



# Full wwPDB NMR Structure Validation Report ⓘ

Apr 26, 2016 – 09:01 PM BST

PDB ID : 2J5D  
Title : NMR STRUCTURE OF BNIP3 TRANSMEMBRANE DOMAIN IN LIPID BICELLES  
Authors : Bocharov, E.V.; Pustovalova, Y.E.; Volynsky, P.E.; Maslennikov, I.V.; Goncharuk, M.V.; Ermolyuk, Y.S.; Arseniev, A.S.  
Deposited on : 2006-09-14

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We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/NMRValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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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 : unknown  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
RCI : v\_1n\_11\_5\_13\_A (Berjanski et al., 2005)  
PANAV : Wang et al. (2010)  
ShiftChecker : rb-20027457  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : rb-20027457

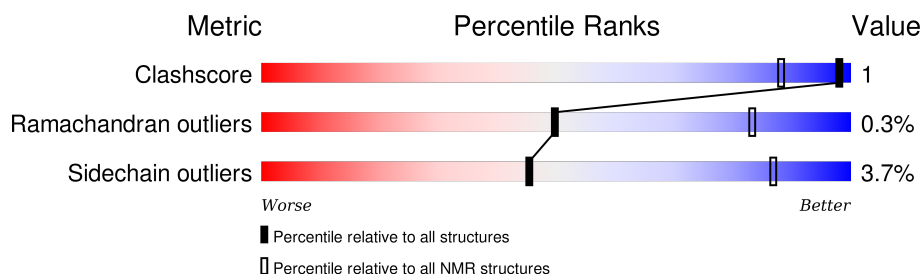
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*SOLUTION NMR*

The overall completeness of chemical shifts assignment is 74%.

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	114402	11133
Ramachandran outliers	111179	9975
Sidechain outliers	111093	9958

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  $\geq 3$ , 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	45	 40% • 56%
1	B	45	 38% • 58%

## 2 Ensemble composition and analysis

This entry contains 16 models. Model 7 is the overall representative, medoid model (most similar to other models).

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:166-A:185, B:165-B:183 (39)	0.43	7

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 3 single-model clusters were found.

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

### 3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 1114 atoms, of which 420 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called BCL2/ADENOVIRUS E1B 19 KDA PROTEIN-INTERACTING PROTEIN 3.

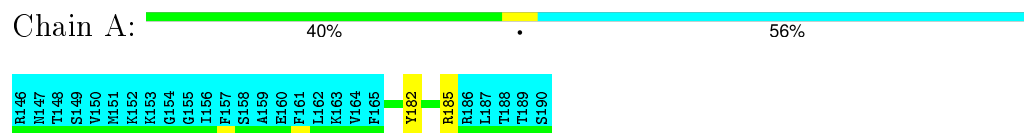
Mol	Chain	Residues	Atoms						Trace
1	A	45	Total	C	H	N	O	S	0
			557	228	210	60	58	1	
1	B	45	Total	C	H	N	O	S	0
			557	228	210	60	58	1	

## 4 Residue-property plots [i](#)

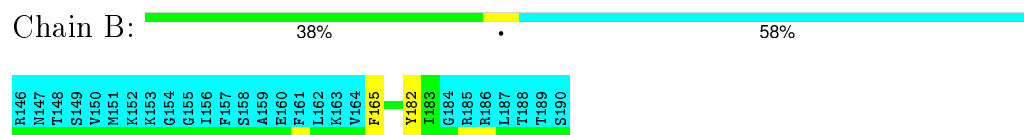
### 4.1 Average score per residue in the NMR ensemble

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: BCL2/ADENOVIRUS E1B 19 KDA PROTEIN-INTERACTING PROTEIN 3



- Molecule 1: BCL2/ADENOVIRUS E1B 19 KDA PROTEIN-INTERACTING PROTEIN 3

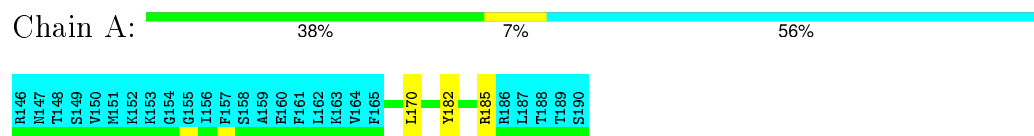


### 4.2 Scores per residue for each member of the ensemble

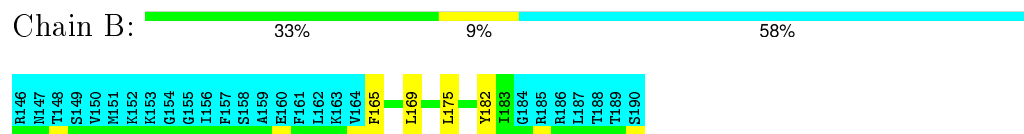
Colouring as in section 4.1 above.

#### 4.2.1 Score per residue for model 1

- Molecule 1: BCL2/ADENOVIRUS E1B 19 KDA PROTEIN-INTERACTING PROTEIN 3

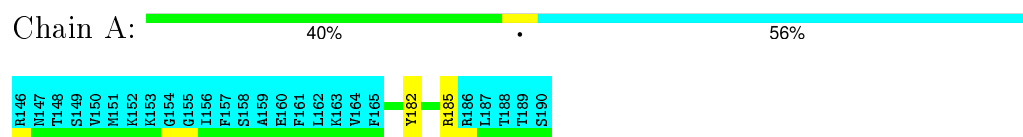


- Molecule 1: BCL2/ADENOVIRUS E1B 19 KDA PROTEIN-INTERACTING PROTEIN 3

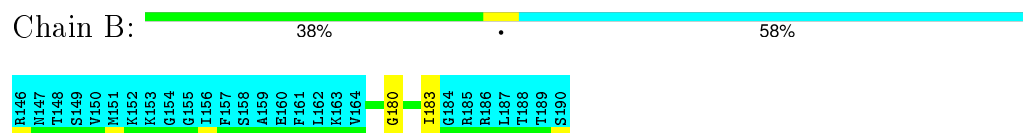


### 4.2.2 Score per residue for model 2

- Molecule 1: BCL2/ADENOVIRUS E1B 19 KDA PROTEIN-INTERACTING PROTEIN 3

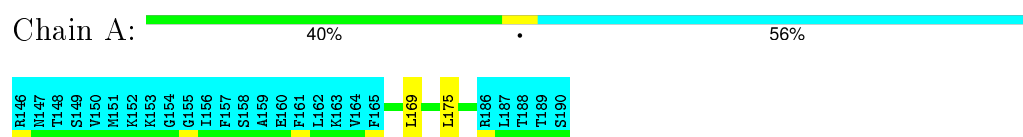


- Molecule 1: BCL2/ADENOVIRUS E1B 19 KDA PROTEIN-INTERACTING PROTEIN 3

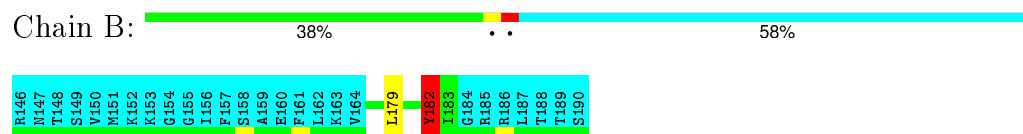


### 4.2.3 Score per residue for model 3

- Molecule 1: BCL2/ADENOVIRUS E1B 19 KDA PROTEIN-INTERACTING PROTEIN 3

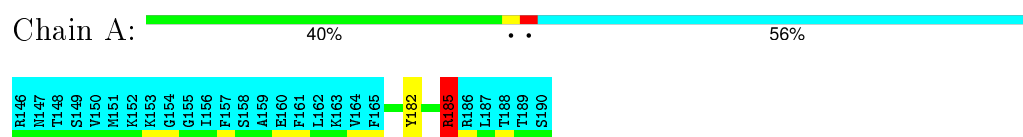


- Molecule 1: BCL2/ADENOVIRUS E1B 19 KDA PROTEIN-INTERACTING PROTEIN 3

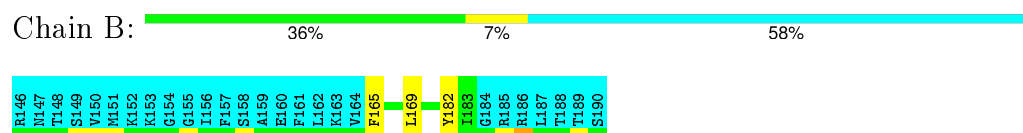


### 4.2.4 Score per residue for model 4

- Molecule 1: BCL2/ADENOVIRUS E1B 19 KDA PROTEIN-INTERACTING PROTEIN 3

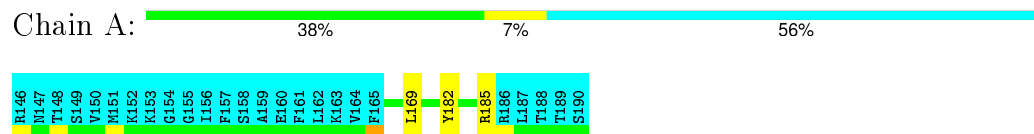


- Molecule 1: BCL2/ADENOVIRUS E1B 19 KDA PROTEIN-INTERACTING PROTEIN 3

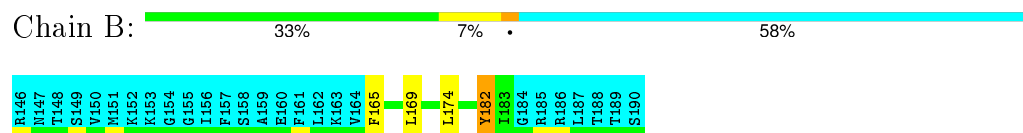


### 4.2.5 Score per residue for model 5

- Molecule 1: BCL2/ADENOVIRUS E1B 19 KDA PROTEIN-INTERACTING PROTEIN 3

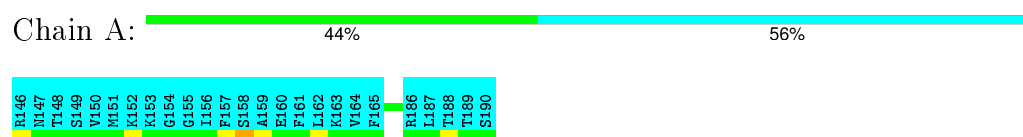


- Molecule 1: BCL2/ADENOVIRUS E1B 19 KDA PROTEIN-INTERACTING PROTEIN 3

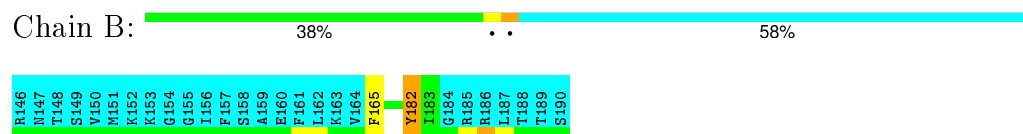


### 4.2.6 Score per residue for model 6

- Molecule 1: BCL2/ADENOVIRUS E1B 19 KDA PROTEIN-INTERACTING PROTEIN 3

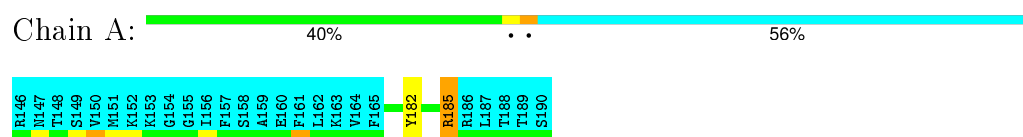


- Molecule 1: BCL2/ADENOVIRUS E1B 19 KDA PROTEIN-INTERACTING PROTEIN 3

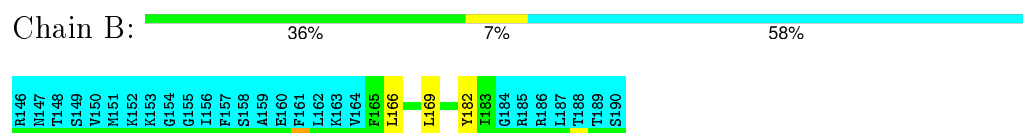


### 4.2.7 Score per residue for model 7 (medoid)

- Molecule 1: BCL2/ADENOVIRUS E1B 19 KDA PROTEIN-INTERACTING PROTEIN 3

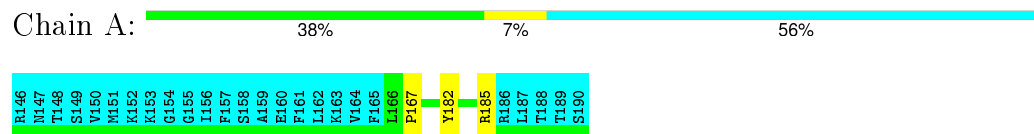


- Molecule 1: BCL2/ADENOVIRUS E1B 19 KDA PROTEIN-INTERACTING PROTEIN 3

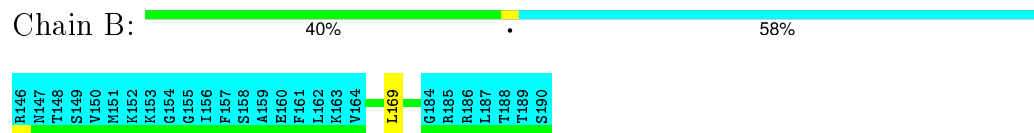


### 4.2.8 Score per residue for model 8

- Molecule 1: BCL2/ADENOVIRUS E1B 19 KDA PROTEIN-INTERACTING PROTEIN 3

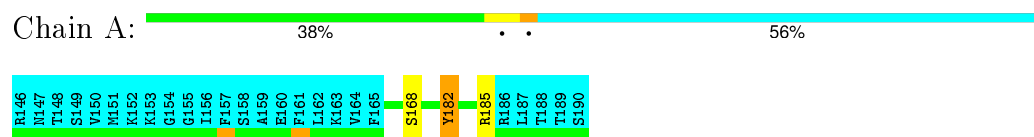


- Molecule 1: BCL2/ADENOVIRUS E1B 19 KDA PROTEIN-INTERACTING PROTEIN 3

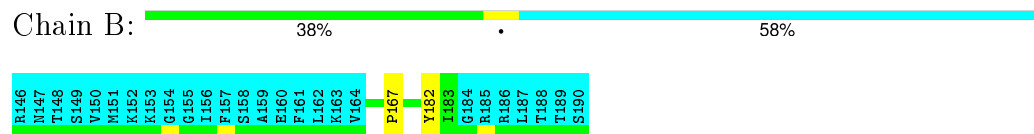


### 4.2.9 Score per residue for model 9

- Molecule 1: BCL2/ADENOVIRUS E1B 19 KDA PROTEIN-INTERACTING PROTEIN 3

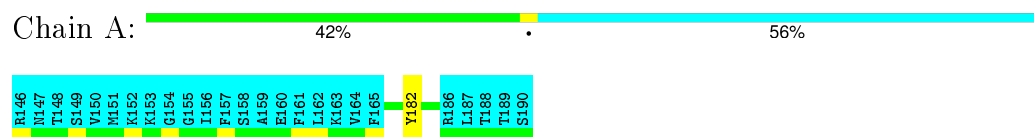


- Molecule 1: BCL2/ADENOVIRUS E1B 19 KDA PROTEIN-INTERACTING PROTEIN 3

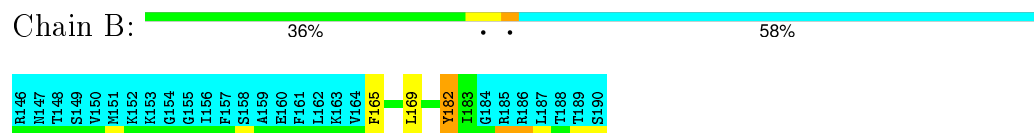


### 4.2.10 Score per residue for model 10

- Molecule 1: BCL2/ADENOVIRUS E1B 19 KDA PROTEIN-INTERACTING PROTEIN 3

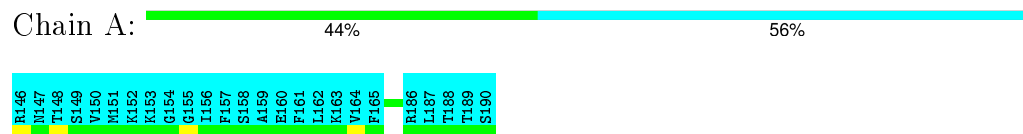


- Molecule 1: BCL2/ADENOVIRUS E1B 19 KDA PROTEIN-INTERACTING PROTEIN 3

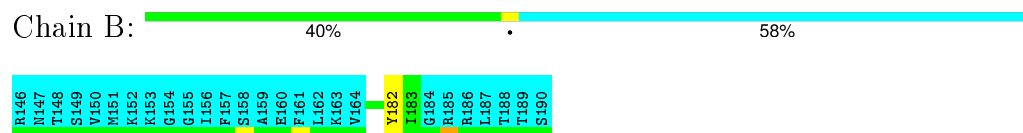


### 4.2.11 Score per residue for model 11

- Molecule 1: BCL2/ADENOVIRUS E1B 19 KDA PROTEIN-INTERACTING PROTEIN 3

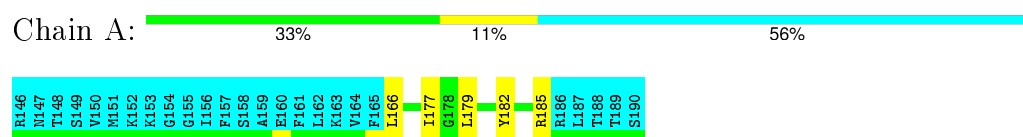


- Molecule 1: BCL2/ADENOVIRUS E1B 19 KDA PROTEIN-INTERACTING PROTEIN 3

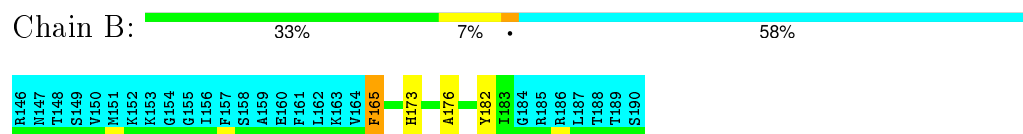


### 4.2.12 Score per residue for model 12

- Molecule 1: BCL2/ADENOVIRUS E1B 19 KDA PROTEIN-INTERACTING PROTEIN 3

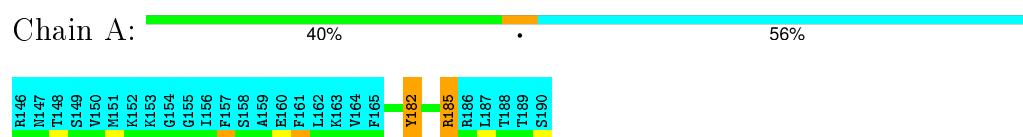


- Molecule 1: BCL2/ADENOVIRUS E1B 19 KDA PROTEIN-INTERACTING PROTEIN 3

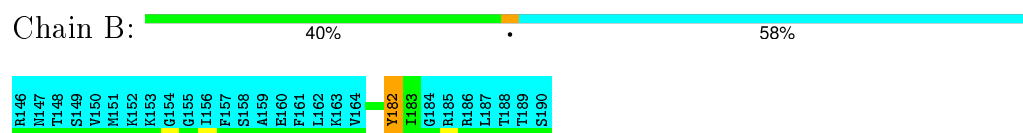


### 4.2.13 Score per residue for model 13

- Molecule 1: BCL2/ADENOVIRUS E1B 19 KDA PROTEIN-INTERACTING PROTEIN 3

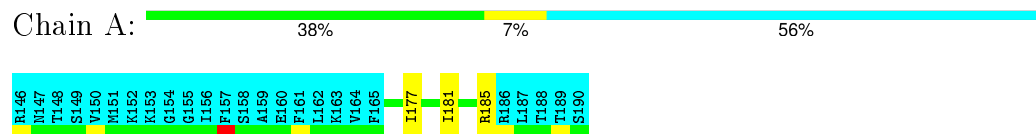


- Molecule 1: BCL2/ADENOVIRUS E1B 19 KDA PROTEIN-INTERACTING PROTEIN 3

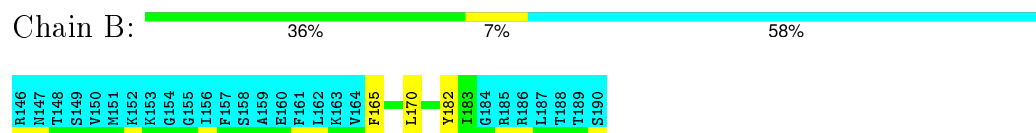


#### 4.2.14 Score per residue for model 14

- Molecule 1: BCL2/ADENOVIRUS E1B 19 KDA PROTEIN-INTERACTING PROTEIN 3

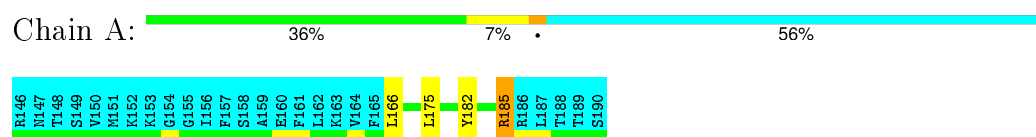


- Molecule 1: BCL2/ADENOVIRUS E1B 19 KDA PROTEIN-INTERACTING PROTEIN 3

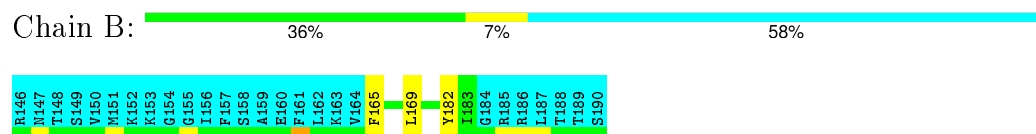


#### 4.2.15 Score per residue for model 15

- Molecule 1: BCL2/ADENOVIRUS E1B 19 KDA PROTEIN-INTERACTING PROTEIN 3

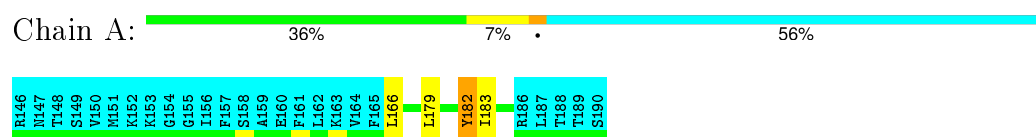


- Molecule 1: BCL2/ADENOVIRUS E1B 19 KDA PROTEIN-INTERACTING PROTEIN 3

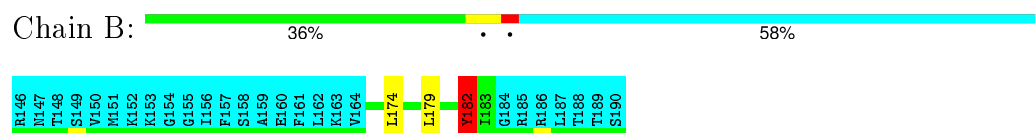


#### 4.2.16 Score per residue for model 16

- Molecule 1: BCL2/ADENOVIRUS E1B 19 KDA PROTEIN-INTERACTING PROTEIN 3



- Molecule 1: BCL2/ADENOVIRUS E1B 19 KDA PROTEIN-INTERACTING PROTEIN 3



## 5 Refinement protocol and experimental data overview

The models were refined using the following method: *TAD*.

Of the 200 calculated structures, 16 were deposited, based on the following criterion: *THE BEST TARGET FUNCTION*.

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

Software name	Classification	Version
GROMACS	refinement	
CYANA	structure solution	

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)	BMRB entry 7288
Number of chemical shift lists	1
Total number of shifts	964
Number of shifts mapped to atoms	964
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	74%

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

## 6 Model quality

### 6.1 Standard geometry

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the (average) root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#Z>5	RMSZ	#Z>5
1	A	0.83±0.08	0±0/152 (0.0±0.2%)	1.02±0.11	1±1/207 (0.4±0.4%)
1	B	0.88±0.07	0±0/149 (0.0±0.0%)	1.03±0.12	1±1/204 (0.3±0.3%)
All	All	0.86	1/4816 (0.0%)	1.03	24/6576 (0.4%)

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
1	A	0.0±0.0	1.0±0.7
1	B	0.0±0.0	1.4±0.7
All	All	0	38

All unique bond outliers are listed below.

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
1	A	182	TYR	CE1-CZ	5.04	1.45	1.38	13	1

All unique angle outliers are listed below. They are sorted according to the Z-score of the worst occurrence in the ensemble.

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	185	ARG	NE-CZ-NH1	8.73	124.66	120.30	8	6
1	B	182	TYR	CB-CG-CD2	-7.74	116.36	121.00	3	4
1	B	165	PHE	CB-CG-CD2	-6.40	116.32	120.80	4	5
1	A	182	TYR	CB-CG-CD2	-5.87	117.48	121.00	12	2
1	A	185	ARG	NE-CZ-NH2	-5.79	117.41	120.30	8	4
1	B	182	TYR	CB-CG-CD1	-5.38	117.77	121.00	16	1
1	A	182	TYR	CB-CG-CD1	-5.36	117.79	121.00	16	2

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)
1	B	182	TYR	Sidechain	14
1	A	182	TYR	Sidechain	10
1	B	169	LEU	Mainchain	5
1	A	185	ARG	Sidechain	5
1	B	165	PHE	Sidechain	3
1	A	169	LEU	Mainchain	1

## 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	149	87	170	0±0
1	B	145	83	163	0±0
All	All	4704	2720	5328	6

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 1.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:179:LEU:O	1:B:182:TYR:HB3	0.44	2.13	3	2
1:A:177:ILE:O	1:A:181:ILE:HD12	0.44	2.13	14	1
1:A:179:LEU:O	1:A:183:ILE:HG12	0.42	2.14	16	1
1:A:177:ILE:HG13	1:B:176:ALA:HB1	0.42	1.91	12	1
1:B:180:GLY:HA2	1:B:183:ILE:HD12	0.41	1.92	2	1

## 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	20/45 (44%)	18±1 (92±5%)	2±1 (8±5%)	0±0 (0±1%)	50	83
1	B	19/45 (42%)	18±1 (94±6%)	1±1 (6±6%)	0±0 (0±1%)	50	83
All	All	624/1440 (43%)	580 (93%)	42 (7%)	2 (0%)	50	83

All 2 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	167	PRO	1
1	B	167	PRO	1

### 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	16/38 (42%)	15±1 (96±4%)	1±1 (4±4%)	43	85
1	B	16/38 (42%)	15±0 (96±3%)	1±0 (4±3%)	47	88
All	All	512/1216 (42%)	493 (96%)	19 (4%)	45	87

All 14 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	185	ARG	2
1	A	175	LEU	2
1	B	169	LEU	2
1	A	166	LEU	2
1	B	174	LEU	2
1	B	166	LEU	1
1	A	168	SER	1
1	B	175	LEU	1
1	A	179	LEU	1
1	B	170	LEU	1
1	A	169	LEU	1
1	A	170	LEU	1

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Models (Total)
1	B	182	TYR	1
1	B	173	HIS	1

### 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 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

The completeness of assignment taking into account all chemical shift lists is 74% for the well-defined parts and 73% for the entire structure.

### 7.1 Chemical shift list 1

File name: BMRB entry 7288

Chemical shift list name: *assigned\_chem\_shift\_list\_1*

#### 7.1.1 Bookkeeping

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	964
Number of shifts mapped to atoms	964
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	0

#### 7.1.2 Chemical shift referencing

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction $\pm$ precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	88	$1.14 \pm 0.07$	Should be applied
$^{13}\text{C}_\beta$	70	$1.93 \pm 0.10$	Should be applied
$^{13}\text{C}'$	0	—	—
$^{15}\text{N}$	84	$2.70 \pm 0.19$	Should be applied

#### 7.1.3 Completeness of resonance assignments

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 74%, i.e. 353 atoms were assigned a chemical shift out of a possible 475. 0 out of 14 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	$^1\text{H}$	$^{13}\text{C}$	$^{15}\text{N}$
Backbone	152/191 (80%)	76/76 (100%)	39/78 (50%)	37/37 (100%)
Sidechain	180/247 (73%)	123/143 (86%)	56/101 (55%)	1/3 (33%)

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	Total	<sup>1</sup> H	<sup>13</sup> C	<sup>15</sup> N
Aromatic	21/37 (57%)	17/21 (81%)	4/16 (25%)	0/0 (—%)
Overall	353/475 (74%)	216/240 (90%)	99/195 (51%)	38/40 (95%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 73%, i.e. 820 atoms were assigned a chemical shift out of a possible 1126. 2 out of 22 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	<sup>1</sup> H	<sup>13</sup> C	<sup>15</sup> N
Backbone	346/446 (78%)	174/178 (98%)	88/180 (49%)	84/88 (95%)
Sidechain	428/598 (72%)	292/350 (83%)	130/222 (59%)	6/26 (23%)
Aromatic	46/82 (56%)	42/46 (91%)	4/36 (11%)	0/0 (—%)
Overall	820/1126 (73%)	508/574 (89%)	222/438 (51%)	90/114 (79%)

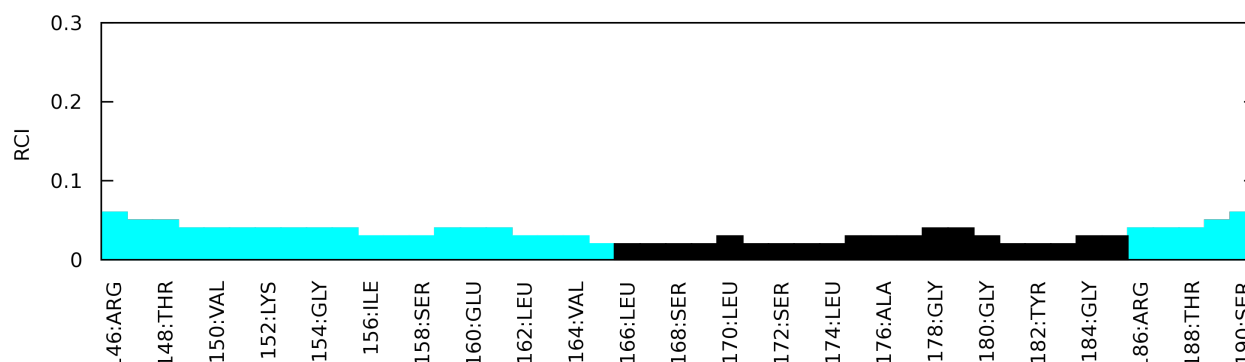
#### 7.1.4 Statistically unusual chemical shifts [i](#)

There are no statistically unusual chemical shifts.

#### 7.1.5 Random Coil Index (RCI) plots [i](#)

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:

