



wwPDB X-ray Structure Validation Summary Report

Feb 28, 2014 – 05:21 AM 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 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/ValidationPDFNotes.html>

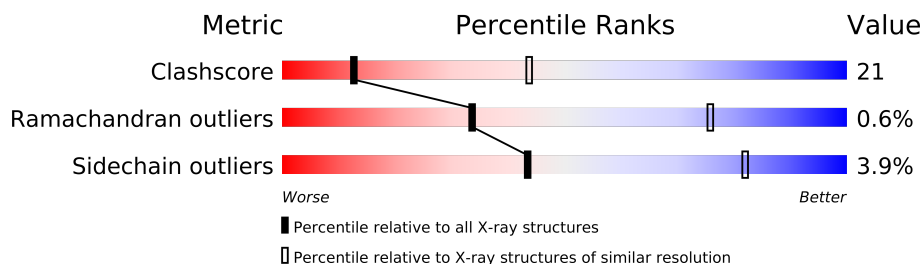
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.15 2013
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	21963
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	stable22683

1 Overall quality at a glance

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	79885	1326 (2.90-2.90)
Ramachandran outliers	78287	1290 (2.90-2.90)
Sidechain outliers	78261	1292 (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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

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 hydrogen and 0 are deuterium.

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		

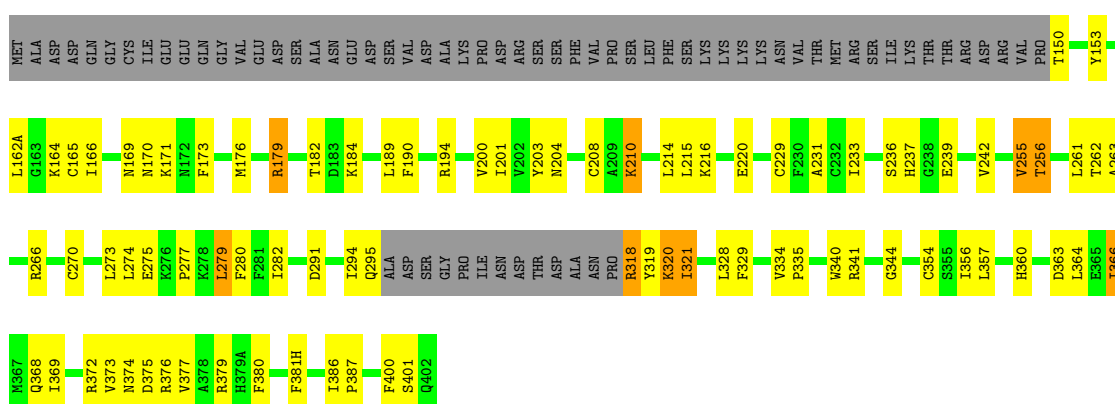
3 Residue-property plots

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.

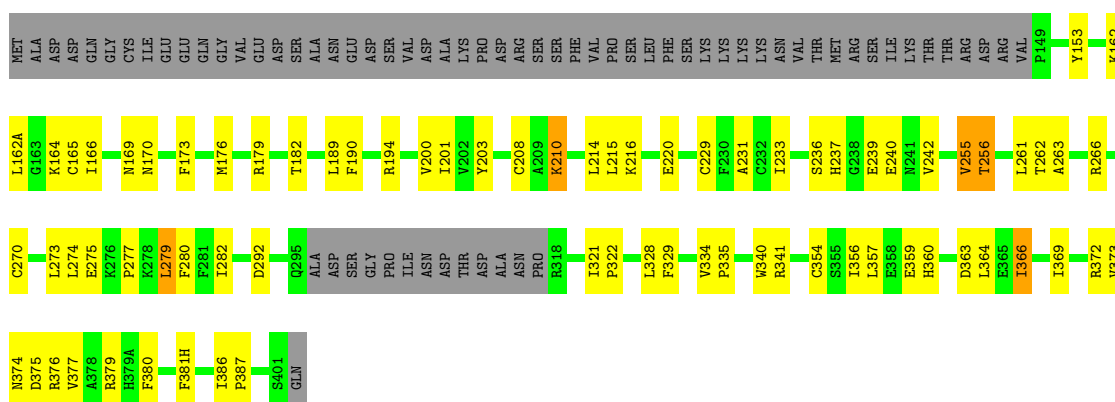
• Molecule 1: Caspase-7

Chain A:



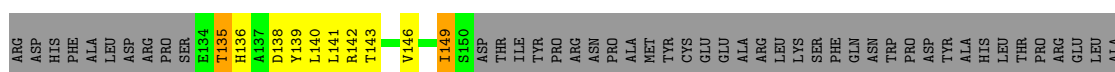
• Molecule 1: Caspase-7

Chain B:



• Molecule 2: X-LINKED INHIBITOR OF APOPTOSIS PROTEIN

Chain C:



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	ILE	ARG	SER	GLU	SER	ASP
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● Molecule 2: X-LINKED INHIBITOR OF APOPTOSIS PROTEIN

Chain D: 

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	ASN	PRO	ALA	MET	TYR	CYS	GLU	GLU	ALA	ARG	LEU	LYS	SER	PHE	GLN	ASN	TRP	PRO	ASP	TYR	ALA	HIS	LEU	THR	PRO	ARG	GLU	LEU	ALA	SER	ALA
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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	HIS	PHE	PRO	ASN	CYS	PHE	PHE	VAL	LEU	GLY	ARG	ASN	LEU	ASN	ASN	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 will therefore be 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	0.40	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 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	134	0	128	10	0
2	D	134	0	128	11	0
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

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 21.

The worst 5 of 158 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(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

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	230/303 (76%)	212 (92%)	16 (7%)	2 (1%)	25	66
1	B	230/303 (76%)	215 (94%)	15 (6%)	0	100	100
2	C	15/119 (13%)	13 (87%)	1 (7%)	1 (7%)	2	5
2	D	15/119 (13%)	14 (93%)	1 (7%)	0	100	100
All	All	490/844 (58%)	454 (93%)	33 (7%)	3 (1%)	33	76

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%)	43	82
1	B	205/266 (77%)	199 (97%)	6 (3%)	55	89
2	C	15/104 (14%)	14 (93%)	1 (7%)	23	56
2	D	15/104 (14%)	13 (87%)	2 (13%)	6	16
All	All	440/740 (60%)	423 (96%)	17 (4%)	43	82

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 ⓘ

There are no RNA chains 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 ⓘ

There are no ligands in this entry.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

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.