Full wwPDB X-ray Structure Validation Report (i)

Oct 2, 2023 – 04:52 AM EDT

PDB ID	:	6NFJ
Title	:	Structure of Beta-Klotho in Complex with FGF19 C-terminal peptide
Authors	:	Kuzina, E.; Schlessinger, J.; Lee, S.
Deposited on	:	2018-12-20
Resolution	:	3.19 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 (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 (i)

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

The reported resolution of this entry is 3.19 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 14271 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 Beta-klotho.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	844	Total	C	N	O	S	0	0	0
			6373	4149	1076	1126	22			
1	D	846	Total	C	N	O	S	0	0	0
			6129	3969	1051	1088	21			

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	308	GLN	ASN	engineered mutation	UNP Q86Z14
A	611	GLN	ASN	engineered mutation	UNP Q86Z14
A	985	ASN	-	expression tag	UNP Q86Z14
A	986	LEU	-	expression tag	UNP Q86Z14
A	987	TYR	-	expression tag	UNP Q86Z14
A	988	PHE	-	expression tag	UNP Q86Z14
A	989	GLN	-	expression tag	UNP Q86Z14
D	308	GLN	ASN	engineered mutation	UNP Q86Z14
D	611	GLN	ASN	engineered mutation	UNP Q86Z14
D	985	ASN	-	expression tag	UNP Q86Z14
D	986	LEU	-	expression tag	UNP Q86Z14
D	987	TYR	-	expression tag	UNP Q86Z14
D	988	PHE	-	expression tag	UNP Q86Z14
D	989	GLN	-	expression tag	UNP Q86Z14

- Molecule 2 is a protein called Nanobody 30.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	111	Total	C	N	O	S	0	0	0
			762	490	136	132	4			
2	E	113	Total	C	N	O	S	0	0	0
			763	488	135	136	4			

- Molecule 3 is a protein called Fibroblast growth factor 19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	19	Total	C	N	O	S	0	0	0
			122	77	19	25	1			
3	F	19	Total	C	N	O	S	0	0	0
			122	77	19	25	1			

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	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	130.09Å 143.90Å 141.05Å 90.00° 90.90° 90.00°	Depositor
Resolution (Å)	59.42 – 3.19	Depositor
% Data completeness (in resolution range)	97.8 (59.42-3.19)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.11 (at 3.19Å)	Xtriage
Refinement program	PHENIX (1.13_2998: ???)	Depositor
R, R_{free}	0.280 , 0.320	Depositor
Wilson B-factor (Å^2)	77.8	Xtriage
Anisotropy	0.438	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.38$, $< L^2 > = 0.21$	Xtriage
Estimated twinning fraction	0.064 for -h,-k,l	Xtriage
Total number of atoms	14271	wwPDB-VP
Average B, all atoms (Å^2)	80.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 55.18 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 3.2847e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[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

There are no ligands in this entry.

4.7 Other polymers

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.