



Full wwPDB NMR Structure Validation Report ⓘ

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PDB ID : 1JQ2 / pdb_00001jq2
Title : POTASSIUM CHANNEL (KCSA) OPEN GATE MODEL
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Deposited on : 2001-08-03

This is a Full wwPDB NMR Structure Validation 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/NMRValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
wwPDB-RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
wwPDB-ShiftChecker	:	v1.2
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

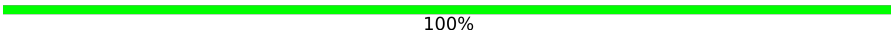
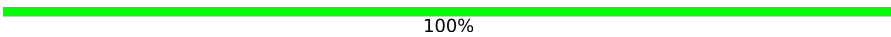
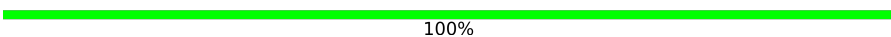
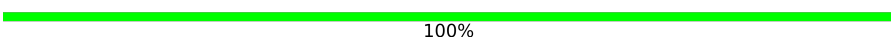
The overall completeness of chemical shifts assignment was not calculated.

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)	NMR archive (#Entries)
Clashscore	229148	14424

The table below summarises the geometric issues observed across the polymeric chains and their fit to the experimental data. The red, orange, yellow and green segments indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A cyan segment indicates the fraction of residues that are not part of the well-defined cores, and 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 $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	A	34	 100%
1	B	34	 100%
1	C	34	 100%
1	D	34	 100%

2 Ensemble composition and analysis ⓘ

This entry contains 50 models.

Cyrange was unable to find well-defined residues.

Error message: No core atoms could be determined.

NmrClust was unable to cluster the ensemble.

Error message: Wrapper check: not enough residues in core to run NmrClust

3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 136 atoms, of which 0 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called VOLTAGE-GATED POTASSIUM CHANNEL.

Mol	Chain	Residues	Atoms		Trace
1	A	34	Total 34	C 34	34
1	B	34	Total 34	C 34	34
1	C	34	Total 34	C 34	34
1	D	34	Total 34	C 34	34

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	90	CYS	LEU	engineered mutation	UNP P0A334
B	90	CYS	LEU	engineered mutation	UNP P0A334
C	90	CYS	LEU	engineered mutation	UNP P0A334
D	90	CYS	LEU	engineered mutation	UNP P0A334

4 Residue-property plots

4.1 Average score per residue in the NMR ensemble

These plots are provided for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic is the same as shown in the summary in section 1 of this report. The second graphic shows the sequence where residues are colour-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 outliers are shown as green connectors. Residues which are classified as ill-defined in the NMR ensemble, are shown in cyan with an underline colour-coded according to the previous scheme. Residues which were present in the experimental sample, but not modelled in the final structure are shown in grey.

- Molecule 1: VOLTAGE-GATED POTASSIUM CHANNEL

Chain A:  100%

There are no outlier residues in this chain.

- Molecule 1: VOLTAGE-GATED POTASSIUM CHANNEL

Chain B:  100%

There are no outlier residues in this chain.

- Molecule 1: VOLTAGE-GATED POTASSIUM CHANNEL

Chain C:  100%

There are no outlier residues in this chain.

- Molecule 1: VOLTAGE-GATED POTASSIUM CHANNEL

Chain D:  100%

There are no outlier residues in this chain.

4.2 Scores per residue for each member of the ensemble

Colouring as in section [4.1](#) above.

4.2.1 Score per residue for model 1

- Molecule 1: VOLTAGE-GATED POTASSIUM CHANNEL

Chain A:  100%

There are no outlier residues in this chain.

- Molecule 1: VOLTAGE-GATED POTASSIUM CHANNEL

Chain B:  100%

There are no outlier residues in this chain.

- Molecule 1: VOLTAGE-GATED POTASSIUM CHANNEL

Chain C:  100%

There are no outlier residues in this chain.

- Molecule 1: VOLTAGE-GATED POTASSIUM CHANNEL

Chain D:  100%

There are no outlier residues in this chain.

4.2.2 Score per residue for model 2

- Molecule 1: VOLTAGE-GATED POTASSIUM CHANNEL

Chain A:  100%

There are no outlier residues in this chain.

- Molecule 1: VOLTAGE-GATED POTASSIUM CHANNEL

Chain B:  100%

There are no outlier residues in this chain.

- Molecule 1: VOLTAGE-GATED POTASSIUM CHANNEL

Chain C:  100%

There are no outlier residues in this chain.

- Molecule 1: VOLTAGE-GATED POTASSIUM CHANNEL

Chain D:  100%

There are no outlier residues in this chain.

4.2.3 Score per residue for model 3

- Molecule 1: VOLTAGE-GATED POTASSIUM CHANNEL

Chain A:  100%

There are no outlier residues in this chain.

- Molecule 1: VOLTAGE-GATED POTASSIUM CHANNEL

Chain B:  100%

There are no outlier residues in this chain.

- Molecule 1: VOLTAGE-GATED POTASSIUM CHANNEL

Chain C:  100%

There are no outlier residues in this chain.

- Molecule 1: VOLTAGE-GATED POTASSIUM CHANNEL

Chain D:  100%

There are no outlier residues in this chain.

4.2.4 Score per residue for model 4

- Molecule 1: VOLTAGE-GATED POTASSIUM CHANNEL

Chain A:  100%

There are no outlier residues in this chain.

- Molecule 1: VOLTAGE-GATED POTASSIUM CHANNEL

Chain B:  100%

There are no outlier residues in this chain.

- Molecule 1: VOLTAGE-GATED POTASSIUM CHANNEL

Chain C:  100%

There are no outlier residues in this chain.

- Molecule 1: VOLTAGE-GATED POTASSIUM CHANNEL

Chain D:  100%

There are no outlier residues in this chain.

4.2.5 Score per residue for model 5

- Molecule 1: VOLTAGE-GATED POTASSIUM CHANNEL

Chain A:  100%

There are no outlier residues in this chain.

- Molecule 1: VOLTAGE-GATED POTASSIUM CHANNEL

Chain B:  100%

There are no outlier residues in this chain.

- Molecule 1: VOLTAGE-GATED POTASSIUM CHANNEL

Chain C:  100%

There are no outlier residues in this chain.

- Molecule 1: VOLTAGE-GATED POTASSIUM CHANNEL

Chain D:  100%

There are no outlier residues in this chain.

4.2.6 Score per residue for model 6

- Molecule 1: VOLTAGE-GATED POTASSIUM CHANNEL

Chain A:  100%

There are no outlier residues in this chain.

- Molecule 1: VOLTAGE-GATED POTASSIUM CHANNEL

Chain B:  100%

There are no outlier residues in this chain.

- Molecule 1: VOLTAGE-GATED POTASSIUM CHANNEL

Chain C:  100%

There are no outlier residues in this chain.

- Molecule 1: VOLTAGE-GATED POTASSIUM CHANNEL

Chain D:  100%

There are no outlier residues in this chain.

4.2.7 Score per residue for model 7

- Molecule 1: VOLTAGE-GATED POTASSIUM CHANNEL

Chain A:  100%

There are no outlier residues in this chain.

- Molecule 1: VOLTAGE-GATED POTASSIUM CHANNEL

Chain B:  100%

There are no outlier residues in this chain.

- Molecule 1: VOLTAGE-GATED POTASSIUM CHANNEL

Chain C:  100%

There are no outlier residues in this chain.

- Molecule 1: VOLTAGE-GATED POTASSIUM CHANNEL

Chain D:  100%

There are no outlier residues in this chain.

4.2.8 Score per residue for model 8

- Molecule 1: VOLTAGE-GATED POTASSIUM CHANNEL

Chain A:  100%

There are no outlier residues in this chain.

- Molecule 1: VOLTAGE-GATED POTASSIUM CHANNEL

Chain B:  100%

There are no outlier residues in this chain.

- Molecule 1: VOLTAGE-GATED POTASSIUM CHANNEL

Chain C:  100%

There are no outlier residues in this chain.

- Molecule 1: VOLTAGE-GATED POTASSIUM CHANNEL

Chain D:  100%

There are no outlier residues in this chain.

4.2.9 Score per residue for model 9

- Molecule 1: VOLTAGE-GATED POTASSIUM CHANNEL

Chain A:  100%

There are no outlier residues in this chain.

- Molecule 1: VOLTAGE-GATED POTASSIUM CHANNEL

Chain B:  100%

There are no outlier residues in this chain.

- Molecule 1: VOLTAGE-GATED POTASSIUM CHANNEL

Chain C:  100%

There are no outlier residues in this chain.

- Molecule 1: VOLTAGE-GATED POTASSIUM CHANNEL

Chain D:  100%

There are no outlier residues in this chain.

4.2.10 Score per residue for model 10

- Molecule 1: VOLTAGE-GATED POTASSIUM CHANNEL

Chain A:  100%

There are no outlier residues in this chain.

- Molecule 1: VOLTAGE-GATED POTASSIUM CHANNEL

Chain B:  100%

There are no outlier residues in this chain.

- Molecule 1: VOLTAGE-GATED POTASSIUM CHANNEL

Chain C:  100%

There are no outlier residues in this chain.

- Molecule 1: VOLTAGE-GATED POTASSIUM CHANNEL

Chain D:  100%

There are no outlier residues in this chain.

4.2.11 Score per residue for model 11

- Molecule 1: VOLTAGE-GATED POTASSIUM CHANNEL

Chain A:  100%

There are no outlier residues in this chain.

- Molecule 1: VOLTAGE-GATED POTASSIUM CHANNEL

Chain B:  100%

There are no outlier residues in this chain.

- Molecule 1: VOLTAGE-GATED POTASSIUM CHANNEL

Chain C:  100%

There are no outlier residues in this chain.

- Molecule 1: VOLTAGE-GATED POTASSIUM CHANNEL

Chain D:  100%

There are no outlier residues in this chain.

4.2.12 Score per residue for model 12

- Molecule 1: VOLTAGE-GATED POTASSIUM CHANNEL

Chain A:  100%

There are no outlier residues in this chain.

- Molecule 1: VOLTAGE-GATED POTASSIUM CHANNEL

Chain B:  100%

There are no outlier residues in this chain.

- Molecule 1: VOLTAGE-GATED POTASSIUM CHANNEL

Chain C:  100%

There are no outlier residues in this chain.

- Molecule 1: VOLTAGE-GATED POTASSIUM CHANNEL

Chain D:  100%

There are no outlier residues in this chain.

4.2.13 Score per residue for model 13

- Molecule 1: VOLTAGE-GATED POTASSIUM CHANNEL

Chain A:  100%

There are no outlier residues in this chain.

- Molecule 1: VOLTAGE-GATED POTASSIUM CHANNEL

Chain B:  100%

There are no outlier residues in this chain.

- Molecule 1: VOLTAGE-GATED POTASSIUM CHANNEL

Chain C:  100%

There are no outlier residues in this chain.

- Molecule 1: VOLTAGE-GATED POTASSIUM CHANNEL

Chain D:  100%

There are no outlier residues in this chain.

4.2.14 Score per residue for model 14

- Molecule 1: VOLTAGE-GATED POTASSIUM CHANNEL

Chain A:  100%

There are no outlier residues in this chain.

- Molecule 1: VOLTAGE-GATED POTASSIUM CHANNEL

Chain B:  100%

There are no outlier residues in this chain.

- Molecule 1: VOLTAGE-GATED POTASSIUM CHANNEL

Chain C:  100%

There are no outlier residues in this chain.

- Molecule 1: VOLTAGE-GATED POTASSIUM CHANNEL

Chain D:  100%

There are no outlier residues in this chain.

4.2.15 Score per residue for model 15

- Molecule 1: VOLTAGE-GATED POTASSIUM CHANNEL

Chain A:  100%

There are no outlier residues in this chain.

- Molecule 1: VOLTAGE-GATED POTASSIUM CHANNEL

Chain B:  100%

There are no outlier residues in this chain.

- Molecule 1: VOLTAGE-GATED POTASSIUM CHANNEL

Chain C:  100%

There are no outlier residues in this chain.

- Molecule 1: VOLTAGE-GATED POTASSIUM CHANNEL

Chain D:  100%

There are no outlier residues in this chain.

4.2.16 Score per residue for model 16

- Molecule 1: VOLTAGE-GATED POTASSIUM CHANNEL

Chain A:  100%

There are no outlier residues in this chain.

- Molecule 1: VOLTAGE-GATED POTASSIUM CHANNEL

Chain B:  100%

There are no outlier residues in this chain.

- Molecule 1: VOLTAGE-GATED POTASSIUM CHANNEL

Chain C:  100%

There are no outlier residues in this chain.

- Molecule 1: VOLTAGE-GATED POTASSIUM CHANNEL

Chain D:  100%

There are no outlier residues in this chain.

4.2.17 Score per residue for model 17

- Molecule 1: VOLTAGE-GATED POTASSIUM CHANNEL

Chain A:  100%

There are no outlier residues in this chain.

- Molecule 1: VOLTAGE-GATED POTASSIUM CHANNEL

Chain B:  100%

There are no outlier residues in this chain.

- Molecule 1: VOLTAGE-GATED POTASSIUM CHANNEL

Chain C:  100%

There are no outlier residues in this chain.

- Molecule 1: VOLTAGE-GATED POTASSIUM CHANNEL

Chain D:  100%

There are no outlier residues in this chain.

4.2.18 Score per residue for model 18

- Molecule 1: VOLTAGE-GATED POTASSIUM CHANNEL

Chain A:  100%

There are no outlier residues in this chain.

- Molecule 1: VOLTAGE-GATED POTASSIUM CHANNEL

Chain B:  100%

There are no outlier residues in this chain.

- Molecule 1: VOLTAGE-GATED POTASSIUM CHANNEL

Chain C:  100%

There are no outlier residues in this chain.

- Molecule 1: VOLTAGE-GATED POTASSIUM CHANNEL

Chain D:  100%

There are no outlier residues in this chain.

4.2.19 Score per residue for model 19

- Molecule 1: VOLTAGE-GATED POTASSIUM CHANNEL

Chain A:  100%

There are no outlier residues in this chain.

- Molecule 1: VOLTAGE-GATED POTASSIUM CHANNEL

Chain B:  100%

There are no outlier residues in this chain.

- Molecule 1: VOLTAGE-GATED POTASSIUM CHANNEL

Chain C:  100%

There are no outlier residues in this chain.

- Molecule 1: VOLTAGE-GATED POTASSIUM CHANNEL

Chain D:  100%

There are no outlier residues in this chain.

4.2.20 Score per residue for model 20

- Molecule 1: VOLTAGE-GATED POTASSIUM CHANNEL

Chain A:  100%

There are no outlier residues in this chain.

- Molecule 1: VOLTAGE-GATED POTASSIUM CHANNEL

Chain B:  100%

There are no outlier residues in this chain.

- Molecule 1: VOLTAGE-GATED POTASSIUM CHANNEL

Chain C:  100%

There are no outlier residues in this chain.

- Molecule 1: VOLTAGE-GATED POTASSIUM CHANNEL

Chain D:  100%

There are no outlier residues in this chain.

4.2.21 Score per residue for model 21

- Molecule 1: VOLTAGE-GATED POTASSIUM CHANNEL

Chain A:  100%

There are no outlier residues in this chain.

- Molecule 1: VOLTAGE-GATED POTASSIUM CHANNEL

Chain B:  100%

There are no outlier residues in this chain.

- Molecule 1: VOLTAGE-GATED POTASSIUM CHANNEL

Chain C:  100%

There are no outlier residues in this chain.

- Molecule 1: VOLTAGE-GATED POTASSIUM CHANNEL

Chain D:  100%

There are no outlier residues in this chain.

4.2.22 Score per residue for model 22

- Molecule 1: VOLTAGE-GATED POTASSIUM CHANNEL

Chain A:  100%

There are no outlier residues in this chain.

- Molecule 1: VOLTAGE-GATED POTASSIUM CHANNEL

Chain B:  100%

There are no outlier residues in this chain.

- Molecule 1: VOLTAGE-GATED POTASSIUM CHANNEL

Chain C:  100%

There are no outlier residues in this chain.

- Molecule 1: VOLTAGE-GATED POTASSIUM CHANNEL

Chain D:  100%

There are no outlier residues in this chain.

4.2.23 Score per residue for model 23

- Molecule 1: VOLTAGE-GATED POTASSIUM CHANNEL

Chain A:  100%

There are no outlier residues in this chain.

- Molecule 1: VOLTAGE-GATED POTASSIUM CHANNEL

Chain B:  100%

There are no outlier residues in this chain.

- Molecule 1: VOLTAGE-GATED POTASSIUM CHANNEL

Chain C:  100%

There are no outlier residues in this chain.

- Molecule 1: VOLTAGE-GATED POTASSIUM CHANNEL

Chain D:  100%

There are no outlier residues in this chain.

4.2.24 Score per residue for model 24

- Molecule 1: VOLTAGE-GATED POTASSIUM CHANNEL

Chain A:  100%

There are no outlier residues in this chain.

- Molecule 1: VOLTAGE-GATED POTASSIUM CHANNEL

Chain B:  100%

There are no outlier residues in this chain.

- Molecule 1: VOLTAGE-GATED POTASSIUM CHANNEL

Chain C:  100%

There are no outlier residues in this chain.

- Molecule 1: VOLTAGE-GATED POTASSIUM CHANNEL

Chain D:  100%

There are no outlier residues in this chain.

4.2.25 Score per residue for model 25

- Molecule 1: VOLTAGE-GATED POTASSIUM CHANNEL

Chain A:  100%

There are no outlier residues in this chain.

- Molecule 1: VOLTAGE-GATED POTASSIUM CHANNEL

Chain B:  100%

There are no outlier residues in this chain.

- Molecule 1: VOLTAGE-GATED POTASSIUM CHANNEL

Chain C:  100%

There are no outlier residues in this chain.

- Molecule 1: VOLTAGE-GATED POTASSIUM CHANNEL

Chain D:  100%

There are no outlier residues in this chain.

4.2.26 Score per residue for model 26

- Molecule 1: VOLTAGE-GATED POTASSIUM CHANNEL

Chain A:  100%

There are no outlier residues in this chain.

- Molecule 1: VOLTAGE-GATED POTASSIUM CHANNEL

Chain B:  100%

There are no outlier residues in this chain.

- Molecule 1: VOLTAGE-GATED POTASSIUM CHANNEL

Chain C:  100%

There are no outlier residues in this chain.

- Molecule 1: VOLTAGE-GATED POTASSIUM CHANNEL

Chain D:  100%

There are no outlier residues in this chain.

4.2.27 Score per residue for model 27

- Molecule 1: VOLTAGE-GATED POTASSIUM CHANNEL

Chain A:  100%

There are no outlier residues in this chain.

- Molecule 1: VOLTAGE-GATED POTASSIUM CHANNEL

Chain B:  100%

There are no outlier residues in this chain.

- Molecule 1: VOLTAGE-GATED POTASSIUM CHANNEL

Chain C:  100%

There are no outlier residues in this chain.

- Molecule 1: VOLTAGE-GATED POTASSIUM CHANNEL

Chain D:  100%

There are no outlier residues in this chain.

4.2.28 Score per residue for model 28

- Molecule 1: VOLTAGE-GATED POTASSIUM CHANNEL

Chain A:  100%

There are no outlier residues in this chain.

- Molecule 1: VOLTAGE-GATED POTASSIUM CHANNEL

Chain B:  100%

There are no outlier residues in this chain.

- Molecule 1: VOLTAGE-GATED POTASSIUM CHANNEL

Chain C:  100%

There are no outlier residues in this chain.

- Molecule 1: VOLTAGE-GATED POTASSIUM CHANNEL

Chain D:  100%

There are no outlier residues in this chain.

4.2.29 Score per residue for model 29

- Molecule 1: VOLTAGE-GATED POTASSIUM CHANNEL

Chain A:  100%

There are no outlier residues in this chain.

- Molecule 1: VOLTAGE-GATED POTASSIUM CHANNEL

Chain B:  100%

There are no outlier residues in this chain.

- Molecule 1: VOLTAGE-GATED POTASSIUM CHANNEL

Chain C:  100%

There are no outlier residues in this chain.

- Molecule 1: VOLTAGE-GATED POTASSIUM CHANNEL

Chain D:  100%

There are no outlier residues in this chain.

4.2.30 Score per residue for model 30

- Molecule 1: VOLTAGE-GATED POTASSIUM CHANNEL

Chain A:  100%

There are no outlier residues in this chain.

- Molecule 1: VOLTAGE-GATED POTASSIUM CHANNEL

Chain B:  100%

There are no outlier residues in this chain.

- Molecule 1: VOLTAGE-GATED POTASSIUM CHANNEL

Chain C:  100%

There are no outlier residues in this chain.

- Molecule 1: VOLTAGE-GATED POTASSIUM CHANNEL

Chain D:  100%

There are no outlier residues in this chain.

4.2.31 Score per residue for model 31

- Molecule 1: VOLTAGE-GATED POTASSIUM CHANNEL

Chain A:  100%

There are no outlier residues in this chain.

- Molecule 1: VOLTAGE-GATED POTASSIUM CHANNEL

Chain B:  100%

There are no outlier residues in this chain.

- Molecule 1: VOLTAGE-GATED POTASSIUM CHANNEL

Chain C:  100%

There are no outlier residues in this chain.

- Molecule 1: VOLTAGE-GATED POTASSIUM CHANNEL

Chain D:  100%

There are no outlier residues in this chain.

4.2.32 Score per residue for model 32

- Molecule 1: VOLTAGE-GATED POTASSIUM CHANNEL

Chain A:  100%

There are no outlier residues in this chain.

- Molecule 1: VOLTAGE-GATED POTASSIUM CHANNEL

Chain B:  100%

There are no outlier residues in this chain.

- Molecule 1: VOLTAGE-GATED POTASSIUM CHANNEL

Chain C:  100%

There are no outlier residues in this chain.

- Molecule 1: VOLTAGE-GATED POTASSIUM CHANNEL

Chain D:  100%

There are no outlier residues in this chain.

4.2.33 Score per residue for model 33

- Molecule 1: VOLTAGE-GATED POTASSIUM CHANNEL

Chain A:  100%

There are no outlier residues in this chain.

- Molecule 1: VOLTAGE-GATED POTASSIUM CHANNEL

Chain B:  100%

There are no outlier residues in this chain.

- Molecule 1: VOLTAGE-GATED POTASSIUM CHANNEL

Chain C:  100%

There are no outlier residues in this chain.

- Molecule 1: VOLTAGE-GATED POTASSIUM CHANNEL

Chain D:  100%

There are no outlier residues in this chain.

4.2.34 Score per residue for model 34

- Molecule 1: VOLTAGE-GATED POTASSIUM CHANNEL

Chain A:  100%

There are no outlier residues in this chain.

- Molecule 1: VOLTAGE-GATED POTASSIUM CHANNEL

Chain B:  100%

There are no outlier residues in this chain.

- Molecule 1: VOLTAGE-GATED POTASSIUM CHANNEL

Chain C:  100%

There are no outlier residues in this chain.

- Molecule 1: VOLTAGE-GATED POTASSIUM CHANNEL

Chain D:  100%

There are no outlier residues in this chain.

4.2.35 Score per residue for model 35

- Molecule 1: VOLTAGE-GATED POTASSIUM CHANNEL

Chain A:  100%

There are no outlier residues in this chain.

- Molecule 1: VOLTAGE-GATED POTASSIUM CHANNEL

Chain B:  100%

There are no outlier residues in this chain.

- Molecule 1: VOLTAGE-GATED POTASSIUM CHANNEL

Chain C:  100%

There are no outlier residues in this chain.

- Molecule 1: VOLTAGE-GATED POTASSIUM CHANNEL

Chain D:  100%

There are no outlier residues in this chain.

4.2.36 Score per residue for model 36

- Molecule 1: VOLTAGE-GATED POTASSIUM CHANNEL

Chain A:  100%

There are no outlier residues in this chain.

- Molecule 1: VOLTAGE-GATED POTASSIUM CHANNEL

Chain B:  100%

There are no outlier residues in this chain.

- Molecule 1: VOLTAGE-GATED POTASSIUM CHANNEL

Chain C:  100%

There are no outlier residues in this chain.

- Molecule 1: VOLTAGE-GATED POTASSIUM CHANNEL

Chain D:  100%

There are no outlier residues in this chain.

4.2.37 Score per residue for model 37

- Molecule 1: VOLTAGE-GATED POTASSIUM CHANNEL

Chain A:  100%

There are no outlier residues in this chain.

- Molecule 1: VOLTAGE-GATED POTASSIUM CHANNEL

Chain B:  100%

There are no outlier residues in this chain.

- Molecule 1: VOLTAGE-GATED POTASSIUM CHANNEL

Chain C:  100%

There are no outlier residues in this chain.

- Molecule 1: VOLTAGE-GATED POTASSIUM CHANNEL

Chain D:  100%

There are no outlier residues in this chain.

4.2.38 Score per residue for model 38

- Molecule 1: VOLTAGE-GATED POTASSIUM CHANNEL

Chain A:  100%

There are no outlier residues in this chain.

- Molecule 1: VOLTAGE-GATED POTASSIUM CHANNEL

Chain B:  100%

There are no outlier residues in this chain.

- Molecule 1: VOLTAGE-GATED POTASSIUM CHANNEL

Chain C:  100%

There are no outlier residues in this chain.

- Molecule 1: VOLTAGE-GATED POTASSIUM CHANNEL

Chain D:  100%

There are no outlier residues in this chain.

4.2.39 Score per residue for model 39

- Molecule 1: VOLTAGE-GATED POTASSIUM CHANNEL

Chain A:  100%

There are no outlier residues in this chain.

- Molecule 1: VOLTAGE-GATED POTASSIUM CHANNEL

Chain B:  100%

There are no outlier residues in this chain.

- Molecule 1: VOLTAGE-GATED POTASSIUM CHANNEL

Chain C:  100%

There are no outlier residues in this chain.

- Molecule 1: VOLTAGE-GATED POTASSIUM CHANNEL

Chain D:  100%

There are no outlier residues in this chain.

4.2.40 Score per residue for model 40

- Molecule 1: VOLTAGE-GATED POTASSIUM CHANNEL

Chain A:  100%

There are no outlier residues in this chain.

- Molecule 1: VOLTAGE-GATED POTASSIUM CHANNEL

Chain B:  100%

There are no outlier residues in this chain.

- Molecule 1: VOLTAGE-GATED POTASSIUM CHANNEL

Chain C:  100%

There are no outlier residues in this chain.

- Molecule 1: VOLTAGE-GATED POTASSIUM CHANNEL

Chain D:  100%

There are no outlier residues in this chain.

4.2.41 Score per residue for model 41

- Molecule 1: VOLTAGE-GATED POTASSIUM CHANNEL

Chain A:  100%

There are no outlier residues in this chain.

- Molecule 1: VOLTAGE-GATED POTASSIUM CHANNEL

Chain B:  100%

There are no outlier residues in this chain.

- Molecule 1: VOLTAGE-GATED POTASSIUM CHANNEL

Chain C:  100%

There are no outlier residues in this chain.

- Molecule 1: VOLTAGE-GATED POTASSIUM CHANNEL

Chain D:  100%

There are no outlier residues in this chain.

4.2.42 Score per residue for model 42

- Molecule 1: VOLTAGE-GATED POTASSIUM CHANNEL

Chain A:  100%

There are no outlier residues in this chain.

- Molecule 1: VOLTAGE-GATED POTASSIUM CHANNEL

Chain B:  100%

There are no outlier residues in this chain.

- Molecule 1: VOLTAGE-GATED POTASSIUM CHANNEL

Chain C:  100%

There are no outlier residues in this chain.

- Molecule 1: VOLTAGE-GATED POTASSIUM CHANNEL

Chain D:  100%

There are no outlier residues in this chain.

4.2.43 Score per residue for model 43

- Molecule 1: VOLTAGE-GATED POTASSIUM CHANNEL

Chain A:  100%

There are no outlier residues in this chain.

- Molecule 1: VOLTAGE-GATED POTASSIUM CHANNEL

Chain B:  100%

There are no outlier residues in this chain.

- Molecule 1: VOLTAGE-GATED POTASSIUM CHANNEL

Chain C:  100%

There are no outlier residues in this chain.

- Molecule 1: VOLTAGE-GATED POTASSIUM CHANNEL

Chain D:  100%

There are no outlier residues in this chain.

4.2.44 Score per residue for model 44

- Molecule 1: VOLTAGE-GATED POTASSIUM CHANNEL

Chain A:  100%

There are no outlier residues in this chain.

- Molecule 1: VOLTAGE-GATED POTASSIUM CHANNEL

Chain B:  100%

There are no outlier residues in this chain.

- Molecule 1: VOLTAGE-GATED POTASSIUM CHANNEL

Chain C:  100%

There are no outlier residues in this chain.

- Molecule 1: VOLTAGE-GATED POTASSIUM CHANNEL

Chain D:  100%

There are no outlier residues in this chain.

4.2.45 Score per residue for model 45

- Molecule 1: VOLTAGE-GATED POTASSIUM CHANNEL

Chain A:  100%

There are no outlier residues in this chain.

- Molecule 1: VOLTAGE-GATED POTASSIUM CHANNEL

Chain B:  100%

There are no outlier residues in this chain.

- Molecule 1: VOLTAGE-GATED POTASSIUM CHANNEL

Chain C:  100%

There are no outlier residues in this chain.

- Molecule 1: VOLTAGE-GATED POTASSIUM CHANNEL

Chain D:  100%

There are no outlier residues in this chain.

4.2.46 Score per residue for model 46

- Molecule 1: VOLTAGE-GATED POTASSIUM CHANNEL

Chain A:  100%

There are no outlier residues in this chain.

- Molecule 1: VOLTAGE-GATED POTASSIUM CHANNEL

Chain B:  100%

There are no outlier residues in this chain.

- Molecule 1: VOLTAGE-GATED POTASSIUM CHANNEL

Chain C:  100%

There are no outlier residues in this chain.

- Molecule 1: VOLTAGE-GATED POTASSIUM CHANNEL

Chain D:  100%

There are no outlier residues in this chain.

4.2.47 Score per residue for model 47

- Molecule 1: VOLTAGE-GATED POTASSIUM CHANNEL

Chain A:  100%

There are no outlier residues in this chain.

- Molecule 1: VOLTAGE-GATED POTASSIUM CHANNEL

Chain B:  100%

There are no outlier residues in this chain.

- Molecule 1: VOLTAGE-GATED POTASSIUM CHANNEL

Chain C:  100%

There are no outlier residues in this chain.

- Molecule 1: VOLTAGE-GATED POTASSIUM CHANNEL

Chain D:  100%

There are no outlier residues in this chain.

4.2.48 Score per residue for model 48

- Molecule 1: VOLTAGE-GATED POTASSIUM CHANNEL

Chain A:  100%

There are no outlier residues in this chain.

- Molecule 1: VOLTAGE-GATED POTASSIUM CHANNEL

Chain B:  100%

There are no outlier residues in this chain.

- Molecule 1: VOLTAGE-GATED POTASSIUM CHANNEL

Chain C:  100%

There are no outlier residues in this chain.

- Molecule 1: VOLTAGE-GATED POTASSIUM CHANNEL

Chain D:  100%

There are no outlier residues in this chain.

4.2.49 Score per residue for model 49

- Molecule 1: VOLTAGE-GATED POTASSIUM CHANNEL

Chain A:  100%

There are no outlier residues in this chain.

- Molecule 1: VOLTAGE-GATED POTASSIUM CHANNEL

Chain B:  100%

There are no outlier residues in this chain.

- Molecule 1: VOLTAGE-GATED POTASSIUM CHANNEL

Chain C:  100%

There are no outlier residues in this chain.

- Molecule 1: VOLTAGE-GATED POTASSIUM CHANNEL

Chain D:  100%

There are no outlier residues in this chain.

4.2.50 Score per residue for model 50

- Molecule 1: VOLTAGE-GATED POTASSIUM CHANNEL

Chain A:  100%

There are no outlier residues in this chain.

- Molecule 1: VOLTAGE-GATED POTASSIUM CHANNEL

Chain B:  100%

There are no outlier residues in this chain.

- Molecule 1: VOLTAGE-GATED POTASSIUM CHANNEL

Chain C:  100%

There are no outlier residues in this chain.

- Molecule 1: VOLTAGE-GATED POTASSIUM CHANNEL

Chain D:  100%

There are no outlier residues in this chain.

5 Refinement protocol and experimental data overview

The models were refined using the following method: *FOURIER DECONVOLUTION, CONFORMATIONAL GRID SEARCH A CARTESAIN REPRESENTATION MOLECULAR MECHANIC ENERGY MINIMIZATION*.

Of the 50 calculated structures, 50 were deposited, based on the following criterion: *STRUCTURES WITH THE LOWEST PENALTY*.

The following table shows the software used for structure solution, optimisation and refinement.

Software name	Classification	Version
Amber	refinement	6.0
REDCAT	structure solution	

No chemical shift data was provided.

6 Model quality [i](#)

6.1 Standard geometry [i](#)

There are no covalent bond-length or bond-angle outliers.

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

There are no planarity outliers.

6.2 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 each 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 averaged over the ensemble.

Mol	Chain	Non-H	H(model)	H(added)	Clashes
All	All	6800	0	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 -.

There are no clashes.

6.3 Torsion angles [i](#)

6.3.1 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 PDB entries followed by that with respect to all NMR entries. 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	0	-	-	-	-
1	B	0	-	-	-	-
1	C	0	-	-	-	-
1	D	0	-	-	-	-
All	All	0	-	-	-	-

There are no Ramachandran outliers.

6.3.2 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 PDB entries followed by that with respect to all NMR entries. 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	0	-	-	-
1	B	0	-	-	-
1	C	0	-	-	-
1	D	0	-	-	-
All	All	0	-	-	-

There are no protein residues with a non-rotameric sidechain to report.

6.3.3 RNA [i](#)

There are no RNA molecules in this entry.

6.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.6 Ligand geometry [i](#)

There are no ligands in this entry.

6.7 Other polymers [i](#)

There are no such molecules in this entry.

6.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

7 Chemical shift validation

No chemical shift data were provided