



# wwPDB X-ray Structure Validation Summary Report

Jun 17, 2024 – 08:05 AM EDT

PDB ID : 5NBT  
Title : Apo structure of p60N/p80C katanin  
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Deposited on : 2017-03-02  
Resolution : 2.40 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  
Xtriage (Phenix) : 1.13  
EDS : 2.37.1  
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) : 2.37.1

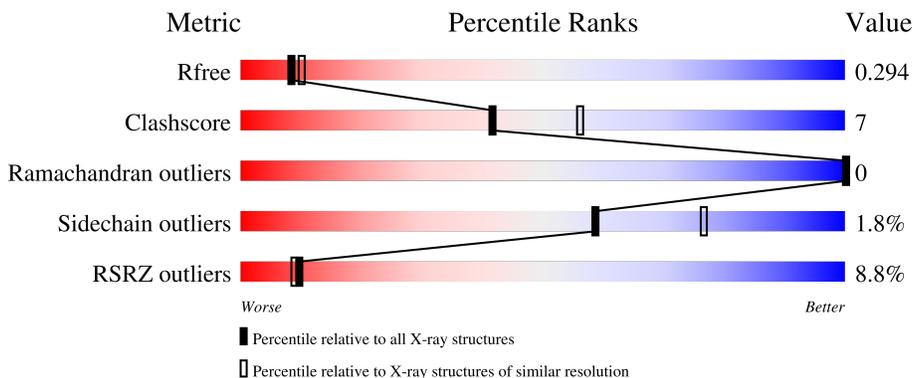
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.40 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	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (2.40-2.40)

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	212	 4% 61% 7% 28%
1	C	212	 4% 55% 15% 26%
2	B	80	 10% 66% 15% 9%
2	D	80	 15% 65% 21% 14%

## 2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 3532 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 Katanin p80 WD40 repeat-containing subunit B1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	146	1153	734	200	212	7	0	0	0
1	C	151	1188	755	208	218	7	0	0	0

There are 68 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	447	MET	-	initiating methionine	UNP Q8BG40
A	448	GLY	-	expression tag	UNP Q8BG40
A	449	SER	-	expression tag	UNP Q8BG40
A	450	SER	-	expression tag	UNP Q8BG40
A	451	HIS	-	expression tag	UNP Q8BG40
A	452	HIS	-	expression tag	UNP Q8BG40
A	453	HIS	-	expression tag	UNP Q8BG40
A	454	HIS	-	expression tag	UNP Q8BG40
A	455	HIS	-	expression tag	UNP Q8BG40
A	456	HIS	-	expression tag	UNP Q8BG40
A	457	SER	-	expression tag	UNP Q8BG40
A	458	SER	-	expression tag	UNP Q8BG40
A	459	GLY	-	expression tag	UNP Q8BG40
A	460	LEU	-	expression tag	UNP Q8BG40
A	461	VAL	-	expression tag	UNP Q8BG40
A	462	PRO	-	expression tag	UNP Q8BG40
A	463	ARG	-	expression tag	UNP Q8BG40
A	464	GLY	-	expression tag	UNP Q8BG40
A	465	SER	-	expression tag	UNP Q8BG40
A	466	HIS	-	expression tag	UNP Q8BG40
A	467	MET	-	expression tag	UNP Q8BG40
A	468	ALA	-	expression tag	UNP Q8BG40
A	469	SER	-	expression tag	UNP Q8BG40
A	470	MET	-	expression tag	UNP Q8BG40
A	471	THR	-	expression tag	UNP Q8BG40

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Chain	Residue	Modelled	Actual	Comment	Reference
A	472	GLY	-	expression tag	UNP Q8BG40
A	473	GLY	-	expression tag	UNP Q8BG40
A	474	GLN	-	expression tag	UNP Q8BG40
A	475	GLN	-	expression tag	UNP Q8BG40
A	476	MET	-	expression tag	UNP Q8BG40
A	477	GLY	-	expression tag	UNP Q8BG40
A	478	ARG	-	expression tag	UNP Q8BG40
A	479	GLY	-	expression tag	UNP Q8BG40
A	480	SER	-	expression tag	UNP Q8BG40
C	447	MET	-	initiating methionine	UNP Q8BG40
C	448	GLY	-	expression tag	UNP Q8BG40
C	449	SER	-	expression tag	UNP Q8BG40
C	450	SER	-	expression tag	UNP Q8BG40
C	451	HIS	-	expression tag	UNP Q8BG40
C	452	HIS	-	expression tag	UNP Q8BG40
C	453	HIS	-	expression tag	UNP Q8BG40
C	454	HIS	-	expression tag	UNP Q8BG40
C	455	HIS	-	expression tag	UNP Q8BG40
C	456	HIS	-	expression tag	UNP Q8BG40
C	457	SER	-	expression tag	UNP Q8BG40
C	458	SER	-	expression tag	UNP Q8BG40
C	459	GLY	-	expression tag	UNP Q8BG40
C	460	LEU	-	expression tag	UNP Q8BG40
C	461	VAL	-	expression tag	UNP Q8BG40
C	462	PRO	-	expression tag	UNP Q8BG40
C	463	ARG	-	expression tag	UNP Q8BG40
C	464	GLY	-	expression tag	UNP Q8BG40
C	465	SER	-	expression tag	UNP Q8BG40
C	466	HIS	-	expression tag	UNP Q8BG40
C	467	MET	-	expression tag	UNP Q8BG40
C	468	ALA	-	expression tag	UNP Q8BG40
C	469	SER	-	expression tag	UNP Q8BG40
C	470	MET	-	expression tag	UNP Q8BG40
C	471	THR	-	expression tag	UNP Q8BG40
C	472	GLY	-	expression tag	UNP Q8BG40
C	473	GLY	-	expression tag	UNP Q8BG40
C	474	GLN	-	expression tag	UNP Q8BG40
C	475	GLN	-	expression tag	UNP Q8BG40
C	476	MET	-	expression tag	UNP Q8BG40
C	477	GLY	-	expression tag	UNP Q8BG40
C	478	ARG	-	expression tag	UNP Q8BG40
C	479	GLY	-	expression tag	UNP Q8BG40

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Chain	Residue	Modelled	Actual	Comment	Reference
C	480	SER	-	expression tag	UNP Q8BG40

- Molecule 2 is a protein called Katanin p60 ATPase-containing subunit A1.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace	
2	B	65	Total	C	N	O	S	0	0	0
			542	348	90	100	4			
2	D	69	Total	C	N	O	S	0	0	0
			575	368	96	107	4			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-1	MET	-	initiating methionine	UNP Q9WV86
B	0	GLY	-	expression tag	UNP Q9WV86
B	40	PRO	LEU	conflict	UNP Q9WV86
D	-1	MET	-	initiating methionine	UNP Q9WV86
D	0	GLY	-	expression tag	UNP Q9WV86
D	40	PRO	LEU	conflict	UNP Q9WV86

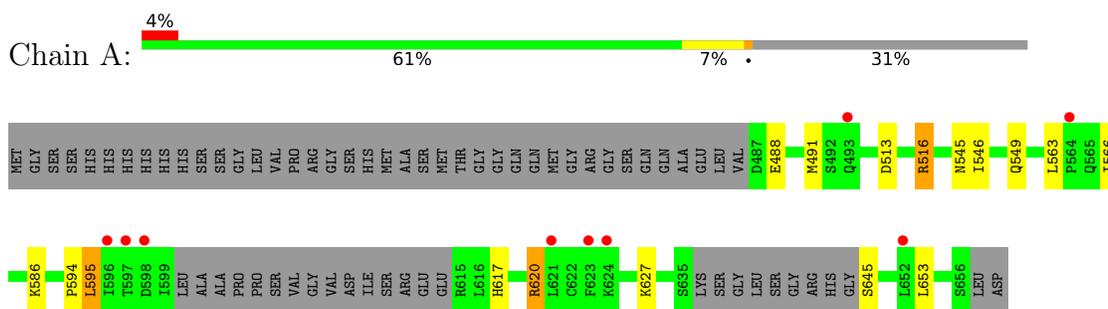
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	24	Total	O	0	0
			24	24		
3	B	8	Total	O	0	0
			8	8		
3	C	36	Total	O	0	0
			36	36		
3	D	6	Total	O	0	0
			6	6		

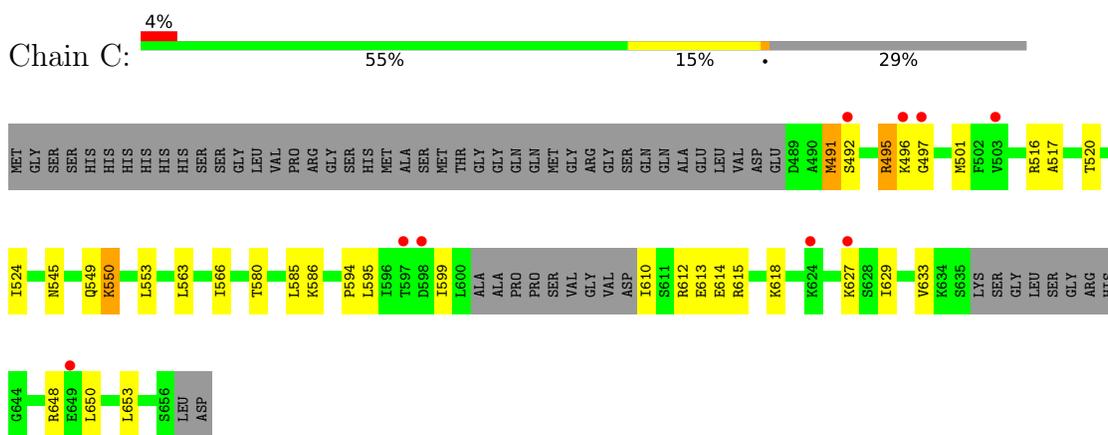
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-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. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

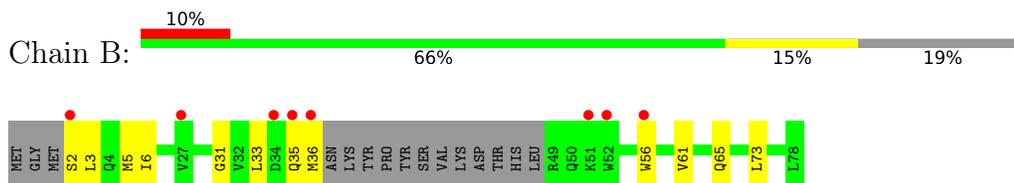
- Molecule 1: Katanin p80 WD40 repeat-containing subunit B1



- Molecule 1: Katanin p80 WD40 repeat-containing subunit B1



- Molecule 2: Katanin p60 ATPase-containing subunit A1



- Molecule 2: Katanin p60 ATPase-containing subunit A1





## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	146.14Å 37.76Å 103.09Å 90.00° 93.37° 90.00°	Depositor
Resolution (Å)	43.26 – 2.40 43.26 – 2.40	Depositor EDS
% Data completeness (in resolution range)	99.8 (43.26-2.40) 99.9 (43.26-2.40)	Depositor EDS
$R_{merge}$	0.17	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.32 (at 2.39Å)	Xtrriage
Refinement program	PHENIX (1.10.1_2155: ???)	Depositor
R, $R_{free}$	0.244 , 0.294 0.245 , 0.294	Depositor DCC
$R_{free}$ test set	1126 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	48.0	Xtrriage
Anisotropy	0.428	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 59.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	3532	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	64.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 11.56% 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](#)

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	0.27	0/1166	0.43	0/1572
1	C	0.27	0/1201	0.42	0/1618
2	B	0.26	0/549	0.38	0/736
2	D	0.26	0/583	0.38	0/783
All	All	0.27	0/3499	0.41	0/4709

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 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	1153	0	1214	12	0
1	C	1188	0	1250	25	0
2	B	542	0	548	8	0
2	D	575	0	577	10	0
3	A	24	0	0	1	0
3	B	8	0	0	0	0
3	C	36	0	0	2	0
3	D	6	0	0	0	0
All	All	3532	0	3589	49	0

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 7.

The worst 5 of 49 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:C:550:LYS:HG2	1:C:553:LEU:HG	1.71	0.73
1:C:545:ASN:O	1:C:549:GLN:NE2	2.24	0.70
1:A:545:ASN:O	1:A:549:GLN:NE2	2.27	0.66
1:A:594:PRO:O	1:A:595:LEU:HB3	1.97	0.63
1:A:620:ARG:NH1	1:C:613:GLU:OE2	2.32	0.62

There are no symmetry-related clashes.

## 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	140/212 (66%)	138 (99%)	2 (1%)	0	100	100
1	C	145/212 (68%)	143 (99%)	2 (1%)	0	100	100
2	B	61/80 (76%)	61 (100%)	0	0	100	100
2	D	65/80 (81%)	64 (98%)	1 (2%)	0	100	100
All	All	411/584 (70%)	406 (99%)	5 (1%)	0	100	100

There are no Ramachandran outliers to report.

### 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	135/186 (73%)	132 (98%)	3 (2%)	52	71
1	C	138/186 (74%)	134 (97%)	4 (3%)	42	62
2	B	59/73 (81%)	59 (100%)	0	100	100
2	D	63/73 (86%)	63 (100%)	0	100	100
All	All	395/518 (76%)	388 (98%)	7 (2%)	59	76

5 of 7 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	491	MET
1	C	495	ARG
1	C	648	ARG
1	C	550	LYS
1	A	620	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
2	D	53	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 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	146/212 (68%)	0.64	9 (6%) 20 19	35, 56, 91, 111	0
1	C	151/212 (71%)	0.67	9 (5%) 21 20	37, 59, 95, 114	0
2	B	65/80 (81%)	0.85	8 (12%) 4 3	40, 63, 99, 117	0
2	D	69/80 (86%)	0.97	12 (17%) 1 1	43, 66, 109, 132	0
All	All	431/584 (73%)	0.74	38 (8%) 10 9	35, 60, 99, 132	0

The worst 5 of 38 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	27	VAL	4.3
2	D	2	SER	4.2
1	C	496	LYS	4.1
2	D	54	GLN	3.6
2	B	34	ASP	3.3

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

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

### 6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

### 6.4 Ligands [i](#)

There are no ligands in this entry.

## 6.5 Other polymers [i](#)

There are no such residues in this entry.