wwPDB X-ray Structure Validation Summary Report (i)

May 18, 2020 – 01:51 am BST

PDB ID	:	3NAF
Title	:	Structure of the Intracellular Gating Ring from the Human High-conductance Ca2+ gated K+ Channel (BK Channel)
Authors	:	Wu, Y.; Yang, Y.; Ye, S.; Jiang, Y.
Deposited on	:	2010-06-01
Resolution	:	3.10 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 following versions of software and data (see references (1)) were used in the production of this report:

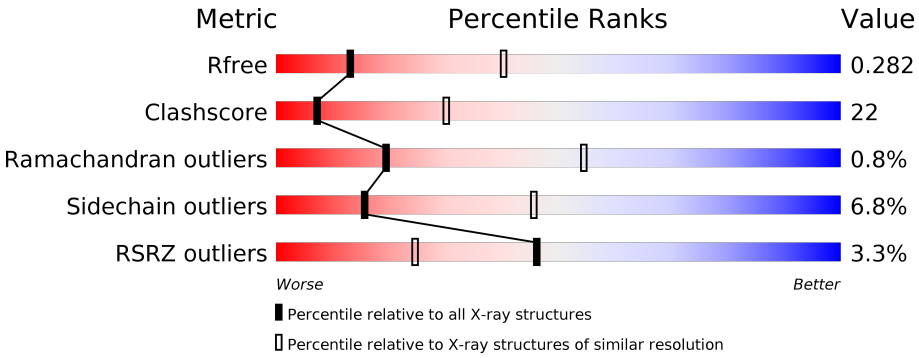
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation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

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.10 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	1094 (3.10-3.10)
Clashscore	141614	1184 (3.10-3.10)
Ramachandran outliers	138981	1141 (3.10-3.10)
Sidechain outliers	138945	1141 (3.10-3.10)
RSRZ outliers	127900	1067 (3.10-3.10)

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 <=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	798	3% 45% 32% . 19%

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 5076 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 Calcium-activated potassium channel subunit alpha-1,Calcium -activated potassium channel subunit alpha-1,Calcium-activated potassium channel subunit alpha-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	648	5076	3237	855	948	36	0	0	0

There are 39 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	290	GLY	-	expression tag	UNP Q12791
A	291	ALA	-	expression tag	UNP Q12791
A	292	MET	-	expression tag	UNP Q12791
A	293	PRO	-	expression tag	UNP Q12791
A	294	ASP	-	expression tag	UNP Q12791
A	295	GLU	-	expression tag	UNP Q12791
A	296	PHE	-	expression tag	UNP Q12791
A	297	ARG	-	expression tag	UNP Q12791
A	298	MET	-	expression tag	UNP Q12791
A	299	LYS	-	expression tag	UNP Q12791
A	300	GLN	-	expression tag	UNP Q12791
A	301	ILE	-	expression tag	UNP Q12791
A	302	GLU	-	expression tag	UNP Q12791
A	303	ASP	-	expression tag	UNP Q12791
A	304	LYS	-	expression tag	UNP Q12791
A	305	LEU	-	expression tag	UNP Q12791
A	306	GLU	-	expression tag	UNP Q12791
A	307	GLU	-	expression tag	UNP Q12791
A	308	ILE	-	expression tag	UNP Q12791
A	309	LEU	-	expression tag	UNP Q12791
A	310	SER	-	expression tag	UNP Q12791
A	311	LYS	-	expression tag	UNP Q12791
A	312	LEU	-	expression tag	UNP Q12791
A	313	TYR	-	expression tag	UNP Q12791
A	314	HIS	-	expression tag	UNP Q12791

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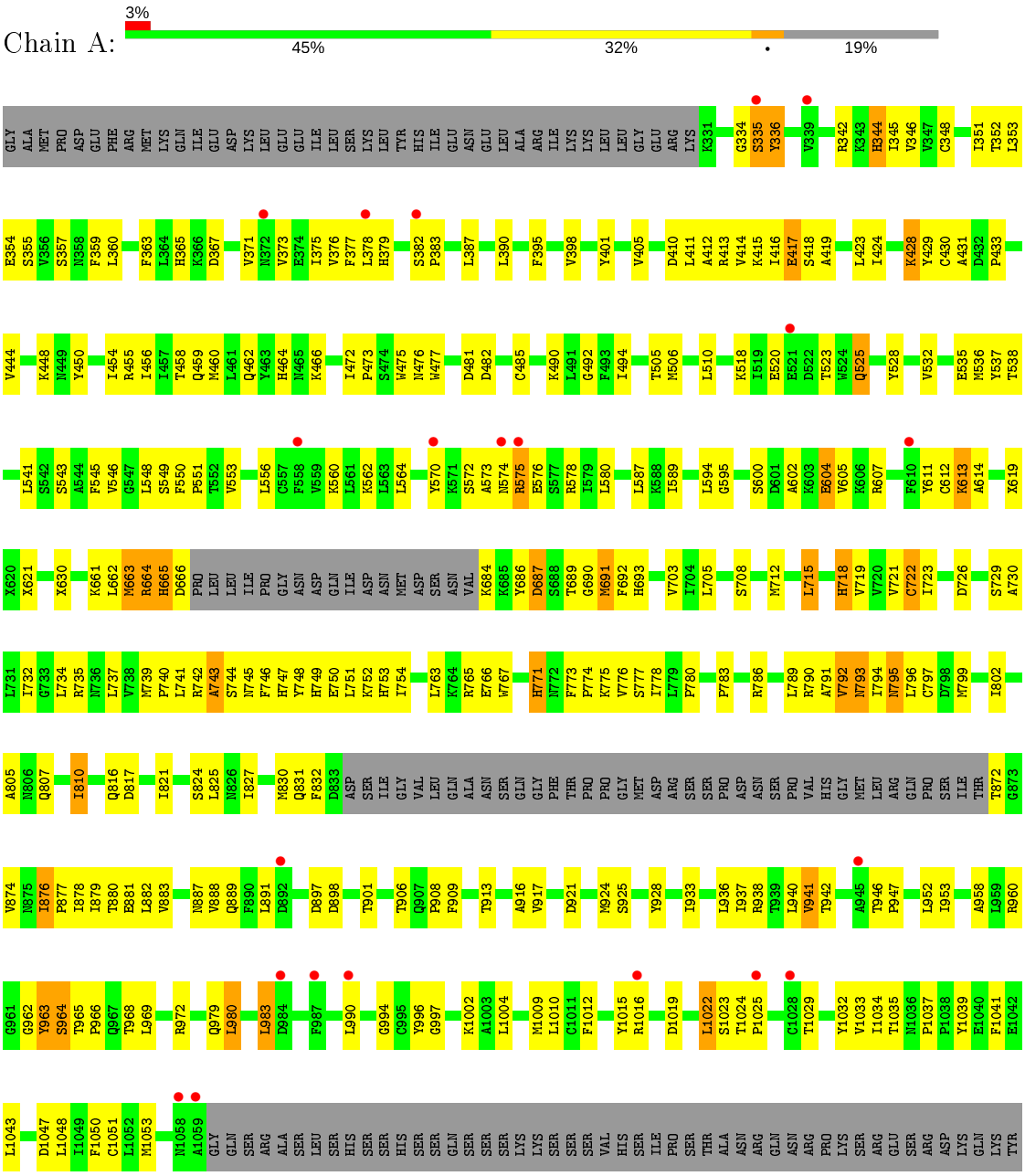
Chain	Residue	Modelled	Actual	Comment	Reference
A	315	ILE	-	expression tag	UNP Q12791
A	316	GLU	-	expression tag	UNP Q12791
A	317	ASN	-	expression tag	UNP Q12791
A	318	GLU	-	expression tag	UNP Q12791
A	319	LEU	-	expression tag	UNP Q12791
A	320	ALA	-	expression tag	UNP Q12791
A	321	ARG	-	expression tag	UNP Q12791
A	322	ILE	-	expression tag	UNP Q12791
A	323	LYS	-	expression tag	UNP Q12791
A	324	LYS	-	expression tag	UNP Q12791
A	325	LEU	-	expression tag	UNP Q12791
A	326	LEU	-	expression tag	UNP Q12791
A	327	GLY	-	expression tag	UNP Q12791
A	328	GLU	-	expression tag	UNP Q12791

3 Residue-property plots (i)

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 (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.

• Molecule 1: Calcium-activated potassium channel subunit alpha-1,Calcium-activated potassium channel subunit alpha-1,Calcium-activated potassium channel subunit alpha-1

Chain A:




VAL
GLN
GLU
GLU
ARG
LEU

4 Data and refinement statistics (i)

Property	Value	Source
Space group	I 4 2 2	Depositor
Cell constants a, b, c, α, β, γ	134.40Å 134.40Å 231.84Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.48 – 3.10 49.48 – 3.05	Depositor EDS
% Data completeness (in resolution range)	88.2 (49.48-3.10) 86.5 (49.48-3.05)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	0.06	Depositor
$< I/\sigma(I) >$ [1]	2.46 (at 3.07Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.6.1_357)	Depositor
R, R_{free}	0.238 , 0.289 0.228 , 0.282	Depositor DCC
R_{free} test set	1977 reflections (10.00%)	wwPDB-VP
Wilson B-factor (Å^2)	99.7	Xtriage
Anisotropy	0.505	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 101.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	5076	wwPDB-VP
Average B, all atoms (Å^2)	139.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.64% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

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	0.24	0/5100	0.49	5/6909 (0.1%)

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	1

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	691	MET	CG-SD-CE	13.79	122.26	100.20
1	A	661	LYS	CB-CA-C	-6.33	97.73	110.40
1	A	964	SER	CB-CA-C	5.92	121.35	110.10
1	A	964	SER	N-CA-C	-5.15	97.08	111.00
1	A	661	LYS	N-CA-C	5.04	124.61	111.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	663	MET	Peptide

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	5076	0	4981	225	0
All	All	5076	0	4981	225	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 22.

The worst 5 of 225 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:665:HIS:O	1:A:665:HIS:HD2	1.31	1.12
1:A:665:HIS:O	1:A:665:HIS:CD2	2.02	1.12
1:A:664:ARG:HG2	1:A:664:ARG:NH1	1.47	1.08
1:A:664:ARG:HH11	1:A:664:ARG:CG	1.61	1.05
1:A:664:ARG:HD3	1:A:665:HIS:N	1.82	0.94

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	Percentiles
1	A	624/798 (78%)	549 (88%)	70 (11%)	5 (1%)	19 54

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	335	SER
1	A	792	VAL
1	A	743	ALA
1	A	793	ASN
1	A	810	ILE

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	555/692 (80%)	517 (93%)	38 (7%)	16 45

5 of 38 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	718	HIS
1	A	771	HIS
1	A	1022	LEU
1	A	745	ASN
1	A	795	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	397	GLN
1	A	616	HIS
1	A	665	HIS
1	A	747	HIS
1	A	831	GLN

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

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	2

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	633:UNK	C	659:SER	N	45.20
1	A	616:HIS	C	618:UNK	N	5.87

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, 95^{th} 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	632/798 (79%)	0.22	21 (3%) 46 24	82, 132, 210, 281	0

The worst 5 of 21 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	574	ASN	4.4
1	A	984	ASP	3.4
1	A	521	GLU	3.3
1	A	575	ARG	3.3
1	A	1059	ALA	3.2

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

There are no ligands in this entry.

6.5 Other polymers

There are no such residues in this entry.