

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

#### Oct 23, 2023 - 08:10 AM EDT

PDB ID	:	2ZBE
Title	:	Calcium pump crystal structure with bound BeF3 in the absence of calcium
		and TG
Authors	:	Toyoshima, C.; Ogawa, H.; Norimatsu, Y.
Deposited on	:	2007-10-20
Resolution	:	3.80  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 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	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
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)	:	2.36

## 1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:  $X\text{-}RAY \, DIFFRACTION$ 

The reported resolution of this entry is 3.80 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.



Motria	Whole archive	Similar resolution				
wietric	$(\# {\rm Entries})$	$(\# { m Entries}, { m resolution} { m range}({ m \AA}))$				
Clashscore	141614	1288 (4.00-3.60)				
Ramachandran outliers	138981	1243 (4.00-3.60)				
Sidechain outliers	138945	1237 (4.00-3.60)				

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 of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. 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 <=5%

Note EDS was not executed.

Mol	Chain	Length	Qualit	y of chain	
1	А	995	49%	43%	8%
1	В	995	49%	43%	8%



# 2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 15358 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		Α	toms		ZeroOcc	AltConf	Trace	
1	А	995	Total 7674	C 4878	N 1287	O 1452	${ m S}\ 57$	1	0	0
1	В	995	Total 7674	C 4878	N 1287	O 1452	S 57	1	0	0

There are 2 discrepancies between the modelled and reference sequences:

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

• Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	А	1	Total Mg 1 1	0	0
2	В	1	Total Mg 1 1	0	0

• Molecule 3 is BERYLLIUM TRIFLUORIDE ION (three-letter code: BEF) (formula: BeF<sub>3</sub>).





Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	
3	Λ	1	Total Be F	0	0	
0	Λ	1	4 1 3	0	0	
2	В	1	Total Be F	0	0	
0	D	T	4 1 3	0	0	



# 3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. 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. 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



# 1931 1931 1933 1933 1933 1934 1933 1934 1935 1934 1947 1947 1947 1946 1947 1947 1946 1946 1947 1956 1956 1956 1956 1956 1956 1956 1956 1956 1956 1956 1957 1956 1956 1956 1957 1956 1956 1956 1957 1957 1957 1956 1956 1956 1957 1956 1956 1956 1957 1957 1957 1957 1957 1958 1958 1958 1957 1954 1958 1958 1958 1954 1957 1954 1958</t

 $\bullet$  Molecule 1: Sarcoplasmic/endoplasmic reticulum calcium ATPase 1

Chain	B:						4	9%	1													4	439	%							89	%			
ACEO M1 E2 A3	E10	V18	623 L24 T25		07h	R31	Y36	H38	N39 E40	E40 L41	P42	A43 E44	E45	G46 V 17	548 S48	L49	W50 FE1	L52	V53 T54	E55	056 857	E58	D59	L61	V62 R63	164	L65 1 66	L67	A68	A69 C70	171	572 F73	V74	L75 A76	<mark>W77</mark> F78
E79 E80 G81 E82	E03 T84 I85	T86 A87	F88 V89 F90	P91	r92 V93	194 L95	L96 107	19/ L98	199 100	N101	A102	1103 V104	G105	V106	0108 0108	E109	R110 N111	A112	E113 N114	A115	1116 5117	A118	L119	E121	F1 OF	M126	G127	V129		A132 D133	R134	I140	-	R143 D144	1145
D149 1150 V151	0155 0156 0157	A161	R164	T172	L1/3 R174	V175	1188	P193	V194	OPTA	S210	1214		1222	T226		E231	1232 G233	K234 1235	1236 R236	D237	4230 M239	C S C S C S C S C S C S C S C S C S C S	1242 E243	0244 D245	K246	T247	r 240 L249	Q250	4251 K252		E255 F256	G257	E258 Q259	L260 S261
K262 V263 1264 S265	1267 1267 C268	V269	W272 L273 T274		1070	H284	R290	4291 A292	1293 V004	1234 Y295	F296	K297 1298	A299	V300	L302	A303	V304 A305	A306	1307 P308	E309	G310	P312	A313	V314 I315	T316 T317	C318	L319 A270	L321	G322	1323 R324	R325	M326	K329	N330 A331	1332 V333
R334 S335 L336 P337	5339 V339 E340	T341 L342	T345	C349	D351	K352 T353	G354 T356	1 355 L356	T357 T350	1 200	M361	5362 V363	C364	K365 M366	F367	I368	1369	N380	<b>3383</b>	I384		P391	1000 1	1402 R403	F419	L413	111 C	01741	N421	D422 S423		D426	V437	G438 E439	T443
T447 L448 V449	R450 N456	T457 E458	V459 R460 N461	L462	X464	V465 E466	E C	1404	S488 P460	D490	R491	V496		R505	V508		P518 F510	G520	V521 1522	D523	R524	Y527	V528	67 QN	R534	V541	TE AE	0 <sup>1</sup> 0 <sup>1</sup>	15 <mark>49</mark>	G553	<b>T554</b>	G555 R556	D557	1559 L559	<mark>R560</mark> C561
L562 A563 L564 A565 Treee		P570 P571	K572 R573 F574	E575 ME76	V577	L578 D579		F584		00001	F593	V596		L600	P602		E606	1611	A617	104	R620	1622 1622	M623	1024 T625	G626 D627		1633	I639	G640	1641 F642	G643	E644	R651	A652 Y653	T654
E657 P662 L663	A004 E665	R671	C675	E680	5682	H683 K684	S685 7666	VOOD	L691	Y694		1697	V705	0 7 0 0	P709		K712 K713	A714	E715 T716	G717	I718	M720	G721	7710	A725 V726		T729	8731	-	L/35 A736	D737	D738 N739	F740	5741 T742	17 <u>43</u>
V747 E748 E749 G750 b751	K/ 51 A752 1753	Y754 N755	N757 K758	0759 1759	r/60 I761	R762 Y763	L764	57.66 S7.66	S767	N/ 60 V7 69	<mark>G770</mark>	E771 V772	V773	C774	L777	T778	1781	G782	L783 P784	E785	A786	L/ 0/ 1788	P789	0791 0791	L792 1.793	W7 94	V795	L797	V7 98	1799 D800	<mark>G</mark> 801	L802 P803	A804	2081 4806	L807
N810 P811 P812 D813 D813	L014 D815 I816	M817 D818 D818	R819 P820 D821	R822	5823 P824	K825 E826	P827	L020 1829	S830	4031 W832	L833	F834 F835	R836	Y837 M020	1030 A839	1840	G841	Y843	V844 G845	A846	A847 Teas	1040 V849	G850	A851 A852	4853 MR54	W855	F856 MGE7	Y858	<u>A859</u>	E860 D861	G862	P863 G864	V865	1866 7867	H868 Q869
L870 T871 H872 F873 M877	E878	D879 H880	F881 H882 F883	E884	1886 L886	F891	E892	P894	E895	M897	T898	M899 A900	L901	S902 V002	1904 L904	V905	T906	E908	M909 C910	N911	A912	L913 N914	S915	2017 S917	E918 N919	<b>Q920</b>	5921	H923	R924	M925 P926	P927	W928 V929	N930	1931 W932	L933
1937 0938 1939	L343 H944	1947	0951	L953	M955	1956 F957	K958	C960	A961	D963	L964	T965 0966	V967	L968 M060	079V	L971	K972 T073	S974	L975 P976	V977	1978	201	E982	1983 L984	4988		L992 E003	G994							



## 4 Data and refinement statistics (i)

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

Property	Value	Source				
Space group	P 21 21 21	Depositor				
Cell constants	133.87Å 91.59Å 248.46Å	Depositor				
a, b, c, $\alpha$ , $\beta$ , $\gamma$	$90.00^{\circ}$ $90.00^{\circ}$ $90.00^{\circ}$	Depositor				
Resolution (Å)	12.00 - 3.80	Depositor				
% Data completeness	90.3 (12.00-3.80)	Depositor				
(in resolution range)	30.3 (12.00 3.00)					
$R_{merge}$	0.09	Depositor				
R <sub>sym</sub>	(Not available)	Depositor				
Refinement program	CNS 1.2	Depositor				
$R, R_{free}$	0.293 , $0.327$	Depositor				
Estimated twinning fraction	No twinning to report.	Xtriage				
Total number of atoms	15358	wwPDB-VP				
Average B, all atoms $(Å^2)$	163.0	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: BEF, ACE, MG

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).

Mal	Chain	Bo	nd lengths	Bond angles							
	Chain	RMSZ	# Z  > 5	RMSZ	# Z  > 5						
1	А	0.74	2/7813~(0.0%)	0.89	25/10594~(0.2%)						
1	В	0.75	1/7813~(0.0%)	0.86	15/10594~(0.1%)						
All	All	0.74	3/15626~(0.0%)	0.88	40/21188~(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	А	0	2
1	В	0	2
All	All	0	4

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	А	107	TRP	CB-CG	5.95	1.60	1.50
1	А	863	PRO	C-N	-5.75	1.22	1.33
1	В	561	CYS	CB-SG	-5.35	1.73	1.81

The worst 5 of 40 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Ζ	$Observed(^{o})$	$Ideal(^{o})$
1	А	671	ARG	NE-CZ-NH1	9.46	125.03	120.30
1	А	822	ARG	NE-CZ-NH2	7.72	124.16	120.30
1	А	651	ARG	NE-CZ-NH2	7.24	123.92	120.30
1	А	762	ARG	NE-CZ-NH2	7.24	123.92	120.30
1	А	290	ARG	NE-CZ-NH2	7.05	123.82	120.30



There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	А	310	GLY	Mainchain
1	А	68	ALA	Mainchain
1	В	284	HIS	Mainchain
1	В	380	ASN	Mainchain

## 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	А	7674	0	7765	645	0
1	В	7674	0	7765	689	0
2	А	1	0	0	0	0
2	В	1	0	0	0	0
3	А	4	0	0	1	0
3	В	4	0	0	0	0
All	All	15358	0	15530	1334	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 43.

The worst 5 of 1334 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:757:MET:CE	1:A:761:ILE:HD11	1.60	1.30
1:B:762:ARG:HE	1:B:833:LEU:HD21	1.02	1.18
1:B:802:LEU:HD13	1:B:939:LEU:CD2	1.74	1.17
1:A:247:THR:OG1	1:A:250:GLN:HB3	1.45	1.17
1:A:802:LEU:HD13	1:A:939:LEU:CD2	1.76	1.15

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	Pe	erc	entile	es
1	А	993/995~(100%)	883~(89%)	84 (8%)	26 (3%)		5	36	
1	В	993/995~(100%)	876~(88%)	91 (9%)	26~(3%)		5	36	
All	All	1986/1990~(100%)	1759~(89%)	175 (9%)	52 (3%)		5	36	

5 of 52 Ramachandran outliers are listed below:

Mol	Chain	$\operatorname{Res}$	Type
1	А	47	LYS
1	А	245	ASP
1	А	292	ALA
1	А	783	LEU
1	А	818	ASP

#### 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 side chain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles		
1	А	840/840~(100%)	757~(90%)	83 (10%)	8 32		
1	В	840/840~(100%)	761 (91%)	79~(9%)	8 35		
All	All	1680/1680~(100%)	1518 (90%)	162 (10%)	8 34		

5 of 162 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	В	296	PHE
	a .:	7	

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Mol	Chain	Res	Type
1	В	757	MET
1	В	338	SER
1	В	488	SER
1	В	813	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 36 such sidechains are listed below:

Mol	Chain	Res	Type
1	В	461	ASN
1	В	966	GLN
1	В	510	ASN
1	В	875	GLN
1	А	869	GLN

#### 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 monosaccharides in this entry.

## 5.6 Ligand geometry (i)

Of 4 ligands modelled in this entry, 2 are monoatomic - leaving 2 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).



Mal Turna C		Chain Bos	Chain	Chain	Chain	Chain	Chain	Chain	Chain	Chain	Chain	Chain	Chain	Chain	Chain	Chain	Chain	Chain	Chain	Chain	Chain	Chain	Chain	Dog	Pog Link	Bond lengths			Bond angles		
INIOI	туре	Unam	nes	LIIIK	Counts	RMSZ	# Z >2	Counts	RMSZ	# Z >2																					
3	BEF	А	998	1	0,3,3	-	-	-																							
3	BEF	В	1098	1	0,3,3	-	-	-																							

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.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	А	998	BEF	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 (i)

## 6.1 Protein, DNA and RNA chains (i)

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

### 6.3 Carbohydrates (i)

EDS was not executed - this section is therefore empty.

## 6.4 Ligands (i)

EDS was not executed - this section is therefore empty.

### 6.5 Other polymers (i)

EDS was not executed - this section is therefore empty.

