



Full wwPDB NMR Structure Validation Report ⓘ

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PDB ID : 1G5J / pdb_00001g5j
Title : COMPLEX OF BCL-XL WITH PEPTIDE FROM BAD
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Deposited on : 2000-11-01

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 ⓘ 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 ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
wwPDB-RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
wwPDB-ShiftChecker	:	v1.2
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

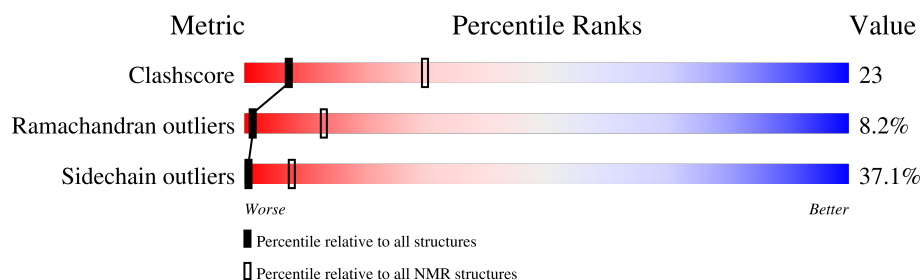
1 Overall quality at a glance

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.



Metric	Whole archive (#Entries)	NMR archive (#Entries)
Clashscore	229148	14424
Ramachandran outliers	224038	12848
Sidechain outliers	223484	12823

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 $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	A	175	
2	B	25	

2 Ensemble composition and analysis ⓘ

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

3 Entry composition

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						Trace
1	A	175	Total	C	H	N	O	S	0
			2731	882	1324	240	279	6	

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	UNP Q07817
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						Trace
2	B	25	Total	C	H	N	O	S	0
			433	137	214	42	39	1	

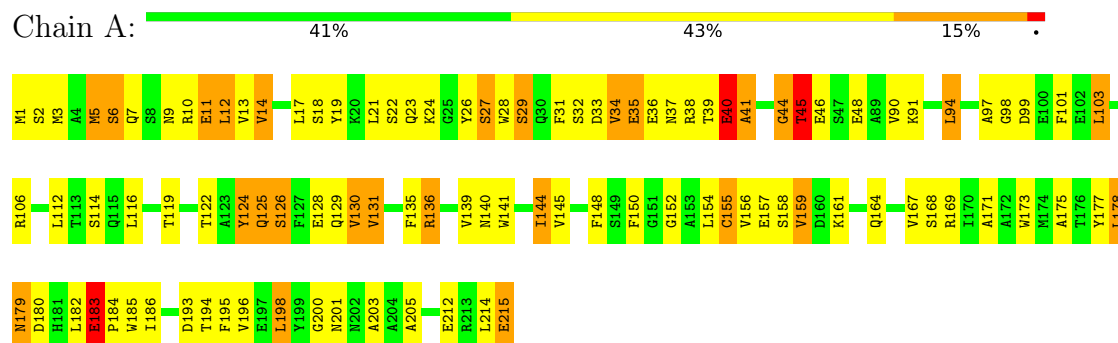
There are 3 discrepancies between the modelled and reference sequences:

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



• Molecule 2: BAD PROTEIN



5 Refinement protocol and experimental data overview ⓘ

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	1407	1324	1324	71
2	B	219	214	211	16
All	All	1626	1538	1535	74

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 23.

All clashes are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Clash(Å)	Distance(Å)
1:A:10:ARG:O	1:A:14:VAL:HG13	0.84	1.72
1:A:21:LEU:HD13	1:A:156:VAL:HG22	0.82	1.51
1:A:46:GLU:O	1:A:90:VAL:HG23	0.79	1.77
1:A:21:LEU:HD12	1:A:26:TYR:CB	0.77	2.10
1:A:5:MET:HE2	1:A:6:SER:N	0.71	1.99
1:A:11:GLU:CD	1:A:39:THR:HG21	0.70	2.11
1:A:101:PHE:CZ	2:B:312:LEU:HD13	0.67	2.24
1:A:5:MET:HE1	1:A:179:ASN:HB2	0.67	1.65
1:A:5:MET:HE2	1:A:6:SER:CA	0.62	2.24
1:A:112:LEU:O	1:A:116:LEU:HD23	0.62	1.93
1:A:94:LEU:HD12	1:A:195:PHE:CZ	0.62	2.29
1:A:44:GLY:O	1:A:45:THR:HG23	0.61	1.95
1:A:116:LEU:HD22	2:B:304:ALA:HB3	0.61	1.70
1:A:159:VAL:HG12	1:A:164:GLN:CG	0.61	2.26

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Atom-1	Atom-2	Clash(Å)	Distance(Å)
1:A:198:LEU:O	1:A:203:ALA:HB2	0.61	1.95
1:A:17:LEU:CD1	1:A:171:ALA:HB2	0.60	2.27
1:A:29:SER:HA	1:A:34:VAL:HG12	0.57	1.74
1:A:94:LEU:HD12	1:A:195:PHE:CE2	0.57	2.35
1:A:144:ILE:HD11	1:A:185:TRP:CZ3	0.55	2.36
1:A:155:CYS:O	1:A:159:VAL:HG22	0.55	2.01
1:A:21:LEU:HD12	1:A:26:TYR:HB3	0.55	1.77
1:A:159:VAL:HG12	1:A:164:GLN:HG2	0.54	1.78
1:A:150:PHE:CE1	2:B:308:TYR:CE2	0.54	2.96
1:A:11:GLU:CG	1:A:39:THR:HG21	0.54	2.32
1:A:116:LEU:HD22	2:B:304:ALA:CB	0.54	2.33
1:A:10:ARG:O	1:A:13:VAL:HG22	0.53	2.04
1:A:11:GLU:HA	1:A:14:VAL:HG22	0.52	1.80
1:A:11:GLU:HG2	1:A:39:THR:HG21	0.52	1.81
1:A:126:SER:O	1:A:130:VAL:HG12	0.52	2.04
2:B:304:ALA:O	2:B:305:ALA:C	0.51	2.53
1:A:214:LEU:HD23	1:A:215:GLU:O	0.50	2.07
1:A:112:LEU:HD22	2:B:308:TYR:CE2	0.49	2.42
1:A:40:GLU:O	1:A:41:ALA:HB2	0.49	2.08
1:A:99:ASP:O	1:A:103:LEU:HD12	0.49	2.07
1:A:13:VAL:HG12	1:A:148:PHE:CE2	0.48	2.43
1:A:177:TYR:CE2	1:A:182:LEU:HD13	0.48	2.43
1:A:150:PHE:CZ	2:B:308:TYR:CE2	0.48	3.01
1:A:112:LEU:HD22	2:B:308:TYR:CZ	0.48	2.43
1:A:5:MET:HE2	1:A:6:SER:CB	0.48	2.38
1:A:141:TRP:CZ3	1:A:185:TRP:CH2	0.47	3.02
1:A:175:ALA:O	1:A:178:LEU:HD12	0.47	2.10
1:A:150:PHE:CZ	2:B:308:TYR:CZ	0.46	3.03
1:A:97:ALA:HB3	1:A:145:VAL:HG11	0.46	1.87
1:A:45:THR:HG22	1:A:48:GLU:CD	0.46	2.34
1:A:116:LEU:HD13	2:B:302:LEU:HD11	0.45	1.86
1:A:144:ILE:HD13	1:A:182:LEU:HD23	0.45	1.88
1:A:12:LEU:HD21	1:A:90:VAL:HG12	0.45	1.88
1:A:112:LEU:CD2	2:B:308:TYR:CZ	0.45	2.99
1:A:18:SER:CB	1:A:28:TRP:CD1	0.45	3.00
1:A:21:LEU:HD12	1:A:26:TYR:HB2	0.45	1.88
1:A:201:ASN:O	1:A:205:ALA:HB2	0.44	2.12
1:A:131:VAL:HG21	1:A:177:TYR:CE1	0.44	2.47
1:A:94:LEU:CD1	1:A:195:PHE:CZ	0.44	2.99
1:A:34:VAL:HG22	1:A:34:VAL:O	0.43	2.12
1:A:94:LEU:CD2	1:A:148:PHE:CD1	0.43	3.00
1:A:17:LEU:HD23	1:A:152:GLY:HA2	0.43	1.91

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Atom-1	Atom-2	Clash(Å)	Distance(Å)
1:A:203:ALA:HB1	2:B:323:PHE:CD1	0.43	2.49
1:A:129:GLN:HB2	2:B:305:ALA:HB1	0.43	1.90
1:A:124:TYR:CG	1:A:125:GLN:N	0.42	2.85
1:A:183:GLU:CB	1:A:184:PRO:CD	0.42	2.96
2:B:304:ALA:O	2:B:306:GLN:N	0.42	2.52
1:A:94:LEU:CD1	1:A:195:PHE:CE2	0.42	3.02
2:B:323:PHE:CD1	2:B:323:PHE:N	0.42	2.84
1:A:97:ALA:CB	1:A:145:VAL:HG11	0.42	2.44
1:A:18:SER:CB	1:A:28:TRP:CG	0.42	3.03
1:A:13:VAL:HG21	1:A:175:ALA:HB2	0.42	1.91
1:A:98:GLY:N	1:A:145:VAL:CG1	0.41	2.83
1:A:101:PHE:CZ	2:B:312:LEU:CD1	0.41	3.00
1:A:135:PHE:CE2	1:A:139:VAL:HG13	0.41	2.50
1:A:27:SER:O	1:A:31:PHE:CE2	0.41	2.73
1:A:130:VAL:HG22	1:A:131:VAL:N	0.41	2.31
1:A:21:LEU:CD1	1:A:156:VAL:HG22	0.41	2.36
1:A:169:ARG:O	1:A:173:TRP:CG	0.41	2.74
1:A:169:ARG:O	1:A:173:TRP:CD2	0.40	2.75

6.3 Torsion angles

6.3.1 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 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	173/175 (99%)	133 (77%)	27 (16%)	13 (8%)	1	15
2	B	23/25 (92%)	18 (78%)	2 (9%)	3 (13%)	0	6
All	All	196/200 (98%)	151 (77%)	29 (15%)	16 (8%)	1	13

All 16 Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type
1	A	33	ASP
1	A	34	VAL
1	A	35	GLU
1	A	37	ASN

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Mol	Chain	Res	Type
1	A	40	GLU
1	A	41	ALA
1	A	44	GLY
1	A	45	THR
1	A	136	ARG
1	A	140	ASN
1	A	167	VAL
1	A	183	GLU
1	A	200	GLY
2	B	304	ALA
2	B	305	ALA
2	B	321	ASP

6.3.2 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 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	148/148 (100%)	93 (63%)	55 (37%)	1	8
2	B	22/22 (100%)	14 (64%)	8 (36%)	1	8
All	All	170/170 (100%)	107 (63%)	63 (37%)	1	8

All 63 residues with a non-rotameric sidechain are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type
1	A	1	MET
1	A	2	SER
1	A	3	MET
1	A	5	MET
1	A	6	SER
1	A	7	GLN
1	A	9	ASN
1	A	11	GLU
1	A	12	LEU
1	A	14	VAL
1	A	19	TYR
1	A	22	SER

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Mol	Chain	Res	Type
1	A	23	GLN
1	A	24	LYS
1	A	27	SER
1	A	29	SER
1	A	32	SER
1	A	35	GLU
1	A	36	GLU
1	A	38	ARG
1	A	40	GLU
1	A	45	THR
1	A	91	LYS
1	A	94	LEU
1	A	103	LEU
1	A	106	ARG
1	A	114	SER
1	A	119	THR
1	A	122	THR
1	A	124	TYR
1	A	125	GLN
1	A	126	SER
1	A	128	GLU
1	A	130	VAL
1	A	131	VAL
1	A	136	ARG
1	A	144	ILE
1	A	154	LEU
1	A	155	CYS
1	A	157	GLU
1	A	158	SER
1	A	159	VAL
1	A	161	LYS
1	A	168	SER
1	A	178	LEU
1	A	179	ASN
1	A	180	ASP
1	A	183	GLU
1	A	186	ILE
1	A	193	ASP
1	A	194	THR
1	A	196	VAL
1	A	198	LEU
1	A	212	GLU

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Mol	Chain	Res	Type
1	A	215	GLU
2	B	301	ASN
2	B	302	LEU
2	B	306	GLN
2	B	311	GLU
2	B	312	LEU
2	B	315	MET
2	B	316	SER
2	B	320	VAL

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 oligosaccharides 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

No chemical shift data were provided