



# wwPDB X-ray Structure Validation Summary Report ⓘ

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PDB ID : 5KTG  
Title : Crystal structure of mouse Bak BH3-in-groove homodimer (GFP)  
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Deposited on : 2016-07-11  
Resolution : 2.80 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

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>.

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.36  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.36

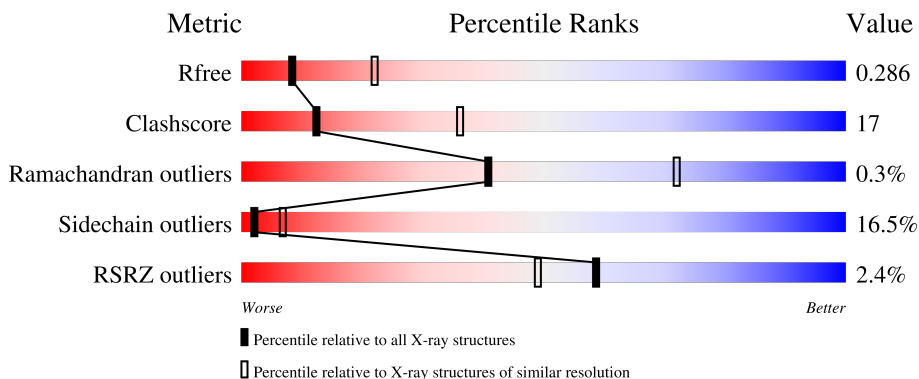
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.80 Å.

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)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. 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  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	309	
1	B	309	

## 2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 4910 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	309	2455	1566	416	465	8	0	0	0
1	B	309	2455	1566	416	465	8	0	0	0

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	66	CR2	SER	chromophore	UNP P42212
A	66	CR2	TYR	chromophore	UNP P42212
A	66	CR2	GLY	chromophore	UNP P42212
A	72	ALA	SER	conflict	UNP P42212
A	206	ASN	ALA	conflict	UNP P42212
A	231	GLY	-	linker	UNP P42212
A	232	SER	-	linker	UNP P42212
A	1084	CYS	ASN	conflict	UNP O08734
B	66	CR2	SER	chromophore	UNP P42212
B	66	CR2	TYR	chromophore	UNP P42212
B	66	CR2	GLY	chromophore	UNP P42212
B	72	ALA	SER	conflict	UNP P42212
B	206	ASN	ALA	conflict	UNP P42212
B	231	GLY	-	linker	UNP P42212
B	232	SER	-	linker	UNP P42212
B	1084	CYS	ASN	conflict	UNP O08734



## 4 Data and refinement statistics i

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	171.64Å 171.64Å 98.19Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	49.55 – 2.80 49.55 – 2.80	Depositor EDS
% Data completeness (in resolution range)	97.0 (49.55-2.80) 94.8 (49.55-2.80)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.15	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.39 (at 2.81Å)	Xtrriage
Refinement program	PHENIX 1.9_1692	Depositor
R, $R_{free}$	0.244 , 0.275 0.257 , 0.286	Depositor DCC
$R_{free}$ test set	1949 reflections (4.86%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	62.9	Xtrriage
Anisotropy	0.299	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.22 , 17.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.41$ , $\langle L^2 \rangle = 0.24$	Xtrriage
Estimated twinning fraction	0.057 for -h,-k,l	Xtrriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	4910	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	91.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.66% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: CR2

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 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	0.90	5/2489 (0.2%)	1.04	2/3363 (0.1%)
1	B	0.88	0/2489	1.03	4/3363 (0.1%)
All	All	0.89	5/4978 (0.1%)	1.03	6/6726 (0.1%)

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 outliers	#Planarity outliers
1	A	0	2
1	B	0	3
All	All	0	5

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1134	TYR	CB-CG	6.10	1.60	1.51
1	A	1134	TYR	CD1-CE1	5.95	1.48	1.39
1	A	34	GLU	CG-CD	5.70	1.60	1.51
1	A	34	GLU	CB-CG	5.64	1.62	1.52
1	A	1134	TYR	CD2-CE2	5.62	1.47	1.39

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	1122	SER	N-CA-C	-6.61	93.16	111.00
1	A	1066	ASN	N-CA-C	-6.37	93.80	111.00
1	A	1134	TYR	CA-CB-CG	5.79	124.40	113.40
1	B	221	LEU	CB-CG-CD1	5.74	120.76	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	122	ARG	NE-CZ-NH2	-5.36	117.62	120.30

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1066	ASN	Peptide
1	A	232	SER	Peptide
1	B	1098	LEU	Peptide
1	B	230	THR	Peptide
1	B	3	LYS	Peptide

## 5.2 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 the 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 within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2455	0	2395	78	2
1	B	2455	0	2395	94	1
All	All	4910	0	4790	164	2

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 17.

The worst 5 of 164 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:133:ASP:O	1:B:140:LYS:NZ	2.03	0.91
1:B:64:PHE:O	1:B:66:CR2:HA31	1.71	0.90
1:B:1088:ASP:OD2	1:B:1135:ARG:NH1	2.18	0.77
1:B:1116:LEU:O	1:B:1119:SER:OG	2.02	0.76
1:B:66:CR2:HD1	1:B:222:GLU:OE2	1.89	0.73

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1099:GLN:NE2	1:B:214:LYS:O[3_664]	2.00	0.20
1:A:164:ASN:OD1	1:A:215:ARG:NH1[2_545]	2.13	0.07

### 5.3 Torsion angles [i](#)

#### 5.3.1 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 X-ray entries followed by that with respect to entries of similar resolution.

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	304/309 (98%)	288 (95%)	15 (5%)	1 (0%)	41	72
1	B	304/309 (98%)	284 (93%)	19 (6%)	1 (0%)	41	72
All	All	608/618 (98%)	572 (94%)	34 (6%)	2 (0%)	41	72

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	1088	ASP
1	A	1113	ALA

#### 5.3.2 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 X-ray entries followed by that with respect to entries of similar resolution.

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	263/264 (100%)	218 (83%)	45 (17%)	2	6
1	B	263/264 (100%)	221 (84%)	42 (16%)	2	7
All	All	526/528 (100%)	439 (84%)	87 (16%)	2	7

5 of 87 residues with a non-rotameric sidechain are listed below:



Mol	Chain	Res	Type
1	B	129	ASP
1	B	208	SER
1	B	141	LEU
1	B	170	ASN
1	B	1081	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 7 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1093	ASN
1	B	80	GLN
1	B	198	ASN
1	B	81	HIS
1	A	185	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or 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 length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
1	CR2	B	66	1	20,20,21	6.30	6 (30%)	25,27,29	4.36	8 (32%)
1	CR2	A	66	1	20,20,21	6.68	5 (25%)	25,27,29	3.41	6 (24%)

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. '2' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	CR2	B	66	1	-	2/6/25/26	0/2/2/2
1	CR2	A	66	1	-	3/6/25/26	0/2/2/2

The worst 5 of 11 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	66	CR2	CB2-CA2	26.01	1.56	1.35
1	B	66	CR2	CB2-CA2	24.38	1.55	1.35
1	A	66	CR2	O2-C2	11.90	1.48	1.23
1	B	66	CR2	O2-C2	10.53	1.45	1.23
1	B	66	CR2	CA2-C2	-7.92	1.40	1.48

The worst 5 of 14 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	66	CR2	CA2-C2-N3	13.27	109.64	103.37
1	A	66	CR2	O2-C2-CA2	-11.11	124.72	130.96
1	B	66	CR2	O2-C2-CA2	-10.71	124.94	130.96
1	A	66	CR2	CA2-C2-N3	8.54	107.41	103.37
1	B	66	CR2	CG2-CB2-CA2	-6.83	121.58	129.94

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	66	CR2	N2-CA2-CB2-CG2
1	A	66	CR2	C2-CA2-CB2-CG2
1	B	66	CR2	C2-CA2-CB2-CG2
1	B	66	CR2	N2-CA2-CB2-CG2
1	A	66	CR2	C3-CA3-N3-C2

There are no ring outliers.

2 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	B	66	CR2	6	0
1	A	66	CR2	1	0

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	308/309 (99%)	-0.29	6 (1%) 66 59	42, 66, 138, 174	0
1	B	308/309 (99%)	-0.09	9 (2%) 51 41	56, 104, 164, 190	0
All	All	616/618 (99%)	-0.19	15 (2%) 59 49	42, 84, 152, 190	0

The worst 5 of 15 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	1144	GLY	6.1
1	B	1138	LEU	5.6
1	A	1120	GLY	3.8
1	A	1068	ILE	3.5
1	B	1142	GLN	3.5

### 6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q < 0.9’ lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
1	CR2	A	66	19/20	0.89	0.23	39,52,76,93	0
1	CR2	B	66	19/20	0.94	0.23	70,77,88,89	0

### 6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 6.4 Ligands

There are no ligands in this entry.

## 6.5 Other polymers

There are no such residues in this entry.