



wwPDB X-ray Structure Validation Summary Report ⓘ

Jan 31, 2016 – 09:49 PM GMT

PDB ID : 1QRQ
Title : STRUCTURE OF A VOLTAGE-DEPENDENT K⁺ CHANNEL BETA SUB-UNIT
Authors : Gulbis, J.M.; Mann, S.; MacKinnon, R.
Deposited on : 1999-06-15
Resolution : 2.80 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
<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
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

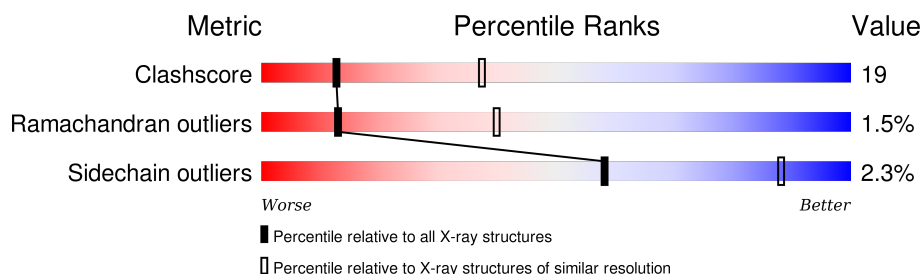
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	102246	2827 (2.80-2.80)
Ramachandran outliers	100387	2782 (2.80-2.80)
Sidechain outliers	100360	2784 (2.80-2.80)

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 ≥ 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	325	
1	B	325	
1	C	325	
1	D	325	

2 Entry composition [i](#)

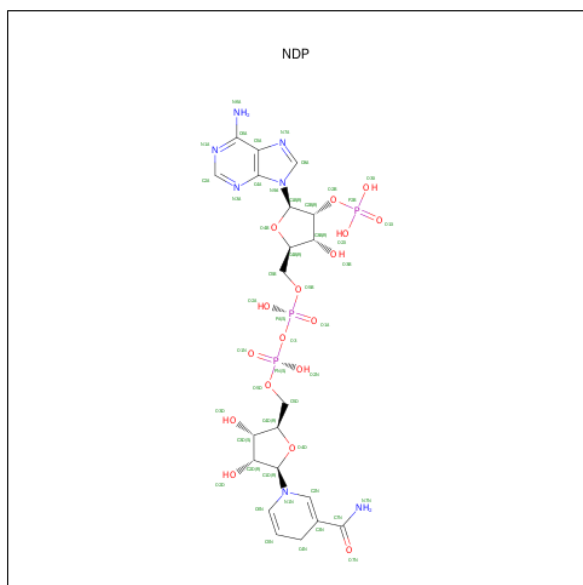
There are 3 unique types of molecules in this entry. The entry contains 10348 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 PROTEIN (KV BETA2 PROTEIN).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	325	Total	C	N	O	S	0	0	0
			2501	1591	436	458	16			
1	B	325	Total	C	N	O	S	0	0	0
			2501	1591	436	458	16			
1	C	325	Total	C	N	O	S	0	0	0
			2501	1591	436	458	16			
1	D	325	Total	C	N	O	S	0	0	0
			2501	1591	436	458	16			

- Molecule 2 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NDP) (formula: C₂₁H₃₀N₇O₁₇P₃).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	B	1	Total	C	N	O	P	0	0
			48	21	7	17	3		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	C	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	D	1	Total	C	N	O	P	0	0
			48	21	7	17	3		

- Molecule 3 is water.

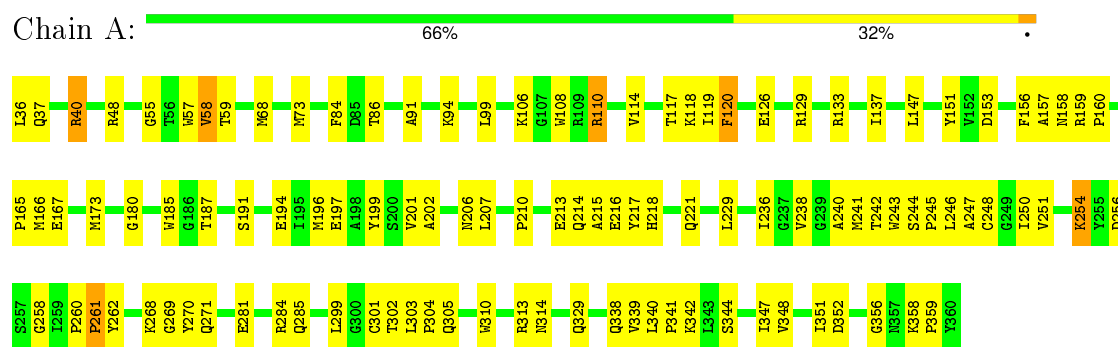
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	38	Total	O	0	0
			38	38		
3	B	38	Total	O	0	0
			38	38		
3	C	38	Total	O	0	0
			38	38		
3	D	38	Total	O	0	0
			38	38		

3 Residue-property plots

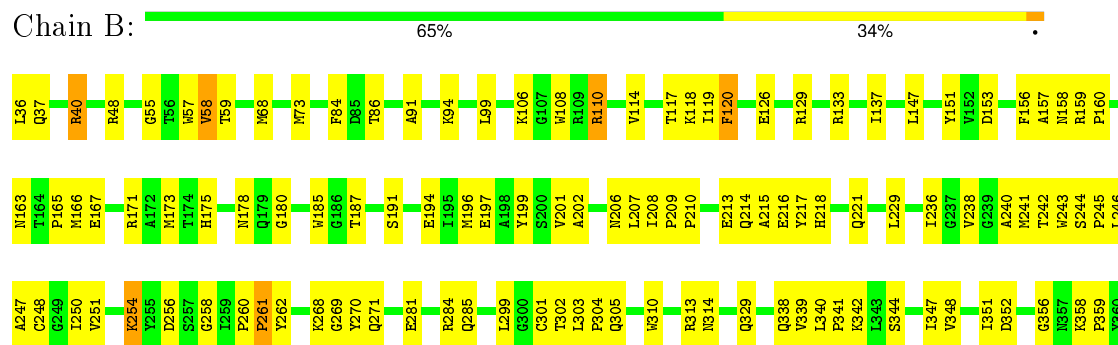
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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.

Note EDS was not executed.

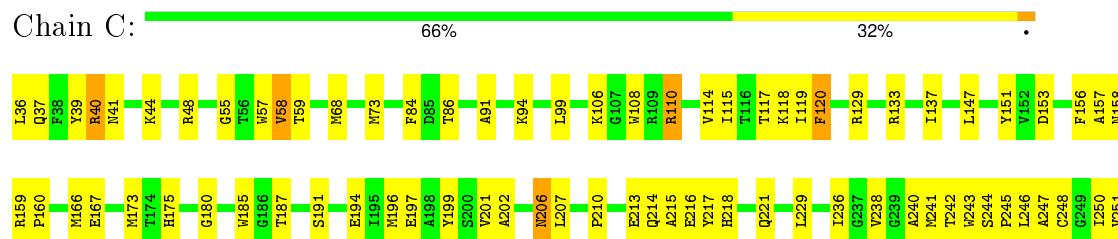
• Molecule 1: PROTEIN (KV BETA2 PROTEIN)

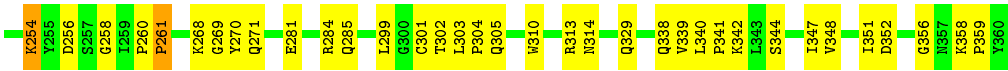


• Molecule 1: PROTEIN (KV BETA2 PROTEIN)

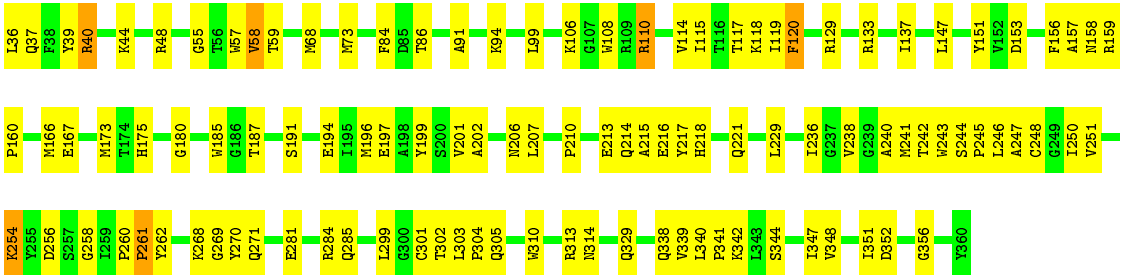


• Molecule 1: PROTEIN (KV BETA2 PROTEIN)





● Molecule 1: PROTEIN (KV BETA2 PROTEIN)



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	156.75Å 114.35Å 93.05Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.00 – 2.80	Depositor
% Data completeness (in resolution range)	97.7 (40.00-2.80)	Depositor
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS	Depositor
R, R_{free}	0.236 , 0.242	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	10348	wwPDB-VP
Average B, all atoms (Å ²)	59.0	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: NDP

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	0.36	0/2550	0.63	2/3451 (0.1%)
1	B	0.36	0/2550	0.63	2/3451 (0.1%)
1	C	0.36	0/2550	0.63	2/3451 (0.1%)
1	D	0.36	0/2550	0.63	2/3451 (0.1%)
All	All	0.36	0/10200	0.63	8/13804 (0.1%)

There are no bond length outliers.

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	157	ALA	N-CA-C	-5.39	96.46	111.00
1	C	157	ALA	N-CA-C	-5.38	96.48	111.00
1	A	157	ALA	N-CA-C	-5.38	96.48	111.00
1	B	157	ALA	N-CA-C	-5.38	96.48	111.00
1	B	260	PRO	N-CA-CB	5.26	109.61	103.30

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	2501	0	2477	93	0
1	B	2501	0	2477	98	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	2501	0	2477	97	0
1	D	2501	0	2477	96	0
2	A	48	0	26	9	0
2	B	48	0	26	9	0
2	C	48	0	26	10	0
2	D	48	0	26	10	0
3	A	38	0	0	0	0
3	B	38	0	0	0	0
3	C	38	0	0	0	0
3	D	38	0	0	0	0
All	All	10348	0	10012	390	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 19.

The worst 5 of 390 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:254:LYS:HA	1:A:258:GLY:HA3	1.40	1.04
1:B:254:LYS:HA	1:B:258:GLY:HA3	1.40	1.03
1:C:254:LYS:HA	1:C:258:GLY:HA3	1.40	1.01
1:D:254:LYS:HA	1:D:258:GLY:HA3	1.40	1.00
2:B:1001:NDP:H52N	2:B:1001:NDP:H6N	1.53	0.90

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	323/325 (99%)	312 (97%)	6 (2%)	5 (2%)	13 40
1	B	323/325 (99%)	312 (97%)	6 (2%)	5 (2%)	13 40

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	323/325 (99%)	312 (97%)	6 (2%)	5 (2%)	13	40
1	D	323/325 (99%)	312 (97%)	6 (2%)	5 (2%)	13	40
All	All	1292/1300 (99%)	1248 (97%)	24 (2%)	20 (2%)	13	40

5 of 20 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	261	PRO
1	B	261	PRO
1	C	261	PRO
1	D	261	PRO
1	A	58	VAL

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	257/272 (94%)	251 (98%)	6 (2%)	58	88
1	B	257/272 (94%)	251 (98%)	6 (2%)	58	88
1	C	257/272 (94%)	251 (98%)	6 (2%)	58	88
1	D	257/272 (94%)	251 (98%)	6 (2%)	58	88
All	All	1028/1088 (94%)	1004 (98%)	24 (2%)	58	88

5 of 24 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	206	ASN
1	C	48	ARG
1	D	206	ASN
1	B	268	LYS
1	C	40	ARG

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

Mol	Chain	Res	Type
1	B	285	GLN
1	C	148	GLN
1	D	271	GLN
1	C	71	HIS
1	C	158	ASN

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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

4 ligands are modelled in this entry.

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).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	NDP	A	1000	-	42,52,52	1.57	8 (19%)	55,80,80	2.32	17 (30%)
2	NDP	B	1001	-	42,52,52	1.57	8 (19%)	55,80,80	2.32	17 (30%)
2	NDP	C	1002	-	42,52,52	1.58	8 (19%)	55,80,80	2.33	16 (29%)
2	NDP	D	1003	-	42,52,52	1.57	8 (19%)	55,80,80	2.33	17 (30%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NDP	A	1000	-	-	0/30/77/77	0/5/5/5
2	NDP	B	1001	-	-	0/30/77/77	0/5/5/5
2	NDP	C	1002	-	-	0/30/77/77	0/5/5/5
2	NDP	D	1003	-	-	0/30/77/77	0/5/5/5

The worst 5 of 32 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	1002	NDP	P2B-O3X	-3.03	1.43	1.54
2	A	1000	NDP	P2B-O3X	-3.03	1.43	1.54
2	B	1001	NDP	P2B-O3X	-3.02	1.43	1.54
2	D	1003	NDP	P2B-O3X	-3.01	1.43	1.54
2	A	1000	NDP	C8A-N7A	-2.12	1.30	1.34

The worst 5 of 67 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	1002	NDP	O2B-P2B-O1X	-5.26	93.98	107.11
2	D	1003	NDP	O2B-P2B-O1X	-5.24	94.02	107.11
2	A	1000	NDP	O2B-P2B-O1X	-5.24	94.03	107.11
2	B	1001	NDP	O2B-P2B-O1X	-5.23	94.06	107.11
2	B	1001	NDP	O2N-PN-O5D	-4.87	83.92	108.46

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 38 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1000	NDP	9	0
2	B	1001	NDP	9	0
2	C	1002	NDP	10	0
2	D	1003	NDP	10	0

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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 will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates ⓘ

EDS was not executed - this section will therefore be empty.

6.4 Ligands ⓘ

EDS was not executed - this section will therefore be empty.

6.5 Other polymers ⓘ

EDS was not executed - this section will therefore be empty.