



# wwPDB X-ray Structure Validation Summary Report ⓘ

Oct 2, 2023 – 11:51 PM EDT

PDB ID : 6OWW  
Title : Crystal structure of a Human Cardiac Calsequestrin Filament Complexed with Ytterbium  
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Deposited on : 2019-05-12  
Resolution : 3.84 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](mailto: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>.

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The following versions of software and data (see [references ⓘ](#)) 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

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.84 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 21808 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 Calsequestrin-2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	329	2715	1771	416	522	6	0	0	0
1	B	329	2715	1771	416	522	6	0	0	0
1	C	329	2715	1771	416	522	6	0	0	0
1	D	329	2715	1771	416	522	6	0	0	0
1	E	329	2715	1771	416	522	6	0	0	0
1	F	329	2715	1771	416	522	6	0	0	0
1	G	329	2715	1771	416	522	6	0	0	0
1	H	329	2715	1771	416	522	6	0	0	0

There are 40 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	13	GLY	-	expression tag	UNP O14958
A	14	HIS	-	expression tag	UNP O14958
A	15	MET	-	expression tag	UNP O14958
A	16	ALA	-	expression tag	UNP O14958
A	17	SER	-	expression tag	UNP O14958
B	13	GLY	-	expression tag	UNP O14958
B	14	HIS	-	expression tag	UNP O14958
B	15	MET	-	expression tag	UNP O14958
B	16	ALA	-	expression tag	UNP O14958
B	17	SER	-	expression tag	UNP O14958
C	13	GLY	-	expression tag	UNP O14958
C	14	HIS	-	expression tag	UNP O14958
C	15	MET	-	expression tag	UNP O14958

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Chain	Residue	Modelled	Actual	Comment	Reference
C	16	ALA	-	expression tag	UNP O14958
C	17	SER	-	expression tag	UNP O14958
D	13	GLY	-	expression tag	UNP O14958
D	14	HIS	-	expression tag	UNP O14958
D	15	MET	-	expression tag	UNP O14958
D	16	ALA	-	expression tag	UNP O14958
D	17	SER	-	expression tag	UNP O14958
E	13	GLY	-	expression tag	UNP O14958
E	14	HIS	-	expression tag	UNP O14958
E	15	MET	-	expression tag	UNP O14958
E	16	ALA	-	expression tag	UNP O14958
E	17	SER	-	expression tag	UNP O14958
F	13	GLY	-	expression tag	UNP O14958
F	14	HIS	-	expression tag	UNP O14958
F	15	MET	-	expression tag	UNP O14958
F	16	ALA	-	expression tag	UNP O14958
F	17	SER	-	expression tag	UNP O14958
G	13	GLY	-	expression tag	UNP O14958
G	14	HIS	-	expression tag	UNP O14958
G	15	MET	-	expression tag	UNP O14958
G	16	ALA	-	expression tag	UNP O14958
G	17	SER	-	expression tag	UNP O14958
H	13	GLY	-	expression tag	UNP O14958
H	14	HIS	-	expression tag	UNP O14958
H	15	MET	-	expression tag	UNP O14958
H	16	ALA	-	expression tag	UNP O14958
H	17	SER	-	expression tag	UNP O14958

- Molecule 2 is YTTERBIUM (III) ION (three-letter code: Yb) (formula: Yb) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	9	Total Yb 9 9	0	0
2	B	7	Total Yb 7 7	0	0
2	C	9	Total Yb 9 9	0	0
2	D	8	Total Yb 8 8	0	0
2	E	9	Total Yb 9 9	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	F	7	Total	Yb	0	0
			7	7		
2	G	8	Total	Yb	0	0
			8	8		
2	H	6	Total	Yb	0	0
			6	6		

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	D	1	Total	O	S	0	0
			5	4	1		
3	F	1	Total	O	S	0	0
			5	4	1		
3	H	1	Total	O	S	0	0
			5	4	1		

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

### 3 Data and refinement statistics

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, $\alpha$ , $\beta$ , $\gamma$	85.83Å 86.02Å 214.34Å 90.00° 89.91° 90.00°	Depositor
Resolution (Å)	214.34 – 3.84	Depositor
% Data completeness (in resolution range)	98.4 (214.34-3.84)	Depositor
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.62 (at 3.89Å)	Xtriage
Refinement program	PHENIX 1.15.2_3472	Depositor
R, $R_{free}$	0.290 , 0.340	Depositor
Wilson B-factor (Å <sup>2</sup> )	79.7	Xtriage
Anisotropy	0.919	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.38$ , $\langle L^2 \rangle = 0.21$	Xtriage
Estimated twinning fraction	0.266 for k,h,-l 0.266 for -k,-h,-l 0.266 for h,-k,-l	Xtriage
Total number of atoms	21808	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	98.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 14.30% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 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 68 ligands modelled in this entry, 63 are monoatomic - leaving 5 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		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
3	SO4	H	407	-	4,4,4	0.16	0	6,6,6	0.19	0
3	SO4	B	408	-	4,4,4	0.15	0	6,6,6	0.06	0
3	SO4	F	408	-	4,4,4	0.14	0	6,6,6	0.08	0
3	SO4	D	409	-	4,4,4	0.17	0	6,6,6	0.12	0
3	SO4	A	410	2	4,4,4	0.15	0	6,6,6	0.15	0

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.