wwPDB X-ray Structure Validation Summary Report (i)

May 16, 2020 – 02:13 am BST

PDB ID	:	4TWD
Title	:	X-ray structure of a pentameric ligand gated ion channel from Erwinia chrysanthemi (ELIC) in complex with memantine
Authors	:	Ulens, C.; Spurny, R.; Thompson, A.J.; Alqazzaz, M.; Debaveye, S.; Lu, H.; Price, K.; Villalgordo, J.M.; Tresadern, G.; Lynch, J.W.; Lummis, S.C.R.
Deposited on	:	2014-06-30
Resolution	:	3.20 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:

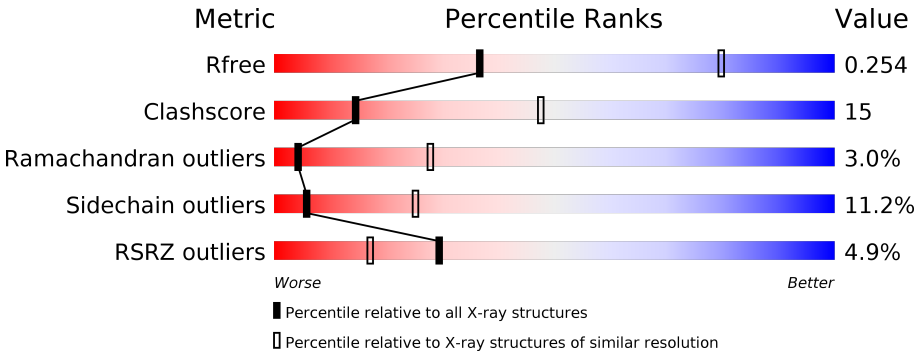
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, 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 3.20 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	1133 (3.20-3.20)
Clashscore	141614	1253 (3.20-3.20)
Ramachandran outliers	138981	1234 (3.20-3.20)
Sidechain outliers	138945	1233 (3.20-3.20)
RSRZ outliers	127900	1095 (3.20-3.20)

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	307	5% 61% 32% 6%
1	B	307	3% 63% 30% 6%
1	C	307	7% 58% 37% 5%
1	D	307	3% 60% 33% 7%
1	E	307	4% 58% 36% 5%
1	F	307	6% 57% 38% 5%

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Mol	Chain	Length	Quality of chain
1	G	307	7% 59% 35% 6%
1	H	307	7% 60% 34% 6%
1	I	307	5% 63% 32% 5%
1	J	307	4% 61% 33% 6%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 25126 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 Cys-loop ligand-gated ion channel.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	307	Total	C	N	O	S	0	0	0
			2497	1624	416	451	6			
1	B	307	Total	C	N	O	S	0	0	0
			2497	1624	416	451	6			
1	C	307	Total	C	N	O	S	0	0	0
			2497	1624	416	451	6			
1	D	307	Total	C	N	O	S	0	0	0
			2497	1624	416	451	6			
1	E	307	Total	C	N	O	S	0	0	0
			2497	1624	416	451	6			
1	F	307	Total	C	N	O	S	0	0	0
			2497	1624	416	451	6			
1	G	307	Total	C	N	O	S	0	0	0
			2497	1624	416	451	6			
1	H	307	Total	C	N	O	S	0	0	0
			2497	1624	416	451	6			
1	I	307	Total	C	N	O	S	0	0	0
			2497	1624	416	451	6			
1	J	307	Total	C	N	O	S	0	0	0
			2497	1624	416	451	6			

There are 40 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	152	ALA	ILE	conflict	UNP P0C7B7
A	164	GLY	-	insertion	UNP P0C7B7
A	247	SER	PHE	engineered mutation	UNP P0C7B7
A	289	ASN	MET	conflict	UNP P0C7B7
B	152	ALA	ILE	conflict	UNP P0C7B7
B	164	GLY	-	insertion	UNP P0C7B7
B	247	SER	PHE	engineered mutation	UNP P0C7B7
B	289	ASN	MET	conflict	UNP P0C7B7
C	152	ALA	ILE	conflict	UNP P0C7B7

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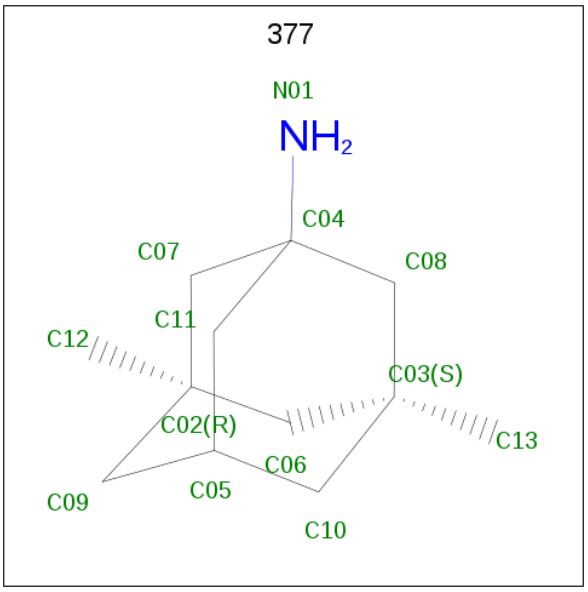
Chain	Residue	Modelled	Actual	Comment	Reference
C	164	GLY	-	insertion	UNP P0C7B7
C	247	SER	PHE	engineered mutation	UNP P0C7B7
C	289	ASN	MET	conflict	UNP P0C7B7
D	152	ALA	ILE	conflict	UNP P0C7B7
D	164	GLY	-	insertion	UNP P0C7B7
D	247	SER	PHE	engineered mutation	UNP P0C7B7
D	289	ASN	MET	conflict	UNP P0C7B7
E	152	ALA	ILE	conflict	UNP P0C7B7
E	164	GLY	-	insertion	UNP P0C7B7
E	247	SER	PHE	engineered mutation	UNP P0C7B7
E	289	ASN	MET	conflict	UNP P0C7B7
F	152	ALA	ILE	conflict	UNP P0C7B7
F	164	GLY	-	insertion	UNP P0C7B7
F	247	SER	PHE	engineered mutation	UNP P0C7B7
F	289	ASN	MET	conflict	UNP P0C7B7
G	152	ALA	ILE	conflict	UNP P0C7B7
G	164	GLY	-	insertion	UNP P0C7B7
G	247	SER	PHE	engineered mutation	UNP P0C7B7
G	289	ASN	MET	conflict	UNP P0C7B7
H	152	ALA	ILE	conflict	UNP P0C7B7
H	164	GLY	-	insertion	UNP P0C7B7
H	247	SER	PHE	engineered mutation	UNP P0C7B7
H	289	ASN	MET	conflict	UNP P0C7B7
I	152	ALA	ILE	conflict	UNP P0C7B7
I	164	GLY	-	insertion	UNP P0C7B7
I	247	SER	PHE	engineered mutation	UNP P0C7B7
I	289	ASN	MET	conflict	UNP P0C7B7
J	152	ALA	ILE	conflict	UNP P0C7B7
J	164	GLY	-	insertion	UNP P0C7B7
J	247	SER	PHE	engineered mutation	UNP P0C7B7
J	289	ASN	MET	conflict	UNP P0C7B7

- Molecule 2 is Memantine (three-letter code: 377) (formula: $C_{12}H_{21}N$).



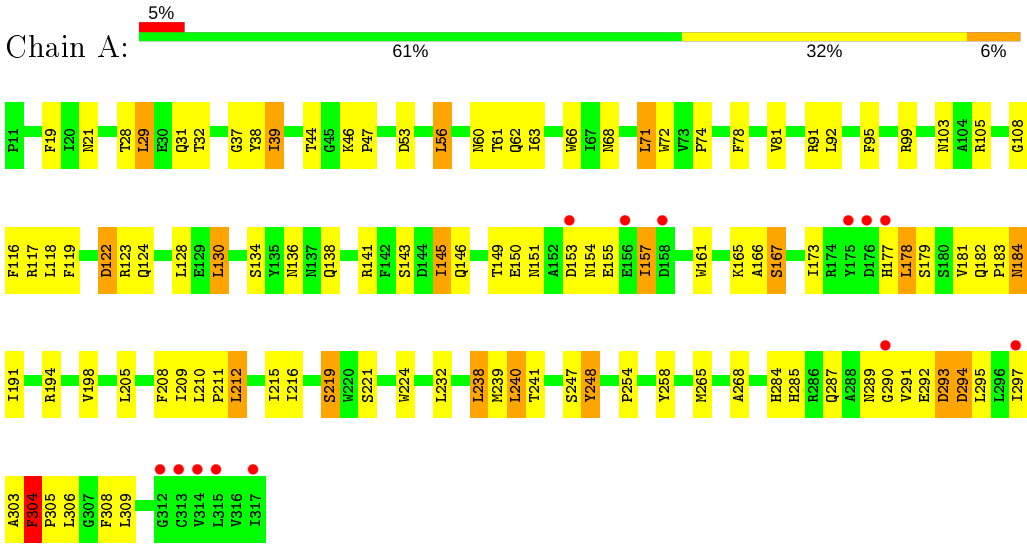
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C N 13 12 1	0	0
2	A	1	Total C N 13 12 1	0	0
2	B	1	Total C N 13 12 1	0	0
2	C	1	Total C N 13 12 1	0	0
2	C	1	Total C N 13 12 1	0	0
2	E	1	Total C N 13 12 1	0	0
2	F	1	Total C N 13 12 1	0	0
2	F	1	Total C N 13 12 1	0	0
2	G	1	Total C N 13 12 1	0	0
2	H	1	Total C N 13 12 1	0	0
2	H	1	Total C N 13 12 1	0	0
2	J	1	Total C N 13 12 1	0	0

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.

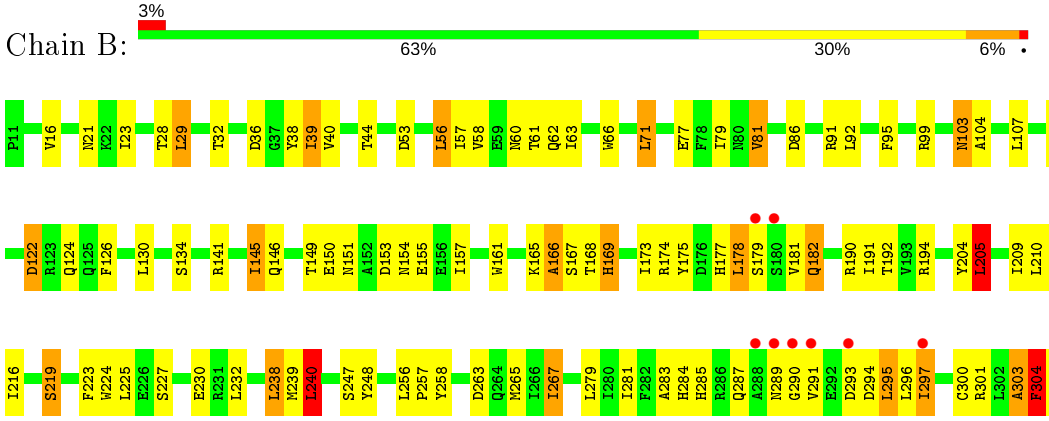
- Molecule 1: Cys-loop ligand-gated ion channel

Chain A:



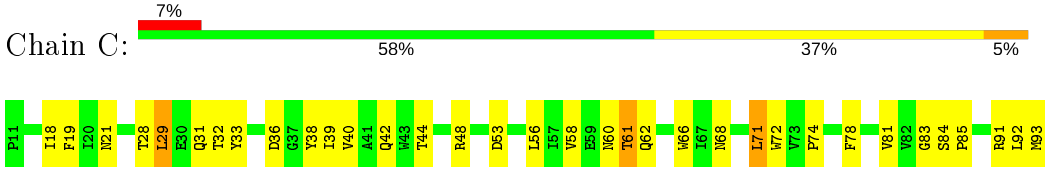
- Molecule 1: Cys-loop ligand-gated ion channel

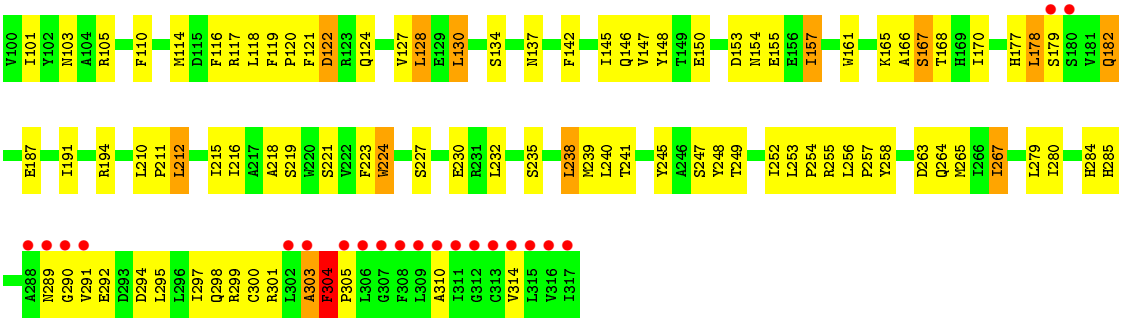
Chain B:



- Molecule 1: Cys-loop ligand-gated ion channel

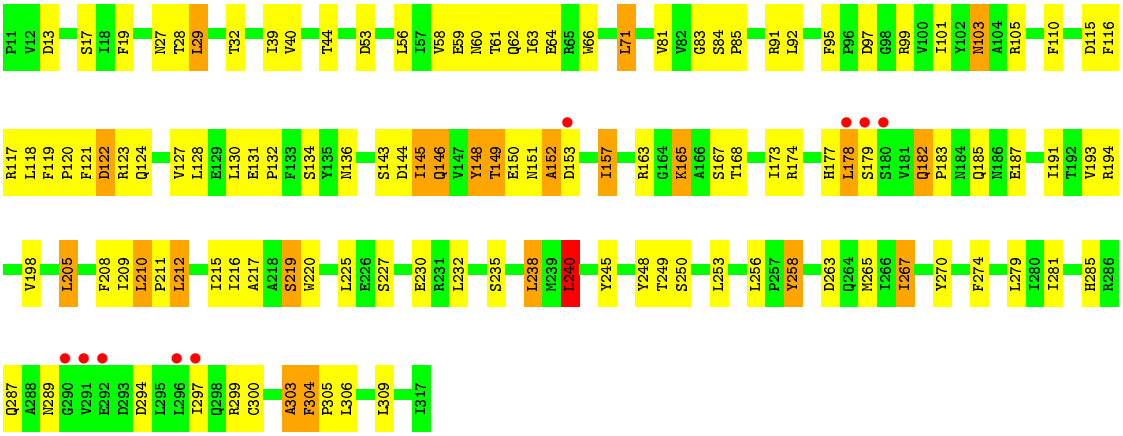
Chain C:





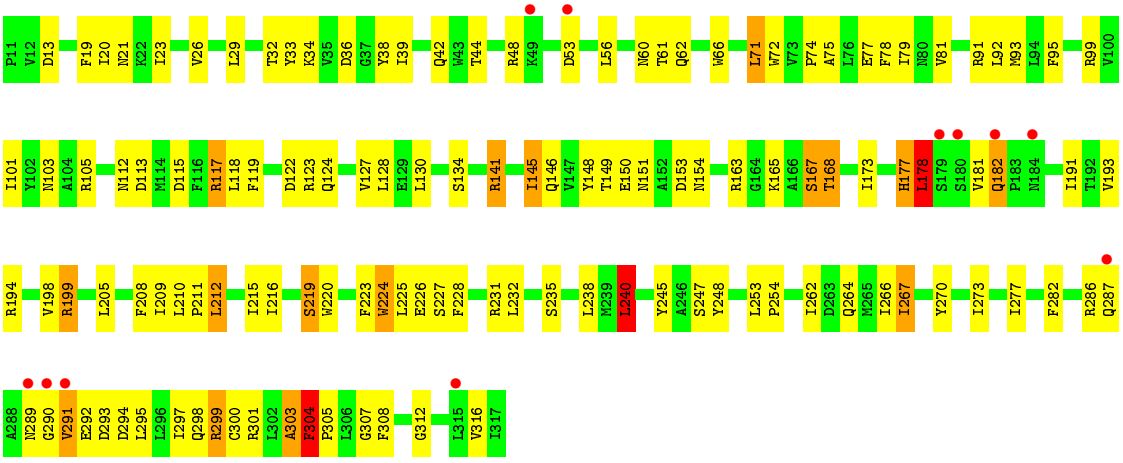
• Molecule 1: Cys-loop ligand-gated ion channel

Chain D:



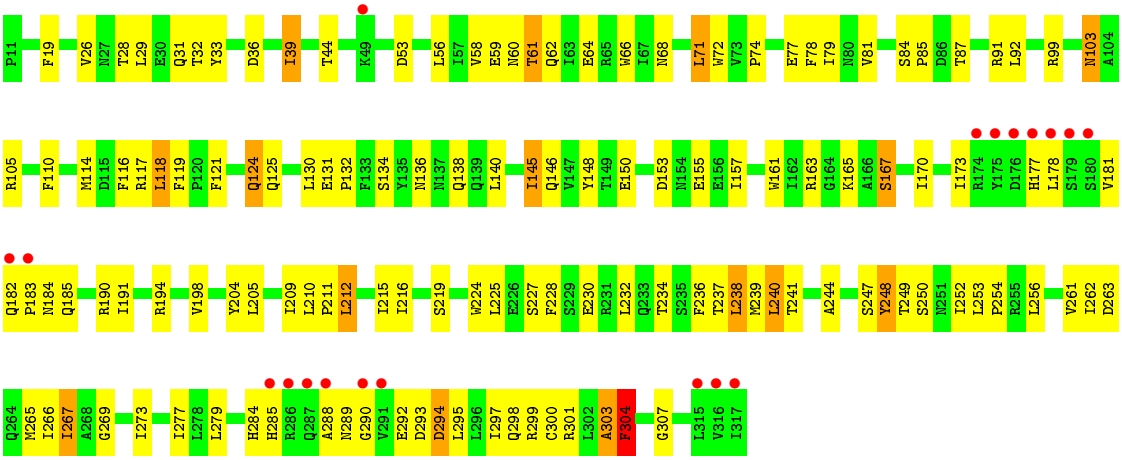
• Molecule 1: Cys-loop ligand-gated ion channel

Chain E:



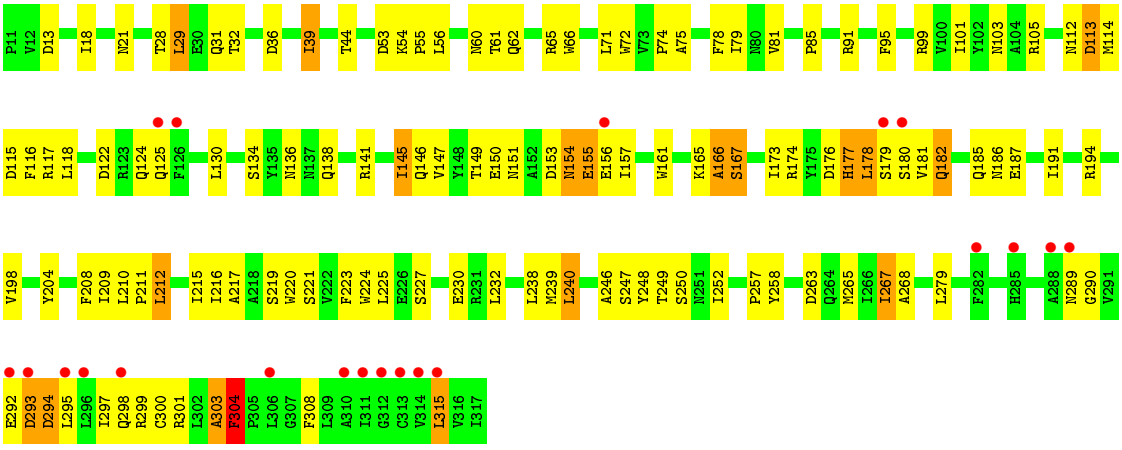
• Molecule 1: Cys-loop ligand-gated ion channel

Chain F:



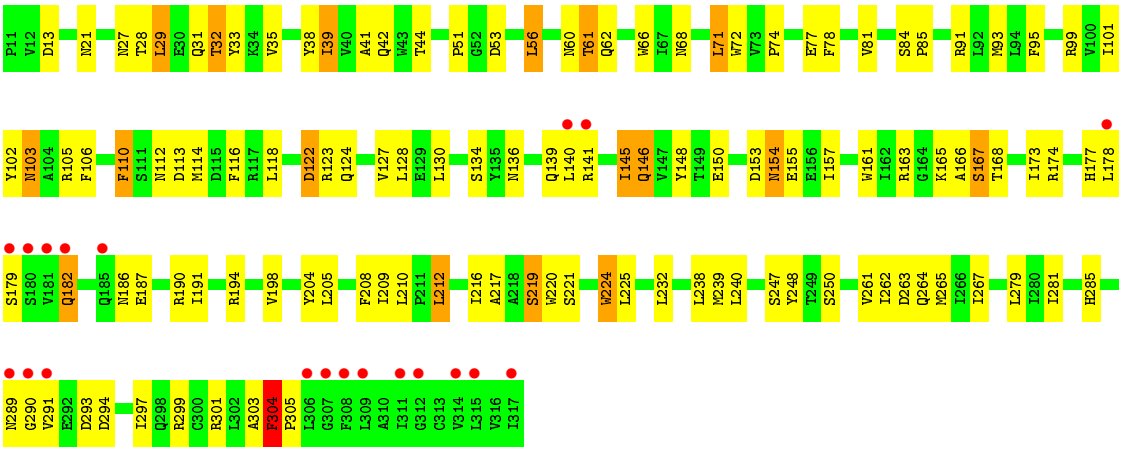
• Molecule 1: Cys-loop ligand-gated ion channel

Chain G:



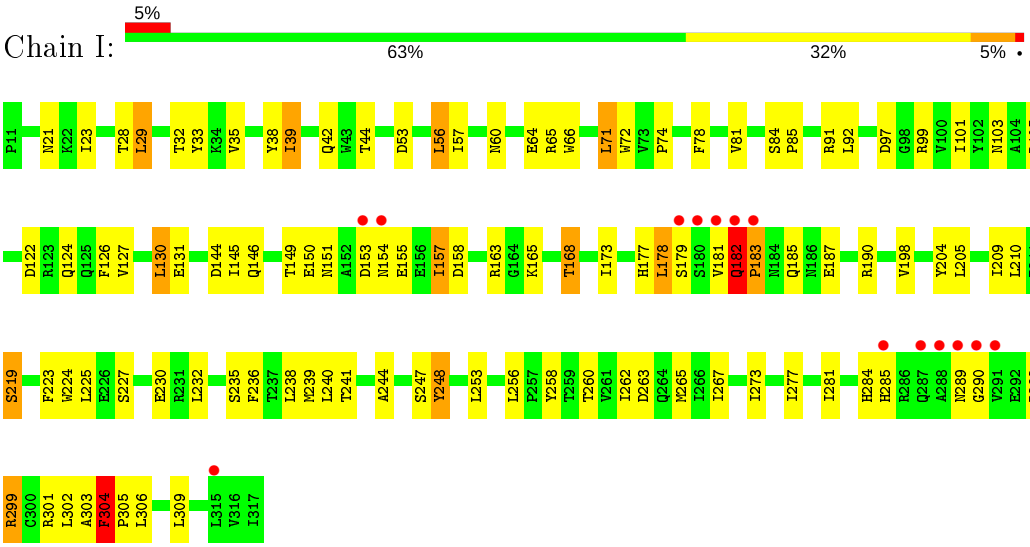
• Molecule 1: Cys-loop ligand-gated ion channel

Chain H:



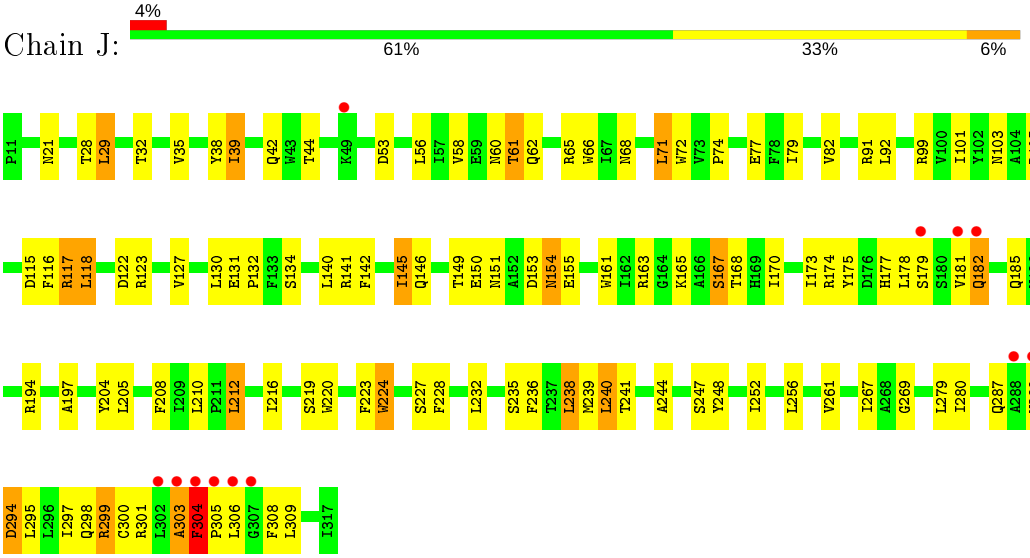
• Molecule 1: Cys-loop ligand-gated ion channel

Chain I:



• Molecule 1: Cys-loop ligand-gated ion channel

Chain J:



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	105.48Å 265.28Å 111.10Å 90.00° 110.28° 90.00°	Depositor
Resolution (Å)	48.63 – 3.20 48.63 – 3.20	Depositor EDS
% Data completeness (in resolution range)	99.8 (48.63-3.20) 91.0 (48.63-3.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.28 (at 3.19Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8_1069)	Depositor
R, R_{free}	0.199 , 0.252 0.202 , 0.254	Depositor DCC
R_{free} test set	4705 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å^2)	84.2	Xtriage
Anisotropy	0.379	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.27 , 73.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.90	EDS
Total number of atoms	25126	wwPDB-VP
Average B, all atoms (Å^2)	120.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.17% 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

Bond lengths and bond angles in the following residue types are not validated in this section: 377

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	0.56	0/2564	0.80	2/3495 (0.1%)
1	B	0.66	0/2564	0.90	3/3495 (0.1%)
1	C	0.67	0/2564	0.86	0/3495
1	D	0.68	0/2564	0.87	2/3495 (0.1%)
1	E	0.58	0/2564	0.80	3/3495 (0.1%)
1	F	0.53	0/2564	0.77	0/3495
1	G	0.65	0/2564	0.87	1/3495 (0.0%)
1	H	0.60	0/2564	0.79	0/3495
1	I	0.61	0/2564	0.81	0/3495
1	J	0.54	0/2564	0.76	1/3495 (0.0%)
All	All	0.61	0/25640	0.82	12/34950 (0.0%)

There are no bond length outliers.

The worst 5 of 12 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	56	LEU	CB-CG-CD1	-6.60	99.78	111.00
1	A	39	ILE	CB-CA-C	-6.29	99.02	111.60
1	B	240	LEU	CA-CB-CG	6.11	129.34	115.30
1	D	205	LEU	CA-CB-CG	-5.98	101.55	115.30
1	E	178	LEU	CA-CB-CG	5.98	129.04	115.30

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	2497	0	2468	77	0
1	B	2497	0	2468	84	0
1	C	2497	0	2468	90	0
1	D	2497	0	2468	90	0
1	E	2497	0	2468	87	0
1	F	2497	0	2468	94	0
1	G	2497	0	2468	98	0
1	H	2497	0	2468	85	0
1	I	2497	0	2468	78	0
1	J	2497	0	2468	81	0
2	A	26	0	42	2	0
2	B	13	0	21	1	0
2	C	26	0	42	2	0
2	E	13	0	21	0	0
2	F	26	0	42	3	0
2	G	13	0	21	0	0
2	H	26	0	42	2	0
2	J	13	0	21	3	0
All	All	25126	0	24932	771	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 15.

The worst 5 of 771 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:E:294:ASP:HB2	1:E:297:ILE:HG22	1.46	0.93
1:G:13:ASP:OD2	1:G:141:ARG:NH1	2.05	0.89
1:G:154:ASN:O	1:G:156:GLU:N	2.10	0.84
1:A:224:TRP:CH2	1:A:301:ARG:HB3	2.13	0.84
1:E:293:ASP:O	1:E:298:GLN:NE2	2.12	0.82

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	305/307 (99%)	279 (92%)	17 (6%)	9 (3%)	4	28
1	B	305/307 (99%)	275 (90%)	19 (6%)	11 (4%)	3	23
1	C	305/307 (99%)	274 (90%)	23 (8%)	8 (3%)	5	31
1	D	305/307 (99%)	278 (91%)	18 (6%)	9 (3%)	4	28
1	E	305/307 (99%)	280 (92%)	16 (5%)	9 (3%)	4	28
1	F	305/307 (99%)	278 (91%)	18 (6%)	9 (3%)	4	28
1	G	305/307 (99%)	278 (91%)	17 (6%)	10 (3%)	4	25
1	H	305/307 (99%)	277 (91%)	19 (6%)	9 (3%)	4	28
1	I	305/307 (99%)	276 (90%)	22 (7%)	7 (2%)	6	34
1	J	305/307 (99%)	279 (92%)	17 (6%)	9 (3%)	4	28
All	All	3050/3070 (99%)	2774 (91%)	186 (6%)	90 (3%)	4	28

5 of 90 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	153	ASP
1	B	166	ALA
1	C	153	ASP
1	C	166	ALA
1	G	154	ASN

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	274/274 (100%)	242 (88%)	32 (12%)	5	23
1	B	274/274 (100%)	243 (89%)	31 (11%)	6	25
1	C	274/274 (100%)	244 (89%)	30 (11%)	6	26
1	D	274/274 (100%)	242 (88%)	32 (12%)	5	23
1	E	274/274 (100%)	243 (89%)	31 (11%)	6	25
1	F	274/274 (100%)	247 (90%)	27 (10%)	8	30
1	G	274/274 (100%)	244 (89%)	30 (11%)	6	26
1	H	274/274 (100%)	242 (88%)	32 (12%)	5	23
1	I	274/274 (100%)	245 (89%)	29 (11%)	6	27
1	J	274/274 (100%)	242 (88%)	32 (12%)	5	23
All	All	2740/2740 (100%)	2434 (89%)	306 (11%)	6	25

5 of 306 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	146	GLN
1	F	167	SER
1	J	118	LEU
1	E	177	HIS
1	E	304	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 17 such sidechains are listed below:

Mol	Chain	Res	Type
1	F	136	ASN
1	F	284	HIS
1	I	89	ASN
1	E	298	GLN
1	I	284	HIS

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)

12 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	377	J	401	-	13,15,15	2.71	10 (76%)	24,27,27	2.75	9 (37%)
2	377	H	402	-	13,15,15	2.58	8 (61%)	24,27,27	2.47	12 (50%)
2	377	F	402	-	13,15,15	3.29	10 (76%)	24,27,27	2.25	7 (29%)
2	377	B	401	-	13,15,15	2.60	9 (69%)	24,27,27	2.73	6 (25%)
2	377	A	401	-	13,15,15	2.69	8 (61%)	24,27,27	2.50	8 (33%)
2	377	C	401	-	13,15,15	2.81	10 (76%)	24,27,27	3.12	12 (50%)
2	377	F	401	-	13,15,15	2.57	9 (69%)	24,27,27	2.21	7 (29%)
2	377	E	401	-	13,15,15	2.90	10 (76%)	24,27,27	2.70	9 (37%)
2	377	C	402	-	13,15,15	2.24	6 (46%)	24,27,27	2.45	9 (37%)
2	377	G	401	-	13,15,15	2.54	8 (61%)	24,27,27	2.27	8 (33%)
2	377	A	402	-	13,15,15	3.25	10 (76%)	24,27,27	3.70	14 (58%)
2	377	H	401	-	13,15,15	2.63	10 (76%)	24,27,27	2.96	6 (25%)

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	377	J	401	-	-	-	0/4/3/3
2	377	H	402	-	-	-	0/4/3/3
2	377	F	402	-	-	-	0/4/3/3
2	377	B	401	-	-	-	0/4/3/3
2	377	A	401	-	-	-	0/4/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	377	C	401	-	-	-	0/4/3/3
2	377	F	401	-	-	-	0/4/3/3
2	377	E	401	-	-	-	0/4/3/3
2	377	C	402	-	-	-	0/4/3/3
2	377	G	401	-	-	-	0/4/3/3
2	377	A	402	-	-	-	0/4/3/3
2	377	H	401	-	-	-	0/4/3/3

The worst 5 of 108 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	402	377	C06-C02	-5.05	1.47	1.53
2	A	402	377	C08-C03	-4.89	1.47	1.53
2	A	402	377	C06-C03	-4.37	1.48	1.53
2	F	402	377	C07-C02	-4.31	1.48	1.53
2	F	402	377	C06-C03	-4.29	1.48	1.53

The worst 5 of 107 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	H	401	377	C04-C07-C02	-10.30	104.52	110.81
2	A	402	377	C07-C02-C09	7.89	113.60	108.68
2	C	401	377	C04-C07-C02	-7.48	106.24	110.81
2	E	401	377	C04-C07-C02	-7.10	106.47	110.81
2	A	402	377	C12-C02-C09	-6.91	103.23	110.47

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

7 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	J	401	377	3	0
2	H	402	377	2	0
2	F	402	377	3	0
2	B	401	377	1	0
2	A	401	377	2	0
2	C	401	377	1	0
2	C	402	377	1	0

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, 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	307/307 (100%)	-0.12	15 (4%) 29 17	74, 118, 193, 267	0
1	B	307/307 (100%)	0.01	9 (2%) 51 36	74, 103, 203, 322	0
1	C	307/307 (100%)	-0.09	21 (6%) 17 10	66, 102, 199, 249	0
1	D	307/307 (100%)	-0.22	9 (2%) 51 36	69, 101, 200, 262	0
1	E	307/307 (100%)	-0.20	11 (3%) 42 27	77, 113, 191, 247	0
1	F	307/307 (100%)	-0.10	19 (6%) 20 11	76, 116, 204, 258	0
1	G	307/307 (100%)	-0.06	21 (6%) 17 10	69, 105, 188, 269	0
1	H	307/307 (100%)	-0.11	20 (6%) 18 11	72, 110, 216, 256	0
1	I	307/307 (100%)	-0.17	14 (4%) 32 20	70, 107, 203, 302	0
1	J	307/307 (100%)	-0.22	12 (3%) 39 25	80, 119, 214, 266	0
All	All	3070/3070 (100%)	-0.13	151 (4%) 29 17	66, 110, 204, 322	0

The worst 5 of 151 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	290	GLY	15.5
1	C	180	SER	12.3
1	E	290	GLY	12.3
1	I	180	SER	9.3
1	I	182	GLN	8.7

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 (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	377	H	401	13/13	0.93	0.27	106,113,120,120	0
2	377	A	402	13/13	0.94	0.34	95,102,109,113	0
2	377	F	401	13/13	0.94	0.37	111,115,119,121	0
2	377	A	401	13/13	0.95	0.48	130,135,138,138	0
2	377	H	402	13/13	0.95	0.22	96,101,107,107	0
2	377	F	402	13/13	0.95	0.27	116,119,130,134	0
2	377	B	401	13/13	0.95	0.23	101,105,109,115	0
2	377	G	401	13/13	0.96	0.22	105,108,116,117	0
2	377	E	401	13/13	0.96	0.31	92,97,104,105	0
2	377	C	402	13/13	0.96	0.25	84,88,91,91	0
2	377	J	401	13/13	0.97	0.31	91,97,98,99	0
2	377	C	401	13/13	0.98	0.43	92,97,106,108	0

6.5 Other polymers (i)

There are no such residues in this entry.