



Full wwPDB NMR Structure Validation Report ⓘ

Feb 17, 2018 – 10:47 pm GMT

PDB ID : 1K3K
Title : Solution Structure of a Bcl-2 Homolog from Kaposi's Sarcoma Virus
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Deposited on : 2001-10-03

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

Cyrange	:	Kirchner and Güntert (2011)
NmrClust	:	Kelley et al. (1996)
MolProbity	:	4.02b-467
Percentile statistics	:	20171227.v01 (using entries in the PDB archive December 27th 2017)
RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
ShiftChecker	:	trunk30686
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk30686

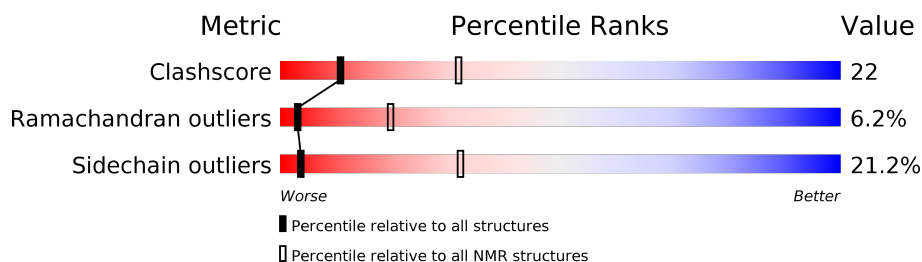
1 Overall quality at a glance

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	136279	12091
Ramachandran outliers	132675	10835
Sidechain outliers	132484	10811

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	158	

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 is only 1 type of molecule in this entry. The entry contains 2277 atoms, of which 1137 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called functional anti-apoptotic factor vBCL-2 homolog.

Mol	Chain	Residues	Atoms						Trace
1	A	146	Total	C	H	N	O	S	0
			2277	737	1137	190	205	8	

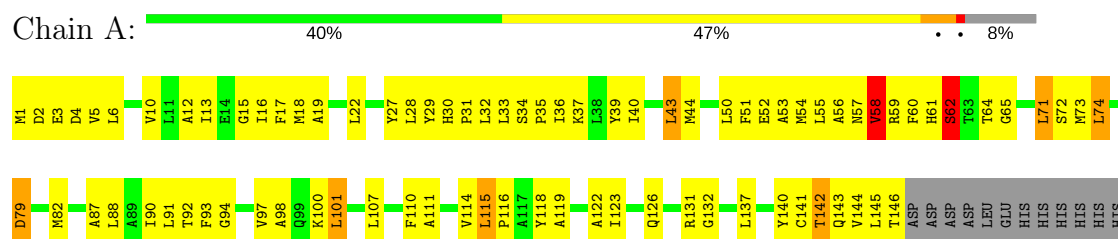
There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	67	ASP	ASN	ENGINEERED	UNP P90504
A	117	ALA	VAL	ENGINEERED	UNP P90504
A	147	ASP	-	EXPRESSION TAG	UNP P90504
A	148	ASP	-	EXPRESSION TAG	UNP P90504
A	149	ASP	-	EXPRESSION TAG	UNP P90504
A	150	ASP	-	EXPRESSION TAG	UNP P90504
A	151	LEU	-	EXPRESSION TAG	UNP P90504
A	152	GLU	-	EXPRESSION TAG	UNP P90504
A	153	HIS	-	EXPRESSION TAG	UNP P90504
A	154	HIS	-	EXPRESSION TAG	UNP P90504
A	155	HIS	-	EXPRESSION TAG	UNP P90504
A	156	HIS	-	EXPRESSION TAG	UNP P90504
A	157	HIS	-	EXPRESSION TAG	UNP P90504
A	158	HIS	-	EXPRESSION TAG	UNP P90504

4 Residue-property plots [i](#)

These plots are provided for all protein, RNA and DNA 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: functional anti-apoptotic factor vBCL-2 homolog



5 Refinement protocol and experimental data overview

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

Of the 100 calculated structures, 1 were deposited, based on the following criterion: *AVERAGE, MINIMIZED*.

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

Software name	Classification	Version
CNX	structure solution	
CNX	refinement	

No chemical shift data was provided. No validations of the models with respect to experimental NMR restraints is performed at this time.

6 Model quality

6.1 Standard geometry

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

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	1140	1137	1134	51
All	All	1140	1137	1134	51

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 22.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)
1:A:74:LEU:HD12	1:A:122:ALA:HB2	0.93	1.37
1:A:93:PHE:CZ	1:A:97:VAL:HG11	0.80	2.10
1:A:54:MET:O	1:A:58:VAL:HG13	0.79	1.77
1:A:39:TYR:CE2	1:A:137:LEU:HD23	0.75	2.16
1:A:71:LEU:HD21	1:A:118:TYR:CD2	0.72	2.20
1:A:12:ALA:O	1:A:16:ILE:HD12	0.71	1.84
1:A:36:ILE:O	1:A:40:ILE:HG23	0.69	1.88
1:A:43:LEU:HB3	1:A:92:THR:HG21	0.67	1.67
1:A:74:LEU:HD12	1:A:122:ALA:CB	0.66	2.18
1:A:93:PHE:CE2	1:A:97:VAL:HG11	0.64	2.27
1:A:93:PHE:O	1:A:97:VAL:HG22	0.62	1.95
1:A:52:GLU:O	1:A:56:ALA:HB3	0.61	1.96
1:A:15:GLY:O	1:A:19:ALA:HB3	0.60	1.96
1:A:101:LEU:HD11	1:A:107:LEU:HB2	0.58	1.74
1:A:93:PHE:O	1:A:97:VAL:HG13	0.56	2.01

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Atom-1	Atom-2	Clash(Å)	Distance(Å)
1:A:142:THR:O	1:A:146:THR:HG23	0.55	2.01
1:A:71:LEU:HD13	1:A:71:LEU:O	0.54	2.02
1:A:43:LEU:HD13	1:A:88:LEU:CD2	0.52	2.34
1:A:119:ALA:O	1:A:123:ILE:HD12	0.52	2.04
1:A:74:LEU:HD13	1:A:118:TYR:CD1	0.52	2.40
1:A:115:LEU:O	1:A:119:ALA:HB2	0.52	2.04
1:A:5:VAL:HG12	1:A:5:VAL:O	0.52	2.05
1:A:141:CYS:O	1:A:144:VAL:HG22	0.51	2.06
1:A:90:ILE:O	1:A:115:LEU:HD11	0.51	2.06
1:A:94:GLY:O	1:A:98:ALA:HB2	0.51	2.05
1:A:10:VAL:HG11	1:A:116:PRO:O	0.50	2.06
1:A:53:ALA:O	1:A:58:VAL:HG12	0.48	2.08
1:A:34:SER:N	1:A:35:PRO:CD	0.48	2.77
1:A:39:TYR:CZ	1:A:137:LEU:HD23	0.47	2.45
1:A:36:ILE:HG22	1:A:40:ILE:CG2	0.47	2.40
1:A:93:PHE:CE1	1:A:97:VAL:HG11	0.47	2.43
1:A:18:MET:CE	1:A:111:ALA:HB1	0.47	2.40
1:A:62:SER:OG	1:A:64:THR:HG22	0.47	2.09
1:A:57:ASN:C	1:A:58:VAL:HG12	0.46	2.30
1:A:32:LEU:HD13	1:A:35:PRO:HD2	0.46	1.87
1:A:107:LEU:O	1:A:110:PHE:CD1	0.45	2.70
1:A:110:PHE:CG	1:A:111:ALA:N	0.45	2.84
1:A:114:VAL:HG12	1:A:115:LEU:N	0.44	2.26
1:A:60:PHE:CG	1:A:107:LEU:CD1	0.43	3.02
1:A:74:LEU:HD13	1:A:118:TYR:HD1	0.43	1.74
1:A:97:VAL:O	1:A:101:LEU:HD13	0.43	2.13
1:A:27:TYR:CD1	1:A:28:LEU:N	0.42	2.87
1:A:60:PHE:CD1	1:A:107:LEU:CD1	0.42	3.02
1:A:50:LEU:CD2	1:A:51:PHE:CD1	0.41	3.03
1:A:55:LEU:HD12	1:A:55:LEU:N	0.41	2.29
1:A:87:ALA:C	1:A:91:LEU:HD12	0.41	2.36
1:A:87:ALA:O	1:A:91:LEU:HD12	0.41	2.16
1:A:13:ILE:O	1:A:17:PHE:CD2	0.41	2.74
1:A:64:THR:HG23	1:A:65:GLY:N	0.40	2.31
1:A:140:TYR:CD1	1:A:140:TYR:O	0.40	2.75
1:A:58:VAL:CG2	1:A:59:ARG:N	0.40	2.84

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	144/158 (91%)	121 (84%)	14 (10%)	9 (6%)	3	20
All	All	144/158 (91%)	121 (84%)	14 (10%)	9 (6%)	3	20

All 9 Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type
1	A	62	SER
1	A	33	LEU
1	A	79	ASP
1	A	132	GLY
1	A	31	PRO
1	A	58	VAL
1	A	82	MET
1	A	3	GLU
1	A	6	LEU

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	118/130 (91%)	93 (79%)	25 (21%)	4	32
All	All	118/130 (91%)	93 (79%)	25 (21%)	4	32

All 25 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	62	SER

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Mol	Chain	Res	Type
1	A	29	TYR
1	A	30	HIS
1	A	143	GLN
1	A	43	LEU
1	A	142	THR
1	A	72	SER
1	A	79	ASP
1	A	2	ASP
1	A	37	LYS
1	A	101	LEU
1	A	1	MET
1	A	73	MET
1	A	71	LEU
1	A	145	LEU
1	A	126	GLN
1	A	100	LYS
1	A	61	HIS
1	A	4	ASP
1	A	58	VAL
1	A	44	MET
1	A	115	LEU
1	A	22	LEU
1	A	74	LEU
1	A	131	ARG

6.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

6.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.6 Ligand geometry ⓘ

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