



wwPDB EM Map/Model Validation Report ⓘ

Apr 10, 2016 – 01:51 PM BST

PDB ID : 3IZN
EMDB ID: : EMD-5250
Title : Mm-cpn deltalid with ATP
Authors : Douglas, N.R.; Reissmann, S.; Zhang, J.; Chen, B.; Jakana, J.; Kumar, R.; Chiu, W.; Frydman, J.
Deposited on : 2010-10-30
Resolution : 6.40 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

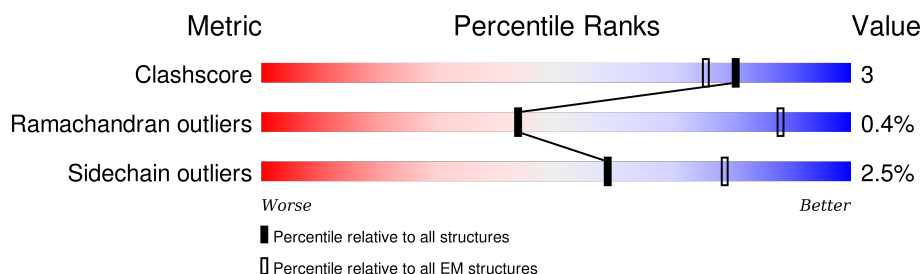
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 6.40 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 $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	A	491	
1	B	491	
1	C	491	
1	D	491	
1	E	491	
1	F	491	
1	G	491	
1	H	491	
1	I	491	

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Mol	Chain	Length	Quality of chain
1	J	491	<div><div></div><div>90%</div><div>9%</div><div></div></div>
1	K	491	<div><div></div><div>90%</div><div>10%</div><div></div></div>
1	L	491	<div><div></div><div>90%</div><div>10%</div><div></div></div>
1	M	491	<div><div></div><div>90%</div><div>9%</div><div></div></div>
1	N	491	<div><div></div><div>90%</div><div>9%</div><div></div></div>
1	O	491	<div><div></div><div>90%</div><div>9%</div><div></div></div>
1	P	491	<div><div></div><div>90%</div><div>9%</div><div></div></div>

2 Entry composition

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 Chaperonin.

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 80 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	235	GLU	-	EXPRESSION TAG	UNP Q877G8
A	236	THR	-	EXPRESSION TAG	UNP Q877G8
A	237	ALA	-	EXPRESSION TAG	UNP Q877G8
A	238	SER	-	EXPRESSION TAG	UNP Q877G8
A	239	GLU	-	EXPRESSION TAG	UNP Q877G8
B	726	GLU	-	EXPRESSION TAG	UNP Q877G8
B	727	THR	-	EXPRESSION TAG	UNP Q877G8
B	728	ALA	-	EXPRESSION TAG	UNP Q877G8
B	729	SER	-	EXPRESSION TAG	UNP Q877G8
B	730	GLU	-	EXPRESSION TAG	UNP Q877G8
C	1217	GLU	-	EXPRESSION TAG	UNP Q877G8
C	1218	THR	-	EXPRESSION TAG	UNP Q877G8
C	1219	ALA	-	EXPRESSION TAG	UNP Q877G8
C	1220	SER	-	EXPRESSION TAG	UNP Q877G8
C	1221	GLU	-	EXPRESSION TAG	UNP Q877G8
D	1708	GLU	-	EXPRESSION TAG	UNP Q877G8
D	1709	THR	-	EXPRESSION TAG	UNP Q877G8
D	1710	ALA	-	EXPRESSION TAG	UNP Q877G8
D	1711	SER	-	EXPRESSION TAG	UNP Q877G8
D	1712	GLU	-	EXPRESSION TAG	UNP Q877G8
E	2199	GLU	-	EXPRESSION TAG	UNP Q877G8
E	2200	THR	-	EXPRESSION TAG	UNP Q877G8
E	2201	ALA	-	EXPRESSION TAG	UNP Q877G8
E	2202	SER	-	EXPRESSION TAG	UNP Q877G8
E	2203	GLU	-	EXPRESSION TAG	UNP Q877G8
F	2690	GLU	-	EXPRESSION TAG	UNP Q877G8
F	2691	THR	-	EXPRESSION TAG	UNP Q877G8
F	2692	ALA	-	EXPRESSION TAG	UNP Q877G8
F	2693	SER	-	EXPRESSION TAG	UNP Q877G8
F	2694	GLU	-	EXPRESSION TAG	UNP Q877G8
G	3181	GLU	-	EXPRESSION TAG	UNP Q877G8
G	3182	THR	-	EXPRESSION TAG	UNP Q877G8
G	3183	ALA	-	EXPRESSION TAG	UNP Q877G8
G	3184	SER	-	EXPRESSION TAG	UNP Q877G8
G	3185	GLU	-	EXPRESSION TAG	UNP Q877G8
H	3672	GLU	-	EXPRESSION TAG	UNP Q877G8
H	3673	THR	-	EXPRESSION TAG	UNP Q877G8
H	3674	ALA	-	EXPRESSION TAG	UNP Q877G8
H	3675	SER	-	EXPRESSION TAG	UNP Q877G8
H	3676	GLU	-	EXPRESSION TAG	UNP Q877G8
I	4163	GLU	-	EXPRESSION TAG	UNP Q877G8
I	4164	THR	-	EXPRESSION TAG	UNP Q877G8
I	4165	ALA	-	EXPRESSION TAG	UNP Q877G8

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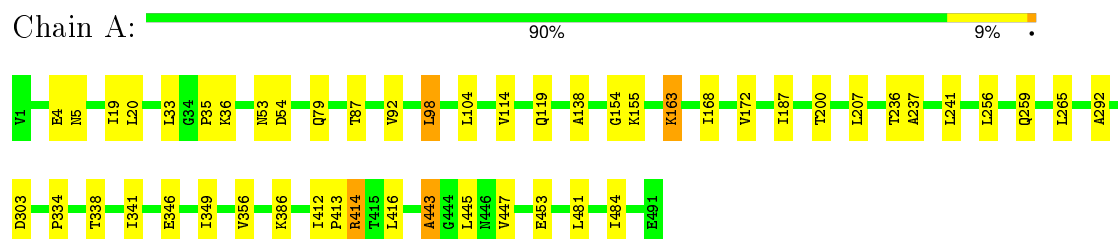
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Chain	Residue	Modelled	Actual	Comment	Reference
I	4166	SER	-	EXPRESSION TAG	UNP Q877G8
I	4167	GLU	-	EXPRESSION TAG	UNP Q877G8
J	4654	GLU	-	EXPRESSION TAG	UNP Q877G8
J	4655	THR	-	EXPRESSION TAG	UNP Q877G8
J	4656	ALA	-	EXPRESSION TAG	UNP Q877G8
J	4657	SER	-	EXPRESSION TAG	UNP Q877G8
J	4658	GLU	-	EXPRESSION TAG	UNP Q877G8
K	5145	GLU	-	EXPRESSION TAG	UNP Q877G8
K	5146	THR	-	EXPRESSION TAG	UNP Q877G8
K	5147	ALA	-	EXPRESSION TAG	UNP Q877G8
K	5148	SER	-	EXPRESSION TAG	UNP Q877G8
K	5149	GLU	-	EXPRESSION TAG	UNP Q877G8
L	5636	GLU	-	EXPRESSION TAG	UNP Q877G8
L	5637	THR	-	EXPRESSION TAG	UNP Q877G8
L	5638	ALA	-	EXPRESSION TAG	UNP Q877G8
L	5639	SER	-	EXPRESSION TAG	UNP Q877G8
L	5640	GLU	-	EXPRESSION TAG	UNP Q877G8
M	6127	GLU	-	EXPRESSION TAG	UNP Q877G8
M	6128	THR	-	EXPRESSION TAG	UNP Q877G8
M	6129	ALA	-	EXPRESSION TAG	UNP Q877G8
M	6130	SER	-	EXPRESSION TAG	UNP Q877G8
M	6131	GLU	-	EXPRESSION TAG	UNP Q877G8
N	6618	GLU	-	EXPRESSION TAG	UNP Q877G8
N	6619	THR	-	EXPRESSION TAG	UNP Q877G8
N	6620	ALA	-	EXPRESSION TAG	UNP Q877G8
N	6621	SER	-	EXPRESSION TAG	UNP Q877G8
N	6622	GLU	-	EXPRESSION TAG	UNP Q877G8
O	7109	GLU	-	EXPRESSION TAG	UNP Q877G8
O	7110	THR	-	EXPRESSION TAG	UNP Q877G8
O	7111	ALA	-	EXPRESSION TAG	UNP Q877G8
O	7112	SER	-	EXPRESSION TAG	UNP Q877G8
O	7113	GLU	-	EXPRESSION TAG	UNP Q877G8
P	7600	GLU	-	EXPRESSION TAG	UNP Q877G8
P	7601	THR	-	EXPRESSION TAG	UNP Q877G8
P	7602	ALA	-	EXPRESSION TAG	UNP Q877G8
P	7603	SER	-	EXPRESSION TAG	UNP Q877G8
P	7604	GLU	-	EXPRESSION TAG	UNP Q877G8

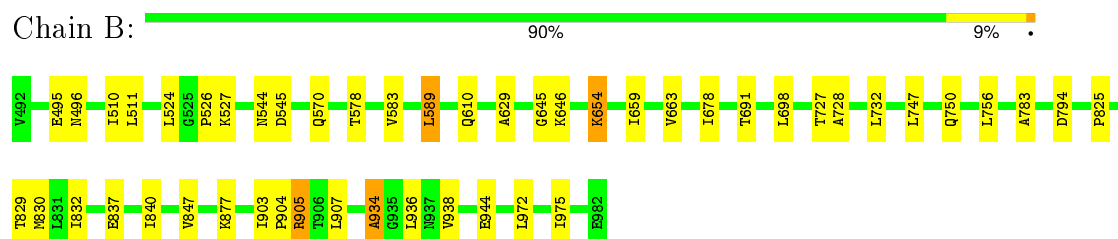
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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.

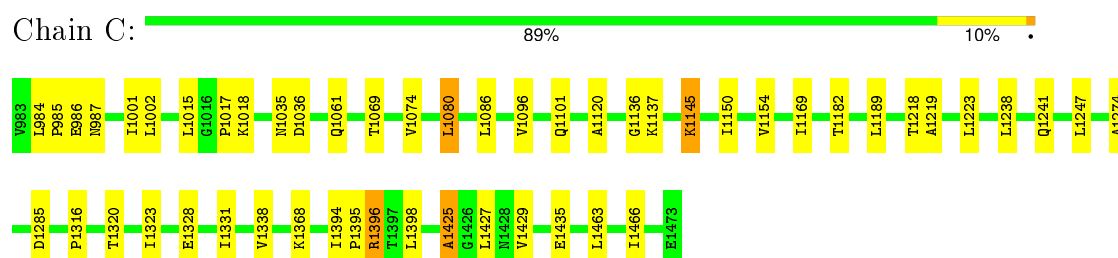
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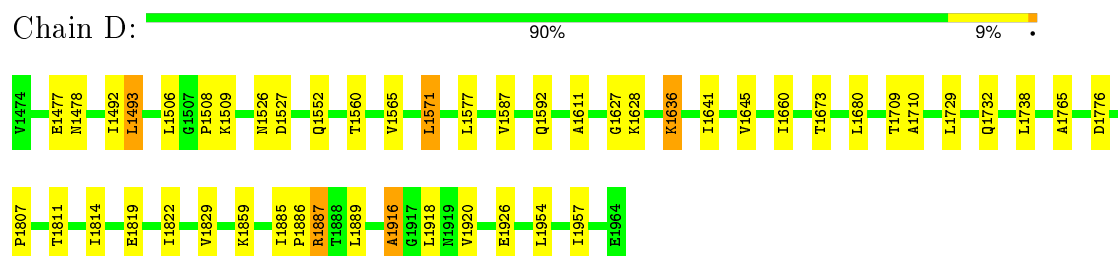
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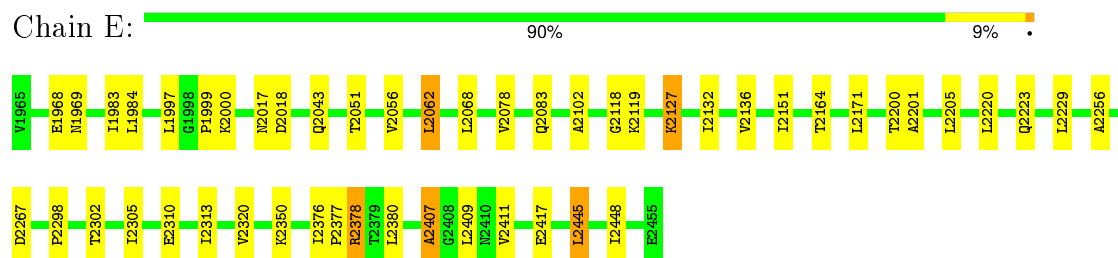
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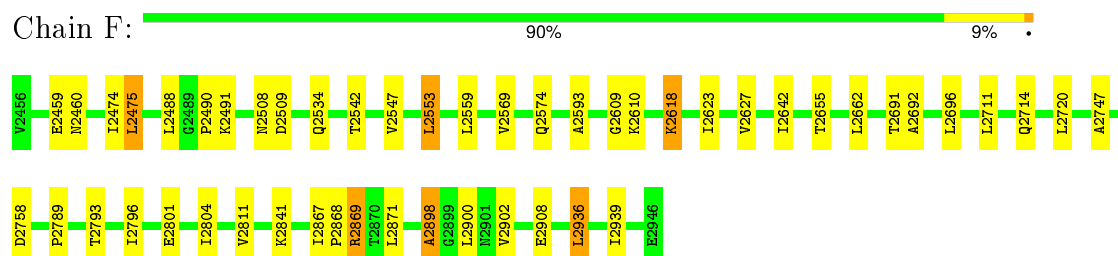
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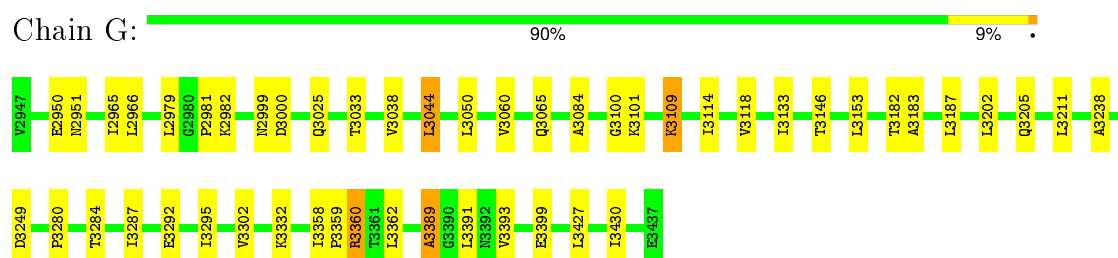
- Molecule 1: Chaperonin



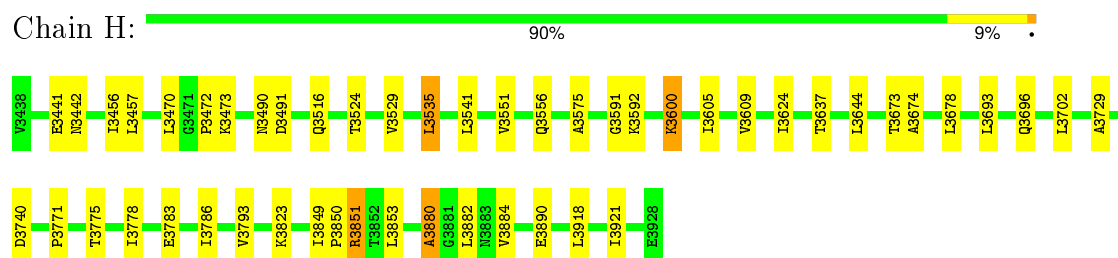
- Molecule 1: Chaperonin



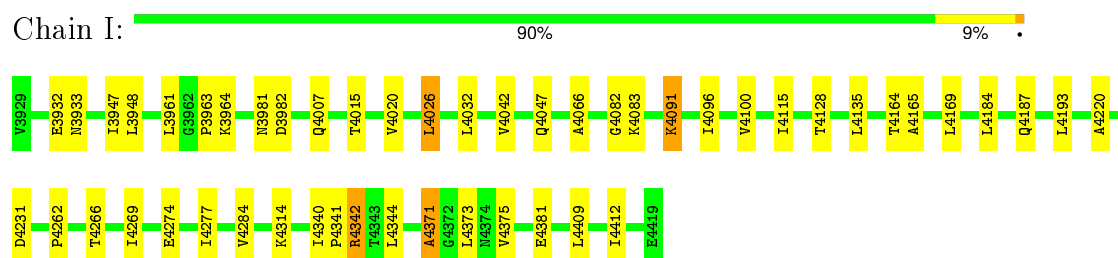
- Molecule 1: Chaperonin



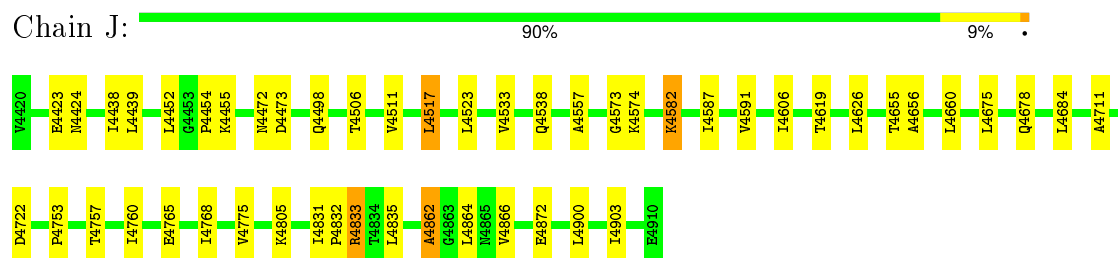
- Molecule 1: Chaperonin



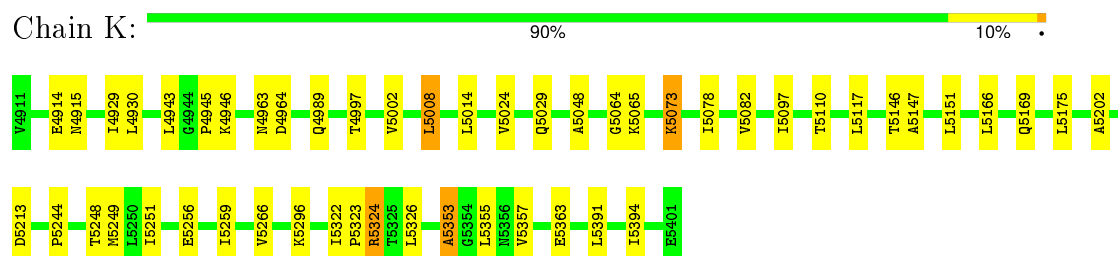
- Molecule 1: Chaperonin



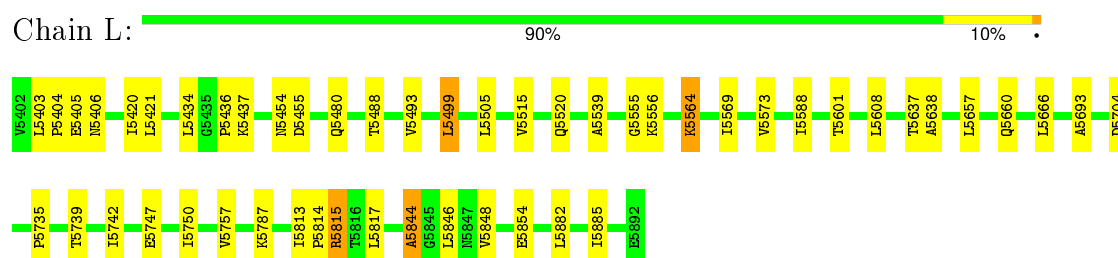
• Molecule 1: Chaperonin



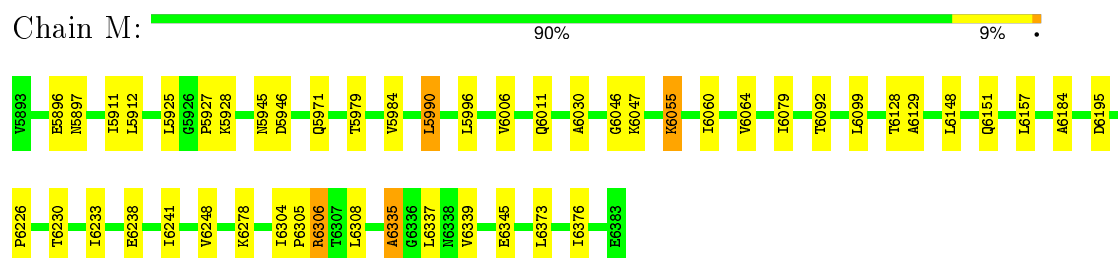
• Molecule 1: Chaperonin



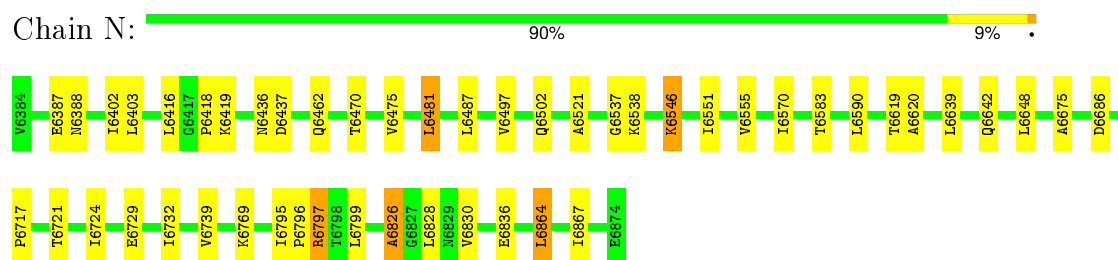
• Molecule 1: Chaperonin



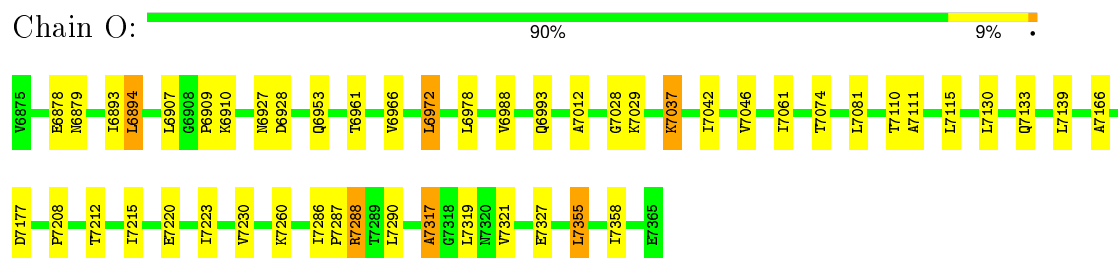
• Molecule 1: Chaperonin



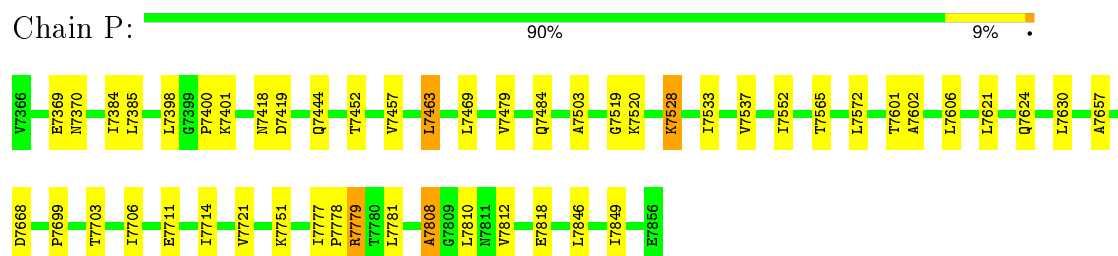
• Molecule 1: Chaperonin



● Molecule 1: Chaperonin



● Molecule 1: Chaperonin



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 10Kx10K CCD camera (binned by 2)	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	0.88	1/3686 (0.0%)	0.76	1/4961 (0.0%)
1	B	0.88	1/3686 (0.0%)	0.76	1/4961 (0.0%)
1	C	0.88	1/3686 (0.0%)	0.76	1/4961 (0.0%)
1	D	0.88	1/3686 (0.0%)	0.76	1/4961 (0.0%)
1	E	0.88	1/3686 (0.0%)	0.76	1/4961 (0.0%)
1	F	0.88	1/3686 (0.0%)	0.76	1/4961 (0.0%)
1	G	0.88	1/3686 (0.0%)	0.76	1/4961 (0.0%)
1	H	0.88	1/3686 (0.0%)	0.75	1/4961 (0.0%)
1	I	0.88	1/3686 (0.0%)	0.76	1/4961 (0.0%)
1	J	0.88	1/3686 (0.0%)	0.76	1/4961 (0.0%)
1	K	0.88	1/3686 (0.0%)	0.76	1/4961 (0.0%)
1	L	0.88	1/3686 (0.0%)	0.76	1/4961 (0.0%)
1	M	0.88	1/3686 (0.0%)	0.76	1/4961 (0.0%)
1	N	0.88	1/3686 (0.0%)	0.76	1/4961 (0.0%)
1	O	0.88	1/3686 (0.0%)	0.76	1/4961 (0.0%)
1	P	0.88	1/3686 (0.0%)	0.75	1/4961 (0.0%)
All	All	0.88	16/58976 (0.0%)	0.76	16/79376 (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	F	2898	ALA	C-O	5.07	1.32	1.23
1	H	3880	ALA	C-O	5.07	1.32	1.23
1	K	5353	ALA	C-O	5.07	1.32	1.23
1	N	6826	ALA	C-O	5.07	1.32	1.23

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	1477	GLU	CA-C-O	-6.63	106.17	120.10
1	O	6878	GLU	CA-C-O	-6.63	106.17	120.10
1	A	4	GLU	CA-C-O	-6.62	106.20	120.10
1	B	495	GLU	CA-C-O	-6.62	106.20	120.10
1	I	3932	GLU	CA-C-O	-6.62	106.20	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	24	0
1	B	3665	0	3801	24	0
1	C	3665	0	3801	25	0
1	D	3665	0	3801	24	0
1	E	3665	0	3801	25	0
1	F	3665	0	3801	26	0
1	G	3665	0	3801	24	0
1	H	3665	0	3801	24	0
1	I	3665	0	3801	24	0
1	J	3665	0	3801	24	0
1	K	3665	0	3801	25	0
1	L	3665	0	3801	24	0
1	M	3665	0	3801	23	0
1	N	3665	0	3801	24	0
1	O	3665	0	3801	26	0
1	P	3665	0	3801	24	0
All	All	58640	0	60819	390	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 390 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:J:4684:LEU:HD23	1:J:4684:LEU:C	2.17	0.65
1:C:1247:LEU:C	1:C:1247:LEU:HD23	2.17	0.65
1:P:7630:LEU:HD23	1:P:7630:LEU:C	2.17	0.65
1:A:265:LEU:HD23	1:A:265:LEU:C	2.17	0.65
1:G:3211:LEU:C	1:G:3211:LEU:HD23	2.17	0.65

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	489/491 (100%)	468 (96%)	19 (4%)	2 (0%)	39	80
1	B	489/491 (100%)	468 (96%)	19 (4%)	2 (0%)	39	80
1	C	489/491 (100%)	468 (96%)	19 (4%)	2 (0%)	39	80
1	D	489/491 (100%)	468 (96%)	19 (4%)	2 (0%)	39	80
1	E	489/491 (100%)	468 (96%)	19 (4%)	2 (0%)	39	80
1	F	489/491 (100%)	468 (96%)	19 (4%)	2 (0%)	39	80
1	G	489/491 (100%)	468 (96%)	19 (4%)	2 (0%)	39	80
1	H	489/491 (100%)	468 (96%)	19 (4%)	2 (0%)	39	80
1	I	489/491 (100%)	468 (96%)	19 (4%)	2 (0%)	39	80
1	J	489/491 (100%)	468 (96%)	19 (4%)	2 (0%)	39	80
1	K	489/491 (100%)	468 (96%)	19 (4%)	2 (0%)	39	80
1	L	489/491 (100%)	468 (96%)	19 (4%)	2 (0%)	39	80
1	M	489/491 (100%)	468 (96%)	19 (4%)	2 (0%)	39	80
1	N	489/491 (100%)	468 (96%)	19 (4%)	2 (0%)	39	80
1	O	489/491 (100%)	468 (96%)	19 (4%)	2 (0%)	39	80
1	P	489/491 (100%)	468 (96%)	19 (4%)	2 (0%)	39	80
All	All	7824/7856 (100%)	7488 (96%)	304 (4%)	32 (0%)	43	80

5 of 32 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 ⓘ

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%)	383 (98%)	10 (2%)	55	81
1	B	393/393 (100%)	383 (98%)	10 (2%)	55	81
1	C	393/393 (100%)	383 (98%)	10 (2%)	55	81
1	D	393/393 (100%)	383 (98%)	10 (2%)	55	81
1	E	393/393 (100%)	383 (98%)	10 (2%)	55	81
1	F	393/393 (100%)	383 (98%)	10 (2%)	55	81
1	G	393/393 (100%)	383 (98%)	10 (2%)	55	81
1	H	393/393 (100%)	383 (98%)	10 (2%)	55	81
1	I	393/393 (100%)	383 (98%)	10 (2%)	55	81
1	J	393/393 (100%)	383 (98%)	10 (2%)	55	81
1	K	393/393 (100%)	383 (98%)	10 (2%)	55	81
1	L	393/393 (100%)	383 (98%)	10 (2%)	55	81
1	M	393/393 (100%)	383 (98%)	10 (2%)	55	81
1	N	393/393 (100%)	383 (98%)	10 (2%)	55	81
1	O	393/393 (100%)	383 (98%)	10 (2%)	55	81
1	P	393/393 (100%)	383 (98%)	10 (2%)	55	81
All	All	6288/6288 (100%)	6128 (98%)	160 (2%)	59	81

5 of 160 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	H	3535	LEU
1	I	4409	LEU
1	O	7288	ARG
1	H	3696	GLN
1	I	3982	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 12 such sidechains are listed below:

Mol	Chain	Res	Type
1	H	3906	GLN
1	I	4397	GLN
1	L	5870	GLN
1	E	2433	GLN
1	K	5379	GLN

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](#)

There are no ligands in this entry.

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.