



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 10:55 AM GMT

PDB ID : 3NKF  
Title : Crystal structure of human ligand-free mature caspase-6 with intersubunit linker attached  
Authors : Vaidya, S.; Hardy, J.A.  
Deposited on : 2010-06-18  
Resolution : 2.90 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  
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

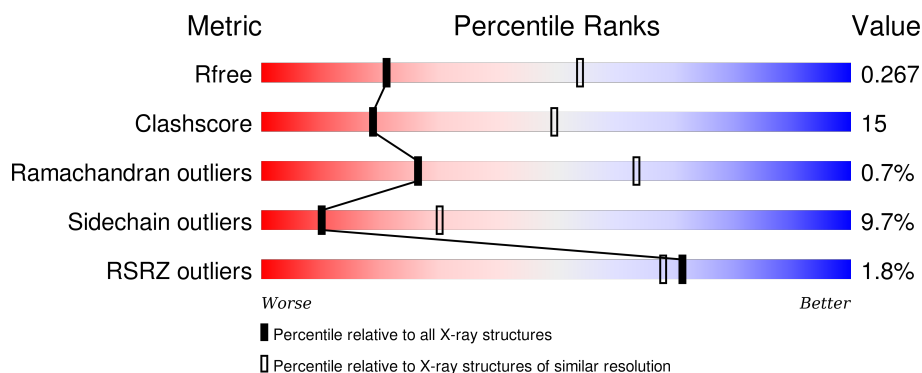
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.90 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	1451 (2.90-2.90)
Clashscore	102246	1668 (2.90-2.90)
Ramachandran outliers	100387	1630 (2.90-2.90)
Sidechain outliers	100360	1632 (2.90-2.90)
RSRZ outliers	91569	1456 (2.90-2.90)

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	277	<div> <div>2%</div> <div>58% 18% • 21%</div> </div>
1	B	277	<div> <div>2%</div> <div>54% 20% • 23%</div> </div>
1	C	277	<div> <div>%</div> <div>53% 22% 5% 20%</div> </div>
1	D	277	<div> <div>%</div> <div>55% 21% • 21%</div> </div>

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 6692 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-6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	219	Total	C	N	O	S	0	0	0
			1665	1073	280	299	13			
1	B	213	Total	C	N	O	S	0	0	0
			1599	1019	273	294	13			
1	C	222	Total	C	N	O	S	0	0	0
			1722	1104	297	308	13			
1	D	220	Total	C	N	O	S	0	0	0
			1679	1075	286	305	13			

There are 28 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	23	MET	-	EXPRESSION TAG	UNP P55212
A	294	HIS	-	EXPRESSION TAG	UNP P55212
A	295	HIS	-	EXPRESSION TAG	UNP P55212
A	296	HIS	-	EXPRESSION TAG	UNP P55212
A	297	HIS	-	EXPRESSION TAG	UNP P55212
A	298	HIS	-	EXPRESSION TAG	UNP P55212
A	299	HIS	-	EXPRESSION TAG	UNP P55212
B	23	MET	-	EXPRESSION TAG	UNP P55212
B	294	HIS	-	EXPRESSION TAG	UNP P55212
B	295	HIS	-	EXPRESSION TAG	UNP P55212
B	296	HIS	-	EXPRESSION TAG	UNP P55212
B	297	HIS	-	EXPRESSION TAG	UNP P55212
B	298	HIS	-	EXPRESSION TAG	UNP P55212
B	299	HIS	-	EXPRESSION TAG	UNP P55212
C	23	MET	-	EXPRESSION TAG	UNP P55212
C	294	HIS	-	EXPRESSION TAG	UNP P55212
C	295	HIS	-	EXPRESSION TAG	UNP P55212
C	296	HIS	-	EXPRESSION TAG	UNP P55212
C	297	HIS	-	EXPRESSION TAG	UNP P55212
C	298	HIS	-	EXPRESSION TAG	UNP P55212
C	299	HIS	-	EXPRESSION TAG	UNP P55212

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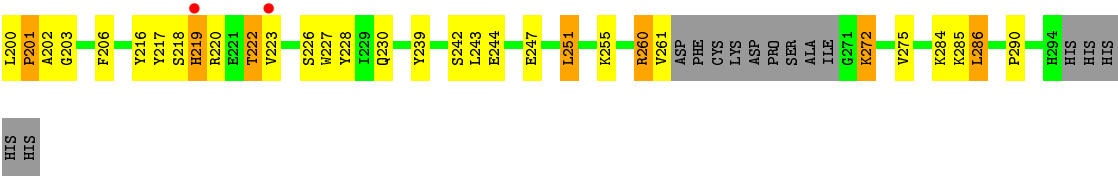
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Chain	Residue	Modelled	Actual	Comment	Reference
D	23	MET	-	EXPRESSION TAG	UNP P55212
D	294	HIS	-	EXPRESSION TAG	UNP P55212
D	295	HIS	-	EXPRESSION TAG	UNP P55212
D	296	HIS	-	EXPRESSION TAG	UNP P55212
D	297	HIS	-	EXPRESSION TAG	UNP P55212
D	298	HIS	-	EXPRESSION TAG	UNP P55212
D	299	HIS	-	EXPRESSION TAG	UNP P55212

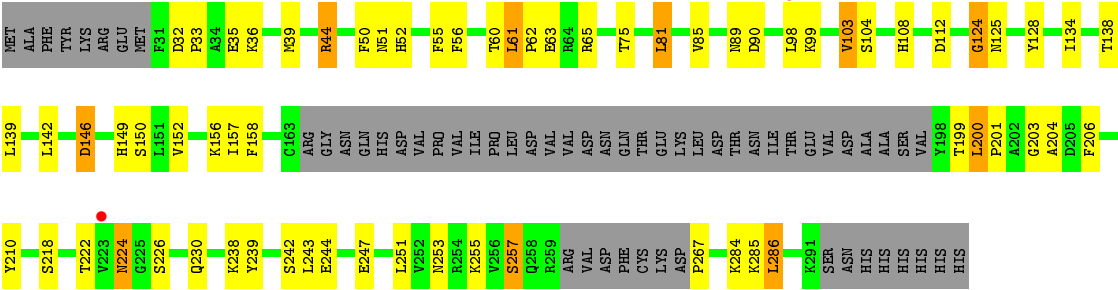
- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	8	Total O 8 8	0	0
2	B	6	Total O 6 6	0	0
2	C	5	Total O 5 5	0	0
2	D	8	Total O 8 8	0	0





● Molecule 1: Caspase-6



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	63.29Å 90.81Å 85.91Å 90.00° 91.04° 90.00°	Depositor
Resolution (Å)	29.50 – 2.90 29.52 – 2.80	Depositor EDS
% Data completeness (in resolution range)	99.7 (29.50-2.90) 94.6 (29.52-2.80)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.45 (at 2.80Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, $R_{free}$	0.216 , 0.270 0.214 , 0.267	Depositor DCC
$R_{free}$ test set	1292 reflections (6.35%)	DCC
Wilson B-factor (Å <sup>2</sup> )	62.5	Xtriage
Anisotropy	0.415	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 77.1	EDS
Estimated twinning fraction	0.205 for h,-k,-l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.34$	Xtriage
Outliers	0 of 24005 reflections	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	6692	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	83.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.71% 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 [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	0.51	0/1702	0.61	1/2298 (0.0%)
1	B	0.55	0/1631	0.61	0/2203
1	C	0.54	0/1760	0.64	0/2371
1	D	0.53	0/1715	0.63	1/2316 (0.0%)
All	All	0.53	0/6808	0.63	2/9188 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	267	PRO	N-CA-CB	6.09	110.61	103.30
1	A	201	PRO	N-CA-CB	5.83	110.30	103.30

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	1665	0	1559	38	0
1	B	1599	0	1465	63	0
1	C	1722	0	1638	61	0
1	D	1679	0	1584	46	0
2	A	8	0	0	2	0
2	B	6	0	0	2	0
2	C	5	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	8	0	0	0	0
All	All	6692	0	6246	197	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 197 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:B:287:HIS:HE1	2:B:9:HOH:O	1.49	0.93
1:C:219:HIS:HD2	1:C:227:TRP:HB2	1.34	0.92
1:B:287:HIS:CE1	2:B:9:HOH:O	2.24	0.90
1:C:52:HIS:HD2	1:C:90:ASP:OD2	1.53	0.90
1:C:219:HIS:CD2	1:C:227:TRP:HB2	2.12	0.84

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	213/277 (77%)	193 (91%)	18 (8%)	2 (1%)	21	57
1	B	205/277 (74%)	193 (94%)	11 (5%)	1 (0%)	34	71
1	C	216/277 (78%)	199 (92%)	15 (7%)	2 (1%)	21	57
1	D	214/277 (77%)	197 (92%)	16 (8%)	1 (0%)	34	71
All	All	848/1108 (76%)	782 (92%)	60 (7%)	6 (1%)	26	63

5 of 6 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	201	PRO

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Mol	Chain	Res	Type
1	A	124	GLY
1	B	124	GLY
1	C	124	GLY
1	D	124	GLY

### 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	163/245 (66%)	149 (91%)	14 (9%)	13	36
1	B	156/245 (64%)	141 (90%)	15 (10%)	10	31
1	C	173/245 (71%)	154 (89%)	19 (11%)	8	23
1	D	169/245 (69%)	153 (90%)	16 (10%)	11	31
All	All	661/980 (67%)	597 (90%)	64 (10%)	10	30

5 of 64 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	286	LEU
1	C	92	LYS
1	D	242	SER
1	C	42	ARG
1	C	61	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 13 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	108	HIS
1	B	230	GLN
1	C	258	GLN
1	B	52	HIS
1	C	219	HIS

### 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	219/277 (79%)	0.04	5 (2%) 64 59	57, 85, 143, 173	0
1	B	213/277 (76%)	0.05	5 (2%) 64 59	56, 89, 139, 181	0
1	C	222/277 (80%)	-0.15	4 (1%) 71 68	29, 69, 128, 214	0
1	D	220/277 (79%)	-0.17	2 (0%) 85 84	30, 71, 127, 191	0
All	All	874/1108 (78%)	-0.06	16 (1%) 71 68	29, 79, 138, 214	0

The worst 5 of 16 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	62	PRO	4.2
1	A	145	GLY	3.9
1	A	148	CYS	3.3
1	A	215	GLY	3.3
1	D	223	VAL	3.2

### 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.