



# wwPDB X-ray Structure Validation Summary Report

Feb 28, 2014 – 08:22 AM GMT

PDB ID : 2EAS  
Title : Crystal structure of the SR CA2+-ATPASE with bound CPA  
Authors : Takahashi, M.; Kondou, Y.; Toyoshima, C.  
Deposited on : 2007-02-02  
Resolution : 3.40 Å(reported)

This is a wwPDB 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/ValidationPDFNotes.html>

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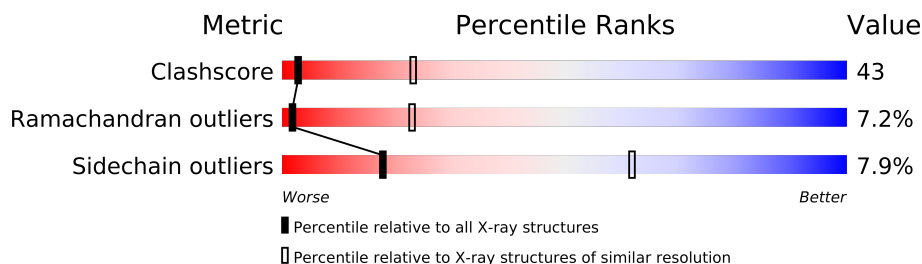
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.15 2013
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	21963
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	stable22683

# 1 Overall quality at a glance

The reported resolution of this entry is 3.40 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	79885	1214 (3.50-3.30)
Ramachandran outliers	78287	1177 (3.50-3.30)
Sidechain outliers	78261	1177 (3.50-3.30)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	995	

## 2 Entry composition i

There are 2 unique types of molecules in this entry. The entry contains 7699 atoms, of which 0 are hydrogen and 0 are deuterium.

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.

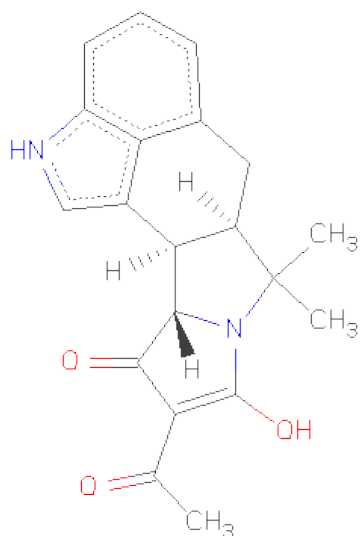
- Molecule 1 is a protein called Sarcoplasmic/endoplasmicreticulum calcium ATPase 1.

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

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<sub>20</sub>H<sub>20</sub>N<sub>2</sub>O<sub>3</sub>).



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

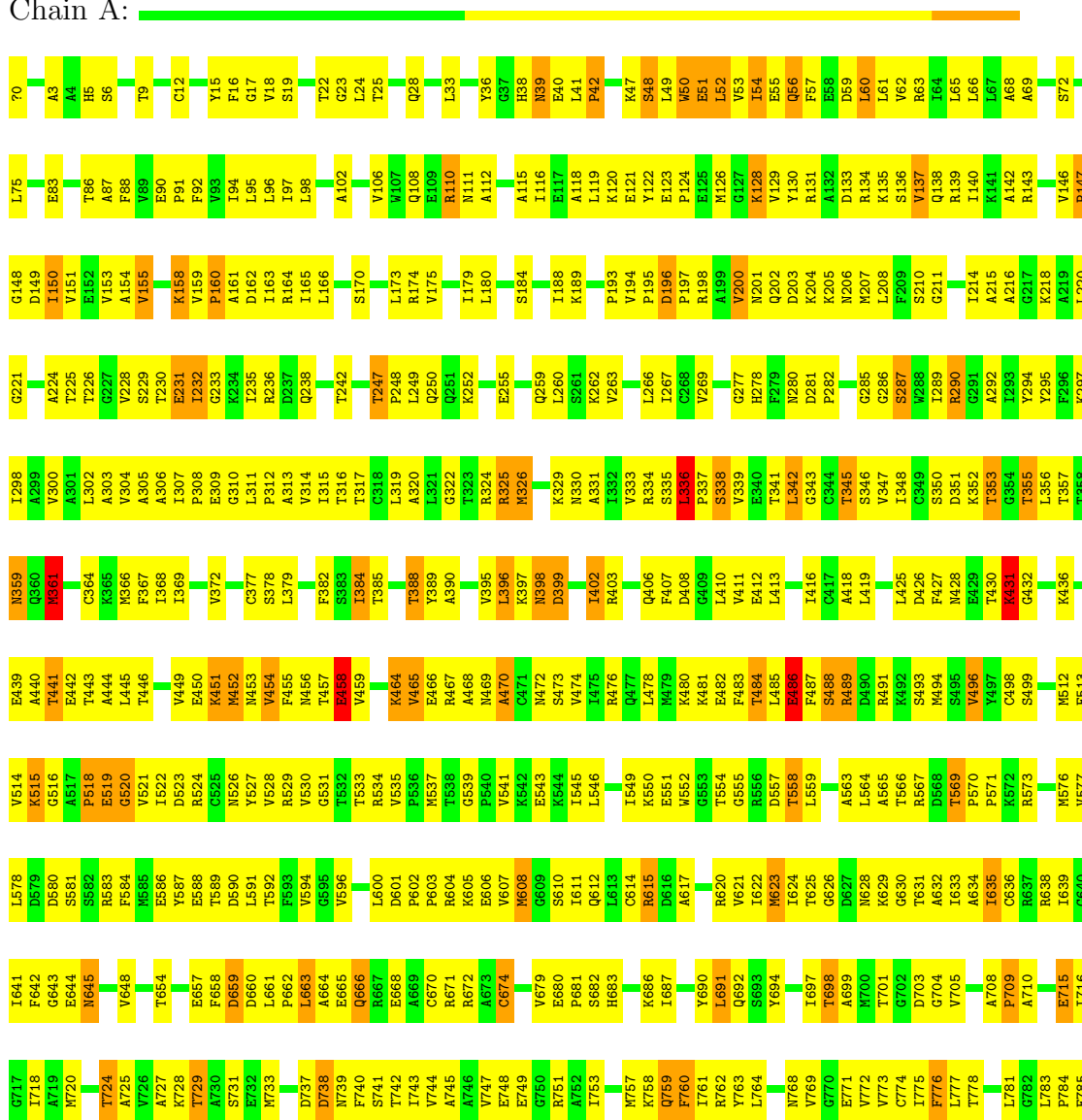
### 3 Residue-property plots

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 ( $RSRZ > 2$ ). 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/endoplasmicreticulum calcium ATPase 1

Chain A:



S936	L786	C864	A786
I937	L787	V865	L787
C938	L788	H868	L788
L939	P789	Q869	P789
S940	Q790		Q790
N941	Q791		Q791
S942	L792	H872	L792
L943	L793	F873	L793
	W794	M874	W794
	V795	Q875	V795
L946	W796		W796
L947	L797	E878	L797
L948	W798	D879	W798
Y949	W799	H880	W799
V950	D800	P881	D800
D951	G801		G801
P952	L802	E884	L802
L953	P803	G885	P803
P954			
	L807	C888	L807
K958	E889	E899	E889
L959	N810		N810
K960	E895	E895	E895
A961	P896	P896	P896
L962	M897	M897	M897
	T898	T898	T898
W967	D816		D816
L968	M817		M817
Y969	D818		D818
Y970	R819		R819
L971	P820	A900	P820
K972	L901	S902	L901
L973	R822		R822
S974	V903		V903
L975	L904		L904
P976	V905		V905
Y977	T906		T906
T978	I907		I907
G979	E908	M909	E908
L980	F834	C910	F834
D981	R836	N911	R836
E982	T837	A912	T837
L983	M838	L913	M838
L984	A839	N914	A839
K985	L840	S915	K985
P986	Y843	L916	P986
L987	V844	S917	L987
A988		E918	A988
R989	A847		R989
	T848	L922	
	W849	M923	
	G850	R924	
	A851	M925	
		P926	
	W854	P927	
	W855	W928	
	F856	V929	
	M857	N930	
	T858		
	A859	L933	
	P863	L934	
		G935	

## 4 Data and refinement statistics

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

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	63.04Å 96.03Å 155.42Å 90.00° 95.09° 90.00°	Depositor
Resolution (Å)	15.00 – 3.40	Depositor
% Data completeness (in resolution range)	99.9 (15.00-3.40)	Depositor
$R_{merge}$	0.05	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.267 , 0.324	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	7699	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	106.0	wwPDB-VP

## 5 Model quality

### 5.1 Standard geometry

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

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	0.62	0/7813	0.79	19/10594 (0.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2

There are no bond length outliers.

The worst 5 of 19 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	989	ARG	NE-CZ-NH2	7.63	124.11	120.30
1	A	290	ARG	NE-CZ-NH2	7.49	124.05	120.30
1	A	836	ARG	NE-CZ-NH2	7.33	123.96	120.30
1	A	325	ARG	NE-CZ-NH2	6.54	123.57	120.30
1	A	324	ARG	NE-CZ-NH2	6.53	123.56	120.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	196	ASP	Mainchain
1	A	287	SER	Mainchain

## 5.2 Close contacts ⓘ

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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	7674	0	7765	666	0
2	A	25	0	19	2	0
All	All	7699	0	7784	666	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 43.

The worst 5 of 666 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:281:ASP:HB3	1:A:282:PRO:HD3	1.31	1.13
1:A:294:TYR:CZ	1:A:298:ILE:HD11	1.85	1.11
1:A:124:PRO:HG3	1:A:160:PRO:HA	1.36	1.06
1:A:802:LEU:HG	1:A:936:SER:HB2	1.12	1.06
1:A:984:LEU:O	1:A:987:ILE:HG22	1.54	1.05

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone ⓘ

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%)	743 (75%)	179 (18%)	71 (7%)	<b>2</b> <b>23</b>

5 of 71 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	52	LEU

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Mol	Chain	Res	Type
1	A	464	LYS
1	A	519	GLU
1	A	873	PHE
1	A	905	VAL

### 5.3.2 Protein sidechains ⓘ

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%)	774 (92%)	66 (8%)	18 62

5 of 66 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	431	LYS
1	A	494	MET
1	A	889	GLU
1	A	441	THR
1	A	486	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 14 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	461	ASN
1	A	472	ASN
1	A	875	GLN
1	A	398	ASN
1	A	872	HIS

### 5.3.3 RNA ⓘ

There are no RNA chains in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

1 ligand is 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	-	29,29,29	2.67	12 (41%)	47,48,48	2.72	16 (34%)

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	0/0/5/5

The worst 5 of 12 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1005	CZA	O1-C2	8.92	1.42	1.23
2	A	1005	CZA	C12-C8	4.12	1.59	1.53
2	A	1005	CZA	C3-C4	3.94	1.47	1.40
2	A	1005	CZA	C9-N1	3.87	1.56	1.49
2	A	1005	CZA	C19-C20	3.83	1.47	1.39

The worst 5 of 16 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1005	CZA	C7-C15-C14	-10.36	119.31	124.56
2	A	1005	CZA	C13-C14-C15	6.29	130.30	123.54
2	A	1005	CZA	C12-C13-C14	-5.42	115.77	119.33
2	A	1005	CZA	C13-C14-C17	5.13	120.81	118.30
2	A	1005	CZA	C8-C9-N1	4.37	106.39	100.97

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.

## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues

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.