

# Full wwPDB NMR Structure Validation Report (i)

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PDB ID : 1G5J

Title : COMPLEX OF BCL-XL WITH PEPTIDE FROM BAD

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This is a Full wwPDB NMR Structure Validation 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 types of validation reports are described at http://www.wwpdb.org/validation/2017/FAQs#types.

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 : 2.29

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

Validation Pipeline (wwPDB-VP) : 2.29

## 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.

There are no overall percentile quality scores available for this entry.

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	175	100%
2	В	25	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 2 unique types of molecules in this entry. The entry contains 3164 atoms, of which 1538 are hydrogens and 0 are deuteriums.

• Molecule 1 is a protein called APOPTOSIS REGULATOR BCL-X.

Mol	Chain	Residues		Atoms						
1	Λ	175	Total	С	Н	N	О	S	0	
1	A	173	2731	882	1324	240	279	6	U	

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	cloning artifact	UNP Q07817
A	2	SER	-	cloning artifact	UNP Q07817
A	3	MET	-	cloning artifact	_
A	4	ALA	-	cloning artifact	UNP Q07817
A	214	LEU	-	cloning artifact	UNP Q07817
A	215	GLU	-	cloning artifact	UNP Q07817

• Molecule 2 is a protein called BAD PROTEIN.

Mol	Chain	Residues		Atoms							
9	D	25	Total	С	Н	N	О	S	0		
	D	20	433	137	214	42	39	1	U		

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference				
В	320	VAL	GLU	engineered mutation	UNP Q07817				
В	321	ASP	GLY	engineered mutation	UNP Q07817				
В	325	LYS	GLY	engineered mutation	UNP Q07817				



## 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: APOPTOSIS REGULATOR BCL-X

Chain .	A:													10	00%	ò																		
M1 S2 M3 A4 M5	S6 Q7 S8	R10 E11	L12 V13	V14 D15	F16	S18	Y19 K20	L21	<b>Q23</b>	K24 G25	Y26	S27 W28	829	(130 F31	832	U33	E35	E36	R38	T39	A41	P42 E43	G44	T45	S47	E48	V90	K91	765	L94	R95	E96 A97	869	E100
F101 E102 L103 R104 Y105	R107 A108	\$110 D111	L112 T113	S114 0115	L116	1118 1118	T119 P120			Y124 0125		F127 E128				E133		R136		V139 N140		G142 R143		V145	F147	F148	S149 F150	G151	6152	A153 L154	C155	V156 E157	S158	0160
K161 E162 M163 Q164 V165	L166 V167 S168	1170 A171	A172 W173	M174 A175	T176	L178	N179 D180			P184 W185		Q187 E188	- ←	G190 G191		D193	F195	V196	L198	Y199	N201	N202 A203	A204	A205	8207	R208	K209 G210	Q211	E212	L214	E215			
• Mole	cule	2:	ВА	D	PΕ	RO	T	ΕI	N																									
Chain	В:													10	00%	)																		
301 302 303 304 305	306	310	312	314	316	318	319	321	323	324																								



#### 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
X-PLOR	refinement	3.1

No chemical shift data was provided.



## 6 Model quality (i)

### 6.1 Standard geometry (i)

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	0	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	Analysed   Favoured   Allowed		Outliers	Percentiles
1	A	0	-	-	-	-
2	В	0	-	=	-	-
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)

There are no ligands in this entry.

### 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

