



## wwPDB EM Map/Model Validation Report ⓘ

Apr 10, 2016 – 01:51 PM BST

PDB ID : 3IZJ  
EMDB ID: : EMD-5246  
Title : Mm-cpn rls with ATP and AlFx  
Authors : Douglas, N.R.; Reissmann, S.; Zhang, J.; Chen, B.; Jakana, J.; Kumar, R.; Chiu, W.; Frydman, J.  
Deposited on : 2010-10-29  
Resolution : 6.90 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](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/EMValidationReportHelp>

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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

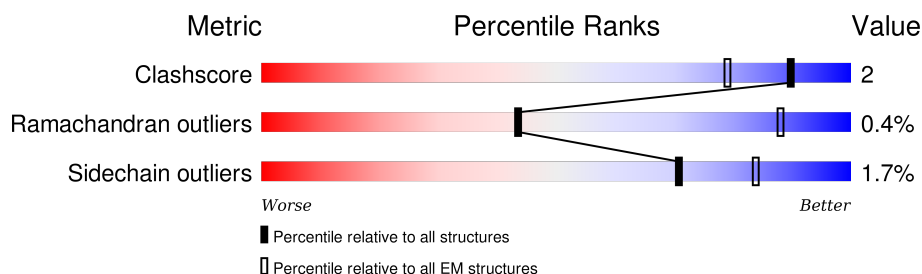
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 6.90 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  $\geq 3$ , 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	513	93% 6% .
1	B	513	93% 6% .
1	C	513	93% 7% .
1	D	513	92% 7% .
1	E	513	93% 7% .
1	F	513	93% 7% .
1	G	513	93% 6% .
1	H	513	93% 7% .
1	I	513	93% 6% .

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Mol	Chain	Length	Quality of chain
1	J	513	<div><div></div><div>93%</div><div>7%</div></div>
1	K	513	<div><div></div><div>93%</div><div>6%</div></div>
1	L	513	<div><div></div><div>93%</div><div>7%</div></div>
1	M	513	<div><div></div><div>93%</div><div>7%</div></div>
1	N	513	<div><div></div><div>92%</div><div>7%</div></div>
1	O	513	<div><div></div><div>93%</div><div>7%</div></div>
1	P	513	<div><div></div><div>93%</div><div>7%</div></div>

## 2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 61440 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 Chaperonin.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	513	Total	C	N	O	S	0	0
			3840	2385	662	768	25		
1	B	513	Total	C	N	O	S	0	0
			3840	2385	662	768	25		
1	C	513	Total	C	N	O	S	0	0
			3840	2385	662	768	25		
1	D	513	Total	C	N	O	S	0	0
			3840	2385	662	768	25		
1	E	513	Total	C	N	O	S	0	0
			3840	2385	662	768	25		
1	F	513	Total	C	N	O	S	0	0
			3840	2385	662	768	25		
1	G	513	Total	C	N	O	S	0	0
			3840	2385	662	768	25		
1	H	513	Total	C	N	O	S	0	0
			3840	2385	662	768	25		
1	I	513	Total	C	N	O	S	0	0
			3840	2385	662	768	25		
1	J	513	Total	C	N	O	S	0	0
			3840	2385	662	768	25		
1	K	513	Total	C	N	O	S	0	0
			3840	2385	662	768	25		
1	L	513	Total	C	N	O	S	0	0
			3840	2385	662	768	25		
1	M	513	Total	C	N	O	S	0	0
			3840	2385	662	768	25		
1	N	513	Total	C	N	O	S	0	0
			3840	2385	662	768	25		
1	O	513	Total	C	N	O	S	0	0
			3840	2385	662	768	25		
1	P	513	Total	C	N	O	S	0	0
			3840	2385	662	768	25		

There are 64 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	321	ALA	THR	ENGINEERED MUTATION	UNP Q877G8
A	322	ALA	ASN	ENGINEERED MUTATION	UNP Q877G8
A	324	ALA	LYS	ENGINEERED MUTATION	UNP Q877G8
A	325	ALA	ASP	ENGINEERED MUTATION	UNP Q877G8
B	834	ALA	THR	ENGINEERED MUTATION	UNP Q877G8
B	835	ALA	ASN	ENGINEERED MUTATION	UNP Q877G8
B	837	ALA	LYS	ENGINEERED MUTATION	UNP Q877G8
B	838	ALA	ASP	ENGINEERED MUTATION	UNP Q877G8
C	1347	ALA	THR	ENGINEERED MUTATION	UNP Q877G8
C	1348	ALA	ASN	ENGINEERED MUTATION	UNP Q877G8
C	1350	ALA	LYS	ENGINEERED MUTATION	UNP Q877G8
C	1351	ALA	ASP	ENGINEERED MUTATION	UNP Q877G8
D	1860	ALA	THR	ENGINEERED MUTATION	UNP Q877G8
D	1861	ALA	ASN	ENGINEERED MUTATION	UNP Q877G8
D	1863	ALA	LYS	ENGINEERED MUTATION	UNP Q877G8
D	1864	ALA	ASP	ENGINEERED MUTATION	UNP Q877G8
E	2373	ALA	THR	ENGINEERED MUTATION	UNP Q877G8
E	2374	ALA	ASN	ENGINEERED MUTATION	UNP Q877G8
E	2376	ALA	LYS	ENGINEERED MUTATION	UNP Q877G8
E	2377	ALA	ASP	ENGINEERED MUTATION	UNP Q877G8
F	2886	ALA	THR	ENGINEERED MUTATION	UNP Q877G8
F	2887	ALA	ASN	ENGINEERED MUTATION	UNP Q877G8
F	2889	ALA	LYS	ENGINEERED MUTATION	UNP Q877G8
F	2890	ALA	ASP	ENGINEERED MUTATION	UNP Q877G8
G	3399	ALA	THR	ENGINEERED MUTATION	UNP Q877G8
G	3400	ALA	ASN	ENGINEERED MUTATION	UNP Q877G8
G	3402	ALA	LYS	ENGINEERED MUTATION	UNP Q877G8
G	3403	ALA	ASP	ENGINEERED MUTATION	UNP Q877G8
H	3912	ALA	THR	ENGINEERED MUTATION	UNP Q877G8
H	3913	ALA	ASN	ENGINEERED MUTATION	UNP Q877G8
H	3915	ALA	LYS	ENGINEERED MUTATION	UNP Q877G8
H	3916	ALA	ASP	ENGINEERED MUTATION	UNP Q877G8
I	4425	ALA	THR	ENGINEERED MUTATION	UNP Q877G8
I	4426	ALA	ASN	ENGINEERED MUTATION	UNP Q877G8
I	4428	ALA	LYS	ENGINEERED MUTATION	UNP Q877G8
I	4429	ALA	ASP	ENGINEERED MUTATION	UNP Q877G8
J	4938	ALA	THR	ENGINEERED MUTATION	UNP Q877G8
J	4939	ALA	ASN	ENGINEERED MUTATION	UNP Q877G8
J	4941	ALA	LYS	ENGINEERED MUTATION	UNP Q877G8
J	4942	ALA	ASP	ENGINEERED MUTATION	UNP Q877G8
K	5451	ALA	THR	ENGINEERED MUTATION	UNP Q877G8
K	5452	ALA	ASN	ENGINEERED MUTATION	UNP Q877G8
K	5454	ALA	LYS	ENGINEERED MUTATION	UNP Q877G8

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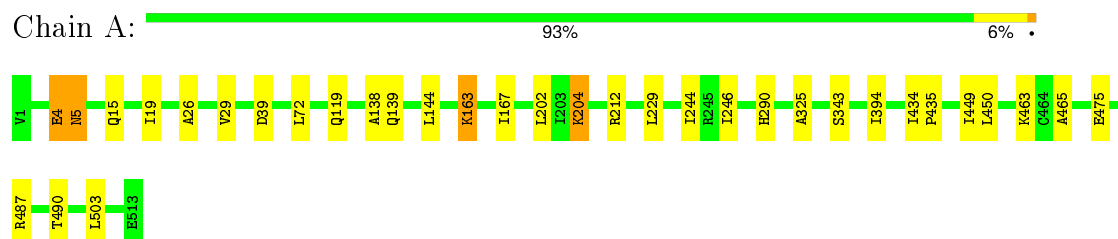
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Chain	Residue	Modelled	Actual	Comment	Reference
K	5455	ALA	ASP	ENGINEERED MUTATION	UNP Q877G8
L	5964	ALA	THR	ENGINEERED MUTATION	UNP Q877G8
L	5965	ALA	ASN	ENGINEERED MUTATION	UNP Q877G8
L	5967	ALA	LYS	ENGINEERED MUTATION	UNP Q877G8
L	5968	ALA	ASP	ENGINEERED MUTATION	UNP Q877G8
M	6477	ALA	THR	ENGINEERED MUTATION	UNP Q877G8
M	6478	ALA	ASN	ENGINEERED MUTATION	UNP Q877G8
M	6480	ALA	LYS	ENGINEERED MUTATION	UNP Q877G8
M	6481	ALA	ASP	ENGINEERED MUTATION	UNP Q877G8
N	6990	ALA	THR	ENGINEERED MUTATION	UNP Q877G8
N	6991	ALA	ASN	ENGINEERED MUTATION	UNP Q877G8
N	6993	ALA	LYS	ENGINEERED MUTATION	UNP Q877G8
N	6994	ALA	ASP	ENGINEERED MUTATION	UNP Q877G8
O	7503	ALA	THR	ENGINEERED MUTATION	UNP Q877G8
O	7504	ALA	ASN	ENGINEERED MUTATION	UNP Q877G8
O	7506	ALA	LYS	ENGINEERED MUTATION	UNP Q877G8
O	7507	ALA	ASP	ENGINEERED MUTATION	UNP Q877G8
P	8016	ALA	THR	ENGINEERED MUTATION	UNP Q877G8
P	8017	ALA	ASN	ENGINEERED MUTATION	UNP Q877G8
P	8019	ALA	LYS	ENGINEERED MUTATION	UNP Q877G8
P	8020	ALA	ASP	ENGINEERED MUTATION	UNP Q877G8

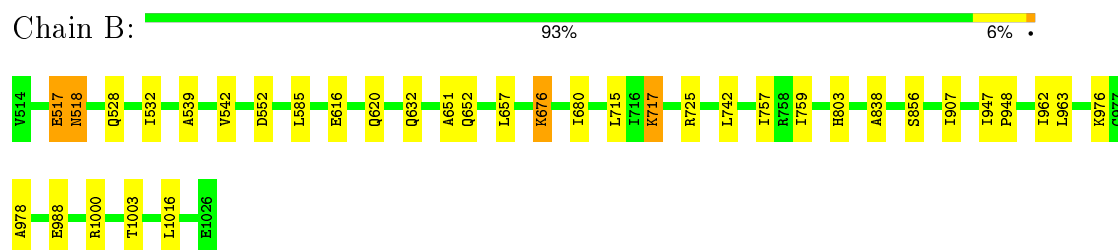
### 3 Residue-property plots [i](#)

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.

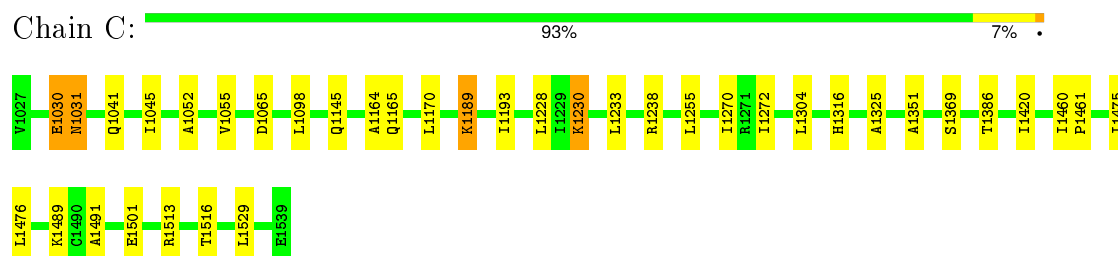
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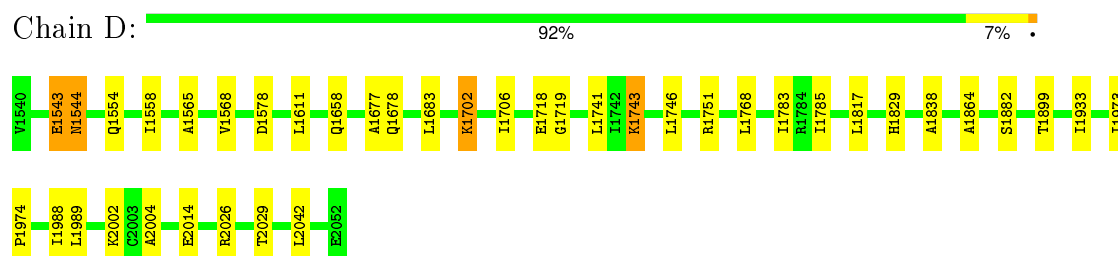
#### • Molecule 1: Chaperonin



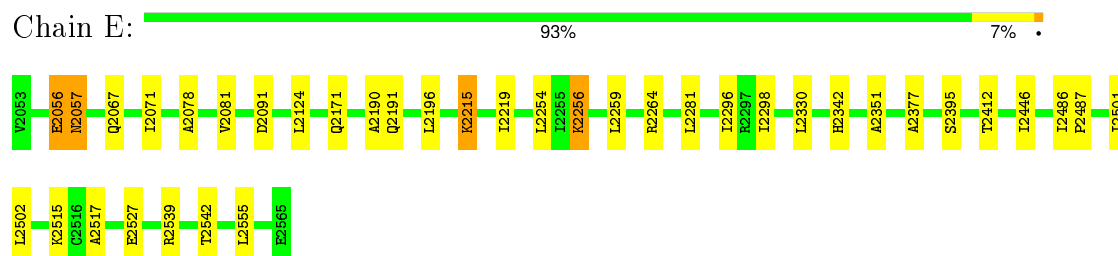
#### • Molecule 1: Chaperonin



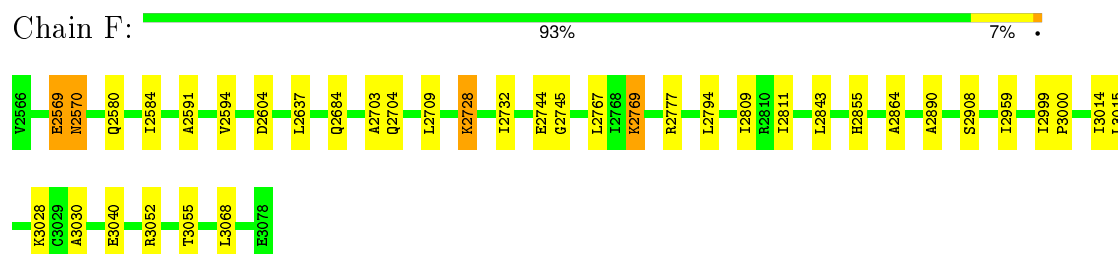
#### • Molecule 1: Chaperonin



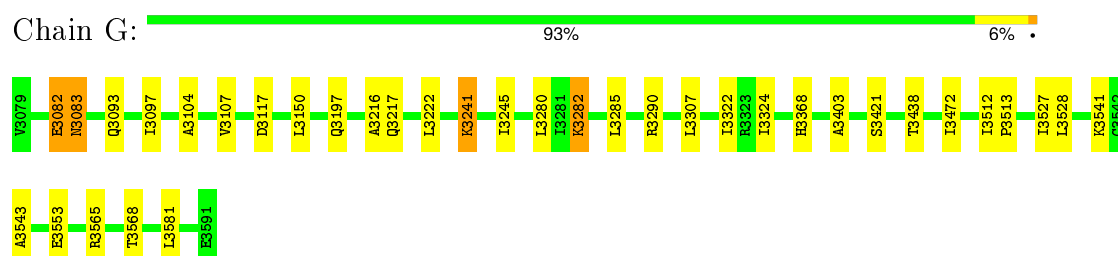
## • Molecule 1: Chaperonin



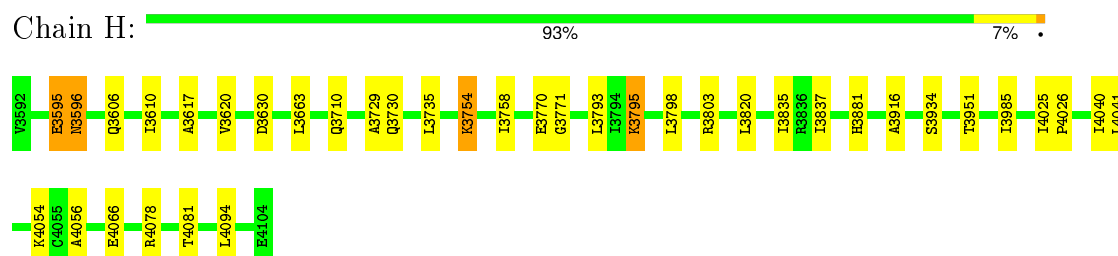
## • Molecule 1: Chaperonin



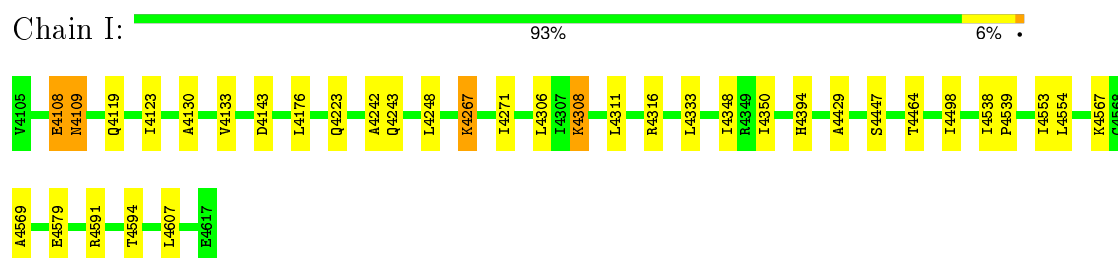
## • Molecule 1: Chaperonin



## • Molecule 1: Chaperonin

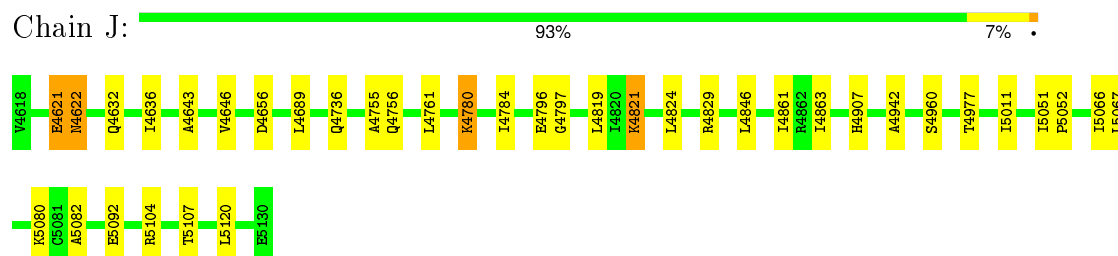


## • Molecule 1: Chaperonin

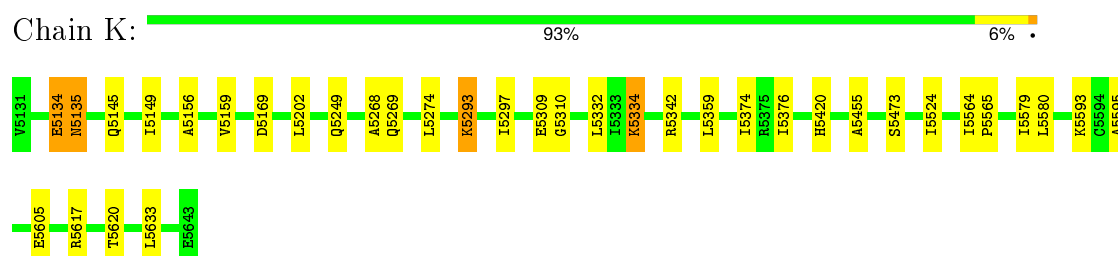




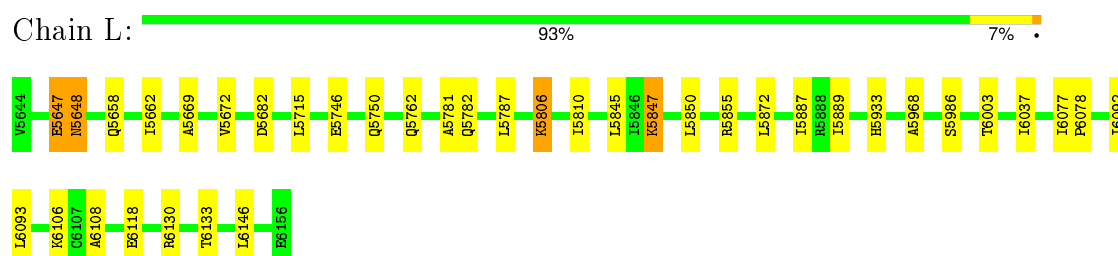
- Molecule 1: Chaperonin



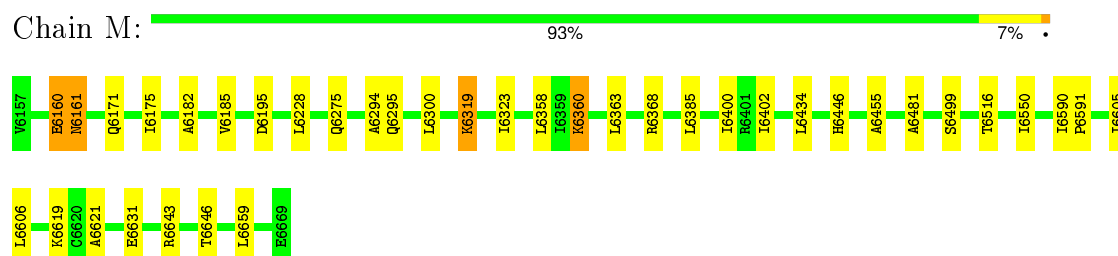
- Molecule 1: Chaperonin



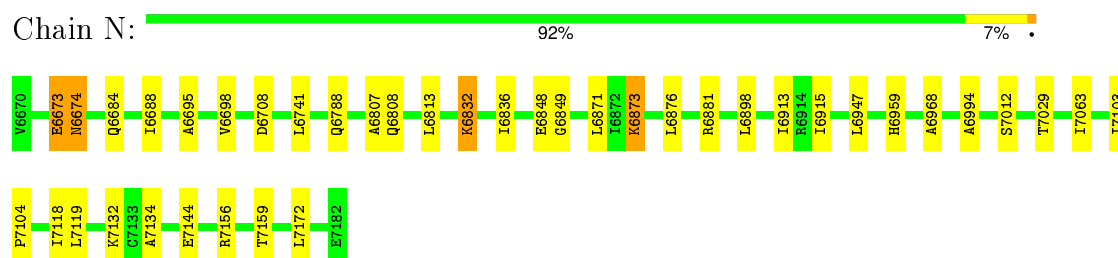
- Molecule 1: Chaperonin



- Molecule 1: Chaperonin

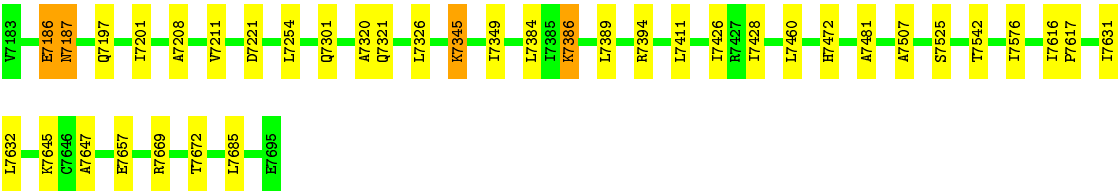


- Molecule 1: Chaperonin




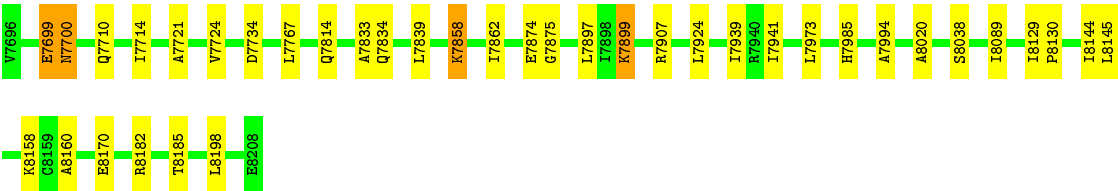
● Molecule 1: Chaperonin

Chain O:  93% 7% .



● Molecule 1: Chaperonin

Chain P:  93% 7% .



## 4 Experimental information

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	Not provided	Depositor
Microscope	JEM3200FSC	Depositor
Voltage (kV)	200	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	Not provided	Depositor
Minimum defocus (nm)	Not provided	Depositor
Maximum defocus (nm)	Not provided	Depositor
Magnification	Not provided	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	0.89	2/3863 (0.1%)	0.78	2/5199 (0.0%)
1	B	0.89	2/3863 (0.1%)	0.78	2/5199 (0.0%)
1	C	0.89	2/3863 (0.1%)	0.78	2/5199 (0.0%)
1	D	0.89	2/3863 (0.1%)	0.78	2/5199 (0.0%)
1	E	0.89	2/3863 (0.1%)	0.78	2/5199 (0.0%)
1	F	0.89	2/3863 (0.1%)	0.78	2/5199 (0.0%)
1	G	0.89	2/3863 (0.1%)	0.78	2/5199 (0.0%)
1	H	0.89	2/3863 (0.1%)	0.78	2/5199 (0.0%)
1	I	0.89	2/3863 (0.1%)	0.78	2/5199 (0.0%)
1	J	0.89	2/3863 (0.1%)	0.78	2/5199 (0.0%)
1	K	0.89	2/3863 (0.1%)	0.78	2/5199 (0.0%)
1	L	0.89	2/3863 (0.1%)	0.78	2/5199 (0.0%)
1	M	0.89	2/3863 (0.1%)	0.78	2/5199 (0.0%)
1	N	0.89	2/3863 (0.1%)	0.78	2/5199 (0.0%)
1	O	0.89	2/3863 (0.1%)	0.78	2/5199 (0.0%)
1	P	0.89	2/3863 (0.1%)	0.78	2/5199 (0.0%)
All	All	0.89	32/61808 (0.1%)	0.78	32/83184 (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 32 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	I	4108	GLU	C-O	-5.99	1.11	1.23
1	K	5134	GLU	C-O	-5.99	1.11	1.23
1	J	4621	GLU	C-O	-5.96	1.12	1.23
1	L	5647	GLU	C-O	-5.96	1.12	1.23
1	A	4	GLU	C-O	-5.95	1.12	1.23

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	725	ARG	NE-CZ-NH2	6.56	123.58	120.30
1	D	1751	ARG	NE-CZ-NH2	6.56	123.58	120.30
1	F	2777	ARG	NE-CZ-NH2	6.56	123.58	120.30
1	H	3803	ARG	NE-CZ-NH2	6.56	123.58	120.30
1	J	4829	ARG	NE-CZ-NH2	6.56	123.58	120.30

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	475	GLU	Mainchain
1	B	632	GLN	Mainchain
1	B	651	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	3840	0	3986	18	0
1	B	3840	0	3983	19	0
1	C	3840	0	3983	20	0
1	D	3840	0	3983	21	0
1	E	3840	0	3983	20	0
1	F	3840	0	3983	19	0
1	G	3840	0	3983	18	0
1	H	3840	0	3983	20	0
1	I	3840	0	3983	18	0
1	J	3840	0	3983	20	0
1	K	3840	0	3983	19	0
1	L	3840	0	3983	20	0
1	M	3840	0	3983	20	0
1	N	3840	0	3983	21	0
1	O	3840	0	3983	20	0
1	P	3840	0	3983	19	0
All	All	61440	0	63731	280	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 280 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:K:5134:GLU:O	1:K:5135:ASN:HB2	2.00	0.61
1:A:4:GLU:O	1:A:5:ASN:HB2	2.00	0.61
1:H:3595:GLU:O	1:H:3596:ASN:HB2	2.00	0.61
1:J:4621:GLU:O	1:J:4622:ASN:HB2	2.00	0.61
1:P:7699:GLU:O	1:P:7700:ASN:HB2	2.00	0.61

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 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	511/513 (100%)	493 (96%)	16 (3%)	2 (0%)	39	80
1	B	511/513 (100%)	493 (96%)	16 (3%)	2 (0%)	39	80
1	C	511/513 (100%)	493 (96%)	16 (3%)	2 (0%)	39	80
1	D	511/513 (100%)	493 (96%)	16 (3%)	2 (0%)	39	80
1	E	511/513 (100%)	493 (96%)	16 (3%)	2 (0%)	39	80
1	F	511/513 (100%)	493 (96%)	16 (3%)	2 (0%)	39	80
1	G	511/513 (100%)	493 (96%)	16 (3%)	2 (0%)	39	80
1	H	511/513 (100%)	493 (96%)	16 (3%)	2 (0%)	39	80
1	I	511/513 (100%)	493 (96%)	16 (3%)	2 (0%)	39	80
1	J	511/513 (100%)	493 (96%)	16 (3%)	2 (0%)	39	80
1	K	511/513 (100%)	493 (96%)	16 (3%)	2 (0%)	39	80
1	L	511/513 (100%)	493 (96%)	16 (3%)	2 (0%)	39	80
1	M	511/513 (100%)	493 (96%)	16 (3%)	2 (0%)	39	80
1	N	511/513 (100%)	493 (96%)	16 (3%)	2 (0%)	39	80
1	O	511/513 (100%)	493 (96%)	16 (3%)	2 (0%)	39	80
1	P	511/513 (100%)	493 (96%)	16 (3%)	2 (0%)	39	80
All	All	8176/8208 (100%)	7888 (96%)	256 (3%)	32 (0%)	43	80

5 of 32 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	5	ASN
1	B	518	ASN
1	C	1031	ASN
1	D	1544	ASN
1	E	2057	ASN

### 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	410/410 (100%)	403 (98%)	7 (2%)	68	87
1	B	410/410 (100%)	403 (98%)	7 (2%)	68	87
1	C	410/410 (100%)	403 (98%)	7 (2%)	68	87
1	D	410/410 (100%)	403 (98%)	7 (2%)	68	87
1	E	410/410 (100%)	403 (98%)	7 (2%)	68	87
1	F	410/410 (100%)	403 (98%)	7 (2%)	68	87
1	G	410/410 (100%)	403 (98%)	7 (2%)	68	87
1	H	410/410 (100%)	403 (98%)	7 (2%)	68	87
1	I	410/410 (100%)	403 (98%)	7 (2%)	68	87
1	J	410/410 (100%)	403 (98%)	7 (2%)	68	87
1	K	410/410 (100%)	403 (98%)	7 (2%)	68	87
1	L	410/410 (100%)	403 (98%)	7 (2%)	68	87
1	M	410/410 (100%)	403 (98%)	7 (2%)	68	87
1	N	410/410 (100%)	403 (98%)	7 (2%)	68	87
1	O	410/410 (100%)	403 (98%)	7 (2%)	68	87
1	P	410/410 (100%)	403 (98%)	7 (2%)	68	87
All	All	6560/6560 (100%)	6448 (98%)	112 (2%)	71	87

5 of 112 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	H	3663	LEU
1	I	4607	LEU
1	O	7525	SER
1	H	3754	LYS
1	I	4143	ASP

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	3698	GLN
1	I	4211	GLN
1	M	6263	GLN
1	G	3185	GLN
1	N	6776	GLN



### 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.