



wwPDB X-ray Structure Validation Summary Report ⓘ

Sep 10, 2023 – 10:05 AM EDT

PDB ID : 4K1N
Title : Crystal structure of full-length mouse alphaE-catenin
Authors : Ishiyama, N.; Ikura, M.
Deposited on : 2013-04-05
Resolution : 6.50 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

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 : 4.02b-467
Xtriage (Phenix) : 1.13
EDS : 2.35.1
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) : 2.35.1

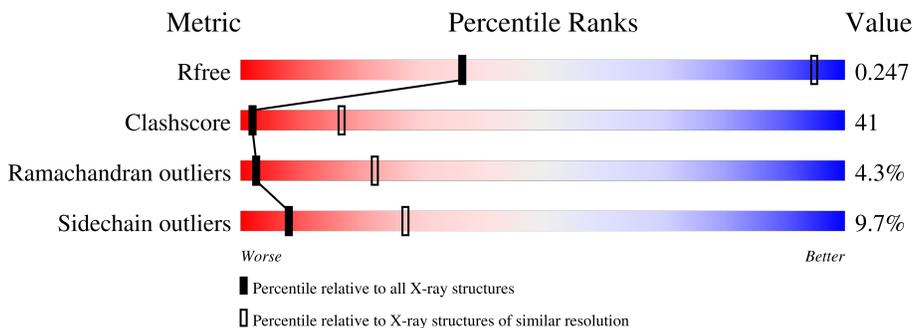
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 6.50 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	1000 (9.00-3.90)
Clashscore	141614	1064 (9.00-3.90)
Ramachandran outliers	138981	1012 (9.00-3.88)
Sidechain outliers	138945	1010 (9.00-3.84)

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 $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	A	912	 25% 28% . . 43%
1	B	912	 25% 28% . . 43%

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 8020 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
			Total	C	N	O	S			
1	A	520	4010	2486	713	789	22	0	0	0
1	B	520	4010	2486	713	789	22	0	0	0

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-5	GLY	-	expression tag	UNP P26231
A	-4	SER	-	expression tag	UNP P26231
A	-3	HIS	-	expression tag	UNP P26231
A	-2	MET	-	expression tag	UNP P26231
A	-1	ALA	-	expression tag	UNP P26231
A	0	SER	-	expression tag	UNP P26231
B	-5	GLY	-	expression tag	UNP P26231
B	-4	SER	-	expression tag	UNP P26231
B	-3	HIS	-	expression tag	UNP P26231
B	-2	MET	-	expression tag	UNP P26231
B	-1	ALA	-	expression tag	UNP P26231
B	0	SER	-	expression tag	UNP P26231

4 Data and refinement statistics

Property	Value	Source
Space group	P 32	Depositor
Cell constants a, b, c, α , β , γ	144.68Å 144.68Å 136.76Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	50.00 – 6.50 47.36 – 6.40	Depositor EDS
% Data completeness (in resolution range)	94.6 (50.00-6.50) 94.2 (47.36-6.40)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.13	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.84 (at 6.67Å)	Xtrriage
Refinement program	CNS	Depositor
R, R_{free}	0.224 , 0.247 0.224 , 0.247	Depositor DCC
R_{free} test set	716 reflections (10.90%)	wwPDB-VP
Wilson B-factor (Å ²)	439.2	Xtrriage
Anisotropy	0.055	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 357.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	0.032 for -h,-k,l 0.051 for h,-h-k,-l 0.023 for -k,-h,-l	Xtrriage
F_o, F_c correlation	0.86	EDS
Total number of atoms	8020	wwPDB-VP
Average B, all atoms (Å ²)	354.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.57% 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	0.22	0/4048	0.46	0/5464
1	B	0.22	0/4048	0.46	0/5464
All	All	0.22	0/8096	0.46	0/10928

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	4010	0	4051	336	0
1	B	4010	0	4051	346	0
All	All	8020	0	8102	666	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 41.

The worst 5 of 666 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:369:ASP:O	1:A:373:LYS:HB3	1.65	0.97
1:A:149:LYS:HG2	1:A:190:MET:HE1	1.47	0.96

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:104:MET:HG2	1:A:131:LEU:HD22	1.48	0.96
1:B:86:LEU:HD22	1:B:87:LYS:H	1.31	0.95
1:B:104:MET:HG2	1:B:131:LEU:HD22	1.48	0.93

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	516/912 (57%)	444 (86%)	49 (10%)	23 (4%)	2	22
1	B	516/912 (57%)	447 (87%)	48 (9%)	21 (4%)	3	23
All	All	1032/1824 (57%)	891 (86%)	97 (9%)	44 (4%)	2	22

5 of 44 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	86	LEU
1	A	291	VAL
1	A	292	ASP
1	A	301	PHE
1	A	393	SER

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	431/766 (56%)	390 (90%)	41 (10%)	8	28
1	B	431/766 (56%)	388 (90%)	43 (10%)	7	26
All	All	862/1532 (56%)	778 (90%)	84 (10%)	8	27

5 of 84 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	347	LEU
1	B	440	ILE
1	B	357	ARG
1	B	399	VAL
1	B	508	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 21 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	226	GLN
1	B	435	ASN
1	B	494	GLN
1	B	456	GLN
1	B	354	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](#)

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

6.1 Protein, DNA and RNA chains

Unable to reproduce the depositors R factor - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains

Unable to reproduce the depositors R factor - this section is therefore empty.

6.3 Carbohydrates

Unable to reproduce the depositors R factor - this section is therefore empty.

6.4 Ligands

Unable to reproduce the depositors R factor - this section is therefore empty.

6.5 Other polymers

Unable to reproduce the depositors R factor - this section is therefore empty.