



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 05:57 PM GMT

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
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

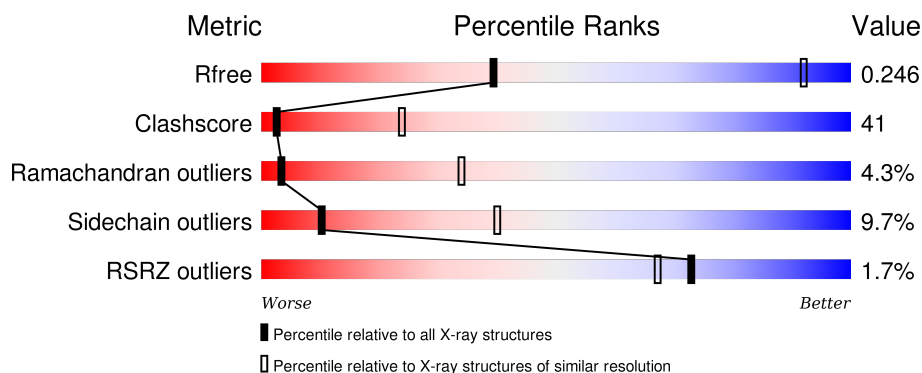
1 Overall quality at a glance

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}	91344	1012 (9.00-3.66)
Clashscore	102246	1060 (9.00-3.70)
Ramachandran outliers	100387	1033 (9.00-3.66)
Sidechain outliers	100360	1004 (9.00-3.66)
RSRZ outliers	91569	1011 (9.00-3.66)

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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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	912	<div> <div></div> <div> <div></div> <div>25%</div> <div>28%</div> <div>• •</div> <div>43%</div> </div> </div>
1	B	912	<div> <div></div> <div> <div></div> <div>25%</div> <div>28%</div> <div>• •</div> <div>43%</div> </div> </div>

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.

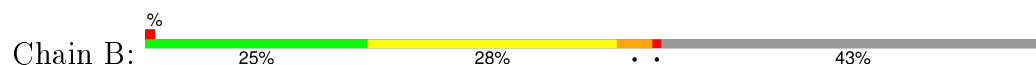
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	520	Total	C	N	O	S	0	0	0
			4010	2486	713	789	22			
1	B	520	Total	C	N	O	S	0	0	0
			4010	2486	713	789	22			

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

LYS ILE LYS ARG ALA SER GLN LYS LYS HIS VAL ASN PRO VAL GLN ALA LEU SER GLU PHE LYS ALA MET ASP SER ILE

- Molecule 1: Catenin alpha-1



ASP	SER	ALA	ALA	MET	SER	LEU	ILE	GLN	ALA	ALA	LYS	ASN	LEU	MET	ASN	VAL	VAL	GLN	THR	VAL	LYS	VAL	ALA	ALA	SER	TYR	VAL	ALA	ALA	SER	THR	LYS	TYR	GLN	LYS	SER	SER	GLN	GLY	MET	ALA	SER	SER	VAL	ASN	LEU	PRO	ALA	ALA	VAL	TRP	LYS	MET	LYS	LYS	PRO	PRO	LEU	VAL	VAL	LYS	ASP
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GLU	LYS	GLN	ASP	GLU	THR	GLN	THR	LYS	ILE	LYS	ARG	ALA	SER	GLN	LYS	LYS	HIS	VAL	ASN	PRO	VAL	GLN	ALA	LEU	SER	GLU	PHE	LYS	ALA	MET	ASP	SER	ILE
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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)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.224 , 0.247 0.224 , 0.246	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å ²)	439.2	Xtriage
Anisotropy	0.055	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 357.9	EDS
Estimated twinning fraction	0.032 for -h,-k,l 0.051 for h,-h-k,-l 0.023 for -k,-h,-l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 6569 reflections	Xtriage
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

Xtriage'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.*

¹ Intensities estimated from amplitudes.

² Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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	0.22	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

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%)	3	33
1	B	516/912 (57%)	447 (87%)	48 (9%)	21 (4%)	3	35
All	All	1032/1824 (57%)	891 (86%)	97 (9%)	44 (4%)	3	34

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%)	11	41
1	B	431/766 (56%)	388 (90%)	43 (10%)	9	38
All	All	862/1532 (56%)	778 (90%)	84 (10%)	10	40

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

Mol	Chain	Res	Type
1	A	584	MET
1	B	141	LEU
1	B	539	ASP
1	A	598	LEU
1	B	86	LEU

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

Mol	Chain	Res	Type
1	A	463	GLN
1	B	203	ASN
1	B	435	ASN
1	A	456	GLN
1	B	456	GLN

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 carbohydrates in this entry.

5.6 Ligand geometry ⓘ

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	520/912 (57%)	0.28	9 (1%) 73 67	355, 355, 355, 355	0
1	B	520/912 (57%)	0.21	9 (1%) 73 67	355, 355, 355, 355	0
All	All	1040/1824 (57%)	0.25	18 (1%) 73 67	355, 355, 355, 355	0

The worst 5 of 18 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	300	ARG	3.9
1	A	470	ALA	3.3
1	B	300	ARG	3.3
1	A	415	GLU	3.0
1	B	348	LEU	2.8

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 carbohydrates 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.