



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 18, 2018 – 07:57 pm GMT

PDB ID : 1KMC
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 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 : 20171227.v01 (using entries in the PDB archive December 27th 2017)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk30686

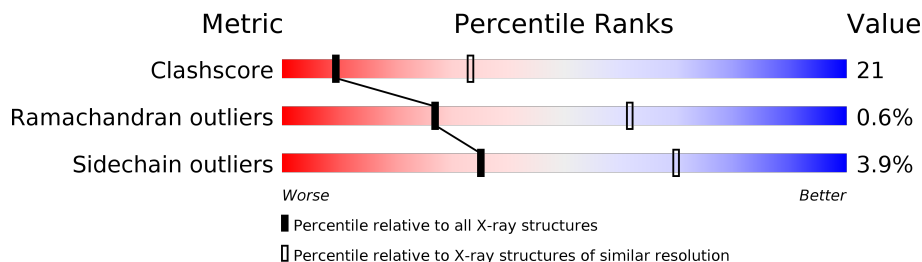
1 Overall quality at a glance

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	122078	1924 (2.90-2.90)
Ramachandran outliers	120005	1884 (2.90-2.90)
Sidechain outliers	119972	1886 (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 ≥ 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	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	UNP P55210
B	285	ALA	CYS	ENGINEERED	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.

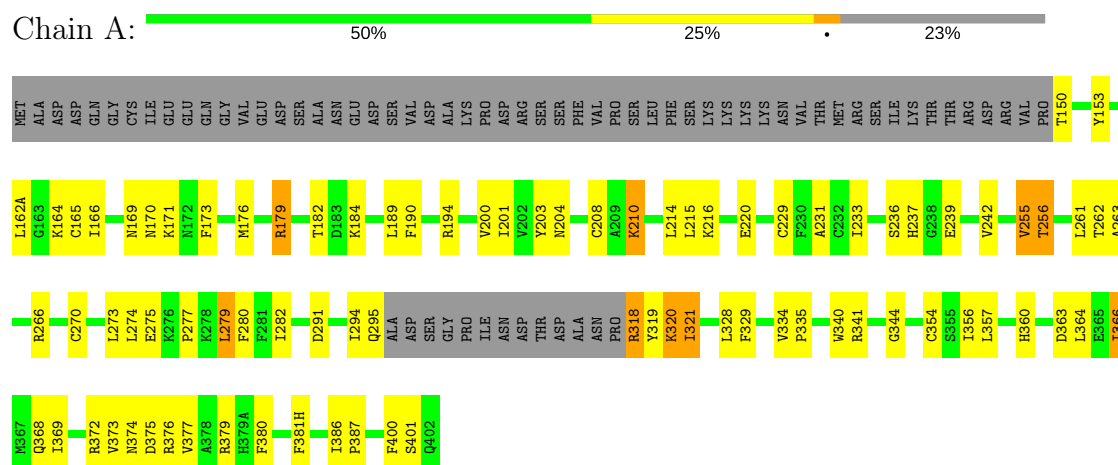
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	16	Total	O	0	0
			16	16		
3	B	8	Total	O	0	0
			8	8		
3	D	1	Total	O	0	0
			1	1		

3 Residue-property plots [i](#)

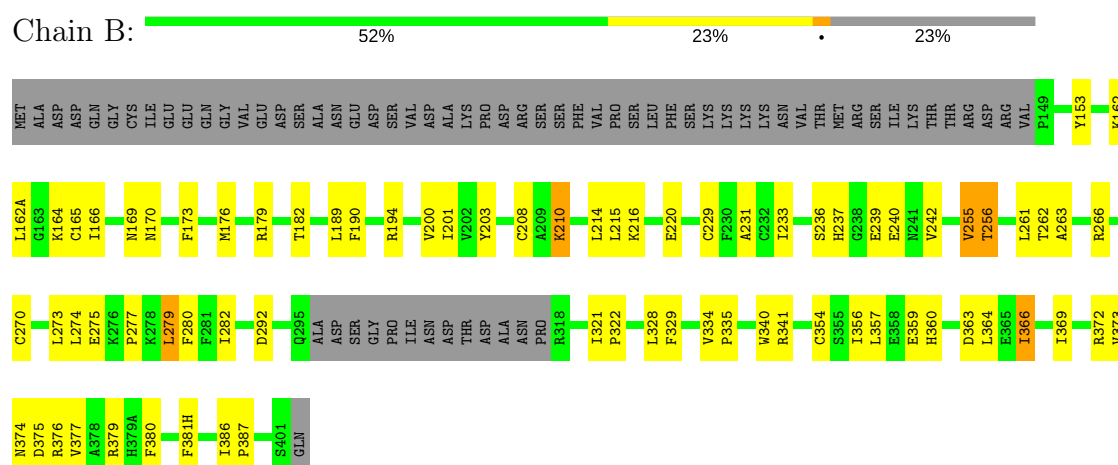
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are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



• Molecule 1: Caspase-7



• Molecule 2: X-LINKED INHIBITOR OF APOPTOSIS PROTEIN



ARG	ASP	HIS	PHE	ALA	LEU	TYR	THR	ASP	ARG	PRO	SER	E134	T135	H136	A137	D138	Y139	L140	L141	R142	T143	V146	I149	S150	ASP	THR	ILE	TYR	PRO	ASN	ARG	ALA	ASP	ASN	PRO	PRO	ALA	TYR	GLU	GLY	GLU	ALA	ARG	LEU	LYS	SER	PHE	GLN	ASN	TRP	ARG	ASP	ASN	LEU	THR	PRO	ASP	GLU	LEU	ALA
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SER	ALA	GLY	HIS	PHE	LEU	TYR	THR	ASP	ARG	PRO	ILE	GLY	ASP	GLN	VAL	GLN	PHE	CYS	CYS	CYS	GLY	GLY	LYS	LEU	ASN	TRP	GLU	PRO	CYS	ASP	ARG	ASN	ALA	TRP	SER	PRO	GLU	HIS	ARG	GLY	ARG	HIS	PHE	ARG	PRO	ALA	GLY	ASN	TRP	GLN	LEU	VAL	PHE	LEU	ARG	GLY	ASN	TRP	ASP	ASN	LEU	ASN	ASN	THR	PRO	GLU	SER	ASP
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● Molecule 2: X-LINKED INHIBITOR OF APOPTOSIS PROTEIN

Chain D: 8% . . 86%

ARG	ASP	HIS	PHE	ALA	LEU	TYR	THR	ASP	ARG	PRO	SER	E134	T135	H136	A137	D138	Y139	L140	T143	G144	Q145	S150	ASP	THR	ILE	TYR	PRO	ASN	ARG	ALA	TRP	SER	PRO	GLU	HIS	ARG	GLY	ARG	HIS	PHE	PRO	ASN	GLY	LEU	LYS	SER	PHE	GLN	ASN	TRP	GLN	LEU	VAL	PHE	LEU	ARG	GLY	ASN	TRP	ASP	ASN	LEU	ASN	ASN	THR	PRO	GLU	SER	ASP	ALA
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GLY	LEU	TYR	THR	GLY	ILE	GLY	ASP	GLN	VAL	GLN	CYS	PHE	CYS	CYS	GLY	LYS	LEU	LYS	ASN	TRP	GLU	PRO	CYS	ASP	ARG	ALA	TRP	SER	GLU	HIS	ARG	GLY	ARG	HIS	PHE	PRO	ASN	GLY	LEU	LYS	SER	PHE	VAL	LEU	GLY	ASN	TRP	ARG	LEU	ASN	ASN	THR	PRO	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 [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	0.40	0/1918	0.82	6/2581 (0.2%)
1	B	0.39	0/1917	0.82	6/2580 (0.2%)
2	C	0.37	0/135	0.56	0/183
2	D	0.36	0/135	0.55	0/183
All	All	0.39	0/4105	0.80	12/5527 (0.2%)

There are no bond length outliers.

The worst 5 of 12 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	376	ARG	NE-CZ-NH1	-14.84	112.88	120.30
1	A	376	ARG	NE-CZ-NH2	13.80	127.20	120.30
1	B	376	ARG	NE-CZ-NH2	-13.48	113.56	120.30
1	B	376	ARG	NE-CZ-NH1	12.89	126.75	120.30
1	B	194	ARG	NE-CZ-NH1	12.33	126.47	120.30

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	1878	0	1839	78	0
1	B	1876	0	1839	68	0
2	C	134	0	128	10	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	158	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 158 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:HD22	2:D:140:LEU:H	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%)	19	52
1	B	230/303 (76%)	215 (94%)	15 (6%)	0	100	100
2	C	15/119 (13%)	13 (87%)	1 (7%)	1 (7%)	1	4
2	D	15/119 (13%)	14 (93%)	1 (7%)	0	100	100
All	All	490/844 (58%)	454 (93%)	33 (7%)	3 (1%)	27	61

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 ⓘ

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%)	197 (96%)	8 (4%)	35	70
1	B	205/266 (77%)	199 (97%)	6 (3%)	45	79
2	C	15/104 (14%)	14 (93%)	1 (7%)	18	46
2	D	15/104 (14%)	13 (87%)	2 (13%)	4	13
All	All	440/740 (60%)	423 (96%)	17 (4%)	35	70

5 of 17 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	366	ILE
1	B	162(A)	LEU
1	B	366	ILE
1	A	321	ILE
2	C	149	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	169	ASN
1	A	360	HIS
1	B	169	ASN
1	B	360	HIS
2	C	136	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

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.