



wwPDB X-ray Structure Validation Summary Report ⓘ

Jan 31, 2016 – 07:58 PM GMT

PDB ID : 1I51
Title : CRYSTAL STRUCTURE OF CASPASE-7 COMPLEXED WITH XIAP
Authors : Chai, J.; Shi, Y.
Deposited on : 2001-02-23
Resolution : 2.45 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
<http://wwpdb.org/validation/2016/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
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

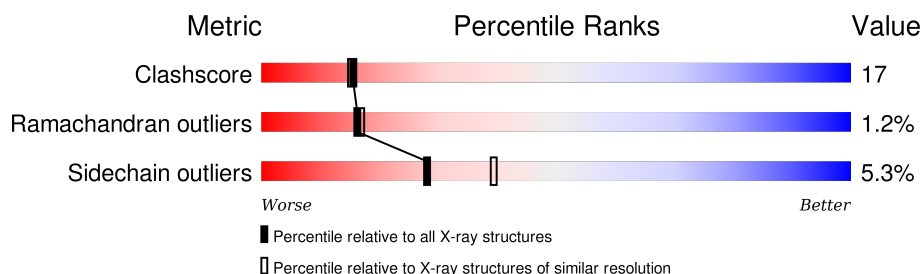
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.45 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	1030 (2.48-2.44)
Ramachandran outliers	100387	1024 (2.48-2.44)
Sidechain outliers	100360	1024 (2.48-2.44)

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. 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	148	 64% 26% 6%
1	C	148	 69% 25% 6%
2	B	105	 65% 22% 12%
2	D	105	 53% 30% 5% 12%
3	E	117	 7% 8% 85%
3	F	117	 7% 8% 85%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 3974 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 SUBUNIT P20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	139	Total	C	N	O	S	0	0	0
			1089	686	187	205	11			
1	C	139	Total	C	N	O	S	0	0	0
			1089	686	187	205	11			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	169	ALA	ASP	ENGINEERED	UNP P55210
C	169	ALA	ASP	ENGINEERED	UNP P55210

- Molecule 2 is a protein called CASPASE-7 SUBUNIT P11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	92	Total	C	N	O	S	0	0	0
			758	487	128	139	4			
2	D	92	Total	C	N	O	S	0	0	0
			758	487	128	139	4			

- Molecule 3 is a protein called X-LINKED INHIBITOR OF APOPTOSIS PROTEIN.

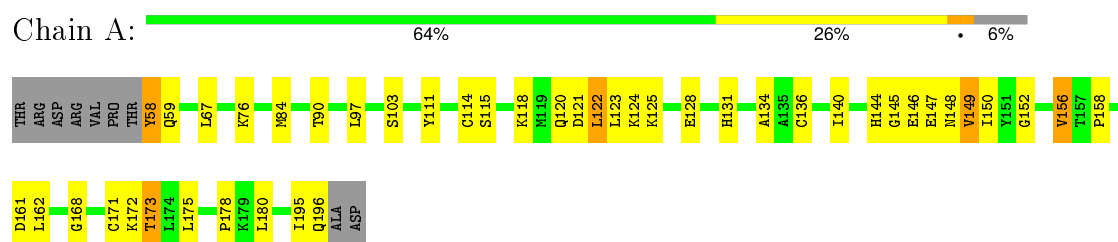
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	E	18	Total	C	N	O	0	0	0
			140	86	24	30			
3	F	18	Total	C	N	O	0	0	0
			140	86	24	30			

3 Residue-property plots [i](#)

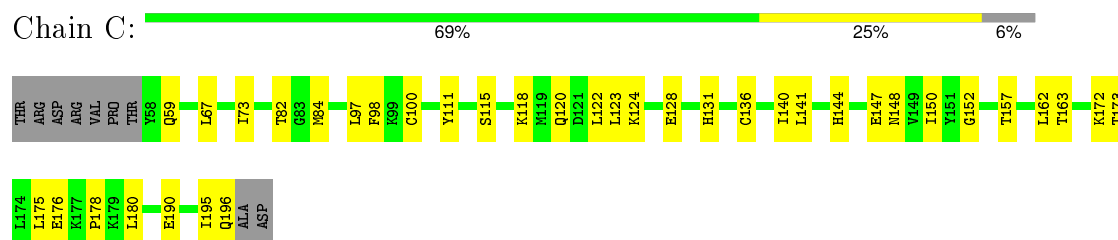
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according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

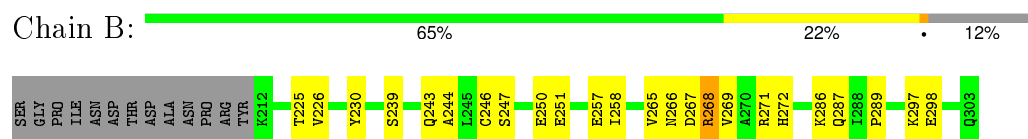
• Molecule 1: CASPASE-7 SUBUNIT P20



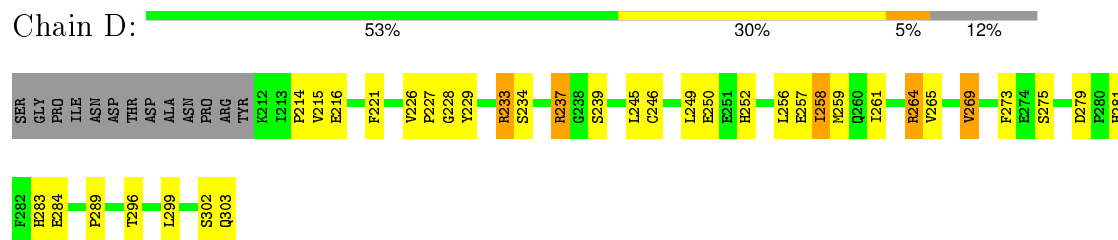
• Molecule 1: CASPASE-7 SUBUNIT P20



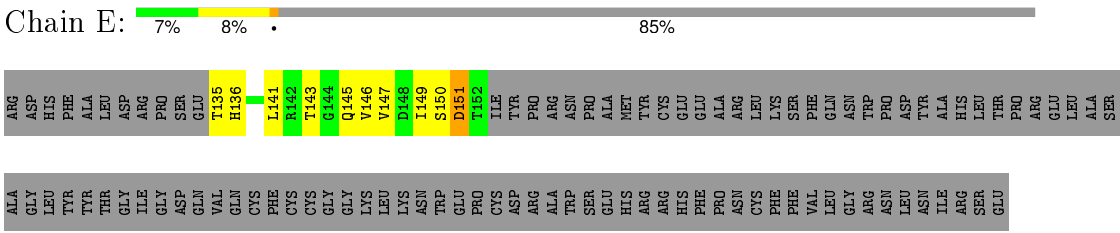
• Molecule 2: CASPASE-7 SUBUNIT P11



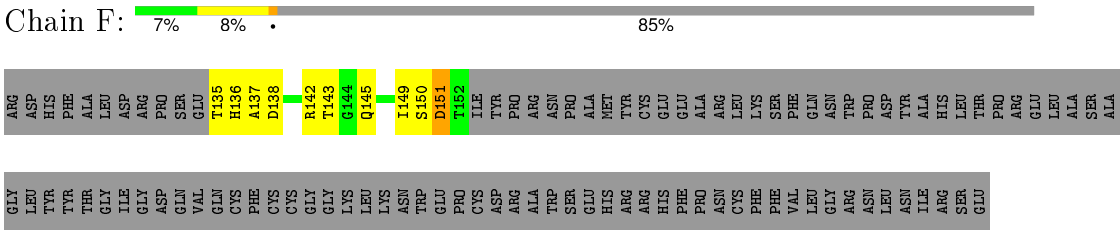
• Molecule 2: CASPASE-7 SUBUNIT P11



• Molecule 3: X-LINKED INHIBITOR OF APOPTOSIS PROTEIN



• Molecule 3: X-LINKED INHIBITOR OF APOPTOSIS PROTEIN



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α , β , γ	89.60Å 89.60Å 185.50Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	20.00 – 2.45	Depositor
% Data completeness (in resolution range)	(Not available) (20.00-2.45)	Depositor
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS	Depositor
R, R_{free}	0.233 , 0.272	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	3974	wwPDB-VP
Average B, all atoms (Å ²)	62.0	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	0.38	0/1106	0.65	1/1482 (0.1%)
1	C	0.40	0/1106	0.64	1/1482 (0.1%)
2	B	0.41	0/780	0.63	0/1054
2	D	0.42	0/780	0.68	0/1054
3	E	0.38	0/141	0.53	0/192
3	F	0.35	0/141	0.51	0/192
All	All	0.40	0/4054	0.64	2/5456 (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	C	152	GLY	N-CA-C	-5.76	98.71	113.10
1	A	152	GLY	N-CA-C	-5.48	99.41	113.10

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	1089	0	1080	35	0
1	C	1089	0	1080	37	0
2	B	758	0	731	19	0
2	D	758	0	731	40	0
3	E	140	0	133	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	F	140	0	133	12	0
All	All	3974	0	3888	135	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 17.

The worst 5 of 135 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:C:115:SER:H	1:C:118:LYS:HD2	1.29	0.94
1:C:111:TYR:CE2	1:C:122:LEU:HD11	2.05	0.91
2:D:258:ILE:CD1	2:D:299:LEU:HB3	2.03	0.88
1:C:131:HIS:H	1:C:173:THR:HG21	1.39	0.87
2:D:233:ARG:HA	2:D:239:SER:HA	1.55	0.87

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	137/148 (93%)	126 (92%)	10 (7%)	1 (1%)	26	32
1	C	137/148 (93%)	130 (95%)	6 (4%)	1 (1%)	26	32
2	B	90/105 (86%)	88 (98%)	2 (2%)	0	100	100
2	D	90/105 (86%)	87 (97%)	3 (3%)	0	100	100
3	E	16/117 (14%)	14 (88%)	0	2 (12%)	0	0
3	F	16/117 (14%)	14 (88%)	0	2 (12%)	0	0
All	All	486/740 (66%)	459 (94%)	21 (4%)	6 (1%)	16	17

5 of 6 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	E	151	ASP
3	F	151	ASP
3	E	150	SER
1	A	171	CYS
1	C	82	THR

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	118/126 (94%)	109 (92%)	9 (8%)	16	21
1	C	118/126 (94%)	114 (97%)	4 (3%)	44	61
2	B	84/95 (88%)	80 (95%)	4 (5%)	31	44
2	D	84/95 (88%)	78 (93%)	6 (7%)	18	24
3	E	16/102 (16%)	16 (100%)	0	100	100
3	F	16/102 (16%)	16 (100%)	0	100	100
All	All	436/646 (68%)	413 (95%)	23 (5%)	28	39

5 of 23 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	258	ILE
2	B	271	ARG
2	D	264	ARG
2	B	268	ARG
1	C	59	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 16 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	112	ASN
1	C	120	GLN
2	D	303	GLN
1	C	74	ASN

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Mol	Chain	Res	Type
3	E	145	GLN

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 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.