



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 10, 2026 – 01:11 PM UTC

PDB ID : 1KMC / pdb_00001kmc
Title : Crystal Structure of the Caspase-7 / XIAP-BIR2 Complex
Authors : Riedl, S.J.; Salvesen, G.S.; Bode, W.
Deposited on : 2001-12-14
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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

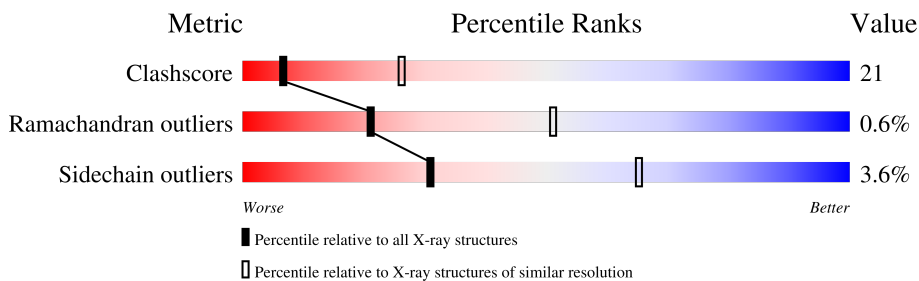
1 Overall quality at a glance

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))
Clashscore	190562	2690 (2.90-2.90)
Ramachandran outliers	187476	2623 (2.90-2.90)
Sidechain outliers	187428	2625 (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 of 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	303	
1	B	303	
2	C	119	
2	D	119	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 4047 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	234	Total	C	N	O	S	64	0	0
			1878	1193	321	350	14			
1	B	234	Total	C	N	O	S	89	0	0
			1876	1193	320	349	14			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	285	ALA	CYS	engineered mutation	UNP P55210
B	285	ALA	CYS	engineered mutation	UNP P55210

- Molecule 2 is a protein called X-LINKED INHIBITOR OF APOPTOSIS PROTEIN.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	C	17	Total	C	N	O	5	0	0
			134	83	23	28			
2	D	17	Total	C	N	O	25	0	0
			134	83	23	28			

- Molecule 3 is water.

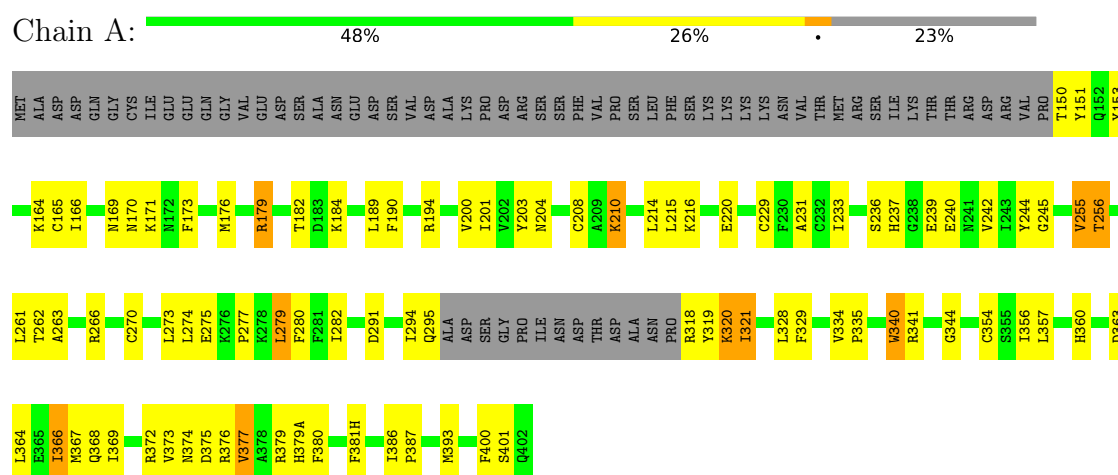
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	16	Total	O	0	0
			16	16		
3	B	8	Total	O	0	0
			8	8		
3	D	1	Total	O	0	0
			1	1		

3 Residue-property plots

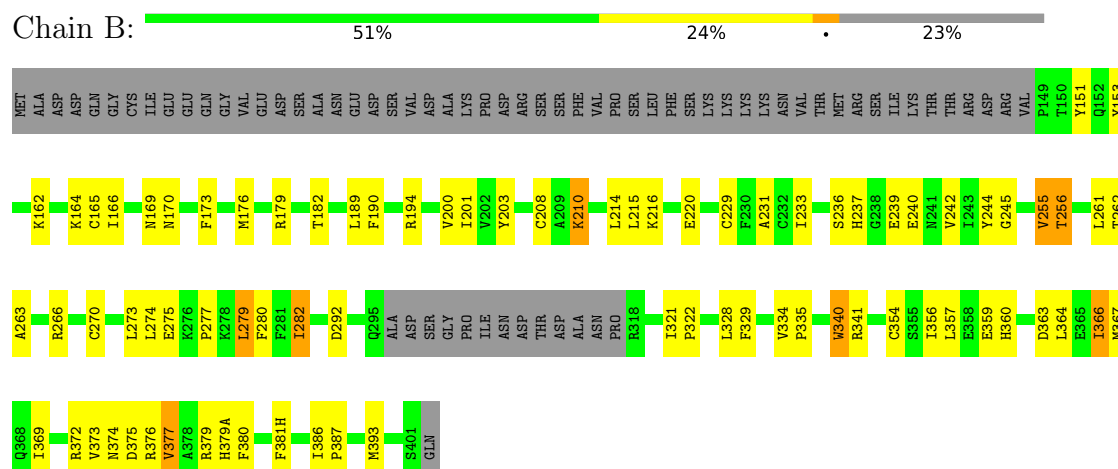
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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



ARG	ASP	HIS	PHE	ALA	LEU	ASP	ARG	PRO	SER	E134	T135	H136	A137	D138	Y139	L140	L141	R142	T143	V146	T149	S150	ASP
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SER	ALA	GLY	LEU	TYR	THR	GLY	ILE	GLY	ASP	GLN	VAL	GLN	CYS	PHE	CYS	CYS	GLY	GLY	LYS	LEU	LYS	ASN	TRP	GLU	PRO	CYS	ASP	ARG	ALA	TRP	SER	GLU	HIS	ARG	ARG	HIS	PHE	PRO	ASN	CYS	PHE	PHE	VAL	LEU	GLY	ARG	ASN	LEU	ASN	ASN	ASP
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● Molecule 2: X-LINKED INHIBITOR OF APOPTOSIS PROTEIN

Chain D: 8% . . 86%

ARG	ASP	HIS	PHE	ALA	LEU	ASP	ARG	PRO	SER	E134	T135	H136	A137	D138	Y139	L140	T143	G144	Q145	S150	ASP	THR	ILE	TYR	PRO	ARG	ALA	ASN	PRO	ALA	TYR	MET	HIS	ARG	CYS	GLU	PHE	PRO	ALA	ASN	ARG	LEU	LYS	PHE	VAL	PHE	LEU	GLN	ASN	TRP	PRO	ASN	LEU	ASP	TYR	ALA	HIS	ARG	THR	GLU	SER	SER	ASP
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GLY	LEU	TYR	THR	ILE	GLY	ASP	GLN	VAL	CYS	PHE	CYS	CYS	GLY	GLY	LYS	LEU	LYS	ASN	TRP	GLU	THR	PRO	CYS	ASP	PRO	ALA	TRP	SER	GLU	HIS	ARG	HIS	PHE	PRO	ASN	CYS	PHE	PHE	VAL	LEU	GLY	ARG	ASN	PRO	LEU	ASN	ASN	TYR	ALA	ILE	ARG	SER	GLU	SER	SER	ASP
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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	88.13Å 88.13Å 186.45Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	50.00 – 2.90	Depositor
% Data completeness (in resolution range)	98.5 (50.00-2.90)	Depositor
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS	Depositor
R, R_{free}	0.234 , 0.275	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	4047	wwPDB-VP
Average B, all atoms (Å ²)	52.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

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	0/1918	0.99	13/2581 (0.5%)
1	B	0.43	0/1917	0.96	13/2580 (0.5%)
2	C	0.48	0/135	0.75	0/183
2	D	0.44	0/135	0.83	0/183
All	All	0.44	0/4105	0.96	26/5527 (0.5%)

There are no bond length outliers.

The worst 5 of 26 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	376	ARG	NE-CZ-NH2	8.89	127.20	119.20
1	A	376	ARG	NE-CZ-NH1	-8.62	112.88	121.50
1	A	194	ARG	NE-CZ-NH2	7.84	126.26	119.20
1	B	376	ARG	CD-NE-CZ	6.70	133.78	124.40
1	B	194	ARG	N-CA-C	-6.64	103.97	111.14

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	1878	0	1839	81	0
1	B	1876	0	1839	70	0
2	C	134	0	128	11	0
2	D	134	0	128	11	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	16	0	0	1	0
3	B	8	0	0	1	0
3	D	1	0	0	0	0
All	All	4047	0	3934	162	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 162 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:274:LEU:HD22	1:B:321:ILE:HD11	1.22	1.09
1:A:210:LYS:HE3	1:A:210:LYS:HA	1.50	0.94
1:A:294:ILE:HG13	1:A:295:GLN:HG2	1.52	0.90
1:A:334:VAL:HG13	1:A:335:PRO:HD2	1.55	0.86
2:D:140:LEU:H	2:D:140:LEU:HD22	1.41	0.86

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	230/303 (76%)	212 (92%)	16 (7%)	2 (1%)	14	41
1	B	230/303 (76%)	215 (94%)	15 (6%)	0	100	100
2	C	15/119 (13%)	13 (87%)	1 (7%)	1 (7%)	1	3
2	D	15/119 (13%)	14 (93%)	1 (7%)	0	100	100
All	All	490/844 (58%)	454 (93%)	33 (7%)	3 (1%)	21	51

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	C	135	THR
1	A	320	LYS
1	A	179	ARG

5.3.2 Protein sidechains [i](#)

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	205/266 (77%)	198 (97%)	7 (3%)	32	66
1	B	205/266 (77%)	199 (97%)	6 (3%)	37	71
2	C	15/104 (14%)	14 (93%)	1 (7%)	15	43
2	D	15/104 (14%)	13 (87%)	2 (13%)	4	12
All	All	440/740 (60%)	424 (96%)	16 (4%)	31	65

5 of 16 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	D	135	THR
2	C	149	ILE
1	B	255	VAL
1	B	377	VAL
1	B	210	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 11 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	351	GLN
1	B	360	HIS
2	D	136	HIS
2	C	145	GLN
1	A	360	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 oligosaccharides 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.