



Full wwPDB NMR Structure Validation Report ⓘ

Mar 5, 2026 – 07:50 PM UTC

PDB ID : 6MIE / pdb_00006mie
BMRB ID : 30517
Title : Solution NMR structure of the KCNQ1 voltage-sensing domain
Authors : Taylor, K.C.; Kuenze, G.; Smith, J.A.; Meiler, J.; McFeeters, R.L.; Sanders, C.R.
Deposited on : 2018-09-19

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

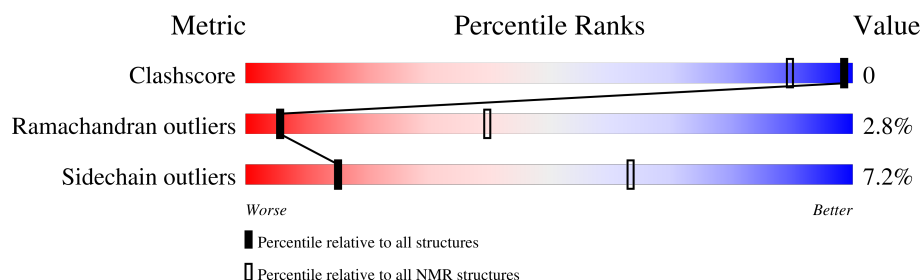
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 72%.

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
Ramachandran outliers	224038	12848
Sidechain outliers	223484	12823

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	159	

2 Ensemble composition and analysis

This entry contains 10 models. Model 1 is the overall representative, medoid model (most similar to other models).

The following residues are included in the computation of the global validation metrics.

Well-defined (core) protein residues			
Well-defined core	Residue range (total)	Backbone RMSD (Å)	Medoid model
1	A:103-A:241 (139)	1.17	1

Ill-defined regions of proteins are excluded from the global statistics.

Ligands and non-protein polymers are included in the analysis.

The models can be grouped into 3 clusters and 1 single-model cluster was found.

Cluster number	Models
1	1, 2, 3, 4, 5
2	6, 7
3	9, 10
Single-model clusters	8

3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 2471 atoms, of which 1263 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Potassium voltage-gated channel subfamily KQT member 1.

Mol	Chain	Residues	Atoms						Trace
1	A	150	Total	C	H	N	O	S	0
			2471	801	1263	210	190	7	

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	91	MET	-	expression tag	UNP P51787
A	92	GLY	-	expression tag	UNP P51787
A	93	HIS	-	expression tag	UNP P51787
A	94	HIS	-	expression tag	UNP P51787
A	95	HIS	-	expression tag	UNP P51787
A	96	HIS	-	expression tag	UNP P51787
A	97	HIS	-	expression tag	UNP P51787
A	98	HIS	-	expression tag	UNP P51787
A	99	GLY	-	expression tag	UNP P51787

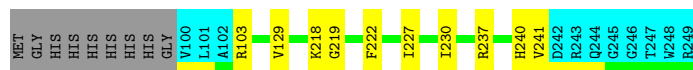
4 Residue-property plots

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: Potassium voltage-gated channel subfamily KQT member 1

Chain A: 



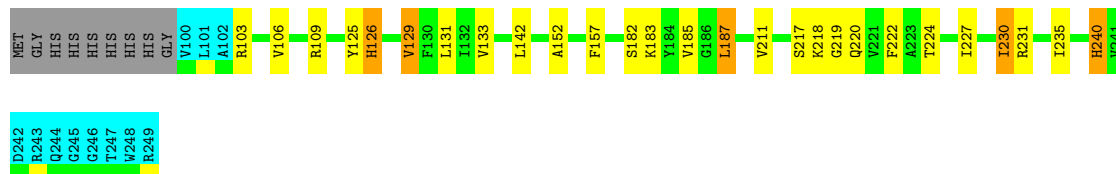
4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1 (medoid)

- Molecule 1: Potassium voltage-gated channel subfamily KQT member 1

Chain A: 



4.2.2 Score per residue for model 2

- Molecule 1: Potassium voltage-gated channel subfamily KQT member 1

Chain A: 



4.2.3 Score per residue for model 3

- Molecule 1: Potassium voltage-gated channel subfamily KQT member 1

Chain A:  78% 9% 7% 6%



4.2.4 Score per residue for model 4

- Molecule 1: Potassium voltage-gated channel subfamily KQT member 1

Chain A:  76% 11% 7% 6%



4.2.5 Score per residue for model 5

- Molecule 1: Potassium voltage-gated channel subfamily KQT member 1

Chain A:  73% 13% 7% 6%



R249

4.2.6 Score per residue for model 6

- Molecule 1: Potassium voltage-gated channel subfamily KQT member 1

Chain A:  76% 10% 7% 6%



4.2.7 Score per residue for model 7

- Molecule 1: Potassium voltage-gated channel subfamily KQT member 1

Chain A:  75% 11% 7% 6%



5 Refinement protocol and experimental data overview

The models were refined using the following method: *molecular dynamics*.

Of the 150 calculated structures, 10 were deposited, based on the following criterion: *structures with the lowest energy*.

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

Software name	Classification	Version
Amber	refinement	16
XPLOR-NIH	structure calculation	2.48

The following table shows chemical shift validation statistics as aggregates over all chemical shift files. Detailed validation can be found in section 7 of this report.

Chemical shift file(s)	working_cs.cif
Number of chemical shift lists	1
Total number of shifts	1581
Number of shifts mapped to atoms	1581
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	72%

6 Model quality

6.1 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 (average) 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	0.84±0.01	0±0/1148 (0.0± 0.0%)	1.48±0.03	5±3/1559 (0.3± 0.2%)
All	All	0.84	0/11480 (0.0%)	1.48	53/15590 (0.3%)

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	Planarity
1	A	0.0±0.0	4.6±1.9
All	All	0	46

There are no bond-length outliers.

All unique angle outliers are listed below. They are sorted according to the Z-score of the worst occurrence in the ensemble.

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	182	SER	CA-C-N	7.45	130.59	120.38	2	2
1	A	182	SER	C-N-CA	7.45	130.59	120.38	2	2
1	A	232	PHE	CA-CB-CG	7.18	120.98	113.80	3	1
1	A	219	GLY	O-C-N	-6.78	118.05	121.85	2	1
1	A	130	PHE	CA-CB-CG	6.57	120.37	113.80	2	1
1	A	146	GLU	CA-C-N	6.51	129.00	120.28	3	1
1	A	146	GLU	C-N-CA	6.51	129.00	120.28	3	1
1	A	240	HIS	CB-CG-CD2	-6.29	123.03	131.20	10	2
1	A	105	HIS	N-CA-C	6.22	119.97	112.38	7	1
1	A	126	HIS	CB-CG-CD2	-6.13	123.23	131.20	1	4
1	A	157	PHE	CA-CB-CG	6.10	119.90	113.80	1	1
1	A	219	GLY	CA-C-N	6.10	132.67	121.70	2	1
1	A	219	GLY	C-N-CA	6.10	132.67	121.70	2	1
1	A	202	ASP	CA-CB-CG	6.00	118.59	112.60	9	2
1	A	219	GLY	N-CA-C	-5.83	104.91	110.21	2	1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	129	VAL	N-CA-CB	5.75	118.36	110.54	1	2
1	A	201	ILE	CA-C-N	5.70	127.91	120.28	2	1
1	A	201	ILE	C-N-CA	5.70	127.91	120.28	2	1
1	A	237	ARG	CA-C-N	5.63	129.70	120.63	10	2
1	A	237	ARG	C-N-CA	5.63	129.70	120.63	10	2
1	A	211	VAL	CA-C-N	5.61	127.62	120.56	1	1
1	A	211	VAL	C-N-CA	5.61	127.62	120.56	1	1
1	A	142	LEU	CA-C-N	5.57	127.74	120.28	1	1
1	A	142	LEU	C-N-CA	5.57	127.74	120.28	1	1
1	A	190	ARG	N-CA-CB	-5.57	101.72	110.30	8	1
1	A	129	VAL	CA-CB-CG2	5.50	119.76	110.40	5	2
1	A	228	ARG	CA-C-N	5.45	125.99	120.00	9	1
1	A	228	ARG	C-N-CA	5.45	125.99	120.00	9	1
1	A	189	GLY	CA-C-N	5.42	129.90	120.68	8	3
1	A	189	GLY	C-N-CA	5.42	129.90	120.68	8	3
1	A	193	PHE	CA-CB-CG	5.33	119.14	113.80	5	1
1	A	156	LEU	CA-C-N	5.30	128.12	120.38	8	1
1	A	156	LEU	C-N-CA	5.30	128.12	120.38	8	1
1	A	147	GLN	OE1-CD-NE2	-5.11	117.50	122.60	10	1
1	A	217	SER	CA-C-N	5.09	131.51	122.45	3	1
1	A	217	SER	C-N-CA	5.09	131.51	122.45	3	1
1	A	107	GLN	OE1-CD-NE2	-5.08	117.52	122.60	9	1
1	A	127	PHE	CA-CB-CG	-5.06	108.74	113.80	9	1

There are no chirality outliers.

All unique planar outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Group	Models (Total)
1	A	218	LYS	Peptide	6
1	A	152	ALA	Peptide	5
1	A	111	TYR	Sidechain	5
1	A	237	ARG	Peptide,Sidechain	4
1	A	241	VAL	Peptide	4
1	A	190	ARG	Sidechain	3
1	A	240	HIS	Peptide	2
1	A	220	GLN	Peptide	2
1	A	125	TYR	Sidechain	1
1	A	126	HIS	Sidechain	1
1	A	230	ILE	Peptide	1
1	A	144	THR	Peptide	1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group	Models (Total)
1	A	239	LEU	Peptide	1
1	A	116	ARG	Peptide	1
1	A	231	ARG	Sidechain	1
1	A	103	ARG	Sidechain,Peptide	1
1	A	174	ARG	Sidechain	1
1	A	171	TYR	Sidechain	1
1	A	194	ALA	Peptide	1
1	A	192	ARG	Peptide	1

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
1	A	1119	1177	1177	0±0
All	All	11190	11770	11770	4

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 0.

All unique clashes are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:187:LEU:HD13	1:A:187:LEU:C	0.43	2.39	1	1
1:A:219:GLY:H	1:A:221:VAL:H	0.43	1.56	2	1
1:A:219:GLY:C	1:A:221:VAL:N	0.40	2.78	10	1
1:A:103:ARG:HA	1:A:106:VAL:HG12	0.40	1.93	8	1

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	139/159 (87%)	126±4 (91±3%)	9±3 (6±2%)	4±2 (3±1%)	6	40
All	All	1390/1590 (87%)	1265 (91%)	86 (6%)	39 (3%)	6	40

All 19 unique Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	A	227	ILE	8
1	A	219	GLY	4
1	A	241	VAL	4
1	A	238	MET	4
1	A	217	SER	3
1	A	179	GLY	2
1	A	194	ALA	2
1	A	106	VAL	1
1	A	182	SER	1
1	A	185	VAL	1
1	A	220	GLN	1
1	A	156	LEU	1
1	A	183	LYS	1
1	A	218	LYS	1
1	A	221	VAL	1
1	A	119	GLY	1
1	A	104	THR	1
1	A	180	CYS	1
1	A	193	PHE	1

6.3.2 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 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	120/135 (89%)	111±3 (93±2%)	9±3 (7±2%)	15	63
All	All	1200/1350 (89%)	1114 (93%)	86 (7%)	15	63

All 38 unique residues with a non-rotameric sidechain are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	A	230	ILE	8
1	A	103	ARG	6
1	A	129	VAL	6
1	A	222	PHE	6
1	A	187	LEU	4
1	A	224	THR	4
1	A	235	ILE	4
1	A	133	VAL	3
1	A	183	LYS	3
1	A	231	ARG	3
1	A	213	LEU	3
1	A	185	VAL	3
1	A	234	GLN	3
1	A	109	ARG	2
1	A	240	HIS	2
1	A	104	THR	2
1	A	218	LYS	2
1	A	110	VAL	2
1	A	131	LEU	1
1	A	156	LEU	1
1	A	211	VAL	1
1	A	232	PHE	1
1	A	121	LYS	1
1	A	127	PHE	1
1	A	118	THR	1
1	A	132	ILE	1
1	A	147	GLN	1
1	A	155	THR	1
1	A	181	ARG	1
1	A	106	VAL	1
1	A	227	ILE	1
1	A	233	LEU	1
1	A	114	LEU	1
1	A	144	THR	1
1	A	236	LEU	1
1	A	157	PHE	1
1	A	145	ILE	1
1	A	221	VAL	1

6.3.3 RNA ⓘ

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

The completeness of assignment taking into account all chemical shift lists is 72% for the well-defined parts and 72% for the entire structure.

7.1 Chemical shift list 1

File name: `working_cs.cif`

Chemical shift list name: *starch_output*

7.1.1 Bookkeeping

The following table shows the results of parsing the chemical shift list and reports the number of nuclei with statistically unusual chemical shifts.

Total number of shifts	1581
Number of shifts mapped to atoms	1581
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	0

7.1.2 Chemical shift referencing

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction $\pm$ precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	135	-0.38 ± 0.15	None needed (< 0.5 ppm)
$^{13}\text{C}_\beta$	113	-0.06 ± 0.08	None needed (< 0.5 ppm)
$^{13}\text{C}'$	129	0.02 ± 0.11	None needed (< 0.5 ppm)
^{15}N	139	0.42 ± 0.16	None needed (< 0.5 ppm)

7.1.3 Completeness of resonance assignments

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 72%, i.e. 1465 atoms were assigned a chemical shift out of a possible 2046. 0 out of 37 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	631/701 (90%)	258/286 (90%)	245/278 (88%)	128/137 (93%)
Sidechain	791/1121 (71%)	562/747 (75%)	228/332 (69%)	1/42 (2%)

Continued on next page...

Continued from previous page...

	Total	¹ H	¹³ C	¹⁵ N
Aromatic	43/224 (19%)	39/111 (35%)	0/106 (0%)	4/7 (57%)
Overall	1465/2046 (72%)	859/1144 (75%)	473/716 (66%)	133/186 (72%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 72%, i.e. 1581 atoms were assigned a chemical shift out of a possible 2201. 0 out of 39 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹ H	¹³ C	¹⁵ N
Backbone	685/758 (90%)	282/310 (91%)	264/300 (88%)	139/148 (94%)
Sidechain	850/1207 (70%)	603/802 (75%)	246/356 (69%)	1/49 (2%)
Aromatic	46/236 (19%)	41/117 (35%)	0/111 (0%)	5/8 (62%)
Overall	1581/2201 (72%)	926/1229 (75%)	510/767 (66%)	145/205 (71%)

7.1.4 Statistically unusual chemical shifts [i](#)

There are no statistically unusual chemical shifts.

7.1.5 Random Coil Index (RCI) plots [i](#)

The image below reports *random coil index* values for the protein chains in the structure. The height of each bar gives a probability of a given residue to be disordered, as predicted from the available chemical shifts and the amino acid sequence. A value above 0.2 is an indication of significant predicted disorder. The colour of the bar shows whether the residue is in the well-defined core (black) or in the ill-defined residue ranges (cyan), as described in section 2 on ensemble composition. If well-defined core and ill-defined regions are not identified then it is shown as gray bars.

Random coil index (RCI) for chain A:

