



wwPDB X-ray Structure Validation Summary Report ⓘ

May 25, 2020 – 11:36 pm BST

PDB ID : 1I4O
Title : CRYSTAL STRUCTURE OF THE XIAP/CASPASE-7 COMPLEX
Authors : Huang, Y.; Park, Y.C.; Rich, R.L.; Segal, D.; Myszka, D.G.; Wu, H.
Deposited on : 2001-02-22
Resolution : 2.40 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

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

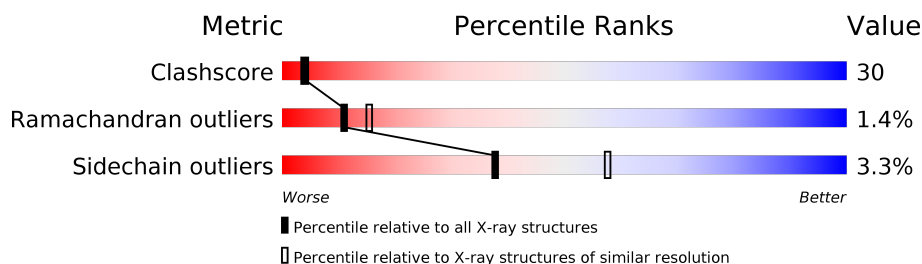
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)

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 ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. 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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	280	
1	B	280	
2	C	141	
2	D	141	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 4124 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	235	Total	C	N	O	S	0	0	0
			1854	1181	313	345	15			
1	B	232	Total	C	N	O	S	0	0	0
			1823	1161	310	337	15			

- Molecule 2 is a protein called BACULOVIRAL IAP REPEAT-CONTAINING PROTEIN 4.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	C	17	Total	C	N	O	0	0	0
			124	78	20	26			
2	D	17	Total	C	N	O	0	0	0
			124	78	20	26			

- Molecule 3 is water.

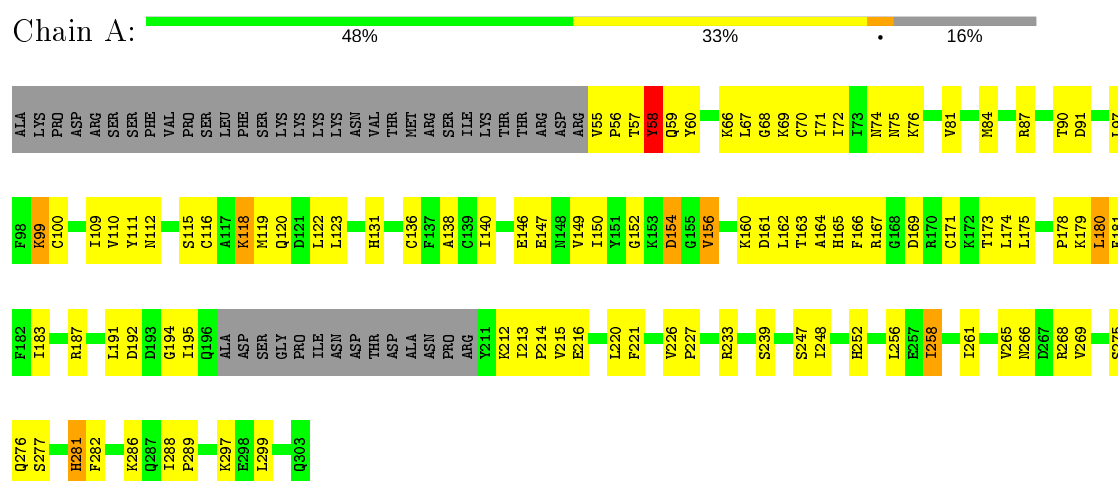
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	87	Total	O	0	0
			87	87		
3	B	98	Total	O	0	0
			98	98		
3	C	6	Total	O	0	0
			6	6		
3	D	8	Total	O	0	0
			8	8		

3 Residue-property plots

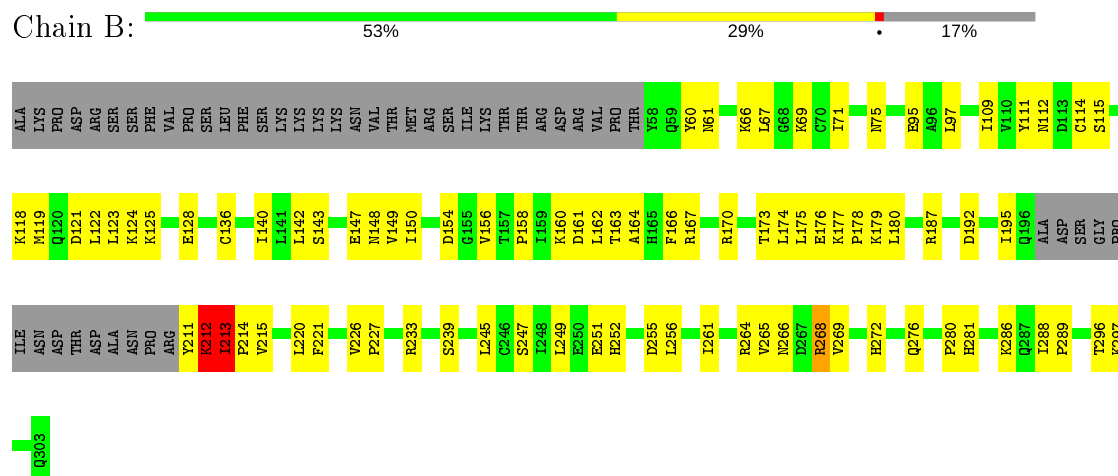
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according 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. 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-7

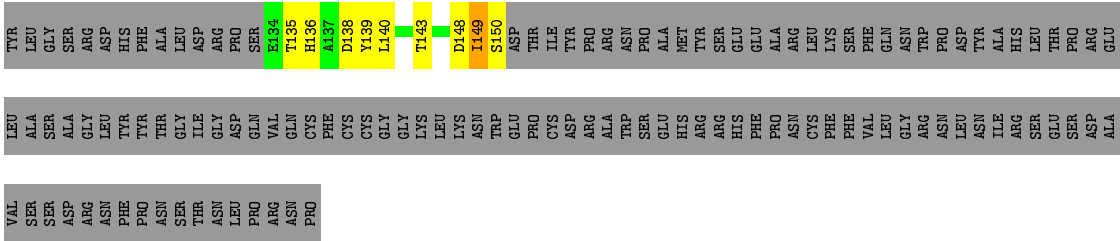


• Molecule 1: CASPASE-7



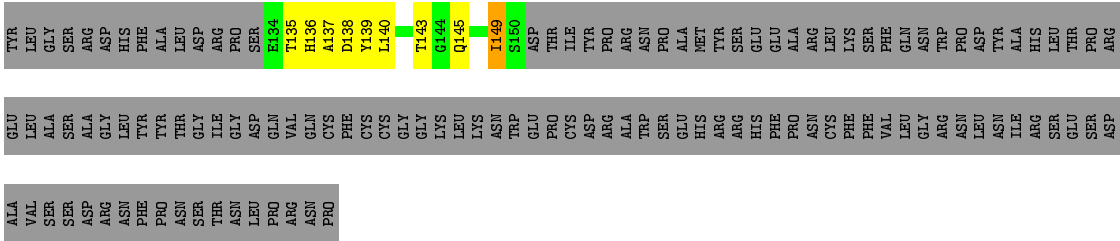
• Molecule 2: BACULOVIRAL IAP REPEAT-CONTAINING PROTEIN 4





● Molecule 2: BACULOVIRAL IAP REPEAT-CONTAINING PROTEIN 4

Chain D: 6% 6% . 88%



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α , β , γ	88.50Å 88.50Å 185.40Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	20.00 – 2.40	Depositor
% Data completeness (in resolution range)	(Not available) (20.00-2.40)	Depositor
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
Refinement program		Depositor
R, R_{free}	0.224 , 0.260	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	4124	wwPDB-VP
Average B, all atoms (Å ²)	51.0	wwPDB-VP

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	0.44	0/1895	0.73	2/2556 (0.1%)
1	B	0.44	0/1862	0.72	2/2510 (0.1%)
2	C	0.77	0/125	0.68	0/171
2	D	0.69	0/125	0.64	0/171
All	All	0.47	0/4007	0.72	4/5408 (0.1%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	213	ILE	N-CA-C	-6.64	93.08	111.00
1	A	152	GLY	N-CA-C	-5.87	98.42	113.10
1	A	58	TYR	N-CA-C	5.08	124.71	111.00
1	B	212	LYS	N-CA-C	-5.05	97.36	111.00

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	1854	0	1793	125	0
1	B	1823	0	1763	106	0
2	C	124	0	113	15	0
2	D	124	0	113	16	0
3	A	87	0	0	9	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	98	0	0	19	0
3	C	6	0	0	2	0
3	D	8	0	0	1	0
All	All	4124	0	3782	230	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 30.

The worst 5 of 230 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:194:GLY:HA2	1:B:211:TYR:CB	1.87	1.04
1:A:276:GLN:O	2:C:149:ILE:HG23	1.63	0.99
1:B:75:ASN:HD21	1:B:119:MET:HE1	1.25	0.99
1:A:286:LYS:HG3	1:B:212:LYS:H	1.30	0.95
2:C:149:ILE:HG12	2:C:149:ILE:O	1.71	0.90

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	231/280 (82%)	210 (91%)	17 (7%)	4 (2%)	9	11
1	B	228/280 (81%)	221 (97%)	6 (3%)	1 (0%)	34	48
2	C	15/141 (11%)	14 (93%)	0	1 (7%)	1	0
2	D	15/141 (11%)	14 (93%)	0	1 (7%)	1	0
All	All	489/842 (58%)	459 (94%)	23 (5%)	7 (1%)	11	15

5 of 7 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	154	ASP
1	A	58	TYR
1	A	275	SER
1	B	213	ILE
1	A	281	HIS

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	200/248 (81%)	192 (96%)	8 (4%)	31	49
1	B	195/248 (79%)	189 (97%)	6 (3%)	40	60
2	C	13/124 (10%)	13 (100%)	0	100	100
2	D	13/124 (10%)	13 (100%)	0	100	100
All	All	421/744 (57%)	407 (97%)	14 (3%)	38	57

5 of 14 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	180	LEU
1	A	258	ILE
1	B	180	LEU
1	A	160	LYS
1	B	95	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 10 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	63	ASN
1	B	74	ASN
1	B	112	ASN
1	B	61	ASN
1	B	75	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 ⓘ

6.1 Protein, DNA and RNA chains ⓘ

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates ⓘ

EDS was not executed - this section is therefore empty.

6.4 Ligands ⓘ

EDS was not executed - this section is therefore empty.

6.5 Other polymers ⓘ

EDS was not executed - this section is therefore empty.