wwPDB X-ray Structure Validation Summary Report (i)

Jun 24, 2024 – 05:54 AM EDT

PDB ID	:	6AKI
Title	:	Calcium release-activated calcium channel protein 1, P288L mutant
Authors	:	Liu, X.; Wu, G.; Yang, X.; Shen, Y.
Deposited on	:	2018-09-01
Resolution	:	4.50 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 types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

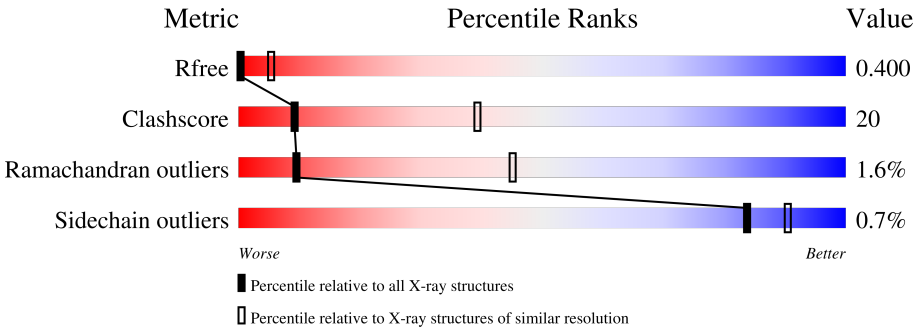
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.20.1
EDS	:	2.37.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

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 4.50 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	1055 (5.20-3.80)
Clashscore	141614	1123 (5.20-3.80)
Ramachandran outliers	138981	1069 (5.20-3.80)
Sidechain outliers	138945	1050 (5.20-3.80)

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 <=5%

Mol	Chain	Length	Quality of chain
1	A	210	46% 25% • 29%
1	B	210	46% 24% • 29%
1	C	210	48% 22% • 29%
1	D	210	50% 21% • 29%
1	E	210	44% 25% • 29%
1	F	210	47% 22% • 29%
1	O	210	50% 21% • 29%

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Mol	Chain	Length	Quality of chain
1	P	210	44% 26% 29%
1	Q	210	47% 24% 29%
1	R	210	48% 21% 29%
1	S	210	40% 30% 29%
1	T	210	50% 21% 29%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	CL	A	401	-	-	X	-
2	CL	D	401	-	-	X	-
2	CL	O	401	-	-	X	-
2	CL	P	401	-	-	X	-

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 12376 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 Calcium release-activated calcium channel protein 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	150	Total	C	N	O	S	0	0	0
			1031	679	166	177	9			
1	B	150	Total	C	N	O	S	0	0	0
			1031	679	166	177	9			
1	C	150	Total	C	N	O	S	0	0	0
			1031	679	166	177	9			
1	D	150	Total	C	N	O	S	0	0	0
			1031	679	166	177	9			
1	E	150	Total	C	N	O	S	0	0	0
			1031	679	166	177	9			
1	F	150	Total	C	N	O	S	0	0	0
			1031	679	166	177	9			
1	O	150	Total	C	N	O	S	0	0	0
			1031	679	166	177	9			
1	P	150	Total	C	N	O	S	0	0	0
			1031	679	166	177	9			
1	Q	150	Total	C	N	O	S	0	0	0
			1031	679	166	177	9			
1	R	150	Total	C	N	O	S	0	0	0
			1031	679	166	177	9			
1	S	150	Total	C	N	O	S	0	0	0
			1031	679	166	177	9			
1	T	150	Total	C	N	O	S	0	0	0
			1031	679	166	177	9			

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	224	SER	CYS	engineered mutation	UNP Q9U6B8
A	283	THR	CYS	engineered mutation	UNP Q9U6B8
A	288	LEU	PRO	engineered mutation	UNP Q9U6B8
B	224	SER	CYS	engineered mutation	UNP Q9U6B8
B	283	THR	CYS	engineered mutation	UNP Q9U6B8

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Chain	Residue	Modelled	Actual	Comment	Reference
B	288	LEU	PRO	engineered mutation	UNP Q9U6B8
C	224	SER	CYS	engineered mutation	UNP Q9U6B8
C	283	THR	CYS	engineered mutation	UNP Q9U6B8
C	288	LEU	PRO	engineered mutation	UNP Q9U6B8
D	224	SER	CYS	engineered mutation	UNP Q9U6B8
D	283	THR	CYS	engineered mutation	UNP Q9U6B8
D	288	LEU	PRO	engineered mutation	UNP Q9U6B8
E	224	SER	CYS	engineered mutation	UNP Q9U6B8
E	283	THR	CYS	engineered mutation	UNP Q9U6B8
E	288	LEU	PRO	engineered mutation	UNP Q9U6B8
F	224	SER	CYS	engineered mutation	UNP Q9U6B8
F	283	THR	CYS	engineered mutation	UNP Q9U6B8
F	288	LEU	PRO	engineered mutation	UNP Q9U6B8
O	224	SER	CYS	engineered mutation	UNP Q9U6B8
O	283	THR	CYS	engineered mutation	UNP Q9U6B8
O	288	LEU	PRO	engineered mutation	UNP Q9U6B8
P	224	SER	CYS	engineered mutation	UNP Q9U6B8
P	283	THR	CYS	engineered mutation	UNP Q9U6B8
P	288	LEU	PRO	engineered mutation	UNP Q9U6B8
Q	224	SER	CYS	engineered mutation	UNP Q9U6B8
Q	283	THR	CYS	engineered mutation	UNP Q9U6B8
Q	288	LEU	PRO	engineered mutation	UNP Q9U6B8
R	224	SER	CYS	engineered mutation	UNP Q9U6B8
R	283	THR	CYS	engineered mutation	UNP Q9U6B8
R	288	LEU	PRO	engineered mutation	UNP Q9U6B8
S	224	SER	CYS	engineered mutation	UNP Q9U6B8
S	283	THR	CYS	engineered mutation	UNP Q9U6B8
S	288	LEU	PRO	engineered mutation	UNP Q9U6B8
T	224	SER	CYS	engineered mutation	UNP Q9U6B8
T	283	THR	CYS	engineered mutation	UNP Q9U6B8
T	288	LEU	PRO	engineered mutation	UNP Q9U6B8

- Molecule 2 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

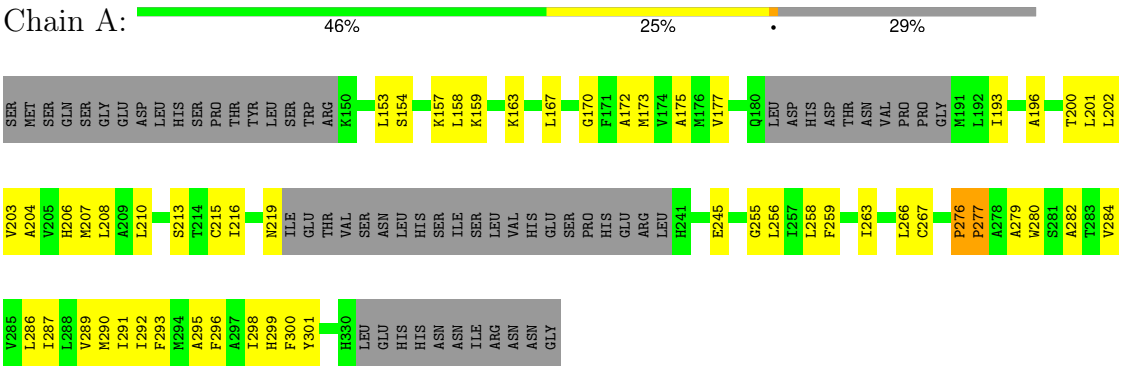
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Cl 1 1	0	0
2	D	1	Total Cl 1 1	0	0
2	O	1	Total Cl 1 1	0	0
2	P	1	Total Cl 1 1	0	0

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. 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.

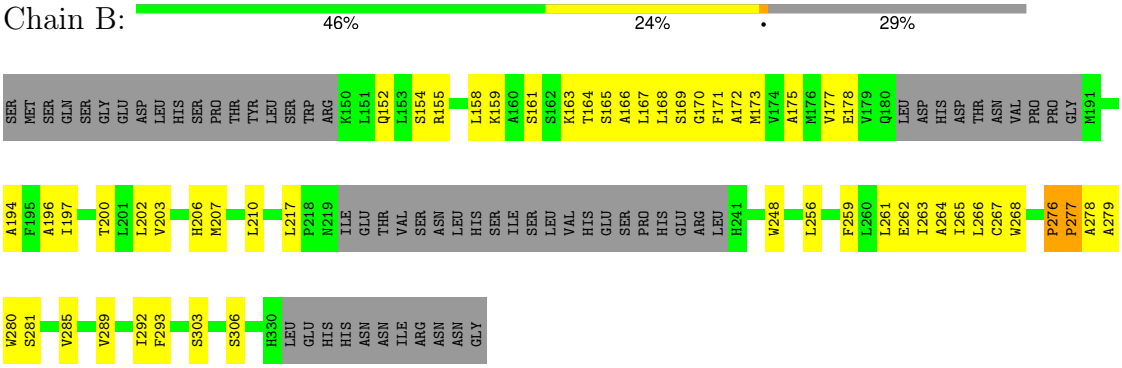
• Molecule 1: Calcium release-activated calcium channel protein 1

Chain A:



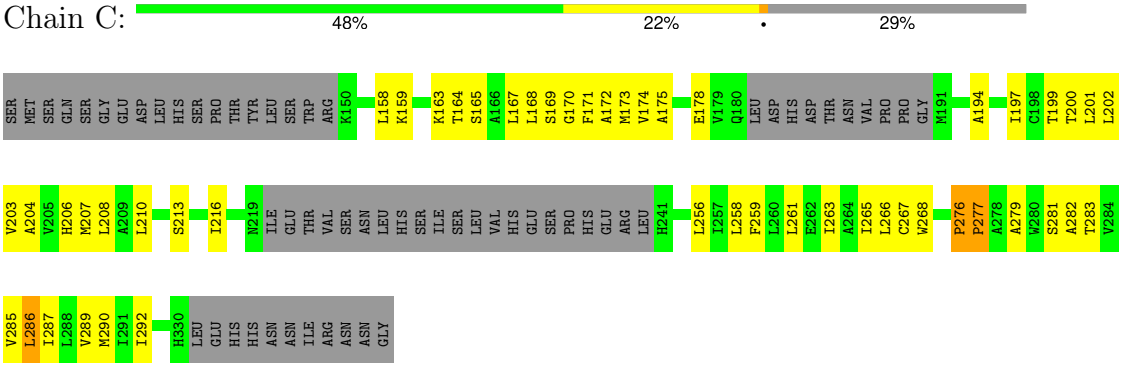
• Molecule 1: Calcium release-activated calcium channel protein 1

Chain B:



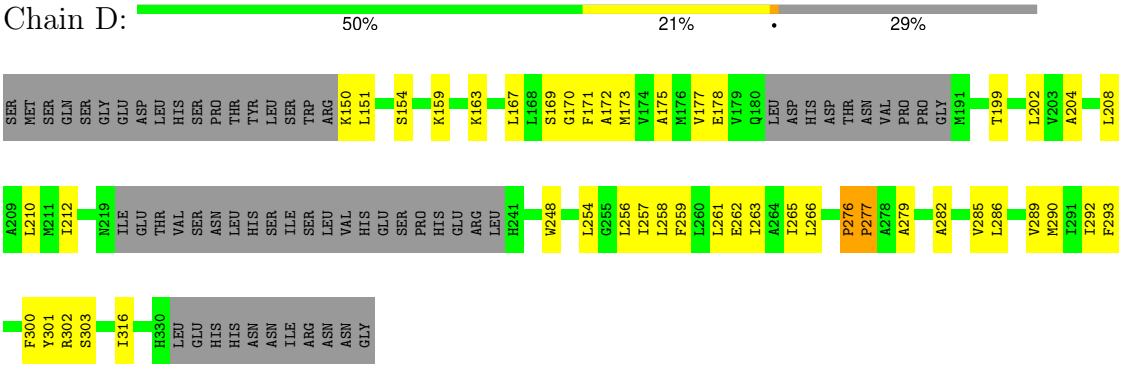
• Molecule 1: Calcium release-activated calcium channel protein 1

Chain C:



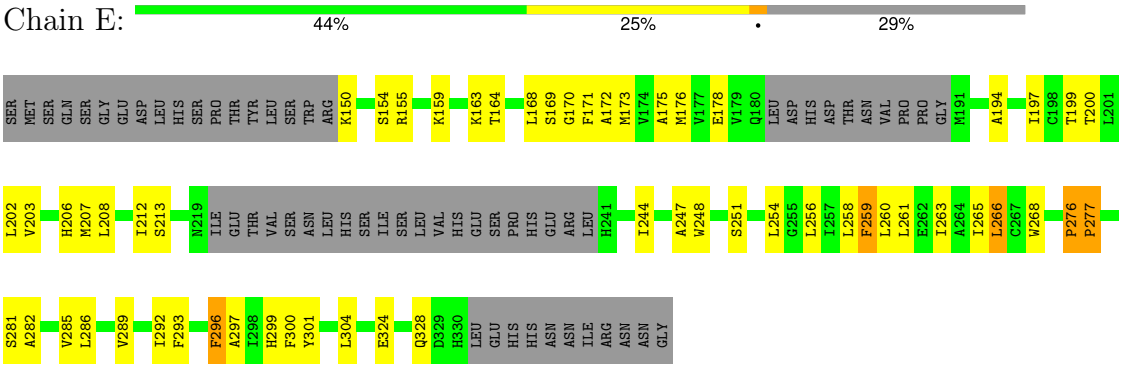
• Molecule 1: Calcium release-activated calcium channel protein 1

Chain D:



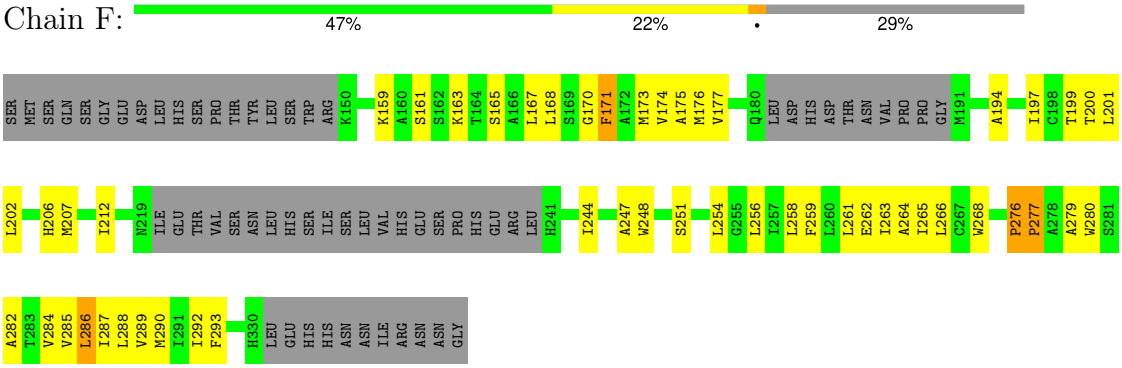
• Molecule 1: Calcium release-activated calcium channel protein 1

Chain E:



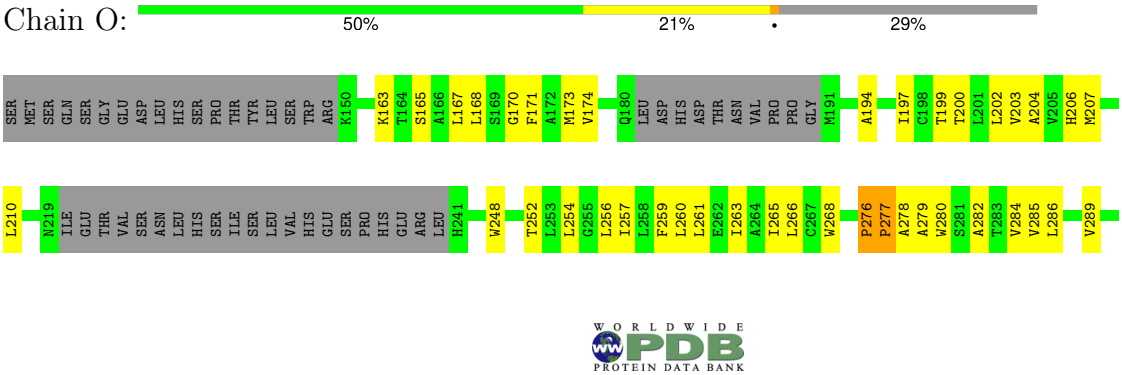
• Molecule 1: Calcium release-activated calcium channel protein 1

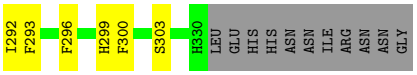
Chain F:



• Molecule 1: Calcium release-activated calcium channel protein 1

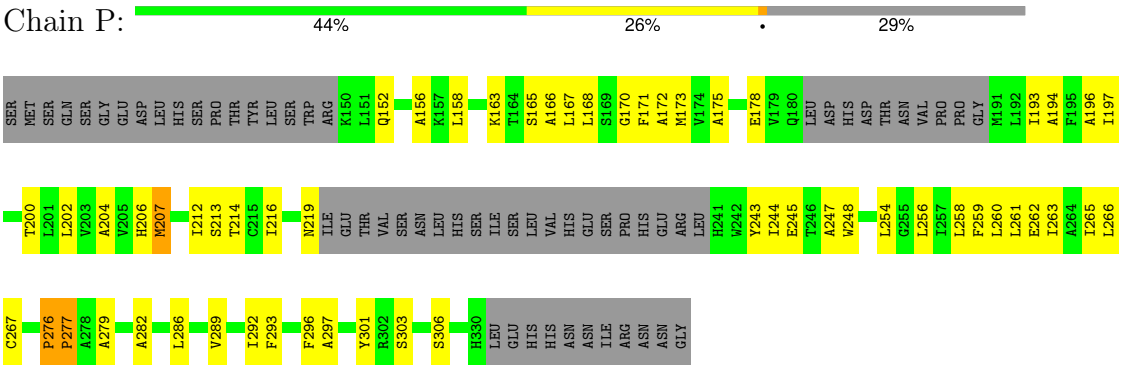
Chain O:





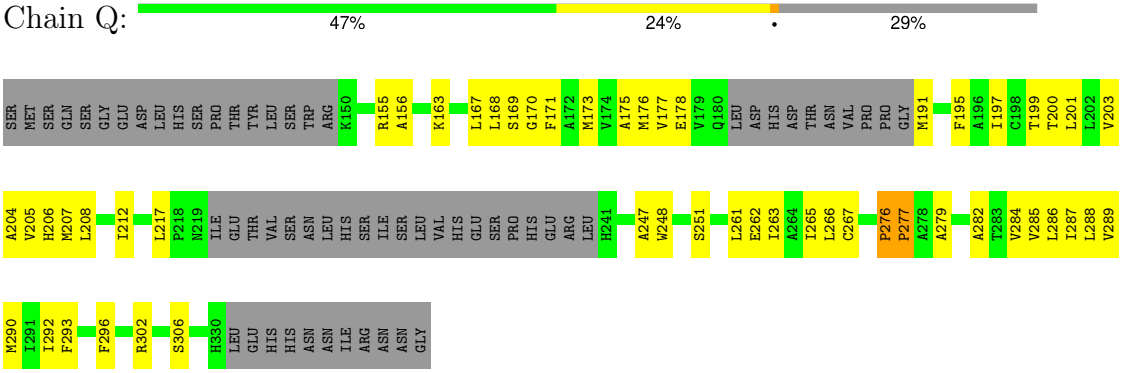
• Molecule 1: Calcium release-activated calcium channel protein 1

Chain P:



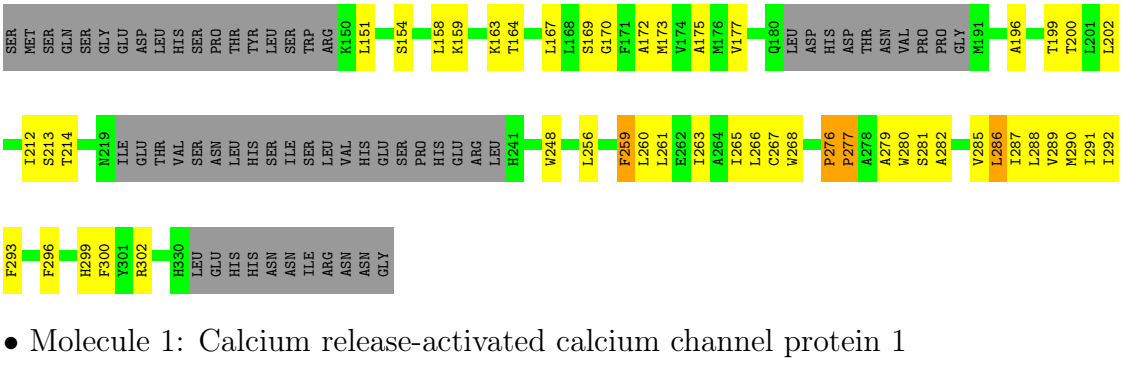
• Molecule 1: Calcium release-activated calcium channel protein 1

Chain Q:



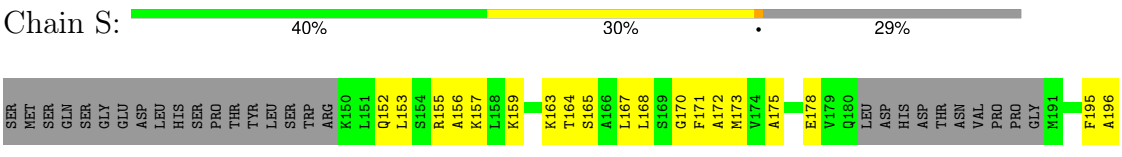
• Molecule 1: Calcium release-activated calcium channel protein 1

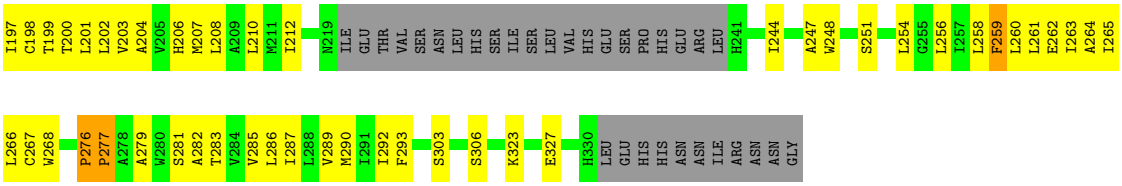
Chain R:



• Molecule 1: Calcium release-activated calcium channel protein 1

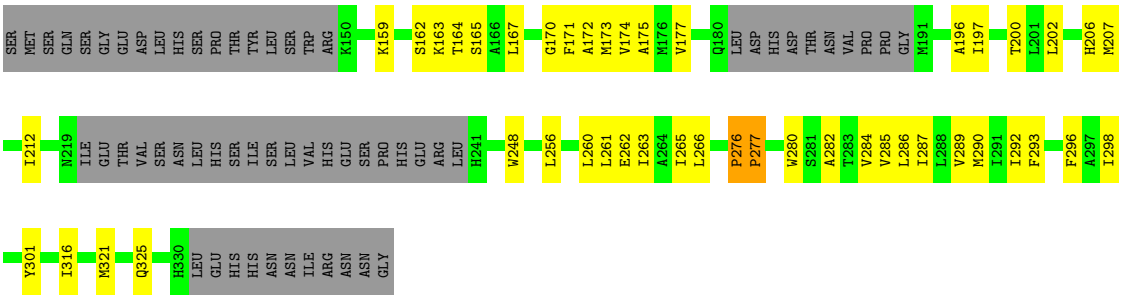
Chain S:





• Molecule 1: Calcium release-activated calcium channel protein 1

Chain T:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	118.11Å 90.66Å 178.72Å 90.00° 106.31° 90.00°	Depositor
Resolution (Å)	26.48 – 4.50 49.81 – 4.50	Depositor EDS
% Data completeness (in resolution range)	69.6 (26.48-4.50) 63.4 (49.81-4.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.19 (at 4.45Å)	Xtriage
Refinement program	PHENIX (1.11.1_2575: ???)	Depositor
R, R_{free}	0.325 , 0.386 0.335 , 0.400	Depositor DCC
R_{free} test set	1754 reflections (10.07%)	wwPDB-VP
Wilson B-factor (Å^2)	0.9	Xtriage
Anisotropy	0.817	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.16 , -10.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	0.013 for h,-k,-h-l	Xtriage
F_o,F_c correlation	0.77	EDS
Total number of atoms	12376	wwPDB-VP
Average B, all atoms (Å^2)	122.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.82% 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: CL

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	0.29	0/1045	0.57	2/1427 (0.1%)
1	B	0.27	0/1045	0.55	2/1427 (0.1%)
1	C	0.29	0/1045	0.58	3/1427 (0.2%)
1	D	0.30	0/1045	0.60	2/1427 (0.1%)
1	E	0.29	0/1045	0.58	3/1427 (0.2%)
1	F	0.31	0/1045	0.59	3/1427 (0.2%)
1	O	0.32	0/1045	0.58	2/1427 (0.1%)
1	P	0.30	0/1045	0.58	2/1427 (0.1%)
1	Q	0.30	0/1045	0.55	2/1427 (0.1%)
1	R	0.31	0/1045	0.64	3/1427 (0.2%)
1	S	0.31	0/1045	0.58	2/1427 (0.1%)
1	T	0.30	0/1045	0.55	2/1427 (0.1%)
All	All	0.30	0/12540	0.58	28/17124 (0.2%)

There are no bond length outliers.

The worst 5 of 28 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	R	286	LEU	CA-CB-CG	-7.43	98.21	115.30
1	D	276	PRO	N-CA-CB	6.54	111.15	103.30
1	Q	276	PRO	N-CA-CB	6.24	110.79	103.30
1	T	276	PRO	N-CA-CB	6.11	110.63	103.30
1	C	276	PRO	N-CA-CB	5.98	110.48	103.30

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	1031	0	974	51	0
1	B	1031	0	974	52	0
1	C	1031	0	974	57	0
1	D	1031	0	974	49	0
1	E	1031	0	974	53	0
1	F	1031	0	974	50	0
1	O	1031	0	974	43	0
1	P	1031	0	974	59	0
1	Q	1031	0	974	49	0
1	R	1031	0	974	53	0
1	S	1031	0	974	72	0
1	T	1031	0	974	47	0
2	A	1	0	0	2	0
2	D	1	0	0	2	0
2	O	1	0	0	2	0
2	P	1	0	0	2	0
All	All	12376	0	11688	479	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 20.

The worst 5 of 479 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:P:243:TYR:O	1:P:247:ALA:HB3	1.66	0.95
1:D:173:MET:HG2	1:E:263:ILE:HD13	1.50	0.94
1:A:263:ILE:HG21	1:E:203:VAL:HG11	1.48	0.92
1:A:200:THR:OG1	1:B:267:CYS:SG	2.29	0.90
1:Q:199:THR:OG1	1:Q:262:GLU:OE1	1.88	0.90

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	144/210 (69%)	137 (95%)	5 (4%)	2 (1%)	11	47
1	B	144/210 (69%)	134 (93%)	7 (5%)	3 (2%)	7	39
1	C	144/210 (69%)	137 (95%)	5 (4%)	2 (1%)	11	47
1	D	144/210 (69%)	134 (93%)	8 (6%)	2 (1%)	11	47
1	E	144/210 (69%)	134 (93%)	8 (6%)	2 (1%)	11	47
1	F	144/210 (69%)	135 (94%)	7 (5%)	2 (1%)	11	47
1	O	144/210 (69%)	134 (93%)	8 (6%)	2 (1%)	11	47
1	P	144/210 (69%)	133 (92%)	8 (6%)	3 (2%)	7	39
1	Q	144/210 (69%)	134 (93%)	7 (5%)	3 (2%)	7	39
1	R	144/210 (69%)	136 (94%)	6 (4%)	2 (1%)	11	47
1	S	144/210 (69%)	136 (94%)	6 (4%)	2 (1%)	11	47
1	T	144/210 (69%)	135 (94%)	7 (5%)	2 (1%)	11	47
All	All	1728/2520 (69%)	1619 (94%)	82 (5%)	27 (2%)	9	45

5 of 27 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	276	PRO
1	C	276	PRO
1	D	276	PRO
1	E	276	PRO
1	P	276	PRO

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	91/187 (49%)	90 (99%)	1 (1%)	73 85
1	B	91/187 (49%)	91 (100%)	0	100 100
1	C	91/187 (49%)	91 (100%)	0	100 100
1	D	91/187 (49%)	91 (100%)	0	100 100
1	E	91/187 (49%)	89 (98%)	2 (2%)	52 71
1	F	91/187 (49%)	90 (99%)	1 (1%)	73 85
1	O	91/187 (49%)	91 (100%)	0	100 100
1	P	91/187 (49%)	89 (98%)	2 (2%)	52 71
1	Q	91/187 (49%)	91 (100%)	0	100 100
1	R	91/187 (49%)	90 (99%)	1 (1%)	73 85
1	S	91/187 (49%)	90 (99%)	1 (1%)	73 85
1	T	91/187 (49%)	91 (100%)	0	100 100
All	All	1092/2244 (49%)	1084 (99%)	8 (1%)	84 90

5 of 8 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	S	259	PHE
1	R	259	PHE
1	P	207	MET
1	F	171	PHE
1	P	296	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	R	206	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 monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 4 ligands modelled in this entry, 4 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.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

Unable to reproduce the depositors R factor - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains

Unable to reproduce the depositors R factor - this section is therefore empty.

6.3 Carbohydrates

Unable to reproduce the depositors R factor - this section is therefore empty.

6.4 Ligands

Unable to reproduce the depositors R factor - this section is therefore empty.

6.5 Other polymers

Unable to reproduce the depositors R factor - this section is therefore empty.