Full wwPDB X-ray Structure Validation Report ⓘ

Oct 2, 2023 – 02:48 AM EDT

PDB ID	:	6N2E
Title	:	Crystal Structure of Human Protocadherin-15 EC1-3 G16D N369D Q370N and Mouse Cadherin-23 EC1-2 T15E
Authors	:	Choudhary, D.; De-la-Torre, P.; Sotomayor, M.
Deposited on	:	2018-11-12
Resolution	:	2.90 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	:	FAILED
Xtriage (Phenix)	:	1.13
EDS	:	FAILED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
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 (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 Å.

There are no overall percentile quality scores available for this entry.

MolProbity and EDS failed to run properly - the sequence quality summary graphics cannot be shown.

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 8779 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 Protocadherin-15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	352	Total	C	N	O	S	0	0	0
			2805	1769	479	546	11			
1	B	365	Total	C	N	O	S	0	0	0
			2899	1826	495	567	11			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	MET	-	initiating methionine	UNP A0A087X1T6
A	16	ASP	GLY	engineered mutation	UNP A0A087X1T6
A	369	ASP	ASN	engineered mutation	UNP A0A087X1T6
A	370	ASN	GLN	engineered mutation	UNP A0A087X1T6
A	371	LEU	-	expression tag	UNP A0A087X1T6
A	372	GLU	-	expression tag	UNP A0A087X1T6
A	373	HIS	-	expression tag	UNP A0A087X1T6
A	374	HIS	-	expression tag	UNP A0A087X1T6
A	375	HIS	-	expression tag	UNP A0A087X1T6
A	376	HIS	-	expression tag	UNP A0A087X1T6
A	377	HIS	-	expression tag	UNP A0A087X1T6
A	378	HIS	-	expression tag	UNP A0A087X1T6
B	0	MET	-	initiating methionine	UNP A0A087X1T6
B	16	ASP	GLY	engineered mutation	UNP A0A087X1T6
B	369	ASP	ASN	engineered mutation	UNP A0A087X1T6
B	370	ASN	GLN	engineered mutation	UNP A0A087X1T6
B	371	LEU	-	expression tag	UNP A0A087X1T6
B	372	GLU	-	expression tag	UNP A0A087X1T6
B	373	HIS	-	expression tag	UNP A0A087X1T6
B	374	HIS	-	expression tag	UNP A0A087X1T6
B	375	HIS	-	expression tag	UNP A0A087X1T6
B	376	HIS	-	expression tag	UNP A0A087X1T6
B	377	HIS	-	expression tag	UNP A0A087X1T6
B	378	HIS	-	expression tag	UNP A0A087X1T6

- Molecule 2 is a protein called Cadherin-23.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	193	Total	C	N	O	S	0	0	0
			1507	956	249	301	1			
2	D	189	Total	C	N	O	S	0	0	0
			1488	945	246	296	1			

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	0	MET	-	initiating methionine	UNP Q99PF4
C	15	GLU	THR	engineered mutation	UNP Q99PF4
C	206	LEU	-	expression tag	UNP Q99PF4
C	207	GLU	-	expression tag	UNP Q99PF4
C	208	HIS	-	expression tag	UNP Q99PF4
C	209	HIS	-	expression tag	UNP Q99PF4
C	210	HIS	-	expression tag	UNP Q99PF4
C	211	HIS	-	expression tag	UNP Q99PF4
C	212	HIS	-	expression tag	UNP Q99PF4
C	213	HIS	-	expression tag	UNP Q99PF4
D	0	MET	-	initiating methionine	UNP Q99PF4
D	15	GLU	THR	engineered mutation	UNP Q99PF4
D	206	LEU	-	expression tag	UNP Q99PF4
D	207	GLU	-	expression tag	UNP Q99PF4
D	208	HIS	-	expression tag	UNP Q99PF4
D	209	HIS	-	expression tag	UNP Q99PF4
D	210	HIS	-	expression tag	UNP Q99PF4
D	211	HIS	-	expression tag	UNP Q99PF4
D	212	HIS	-	expression tag	UNP Q99PF4
D	213	HIS	-	expression tag	UNP Q99PF4

- Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	5	Total	Ca	0	0
			5	5		
3	B	5	Total	Ca	0	0
			5	5		
3	C	4	Total	Ca	0	0
			4	4		
3	D	4	Total	Ca	0	0
			4	4		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	28	Total O 28 28	0	0
4	B	32	Total O 32 32	0	0
4	C	1	Total O 1 1	0	0
4	D	1	Total O 1 1	0	0

MolProbity and EDS failed to run properly - this section is therefore empty.

3 Data and refinement statistics (i)

EDS failed to run properly - this section is therefore incomplete.

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	76.79Å 65.40Å 190.01Å 90.00° 99.12° 90.00°	Depositor
Resolution (Å)	49.52 – 2.90	Depositor
% Data completeness (in resolution range)	92.4 (49.52-2.90)	Depositor
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.57 (at 2.91Å)	Xtriage
Refinement program	REFMAC 5.8.0238	Depositor
R, R_{free}	0.225 , 0.253	Depositor
Wilson B-factor (Å^2)	51.9	Xtriage
Anisotropy	0.512	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	0.028 for h,-k,-h-l	Xtriage
Total number of atoms	8779	wwPDB-VP
Average B, all atoms (Å^2)	82.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.79% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

4 Model quality

4.1 Standard geometry

MolProbity failed to run properly - this section is therefore empty.

4.2 Too-close contacts

MolProbity failed to run properly - this section is therefore empty.

4.3 Torsion angles

4.3.1 Protein backbone

MolProbity failed to run properly - this section is therefore empty.

4.3.2 Protein sidechains

MolProbity failed to run properly - this section is therefore empty.

4.3.3 RNA

MolProbity failed to run properly - this section is therefore empty.

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

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

4.5 Carbohydrates

There are no monosaccharides in this entry.

4.6 Ligand geometry

Of 18 ligands modelled in this entry, 18 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

4.7 Other polymers (i)

There are no such residues in this entry.

4.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

5 Fit of model and data

5.1 Protein, DNA and RNA chains

EDS failed to run properly - this section is therefore empty.

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

EDS failed to run properly - this section is therefore empty.

5.3 Carbohydrates

EDS failed to run properly - this section is therefore empty.

5.4 Ligands

EDS failed to run properly - this section is therefore empty.

5.5 Other polymers

EDS failed to run properly - this section is therefore empty.