

# Full wwPDB X-ray Structure Validation Report (i)

Oct 2, 2023 – 01:25 PM EDT

PDB ID : 6NUF

Title : Structure of Calcineurin in complex with NHE1 peptide

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Deposited on : 2019-01-31

Resolution : 1.90 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 (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

Mogul : 1.8.5 (274361), CSD as541be (2020)

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 1.90 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 11 unique types of molecules in this entry. The entry contains 9109 atoms, of which 4272 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 Serine/threonine-protein phosphatase 2B catalytic subunit alpha isoform.

Mol	Chain	Residues			Atom	ıs			ZeroOcc	AltConf	Trace
1	A	360	Total 5817	C 1896	H 2872	N 492	O 537	S 20	0	5	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	GLY	-	expression tag	UNP Q08209
A	0	HIS	-	expression tag	UNP Q08209

• Molecule 2 is a protein called Calcineurin subunit B type 1.

Mol	Chain	Residues			Atom	ıS			ZeroOcc	AltConf	Trace
2	В	156	Total 2463	C 781	H 1223	N 206	O 246	S 7	0	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
В	15	MET	-	expression tag	UNP P63098

• Molecule 3 is a protein called Sodium/hydrogen exchanger 1.

Mol	Chain	Residues		$\mathbf{A}^{1}$	toms			ZeroOcc	AltConf	Trace
3	С	19	Total 281	C 91	H 139	N	O 30	0	0	0

There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
С	676	GLY	-	expression tag	UNP P19634

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Chain	Residue	Modelled	Actual	Comment	Reference
С	677	HIS	-	expression tag	UNP P19634
С	678	MET	-	expression tag	UNP P19634
С	698	ALA	ARG	engineered mutation	UNP P19634
С	700	ALA	ARG	engineered mutation	UNP P19634

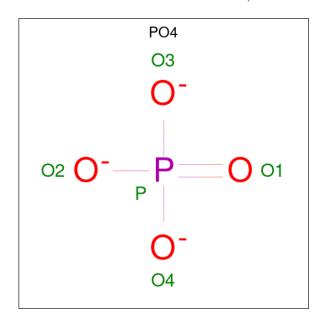
• Molecule 4 is FE (III) ION (three-letter code: FE) (formula: Fe).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total Fe 1 1	0	0

• Molecule 5 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total Zn 1 1	0	0

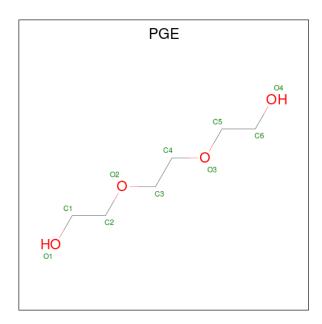
• Molecule 6 is PHOSPHATE ION (three-letter code: PO4) (formula: O<sub>4</sub>P).



Mol	Chain	Residues	Ato	oms		ZeroOcc	AltConf
6	A	1	Total 5	O 4	P 1	0	0

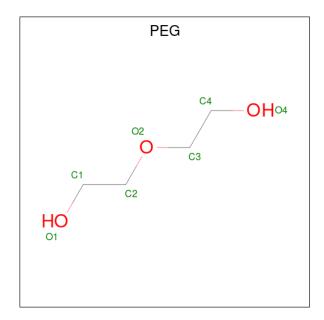
 $\bullet$  Molecule 7 is TRIETHYLENE GLYCOL (three-letter code: PGE) (formula:  $\mathrm{C_6H_{14}O_4}).$ 





M	[ol	Chain	Residues	A	Ator	$\mathbf{n}\mathbf{s}$		ZeroOcc	AltConf
-	7	Δ	1	Total	С	Н	О	0	0
	•	11	1	24	6	14	4	O	
,	7	Λ	1	Total	$\mathbf{C}$	Η	O	0	0
'	1	Λ	1	24	6	14	4	0	

 $\bullet \ \, \text{Molecule 8 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: $C_4H_{10}O_3$)}. \\$ 



Mol	Chain	Residues	A	Ator	ns		ZeroOcc	AltConf
Q	Λ	1	Total	С	Н	О	0	0
0	Λ	1	17	4	10	3	0	

• Molecule 9 is SODIUM ION (three-letter code: NA) (formula: Na).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	A	1	Total Na 1 1	0	0

• Molecule 10 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	В	4	Total Ca 4 4	0	0

• Molecule 11 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
11	A	351	Total O 351 351	0	0
11	В	105	Total O 105 105	0	0
11	С	15	Total O 15 15	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 2 2 21	Depositor
Cell constants	79.48Å 126.81Å 127.43Å	Depositor
a, b, c, $\alpha$ , $\beta$ , $\gamma$	90.00° 90.00° 90.00°	Depositor
Resolution (Å)	16.13 - 1.90	Depositor
% Data completeness	97.5 (16.13-1.90)	Depositor
(in resolution range)	,	-
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$< I/\sigma(I) > 1$	0.64  (at  1.90Å)	Xtriage
Refinement program	PHENIX (1.11.1_2575: ???)	Depositor
$R, R_{free}$	0.169 , $0.209$	Depositor
Wilson B-factor $(A^2)$	15.9	Xtriage
Anisotropy	0.283	Xtriage
L-test for twinning <sup>2</sup>	$ < L > = 0.49, < L^2> = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	9109	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 4.35% of the height of the origin peak. No significant pseudotranslation is detected.

<sup>&</sup>lt;sup>2</sup>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.



<sup>&</sup>lt;sup>1</sup>Intensities 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)

Of 11 ligands modelled in this entry, 7 are monoatomic - leaving 4 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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| > 2 is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol Type		Chain	Res	Link	Bond lengths			Bond angles		
IVIOI	туре	Chain	nes	Lilik	Counts	RMSZ	# Z >2	Counts	RMSZ	# Z  > 2
6	PO4	A	403	5,4	4,4,4	0.76	0	6,6,6	0.60	0
7	PGE	A	405	-	9,9,9	0.55	0	8,8,8	0.50	0
7	PGE	A	404	-	9,9,9	0.55	0	8,8,8	0.58	0
8	PEG	A	406	-	6,6,6	0.55	0	5,5,5	0.60	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	PGE	A	405	-	-	2/7/7/7	-
7	PGE	A	404	-	-	3/7/7/7	-
8	PEG	A	406	-	-	2/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	A	404	PGE	O1-C1-C2-O2
7	A	405	PGE	O2-C3-C4-O3
7	A	404	PGE	C1-C2-O2-C3
8	A	406	PEG	O1-C1-C2-O2
8	A	406	PEG	C1-C2-O2-C3
7	A	404	PGE	C3-C4-O3-C5
7	A	405	PGE	O1-C1-C2-O2

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 (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.

