



Full wwPDB X-ray Structure Validation Report ⓘ

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PDB ID : 4ONS
Title : Structural and thermodynamic characterization of cadherin-beta-catenin-alp
ha-catenincomplex formation
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Deposited on : 2014-01-29
Resolution : 2.80 Å(reported)

This is a full wwPDB validation 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/ValidationPDFNotes.html>

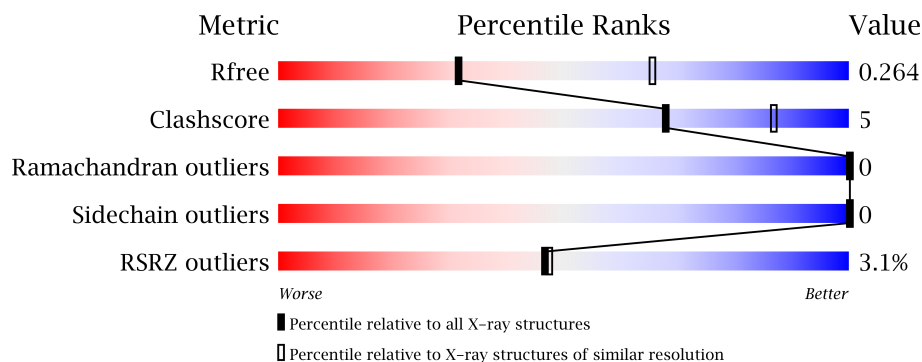
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.16 November 2013
Xtriage (Phenix) : dev-1439
EDS : stable22978
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22978

1 Overall quality at a glance

The reported resolution of this entry is 2.80 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}	66092	1799 (2.80-2.80)
Clashscore	79885	2295 (2.80-2.80)
Ramachandran outliers	78287	2252 (2.80-2.80)
Sidechain outliers	78261	2254 (2.80-2.80)
RSRZ outliers	66119	1802 (2.80-2.80)

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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	248	
1	C	248	
2	B	88	
2	D	88	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 4318 atoms, of which 0 are hydrogen and 0 are deuterium.

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-2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	230	Total	C	N	O	S	0	0	0
			1782	1104	328	341	9			
1	C	205	Total	C	N	O	S	0	0	0
			1590	990	291	302	7			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	17	MET	-	EXPRESSION TAG	UNP Q61301
C	17	MET	-	EXPRESSION TAG	UNP Q61301

- Molecule 2 is a protein called Catenin beta-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	56	Total	C	N	O	S	0	0	0
			443	277	82	81	3			
2	D	61	Total	C	N	O	S	0	0	0
			481	298	88	91	4			

There are 28 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	64	MET	-	EXPRESSION TAG	UNP Q02248
B	65	GLY	-	EXPRESSION TAG	UNP Q02248
B	66	SER	-	EXPRESSION TAG	UNP Q02248
B	67	SER	-	EXPRESSION TAG	UNP Q02248
B	68	HIS	-	EXPRESSION TAG	UNP Q02248
B	69	HIS	-	EXPRESSION TAG	UNP Q02248
B	70	HIS	-	EXPRESSION TAG	UNP Q02248
B	71	HIS	-	EXPRESSION TAG	UNP Q02248
B	72	HIS	-	EXPRESSION TAG	UNP Q02248
B	73	HIS	-	EXPRESSION TAG	UNP Q02248

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Chain	Residue	Modelled	Actual	Comment	Reference
B	74	SER	-	EXPRESSION TAG	UNP Q02248
B	75	GLN	-	EXPRESSION TAG	UNP Q02248
B	76	ASP	-	EXPRESSION TAG	UNP Q02248
B	77	PRO	-	EXPRESSION TAG	UNP Q02248
D	64	MET	-	EXPRESSION TAG	UNP Q02248
D	65	GLY	-	EXPRESSION TAG	UNP Q02248
D	66	SER	-	EXPRESSION TAG	UNP Q02248
D	67	SER	-	EXPRESSION TAG	UNP Q02248
D	68	HIS	-	EXPRESSION TAG	UNP Q02248
D	69	HIS	-	EXPRESSION TAG	UNP Q02248
D	70	HIS	-	EXPRESSION TAG	UNP Q02248
D	71	HIS	-	EXPRESSION TAG	UNP Q02248
D	72	HIS	-	EXPRESSION TAG	UNP Q02248
D	73	HIS	-	EXPRESSION TAG	UNP Q02248
D	74	SER	-	EXPRESSION TAG	UNP Q02248
D	75	GLN	-	EXPRESSION TAG	UNP Q02248
D	76	ASP	-	EXPRESSION TAG	UNP Q02248
D	77	PRO	-	EXPRESSION TAG	UNP Q02248

- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	10	Total O 10 10	0	0
3	B	6	Total O 6 6	0	0
3	C	3	Total O 3 3	0	0
3	D	3	Total O 3 3	0	0

4 Data and refinement statistics

Property	Value	Source
Space group	P 31	Depositor
Cell constants a, b, c, α , β , γ	96.12Å 96.12Å 65.52Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	38.75 – 2.80 38.75 – 2.80	Depositor EDS
% Data completeness (in resolution range)	96.7 (38.75-2.80) 96.7 (38.75-2.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.46 (at 2.81Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.4.1496)	Depositor
R, R_{free}	0.203 , 0.264 0.203 , 0.264	Depositor DCC
R_{free} test set	1146 reflections (7.11%)	DCC
Wilson B-factor (Å ²)	60.4	Xtriage
Anisotropy	0.523	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 38.9	EDS
Estimated twinning fraction	0.022 for -h,-k,l 0.046 for h,-h-k,-l 0.022 for -k,-h,-l	Xtriage
L-test for twinning	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 16528 reflections	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	4318	wwPDB-VP
Average B, all atoms (Å ²)	79.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.96% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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	0/1796	0.36	0/2413
1	C	0.22	0/1598	0.36	0/2141
2	B	0.25	0/451	0.38	0/611
2	D	0.23	0/490	0.38	0/664
All	All	0.22	0/4335	0.36	0/5829

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1782	0	0	8	0
1	C	1590	0	0	10	0
2	B	443	0	0	5	0
2	D	481	0	0	1	0
3	A	10	0	0	0	0
3	B	6	0	0	0	0
3	C	3	0	0	1	0
3	D	3	0	0	0	0
All	All	4318	0	0	21	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 5.

All (21) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:134:HIS:O	2:B:138:ASN:ND2	2.30	0.65
1:A:101:GLU:OE1	1:A:104:ARG:NH1	2.31	0.64
1:A:188:TYR:OH	1:A:192:ARG:NH1	2.33	0.61
1:A:212:ALA:O	1:A:216:ASN:ND2	2.33	0.61
1:A:21:THR:OG1	1:A:136:ARG:NH1	2.35	0.60
1:C:88:GLU:OE2	1:C:136:ARG:NH2	2.37	0.56
2:B:85:GLN:O	2:B:89:THR:OG1	2.24	0.54
1:C:171:ASP:O	1:C:175:ARG:N	2.40	0.54
1:C:54:SER:OG	2:D:142:TYR:OH	2.28	0.51
1:C:33:THR:O	1:C:37:THR:OG1	2.29	0.51
2:B:130:GLN:O	2:B:134:HIS:ND1	2.44	0.50
1:C:212:ALA:O	1:C:216:ASN:ND2	2.45	0.49
1:A:194:GLN:OE1	1:A:210:ARG:NH2	2.46	0.48
1:C:239:ASN:ND2	3:C:301:HOH:O	2.47	0.47
1:A:245:LYS:NZ	1:A:246:GLN:OE1	2.48	0.46
1:A:54:SER:OG	2:B:142:TYR:OH	2.34	0.46
1:C:123:MET:O	1:C:127:ALA:N	2.49	0.46
1:C:215:LYS:O	1:C:218:THR:OG1	2.37	0.43
1:A:142:ASP:OD1	2:B:93:ARG:NE	2.52	0.43
1:C:83:GLN:OE1	1:C:148:ARG:NH1	2.52	0.41
1:C:247:VAL:O	1:C:251:ILE:N	2.53	0.41

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	224/248 (90%)	221 (99%)	3 (1%)	0	100	100
1	C	195/248 (79%)	194 (100%)	1 (0%)	0	100	100
2	B	52/88 (59%)	52 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	D	59/88 (67%)	57 (97%)	2 (3%)	0	100	100
All	All	530/672 (79%)	524 (99%)	6 (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	187/203 (92%)	187 (100%)	0	100	100
1	C	167/203 (82%)	167 (100%)	0	100	100
2	B	47/74 (64%)	47 (100%)	0	100	100
2	D	51/74 (69%)	51 (100%)	0	100	100
All	All	452/554 (82%)	452 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA ⓘ

There are no RNA chains 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 ⓘ

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 ⓘ

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, 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	230/248 (92%)	-0.12	1 (0%) 90 91	30, 69, 111, 146	3 (1%)
1	C	205/248 (82%)	0.30	15 (7%) 15 13	32, 84, 175, 185	3 (1%)
2	B	56/88 (63%)	-0.25	0 100 100	33, 51, 88, 97	0
2	D	61/88 (69%)	-0.02	1 (1%) 68 69	36, 56, 112, 141	0
All	All	552/672 (82%)	0.04	17 (3%) 47 47	30, 70, 163, 185	6 (1%)

All (17) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	244	PHE	5.5
2	D	105	GLU	5.5
1	C	242	TYR	4.7
1	C	212	ALA	4.5
1	C	252	ALA	4.4
1	C	219	MET	4.3
1	C	211	GLY	3.7
1	C	258	ALA	3.6
1	C	241	ASP	3.2
1	A	198	LYS	3.0
1	C	215	LYS	2.9
1	C	237	ARG	2.6
1	C	176	PHE	2.6
1	C	227	PHE	2.5
1	C	248	GLN	2.4
1	C	214	LYS	2.1
1	C	245	LYS	2.0

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

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

There are no ligands in this entry.

6.5 Other polymers ⓘ

There are no such residues in this entry.