)	7 (3%)	6	31
1	B	211/272 (78%)	186 (88%)	17 (8%)	8 (4%)	5	27
All	All	415/544 (76%)	364 (88%)	36 (9%)	15 (4%)	5	29

5 of 15 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	81	VAL
1	A	234	SER
1	B	56	PRO
1	B	186	CYS
1	A	147	GLU

### 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	184/239 (77%)	170 (92%)	14 (8%)	19	57
1	B	191/239 (80%)	181 (95%)	10 (5%)	32	75
All	All	375/478 (78%)	351 (94%)	24 (6%)	25	66

5 of 24 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	220	LEU
1	A	272	HIS
1	B	290	CYS
1	A	229	TYR
1	A	230	TYR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 8 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	243	GLN
1	B	243	GLN
1	A	287	GLN
1	A	120	GLN
1	A	272	HIS

### 5.3.3 RNA ⓘ

There are no RNA chains 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 carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

There are no ligands in this entry.

## 5.7 Other polymers ⓘ

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 ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

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	210/272 (77%)	0.09	0	100 100	43, 69, 96, 101	0
1	B	217/272 (79%)	0.08	2 (0%)	81 24	40, 58, 96, 101	0
All	All	427/544 (78%)	0.09	2 (0%)	88 36	40, 62, 96, 101	0

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	227	PRO	2.5
1	B	287	GLN	2.2

### 6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

### 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

### 6.4 Ligands ⓘ

There are no ligands in this entry.

### 6.5 Other polymers ⓘ

There are no such residues in this entry.