

## wwPDB NMR Structure Validation Summary Report (i)

#### Feb 12, 2022 – 05:06 PM EST

PDB ID : 1G3F

Title : NMR STRUCTURE OF A 9 RESIDUE PEPTIDE FROM SMAC/DIABLO

COMPLEXED TO THE BIR3 DOMAIN OF XIAP

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This is a wwPDB NMR 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/NMRValidationReportHelp with specific help available everywhere you see the (i) symbol.

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

MolProbity: 4.02b-467

Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)

RCI : v 1n 11 5 13 A (Berjanski et al., 2005)

PANAV : Wang et al. (2010)

ShiftChecker : 2.26

Ideal geometry (proteins) : Engh & Huber (2001) Ideal geometry (DNA, RNA) : Parkinson et al. (1996)

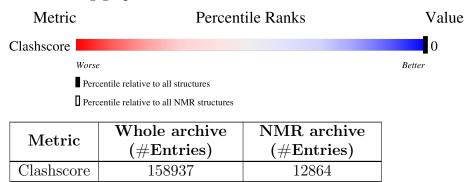
Validation Pipeline (wwPDB-VP) : 2.26

## 1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:  $SOLUTION\ NMR$ 

The overall completeness of chemical shifts assignment was not calculated.

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.



The table below summarises the geometric issues observed across the polymeric chains and their fit to the experimental data. The red, orange, yellow and green segments indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. A cyan segment indicates the fraction of residues that are not part of the well-defined cores, and 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 <=5%

Mol	Chain	Length	Quality of chain
1	A	117	100%
2	В	9	100%



## 2 Ensemble composition and analysis (i)

This entry contains 1 models. Identification of well-defined residues and clustering analysis are not possible.



## 3 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 1970 atoms, of which 958 are hydrogens and 0 are deuteriums.

• Molecule 1 is a protein called INHIBITOR OF APOPTOSIS PROTEIN 3.

Mol	Chain	Residues		Atoms					Trace
1	Λ	117	Total	С	Н	N	О	S	0
1	A	117	1832	597	887	162	180	6	U

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	240	MET	-	cloning artifact	UNP P98170

• Molecule 2 is a protein called SMAC.

Mol	Chain	Residues	Atoms				Trace	
9	D	0	Total	С	Н	N	О	0
2	Б	9	137	41	71	11	14	U

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

Mol	Chain	Residues	Atoms
2	2 Λ 1		Total Zn
3	A	1	1 1



## 4 Residue-property plots (i)

These plots are provided for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic is the same as shown in the summary in section 1 of this report. The second graphic shows the sequence where residues are colour-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 outliers are shown as green connectors. Residues which are classified as ill-defined in the NMR ensemble, are shown in cyan with an underline colour-coded according to the previous scheme. Residues which were present in the experimental sample, but not modelled in the final structure are shown in grey.

• Molecule 1: INHIBITOR OF APOPTOSIS PROTEIN 3

Chain A:				100%		
M240 8241 D242 A243 V244 S245 S246	D247 R248 N249 F250 P251	N252 8253 17254 N255 1256 P257 R258 N259	P260 8261 M262 A263 D264 Y265 E266 A267 R268	1270 1271 1271 1274 1274 1276 1276 1276 1277 8278 1280 1280 1280 1280 1280 1280 1280 128	1284 A285 A286 A287 (2288 Y290 A291 (2292 (2293 (2293 (2294 (2295	M297 W298 W298 K299
C300 F301 H302 C303 G304 G306	L307 T308 D309 W310 K311	S313 S313 D315 D316 W317 Q319	H320 K321 W322 W323 Y324 P326 G326 G327 K328	1330 1331 1331 1333 1333 1338 1339 1339 1339	1344 1345 1348 1348 1349 1350 1351 1352 1355	T356
• Molecul	e 2: SN	ИАС				
Chain B:				100%		
901 902 903 904 905 906	808 806					



#### Refinement protocol and experimental data overview (i) 5



The models were refined using the following method: simulated annealing.

Of the ? calculated structures, 1 were deposited, based on the following criterion: ?.

The following table shows the software used for structure solution, optimisation and refinement.

Software name	Classification	Version
CNX	refinement	2000

No chemical shift data was provided.



## 6 Model quality (i)

## 6.1 Standard geometry (i)

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

There are no covalent bond-length or bond-angle outliers.

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 6.2 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 each 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 averaged over the ensemble.

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	A	0	0	0	0
2	В	0	0	0	0
All	All	1	0	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 -.

There are no clashes.

### 6.3 Torsion angles (i)

#### 6.3.1 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 PDB entries followed by that with respect to all NMR entries. 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	0	-	-	-	-
2	В	0	-	-	_	-

Continued on next page...



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]	Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
	All	All	0	-	-	-	-

There are no Ramachandran outliers.

#### 6.3.2 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 PDB entries followed by that with respect to all NMR entries. 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	0	-	-	-
2	В	0	-	-	-
All	All	0	-	-	-

There are no protein residues with a non-rotameric sidechain to report.

#### 6.3.3 RNA (i)

There are no RNA molecules in this entry.

### 6.4 Non-standard residues in protein, DNA, RNA chains (i)

There are no non-standard protein/DNA/RNA residues in this entry.

### 6.5 Carbohydrates (i)

There are no monosaccharides in this entry.

## 6.6 Ligand geometry (i)

Of 1 ligands modelled in this entry, 1 is monoatomic - leaving 0 for Mogul analysis.

## 6.7 Other polymers (i)

There are no such molecules in this entry.



## 6.8 Polymer linkage issues (i)

There are no chain breaks in this entry.



# 7 Chemical shift validation (i)

No chemical shift data were provided

