



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 8, 2026 – 05:01 PM UTC

PDB ID : 4NPQ / pdb_00004npq
Title : The resting-state conformation of the GLIC ligand-gated ion channel
Authors : Sauguet, L.; Shahsavar, A.; Poitevin, F.; Huon, C.; Menny, A.; Nemecz, A.;
Haouz, A.; Changeux, J.P.; Corringer, P.J.; Delarue, M.
Deposited on : 2013-11-22
Resolution : 4.35 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 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
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

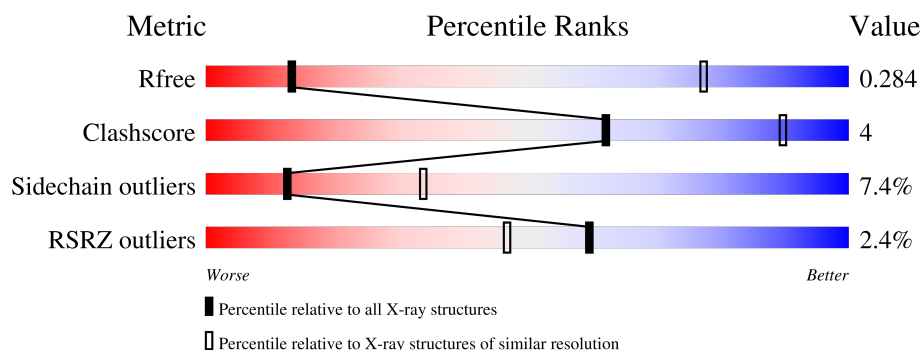
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 4.35 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.



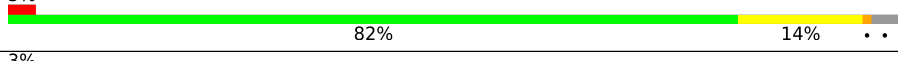
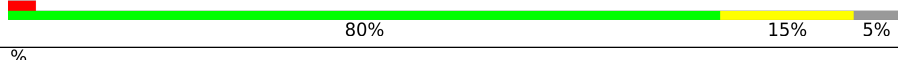
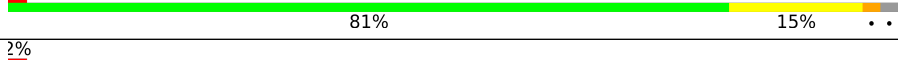
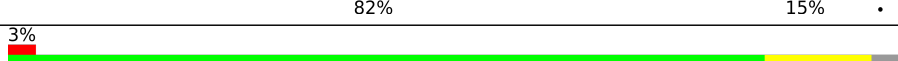
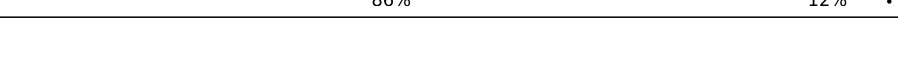
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1059 (4.76-3.90)
Clashscore	190562	1105 (4.76-3.90)
Sidechain outliers	187428	1022 (4.80-3.88)
RSRZ outliers	180081	1056 (4.76-3.90)

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 of 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	318	3% 82%14%..
1	B	318	3% 82%15%..
1	C	318	3% 81%15%..
1	D	318	3% 82%15%..
1	E	318	3% 81%16%..
1	F	318	% 83%14%..

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Mol	Chain	Length	Quality of chain
1	G	318	
1	H	318	
1	I	318	
1	J	318	
1	K	318	
1	L	318	
1	M	318	
1	N	318	
1	O	318	
1	P	318	
1	Q	318	
1	R	318	
1	S	318	
1	T	318	

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 45859 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 Proton-gated ion channel.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	311	Total	C	N	O	S	0	0	0
			2322	1533	355	430	4			
1	B	311	Total	C	N	O	S	0	0	0
			2334	1540	361	429	4			
1	C	311	Total	C	N	O	S	0	0	0
			2341	1551	359	427	4			
1	D	311	Total	C	N	O	S	0	0	0
			2330	1543	353	431	3			
1	E	311	Total	C	N	O	S	0	0	0
			2355	1559	359	433	4			
1	F	311	Total	C	N	O	S	0	0	0
			2334	1546	361	423	4			
1	G	311	Total	C	N	O	S	0	0	0
			2325	1538	361	422	4			
1	H	309	Total	C	N	O	S	0	0	0
			2199	1440	350	406	3			
1	I	307	Total	C	N	O	S	0	0	0
			2145	1408	344	389	4			
1	J	311	Total	C	N	O	S	0	0	0
			2257	1485	362	407	3			
1	K	309	Total	C	N	O	S	0	0	0
			2312	1530	360	418	4			
1	L	302	Total	C	N	O	S	0	0	0
			2274	1505	344	421	4			
1	M	308	Total	C	N	O	S	0	0	0
			2271	1501	353	413	4			
1	N	311	Total	C	N	O	S	0	0	0
			2359	1564	364	427	4			
1	O	311	Total	C	N	O	S	0	0	0
			2366	1565	362	435	4			
1	P	311	Total	C	N	O	S	0	0	0
			2280	1499	357	420	4			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	Q	311	Total	C	N	O	S	0	0	0
			2345	1555	357	429	4			
1	R	311	Total	C	N	O	S	0	0	0
			2293	1511	362	417	3			
1	S	309	Total	C	N	O	S	0	0	0
			2268	1497	359	408	4			
1	T	311	Total	C	N	O	S	0	0	0
			2149	1410	352	384	3			

There are 40 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	ALA	-	expression tag	UNP Q7NDN8
A	318	GLY	-	expression tag	UNP Q7NDN8
B	1	ALA	-	expression tag	UNP Q7NDN8
B	318	GLY	-	expression tag	UNP Q7NDN8
C	1	ALA	-	expression tag	UNP Q7NDN8
C	318	GLY	-	expression tag	UNP Q7NDN8
D	1	ALA	-	expression tag	UNP Q7NDN8
D	318	GLY	-	expression tag	UNP Q7NDN8
E	1	ALA	-	expression tag	UNP Q7NDN8
E	318	GLY	-	expression tag	UNP Q7NDN8
F	1	ALA	-	expression tag	UNP Q7NDN8
F	318	GLY	-	expression tag	UNP Q7NDN8
G	1	ALA	-	expression tag	UNP Q7NDN8
G	318	GLY	-	expression tag	UNP Q7NDN8
H	1	ALA	-	expression tag	UNP Q7NDN8
H	318	GLY	-	expression tag	UNP Q7NDN8
I	1	ALA	-	expression tag	UNP Q7NDN8
I	318	GLY	-	expression tag	UNP Q7NDN8
J	1	ALA	-	expression tag	UNP Q7NDN8
J	318	GLY	-	expression tag	UNP Q7NDN8
K	1	ALA	-	expression tag	UNP Q7NDN8
K	318	GLY	-	expression tag	UNP Q7NDN8
L	1	ALA	-	expression tag	UNP Q7NDN8
L	318	GLY	-	expression tag	UNP Q7NDN8
M	1	ALA	-	expression tag	UNP Q7NDN8
M	318	GLY	-	expression tag	UNP Q7NDN8
N	1	ALA	-	expression tag	UNP Q7NDN8
N	318	GLY	-	expression tag	UNP Q7NDN8
O	1	ALA	-	expression tag	UNP Q7NDN8
O	318	GLY	-	expression tag	UNP Q7NDN8
P	1	ALA	-	expression tag	UNP Q7NDN8

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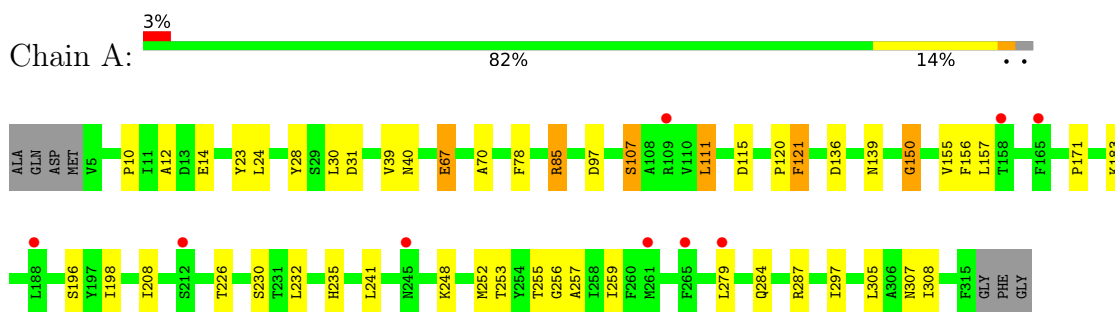
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Chain	Residue	Modelled	Actual	Comment	Reference
P	318	GLY	-	expression tag	UNP Q7NDN8
Q	1	ALA	-	expression tag	UNP Q7NDN8
Q	318	GLY	-	expression tag	UNP Q7NDN8
R	1	ALA	-	expression tag	UNP Q7NDN8
R	318	GLY	-	expression tag	UNP Q7NDN8
S	1	ALA	-	expression tag	UNP Q7NDN8
S	318	GLY	-	expression tag	UNP Q7NDN8
T	1	ALA	-	expression tag	UNP Q7NDN8
T	318	GLY	-	expression tag	UNP Q7NDN8

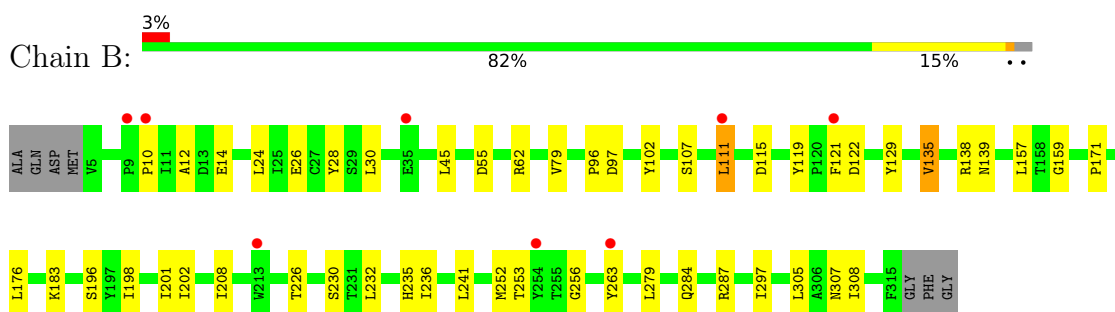
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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.

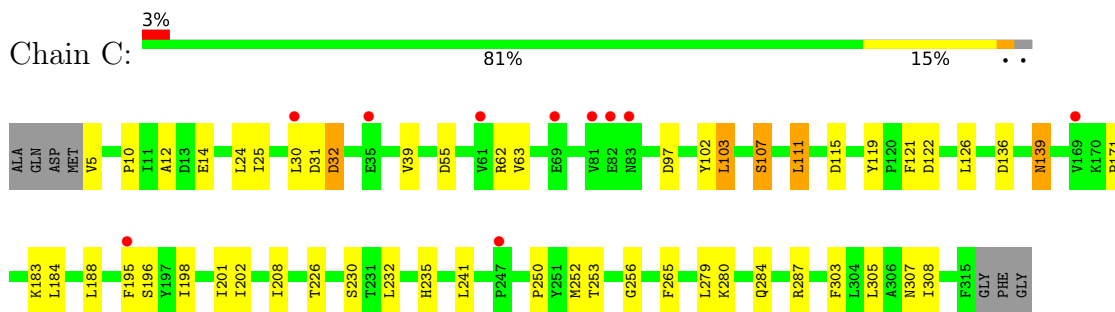
- Molecule 1: Proton-gated ion channel



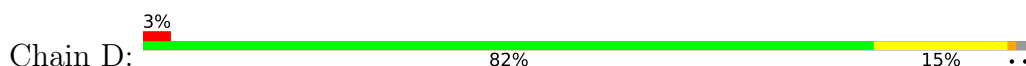
- Molecule 1: Proton-gated ion channel

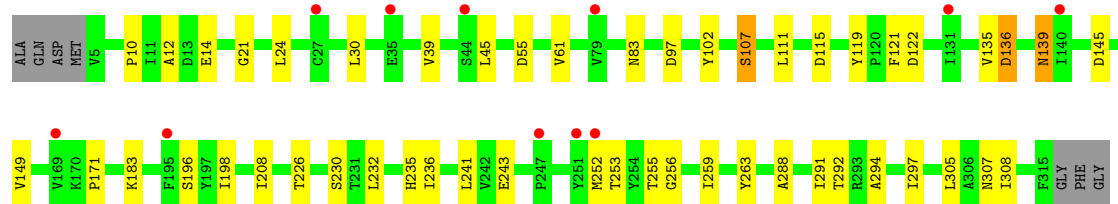


- Molecule 1: Proton-gated ion channel

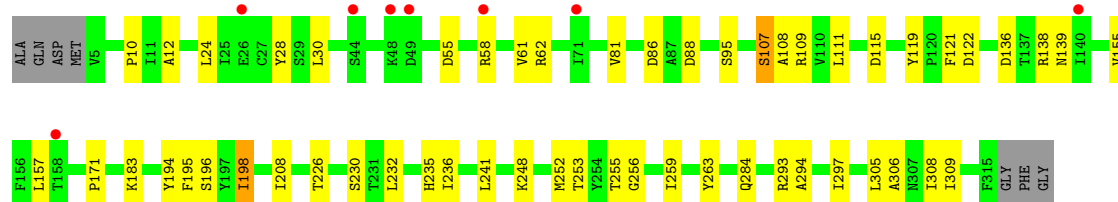
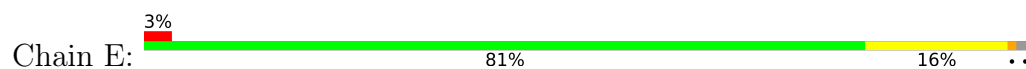


- Molecule 1: Proton-gated ion channel

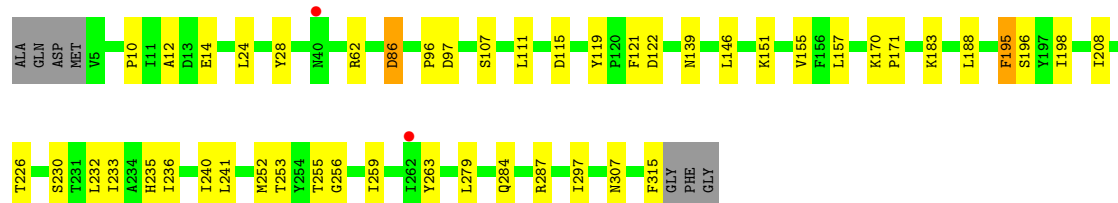
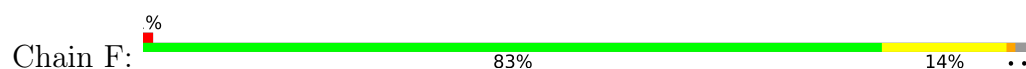




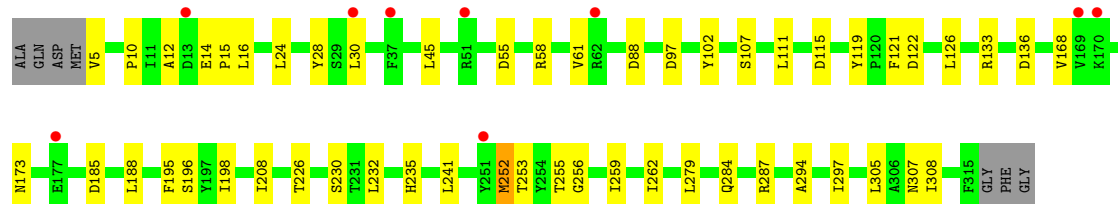
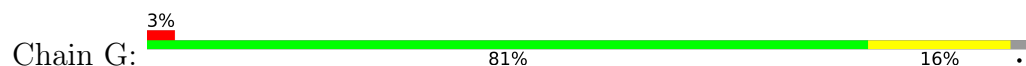
• Molecule 1: Proton-gated ion channel



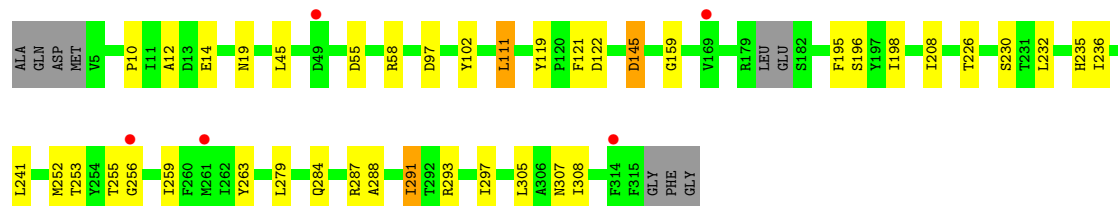
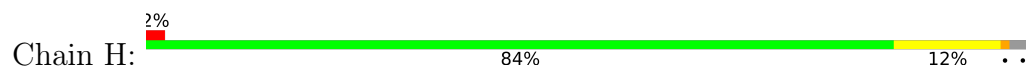
• Molecule 1: Proton-gated ion channel



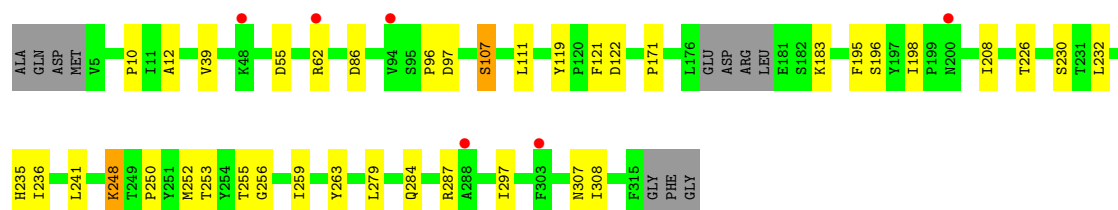
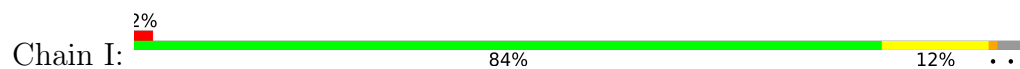
• Molecule 1: Proton-gated ion channel



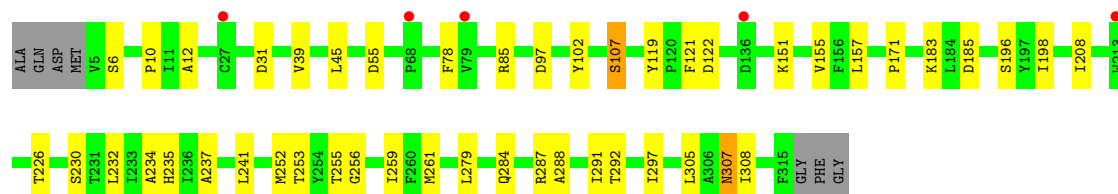
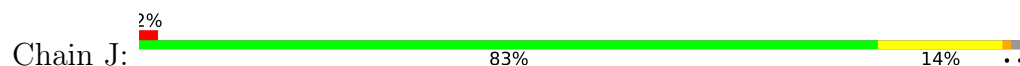
• Molecule 1: Proton-gated ion channel



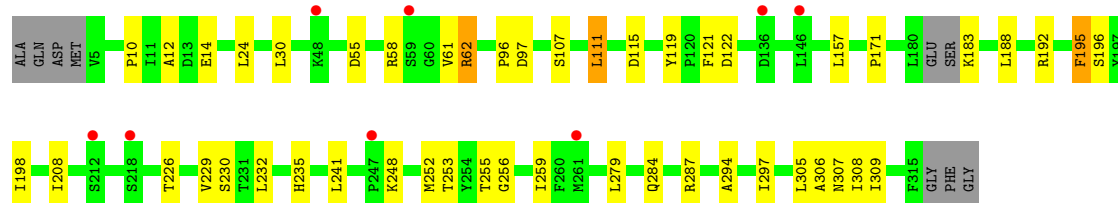
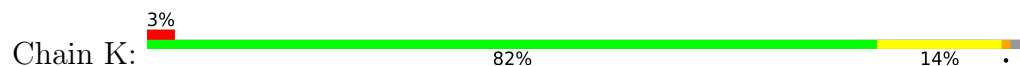
● Molecule 1: Proton-gated ion channel



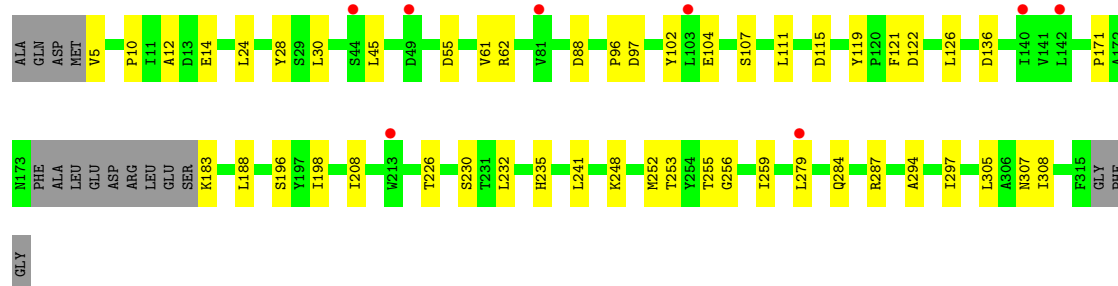
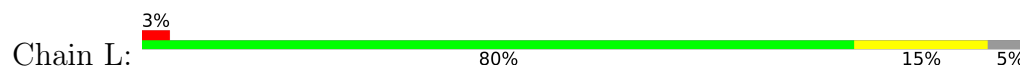
● Molecule 1: Proton-gated ion channel



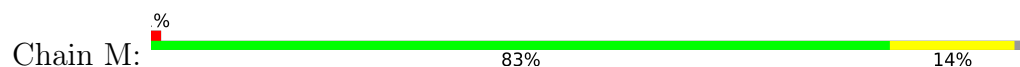
● Molecule 1: Proton-gated ion channel



● Molecule 1: Proton-gated ion channel



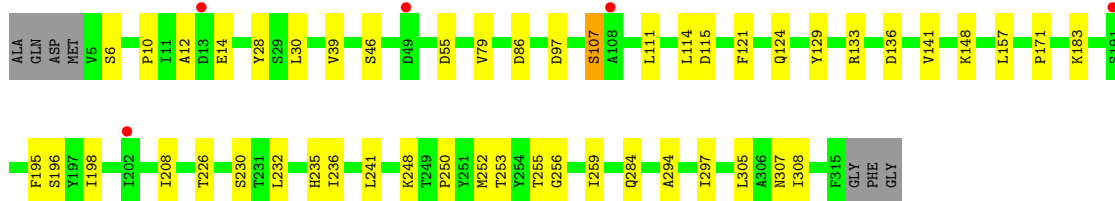
● Molecule 1: Proton-gated ion channel



GLY
PHE
GLY

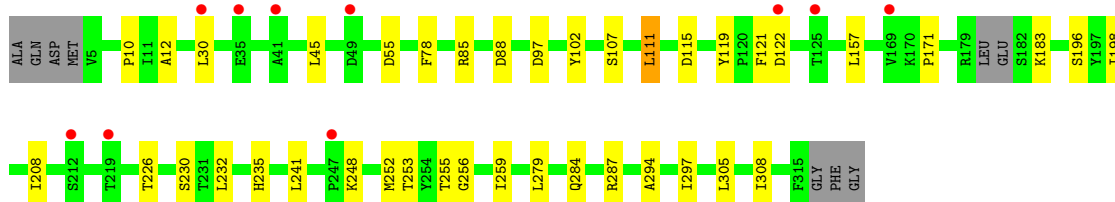
• Molecule 1: Proton-gated ion channel

Chain R:  2% 82% 15% .



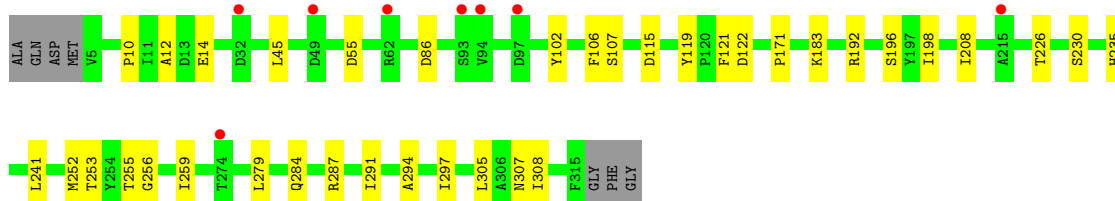
• Molecule 1: Proton-gated ion channel

Chain S:  3% 85% 12% .



• Molecule 1: Proton-gated ion channel

Chain T:  3% 86% 12% .



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	131.53Å 384.10Å 148.44Å 90.00° 98.47° 90.00°	Depositor
Resolution (Å)	20.00 – 4.35 20.00 – 4.35	Depositor EDS
% Data completeness (in resolution range)	99.7 (20.00-4.35) 98.7 (20.00-4.35)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	0.05	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.54 (at 4.36Å)	Xtriage
Refinement program	BUSTER 2.11.4	Depositor
R, R_{free}	0.240 , 0.244 (Not available) , 0.284	Depositor DCC
R_{free} test set	4703 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	218.1	Xtriage
Anisotropy	0.177	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.21 , 134.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.36$, $\langle L^2 \rangle = 0.20$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	45859	wwPDB-VP
Average B, all atoms (Å ²)	239.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.09% 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 ⓘ

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	0.67	0/2385	1.21	3/3291 (0.1%)
1	B	0.69	0/2398	1.25	4/3306 (0.1%)
1	C	0.68	0/2406	1.26	10/3317 (0.3%)
1	D	0.65	0/2394	1.25	6/3306 (0.2%)
1	E	0.66	0/2419	1.20	4/3335 (0.1%)
1	F	0.68	0/2399	1.25	4/3304 (0.1%)
1	G	0.72	0/2389	1.27	9/3293 (0.3%)
1	H	0.67	0/2255	1.23	4/3115 (0.1%)
1	I	0.67	0/2201	1.24	4/3043 (0.1%)
1	J	0.68	0/2318	1.22	3/3197 (0.1%)
1	K	0.68	1/2375 (0.0%)	1.23	5/3273 (0.2%)
1	L	0.65	0/2337	1.20	3/3226 (0.1%)
1	M	0.67	0/2333	1.20	3/3221 (0.1%)
1	N	0.67	0/2425	1.23	7/3342 (0.2%)
1	O	0.68	1/2432 (0.0%)	1.21	2/3354 (0.1%)
1	P	0.67	0/2342	1.28	7/3234 (0.2%)
1	Q	0.69	0/2411	1.25	5/3326 (0.2%)
1	R	0.66	0/2355	1.22	4/3250 (0.1%)
1	S	0.66	1/2330 (0.0%)	1.21	2/3214 (0.1%)
1	T	0.67	0/2206	1.23	4/3050 (0.1%)
All	All	0.67	3/47110 (0.0%)	1.23	93/64997 (0.1%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	O	7	PRO	CA-C	5.90	1.55	1.51
1	K	121	PHE	CA-C	-5.50	1.45	1.52
1	S	121	PHE	CA-C	-5.23	1.45	1.52

The worst 5 of 93 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	195	PHE	CA-CB-CG	12.74	126.54	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	121	PHE	N-CA-C	-12.18	96.98	113.30
1	Q	159	GLY	N-CA-C	-12.13	99.39	115.40
1	P	309	ILE	N-CA-C	-12.01	102.13	111.62
1	G	195	PHE	CA-CB-CG	11.03	124.83	113.80

There are no chirality outliers.

There are no planarity outliers.

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	2322	0	2154	22	0
1	B	2334	0	2173	24	0
1	C	2341	0	2196	21	0
1	D	2330	0	2181	22	0
1	E	2355	0	2213	20	0
1	F	2334	0	2181	23	0
1	G	2325	0	2175	16	0
1	H	2199	0	1930	19	0
1	I	2145	0	1855	16	0
1	J	2257	0	2033	22	0
1	K	2312	0	2156	18	0
1	L	2274	0	2128	22	0
1	M	2271	0	2086	16	0
1	N	2359	0	2238	20	0
1	O	2366	0	2233	30	0
1	P	2280	0	2054	16	0
1	Q	2345	0	2193	27	0
1	R	2293	0	2109	26	0
1	S	2268	0	2072	16	0
1	T	2149	0	1832	14	0
All	All	45859	0	42192	357	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 4.

The worst 5 of 357 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:L:12:ALA:HB2	1:R:141:VAL:HG11	1.24	1.13
1:H:19:ASN:HB3	1:H:145:ASP:OD1	1.55	1.06
1:L:12:ALA:HB2	1:R:141:VAL:CG1	1.98	0.94
1:Q:10:PRO:HB2	1:Q:12:ALA:O	1.73	0.89
1:L:12:ALA:CB	1:R:141:VAL:HG11	2.03	0.88

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

There are no protein backbone outliers to report in this entry.

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	230/284 (81%)	209 (91%)	21 (9%)	9	28
1	B	232/284 (82%)	218 (94%)	14 (6%)	17	40
1	C	233/284 (82%)	213 (91%)	20 (9%)	10	30
1	D	235/284 (83%)	221 (94%)	14 (6%)	17	40
1	E	239/284 (84%)	220 (92%)	19 (8%)	11	32
1	F	229/284 (81%)	213 (93%)	16 (7%)	14	36
1	G	229/284 (81%)	208 (91%)	21 (9%)	8	27
1	H	194/284 (68%)	181 (93%)	13 (7%)	15	37
1	I	181/284 (64%)	169 (93%)	12 (7%)	15	37
1	J	205/284 (72%)	192 (94%)	13 (6%)	16	38
1	K	226/284 (80%)	206 (91%)	20 (9%)	9	29
1	L	231/284 (81%)	215 (93%)	16 (7%)	14	37

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	M	217/284 (76%)	200 (92%)	17 (8%)	11	32
1	N	239/284 (84%)	220 (92%)	19 (8%)	11	32
1	O	242/284 (85%)	225 (93%)	17 (7%)	14	36
1	P	214/284 (75%)	197 (92%)	17 (8%)	11	32
1	Q	234/284 (82%)	216 (92%)	18 (8%)	12	32
1	R	219/284 (77%)	203 (93%)	16 (7%)	13	34
1	S	214/284 (75%)	200 (94%)	14 (6%)	15	38
1	T	173/284 (61%)	163 (94%)	10 (6%)	18	41
All	All	4416/5680 (78%)	4089 (93%)	327 (7%)	13	34

5 of 327 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	N	284	GLN
1	Q	308	ILE
1	O	30	LEU
1	P	196	SER
1	R	305	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 82 such sidechains are listed below:

Mol	Chain	Res	Type
1	N	284	GLN
1	R	235	HIS
1	O	239	ASN
1	P	277	HIS
1	R	307	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

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	311/318 (97%)	0.24	9 (2%) 53 41	161, 244, 294, 300	0
1	B	311/318 (97%)	0.17	8 (2%) 57 44	166, 242, 293, 300	0
1	C	311/318 (97%)	0.22	10 (3%) 50 39	148, 226, 278, 290	0
1	D	311/318 (97%)	0.27	11 (3%) 47 37	146, 232, 285, 295	0
1	E	311/318 (97%)	0.20	8 (2%) 57 44	145, 222, 269, 287	0
1	F	311/318 (97%)	0.17	2 (0%) 85 73	168, 232, 285, 296	0
1	G	311/318 (97%)	0.18	9 (2%) 53 41	174, 232, 296, 300	0
1	H	309/318 (97%)	0.08	5 (1%) 70 55	162, 268, 300, 300	0
1	I	307/318 (96%)	0.17	6 (1%) 65 50	178, 265, 300, 300	0
1	J	311/318 (97%)	0.16	5 (1%) 70 55	171, 262, 300, 300	0
1	K	309/318 (97%)	0.19	8 (2%) 57 44	163, 239, 290, 300	0
1	L	302/318 (94%)	0.13	8 (2%) 57 44	167, 247, 290, 300	0
1	M	308/318 (96%)	-0.06	3 (0%) 79 64	172, 256, 291, 299	0
1	N	311/318 (97%)	0.19	5 (1%) 70 55	173, 255, 293, 299	0
1	O	311/318 (97%)	0.10	6 (1%) 66 52	161, 224, 278, 288	0
1	P	311/318 (97%)	0.14	10 (3%) 50 39	168, 268, 300, 300	0
1	Q	311/318 (97%)	0.12	11 (3%) 47 37	172, 232, 287, 300	0
1	R	311/318 (97%)	0.16	5 (1%) 70 55	178, 239, 288, 296	0
1	S	309/318 (97%)	0.22	10 (3%) 50 39	173, 269, 300, 300	0
1	T	311/318 (97%)	0.24	8 (2%) 57 44	179, 270, 300, 300	0
All	All	6198/6360 (97%)	0.16	147 (2%) 59 47	145, 245, 299, 300	0

The worst 5 of 147 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	Q	169	VAL	7.7
1	B	9	PRO	5.2
1	P	252	MET	4.5
1	B	111	LEU	4.4
1	S	169	VAL	4.4

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.