wwPDB X-ray Structure Validation Summary Report (i)

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PDB ID	:	6N22
Title	:	Crystal structure of mouse Protocadherin-15 EC1-2 BAP
Authors	:	Narui, Y.; Sotomayor, M.
Deposited on	:	2018-11-12
Resolution	:	2.40 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 (i) 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 (i)) 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

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

The reported resolution of this entry is 2.40 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 3 unique types of molecules in this entry. The entry contains 1894 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
			Total	C	N	O	S			
1	A	231	1842	1153	319	364	6	0	2	0

There are 23 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	240	GLY	-	expression tag	UNP Q99PJ1
A	241	LEU	-	expression tag	UNP Q99PJ1
A	242	ASN	-	expression tag	UNP Q99PJ1
A	243	ASP	-	expression tag	UNP Q99PJ1
A	244	ILE	-	expression tag	UNP Q99PJ1
A	245	PHE	-	expression tag	UNP Q99PJ1
A	246	GLU	-	expression tag	UNP Q99PJ1
A	247	ALA	-	expression tag	UNP Q99PJ1
A	248	GLN	-	expression tag	UNP Q99PJ1
A	249	LYS	-	expression tag	UNP Q99PJ1
A	250	ILE	-	expression tag	UNP Q99PJ1
A	251	GLU	-	expression tag	UNP Q99PJ1
A	252	TRP	-	expression tag	UNP Q99PJ1
A	253	HIS	-	expression tag	UNP Q99PJ1
A	254	GLU	-	expression tag	UNP Q99PJ1
A	255	LEU	-	expression tag	UNP Q99PJ1
A	256	GLU	-	expression tag	UNP Q99PJ1
A	257	HIS	-	expression tag	UNP Q99PJ1
A	258	HIS	-	expression tag	UNP Q99PJ1
A	259	HIS	-	expression tag	UNP Q99PJ1
A	260	HIS	-	expression tag	UNP Q99PJ1
A	261	HIS	-	expression tag	UNP Q99PJ1
A	262	HIS	-	expression tag	UNP Q99PJ1

- Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	3	Total Ca 3 3	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	49	Total O 49 49	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 64	Depositor
Cell constants a, b, c, α, β, γ	99.62Å 99.62Å 58.56Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	49.86 – 2.40	Depositor
% Data completeness (in resolution range)	99.9 (49.86-2.40)	Depositor
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.06 (at 2.39Å)	Xtriage
Refinement program	REFMAC 5.8.0232	Depositor
R, R_{free}	0.170 , 0.233	Depositor
Wilson B-factor (Å^2)	39.2	Xtriage
Anisotropy	0.472	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	0.049 for h,-h-k,-l	Xtriage
Total number of atoms	1894	wwPDB-VP
Average B, all atoms (Å^2)	47.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.07% 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 3 ligands modelled in this entry, 3 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.