



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 7, 2026 – 03:44 AM UTC

PDB ID : 4HM9 / pdb_00004hm9
Title : Crystal structure of full-length human catenin-beta-like 1
Authors : Du, Z.; Huang, X.; Wang, G.; Wu, Y.
Deposited on : 2012-10-18
Resolution : 3.10 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

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>.

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

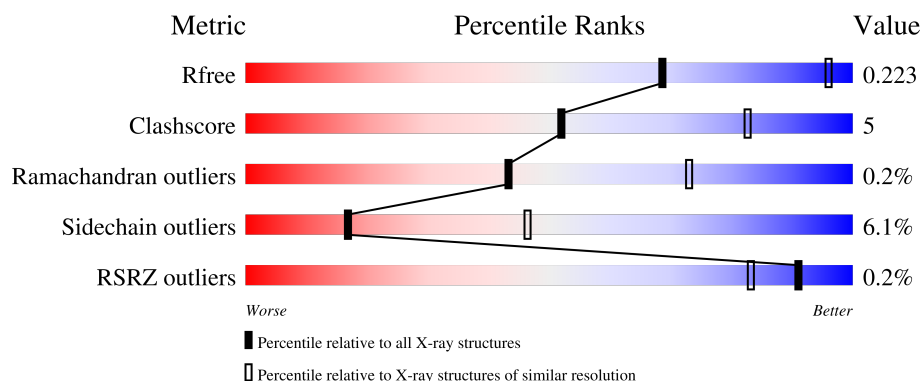
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.10 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	1456 (3.10-3.10)
Clashscore	190562	1539 (3.10-3.10)
Ramachandran outliers	187476	1467 (3.10-3.10)
Sidechain outliers	187428	1467 (3.10-3.10)
RSRZ outliers	180081	1456 (3.10-3.10)

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 ≥ 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	568	 74% 15% 10%

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 4117 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 Beta-catenin-like protein 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	511	Total	C	N	O	S	0	0	0
			4117	2574	717	799	27			

There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-4	GLY	-	expression tag	UNP Q8WYA6
A	-3	PRO	-	expression tag	UNP Q8WYA6
A	-2	SER	-	expression tag	UNP Q8WYA6
A	-1	SER	-	expression tag	UNP Q8WYA6
A	0	PRO	-	expression tag	UNP Q8WYA6

i

- Molecule 1: Beta-catenin-like protein 1

GLY	PRO	SER	SER	MET	ASP	VAL	GLY	GLU	LEU	SER	THR	GLN	PRO	ASN	ARG	GLY	THR	LYS	ARG	ASP	GLU	GLU	GLU	GLN	MET	ARG	LYS	GLN	THR	THR	ARG	GLU	ARG	GLY	TYR	ARG	GLU	GLU	MET	THR	VAL	VAL	E50	D55	L60	D61																																																																				
																																															K395	V396	G397	E405	L415	L418	L426	M442	R485	V492	M500	A501	E502	M505	A506	M507	V508	R512	V515	L519	I526	R530	E535	I540	E547	M551	I556	E561	M562	F563	A181	E182	L183	I184	I185	D186	V193	R203	E210	G214	V222	M225	R229	M232	C233	T234	L241	L242	D256	L270	D274	E275	M276	R277	L280	E305	C318	M339	I343	K355	E365	I376	L377	G378	L379	K392	I393	V394
																																															I62	I63	R65	E68	E69	E70	GLU	GLU	GLU	E74	E75	P76	L77	D78	E79	R82	R100	F103	N106	P107	E108	K109	M110	M111	S112	E114	L115	D116	I121	A128	D132	L133	L136	L137	V138	H152	T155	I159	A160	V161	L168	I171	F178																									

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	48.99Å 116.36Å 137.40Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	42.62 – 3.10 42.62 – 3.10	Depositor EDS
% Data completeness (in resolution range)	98.6 (42.62-3.10) 97.7 (42.62-3.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.24	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.54 (at 3.12Å)	Xtriage
Refinement program	PHENIX 1.8_1069	Depositor
R, R_{free}	0.174 , 0.225 0.176 , 0.223	Depositor DCC
R_{free} test set	892 reflections (5.99%)	wwPDB-VP
Wilson B-factor (Å ²)	61.0	Xtriage
Anisotropy	0.273	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 22.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	4117	wwPDB-VP
Average B, all atoms (Å ²)	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.88% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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	0.28	0/4168	0.72	2/5600 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	508	VAL	CA-C-N	5.27	124.90	119.05
1	A	508	VAL	C-N-CA	5.27	124.90	119.05

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	4117	0	4139	42	0
All	All	4117	0	4139	42	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 5.

All (42) 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:A:62:ILE:HG23	1:A:65:ARG:HH12	1.53	0.72

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:92:ARG:HD3	1:A:116:ASP:HB3	1.81	0.63
1:A:415:LEU:HB3	1:A:502:GLU:HG2	1.82	0.62
1:A:186:ASP:OD1	1:A:229:ARG:NH2	2.35	0.59
1:A:152:HIS:O	1:A:203:ARG:NH2	2.34	0.59
1:A:485:ARG:NH2	1:A:535:GLU:OE2	2.34	0.57
1:A:274:ASP:HA	1:A:277:ARG:HD2	1.87	0.56
1:A:256:ASP:OD1	1:A:256:ASP:N	2.39	0.56
1:A:392:LYS:NZ	1:A:397:GLY:O	2.38	0.54
1:A:159:ILE:HD12	1:A:214:GLY:HA3	1.90	0.53
1:A:405:GLU:HG3	1:A:492:VAL:HG22	1.93	0.49
1:A:132:ASP:OD1	1:A:132:ASP:N	2.45	0.49
1:A:547:GLU:O	1:A:551:ASN:ND2	2.46	0.48
1:A:75:GLU:CD	1:A:76:PRO:HD2	2.39	0.48
1:A:512:ARG:NE	1:A:563:PHE:O	2.45	0.47
1:A:121:ILE:HD13	1:A:161:VAL:HG12	1.96	0.47
1:A:128:ALA:HB2	1:A:168:LEU:HD23	1.95	0.47
1:A:547:GLU:H	1:A:547:GLU:HG3	1.42	0.46
1:A:270:LEU:HD11	1:A:280:LEU:HD13	1.99	0.44
1:A:242:LEU:HD21	1:A:280:LEU:HD12	1.99	0.44
1:A:234:THR:HG23	1:A:275:GLU:HG2	2.00	0.43
1:A:418:LEU:HD12	1:A:426:LEU:HD22	2.00	0.43
1:A:100:ARG:NH1	1:A:114:GLU:OE2	2.49	0.43
1:A:185:ILE:HG21	1:A:229:ARG:HG3	1.99	0.43
1:A:181:ALA:O	1:A:185:ILE:HG12	2.19	0.43
1:A:365:GLU:H	1:A:365:GLU:CD	2.26	0.43
1:A:442:MET:HE1	1:A:500:MET:HG3	2.01	0.42
1:A:442:MET:HE3	1:A:515:VAL:HG22	2.00	0.42
1:A:222:VAL:HG11	1:A:241:LEU:HD22	2.02	0.42
1:A:519:LEU:HD23	1:A:519:LEU:HA	1.85	0.41
1:A:540:ILE:HD12	1:A:556:ILE:HD11	2.02	0.41
1:A:107:PRO:HA	1:A:110:PHE:CZ	2.56	0.41
1:A:171:ILE:HD13	1:A:171:ILE:HA	1.95	0.41
1:A:60:LEU:HD23	1:A:63:ILE:HD11	2.03	0.40
1:A:225:MET:HE2	1:A:232:MET:HE1	2.03	0.40
1:A:55:ASP:OD1	1:A:55:ASP:N	2.54	0.40
1:A:318:CYS:SG	1:A:355:LYS:HE3	2.62	0.40
1:A:103:PHE:HB3	1:A:106:ASN:HB2	2.04	0.40
1:A:138:VAL:HG21	1:A:183:VAL:HG22	2.04	0.40
1:A:155:THR:O	1:A:159:ILE:HG12	2.21	0.40
1:A:133:LEU:HB3	1:A:136:LEU:HD12	2.03	0.40
1:A:526:ILE:O	1:A:530:ARG:HG3	2.21	0.40

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	507/568 (89%)	496 (98%)	10 (2%)	1 (0%)	43 73

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	376	ILE

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	462/514 (90%)	434 (94%)	28 (6%)	17 46

All (28) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	68	GLU
1	A	77	LEU
1	A	79	GLU
1	A	108	GLU
1	A	111	MET
1	A	112	GLU
1	A	132	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	155	THR
1	A	161	VAL
1	A	171	ILE
1	A	178	GLU
1	A	193	VAL
1	A	210	GLU
1	A	222	VAL
1	A	229	ARG
1	A	305	GLU
1	A	339	MET
1	A	348	ILE
1	A	377	LEU
1	A	379	LEU
1	A	394	LYS
1	A	396	VAL
1	A	492	VAL
1	A	505	ASN
1	A	507	ASN
1	A	540	ILE
1	A	547	GLU
1	A	561	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	125	HIS
1	A	292	GLN
1	A	340	ASN
1	A	505	ASN
1	A	507	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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 [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, 95th 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 ²)	Q<0.9
1	A	511/568 (89%)	-0.74	1 (0%) 91 83	6, 24, 65, 111	0

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	396	VAL	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.