



wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 3, 2017 – 09:42 AM EDT

PDB ID : 5Y0B
Title : PIG GASTRIC H⁺,K⁺ - ATPASE IN COMPLEX with BYK99
Authors : Abe, K.; Shimokawa, J.; Natio, M.; Munson, K.; Vagin, O.; Sachs, G.; Suzuki, H.; Tani, K.; Fujiyoshi, Y.
Deposited on : unknown
Resolution : 6.70 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

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20029824

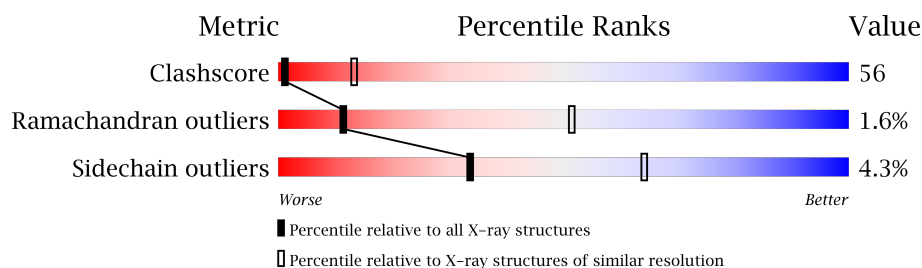
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON CRYSTALLOGRAPHY

The reported resolution of this entry is 6.70 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	112137	1033 (9.50-3.80)
Ramachandran outliers	110173	1002 (9.50-3.76)
Sidechain outliers	110143	1097 (9.50-3.70)

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 ≥ 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	1034	
2	B	290	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 9101 atoms, of which 0 are hydrogens and 0 are deuteriums.

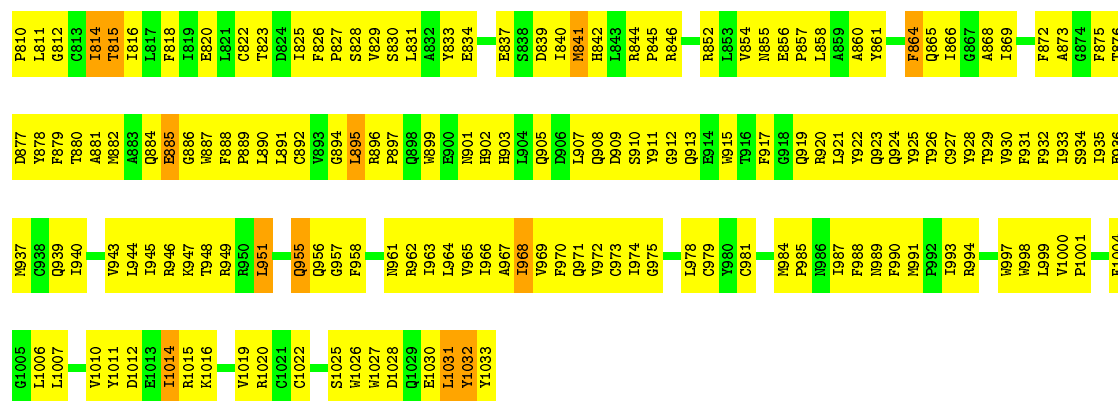
In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Potassium-transporting ATPase alpha chain 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	986	Total	C	N	O	S	0	0	0
			7658	4890	1294	1422	52			

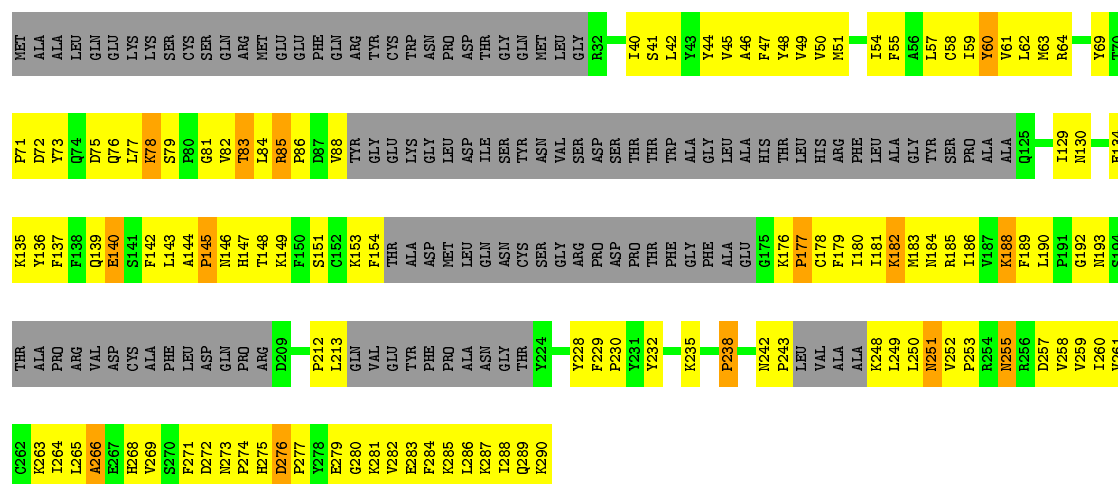
- Molecule 2 is a protein called Potassium-transporting ATPase subunit beta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	175	Total	C	N	O	S	0	0	0
			1443	949	237	249	8			



• Molecule 2: Potassium-transporting ATPase subunit beta

Chain B: 19% 36% 5% 40%



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	142.60Å 112.00Å 320.00Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	200.00 – 6.70	Depositor
% Data completeness (in resolution range)	50.1 (200.00-6.70)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	unknown	Depositor
R, R_{free}	(Not available) , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	9101	wwPDB-VP
Average B, all atoms (Å ²)	30.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

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	0.26	0/7816	0.53	0/10616
2	B	0.29	0/1486	0.53	0/2008
All	All	0.27	0/9302	0.53	0/12624

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-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 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	7658	0	7689	861	1
2	B	1443	0	1431	187	0
All	All	9101	0	9120	1018	1

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 56.

The worst 5 of 1018 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)
2:B:83:THR:HG23	2:B:182:LYS:HD3	1.28	1.10
1:A:837:GLU:HB3	1:A:951:LEU:HD21	1.32	1.09

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:951:LEU:H	1:A:951:LEU:HD23	1.15	1.08
1:A:1027:TRP:HB3	1:A:1031:LEU:CD1	1.84	1.06
1:A:431:CYS:HB3	1:A:473:LEU:HD13	1.32	1.04

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:187:PHE:CZ	1:A:457:ILE:CD1[2_565]	1.04	1.16

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	984/1034 (95%)	913 (93%)	60 (6%)	11 (1%)	17	60
2	B	163/290 (56%)	135 (83%)	21 (13%)	7 (4%)	3	29
All	All	1147/1324 (87%)	1048 (91%)	81 (7%)	18 (2%)	11	51

5 of 18 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	140	GLU
2	B	251	ASN
1	A	93	ARG
1	A	134	THR
1	A	955	GLN

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	833/869 (96%)	801 (96%)	32 (4%)	38	67
2	B	162/254 (64%)	151 (93%)	11 (7%)	18	51
All	All	995/1123 (89%)	952 (96%)	43 (4%)	33	64

5 of 43 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	728	VAL
1	A	841	MET
2	B	182	LYS
1	A	762	ASP
1	A	796	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 30 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	675	ASN
1	A	729	ASN
2	B	268	HIS
1	A	706	GLN
1	A	842	HIS

5.3.3 RNA ⓘ

There are no RNA molecules 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 [i](#)

There are no ligands in this entry.

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 is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates ⓘ

EDS was not executed - this section is therefore empty.

6.4 Ligands ⓘ

EDS was not executed - this section is therefore empty.

6.5 Other polymers ⓘ

EDS was not executed - this section is therefore empty.