



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 1, 2014 – 03:39 AM GMT

PDB ID : 3E4C  
Title : Procaspase-1 zymogen domain crystal strucutre  
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Deposited on : 2008-08-11  
Resolution : 2.05 Å(reported)

This is a full wwPDB 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/ValidationPDFNotes.html>

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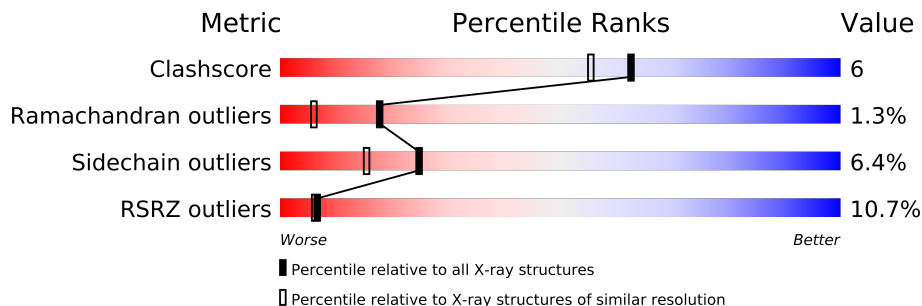
The following versions of software and data (see [references](#)) were used in the production of this report:

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 2.05 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	79885	1577 (2.06-2.02)
Ramachandran outliers	78287	1565 (2.06-2.02)
Sidechain outliers	78261	1565 (2.06-2.02)
RSRZ outliers	66119	1381 (2.06-2.02)

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	302	
1	B	302	

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 4423 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-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	271	Total	C	N	O	S	0	12	0
			2149	1351	371	410	17			
1	B	269	Total	C	N	O	S	0	12	0
			2137	1345	369	406	17			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	103	GLN	-	EXPRESSION TAG	UNP P29466
A	285	ALA	CYS	ENGINEERED	UNP P29466
B	103	GLN	-	EXPRESSION TAG	UNP P29466
B	285	ALA	CYS	ENGINEERED	UNP P29466

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	Mg	0	0
			1	1		

- Molecule 3 is water.

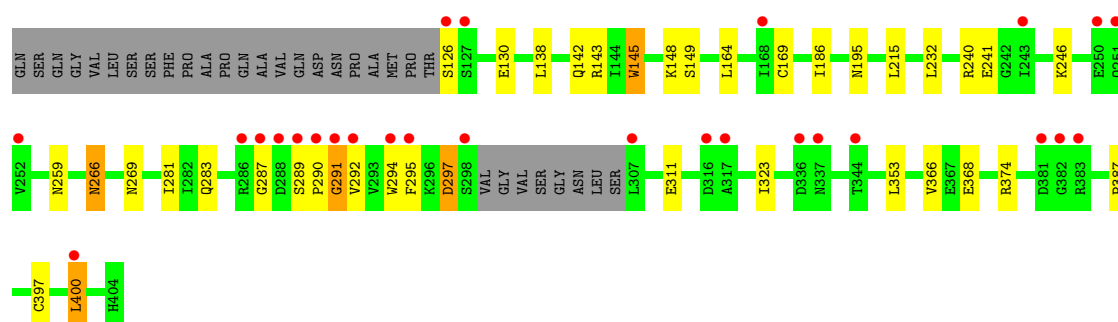
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	69	Total	O	0	0
			69	69		
3	B	67	Total	O	0	0
			67	67		

### 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 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 ( $RSRZ > 2$ ). 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.

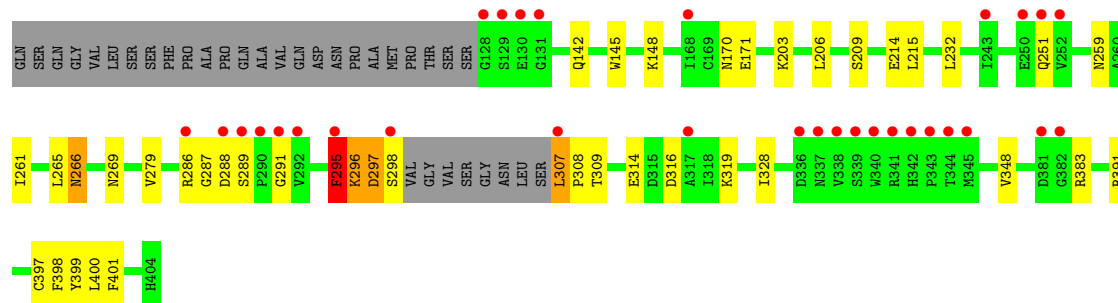
#### • Molecule 1: Caspase-1

Chain A: 



#### • Molecule 1: Caspase-1

Chain B: 



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	56.10Å 58.00Å 60.12Å 105.95° 119.60° 92.77°	Depositor
Resolution (Å)	20.00 – 2.05 19.78 – 2.05	Depositor EDS
% Data completeness (in resolution range)	96.6 (20.00-2.05) 96.6 (19.78-2.05)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.06	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.78 (at 2.06Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, $R_{free}$	0.200 , 0.263 0.212 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	DCC
Wilson B-factor (Å <sup>2</sup> )	35.6	Xtriage
Anisotropy	0.133	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 51.9	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 37221 reflections	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	4423	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.58% 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

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

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	0.56	0/2193	0.69	0/2957
1	B	0.61	0/2181	0.73	0/2941
All	All	0.59	0/4374	0.71	0/5898

There are no bond length outliers.

There are no bond angle outliers.

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	2149	0	2116	18	0
1	B	2137	0	2103	31	0
2	B	1	0	0	0	0
3	A	69	0	0	1	0
3	B	67	0	0	2	0
All	All	4423	0	4219	48	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 6.

All (48) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:148:LYS:NZ	1:B:397:CYS:SG	2.26	1.08
1:A:148:LYS:NZ	1:A:397:CYS:SG	2.27	1.07
1:B:142:GLN:HG3	3:B:405:HOH:O	1.72	0.88
1:B:259:ASN:HD22	1:B:391:ARG:HH22	1.20	0.87
1:A:290[A]:PRO:O	1:A:291[A]:GLY:O	1.92	0.85
1:B:266:ASN:C	1:B:266:ASN:HD22	1.86	0.77
1:B:295[B]:PHE:O	1:B:296[B]:LYS:CB	2.37	0.72
1:B:297[B]:ASP:O	1:B:298[B]:SER:HB3	1.89	0.72
1:A:266:ASN:HD22	1:A:266:ASN:C	1.93	0.71
1:B:297[B]:ASP:O	1:B:298[B]:SER:CB	2.39	0.71
1:B:287[B]:GLY:O	1:B:289[B]:SER:N	2.26	0.69
1:B:295[B]:PHE:O	1:B:296[B]:LYS:HB2	1.93	0.68
1:A:266:ASN:ND2	1:A:269:ASN:H	1.93	0.66
1:B:295[B]:PHE:O	1:B:296[B]:LYS:HG2	1.98	0.64
1:B:142:GLN:HE21	1:B:142:GLN:HA	1.63	0.64
1:B:295[B]:PHE:O	1:B:296[B]:LYS:CG	2.48	0.62
1:B:251:GLN:OE1	1:B:251:GLN:N	2.34	0.61
1:A:266:ASN:HD21	1:A:269:ASN:H	1.51	0.58
1:B:266:ASN:C	1:B:266:ASN:ND2	2.56	0.58
1:B:297[B]:ASP:OD1	1:B:297[B]:ASP:N	2.36	0.58
1:A:145:TRP:O	1:A:149:SER:HB3	2.07	0.54
1:B:286:ARG:HG2	1:B:291[B]:GLY:HA2	1.89	0.54
1:A:374:ARG:HD3	1:A:387:PRO:O	2.09	0.52
1:B:328:ILE:O	1:B:328:ILE:HG23	2.09	0.51
1:B:142:GLN:NE2	1:B:142:GLN:HA	2.27	0.50
1:A:368:GLU:OE1	1:B:148:LYS:NZ	2.40	0.49
1:B:142:GLN:CG	3:B:405:HOH:O	2.43	0.49
1:A:289[A]:SER:HB2	1:A:290[A]:PRO:HD2	1.93	0.49
1:A:366:VAL:HG12	1:A:400:LEU:CD2	2.44	0.48
1:A:126:SER:N	3:A:434:HOH:O	2.47	0.48
1:B:266:ASN:ND2	1:B:269:ASN:H	2.11	0.47
1:B:399:TYR:HB2	1:B:401:PHE:CE2	2.48	0.47
1:B:287[B]:GLY:C	1:B:289[B]:SER:N	2.69	0.46
1:B:279:VAL:CG2	1:B:398:PHE:HE2	2.28	0.46
1:B:314:GLU:O	1:B:319:LYS:HE3	2.16	0.46
1:B:148:LYS:CE	1:B:397:CYS:SG	3.04	0.45
1:B:170:ASN:ND2	1:B:206:LEU:H	2.16	0.44
1:B:307:LEU:N	1:B:308:PRO:CD	2.82	0.43
1:A:169:CYS:HB3	1:A:186:ILE:HD11	2.01	0.42
1:B:203:LYS:HB3	1:B:206:LEU:HD11	2.00	0.42
1:A:130:GLU:O	1:A:195:ASN:HB3	2.19	0.42
1:A:266:ASN:HB2	1:A:323:ILE:O	2.20	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:240:ARG:HB3	1:A:241:GLU:OE1	2.19	0.42
1:A:266:ASN:ND2	1:A:266:ASN:C	2.66	0.42
1:A:148:LYS:CE	1:A:397:CYS:SG	3.08	0.41
1:B:328:ILE:CG2	1:B:328:ILE:O	2.67	0.41
1:B:261:ILE:O	1:B:265:LEU:HD23	2.21	0.41
1:A:281:ILE:HD13	1:A:353:LEU:HD21	2.03	0.41

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	267/302 (88%)	246 (92%)	17 (6%)	4 (2%)	15	4
1	B	265/302 (88%)	249 (94%)	13 (5%)	3 (1%)	21	8
All	All	532/604 (88%)	495 (93%)	30 (6%)	7 (1%)	18	6

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	291[A]	GLY
1	A	297[A]	ASP
1	A	287[A]	GLY
1	B	288[B]	ASP
1	B	296[B]	LYS
1	A	294[A]	TRP
1	B	295[B]	PHE

### 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	242/267 (91%)	226 (93%)	16 (7%)	24	14
1	B	240/267 (90%)	225 (94%)	15 (6%)	25	16
All	All	482/534 (90%)	451 (94%)	31 (6%)	25	15

All (31) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	138	LEU
1	A	142	GLN
1	A	143	ARG
1	A	145	TRP
1	A	164	LEU
1	A	215	LEU
1	A	232	LEU
1	A	246	LYS
1	A	259	ASN
1	A	266	ASN
1	A	283	GLN
1	A	292[A]	VAL
1	A	295[A]	PHE
1	A	297[A]	ASP
1	A	311	GLU
1	A	400	LEU
1	B	145	TRP
1	B	171	GLU
1	B	209	SER
1	B	214	GLU
1	B	215	LEU
1	B	232	LEU
1	B	266	ASN
1	B	295[B]	PHE
1	B	297[B]	ASP
1	B	307	LEU
1	B	309	THR
1	B	316	ASP
1	B	348	VAL
1	B	383	ARG
1	B	400	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	170	ASN
1	A	195	ASN
1	A	263	ASN
1	A	266	ASN
1	A	269	ASN
1	A	385	GLN
1	B	142	GLN
1	B	147	GLN
1	B	170	ASN
1	B	259	ASN
1	B	263	ASN
1	B	266	ASN
1	B	269	ASN
1	B	283	GLN

### 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 ⓘ

Of 1 ligands modelled in this entry, 1 is monoatomic - leaving 0 for Mogul analysis.

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.

## 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	271/302 (89%)	0.40	27 (9%) 8 7	22, 36, 69, 96	12 (4%)
1	B	269/302 (89%)	0.65	31 (11%) 5 5	8, 34, 77, 123	12 (4%)
All	All	540/604 (89%)	0.52	58 (10%) 6 6	8, 35, 75, 123	24 (4%)

All (58) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	340	TRP	12.7
1	B	338	VAL	12.1
1	B	343	PRO	10.5
1	B	341	ARG	8.5
1	B	130	GLU	7.0
1	B	344	THR	6.8
1	B	298[B]	SER	6.0
1	B	342	HIS	5.9
1	B	290[B]	PRO	5.8
1	A	344	THR	5.8
1	B	337	ASN	5.5
1	B	129	SER	5.2
1	B	128	GLY	5.0
1	A	288[A]	ASP	5.0
1	B	345	MET	4.9
1	B	288[B]	ASP	4.8
1	A	298[A]	SER	4.5
1	A	317	ALA	4.4
1	B	289[B]	SER	4.3
1	A	382	GLY	4.2
1	A	290[A]	PRO	4.2
1	B	252	VAL	4.1
1	A	250	GLU	4.0
1	B	381	ASP	3.9

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Mol	Chain	Res	Type	RSRZ
1	B	339	SER	3.9
1	A	287[A]	GLY	3.8
1	B	307	LEU	3.8
1	A	337	ASN	3.5
1	B	382	GLY	3.4
1	B	286	ARG	3.3
1	A	126	SER	3.2
1	B	250	GLU	3.2
1	A	294[A]	TRP	3.2
1	A	291[A]	GLY	3.1
1	B	336	ASP	3.1
1	A	251	GLN	3.1
1	A	292[A]	VAL	3.0
1	B	251	GLN	3.0
1	A	286	ARG	2.9
1	A	383	ARG	2.8
1	B	131	GLY	2.8
1	A	289[A]	SER	2.8
1	B	291[B]	GLY	2.7
1	B	243	ILE	2.7
1	B	317	ALA	2.6
1	B	168	ILE	2.6
1	A	295[A]	PHE	2.6
1	A	400	LEU	2.6
1	B	292[B]	VAL	2.5
1	A	127	SER	2.5
1	A	252	VAL	2.5
1	A	243	ILE	2.4
1	A	381	ASP	2.4
1	B	295[B]	PHE	2.4
1	A	316	ASP	2.2
1	A	307	LEU	2.1
1	A	168	ILE	2.1
1	A	336	ASP	2.0

## 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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
2	MG	B	1	1/1	0.03	-2.65	34,34,34,34	0

### 6.5 Other polymers

There are no such residues in this entry.