



Full wwPDB X-ray Structure Validation Report ⓘ

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PDB ID : 6O3E / pdb_00006o3e
Title : mouse aE-catenin 82-883
Authors : Pokutta, S.; Weis, W.I.
Deposited on : 2019-02-26
Resolution : 4.00 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

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

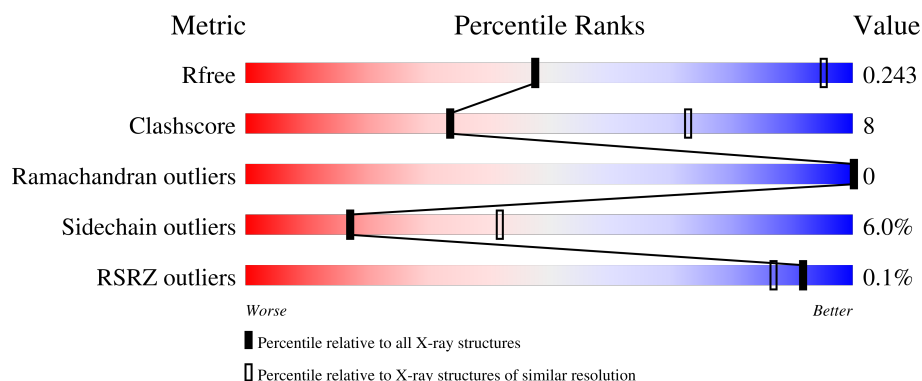
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 4.00 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	1082 (4.20-3.80)
Clashscore	190562	1129 (4.20-3.80)
Ramachandran outliers	187476	1064 (4.20-3.80)
Sidechain outliers	187428	1055 (4.20-3.80)
RSRZ outliers	180081	1082 (4.20-3.80)

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 ≥ 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	806	
1	B	806	

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 8070 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 alpha-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	536	Total	C	N	O	S	0	0	0
			4004	2485	707	793	19			
1	B	541	Total	C	N	O	S	0	0	0
			4066	2515	724	807	20			

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	78	GLY	-	expression tag	UNP P26231
A	79	GLY	-	expression tag	UNP P26231
A	80	ILE	-	expression tag	UNP P26231
A	81	LEU	-	expression tag	UNP P26231
A	116	SER	CYS	engineered mutation	UNP P26231
B	78	GLY	-	expression tag	UNP P26231
B	79	GLY	-	expression tag	UNP P26231
B	80	ILE	-	expression tag	UNP P26231
B	81	LEU	-	expression tag	UNP P26231
B	116	SER	CYS	engineered mutation	UNP P26231

[illegible]

4 Data and refinement statistics

Property	Value	Source
Space group	P 32	Depositor
Cell constants a, b, c, α , β , γ	145.26Å 145.26Å 136.27Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	19.97 – 4.00 19.97 – 4.00	Depositor EDS
% Data completeness (in resolution range)	97.8 (19.97-4.00) 97.1 (19.97-4.00)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.40 (at 4.07Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.213 , 0.243 0.215 , 0.243	Depositor DCC
R_{free} test set	1324 reflections (4.88%)	wwPDB-VP
Wilson B-factor (Å ²)	200.8	Xtriage
Anisotropy	0.288	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.22 , 127.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.039 for -h,-k,l 0.053 for h,-h-k,-l 0.036 for -k,-h,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	8070	wwPDB-VP
Average B, all atoms (Å ²)	209.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.63% 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	0.15	0/4043	0.34	0/5486
1	B	0.15	0/4105	0.33	0/5566
All	All	0.15	0/8148	0.34	0/11052

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	4004	0	3922	71	0
1	B	4066	0	3988	55	0
All	All	8070	0	7910	123	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 8.

All (123) 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:376:ARG:HE	1:B:380:ARG:HH11	1.24	0.84
1:B:319:MET:HE2	1:B:436:LEU:HB3	1.70	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:584:MET:HE1	1:A:618:VAL:HG23	1.70	0.72
1:B:195:GLN:HB2	1:B:207:MET:HG2	1.72	0.71
1:A:104:MET:HE3	1:A:128:ALA:HB2	1.74	0.69
1:A:387:MET:HE1	1:A:506:THR:HB	1.74	0.69
1:B:563:TYR:OH	1:B:633:ARG:NH2	2.29	0.65
1:B:278:LEU:HD13	1:B:439:SER:HB3	1.78	0.64
1:A:243:LEU:HD21	1:A:462:PRO:HB2	1.81	0.61
1:A:467:ALA:HB2	1:A:487:PHE:HD2	1.66	0.60
1:A:509:ASP:N	1:A:509:ASP:OD1	2.33	0.60
1:A:530:LEU:HD12	1:A:538:LEU:HD21	1.85	0.59
1:B:387:MET:HA	1:B:387:MET:HE2	1.86	0.58
1:A:160:GLY:HA3	1:A:180:LEU:HD11	1.88	0.56
1:A:530:LEU:HD21	1:A:608:GLU:HG2	1.86	0.56
1:B:389:HIS:HB3	1:B:433:VAL:HG13	1.86	0.56
1:B:509:ASP:OD1	1:B:509:ASP:N	2.38	0.55
1:A:592:GLU:HA	1:A:595:VAL:HG22	1.89	0.55
1:B:309:LEU:O	1:B:313:ILE:HG12	2.06	0.55
1:B:503:ASP:OD1	1:B:551:ARG:NH2	2.40	0.54
1:B:577:LYS:HA	1:B:580:SER:HB3	1.90	0.54
1:B:220:ILE:HG22	1:B:244:ILE:HG12	1.89	0.54
1:B:512:LEU:HD13	1:B:626:ARG:HA	1.90	0.54
1:B:379:ARG:O	1:B:383:ARG:HG3	2.09	0.53
1:A:511:PHE:HZ	1:A:551:ARG:HG3	1.73	0.53
1:A:542:ALA:HB2	1:A:591:VAL:HG21	1.89	0.53
1:A:135:VAL:HG11	1:B:131:LEU:HD21	1.91	0.53
1:B:218:VAL:HB	1:B:219:PRO:HD3	1.92	0.51
1:B:169:ASN:ND2	1:B:172:ASP:H	2.08	0.51
1:A:523:VAL:HG13	1:A:615:SER:HB3	1.93	0.51
1:A:401:LEU:HD22	1:A:491:TRP:CD1	2.46	0.50
1:B:150:LEU:HD11	1:B:191:ALA:HA	1.93	0.50
1:B:457:LEU:HD12	1:B:494:GLN:HB3	1.94	0.50
1:A:397:THR:HB	1:A:495:VAL:HG11	1.94	0.50
1:A:399:VAL:O	1:A:403:VAL:HG23	2.12	0.50
1:A:568:TYR:OH	1:A:629:VAL:O	2.27	0.50
1:B:538:LEU:HD11	1:B:611:PHE:CZ	2.47	0.49
1:A:579:LEU:HG	1:A:584:MET:HE2	1.95	0.49
1:A:478:LYS:O	1:A:481:GLN:NE2	2.46	0.49
1:B:478:LYS:O	1:B:482:GLU:HG2	2.14	0.48
1:B:319:MET:HE1	1:B:440:ILE:HG23	1.94	0.48
1:A:225:SER:HA	1:A:241:ARG:HD3	1.96	0.47
1:A:394:PHE:HD2	1:A:499:THR:HG23	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:412:ASN:N	1:A:412:ASN:OD1	2.46	0.47
1:A:478:LYS:HA	1:A:481:GLN:HE22	1.78	0.47
1:A:320:ALA:HB2	1:A:333:ILE:HG21	1.95	0.47
1:A:332:ARG:HD2	1:A:332:ARG:HA	1.50	0.47
1:A:387:MET:HE3	1:A:510:ASP:HB2	1.96	0.47
1:B:438:CYS:SG	1:B:447:VAL:HG13	2.55	0.47
1:A:372:THR:HA	1:A:375:THR:HG22	1.95	0.46
1:A:578:LEU:O	1:A:582:THR:HB	2.16	0.46
1:B:289:ILE:HG22	1:B:305:LEU:HD13	1.96	0.46
1:B:169:ASN:HD22	1:B:171:GLN:H	1.63	0.46
1:A:466:ASN:HA	1:A:469:LEU:HB2	1.98	0.46
1:B:309:LEU:HD11	1:B:340:VAL:HG13	1.98	0.46
1:B:634:THR:H	1:B:635:PRO:HD2	1.80	0.46
1:A:471:LEU:HD11	1:A:480:ALA:O	2.16	0.46
1:B:161:ILE:HD11	1:B:218:VAL:HG22	1.97	0.46
1:A:508:ILE:O	1:A:512:LEU:HG	2.15	0.46
1:A:309:LEU:HD11	1:A:340:VAL:HG13	1.98	0.45
1:B:579:LEU:HD12	1:B:621:GLY:HA3	1.98	0.45
1:A:319:MET:HE3	1:A:319:MET:HB2	1.86	0.45
1:A:394:PHE:HE1	1:A:433:VAL:HG11	1.81	0.45
1:B:399:VAL:H	1:B:400:PRO:HD2	1.81	0.45
1:B:546:ARG:HA	1:B:584:MET:HE2	1.99	0.45
1:A:309:LEU:O	1:A:313:ILE:HG12	2.16	0.45
1:A:582:THR:O	1:A:586:ARG:HG2	2.17	0.45
1:A:320:ALA:HB1	1:A:330:ARG:HB2	2.00	0.44
1:B:471:LEU:HA	1:B:480:ALA:HB1	2.00	0.44
1:A:419:TYR:HA	1:A:422:VAL:HG12	1.98	0.44
1:B:583:VAL:HG13	1:B:617:LEU:HG	2.00	0.44
1:A:620:ASP:O	1:A:624:ASP:HB2	2.18	0.44
1:A:286:ASP:OD1	1:A:375:THR:HG21	2.18	0.44
1:A:313:ILE:HG13	1:A:341:ARG:HH11	1.82	0.43
1:A:350:GLU:HG3	1:A:367:ALA:HB2	2.00	0.43
1:B:373:LYS:HD3	1:B:373:LYS:HA	1.68	0.43
1:B:161:ILE:HD13	1:B:180:LEU:HD21	1.99	0.43
1:A:615:SER:O	1:A:618:VAL:HG12	2.18	0.43
1:B:387:MET:HG3	1:B:510:ASP:HB3	2.00	0.43
1:B:530:LEU:HD13	1:B:611:PHE:CD2	2.54	0.43
1:A:88:GLU:H	1:A:88:GLU:HG2	1.61	0.43
1:A:285:PHE:HZ	1:A:344:LEU:HD12	1.84	0.43
1:A:386:VAL:O	1:A:390:VAL:HG23	2.19	0.43
1:A:467:ALA:HB2	1:A:487:PHE:CD2	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:496:ARG:HD2	1:A:554:HIS:NE2	2.34	0.43
1:A:104:MET:HA	1:A:127:ALA:HB1	2.01	0.42
1:A:313:ILE:HG13	1:A:341:ARG:NH1	2.33	0.42
1:B:494:GLN:HA	1:B:497:VAL:HG12	2.01	0.42
1:A:347:LEU:HD11	1:A:368:ILE:HG12	2.01	0.42
1:A:583:VAL:HG13	1:A:617:LEU:HB3	2.01	0.42
1:B:160:GLY:HA3	1:B:180:LEU:HD13	2.02	0.42
1:A:131:LEU:O	1:A:135:VAL:HG13	2.20	0.42
1:B:505:ILE:HG23	1:B:506:THR:HG23	2.01	0.42
1:A:292:ASP:OD2	1:A:295:SER:OG	2.26	0.42
1:A:626:ARG:O	1:A:630:LEU:HG	2.19	0.42
1:A:285:PHE:O	1:A:289:ILE:HG23	2.20	0.42
1:B:230:GLN:C	1:B:232:PRO:HD3	2.44	0.42
1:A:128:ALA:HB3	1:B:139:LEU:HD21	2.00	0.42
1:B:401:LEU:O	1:B:405:ILE:HG23	2.20	0.42
1:A:106:SER:O	1:A:110:GLU:HG2	2.19	0.41
1:A:132:LEU:HB2	1:B:135:VAL:HG11	2.02	0.41
1:A:471:LEU:HD13	1:A:484:MET:HE2	2.02	0.41
1:A:549:ALA:HB1	1:A:584:MET:HE3	2.01	0.41
1:B:528:ILE:HD13	1:B:528:ILE:HA	1.85	0.41
1:A:169:ASN:HB2	1:A:172:ASP:H	1.84	0.41
1:B:451:ARG:HA	1:B:451:ARG:HD2	1.89	0.41
1:A:461:CYS:HB3	1:A:462:PRO:HD3	2.03	0.41
1:B:305:LEU:HD23	1:B:305:LEU:HA	1.84	0.41
1:A:240:ASN:HA	1:A:466:ASN:HD22	1.84	0.41
1:A:309:LEU:HB2	1:A:344:LEU:HD13	2.03	0.41
1:B:213:ILE:HD13	1:B:213:ILE:HA	1.95	0.41
1:A:90:LEU:O	1:A:94:VAL:HG23	2.20	0.41
1:B:390:VAL:O	1:B:394:PHE:HB2	2.21	0.41
1:B:402:LEU:HA	1:B:405:ILE:HG12	2.03	0.41
1:B:91:VAL:O	1:B:94:VAL:HG12	2.20	0.41
1:B:309:LEU:HD22	1:B:344:LEU:HD22	2.03	0.41
1:B:319:MET:HE3	1:B:319:MET:HB2	1.82	0.41
1:A:511:PHE:CE2	1:A:555:VAL:HG11	2.55	0.41
1:A:595:VAL:O	1:A:599:SER:HB3	2.21	0.40
1:A:566:GLY:H	1:A:569:THR:HB	1.86	0.40
1:B:395:LEU:HD11	1:B:548:ARG:HG3	2.03	0.40
1:A:302:ARG:N	1:A:303:PRO:HD2	2.37	0.40
1:B:207:MET:HE1	1:B:259:ALA:HB2	2.03	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	530/806 (66%)	508 (96%)	22 (4%)	0	100	100
1	B	535/806 (66%)	511 (96%)	24 (4%)	0	100	100
All	All	1065/1612 (66%)	1019 (96%)	46 (4%)	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	413/675 (61%)	390 (94%)	23 (6%)	19	43
1	B	422/675 (62%)	395 (94%)	27 (6%)	16	40
All	All	835/1350 (62%)	785 (94%)	50 (6%)	17	42

All (50) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	103	LEU
1	A	144	MET
1	A	146	ASP
1	A	175	ILE
1	A	180	LEU
1	A	207	MET
1	A	214	LEU
1	A	284	ASN

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Mol	Chain	Res	Type
1	A	332	ARG
1	A	365	ASN
1	A	395	LEU
1	A	404	LEU
1	A	412	ASN
1	A	442	ASN
1	A	481	GLN
1	A	490	GLN
1	A	509	ASP
1	A	510	ASP
1	A	515	SER
1	A	518	HIS
1	A	535	VAL
1	A	548	ARG
1	A	572	VAL
1	B	119	VAL
1	B	131	LEU
1	B	150	LEU
1	B	153	GLN
1	B	169	ASN
1	B	243	LEU
1	B	248	LEU
1	B	277	GLU
1	B	311	SER
1	B	312	ILE
1	B	318	LEU
1	B	368	ILE
1	B	378	LEU
1	B	386	VAL
1	B	440	ILE
1	B	461	CYS
1	B	469	LEU
1	B	483	ASN
1	B	509	ASP
1	B	515	SER
1	B	519	ILE
1	B	528	ILE
1	B	530	LEU
1	B	535	VAL
1	B	541	THR
1	B	548	ARG
1	B	558	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	217	ASN
1	A	230	GLN
1	A	283	ASN
1	A	354	ASN
1	A	456	GLN
1	A	466	ASN
1	A	481	GLN
1	A	483	ASN
1	A	490	GLN
1	B	169	ASN
1	B	230	GLN
1	B	284	ASN
1	B	381	GLN
1	B	481	GLN
1	B	490	GLN
1	B	554	HIS

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 ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

There are no ligands in this entry.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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	536/806 (66%)	-0.14	1 (0%) 91 81	153, 204, 280, 494	0
1	B	541/806 (67%)	-0.10	0 100 100	147, 202, 269, 461	0
All	All	1077/1612 (66%)	-0.12	1 (0%) 92 87	147, 203, 273, 494	0

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	363	ALA	2.5

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.