



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 01:46 AM GMT

PDB ID : 2EAU  
Title : Crystal structure of the SR CA2+-ATPASE with bound CPA in the presence of curcumin  
Authors : Takahashi, M.; Kondou, Y.; Toyoshima, C.  
Deposited on : 2007-02-02  
Resolution : 2.80 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  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

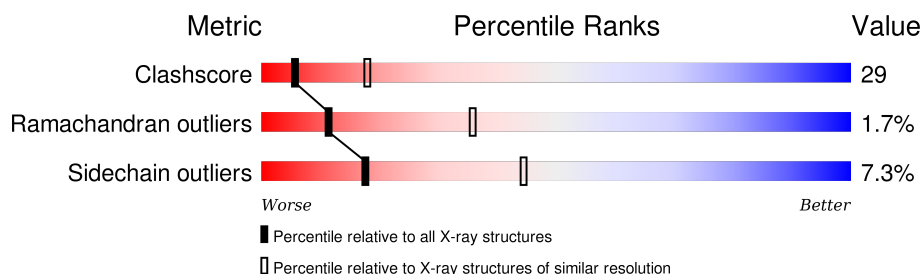
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.80 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	102246	2827 (2.80-2.80)
Ramachandran outliers	100387	2782 (2.80-2.80)
Sidechain outliers	100360	2784 (2.80-2.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	995	<div> <div style="width: 53%; background-color: green;"></div> <div style="width: 42%; background-color: yellow;"></div> <div style="width: 5%; background-color: orange;"></div> </div> <div>53% 42% 5%</div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	CZA	A	1005	X	-	X	-

## 2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 7756 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.

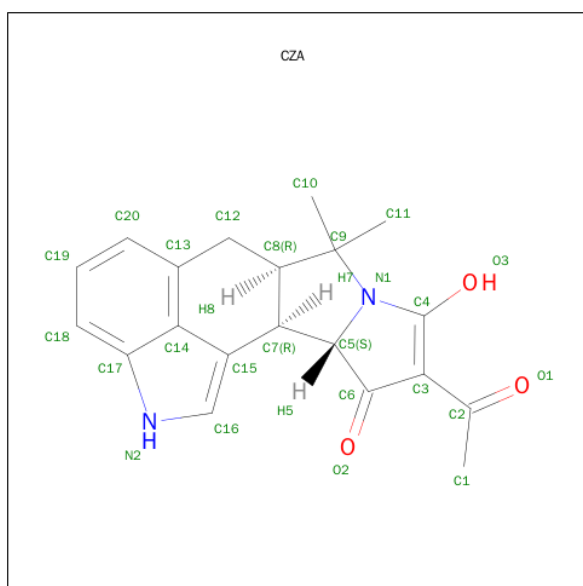
- Molecule 1 is a protein called Sarcoplasmic/endoplasmic reticulum calcium ATPase 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	995	Total	C	N	O	S	1	0	0
			7674	4878	1287	1452	57			

There is a discrepancy between the modelled and reference sequences:

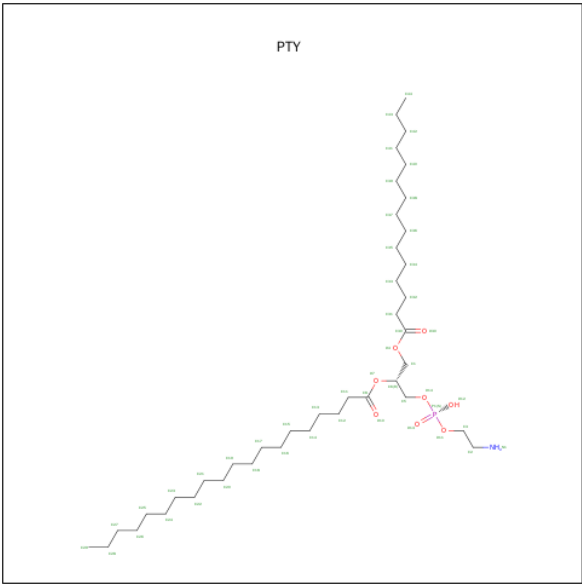
Chain	Residue	Modelled	Actual	Comment	Reference
A	994	GLY	-	SEE REMARK 999	UNP P04191

- Molecule 2 is (6AR,11AS,11BR)-10-ACETYL-9-HYDROXY-7,7-DIMETHYL-2,6,6A,7,11A,11B-HEXAHYDRO-11H-PYRROLO[1',2':2,3]ISOINDOLO[4,5,6-CD]INDOL-11-ONE (three-letter code: CZA) (formula:  $C_{20}H_{20}N_2O_3$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			25	20	2	3		

- Molecule 3 is PHOSPHATIDYLETHANOLAMINE (three-letter code: PTY) (formula: C<sub>40</sub>H<sub>80</sub>NO<sub>8</sub>P).



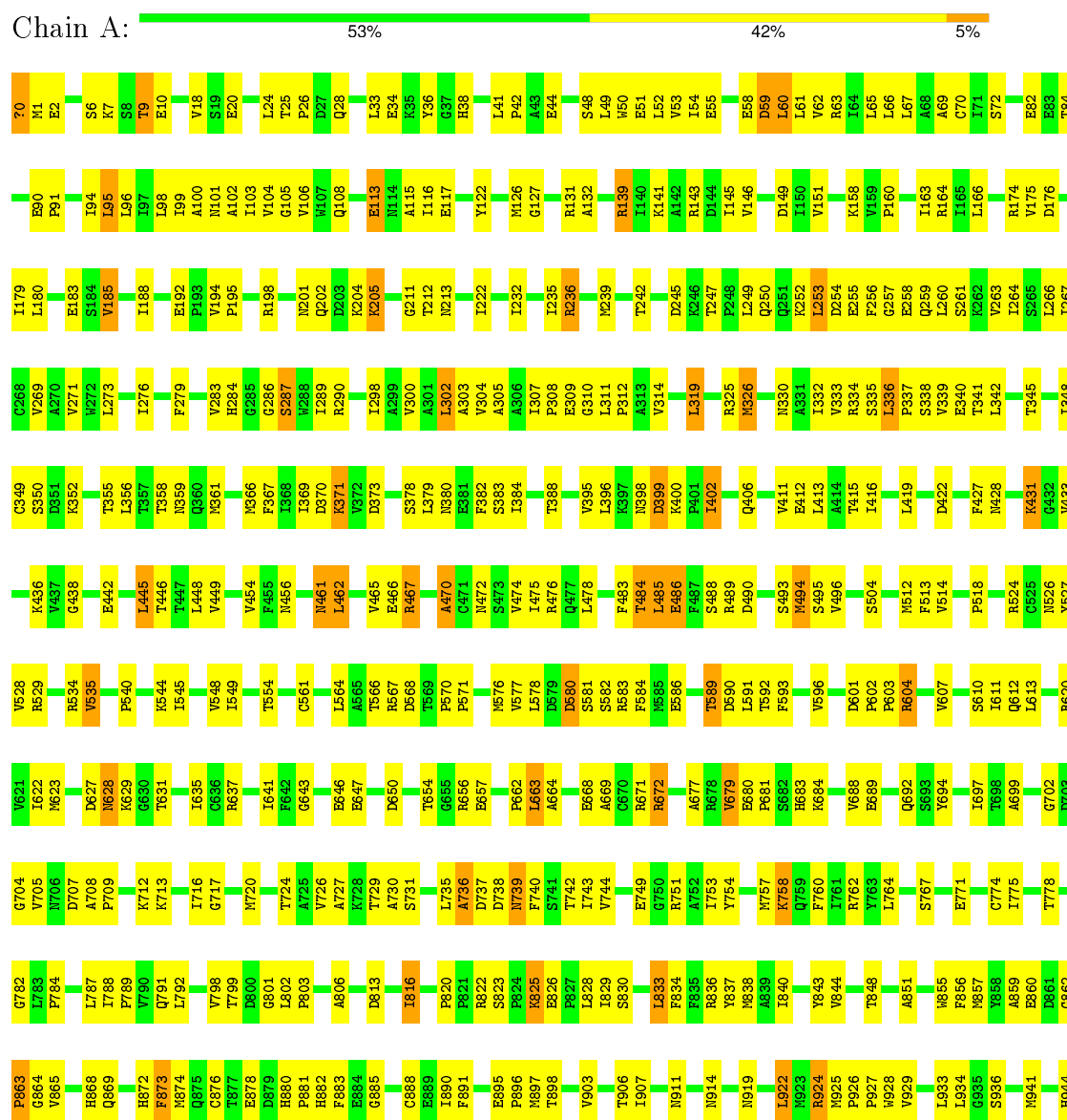
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			19	9	1	8	1		
3	A	1	Total	C	N	O	P	0	0
			19	9	1	8	1		
3	A	1	Total	C	N	O	P	0	0
			19	9	1	8	1		

### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $\text{RSRZ} > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

Note EDS was not executed.

- Molecule 1: Sarcoplasmic/endoplasmic reticulum calcium ATPase 1



P945	P946	P947	P950	P951	P952	P953	P954	P955	P956	P957	P958	P959	P960	P963	P964	P965	P966	P967	P968	P971	P972	P973	P974	P975	P976	P977	P978	P979	P980	P981	P982	P983	P984	P985	P986	P987	P988	P989	P992	P993	P994
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## 4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section will therefore be incomplete.

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	71.65Å 71.65Å 586.25Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	15.00 – 2.80	Depositor
% Data completeness (in resolution range)	97.6 (15.00-2.80)	Depositor
$R_{merge}$	0.14	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.247 , 0.272	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	7756	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	62.0	wwPDB-VP

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: CZA, ACE, PTY

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  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	A	0.53	1/7813 (0.0%)	0.66	2/10594 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	0	ACE	C-N	-24.41	0.78	1.34

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	0	ACE	C-N-CA	9.78	146.16	121.70
1	A	0	ACE	O-C-N	-6.93	111.62	122.70

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	7674	0	7767	453	0
2	A	25	0	19	23	0
3	A	57	0	33	2	0
All	All	7756	0	7819	453	0



The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 29.

The worst 5 of 453 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:101:ASN:HB3	2:A:1005:CZA:C18	1.69	1.21
1:A:0:ACE:CH3	1:A:1:MET:N	2.07	1.18
1:A:0:ACE:C	1:A:1:MET:CA	2.19	1.11
1:A:101:ASN:CB	2:A:1005:CZA:C18	2.34	1.04
1:A:101:ASN:HD22	2:A:1005:CZA:C19	1.77	0.98

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	993/995 (100%)	863 (87%)	113 (11%)	17 (2%)	11	36

5 of 17 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	951	ASP
1	A	663	LEU
1	A	736	ALA
1	A	950	VAL
1	A	185	VAL

### 5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	840/840 (100%)	779 (93%)	61 (7%)	17	44

5 of 61 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	461	ASN
1	A	540	PRO
1	A	888	CYS
1	A	467	ARG
1	A	485	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 12 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	628	ASN
1	A	706	ASN
1	A	914	ASN
1	A	510	ASN
1	A	880	HIS

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

4 ligands are modelled in this entry.

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$
2	CZA	A	1005	-	25,29,29	2.49	9 (36%)	22,48,48	2.17	5 (22%)
3	PTY	A	1011	-	17,18,49	1.48	4 (23%)	18,23,54	1.50	3 (16%)
3	PTY	A	1012	-	17,18,49	1.46	4 (23%)	18,23,54	1.28	2 (11%)
3	PTY	A	1013	-	17,18,49	1.33	3 (17%)	18,23,54	1.53	3 (16%)

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
2	CZA	A	1005	-	3/3/9/9	0/4/52/52	0/5/5/5
3	PTY	A	1011	-	-	0/20/20/53	0/0/0/0
3	PTY	A	1012	-	-	0/20/20/53	0/0/0/0
3	PTY	A	1013	-	-	0/20/20/53	0/0/0/0

The worst 5 of 20 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1005	CZA	C3-C2	-3.83	1.34	1.46
2	A	1005	CZA	C1-C2	-3.53	1.42	1.50
2	A	1005	CZA	O3-C4	-2.65	1.23	1.31
2	A	1005	CZA	C4-N1	-2.50	1.36	1.39
2	A	1005	CZA	C13-C14	-2.39	1.39	1.44

The worst 5 of 13 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1005	CZA	C12-C13-C14	-5.08	115.07	119.49
3	A	1011	PTY	O12-P1-O13	-2.98	96.38	112.53
3	A	1013	PTY	C5-C6-C1	-2.97	105.14	112.07
2	A	1005	CZA	C19-C18-C17	-2.68	115.77	120.06
2	A	1005	CZA	O3-C4-C3	-2.02	124.59	130.14

All (3) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	A	1005	CZA	C5
2	A	1005	CZA	C8
2	A	1005	CZA	C7

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 25 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1005	CZA	23	0
3	A	1011	PTY	1	0
3	A	1012	PTY	1	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

EDS was not executed - this section will therefore be empty.

### 6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

EDS was not executed - this section will therefore be empty.

### 6.3 Carbohydrates ⓘ

EDS was not executed - this section will therefore be empty.

### 6.4 Ligands ⓘ

EDS was not executed - this section will therefore be empty.

### 6.5 Other polymers ⓘ

EDS was not executed - this section will therefore be empty.