



# wwPDB X-ray Structure Validation Summary Report ⓘ

Jan 31, 2016 – 07:58 PM GMT

PDB ID : 1I3O  
Title : CRYSTAL STRUCTURE OF THE COMPLEX OF XIAP-BIR2 AND CAS-PASE 3  
Authors : Riedl, S.J.; Renatus, M.; Schwarzenbacher, R.; Zhou, Q.; Sun, C.; Fesik, S.W.; Liddington, R.C.; Salvesen, G.S.  
Deposited on : 2001-02-15  
Resolution : 2.70 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) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

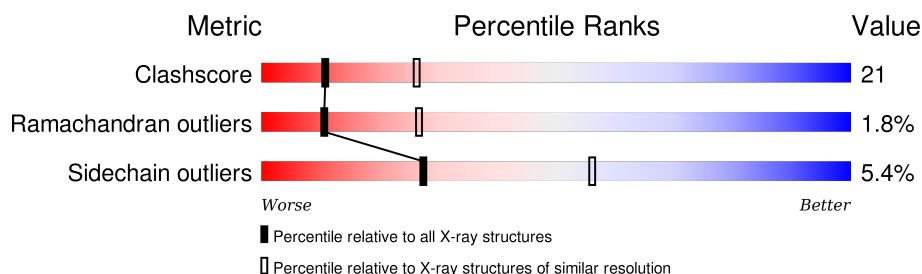
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.70 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	102246	2422 (2.70-2.70)
Ramachandran outliers	100387	2382 (2.70-2.70)
Sidechain outliers	100360	2382 (2.70-2.70)

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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	175	
1	C	175	
2	B	110	
2	D	110	
3	E	121	
3	F	121	

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 5593 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 3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	143	Total	C	N	O	S	11	0	0
			1133	701	204	220	8			
1	C	144	Total	C	N	O	S	6	0	0
			1142	705	205	224	8			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	285	ALA	CYS	ENGINEERED	UNP P42574
C	285	ALA	CYS	ENGINEERED	UNP P42574

- Molecule 2 is a protein called CASPASE 3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	101	Total	C	N	O	S	5	0	0
			827	538	131	151	7			
2	D	101	Total	C	N	O	S	12	0	0
			827	538	131	151	7			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	403	LEU	-	EXPRESSION TAG	UNP P42574
B	404	GLU	-	EXPRESSION TAG	UNP P42574
B	405	HIS	-	EXPRESSION TAG	UNP P42574
B	406	HIS	-	EXPRESSION TAG	UNP P42574
B	407	HIS	-	EXPRESSION TAG	UNP P42574
B	408	HIS	-	EXPRESSION TAG	UNP P42574
B	409	HIS	-	EXPRESSION TAG	UNP P42574
B	410	HIS	-	EXPRESSION TAG	UNP P42574
D	403	LEU	-	EXPRESSION TAG	UNP P42574
D	404	GLU	-	EXPRESSION TAG	UNP P42574

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Chain	Residue	Modelled	Actual	Comment	Reference
D	405	HIS	-	EXPRESSION TAG	UNP P42574
D	406	HIS	-	EXPRESSION TAG	UNP P42574
D	407	HIS	-	EXPRESSION TAG	UNP P42574
D	408	HIS	-	EXPRESSION TAG	UNP P42574
D	409	HIS	-	EXPRESSION TAG	UNP P42574
D	410	HIS	-	EXPRESSION TAG	UNP P42574

- Molecule 3 is a protein called BACULOVIRAL IAP REPEAT-CONTAINING PROTEIN 4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	111	Total	C	N	O	S	0	0	0
			903	573	162	164	4			
3	F	93	Total	C	N	O	S	7	0	0
			746	470	136	136	4			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	120	GLY	-	CLONING ARTIFACT	UNP P98170
E	121	SER	-	CLONING ARTIFACT	UNP P98170
E	122	HIS	-	CLONING ARTIFACT	UNP P98170
E	123	MET	-	CLONING ARTIFACT	UNP P98170
E	202	ALA	CYS	ENGINEERED	UNP P98170
E	213	GLY	CYS	ENGINEERED	UNP P98170
F	120	GLY	-	CLONING ARTIFACT	UNP P98170
F	121	SER	-	CLONING ARTIFACT	UNP P98170
F	122	HIS	-	CLONING ARTIFACT	UNP P98170
F	123	MET	-	CLONING ARTIFACT	UNP P98170
F	202	ALA	CYS	ENGINEERED	UNP P98170
F	213	GLY	CYS	ENGINEERED	UNP P98170

- Molecule 4 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	F	1	Total	Zn	0	0
			1	1		
4	E	1	Total	Zn	0	0
			1	1		

- Molecule 5 is water.

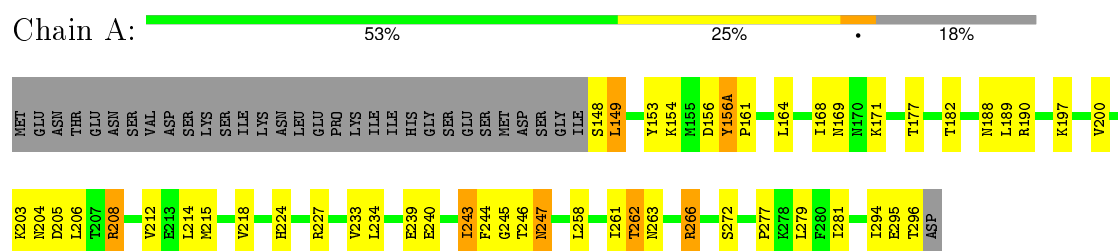
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	3	Total 3	O 3	0	0
5	B	4	Total 4	O 4	0	0
5	C	3	Total 3	O 3	0	0
5	D	2	Total 2	O 2	0	0
5	E	1	Total 1	O 1	0	0

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

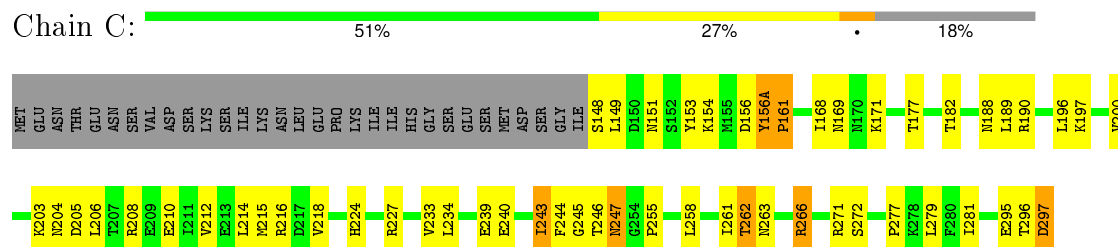
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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 ( $RSRZ > 2$ ). 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.

Note EDS was not executed.

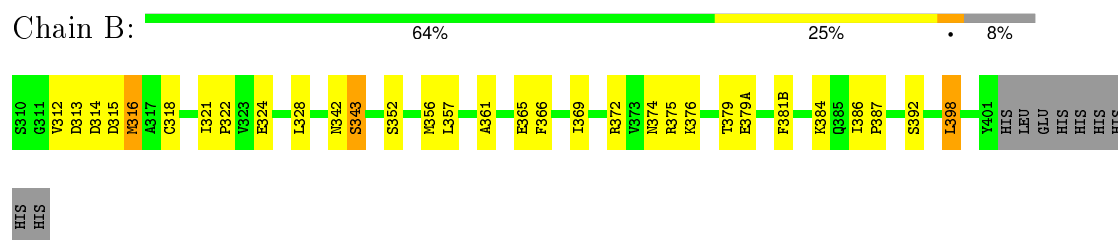
#### • Molecule 1: CASPASE 3



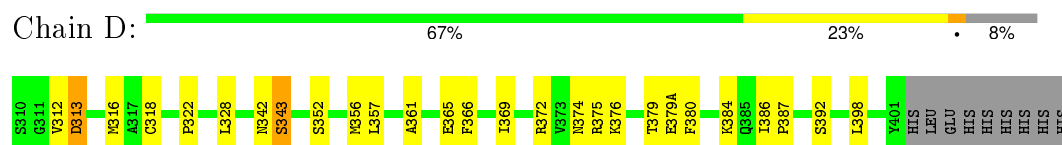
#### • Molecule 1: CASPASE 3



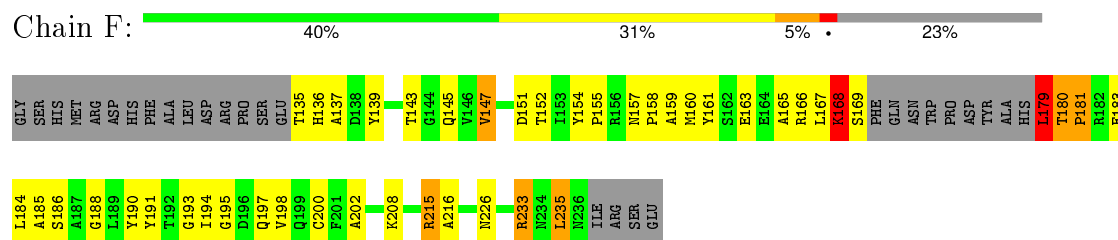
#### • Molecule 2: CASPASE 3



#### • Molecule 2: CASPASE 3



#### • Molecule 3: BACULOVIRAL IAP REPEAT-CONTAINING PROTEIN 4



## 4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section will therefore be incomplete.

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	70.70 Å 95.50 Å 144.20 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	500.00 – 2.70	Depositor
% Data completeness (in resolution range)	98.6 (500.00-2.70)	Depositor
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	CNS 1.0	Depositor
R, $R_{free}$	0.248 , 0.278	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	5593	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	55.0	wwPDB-VP



## 5 Model quality

### 5.1 Standard geometry

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

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	0.45	0/1148	0.67	1/1538 (0.1%)
1	C	0.44	0/1157	0.65	1/1549 (0.1%)
2	B	0.46	0/851	0.63	0/1149
2	D	0.45	0/851	0.63	0/1149
3	E	0.46	0/931	0.63	1/1265 (0.1%)
3	F	0.70	2/765 (0.3%)	0.77	2/1035 (0.2%)
All	All	0.49	2/5703 (0.0%)	0.66	5/7685 (0.1%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	181	PRO	N-CD	10.09	1.61	1.47
3	F	181	PRO	N-CA	-6.71	1.35	1.47

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	179	LEU	CB-CA-C	-8.87	93.34	110.20
3	F	179	LEU	N-CA-C	6.40	128.28	111.00
1	C	245	GLY	N-CA-C	-5.82	98.55	113.10
1	A	245	GLY	N-CA-C	-5.72	98.80	113.10
3	E	179	LEU	N-CA-CB	5.57	121.53	110.40

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	1133	0	1130	45	0
1	C	1142	0	1134	56	0
2	B	827	0	795	33	0
2	D	827	0	795	28	0
3	E	903	0	847	47	0
3	F	746	0	710	52	0
4	E	1	0	0	0	0
4	F	1	0	0	0	0
5	A	3	0	0	0	0
5	B	4	0	0	1	0
5	C	3	0	0	0	0
5	D	2	0	0	0	0
5	E	1	0	0	0	0
All	All	5593	0	5411	229	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 21.

The worst 5 of 229 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)
3:F:180:THR:OG1	3:F:183:GLU:HB3	1.54	1.05
3:F:215:ARG:HA	3:F:215:ARG:NH1	1.82	0.93
1:C:177:THR:HG21	3:F:145:GLN:HG2	1.48	0.92
3:F:168:LYS:HD3	3:F:169:SER:H	1.34	0.90
1:A:247:ASN:H	1:A:247:ASN:HD22	1.22	0.87

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	141/175 (81%)	130 (92%)	8 (6%)	3 (2%)	9	23
1	C	142/175 (81%)	130 (92%)	10 (7%)	2 (1%)	14	35
2	B	99/110 (90%)	93 (94%)	4 (4%)	2 (2%)	9	24
2	D	99/110 (90%)	91 (92%)	7 (7%)	1 (1%)	19	45
3	E	109/121 (90%)	98 (90%)	10 (9%)	1 (1%)	21	49
3	F	89/121 (74%)	80 (90%)	6 (7%)	3 (3%)	5	10
All	All	679/812 (84%)	622 (92%)	45 (7%)	12 (2%)	11	27

5 of 12 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	F	168	LYS
3	F	167	LEU
1	A	156(A)	TYR
2	B	343	SER
1	C	156(A)	TYR

### 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	128/158 (81%)	120 (94%)	8 (6%)	22	48
1	C	129/158 (82%)	122 (95%)	7 (5%)	27	56
2	B	89/98 (91%)	88 (99%)	1 (1%)	80	94
2	D	89/98 (91%)	88 (99%)	1 (1%)	80	94
3	E	94/103 (91%)	84 (89%)	10 (11%)	8	19
3	F	78/103 (76%)	72 (92%)	6 (8%)	16	36
All	All	607/718 (84%)	574 (95%)	33 (5%)	27	56

5 of 33 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	266	ARG
3	E	131	ARG
3	F	215	ARG
1	C	297	ASP
2	D	313	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 18 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	195	ASN
1	C	247	ASN
3	E	236	ASN
1	C	169	ASN
1	C	188	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules 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 2 ligands modelled in this entry, 2 are 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.

No monomer is involved in short contacts.

## 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 ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

### 6.3 Carbohydrates ⓘ

EDS was not executed - this section will therefore be empty.

### 6.4 Ligands ⓘ

EDS was not executed - this section will therefore be empty.

### 6.5 Other polymers ⓘ

EDS was not executed - this section will therefore be empty.