



wwPDB X-ray Structure Validation Summary Report ⓘ

May 29, 2020 – 04:02 am BST

PDB ID : 3U6N
Title : Open Structure of the BK channel Gating Ring
Authors : Yuan, P.; MacKinnon, R.
Deposited on : 2011-10-12
Resolution : 3.61 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 ⓘ symbol.

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

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

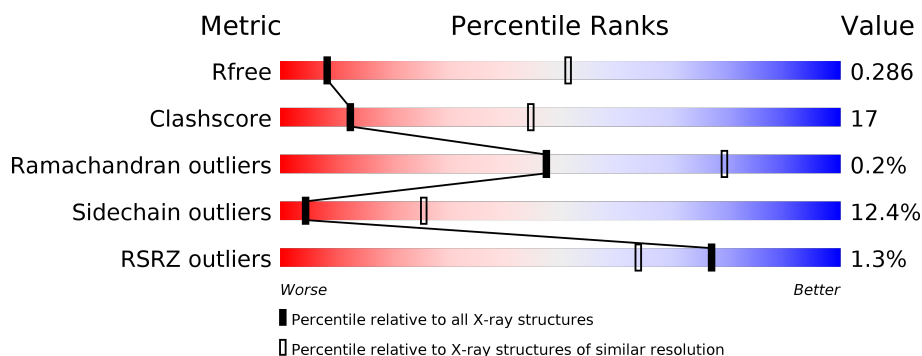
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.61 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))
R_{free}	130704	1290 (3.74-3.50)
Clashscore	141614	1387 (3.74-3.50)
Ramachandran outliers	138981	1339 (3.74-3.50)
Sidechain outliers	138945	1339 (3.74-3.50)
RSRZ outliers	127900	1191 (3.74-3.50)

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 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 $\leq 5\%$. 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.

Mol	Chain	Length	Quality of chain
1	A	696	<div> <div>%</div> <div> <div></div> <div>56%</div> <div>25%</div> <div>•</div> <div>16%</div> </div> </div>
1	B	696	<div> <div>%</div> <div> <div></div> <div>56%</div> <div>25%</div> <div>•</div> <div>16%</div> </div> </div>
1	C	696	<div> <div></div> <div> <div>55%</div> <div>26%</div> <div>•</div> <div>16%</div> </div> </div>
1	D	696	<div> <div>%</div> <div> <div></div> <div>56%</div> <div>24%</div> <div>•</div> <div>16%</div> </div> </div>
1	E	696	<div> <div>%</div> <div> <div></div> <div>56%</div> <div>25%</div> <div>•</div> <div>16%</div> </div> </div>
1	F	696	<div> <div>%</div> <div> <div></div> <div>57%</div> <div>24%</div> <div>•</div> <div>16%</div> </div> </div>

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Mol	Chain	Length	Quality of chain
1	G	696	<div><div><div></div><div></div><div></div><div></div></div><div><div>2%</div><div>56%</div><div>25%</div><div>•</div><div>16%</div></div></div>
1	H	696	<div><div><div></div><div></div><div></div><div></div></div><div><div>2%</div><div>56%</div><div>24%</div><div>•</div><div>16%</div></div></div>

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 34504 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 High-Conductance Ca²⁺-Activated K⁺ Channel protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	585	Total	C	N	O	S	0	0	0
			4312	2756	722	800	34			
1	B	585	Total	C	N	O	S	0	0	0
			4312	2756	722	800	34			
1	C	585	Total	C	N	O	S	0	0	0
			4312	2756	722	800	34			
1	D	585	Total	C	N	O	S	0	0	0
			4312	2756	722	800	34			
1	E	585	Total	C	N	O	S	0	0	0
			4312	2756	722	800	34			
1	F	585	Total	C	N	O	S	0	0	0
			4312	2756	722	800	34			
1	G	585	Total	C	N	O	S	0	0	0
			4312	2756	722	800	34			
1	H	585	Total	C	N	O	S	0	0	0
			4312	2756	722	800	34			

There are 120 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	340	MET	-	initiating methionine	UNP B7ZC96
A	578	ARG	-	see remark 999	UNP B7ZC96
A	579	SER	-	see remark 999	UNP B7ZC96
A	580	ARG	-	see remark 999	UNP B7ZC96
A	581	LYS	-	see remark 999	UNP B7ZC96
A	582	ARG	SER	see remark 999	UNP B7ZC96
A	1061	SER	-	expression tag	UNP F1QYL4
A	1062	ASN	-	expression tag	UNP F1QYL4
A	1063	SER	-	expression tag	UNP F1QYL4
A	1064	LEU	-	expression tag	UNP F1QYL4
A	1065	GLU	-	expression tag	UNP F1QYL4
A	1066	VAL	-	expression tag	UNP F1QYL4
A	1067	LEU	-	expression tag	UNP F1QYL4

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Chain	Residue	Modelled	Actual	Comment	Reference
A	1068	PHE	-	expression tag	UNP F1QYL4
A	1069	GLN	-	expression tag	UNP F1QYL4
B	340	MET	-	initiating methionine	UNP B7ZC96
B	578	ARG	-	see remark 999	UNP B7ZC96
B	579	SER	-	see remark 999	UNP B7ZC96
B	580	ARG	-	see remark 999	UNP B7ZC96
B	581	LYS	-	see remark 999	UNP B7ZC96
B	582	ARG	SER	see remark 999	UNP B7ZC96
B	1061	SER	-	expression tag	UNP F1QYL4
B	1062	ASN	-	expression tag	UNP F1QYL4
B	1063	SER	-	expression tag	UNP F1QYL4
B	1064	LEU	-	expression tag	UNP F1QYL4
B	1065	GLU	-	expression tag	UNP F1QYL4
B	1066	VAL	-	expression tag	UNP F1QYL4
B	1067	LEU	-	expression tag	UNP F1QYL4
B	1068	PHE	-	expression tag	UNP F1QYL4
B	1069	GLN	-	expression tag	UNP F1QYL4
C	340	MET	-	initiating methionine	UNP B7ZC96
C	578	ARG	-	see remark 999	UNP B7ZC96
C	579	SER	-	see remark 999	UNP B7ZC96
C	580	ARG	-	see remark 999	UNP B7ZC96
C	581	LYS	-	see remark 999	UNP B7ZC96
C	582	ARG	SER	see remark 999	UNP B7ZC96
C	1061	SER	-	expression tag	UNP F1QYL4
C	1062	ASN	-	expression tag	UNP F1QYL4
C	1063	SER	-	expression tag	UNP F1QYL4
C	1064	LEU	-	expression tag	UNP F1QYL4
C	1065	GLU	-	expression tag	UNP F1QYL4
C	1066	VAL	-	expression tag	UNP F1QYL4
C	1067	LEU	-	expression tag	UNP F1QYL4
C	1068	PHE	-	expression tag	UNP F1QYL4
C	1069	GLN	-	expression tag	UNP F1QYL4
D	340	MET	-	initiating methionine	UNP B7ZC96
D	578	ARG	-	see remark 999	UNP B7ZC96
D	579	SER	-	see remark 999	UNP B7ZC96
D	580	ARG	-	see remark 999	UNP B7ZC96
D	581	LYS	-	see remark 999	UNP B7ZC96
D	582	ARG	SER	see remark 999	UNP B7ZC96
D	1061	SER	-	expression tag	UNP F1QYL4
D	1062	ASN	-	expression tag	UNP F1QYL4
D	1063	SER	-	expression tag	UNP F1QYL4
D	1064	LEU	-	expression tag	UNP F1QYL4

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Chain	Residue	Modelled	Actual	Comment	Reference
D	1065	GLU	-	expression tag	UNP F1QYL4
D	1066	VAL	-	expression tag	UNP F1QYL4
D	1067	LEU	-	expression tag	UNP F1QYL4
D	1068	PHE	-	expression tag	UNP F1QYL4
D	1069	GLN	-	expression tag	UNP F1QYL4
E	340	MET	-	initiating methionine	UNP B7ZC96
E	578	ARG	-	see remark 999	UNP B7ZC96
E	579	SER	-	see remark 999	UNP B7ZC96
E	580	ARG	-	see remark 999	UNP B7ZC96
E	581	LYS	-	see remark 999	UNP B7ZC96
E	582	ARG	SER	see remark 999	UNP B7ZC96
E	1061	SER	-	expression tag	UNP F1QYL4
E	1062	ASN	-	expression tag	UNP F1QYL4
E	1063	SER	-	expression tag	UNP F1QYL4
E	1064	LEU	-	expression tag	UNP F1QYL4
E	1065	GLU	-	expression tag	UNP F1QYL4
E	1066	VAL	-	expression tag	UNP F1QYL4
E	1067	LEU	-	expression tag	UNP F1QYL4
E	1068	PHE	-	expression tag	UNP F1QYL4
E	1069	GLN	-	expression tag	UNP F1QYL4
F	340	MET	-	initiating methionine	UNP B7ZC96
F	578	ARG	-	see remark 999	UNP B7ZC96
F	579	SER	-	see remark 999	UNP B7ZC96
F	580	ARG	-	see remark 999	UNP B7ZC96
F	581	LYS	-	see remark 999	UNP B7ZC96
F	582	ARG	SER	see remark 999	UNP B7ZC96
F	1061	SER	-	expression tag	UNP F1QYL4
F	1062	ASN	-	expression tag	UNP F1QYL4
F	1063	SER	-	expression tag	UNP F1QYL4
F	1064	LEU	-	expression tag	UNP F1QYL4
F	1065	GLU	-	expression tag	UNP F1QYL4
F	1066	VAL	-	expression tag	UNP F1QYL4
F	1067	LEU	-	expression tag	UNP F1QYL4
F	1068	PHE	-	expression tag	UNP F1QYL4
F	1069	GLN	-	expression tag	UNP F1QYL4
G	340	MET	-	initiating methionine	UNP B7ZC96
G	578	ARG	-	see remark 999	UNP B7ZC96
G	579	SER	-	see remark 999	UNP B7ZC96
G	580	ARG	-	see remark 999	UNP B7ZC96
G	581	LYS	-	see remark 999	UNP B7ZC96
G	582	ARG	SER	see remark 999	UNP B7ZC96
G	1061	SER	-	expression tag	UNP F1QYL4

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Chain	Residue	Modelled	Actual	Comment	Reference
G	1062	ASN	-	expression tag	UNP F1QYL4
G	1063	SER	-	expression tag	UNP F1QYL4
G	1064	LEU	-	expression tag	UNP F1QYL4
G	1065	GLU	-	expression tag	UNP F1QYL4
G	1066	VAL	-	expression tag	UNP F1QYL4
G	1067	LEU	-	expression tag	UNP F1QYL4
G	1068	PHE	-	expression tag	UNP F1QYL4
G	1069	GLN	-	expression tag	UNP F1QYL4
H	340	MET	-	initiating methionine	UNP B7ZC96
H	578	ARG	-	see remark 999	UNP B7ZC96
H	579	SER	-	see remark 999	UNP B7ZC96
H	580	ARG	-	see remark 999	UNP B7ZC96
H	581	LYS	-	see remark 999	UNP B7ZC96
H	582	ARG	SER	see remark 999	UNP B7ZC96
H	1061	SER	-	expression tag	UNP F1QYL4
H	1062	ASN	-	expression tag	UNP F1QYL4
H	1063	SER	-	expression tag	UNP F1QYL4
H	1064	LEU	-	expression tag	UNP F1QYL4
H	1065	GLU	-	expression tag	UNP F1QYL4
H	1066	VAL	-	expression tag	UNP F1QYL4
H	1067	LEU	-	expression tag	UNP F1QYL4
H	1068	PHE	-	expression tag	UNP F1QYL4
H	1069	GLN	-	expression tag	UNP F1QYL4


- Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca).

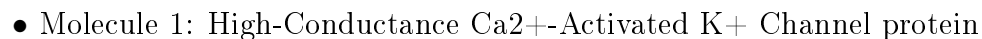
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	G	1	Total Ca 1 1	0	0
2	D	1	Total Ca 1 1	0	0
2	E	1	Total Ca 1 1	0	0
2	H	1	Total Ca 1 1	0	0
2	B	1	Total Ca 1 1	0	0
2	C	1	Total Ca 1 1	0	0
2	A	1	Total Ca 1 1	0	0
2	F	1	Total Ca 1 1	0	0

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 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.

- Chain A:

Position	Residue	Conservation (bits)
1	Met	0.15
2	Gly	0.15
3	Arg	0.15
4	Arg	0.15
5	Arg	0.15
6	Arg	0.15
7	Arg	0.15
8	Arg	0.15
9	Arg	0.15
10	Arg	0.15
11	Arg	0.15
12	Arg	0.15
13	Arg	0.15
14	Arg	0.15
15	Arg	0.15
16	Arg	0.15
17	Arg	0.15
18	Arg	0.15
19	Arg	0.15
20	Arg	0.15

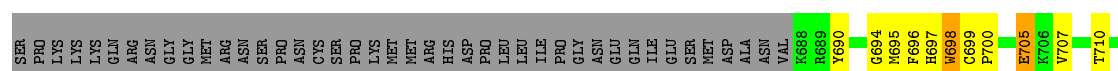
- Chain B: 



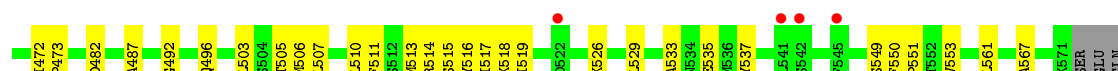
D935	ASN	S720	SER	GLU	H464	MET
N936	ASN	G721	PRO	SER	N465	GLY
I937	ILE	H722	LYS	ARG	N468	ARG
L938	ASP		LYS	SER	H468	K349
L939	ASP	V725	LYS	ARG	N471	H244
L940	A617	C726	GLN	K581		I345
I941	S818	I727	ANG	R582		
R942			ASN	S583		
V945	D821	L735	GLY	N586		I351
A949	L825	L738	MET		D482	T352
THR	L226		ARG	N589	A487	L353
PRO	L829	V742	ASN	H590	G492	E354
GLU	N830	M743	SER		Q496	S355
L953	N830	P744	PRO	M593		V356
E954	N834	L745	ASN		L503	F363
		R746	CYS	F600	S504	L364
A958	D637	A747	SER		T505	H365
E959	S748	N748	PRO	S804	N506	K366
N960	ASP	N749	LYS	D605	L507	
N961	SER	F750	MET	A606	A508	N372
A962	VAL		MET	K607	N509	V376
L963	T875	P757	ARG	E608	L510	
		I758	HIS	V609	F511	H379
S968	I880	V759	ASP	K610	S512	
	P881	F760	PRO	R611	N513	E386
			LEU	A612	B514	
T972	B385	L764	LEU	F613	S515	F395
	L886	D765	ILE	K614	L516	
R976	V687	V766	PRO	TTR	I517	V398
	N888	L767	GLY	CYS	K518	E399
V981	N891	R769	GLU	LVS	L519	F400
	V692	E770	GLN	ALA	Y401	Y401
		N771	ILE	HIS	K526	Q402
Y987	L895	E772	GLU	ASP	L529	V405
D988	D896	I773	SER	ASP	A533	
G989		L774	MET	ILE	N534	R413
F1004	P903	H775	ASP	THR	E535	V414
K1005		N776	ALA	ASP	N536	
A1007	L907		ASN	PRO	N537	E417
L1008	N908	F781	VAL	LVS		S418
T1010	L909	P787	K688	ARG		
	P912	R790	Y690	ILE	F545	L423
L1014	P912			LVS		
G1015	L924	L793	G694	LVS	S549	N427
F1016	L925		N695	CYS	F550	
		V796	F696	GLY	P551	C430
L1021	S926	N797	H697	LVS	T552	A431
A1024	N927	N798	N698	ARG	V553	
HIS	N928	L800	G699	ILE	L561	E436
LEU	N929	C801	P700	GLU		N449
ALA	E930	D802	E705	ASP	A567	Y450
P1029	T931	N803	V707	GLU		H451
				GLU	K571	P452
	Y932			PRO	SER	
	N934	N810	T710	THR	GLU	L461
		G810		LEU	N467	Q462

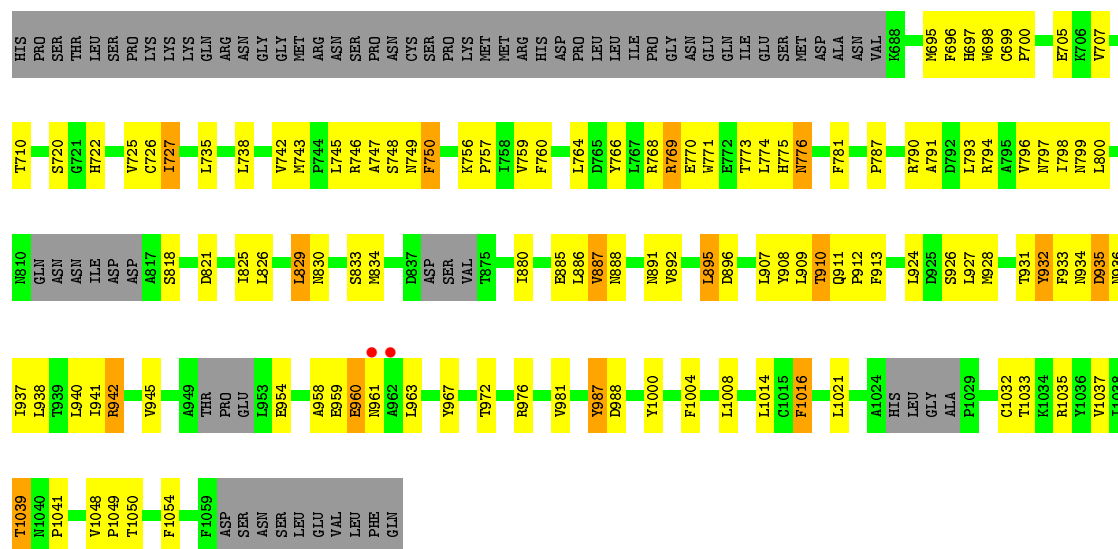


• Molecule 1: High-Conductance Ca²⁺-Activated K⁺ Channel protein

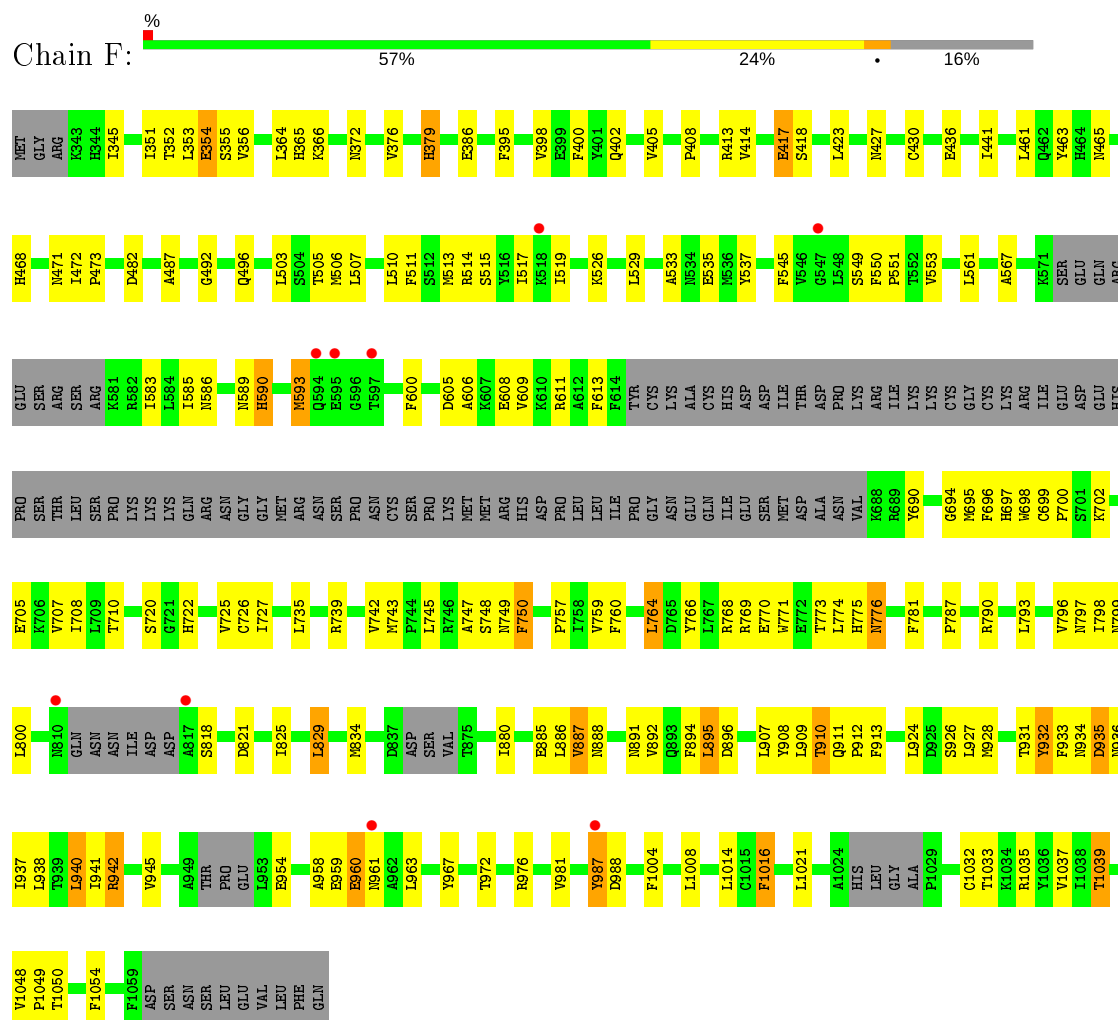


• Molecule 1: High-Conductance Ca²⁺-Activated K⁺ Channel protein

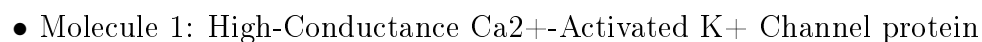


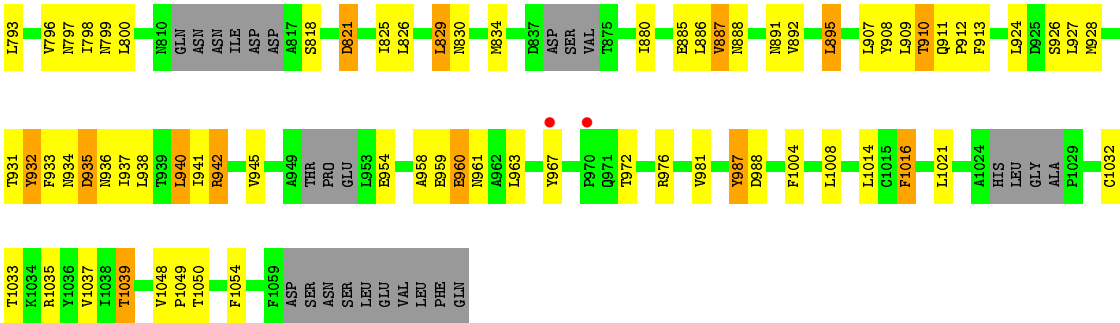


- Molecule 1: High-Conductance Ca^{2+} -Activated K^{+} Channel protein



- Molecule 1: High-Conductance Ca^{2+} -Activated K^{+} Channel protein





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	137.65Å 210.82Å 238.76Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.22 – 3.61 48.21 – 3.61	Depositor EDS
% Data completeness (in resolution range)	89.0 (48.22-3.61) 89.1 (48.21-3.61)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.37 (at 3.57Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.260 , 0.289 0.258 , 0.286	Depositor DCC
R_{free} test set	3620 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	91.1	Xtriage
Anisotropy	0.051	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 49.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.88	EDS
Total number of atoms	34504	wwPDB-VP
Average B, all atoms (Å ²)	104.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.04% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

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:
CA

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	0.42	0/4398	0.56	0/6001
1	B	0.42	1/4398 (0.0%)	0.56	0/6001
1	C	0.43	0/4398	0.56	0/6001
1	D	0.42	1/4398 (0.0%)	0.56	0/6001
1	E	0.43	0/4398	0.57	0/6001
1	F	0.43	0/4398	0.57	0/6001
1	G	0.42	0/4398	0.56	0/6001
1	H	0.41	0/4398	0.56	0/6001
All	All	0.42	2/35184 (0.0%)	0.56	0/48008

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	698	TRP	CD2-CE2	5.27	1.47	1.41
1	D	698	TRP	CD2-CE2	5.12	1.47	1.41

There are no bond angle outliers.

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	4312	0	4016	143	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	4312	0	4016	144	0
1	C	4312	0	4017	145	0
1	D	4312	0	4016	148	1
1	E	4312	0	4017	147	1
1	F	4312	0	4017	147	1
1	G	4312	0	4017	155	1
1	H	4312	0	4017	145	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
2	E	1	0	0	0	0
2	F	1	0	0	0	0
2	G	1	0	0	0	0
2	H	1	0	0	0	0
All	All	34504	0	32133	1117	2

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 17.

The worst 5 of 1117 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:B:511:PHE:CZ	1:B:941:ILE:CG2	2.27	1.17
1:G:511:PHE:CZ	1:G:941:ILE:CG2	2.28	1.17
1:H:511:PHE:CZ	1:H:941:ILE:CG2	2.28	1.16
1:C:511:PHE:CZ	1:C:941:ILE:CG2	2.29	1.15
1:E:511:PHE:CZ	1:E:941:ILE:CG2	2.29	1.15

All (2) 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:D:716:MET:CE	1:G:1005:CYS:CB[3_454]	2.06	0.14
1:E:987:TYR:OH	1:F:702:LYS:C[4_555]	2.17	0.03

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	571/696 (82%)	540 (95%)	30 (5%)	1 (0%)	47	79
1	B	571/696 (82%)	539 (94%)	31 (5%)	1 (0%)	47	79
1	C	571/696 (82%)	538 (94%)	32 (6%)	1 (0%)	47	79
1	D	571/696 (82%)	540 (95%)	30 (5%)	1 (0%)	47	79
1	E	571/696 (82%)	538 (94%)	32 (6%)	1 (0%)	47	79
1	F	571/696 (82%)	539 (94%)	31 (5%)	1 (0%)	47	79
1	G	571/696 (82%)	539 (94%)	31 (5%)	1 (0%)	47	79
1	H	571/696 (82%)	537 (94%)	33 (6%)	1 (0%)	47	79
All	All	4568/5568 (82%)	4310 (94%)	250 (6%)	8 (0%)	47	79

5 of 8 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	799	ASN
1	D	799	ASN
1	F	799	ASN
1	G	799	ASN
1	H	799	ASN

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	432/616 (70%)	378 (88%)	54 (12%)	4	25

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	432/616 (70%)	379 (88%)	53 (12%)	4	26
1	C	432/616 (70%)	378 (88%)	54 (12%)	4	25
1	D	432/616 (70%)	378 (88%)	54 (12%)	4	25
1	E	432/616 (70%)	379 (88%)	53 (12%)	4	26
1	F	432/616 (70%)	379 (88%)	53 (12%)	4	26
1	G	432/616 (70%)	378 (88%)	54 (12%)	4	25
1	H	432/616 (70%)	379 (88%)	53 (12%)	4	26
All	All	3456/4928 (70%)	3028 (88%)	428 (12%)	4	25

5 of 428 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	885	GLU
1	E	768	ARG
1	H	745	LEU
1	D	935	ASP
1	E	365	HIS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 53 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	468	HIS
1	E	468	HIS
1	H	465	ASN
1	D	697	HIS
1	D	891	ASN

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 [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 8 ligands modelled in this entry, 8 are monoatomic - leaving 0 for Mogul analysis.

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.

No monomer is involved in short contacts.

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 ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	585/696 (84%)	-0.23	4 (0%) 87 78	58, 105, 158, 185	0
1	B	585/696 (84%)	-0.22	5 (0%) 84 73	67, 105, 151, 179	0
1	C	585/696 (84%)	-0.31	3 (0%) 91 83	55, 95, 141, 181	0
1	D	585/696 (84%)	-0.22	6 (1%) 82 70	57, 102, 155, 217	0
1	E	585/696 (84%)	-0.28	8 (1%) 75 61	50, 86, 134, 180	0
1	F	585/696 (84%)	-0.22	9 (1%) 73 60	59, 96, 149, 200	0
1	G	585/696 (84%)	-0.09	15 (2%) 56 40	68, 108, 160, 198	0
1	H	585/696 (84%)	-0.08	13 (2%) 62 46	75, 112, 161, 203	0
All	All	4680/5568 (84%)	-0.21	63 (1%) 77 64	50, 101, 154, 217	0

The worst 5 of 63 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	875	THR	4.5
1	F	595	GLU	4.3
1	D	718	VAL	4.1
1	A	966	GLY	3.8
1	G	970	PRO	3.7

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	CA	H	2001	1/1	0.91	0.14	82,82,82,82	0
2	CA	F	2001	1/1	0.91	0.15	72,72,72,72	0
2	CA	C	2001	1/1	0.96	0.08	61,61,61,61	0
2	CA	B	2001	1/1	0.97	0.12	73,73,73,73	0
2	CA	A	2001	1/1	0.97	0.08	68,68,68,68	0
2	CA	D	2001	1/1	0.97	0.10	50,50,50,50	0
2	CA	E	2001	1/1	0.97	0.09	57,57,57,57	0
2	CA	G	2001	1/1	0.98	0.11	57,57,57,57	0

6.5 Other polymers [i](#)

There are no such residues in this entry.