



# Full wwPDB X-ray Structure Validation Report ⓘ

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PDB ID : 9I8K / pdb\_00009i8k  
Title : Beta-catenin armadillo (150-663)  
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Deposited on : 2025-02-05  
Resolution : 2.00 Å(reported)

This is a Full wwPDB X-ray Structure Validation 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	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

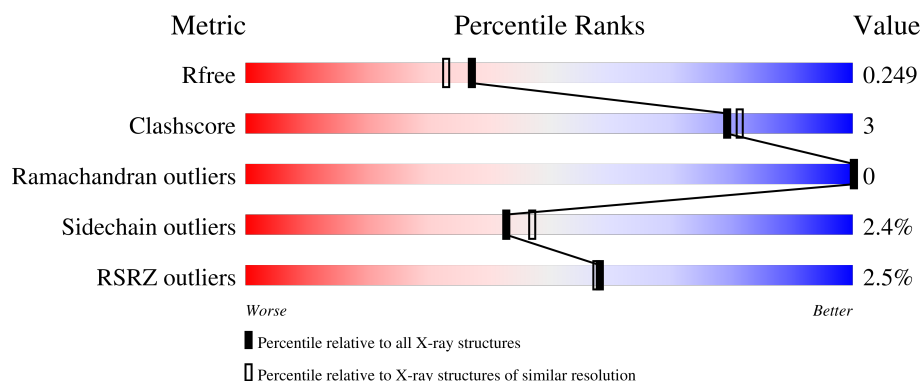
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.00 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))
$R_{free}$	180053	10052 (2.00-2.00)
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (2.00-2.00)

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	514	<div> <div>2%</div> <div> <div></div> <div>90%</div> <div>8%</div> <div>.</div> </div> </div>
1	B	514	<div> <div>3%</div> <div> <div></div> <div>88%</div> <div>9%</div> <div>..</div> </div> </div>

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 8023 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 Catenin beta-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	504	Total	C	N	O	S	0	0	0
			3847	2418	700	703	26			
1	B	504	Total	C	N	O	S	0	2	0
			3863	2428	704	704	27			

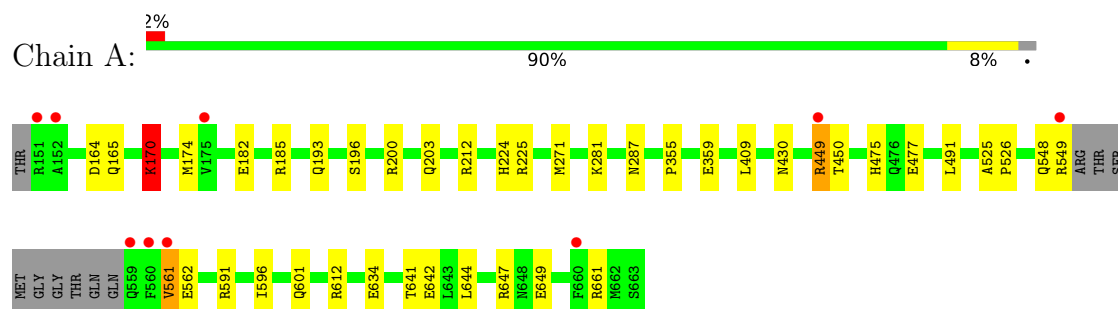
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	159	Total	O	0	0
			159	159		
2	B	154	Total	O	0	0
			154	154		

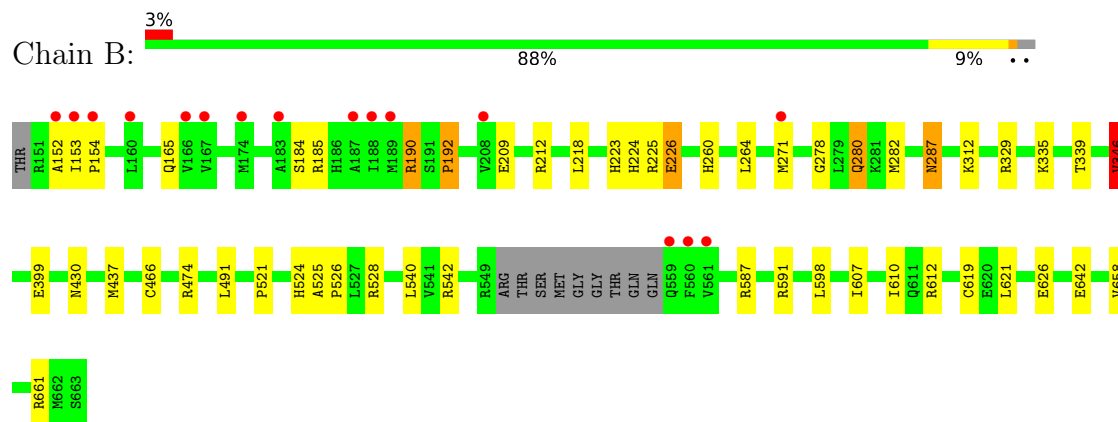
### 3 Residue-property plots

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: Catenin beta-1



#### • Molecule 1: Catenin beta-1



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	84.02Å 205.06Å 64.74Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.00 – 2.00 47.00 – 2.00	Depositor EDS
% Data completeness (in resolution range)	99.3 (47.00-2.00) 99.5 (47.00-2.00)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.20 (at 2.00Å)	Xtriage
Refinement program	REFMAC 5.8.0425	Depositor
R, $R_{free}$	0.202 , 0.239 0.211 , 0.249	Depositor DCC
$R_{free}$ test set	2101 reflections (2.75%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	33.1	Xtriage
Anisotropy	0.134	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 27.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	8023	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 41.31 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 2.4054e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<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

### 5.1 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 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	0.59	0/3901	1.08	7/5291 (0.1%)
1	B	0.60	0/3920	1.06	5/5315 (0.1%)
All	All	0.59	0/7821	1.07	12/10606 (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	6
1	B	0	6
All	All	0	12

There are no bond length outliers.

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	649	GLU	CB-CA-C	-6.08	100.70	110.79
1	B	346	VAL	N-CA-CB	-5.71	103.33	110.47
1	B	152	ALA	CA-C-N	5.66	123.81	120.24
1	B	152	ALA	C-N-CA	5.66	123.81	120.24
1	A	170	LYS	N-CA-CB	5.60	118.96	110.28
1	B	466	CYS	CB-CA-C	-5.60	101.50	110.79
1	A	271	MET	CG-SD-CE	5.59	113.19	100.90
1	A	649	GLU	N-CA-CB	5.47	118.17	110.12
1	B	626	GLU	CB-CA-C	5.40	121.03	110.67
1	A	561	VAL	N-CA-CB	5.35	117.47	111.21
1	A	164	ASP	CA-CB-CG	5.20	117.80	112.60
1	A	281	LYS	N-CA-CB	5.15	117.53	110.07

There are no chirality outliers.

All (12) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	212	ARG	Sidechain
1	A	225	ARG	Sidechain
1	A	449	ARG	Sidechain
1	A	549	ARG	Sidechain
1	A	591	ARG	Sidechain
1	A	612	ARG	Sidechain
1	B	329	ARG	Sidechain
1	B	474	ARG	Sidechain
1	B	528	ARG	Sidechain
1	B	542	ARG	Sidechain
1	B	591	ARG	Sidechain
1	B	612	ARG	Sidechain

## 5.2 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 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	3847	0	3996	19	0
1	B	3863	0	4017	24	0
2	A	159	0	0	2	0
2	B	154	0	0	3	0
All	All	8023	0	8013	43	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 3.

All (43) 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:280:GLN:HE21	1:B:280:GLN:H	1.28	0.80
1:B:209:GLU:OE2	1:B:212:ARG:NH1	2.21	0.74
1:A:642:GLU:OE1	2:A:701:HOH:O	2.05	0.74
1:A:165:GLN:OE1	2:A:702:HOH:O	2.11	0.68
1:B:335:LYS:O	1:B:339:THR:HG23	1.99	0.63
1:A:641:THR:O	1:A:644:LEU:HB2	2.02	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:312:LYS:HE2	1:B:346:VAL:HG13	1.87	0.57
1:A:196:SER:OG	1:A:200:ARG:NH2	2.40	0.55
1:A:185:ARG:HD3	1:A:224:HIS:CE1	2.41	0.55
1:A:475:HIS:CE1	1:A:477:GLU:HB2	2.43	0.54
1:A:185:ARG:CD	1:A:224:HIS:CE1	2.91	0.53
1:B:540:LEU:HG	1:B:598:LEU:HD21	1.91	0.53
1:B:619:CYS:HA	1:B:658:VAL:HG22	1.92	0.52
1:A:548:GLN:NE2	1:A:601:GLN:OE1	2.45	0.50
1:A:491:LEU:CD1	1:A:526:PRO:HB2	2.42	0.50
1:B:190:ARG:O	1:B:192:PRO:HD3	2.11	0.50
1:B:619:CYS:O	1:B:661:ARG:NH1	2.44	0.49
1:B:642:GLU:OE2	2:B:701:HOH:O	2.20	0.49
1:B:339:THR:HG22	2:B:779:HOH:O	2.12	0.49
1:B:223:HIS:CE1	2:B:799:HOH:O	2.65	0.48
1:B:587:ARG:HG2	1:B:621:LEU:HD23	1.94	0.48
1:B:607:ILE:HD12	1:B:610:ILE:HD12	1.95	0.48
1:A:647:ARG:HH11	1:A:647:ARG:HG3	1.80	0.47
1:B:525:ALA:HB3	1:B:526:PRO:HD3	1.96	0.47
1:B:278:GLY:O	1:B:282:MET:HG3	2.15	0.47
1:B:491:LEU:CD1	1:B:526:PRO:HB2	2.45	0.46
1:B:224:HIS:HB3	1:B:226:GLU:OE2	2.16	0.46
1:B:287:ASN:HD22	1:B:287:ASN:H	1.63	0.46
1:B:521:PRO:HA	1:B:524:HIS:CE1	2.51	0.45
1:A:525:ALA:HB3	1:A:526:PRO:HD3	1.99	0.44
1:B:153:ILE:N	1:B:154:PRO:CD	2.81	0.43
1:B:399:GLU:HB3	1:B:437:MET:HE2	1.99	0.43
1:A:596:ILE:HG22	1:A:634:GLU:HG3	2.01	0.42
1:A:561:VAL:HG12	1:A:562:GLU:HG3	2.02	0.42
1:B:271[A]:MET:HE3	1:B:271[A]:MET:HB2	1.73	0.42
1:A:185:ARG:HD2	1:A:224:HIS:CE1	2.55	0.42
1:B:260:HIS:CE1	1:B:264:LEU:HD11	2.54	0.42
1:A:355:PRO:O	1:A:359:GLU:HG2	2.21	0.41
1:B:185:ARG:HD2	1:B:224:HIS:CE1	2.55	0.41
1:A:409:LEU:HB3	1:A:450:THR:OG1	2.20	0.41
1:A:170:LYS:HB3	1:A:170:LYS:HE2	1.90	0.40
1:A:491:LEU:HD13	1:A:526:PRO:HB2	2.02	0.40
1:A:525:ALA:N	1:A:526:PRO:CD	2.84	0.40

There are no symmetry-related clashes.



## 5.3 Torsion angles

### 5.3.1 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 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	500/514 (97%)	497 (99%)	3 (1%)	0	100	100
1	B	502/514 (98%)	497 (99%)	5 (1%)	0	100	100
All	All	1002/1028 (98%)	994 (99%)	8 (1%)	0	100	100

There are no Ramachandran outliers to report.

### 5.3.2 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 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	418/426 (98%)	409 (98%)	9 (2%)	45	50
1	B	420/426 (99%)	409 (97%)	11 (3%)	40	44
All	All	838/852 (98%)	818 (98%)	20 (2%)	43	47

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	170	LYS
1	A	174	MET
1	A	182	GLU
1	A	193	GLN
1	A	203	GLN
1	A	287	ASN
1	A	430	ASN
1	A	449	ARG

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Mol	Chain	Res	Type
1	A	661	ARG
1	B	165	GLN
1	B	184	SER
1	B	190	ARG
1	B	192	PRO
1	B	218	LEU
1	B	225	ARG
1	B	226	GLU
1	B	280	GLN
1	B	287	ASN
1	B	346	VAL
1	B	430	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	193	GLN
1	A	224	HIS
1	A	265	HIS
1	A	266	GLN
1	A	287	ASN
1	A	322	GLN
1	A	326	ASN
1	A	380	ASN
1	A	470	HIS
1	A	476	GLN
1	A	499	HIS
1	B	224	HIS
1	B	280	GLN
1	B	287	ASN
1	B	379	GLN
1	B	407	GLN
1	B	415	ASN
1	B	440	GLN

### 5.3.3 RNA ⓘ

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 oligosaccharides 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

### 6.1 Protein, DNA and RNA chains

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	504/514 (98%)	0.06	9 (1%) 67 67	22, 34, 56, 81	0
1	B	504/514 (98%)	0.14	16 (3%) 50 49	16, 33, 66, 96	2 (0%)
All	All	1008/1028 (98%)	0.10	25 (2%) 58 58	16, 33, 62, 96	2 (0%)

All (25) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	271[A]	MET	3.8
1	B	560	PHE	3.3
1	B	154	PRO	2.9
1	B	559	GLN	2.8
1	B	208	VAL	2.7
1	A	152	ALA	2.7
1	A	549	ARG	2.6
1	A	151	ARG	2.5
1	B	152	ALA	2.4
1	B	561	VAL	2.4
1	B	183	ALA	2.4
1	B	187	ALA	2.4
1	A	559	GLN	2.4
1	A	561	VAL	2.3
1	B	174	MET	2.3
1	A	560	PHE	2.3
1	B	167	VAL	2.2
1	B	189	MET	2.2
1	A	175	VAL	2.1
1	B	188	ILE	2.1
1	B	166	VAL	2.1
1	B	153	ILE	2.1
1	A	660	PHE	2.1
1	B	160	LEU	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	449	ARG	2.0

## 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 oligosaccharides 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.