



wwPDB/EMDataBank EM Map/Model Validation Summary Report ⓘ

Nov 23, 2019 – 09:41 PM EST

PDB ID : 6V00
EMDB ID: : EMD-20966
Title : structure of human KCNQ1-KCNE3-CaM complex
Authors : Mackinnon, R.; Sun, J.
Deposited on : 2019-11-16
Resolution : 3.10 Å(reported)

This is a wwPDB/EMDataBank EM Map/Model Validation Summary Report
for a publicly released PDB/EMDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

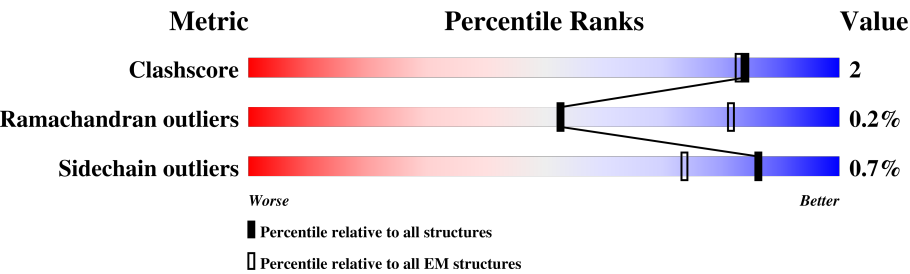
MolProbity : 4.02b-467
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : 2.4

1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 3.10 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)	EM structures (#Entries)
Clashscore	136327	1886
Ramachandran outliers	132723	1663
Sidechain outliers	132532	1531

The table below summarises the geometric issues observed across the polymeric chains. The red, orange, yellow and green segments on the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	A	557	
1	D	557	
1	G	557	
1	J	557	
2	B	149	
2	E	149	
2	H	149	
2	K	149	
3	C	355	

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Mol	Chain	Length	Quality of chain
3	F	355	<div><div></div><div>12%</div><div></div><div>87%</div></div>
3	I	355	<div><div></div><div>13%</div><div></div><div>87%</div></div>
3	L	355	<div><div></div><div>13%</div><div></div><div>87%</div></div>

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 17460 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, 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 Potassium voltage-gated channel subfamily KQT member 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	354	Total	C	N	O	S	0	0
			2864	1879	499	475	11		
1	D	354	Total	C	N	O	S	0	0
			2864	1879	499	475	11		
1	G	354	Total	C	N	O	S	0	0
			2864	1879	499	475	11		
1	J	354	Total	C	N	O	S	0	0
			2864	1879	499	475	11		

There are 48 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	75	MET	-	expression tag	UNP P51787
A	621	SER	-	expression tag	UNP P51787
A	622	ASN	-	expression tag	UNP P51787
A	623	SER	-	expression tag	UNP P51787
A	624	LEU	-	expression tag	UNP P51787
A	625	GLU	-	expression tag	UNP P51787
A	626	VAL	-	expression tag	UNP P51787
A	627	LEU	-	expression tag	UNP P51787
A	628	PHE	-	expression tag	UNP P51787
A	629	GLN	-	expression tag	UNP P51787
A	630	GLY	-	expression tag	UNP P51787
A	631	PRO	-	expression tag	UNP P51787
D	75	MET	-	expression tag	UNP P51787
D	621	SER	-	expression tag	UNP P51787
D	622	ASN	-	expression tag	UNP P51787
D	623	SER	-	expression tag	UNP P51787
D	624	LEU	-	expression tag	UNP P51787
D	625	GLU	-	expression tag	UNP P51787
D	626	VAL	-	expression tag	UNP P51787
D	627	LEU	-	expression tag	UNP P51787
D	628	PHE	-	expression tag	UNP P51787
D	629	GLN	-	expression tag	UNP P51787

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Chain	Residue	Modelled	Actual	Comment	Reference
D	630	GLY	-	expression tag	UNP P51787
D	631	PRO	-	expression tag	UNP P51787
G	75	MET	-	expression tag	UNP P51787
G	621	SER	-	expression tag	UNP P51787
G	622	ASN	-	expression tag	UNP P51787
G	623	SER	-	expression tag	UNP P51787
G	624	LEU	-	expression tag	UNP P51787
G	625	GLU	-	expression tag	UNP P51787
G	626	VAL	-	expression tag	UNP P51787
G	627	LEU	-	expression tag	UNP P51787
G	628	PHE	-	expression tag	UNP P51787
G	629	GLN	-	expression tag	UNP P51787
G	630	GLY	-	expression tag	UNP P51787
G	631	PRO	-	expression tag	UNP P51787
J	75	MET	-	expression tag	UNP P51787
J	621	SER	-	expression tag	UNP P51787
J	622	ASN	-	expression tag	UNP P51787
J	623	SER	-	expression tag	UNP P51787
J	624	LEU	-	expression tag	UNP P51787
J	625	GLU	-	expression tag	UNP P51787
J	626	VAL	-	expression tag	UNP P51787
J	627	LEU	-	expression tag	UNP P51787
J	628	PHE	-	expression tag	UNP P51787
J	629	GLN	-	expression tag	UNP P51787
J	630	GLY	-	expression tag	UNP P51787
J	631	PRO	-	expression tag	UNP P51787

- Molecule 2 is a protein called Calmodulin-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	144	Total	C	N	O	S	0	0
			1105	681	180	235	9		
2	E	144	Total	C	N	O	S	0	0
			1105	681	180	235	9		
2	H	144	Total	C	N	O	S	0	0
			1105	681	180	235	9		
2	K	144	Total	C	N	O	S	0	0
			1105	681	180	235	9		

- Molecule 3 is a protein called MCherry fluorescent protein,Potassium voltage-gated channel subfamily E member 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	47	Total 394	C 256	N 68	O 68	S 2	0	0
3	F	47	Total 394	C 256	N 68	O 68	S 2	0	0
3	I	47	Total 394	C 256	N 68	O 68	S 2	0	0
3	L	47	Total 394	C 256	N 68	O 68	S 2	0	0

There are 88 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	-251	GLY	-	expression tag	UNP X5DSL3
C	-250	GLY	-	expression tag	UNP X5DSL3
C	-153	ASN	LYS	conflict	UNP X5DSL3
C	-107	CYS	LYS	conflict	UNP X5DSL3
C	-106	ARG	LYS	conflict	UNP X5DSL3
C	-98	THR	SER	conflict	UNP X5DSL3
C	-49	ASP	ASN	conflict	UNP X5DSL3
C	-43	LEU	THR	conflict	UNP X5DSL3
C	-13	GLY	-	linker	UNP X5DSL3
C	-12	SER	-	linker	UNP X5DSL3
C	-11	GLY	-	linker	UNP X5DSL3
C	-10	GLU	-	linker	UNP X5DSL3
C	-9	ASN	-	linker	UNP X5DSL3
C	-8	LEU	-	linker	UNP X5DSL3
C	-7	TYR	-	linker	UNP X5DSL3
C	-6	PHE	-	linker	UNP X5DSL3
C	-5	GLN	-	linker	UNP X5DSL3
C	-4	SER	-	linker	UNP X5DSL3
C	-3	SER	-	linker	UNP X5DSL3
C	-2	ARG	-	linker	UNP X5DSL3
C	-1	ALA	-	linker	UNP X5DSL3
C	0	THR	-	linker	UNP X5DSL3
F	-251	GLY	-	expression tag	UNP X5DSL3
F	-250	GLY	-	expression tag	UNP X5DSL3
F	-153	ASN	LYS	conflict	UNP X5DSL3
F	-107	CYS	LYS	conflict	UNP X5DSL3
F	-106	ARG	LYS	conflict	UNP X5DSL3
F	-98	THR	SER	conflict	UNP X5DSL3
F	-49	ASP	ASN	conflict	UNP X5DSL3
F	-43	LEU	THR	conflict	UNP X5DSL3
F	-13	GLY	-	linker	UNP X5DSL3

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Chain	Residue	Modelled	Actual	Comment	Reference
F	-12	SER	-	linker	UNP X5DSL3
F	-11	GLY	-	linker	UNP X5DSL3
F	-10	GLU	-	linker	UNP X5DSL3
F	-9	ASN	-	linker	UNP X5DSL3
F	-8	LEU	-	linker	UNP X5DSL3
F	-7	TYR	-	linker	UNP X5DSL3
F	-6	PHE	-	linker	UNP X5DSL3
F	-5	GLN	-	linker	UNP X5DSL3
F	-4	SER	-	linker	UNP X5DSL3
F	-3	SER	-	linker	UNP X5DSL3
F	-2	ARG	-	linker	UNP X5DSL3
F	-1	ALA	-	linker	UNP X5DSL3
F	0	THR	-	linker	UNP X5DSL3
I	-251	GLY	-	expression tag	UNP X5DSL3
I	-250	GLY	-	expression tag	UNP X5DSL3
I	-153	ASN	LYS	conflict	UNP X5DSL3
I	-107	CYS	LYS	conflict	UNP X5DSL3
I	-106	ARG	LYS	conflict	UNP X5DSL3
I	-98	THR	SER	conflict	UNP X5DSL3
I	-49	ASP	ASN	conflict	UNP X5DSL3
I	-43	LEU	THR	conflict	UNP X5DSL3
I	-13	GLY	-	linker	UNP X5DSL3
I	-12	SER	-	linker	UNP X5DSL3
I	-11	GLY	-	linker	UNP X5DSL3
I	-10	GLU	-	linker	UNP X5DSL3
I	-9	ASN	-	linker	UNP X5DSL3
I	-8	LEU	-	linker	UNP X5DSL3
I	-7	TYR	-	linker	UNP X5DSL3
I	-6	PHE	-	linker	UNP X5DSL3
I	-5	GLN	-	linker	UNP X5DSL3
I	-4	SER	-	linker	UNP X5DSL3
I	-3	SER	-	linker	UNP X5DSL3
I	-2	ARG	-	linker	UNP X5DSL3
I	-1	ALA	-	linker	UNP X5DSL3
I	0	THR	-	linker	UNP X5DSL3
L	-251	GLY	-	expression tag	UNP X5DSL3
L	-250	GLY	-	expression tag	UNP X5DSL3
L	-153	ASN	LYS	conflict	UNP X5DSL3
L	-107	CYS	LYS	conflict	UNP X5DSL3
L	-106	ARG	LYS	conflict	UNP X5DSL3
L	-98	THR	SER	conflict	UNP X5DSL3
L	-49	ASP	ASN	conflict	UNP X5DSL3

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Chain	Residue	Modelled	Actual	Comment	Reference
L	-43	LEU	THR	conflict	UNP X5DSL3
L	-13	GLY	-	linker	UNP X5DSL3
L	-12	SER	-	linker	UNP X5DSL3
L	-11	GLY	-	linker	UNP X5DSL3
L	-10	GLU	-	linker	UNP X5DSL3
L	-9	ASN	-	linker	UNP X5DSL3
L	-8	LEU	-	linker	UNP X5DSL3
L	-7	TYR	-	linker	UNP X5DSL3
L	-6	PHE	-	linker	UNP X5DSL3
L	-5	GLN	-	linker	UNP X5DSL3
L	-4	SER	-	linker	UNP X5DSL3
L	-3	SER	-	linker	UNP X5DSL3
L	-2	ARG	-	linker	UNP X5DSL3
L	-1	ALA	-	linker	UNP X5DSL3
L	0	THR	-	linker	UNP X5DSL3

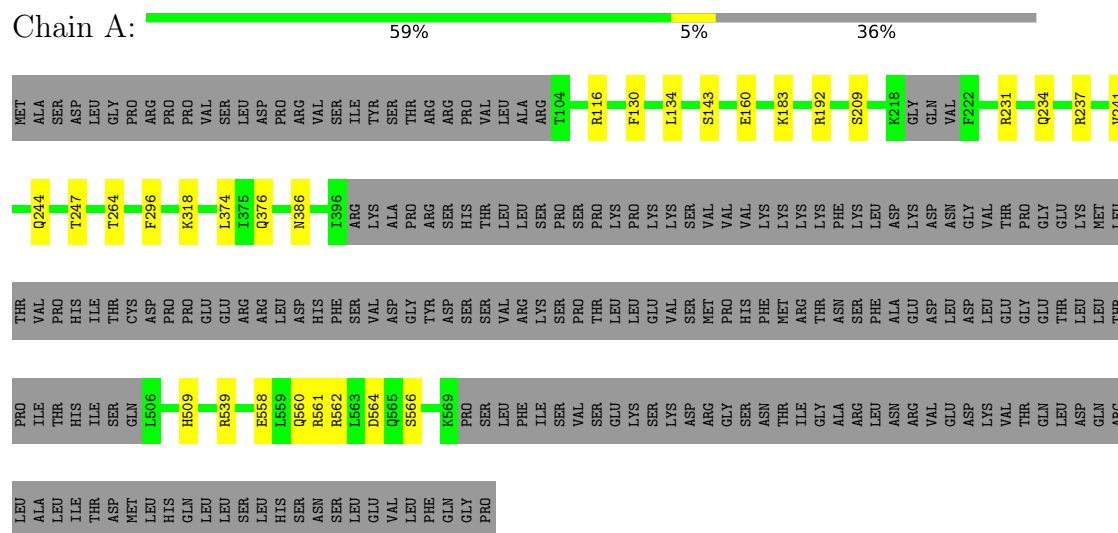
- Molecule 4 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	AltConf
4	H	2	Total Ca 2 2	0
4	B	2	Total Ca 2 2	0
4	K	2	Total Ca 2 2	0
4	E	2	Total Ca 2 2	0

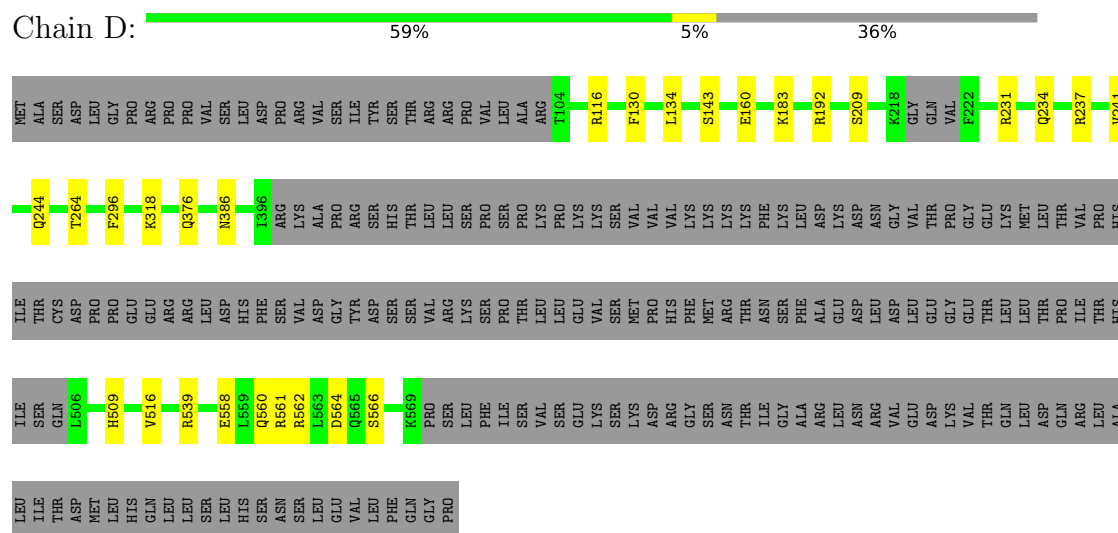
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. 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. 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: Potassium voltage-gated channel subfamily KQT member 1

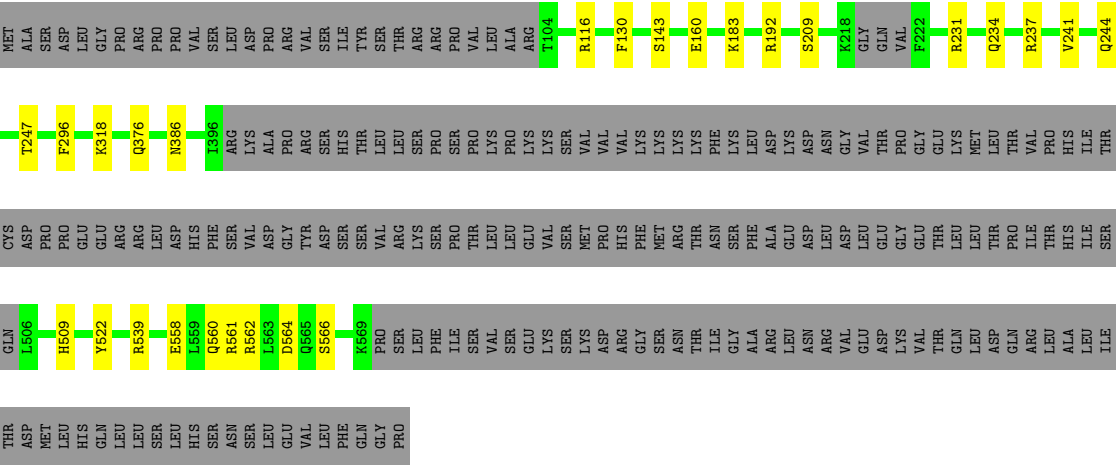


- Molecule 1: Potassium voltage-gated channel subfamily KQT member 1



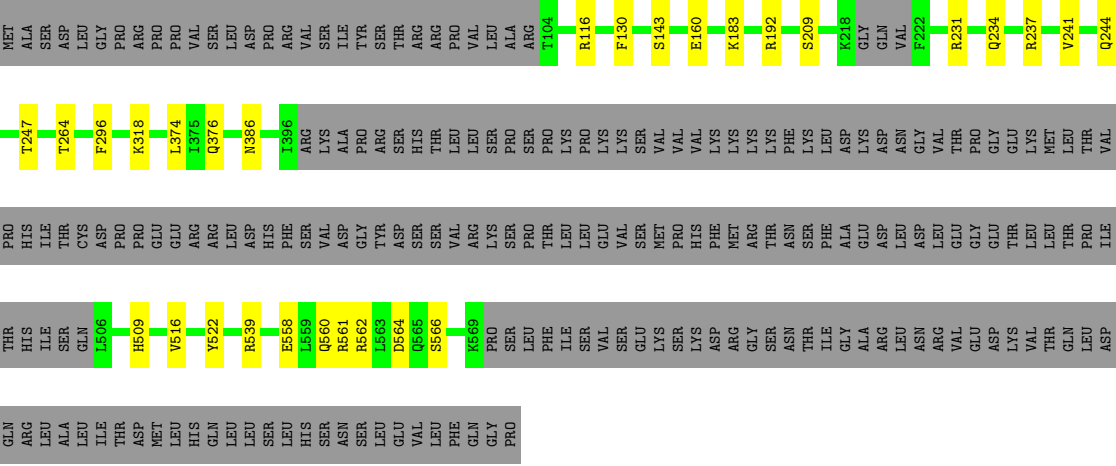
- Molecule 1: Potassium voltage-gated channel subfamily KQT member 1





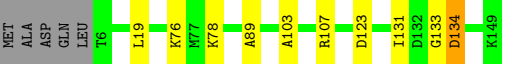
● Molecule 1: Potassium voltage-gated channel subfamily KQT member 1

Chain J: 58% 5% 36%



● Molecule 2: Calmodulin-1

Chain B: 90% 6% ..



● Molecule 2: Calmodulin-1

Chain E: 90% 6% ..



● Molecule 2: Calmodulin-1

Chain H: 90% 6% ..



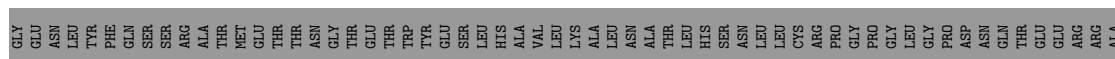
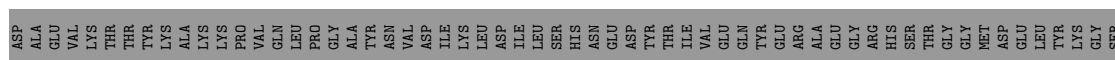
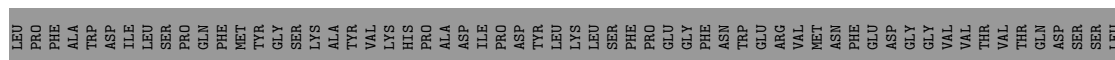
- Molecule 2: Calmodulin-1

Chain K: 89% 7% . .



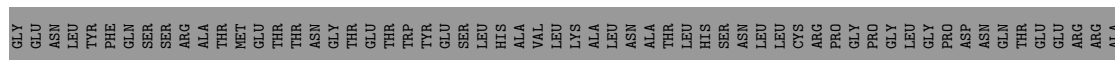
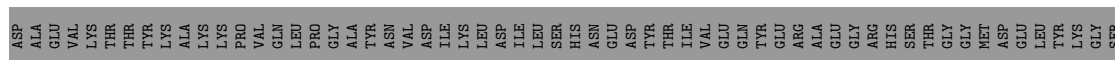
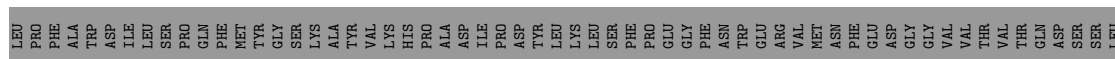
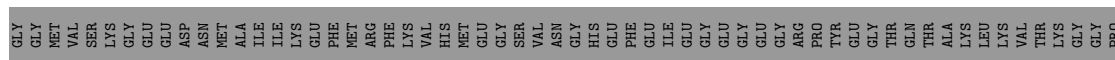
- Molecule 3: MCherry fluorescent protein,Potassium voltage-gated channel subfamily E member 3

Chain C: 12% . 87%



- Molecule 3: MCherry fluorescent protein,Potassium voltage-gated channel subfamily E member 3

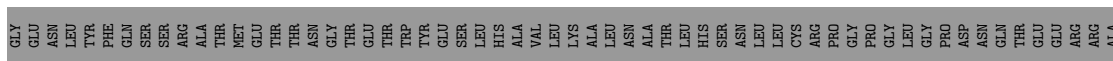
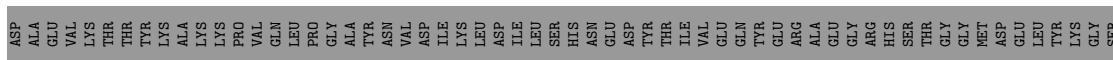
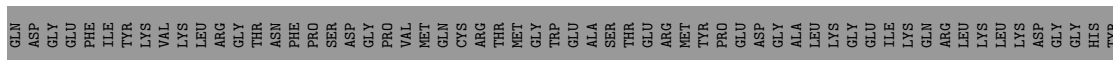
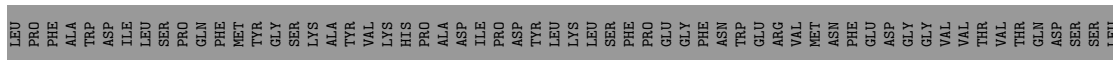
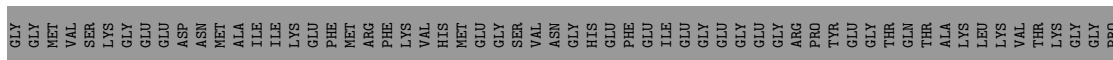
Chain F: 12% . 87%





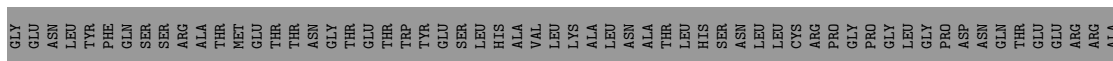
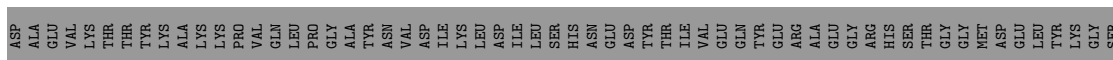
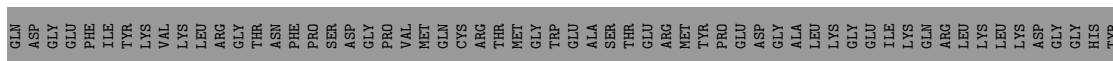
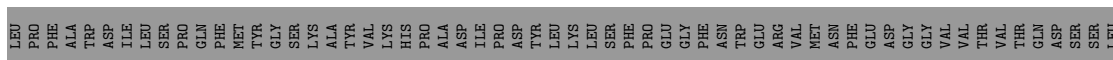
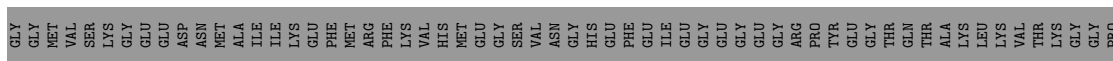
- Molecule 3: MCherry fluorescent protein, Potassium voltage-gated channel subfamily E member

Chain I: 13% . 87%



- Molecule 3: MCherry fluorescent protein, Potassium voltage-gated channel subfamily E member 3

Chain L:  13% • 87%



4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of particles used	39074	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	94	Depositor
Minimum defocus (nm)	Not provided	Depositor
Maximum defocus (nm)	Not provided	Depositor
Magnification	Not provided	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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	$\# Z > 2$	RMSZ	$\# Z > 2$
1	A	0.40	0/2935	0.57	0/3972
1	D	0.40	0/2935	0.57	0/3972
1	G	0.40	0/2935	0.57	0/3972
1	J	0.40	0/2935	0.56	0/3972
2	B	0.32	0/1117	0.53	0/1503
2	E	0.32	0/1117	0.53	0/1503
2	H	0.32	0/1117	0.53	0/1503
2	K	0.32	0/1117	0.53	0/1503
3	C	0.40	0/403	0.58	0/543
3	F	0.40	0/403	0.58	0/543
3	I	0.40	0/403	0.58	0/543
3	L	0.40	0/403	0.58	0/543
All	All	0.38	0/17820	0.56	0/24072

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2864	0	2929	17	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	2864	0	2929	16	0
1	G	2864	0	2929	15	0
1	J	2864	0	2929	18	0
2	B	1105	0	1020	6	0
2	E	1105	0	1020	6	0
2	H	1105	0	1020	6	0
2	K	1105	0	1020	8	0
3	C	394	0	391	3	0
3	F	394	0	391	3	0
3	I	394	0	391	2	0
3	L	394	0	391	2	0
4	B	2	0	0	0	0
4	E	2	0	0	0	0
4	H	2	0	0	0	0
4	K	2	0	0	0	0
All	All	17460	0	17360	87	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 2.

The worst 5 of 87 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)
2:H:133:GLY:O	2:H:134:ASP:CB	2.46	0.64
2:K:133:GLY:O	2:K:134:ASP:CB	2.46	0.64
2:E:133:GLY:O	2:E:134:ASP:CB	2.46	0.63
2:B:133:GLY:O	2:B:134:ASP:CB	2.45	0.62
1:A:183:LYS:O	1:A:192:ARG:NH2	2.36	0.59

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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 EM 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	348/557 (62%)	335 (96%)	13 (4%)	0	100	100
1	D	348/557 (62%)	335 (96%)	13 (4%)	0	100	100
1	G	348/557 (62%)	335 (96%)	13 (4%)	0	100	100
1	J	348/557 (62%)	335 (96%)	13 (4%)	0	100	100
2	B	142/149 (95%)	135 (95%)	6 (4%)	1 (1%)	24	61
2	E	142/149 (95%)	135 (95%)	6 (4%)	1 (1%)	24	61
2	H	142/149 (95%)	135 (95%)	6 (4%)	1 (1%)	24	61
2	K	142/149 (95%)	135 (95%)	6 (4%)	1 (1%)	24	61
3	C	45/355 (13%)	41 (91%)	4 (9%)	0	100	100
3	F	45/355 (13%)	41 (91%)	4 (9%)	0	100	100
3	I	45/355 (13%)	41 (91%)	4 (9%)	0	100	100
3	L	45/355 (13%)	41 (91%)	4 (9%)	0	100	100
All	All	2140/4244 (50%)	2044 (96%)	92 (4%)	4 (0%)	53	81

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	134	ASP
2	E	134	ASP
2	H	134	ASP
2	K	134	ASP

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM 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	301/490 (61%)	298 (99%)	3 (1%)	78	91
1	D	301/490 (61%)	298 (99%)	3 (1%)	78	91
1	G	301/490 (61%)	298 (99%)	3 (1%)	78	91
1	J	301/490 (61%)	298 (99%)	3 (1%)	78	91
2	B	114/127 (90%)	114 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	E	114/127 (90%)	114 (100%)	0	100	100
2	H	114/127 (90%)	114 (100%)	0	100	100
2	K	114/127 (90%)	114 (100%)	0	100	100
3	C	43/302 (14%)	43 (100%)	0	100	100
3	F	43/302 (14%)	43 (100%)	0	100	100
3	I	43/302 (14%)	43 (100%)	0	100	100
3	L	43/302 (14%)	43 (100%)	0	100	100
All	All	1832/3676 (50%)	1820 (99%)	12 (1%)	86	94

5 of 12 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	539	ARG
1	G	376	GLN
1	J	376	GLN
1	D	386	ASN
1	G	539	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 8 such sidechains are listed below:

Mol	Chain	Res	Type
3	F	93	HIS
3	L	93	HIS
3	I	93	HIS
1	D	386	ASN
1	G	386	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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 8 ligands modelled in this entry, 8 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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.