



# wwPDB Geometry-Only Validation Summary Report ⓘ

Mar 11, 2018 – 05:17 pm GMT

PDB ID : 4UX2  
Title : Cryo-EM structure of antagonist-bound E2P gastric H,K-ATPase (SCH.E2. MgF)  
Authors : Abe, K.; Tani, K.; Fujiyoshi, Y.  
Deposited on : 2014-08-18  
Resolution : 7.00 Å(reported)

This is a wwPDB Geometry-Only 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk31020

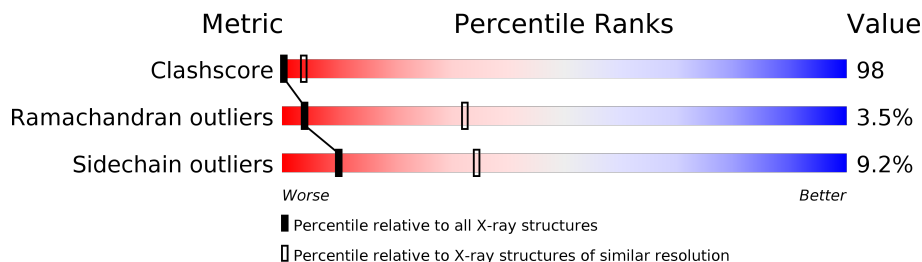
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON CRYSTALLOGRAPHY*

The reported resolution of this entry is 7.00 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	122126	1146 (10.00-3.80)
Ramachandran outliers	120053	1071 (10.00-3.80)
Sidechain outliers	120020	1038 (10.00-3.80)

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  $\leq 5\%$ .

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 9161 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	993	Total	C	N	O	S	0	0	0
			7718	4927	1304	1434	53			

- Molecule 2 is a protein called POTASSIUM-TRANSPORTING ATPASE SUBUNIT BETA.

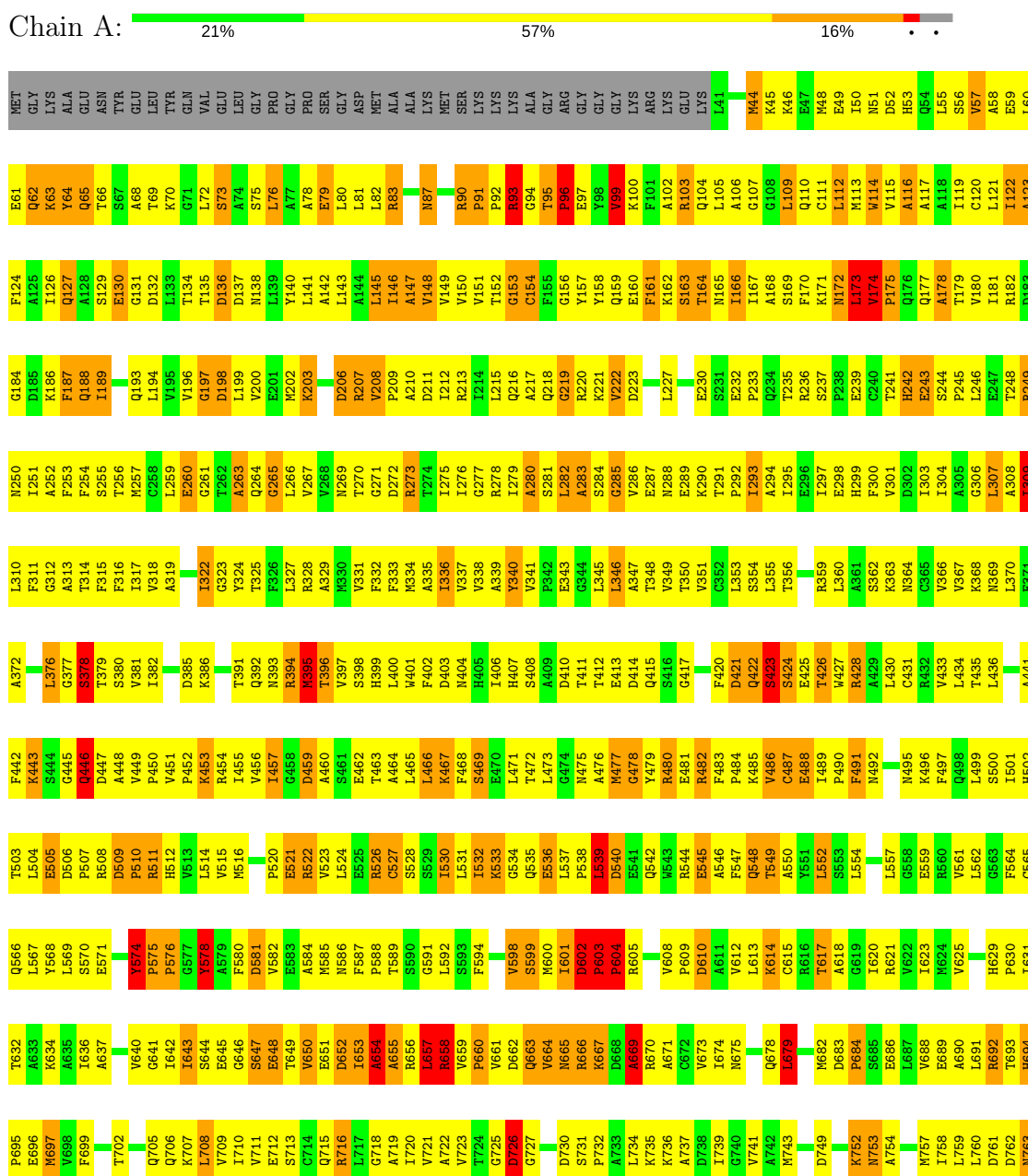
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	175	Total	C	N	O	S	0	0	0
			1443	949	237	249	8			

### 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 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: POTASSIUM-TRANSPORTING ATPASE ALPHA CHAIN 1





## 4 Model quality

### 4.1 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	1.15	3/7876 (0.0%)	1.39	37/10694 (0.3%)
2	B	1.13	1/1486 (0.1%)	1.42	11/2008 (0.5%)
All	All	1.14	4/9362 (0.0%)	1.40	48/12702 (0.4%)

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	160
2	B	0	52
All	All	0	212

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	254	ARG	CZ-NH2	5.23	1.39	1.33
1	A	950	ARG	CZ-NH1	5.07	1.39	1.33
1	A	511	ARG	NE-CZ	5.06	1.39	1.33
1	A	273	ARG	NE-CZ	5.03	1.39	1.33

The worst 5 of 48 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	140	TYR	CB-CG-CD1	10.11	127.07	121.00
2	B	68	PRO	CA-N-CD	-9.05	98.84	111.50
1	A	960	ARG	NE-CZ-NH1	7.32	123.96	120.30
1	A	950	ARG	NE-CZ-NH2	7.29	123.95	120.30
1	A	692	ARG	NE-CZ-NH1	-7.25	116.67	120.30

There are no chirality outliers.

5 of 212 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	44	MET	Mainchain
1	A	62	GLN	Mainchain
1	A	63	LYS	Mainchain
1	A	73	SER	Mainchain
1	A	75	SER	Mainchain

## 4.2 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	7718	0	7746	1572	0
2	B	1443	0	1430	358	0
All	All	9161	0	9176	1793	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 98.

The worst 5 of 1793 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:901:ASN:HB3	1:A:904:LEU:CD1	1.26	1.65
1:A:398:SER:CB	1:A:600:MET:CA	1.78	1.56
1:A:994:ARG:NH1	2:B:73:TYR:CG	1.70	1.55
1:A:913:GLN:NE2	2:B:77:LEU:HD22	1.25	1.48
1:A:398:SER:HB2	1:A:600:MET:CA	0.96	1.42

There are no symmetry-related clashes.

## 4.3 Torsion angles [i](#)

### 4.3.1 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	991/1034 (96%)	904 (91%)	60 (6%)	27 (3%)	5	38
2	B	163/290 (56%)	133 (82%)	17 (10%)	13 (8%)	1	16
All	All	1154/1324 (87%)	1037 (90%)	77 (7%)	40 (4%)	4	32

5 of 40 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	163	SER
1	A	172	ASN
1	A	175	PRO
1	A	283	ALA
1	A	378	SER

#### 4.3.2 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	840/869 (97%)	778 (93%)	62 (7%)	15	45
2	B	162/254 (64%)	132 (82%)	30 (18%)	2	11
All	All	1002/1123 (89%)	910 (91%)	92 (9%)	10	34

5 of 92 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	679	LEU
1	A	884	GLN
2	B	254	ARG
1	A	683	ASP
1	A	763	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 31 such sidechains are listed below:



Mol	Chain	Res	Type
1	A	773	GLN
1	A	884	GLN
2	B	268	HIS
1	A	847	ASN
1	A	903	HIS

#### 4.3.3 RNA [i](#)

There are no RNA molecules in this entry.

#### 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 carbohydrates in this entry.

#### 4.6 Ligand geometry [i](#)

There are no ligands in this entry.

#### 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.