



wwPDB X-ray Structure Validation Summary Report ⓘ

May 28, 2020 – 08:53 pm BST

PDB ID : 1XB0
Title : Structure of the BIR domain of IAP-like protein 2
Authors : Shin, H.; Renatus, M.; Eckelman, B.P.; Nunes, V.A.; Sampaio, C.A.M.;
Salvesen, G.S.
Deposited on : 2004-08-27
Resolution : 2.20 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

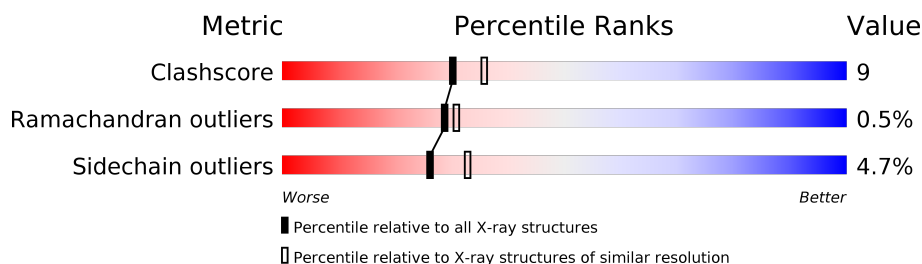
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)

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	108	68% 15% • 15%
1	B	108	72% 19% • 6%
1	C	108	67% 16% • 16%
1	D	108	67% 16% • 16%
1	E	108	72% 11% • 14%
1	F	108	73% 19% • 5%
2	G	7	14% 43% 43%
2	H	7	29% 29% 43%

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Mol	Chain	Length	Quality of chain
2	I	7	<div><div></div><div></div><div></div><div>14%</div><div>43%</div><div>43%</div></div>
2	J	7	<div><div></div><div></div><div></div><div>29%</div><div>43%</div><div>29%</div></div>
2	K	7	<div><div></div><div></div><div></div><div>43%</div><div>14%</div><div>43%</div></div>
2	L	7	<div><div></div><div></div><div></div><div>57%</div><div>43%</div></div>

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 5158 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 Baculoviral IAP repeat-containing protein 8.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	92	Total	C	N	O	S	3	0	0
			751	482	130	134	5			
1	B	101	Total	C	N	O	S	34	0	0
			819	524	142	148	5			
1	C	91	Total	C	N	O	S	18	0	0
			746	479	129	133	5			
1	D	91	Total	C	N	O	S	25	0	0
			746	479	129	133	5			
1	E	93	Total	C	N	O	S	33	0	0
			757	485	131	136	5			
1	F	103	Total	C	N	O	S	47	0	0
			832	531	145	151	5			

There are 78 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	249	GLY	-	CLONING ARTIFACT	UNP Q96P09
A	250	SER	-	CLONING ARTIFACT	UNP Q96P09
A	251	HIS	-	CLONING ARTIFACT	UNP Q96P09
A	252	MET	-	CLONING ARTIFACT	UNP Q96P09
A	253	SER	-	SEE REMARK 999	UNP Q96P09
A	254	THR	-	SEE REMARK 999	UNP Q96P09
A	255	ASN	-	SEE REMARK 999	UNP Q96P09
A	256	LEU	-	SEE REMARK 999	UNP Q96P09
A	257	PRO	-	SEE REMARK 999	UNP Q96P09
A	258	ARG	-	SEE REMARK 999	UNP Q96P09
A	259	ASN	-	SEE REMARK 999	UNP Q96P09
A	260	PRO	-	SEE REMARK 999	UNP Q96P09
A	261	SER	-	SEE REMARK 999	UNP Q96P09
B	249	GLY	-	CLONING ARTIFACT	UNP Q96P09
B	250	SER	-	CLONING ARTIFACT	UNP Q96P09
B	251	HIS	-	CLONING ARTIFACT	UNP Q96P09
B	252	MET	-	CLONING ARTIFACT	UNP Q96P09

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Chain	Residue	Modelled	Actual	Comment	Reference
B	253	SER	-	SEE REMARK 999	UNP Q96P09
B	254	THR	-	SEE REMARK 999	UNP Q96P09
B	255	ASN	-	SEE REMARK 999	UNP Q96P09
B	256	LEU	-	SEE REMARK 999	UNP Q96P09
B	257	PRO	-	SEE REMARK 999	UNP Q96P09
B	258	ARG	-	SEE REMARK 999	UNP Q96P09
B	259	ASN	-	SEE REMARK 999	UNP Q96P09
B	260	PRO	-	SEE REMARK 999	UNP Q96P09
B	261	SER	-	SEE REMARK 999	UNP Q96P09
C	249	GLY	-	CLONING ARTIFACT	UNP Q96P09
C	250	SER	-	CLONING ARTIFACT	UNP Q96P09
C	251	HIS	-	CLONING ARTIFACT	UNP Q96P09
C	252	MET	-	CLONING ARTIFACT	UNP Q96P09
C	253	SER	-	SEE REMARK 999	UNP Q96P09
C	254	THR	-	SEE REMARK 999	UNP Q96P09
C	255	ASN	-	SEE REMARK 999	UNP Q96P09
C	256	LEU	-	SEE REMARK 999	UNP Q96P09
C	257	PRO	-	SEE REMARK 999	UNP Q96P09
C	258	ARG	-	SEE REMARK 999	UNP Q96P09
C	259	ASN	-	SEE REMARK 999	UNP Q96P09
C	260	PRO	-	SEE REMARK 999	UNP Q96P09
C	261	SER	-	SEE REMARK 999	UNP Q96P09
D	249	GLY	-	CLONING ARTIFACT	UNP Q96P09
D	250	SER	-	CLONING ARTIFACT	UNP Q96P09
D	251	HIS	-	CLONING ARTIFACT	UNP Q96P09
D	252	MET	-	CLONING ARTIFACT	UNP Q96P09
D	253	SER	-	SEE REMARK 999	UNP Q96P09
D	254	THR	-	SEE REMARK 999	UNP Q96P09
D	255	ASN	-	SEE REMARK 999	UNP Q96P09
D	256	LEU	-	SEE REMARK 999	UNP Q96P09
D	257	PRO	-	SEE REMARK 999	UNP Q96P09
D	258	ARG	-	SEE REMARK 999	UNP Q96P09
D	259	ASN	-	SEE REMARK 999	UNP Q96P09
D	260	PRO	-	SEE REMARK 999	UNP Q96P09
D	261	SER	-	SEE REMARK 999	UNP Q96P09
E	249	GLY	-	CLONING ARTIFACT	UNP Q96P09
E	250	SER	-	CLONING ARTIFACT	UNP Q96P09
E	251	HIS	-	CLONING ARTIFACT	UNP Q96P09
E	252	MET	-	CLONING ARTIFACT	UNP Q96P09
E	253	SER	-	SEE REMARK 999	UNP Q96P09
E	254	THR	-	SEE REMARK 999	UNP Q96P09
E	255	ASN	-	SEE REMARK 999	UNP Q96P09

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Chain	Residue	Modelled	Actual	Comment	Reference
E	256	LEU	-	SEE REMARK 999	UNP Q96P09
E	257	PRO	-	SEE REMARK 999	UNP Q96P09
E	258	ARG	-	SEE REMARK 999	UNP Q96P09
E	259	ASN	-	SEE REMARK 999	UNP Q96P09
E	260	PRO	-	SEE REMARK 999	UNP Q96P09
E	261	SER	-	SEE REMARK 999	UNP Q96P09
F	249	GLY	-	CLONING ARTIFACT	UNP Q96P09
F	250	SER	-	CLONING ARTIFACT	UNP Q96P09
F	251	HIS	-	CLONING ARTIFACT	UNP Q96P09
F	252	MET	-	CLONING ARTIFACT	UNP Q96P09
F	253	SER	-	SEE REMARK 999	UNP Q96P09
F	254	THR	-	SEE REMARK 999	UNP Q96P09
F	255	ASN	-	SEE REMARK 999	UNP Q96P09
F	256	LEU	-	SEE REMARK 999	UNP Q96P09
F	257	PRO	-	SEE REMARK 999	UNP Q96P09
F	258	ARG	-	SEE REMARK 999	UNP Q96P09
F	259	ASN	-	SEE REMARK 999	UNP Q96P09
F	260	PRO	-	SEE REMARK 999	UNP Q96P09
F	261	SER	-	SEE REMARK 999	UNP Q96P09

- Molecule 2 is a protein called Diablo homolog, mitochondrial.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	G	4	Total	C	N	O	0	0	0
			27	19	4	4			
2	H	4	Total	C	N	O	0	0	0
			27	19	4	4			
2	I	4	Total	C	N	O	0	0	0
			27	19	4	4			
2	J	5	Total	C	N	O	0	0	0
			32	22	5	5			
2	K	4	Total	C	N	O	0	0	0
			27	19	4	4			
2	L	4	Total	C	N	O	0	0	0
			27	19	4	4			

- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	D	4	Total	Zn	0	0
			4	4		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	E	4	Total 4	Zn 4	0	0
3	B	4	Total 4	Zn 4	0	0
3	C	4	Total 4	Zn 4	0	0
3	A	4	Total 4	Zn 4	0	0
3	F	4	Total 4	Zn 4	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	51	Total 51	O 51	0	0
4	G	1	Total 1	O 1	0	0
4	B	58	Total 58	O 58	0	0
4	H	4	Total 4	O 4	0	0
4	C	43	Total 43	O 43	0	0
4	D	48	Total 48	O 48	0	0
4	J	2	Total 2	O 2	0	0
4	E	44	Total 44	O 44	0	0
4	K	4	Total 4	O 4	0	0
4	F	57	Total 57	O 57	0	0
4	L	4	Total 4	O 4	0	0

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. 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: Baculoviral IAP repeat-containing protein 8

Chain A: 



- Molecule 1: Baculoviral IAP repeat-containing protein 8

Chain B: 



- Molecule 1: Baculoviral IAP repeat-containing protein 8

Chain C: 



- Molecule 1: Baculoviral IAP repeat-containing protein 8

Chain D: 



- Molecule 1: Baculoviral IAP repeat-containing protein 8

Chain E: 



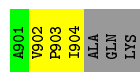
- Molecule 1: Baculoviral IAP repeat-containing protein 8

Chain F:  73% 19% 5%

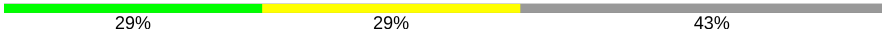


- Molecule 2: Diablo homolog, mitochondrial

Chain G:  14% 43% 43%



- Molecule 2: Diablo homolog, mitochondrial

Chain H:  29% 29% 43%



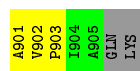
- Molecule 2: Diablo homolog, mitochondrial

Chain I:  14% 43% 43%



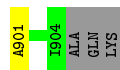
- Molecule 2: Diablo homolog, mitochondrial

Chain J:  29% 43% 29%



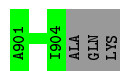
- Molecule 2: Diablo homolog, mitochondrial

Chain K:  43% 14% 43%



- Molecule 2: Diablo homolog, mitochondrial

Chain L:  57% 43%



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α , β , γ	86.40 Å 86.40 Å 226.77 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.20	Depositor
% Data completeness (in resolution range)	98.7 (50.00-2.20)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.223 , 0.244	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	5158	wwPDB-VP
Average B, all atoms (Å ²)	29.0	wwPDB-VP

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: ZN

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	0.36	0/776	0.55	0/1051
1	B	0.33	0/844	0.57	0/1143
1	C	0.36	0/771	0.49	0/1044
1	D	0.34	0/771	0.50	0/1044
1	E	0.33	0/782	0.51	0/1059
1	F	0.35	0/857	0.85	3/1161 (0.3%)
2	G	0.24	0/27	0.52	0/37
2	H	0.40	0/27	0.67	0/37
2	I	0.38	0/27	0.56	0/37
2	J	0.40	0/32	0.62	0/44
2	K	0.33	0/27	0.73	0/37
2	L	0.37	0/27	0.51	0/37
All	All	0.35	0/4968	0.60	3/6731 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	268	ARG	NE-CZ-NH1	-15.52	112.54	120.30
1	F	268	ARG	NE-CZ-NH2	14.82	127.71	120.30
1	F	268	ARG	CD-NE-CZ	6.81	133.14	123.60

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	751	0	703	13	0
1	B	819	0	780	16	0
1	C	746	0	701	13	0
1	D	746	0	701	12	1
1	E	757	0	708	10	0
1	F	832	0	788	16	0
2	G	27	0	31	4	0
2	H	27	0	31	2	0
2	I	27	0	31	3	0
2	J	32	0	36	3	0
2	K	27	0	31	2	0
2	L	27	0	31	0	0
3	A	4	0	0	0	0
3	B	4	0	0	0	0
3	C	4	0	0	0	0
3	D	4	0	0	0	0
3	E	4	0	0	0	0
3	F	4	0	0	0	0
4	A	51	0	0	0	0
4	B	58	0	0	1	0
4	C	43	0	0	0	0
4	D	48	0	0	0	0
4	E	44	0	0	0	1
4	F	57	0	0	0	1
4	G	1	0	0	0	0
4	H	4	0	0	0	0
4	J	2	0	0	0	0
4	K	4	0	0	0	0
4	L	4	0	0	0	0
All	All	5158	0	4572	84	2

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 9.

The worst 5 of 84 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:311:LYS:HB2	1:A:314:GLU:HG3	1.54	0.88
1:A:292:ILE:HD11	1:A:297:LYS:HD3	1.52	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:280:ASN:HD21	1:F:282:GLU:HB2	1.42	0.83
1:F:336:HIS:CE1	1:F:340:ASN:HD21	2.03	0.76
1:F:345:THR:HG21	1:F:356:THR:HG21	1.65	0.76

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:839:HOH:O	4:E:839:HOH:O[7_555]	2.03	0.17
1:D:333:GLU:OE2	4:F:937:HOH:O[7_555]	2.17	0.03

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	90/108 (83%)	86 (96%)	3 (3%)	1 (1%)	14	12
1	B	99/108 (92%)	94 (95%)	5 (5%)	0	100	100
1	C	89/108 (82%)	85 (96%)	4 (4%)	0	100	100
1	D	89/108 (82%)	86 (97%)	3 (3%)	0	100	100
1	E	91/108 (84%)	82 (90%)	8 (9%)	1 (1%)	14	12
1	F	101/108 (94%)	95 (94%)	5 (5%)	1 (1%)	15	14
2	G	2/7 (29%)	2 (100%)	0	0	100	100
2	H	2/7 (29%)	2 (100%)	0	0	100	100
2	I	2/7 (29%)	2 (100%)	0	0	100	100
2	J	3/7 (43%)	3 (100%)	0	0	100	100
2	K	2/7 (29%)	2 (100%)	0	0	100	100
2	L	2/7 (29%)	2 (100%)	0	0	100	100
All	All	572/690 (83%)	541 (95%)	28 (5%)	3 (0%)	29	31

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	255	ASN
1	E	273	GLY
1	F	255	ASN

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	76/90 (84%)	71 (93%)	5 (7%)	16	19
1	B	84/90 (93%)	81 (96%)	3 (4%)	35	45
1	C	76/90 (84%)	72 (95%)	4 (5%)	22	27
1	D	76/90 (84%)	72 (95%)	4 (5%)	22	27
1	E	77/90 (86%)	73 (95%)	4 (5%)	23	28
1	F	85/90 (94%)	82 (96%)	3 (4%)	36	46
2	G	3/5 (60%)	3 (100%)	0	100	100
2	H	3/5 (60%)	3 (100%)	0	100	100
2	I	3/5 (60%)	3 (100%)	0	100	100
2	J	3/5 (60%)	3 (100%)	0	100	100
2	K	3/5 (60%)	3 (100%)	0	100	100
2	L	3/5 (60%)	3 (100%)	0	100	100
All	All	492/570 (86%)	469 (95%)	23 (5%)	26	33

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

Mol	Chain	Res	Type
1	C	269	LEU
1	D	255	ASN
1	F	269	LEU
1	C	307	LEU
1	D	259	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 22 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	341	ASN
1	D	309	ASN
1	F	309	ASN
1	D	259	ASN
1	D	299	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](#)

Of 24 ligands modelled in this entry, 24 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

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 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.