



wwPDB NMR Structure Validation Summary Report ⓘ

Feb 17, 2018 – 03:09 am GMT

PDB ID : 2M5B
Title : The NMR structure of the BID-BAK complex
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Deposited on : 2013-02-19

This is a wwPDB NMR Structure Validation Summary Report for a publicly released PDB entry.

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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
Mogul	:	1.7.3 (157068), CSD as539be (2018)
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

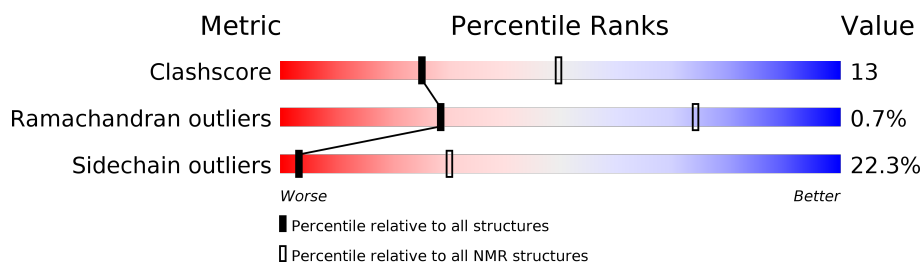
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 77%.

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	169	
2	B	23	

2 Ensemble composition and analysis

This entry contains 20 models. Model 13 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *fewest violations*.

The following residues are included in the computation of the global validation metrics.

Well-defined (core) protein residues			
Well-defined core	Residue range (total)	Backbone RMSD (Å)	Medoid model
1	A:22-A:45, A:66-A:184, B:81-B:91, B:93-B:95, B:98-B:101 (161)	0.36	13

Ill-defined regions of proteins are excluded from the global statistics.

Ligands and non-protein polymers are included in the analysis.

The models can be grouped into 2 clusters and 1 single-model cluster was found.

Cluster number	Models
1	2, 3, 4, 5, 7, 9, 10, 11, 12, 13, 14, 15, 17, 18, 19
2	6, 8, 16, 20
Single-model clusters	1

3 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 2783 atoms, of which 1268 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Bcl-2 homologous antagonist/killer.

Mol	Chain	Residues	Atoms						Trace
1	A	169	Total	C	H	N	O	S	0
			2440	850	1103	234	248	5	

- Molecule 2 is a protein called human_BID_BH3_SAHB.

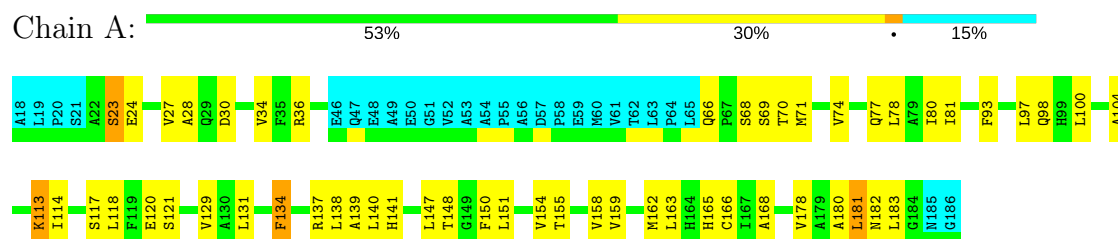
Mol	Chain	Residues	Atoms					Trace
2	B	23	Total	C	H	N	O	1
			343	111	165	35	32	

4 Residue-property plots

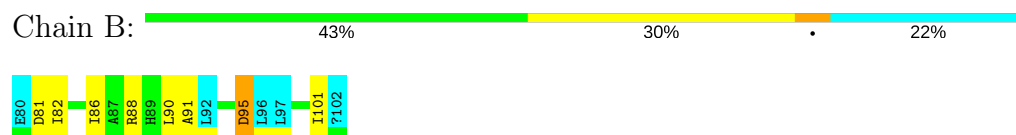
4.1 Average score per residue in the NMR ensemble

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: Bcl-2 homologous antagonist/killer



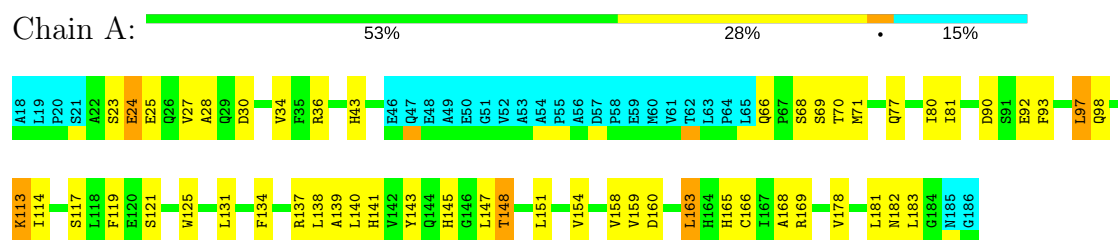
- Molecule 2: human_BID_BH3_SAHB



4.2 Residue scores for the representative (medoid) model from the NMR ensemble

The representative model is number 13. Colouring as in section 4.1 above.

- Molecule 1: Bcl-2 homologous antagonist/killer



- Molecule 2: human_BID_BH3_SAHB



D80	D81	I82	I83	R84	R85	I86	A87	R88	R89	L90	A91	I92	D95	L96	L97	S100	I101	I102
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5 Refinement protocol and experimental data overview

The models were refined using the following method: *torsion angle dynamics, simulated annealing, molecular dynamics*.

Of the 100 calculated structures, 20 were deposited, based on the following criterion: *structures with the lowest energy*.

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

Software name	Classification	Version
TOPSPIN	structure solution	
TOPSPIN	structure solution	
TOPSPIN	structure solution	
CYANA	refinement	

The following table shows chemical shift validation statistics as aggregates over all chemical shift files. Detailed validation can be found in section 7 of this report.

Chemical shift file(s)	2m5b_cs.str
Number of chemical shift lists	1
Total number of shifts	2094
Number of shifts mapped to atoms	2094
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	77%

No validations of the models with respect to experimental NMR restraints is performed at this time.

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: NH2, NLE, MK8

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

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	Chirality	Planarity
2	B	0.0±0.0	2.0±0.0
All	All	0	40

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

All unique planar outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Group	Models (Total)
2	B	91	ALA	Peptide	20
2	B	95	ASP	Peptide	20

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	1156	960	1110	31±5
2	B	142	126	146	8±3
All	All	25960	21720	25120	641

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 13.

5 of 209 unique clashes are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:114:ILE:HD12	2:B:86:ILE:HG21	0.98	1.33	6	10
1:A:70:THR:HG21	1:A:178:VAL:HG13	0.95	1.35	17	8
1:A:183:LEU:HD22	2:B:101:ILE:HD12	0.94	1.32	2	8
1:A:104:ALA:HB2	1:A:147:LEU:HD13	0.94	1.39	6	1
1:A:97:LEU:HD11	1:A:138:LEU:HD12	0.85	1.44	3	3

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	143/169 (85%)	132±2 (92±1%)	10±2 (7±1%)	1±1 (1±1%)	26	72
2	B	18/23 (78%)	15±1 (84±5%)	3±1 (16±5%)	0±0 (0±0%)	100	100
All	All	3220/3840 (84%)	2933 (91%)	264 (8%)	23 (1%)	28	74

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

Mol	Chain	Res	Type	Models (Total)
1	A	146	GLY	4
1	A	166	CYS	4
1	A	149	GLY	4
1	A	148	THR	3
1	A	184	GLY	3

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	118/137 (86%)	92±3 (78±3%)	26±3 (22±3%)	3	31
2	B	15/16 (94%)	11±1 (73±8%)	4±1 (27±8%)	2	22

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	2660/3060 (87%)	2066 (78%)	594 (22%)	3 30

5 of 76 unique residues with a non-rotameric sidechain are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	A	134	PHE	20
1	A	151	LEU	20
1	A	165	HIS	20
1	A	23	SER	17
2	B	88	ARG	17

6.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

3 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds for which Mogul statistics could be retrieved, the number of bonds that are observed in the model and the number of bonds that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length is the number of standard deviations the observed value is removed from the expected value. A bond length with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the average root-mean-square of all Z scores of the bond lengths.

Mol	Type	Chain	Res	Link	Bond lengths		
					Counts	RMSZ	#Z>2
2	MK8	B	92	2	5,8,9	1.10±0.02	0±0 (0±0%)
2	MK8	B	96	2	5,8,9	1.09±0.02	0±0 (0±0%)
2	NLE	B	97	2	7,7,8	1.07±0.02	0±0 (0±0%)

In the following table, the Counts columns list the number of angles for which Mogul statistics could be retrieved, the number of angles that are observed in the model and the number of angles that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond angle is the number of standard deviations the observed value is removed from the expected value. A bond angle with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the average root-mean-square of all Z scores of the bond angles.

Mol	Type	Chain	Res	Link	Bond angles		
					Counts	RMSZ	#Z>2
2	MK8	B	92	2	5,10,12	1.90±0.01	0±0 (0±0%)
2	MK8	B	96	2	5,10,12	2.04±0.01	0±0 (0±0%)
2	NLE	B	97	2	4,7,9	0.94±0.01	0±0 (0±0%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	MK8	B	92	2	-	0±0,6,8,11	0±0,0,0,0
2	MK8	B	96	2	-	0±0,6,8,11	0±0,0,0,0
2	NLE	B	97	2	-	0±0,4,6,8	0±0,0,0,0

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.

6.5 Carbohydrates [i](#)

There are no carbohydrates 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](#)

The completeness of assignment taking into account all chemical shift lists is 77% for the well-defined parts and 78% for the entire structure.

7.1 Chemical shift list 1

File name: 2m5b_cs.str

Chemical shift list name: *assigned_chem_shift_list_1*

7.1.1 Bookkeeping [i](#)

The following table shows the results of parsing the chemical shift list and reports the number of nuclei with statistically unusual chemical shifts.

Total number of shifts	2094
Number of shifts mapped to atoms	2094
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	9

7.1.2 Chemical shift referencing [i](#)

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction \pm precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	168	-0.31 ± 0.08	None needed (< 0.5 ppm)
$^{13}\text{C}_\beta$	154	0.39 ± 0.06	None needed (< 0.5 ppm)
$^{13}\text{C}'$	0	—	None (insufficient data)
^{15}N	155	0.76 ± 0.33	Should be applied

7.1.3 Completeness of resonance assignments [i](#)

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 77%, i.e. 1560 atoms were assigned a chemical shift out of a possible 2027. 17 out of 26 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	597/801 (75%)	319/320 (100%)	143/322 (44%)	135/159 (85%)
Sidechain	798/1004 (79%)	522/585 (89%)	259/361 (72%)	17/58 (29%)

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	Total	¹ H	¹³ C	¹⁵ N
Aromatic	165/222 (74%)	103/119 (87%)	59/93 (63%)	3/10 (30%)
Overall	1560/2027 (77%)	944/1024 (92%)	461/776 (59%)	155/227 (68%)

7.1.4 Statistically unusual chemical shifts ⓘ

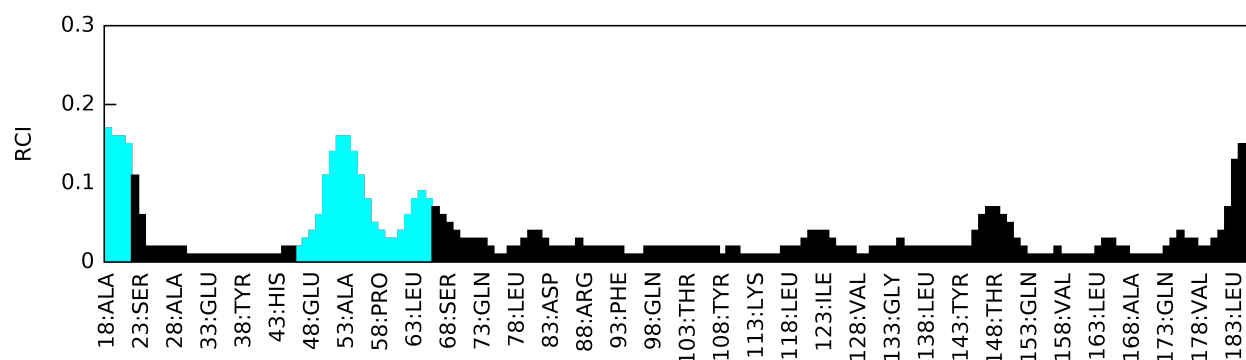
The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

Mol	Chain	Res	Type	Atom	Shift, ppm	Expected range, ppm	Z-score
1	A	127	ARG	NE	117.95	92.63 – 76.73	20.9
1	A	174	ARG	HD3	1.46	4.36 – 1.86	-6.6
1	A	115	ALA	HB3	-0.20	2.61 – 0.11	-6.2
1	A	115	ALA	HB2	-0.20	2.61 – 0.11	-6.2
1	A	115	ALA	HB1	-0.20	2.61 – 0.11	-6.2
1	A	123	ILE	HG22	-0.83	2.13 – -0.57	-6.0
1	A	123	ILE	HG23	-0.83	2.13 – -0.57	-6.0
1	A	123	ILE	HG21	-0.83	2.13 – -0.57	-6.0
1	A	153	GLN	HB3	0.64	3.37 – 0.67	-5.1

7.1.5 Random Coil Index (RCI) plots ⓘ

The images below report *random coil index* values for the protein chains in the structure. The height of each bar gives a probability of a given residue to be disordered, as predicted from the available chemical shifts and the amino acid sequence. A value above 0.2 is an indication of significant predicted disorder. The colour of the bar shows whether the residue is in the well-defined core (black) or in the ill-defined residue ranges (cyan), as described in section 2 on ensemble composition.

Random coil index (RCI) for chain A:



Random coil index (RCI) for chain B:

