wwPDB EM Map/Model Validation Report (i)

Apr 10, 2016 – 01:49 PM BST

PDB ID	:	3J03
EMDB ID:	:	EMD-5138
Title	:	Lidless Mm-cpn in the closed state with ATP/AlFx
Authors	:	Zhang, J.; Ma, B.; DiMaio, F.; Douglas, N.R.; Joachimiak, L.; Baker, D.; Frydman, J.; Levitt, M.; Chiu, W.
Deposited on	:	2011-02-10
Resolution	:	4.80 Å(reported)

This is a wwPDB EM Map/Model Validation Report for a publicly released PDB/EMDB entry.
For rigid body fitted models, validation errors reported here could
stem from errors in the original structure(s) used in the fitting.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
http://wwpdb.org/validation/2016/EMValidationReportHelp

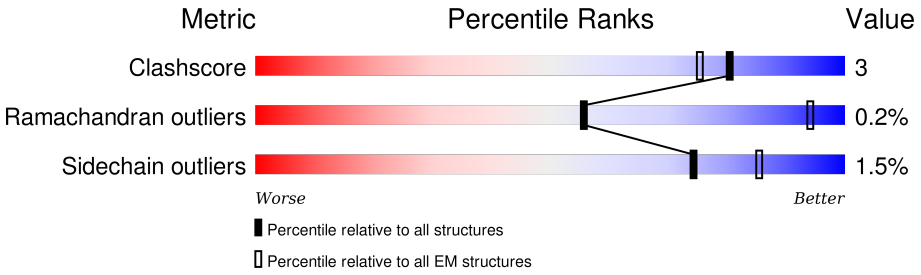
MolProbity	:	4.02b-467
Mogul	:	unknown
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk27241

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 4.80 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	114402	924
Ramachandran outliers	111179	726
Sidechain outliers	111093	686

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 <=5%

Mol	Chain	Length	Quality of chain
1	A	491	90% 10%
1	B	491	90% 10%
1	C	491	90% 9%
1	D	491	90% 9%
1	E	491	91% 8%
1	F	491	90% 10%
1	G	491	90% 9%
1	H	491	90% 9%
1	I	491	90% 10%

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Mol	Chain	Length	Quality of chain
1	J	491	90% 9%
1	K	491	90% 10%
1	L	491	90% 9%
1	M	491	90% 9%
1	N	491	91% 8%
1	O	491	90% 9%
1	P	491	90% 9%

2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 58640 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 Lidless Mm-cpn.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	491	Total	C	N	O	S	0	0
			3665	2272	635	734	24		
1	B	491	Total	C	N	O	S	0	0
			3665	2272	635	734	24		
1	C	491	Total	C	N	O	S	0	0
			3665	2272	635	734	24		
1	D	491	Total	C	N	O	S	0	0
			3665	2272	635	734	24		
1	E	491	Total	C	N	O	S	0	0
			3665	2272	635	734	24		
1	F	491	Total	C	N	O	S	0	0
			3665	2272	635	734	24		
1	G	491	Total	C	N	O	S	0	0
			3665	2272	635	734	24		
1	H	491	Total	C	N	O	S	0	0
			3665	2272	635	734	24		
1	I	491	Total	C	N	O	S	0	0
			3665	2272	635	734	24		
1	J	491	Total	C	N	O	S	0	0
			3665	2272	635	734	24		
1	K	491	Total	C	N	O	S	0	0
			3665	2272	635	734	24		
1	L	491	Total	C	N	O	S	0	0
			3665	2272	635	734	24		
1	M	491	Total	C	N	O	S	0	0
			3665	2272	635	734	24		
1	N	491	Total	C	N	O	S	0	0
			3665	2272	635	734	24		
1	O	491	Total	C	N	O	S	0	0
			3665	2272	635	734	24		
1	P	491	Total	C	N	O	S	0	0
			3665	2272	635	734	24		

There are 96 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	235	GLU	-	LINKER	UNP Q877G8
A	236	THR	-	LINKER	UNP Q877G8
A	237	ALA	-	LINKER	UNP Q877G8
A	238	SER	-	LINKER	UNP Q877G8
A	239	GLU	-	LINKER	UNP Q877G8
A	240	MET	-	LINKER	UNP Q877G8
B	726	GLU	-	LINKER	UNP Q877G8
B	727	THR	-	LINKER	UNP Q877G8
B	728	ALA	-	LINKER	UNP Q877G8
B	729	SER	-	LINKER	UNP Q877G8
B	730	GLU	-	LINKER	UNP Q877G8
B	731	MET	-	LINKER	UNP Q877G8
C	1217	GLU	-	LINKER	UNP Q877G8
C	1218	THR	-	LINKER	UNP Q877G8
C	1219	ALA	-	LINKER	UNP Q877G8
C	1220	SER	-	LINKER	UNP Q877G8
C	1221	GLU	-	LINKER	UNP Q877G8
C	1222	MET	-	LINKER	UNP Q877G8
D	1708	GLU	-	LINKER	UNP Q877G8
D	1709	THR	-	LINKER	UNP Q877G8
D	1710	ALA	-	LINKER	UNP Q877G8
D	1711	SER	-	LINKER	UNP Q877G8
D	1712	GLU	-	LINKER	UNP Q877G8
D	1713	MET	-	LINKER	UNP Q877G8
E	2199	GLU	-	LINKER	UNP Q877G8
E	2200	THR	-	LINKER	UNP Q877G8
E	2201	ALA	-	LINKER	UNP Q877G8
E	2202	SER	-	LINKER	UNP Q877G8
E	2203	GLU	-	LINKER	UNP Q877G8
E	2204	MET	-	LINKER	UNP Q877G8
F	2690	GLU	-	LINKER	UNP Q877G8
F	2691	THR	-	LINKER	UNP Q877G8
F	2692	ALA	-	LINKER	UNP Q877G8
F	2693	SER	-	LINKER	UNP Q877G8
F	2694	GLU	-	LINKER	UNP Q877G8
F	2695	MET	-	LINKER	UNP Q877G8
G	3181	GLU	-	LINKER	UNP Q877G8
G	3182	THR	-	LINKER	UNP Q877G8
G	3183	ALA	-	LINKER	UNP Q877G8
G	3184	SER	-	LINKER	UNP Q877G8
G	3185	GLU	-	LINKER	UNP Q877G8
G	3186	MET	-	LINKER	UNP Q877G8
H	3672	GLU	-	LINKER	UNP Q877G8

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Chain	Residue	Modelled	Actual	Comment	Reference
H	3673	THR	-	LINKER	UNP Q877G8
H	3674	ALA	-	LINKER	UNP Q877G8
H	3675	SER	-	LINKER	UNP Q877G8
H	3676	GLU	-	LINKER	UNP Q877G8
H	3677	MET	-	LINKER	UNP Q877G8
I	4163	GLU	-	LINKER	UNP Q877G8
I	4164	THR	-	LINKER	UNP Q877G8
I	4165	ALA	-	LINKER	UNP Q877G8
I	4166	SER	-	LINKER	UNP Q877G8
I	4167	GLU	-	LINKER	UNP Q877G8
I	4168	MET	-	LINKER	UNP Q877G8
J	4654	GLU	-	LINKER	UNP Q877G8
J	4655	THR	-	LINKER	UNP Q877G8
J	4656	ALA	-	LINKER	UNP Q877G8
J	4657	SER	-	LINKER	UNP Q877G8
J	4658	GLU	-	LINKER	UNP Q877G8
J	4659	MET	-	LINKER	UNP Q877G8
K	5145	GLU	-	LINKER	UNP Q877G8
K	5146	THR	-	LINKER	UNP Q877G8
K	5147	ALA	-	LINKER	UNP Q877G8
K	5148	SER	-	LINKER	UNP Q877G8
K	5149	GLU	-	LINKER	UNP Q877G8
K	5150	MET	-	LINKER	UNP Q877G8
L	5636	GLU	-	LINKER	UNP Q877G8
L	5637	THR	-	LINKER	UNP Q877G8
L	5638	ALA	-	LINKER	UNP Q877G8
L	5639	SER	-	LINKER	UNP Q877G8
L	5640	GLU	-	LINKER	UNP Q877G8
L	5641	MET	-	LINKER	UNP Q877G8
M	6127	GLU	-	LINKER	UNP Q877G8
M	6128	THR	-	LINKER	UNP Q877G8
M	6129	ALA	-	LINKER	UNP Q877G8
M	6130	SER	-	LINKER	UNP Q877G8
M	6131	GLU	-	LINKER	UNP Q877G8
M	6132	MET	-	LINKER	UNP Q877G8
N	6618	GLU	-	LINKER	UNP Q877G8
N	6619	THR	-	LINKER	UNP Q877G8
N	6620	ALA	-	LINKER	UNP Q877G8
N	6621	SER	-	LINKER	UNP Q877G8
N	6622	GLU	-	LINKER	UNP Q877G8
N	6623	MET	-	LINKER	UNP Q877G8
O	7109	GLU	-	LINKER	UNP Q877G8

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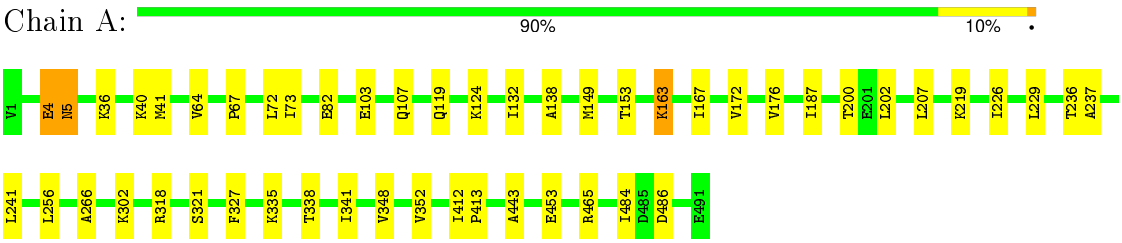
Chain	Residue	Modelled	Actual	Comment	Reference
O	7110	THR	-	LINKER	UNP Q877G8
O	7111	ALA	-	LINKER	UNP Q877G8
O	7112	SER	-	LINKER	UNP Q877G8
O	7113	GLU	-	LINKER	UNP Q877G8
O	7114	MET	-	LINKER	UNP Q877G8
P	7600	GLU	-	LINKER	UNP Q877G8
P	7601	THR	-	LINKER	UNP Q877G8
P	7602	ALA	-	LINKER	UNP Q877G8
P	7603	SER	-	LINKER	UNP Q877G8
P	7604	GLU	-	LINKER	UNP Q877G8
P	7605	MET	-	LINKER	UNP Q877G8

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 errors 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.

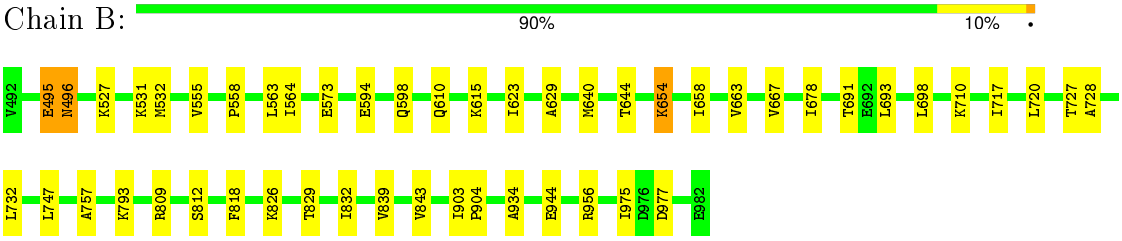
- Molecule 1: Lidless Mm-cpn

Chain A:



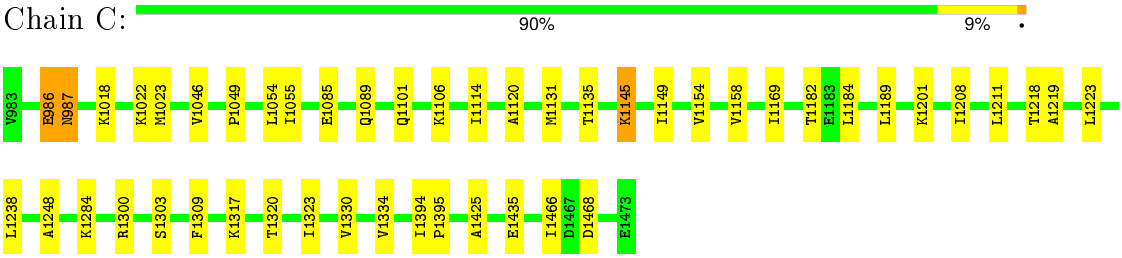
- Molecule 1: Lidless Mm-cpn

Chain B:



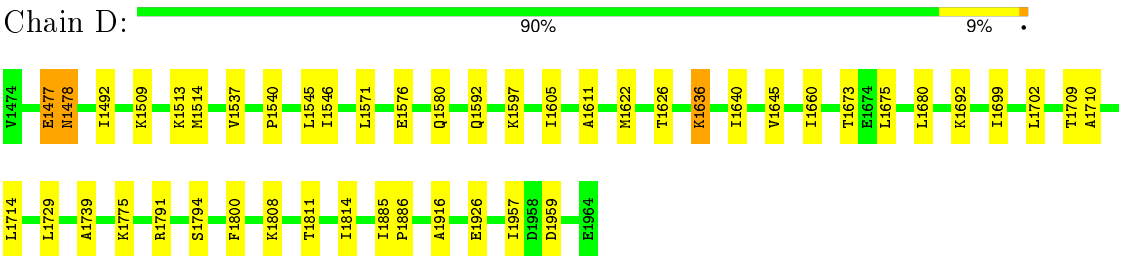
- Molecule 1: Lidless Mm-cpn

Chain C:



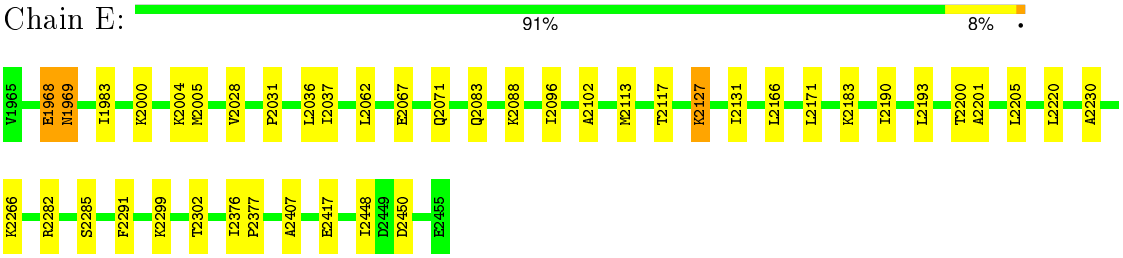
- Molecule 1: Lidless Mm-cpn

Chain D:



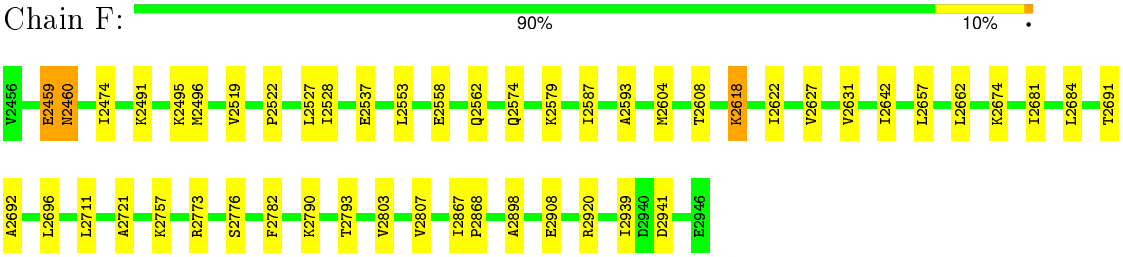
• Molecule 1: Lidless Mm-cpn

Chain E:



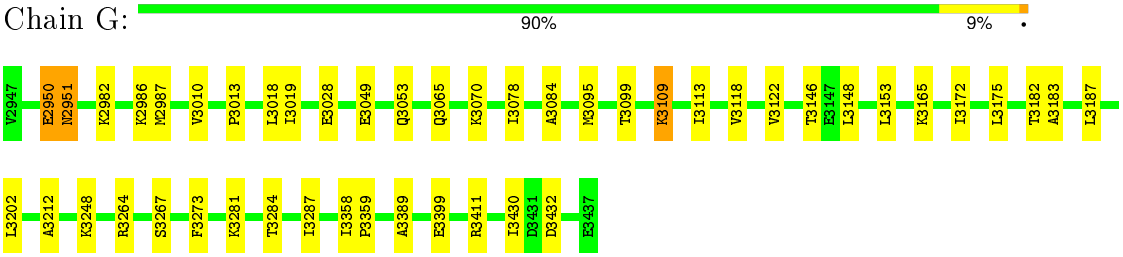
• Molecule 1: Lidless Mm-cpn

Chain F:



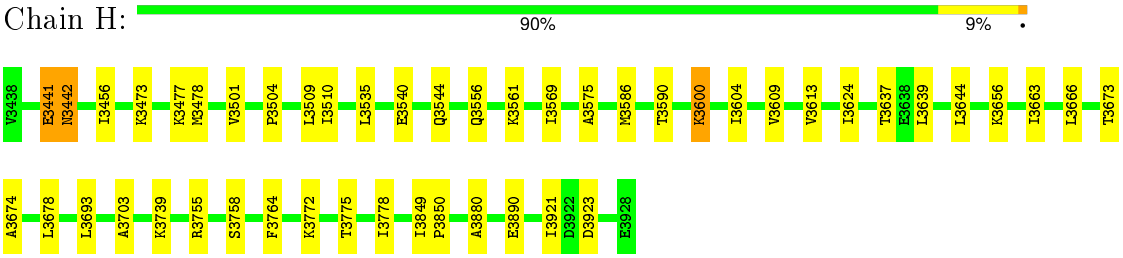
• Molecule 1: Lidless Mm-cpn

Chain G:



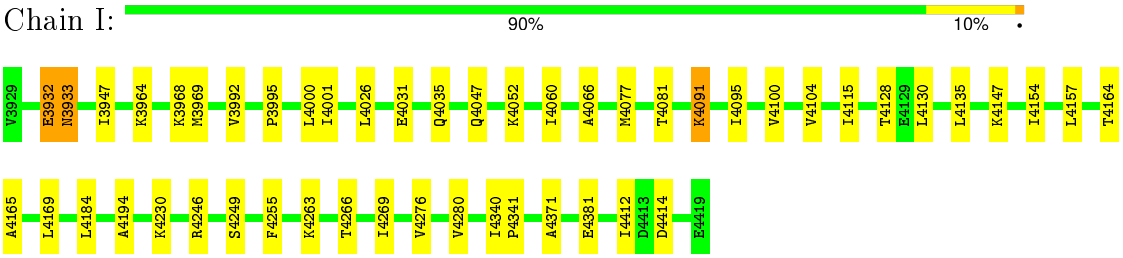
• Molecule 1: Lidless Mm-cpn

Chain H:



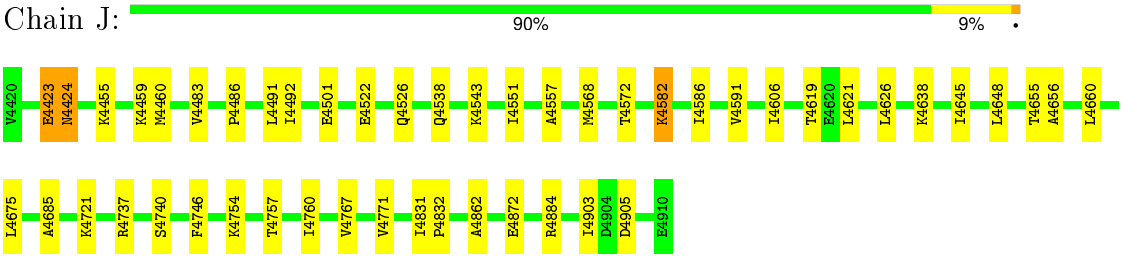
• Molecule 1: Lidless Mm-cpn

Chain I:



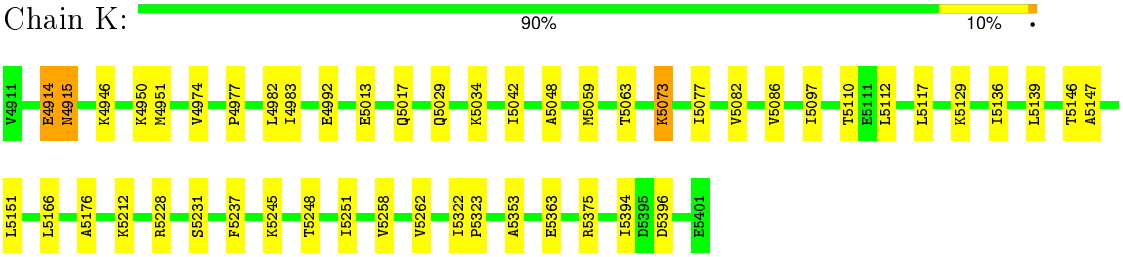
- Molecule 1: Lidless Mm-cpn

Chain J:



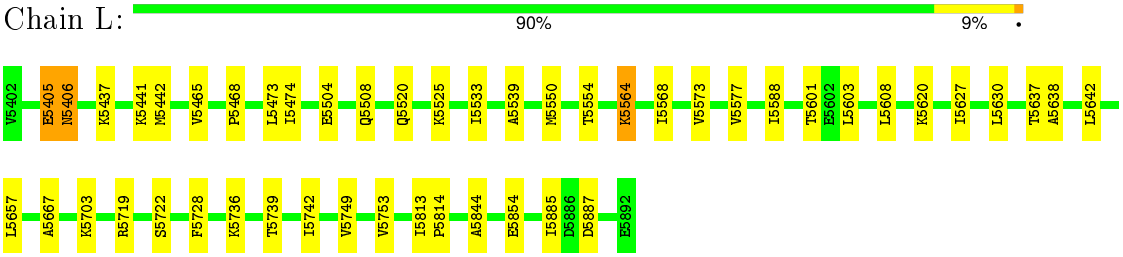
- Molecule 1: Lidless Mm-cpn

Chain K:



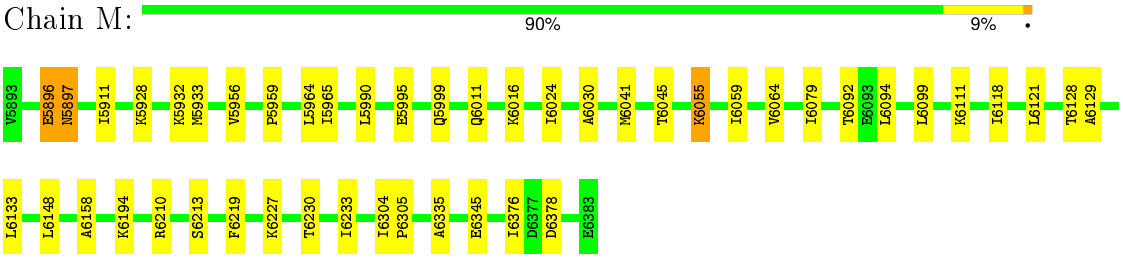
- Molecule 1: Lidless Mm-cpn

Chain L:



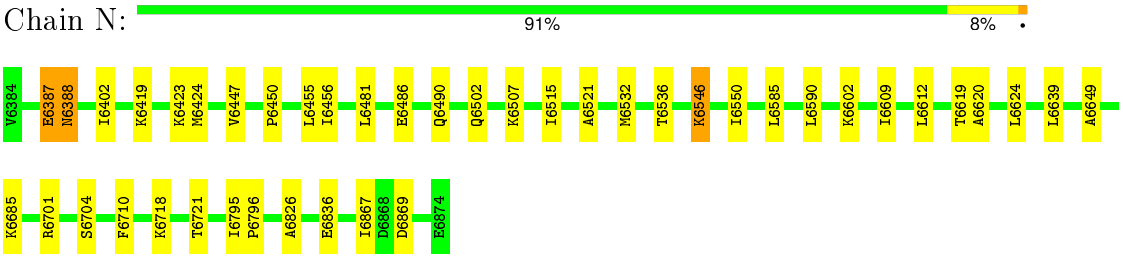
- Molecule 1: Lidless Mm-cpn

Chain M:



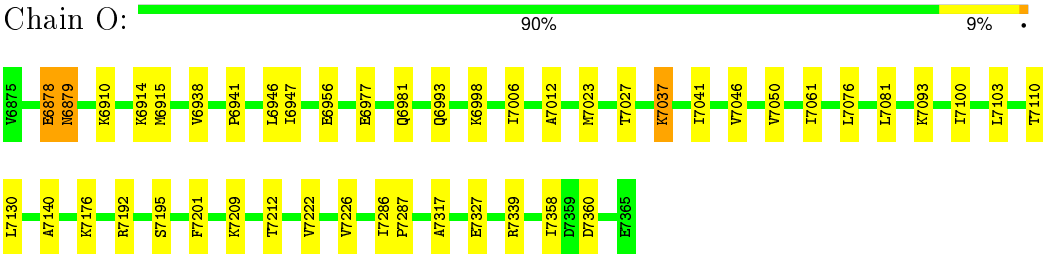
- Molecule 1: Lidless Mm-cpn

Chain N:



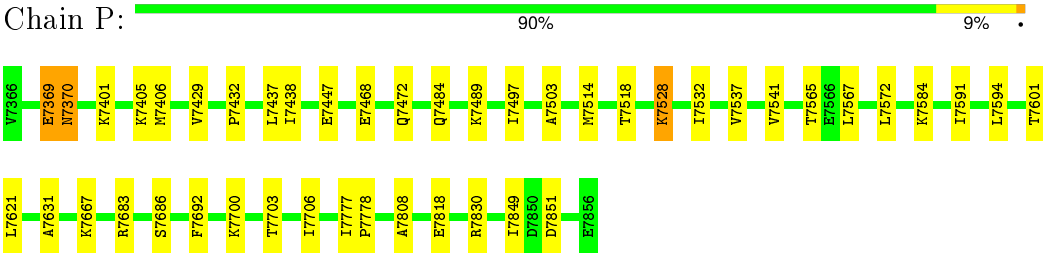
- Molecule 1: Lidless Mm-cpn

Chain O:



- Molecule 1: Lidless Mm-cpn

Chain P:



4 Experimental information (i)

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, D	Depositor
Number of images	Not provided	Depositor
Resolution determination method	FSC at 0.5 cut-off	Depositor
CTF correction method	Each micrograph	Depositor
Microscope	JEM3200FSC	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	20	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	80000	Depositor
Image detector	Gatan 4kX4k CCD Camera	Depositor

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	#$\|Z\|$ >2	RMSZ	#$\|Z\|$ >2
1	A	0.86	1/3686 (0.0%)	0.76	2/4961 (0.0%)
1	B	0.86	1/3686 (0.0%)	0.76	2/4961 (0.0%)
1	C	0.86	1/3686 (0.0%)	0.76	2/4961 (0.0%)
1	D	0.86	1/3686 (0.0%)	0.76	2/4961 (0.0%)
1	E	0.86	1/3686 (0.0%)	0.76	2/4961 (0.0%)
1	F	0.86	1/3686 (0.0%)	0.76	2/4961 (0.0%)
1	G	0.86	1/3686 (0.0%)	0.76	2/4961 (0.0%)
1	H	0.86	1/3686 (0.0%)	0.76	2/4961 (0.0%)
1	I	0.86	1/3686 (0.0%)	0.76	2/4961 (0.0%)
1	J	0.86	1/3686 (0.0%)	0.76	2/4961 (0.0%)
1	K	0.86	1/3686 (0.0%)	0.76	2/4961 (0.0%)
1	L	0.86	1/3686 (0.0%)	0.76	2/4961 (0.0%)
1	M	0.86	1/3686 (0.0%)	0.76	2/4961 (0.0%)
1	N	0.86	1/3686 (0.0%)	0.76	2/4961 (0.0%)
1	O	0.86	1/3686 (0.0%)	0.76	2/4961 (0.0%)
1	P	0.86	1/3686 (0.0%)	0.76	2/4961 (0.0%)
All	All	0.86	16/58976 (0.0%)	0.76	32/79376 (0.0%)

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 outliers	#Planarity outliers
1	A	0	3
1	B	0	3
1	C	0	3
1	D	0	3
1	E	0	3
1	F	0	3
1	G	0	3
1	H	0	3
1	I	0	3

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Mol	Chain	#Chirality outliers	#Planarity outliers
1	J	0	3
1	K	0	3
1	L	0	3
1	M	0	3
1	N	0	3
1	O	0	3
1	P	0	3
All	All	0	48

The worst 5 of 16 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	1916	ALA	C-O	5.10	1.33	1.23
1	B	934	ALA	C-O	5.07	1.32	1.23
1	H	3880	ALA	C-O	5.07	1.32	1.23
1	I	4371	ALA	C-O	5.07	1.32	1.23
1	K	5353	ALA	C-O	5.07	1.32	1.23

The worst 5 of 32 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	N	6387	GLU	CA-C-O	-6.62	106.19	120.10
1	B	495	GLU	CA-C-O	-6.62	106.19	120.10
1	F	2459	GLU	CA-C-O	-6.62	106.19	120.10
1	M	5896	GLU	CA-C-O	-6.62	106.21	120.10
1	G	2950	GLU	CA-C-O	-6.61	106.21	120.10

There are no chirality outliers.

5 of 48 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	119	GLN	Mainchain
1	A	138	ALA	Mainchain
1	A	453	GLU	Mainchain
1	B	610	GLN	Mainchain
1	B	629	ALA	Mainchain

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	3665	0	3804	28	0
1	B	3665	0	3801	28	0
1	C	3665	0	3801	27	0
1	D	3665	0	3801	26	0
1	E	3665	0	3801	24	0
1	F	3665	0	3801	28	0
1	G	3665	0	3801	26	0
1	H	3665	0	3801	27	0
1	I	3665	0	3801	28	0
1	J	3665	0	3801	27	0
1	K	3665	0	3801	28	0
1	L	3665	0	3801	27	0
1	M	3665	0	3801	26	0
1	N	3665	0	3801	24	0
1	O	3665	0	3801	27	0
1	P	3665	0	3801	26	0
All	All	58640	0	60819	395	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 3.

The worst 5 of 395 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:B:615:LYS:HE2	1:B:615:LYS:HA	1.73	0.71
1:P:7489:LYS:HE2	1:P:7489:LYS:HA	1.73	0.71
1:K:5034:LYS:HA	1:K:5034:LYS:HE2	1.73	0.71
1:G:3070:LYS:HA	1:G:3070:LYS:HE2	1.73	0.71
1:A:124:LYS:HE2	1:A:124:LYS:HA	1.73	0.70

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	489/491 (100%)	471 (96%)	17 (4%)	1 (0%)	52	86
1	B	489/491 (100%)	471 (96%)	17 (4%)	1 (0%)	52	86
1	C	489/491 (100%)	471 (96%)	17 (4%)	1 (0%)	52	86
1	D	489/491 (100%)	471 (96%)	17 (4%)	1 (0%)	52	86
1	E	489/491 (100%)	471 (96%)	17 (4%)	1 (0%)	52	86
1	F	489/491 (100%)	471 (96%)	17 (4%)	1 (0%)	52	86
1	G	489/491 (100%)	471 (96%)	17 (4%)	1 (0%)	52	86
1	H	489/491 (100%)	471 (96%)	17 (4%)	1 (0%)	52	86
1	I	489/491 (100%)	471 (96%)	17 (4%)	1 (0%)	52	86
1	J	489/491 (100%)	471 (96%)	17 (4%)	1 (0%)	52	86
1	K	489/491 (100%)	471 (96%)	17 (4%)	1 (0%)	52	86
1	L	489/491 (100%)	471 (96%)	17 (4%)	1 (0%)	52	86
1	M	489/491 (100%)	471 (96%)	17 (4%)	1 (0%)	52	86
1	N	489/491 (100%)	471 (96%)	17 (4%)	1 (0%)	52	86
1	O	489/491 (100%)	471 (96%)	17 (4%)	1 (0%)	52	86
1	P	489/491 (100%)	471 (96%)	17 (4%)	1 (0%)	52	86
All	All	7824/7856 (100%)	7536 (96%)	272 (4%)	16 (0%)	56	86

5 of 16 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	5	ASN
1	B	496	ASN
1	C	987	ASN
1	D	1478	ASN
1	E	1969	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 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	393/393 (100%)	387 (98%)	6 (2%)	72	89
1	B	393/393 (100%)	387 (98%)	6 (2%)	72	89
1	C	393/393 (100%)	387 (98%)	6 (2%)	72	89
1	D	393/393 (100%)	387 (98%)	6 (2%)	72	89
1	E	393/393 (100%)	387 (98%)	6 (2%)	72	89
1	F	393/393 (100%)	387 (98%)	6 (2%)	72	89
1	G	393/393 (100%)	387 (98%)	6 (2%)	72	89
1	H	393/393 (100%)	387 (98%)	6 (2%)	72	89
1	I	393/393 (100%)	387 (98%)	6 (2%)	72	89
1	J	393/393 (100%)	387 (98%)	6 (2%)	72	89
1	K	393/393 (100%)	387 (98%)	6 (2%)	72	89
1	L	393/393 (100%)	387 (98%)	6 (2%)	72	89
1	M	393/393 (100%)	387 (98%)	6 (2%)	72	89
1	N	393/393 (100%)	387 (98%)	6 (2%)	72	89
1	O	393/393 (100%)	387 (98%)	6 (2%)	72	89
1	P	393/393 (100%)	387 (98%)	6 (2%)	72	89
All	All	6288/6288 (100%)	6192 (98%)	96 (2%)	74	89

5 of 96 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	H	3509	LEU
1	I	4263	LYS
1	O	7195	SER
1	H	3600	LYS
1	I	3964	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 16 such sidechains are listed below:

Mol	Chain	Res	Type
1	H	3883	ASN
1	I	4374	ASN
1	M	6338	ASN
1	G	3392	ASN
1	N	6829	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

There are no carbohydrates in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.