

Full wwPDB X-ray Structure Validation Report (i)

Oct 3, 2023 – 12:13 AM EDT

PDB ID : 6PNP

Title : Crystal structure of the splice insert-free neurexin-1 LNS2 domain in complex

with neurexophilin-1

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Deposited on : 2019-07-02

Resolution : 1.94 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 (1)) 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 1.94 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 5175 atoms, of which 2519 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 Neurexin-1.

Mol	Chain	Residues	${f Atoms}$			ZeroOcc	AltConf	Trace			
1	A	193	Total 2943	C 938	H 1460	N 247	O 292	S 6	0	1	0

There are 27 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	280	ASP	-	expression tag	UNP Q9CS84
A	281	ALA	-	expression tag	UNP Q9CS84
A	282	SER	_	expression tag	UNP Q9CS84
A	293	ALA	CYS	engineered mutation	UNP Q9CS84
A	?	-	HIS	deletion	UNP Q9CS84
A	?	-	SER	deletion	UNP Q9CS84
A	?	-	GLY	deletion	UNP Q9CS84
A	?	-	ILE	deletion	UNP Q9CS84
A	?	-	GLY	deletion	UNP Q9CS84
A	?	-	HIS	deletion	UNP Q9CS84
A	?	-	ALA	deletion	UNP Q9CS84
A	?	-	MET	deletion	UNP Q9CS84
A	?	-	VAL	deletion	UNP Q9CS84
A	?	-	ASN	deletion	UNP Q9CS84
A	?	-	LYS	deletion	UNP Q9CS84
A	?	-	LEU	deletion	UNP Q9CS84
A	?	-	HIS	deletion	UNP Q9CS84
A	?	-	CYS	deletion	UNP Q9CS84
A	?	-	SER	deletion	UNP Q9CS84
A	481	ALA	-	expression tag	UNP Q9CS84
A	482	ALA	-	expression tag	UNP Q9CS84
A	483	LEU	-	expression tag	UNP Q9CS84
A	484	GLU	-	expression tag	UNP Q9CS84
A	485	VAL	-	expression tag	UNP Q9CS84
A	486	LEU	-	expression tag	UNP Q9CS84
A	487	PHE	-	expression tag	UNP Q9CS84
A	488	GLN	-	expression tag	UNP Q9CS84



• Molecule 2 is a protein called Neurexophilin-1.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace			
2	В	132	Total 2165	C 709	H 1059	N 180	O 211	S 6	0	5	0

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
В	110	ASP	-	expression tag	UNP Q63366
В	111	ALA	-	expression tag	UNP Q63366
В	112	ALA	-	expression tag	UNP Q63366
В	113	GLN	-	expression tag	UNP Q63366
В	114	PRO	-	expression tag	UNP Q63366
В	115	ALA	-	expression tag	UNP Q63366
В	116	ALA	-	expression tag	UNP Q63366
В	117	ARG	-	expression tag	UNP Q63366
В	118	ASP	-	expression tag	UNP Q63366
В	146	ASP	ASN	engineered mutation	UNP Q63366
В	156	ASP	ASN	engineered mutation	UNP Q63366
В	162	ASP	ASN	engineered mutation	UNP Q63366
В	272	LEU	-	expression tag	UNP Q63366
В	273	GLU	-	expression tag	UNP Q63366
В	274	VAL	-	expression tag	UNP Q63366
В	275	LEU	-	expression tag	UNP Q63366
В	276	PHE	-	expression tag	UNP Q63366
В	277	GLN	-	expression tag	UNP Q63366

• Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	27	Total O 27 27	0	0
3	В	40	Total O 40 40	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	C 1 2 1	Depositor	
Cell constants	71.70Å 60.98Å 79.62Å	Donositor	
a, b, c, α , β , γ	90.00° 106.74° 90.00°	Depositor	
Resolution (Å)	45.60 - 1.94	Depositor	
% Data completeness	95.0 (45.60-1.94)	Depositor	
(in resolution range)	` '		
R_{merge}	0.10	Depositor	
R_{sym}	(Not available)	Depositor	
$< I/\sigma(I) > 1$	1.11 (at 1.94Å)	Xtriage	
Refinement program	PHENIX 1.14_3260	Depositor	
R, R_{free}	0.198 , 0.247	Depositor	
Wilson B-factor (Å ²)	39.4	Xtriage	
Anisotropy	0.301	Xtriage	
L-test for twinning ²	$ < L >=0.50, < L^2>=0.33$	Xtriage	
Estimated twinning fraction	No twinning to report.	Xtriage	
Total number of atoms	5175	wwPDB-VP	
Average B, all atoms (\mathring{A}^2)	84.0	wwPDB-VP	

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 6.62% of the height of the origin peak. No significant pseudotranslation is detected.

²Theoretical 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.



¹Intensities estimated from amplitudes.

4 Model quality (i)

4.1 Standard geometry (i)

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

4.2 Too-close contacts (i)

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

4.3 Torsion angles (i)

4.3.1 Protein backbone (i)

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

4.3.2 Protein sidechains (i)

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

4.3.3 RNA (i)

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

4.4 Non-standard residues in protein, DNA, RNA chains (i)

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

4.5 Carbohydrates (i)

There are no monosaccharides in this entry.

4.6 Ligand geometry (i)

There are no ligands in this entry.

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 (i)

5.1 Protein, DNA and RNA chains (i)

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

5.2 Non-standard residues in protein, DNA, RNA chains (i)

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

5.3 Carbohydrates (i)

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

5.4 Ligands (i)

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

5.5 Other polymers (i)

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

