



wwPDB EM Map/Model Validation Report ⓘ

Apr 10, 2016 – 02:04 PM BST

PDB ID : 3LOS
EMDB ID: : EMD-5137
Title : Atomic Model of Mm-cpn in the Closed State
Authors : Zhang, J.; Baker, M.L.; Schroeder, G.; Douglas, N.R.; Reissmann, S.; Jakana, J.; Dougherty, M.; Fu, C.J.; Levitt, M.; Ludtke, S.J.; Frydman, J.; Chiu, W.
Deposited on : 2010-02-04
Resolution : 4.30 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>

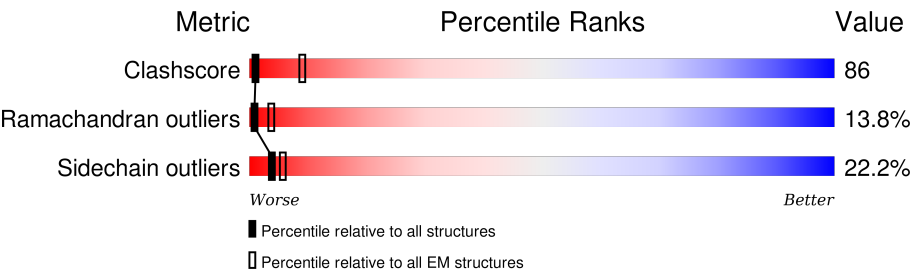
MolProbity : 4.02b-467
Mogul : unknown
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : trunk27241

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 4.30 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	543	22% 50% 23% . .
1	B	543	22% 48% 24% . .
1	C	543	22% 49% 23% . .
1	D	543	22% 49% 24% . .
1	E	543	22% 49% 23% . .
1	F	543	22% 49% 24% . .
1	G	543	22% 49% 23% . .
1	H	543	21% 49% 24% . .
1	I	543	22% 49% 23% . .

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	J	543	<div><div></div><div>22%49%23%<div><div></div><div></div></div></div></div>
1	K	543	<div><div></div><div>22%49%24%<div><div></div><div></div></div></div></div>
1	L	543	<div><div></div><div>22%49%23%<div><div></div><div></div></div></div></div>
1	M	543	<div><div></div><div>22%48%24%<div><div></div><div></div></div></div></div>
1	N	543	<div><div></div><div>22%49%23%<div><div></div><div></div></div></div></div>
1	O	543	<div><div></div><div>22%48%24%<div><div></div><div></div></div></div></div>
1	P	543	<div><div></div><div>22%49%23%<div><div></div><div></div></div></div></div>

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 63712 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.

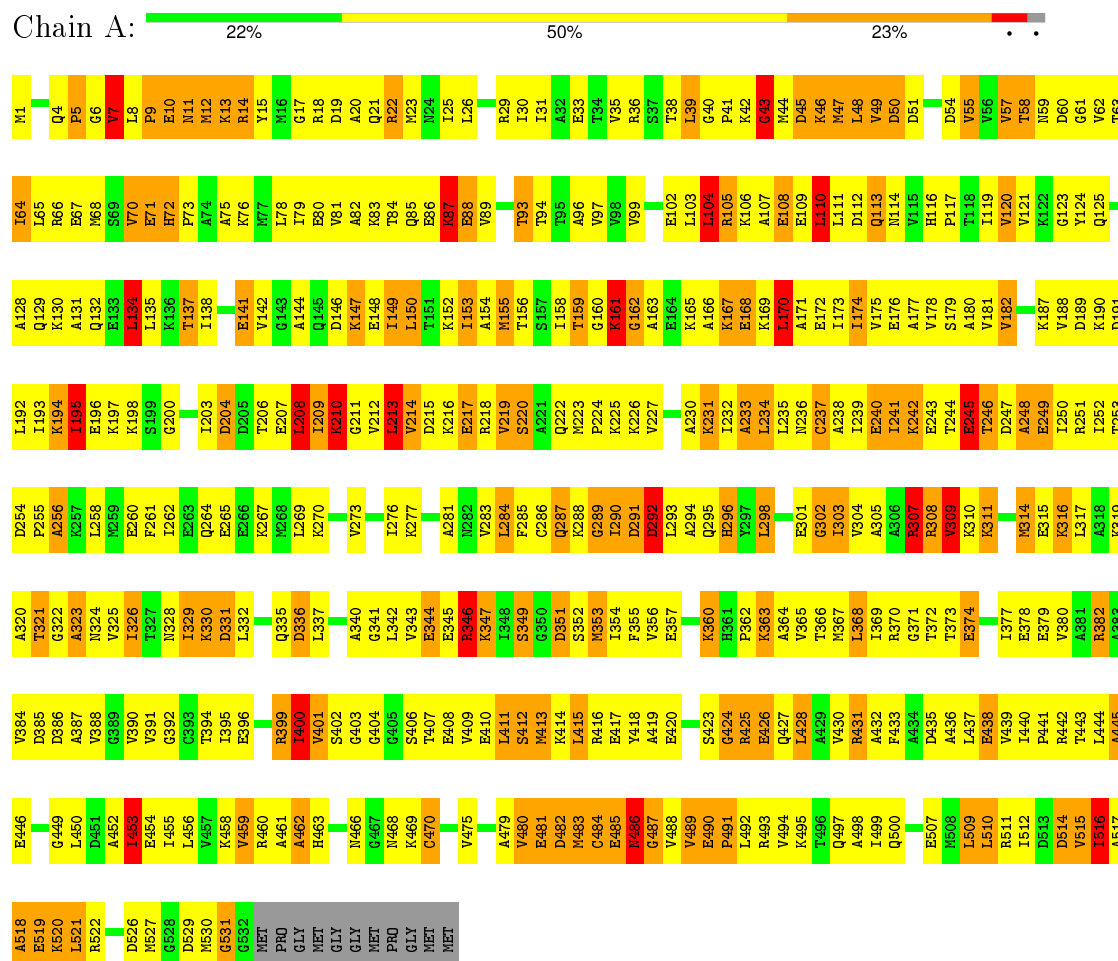
- Molecule 1 is a protein called Chaperonin.

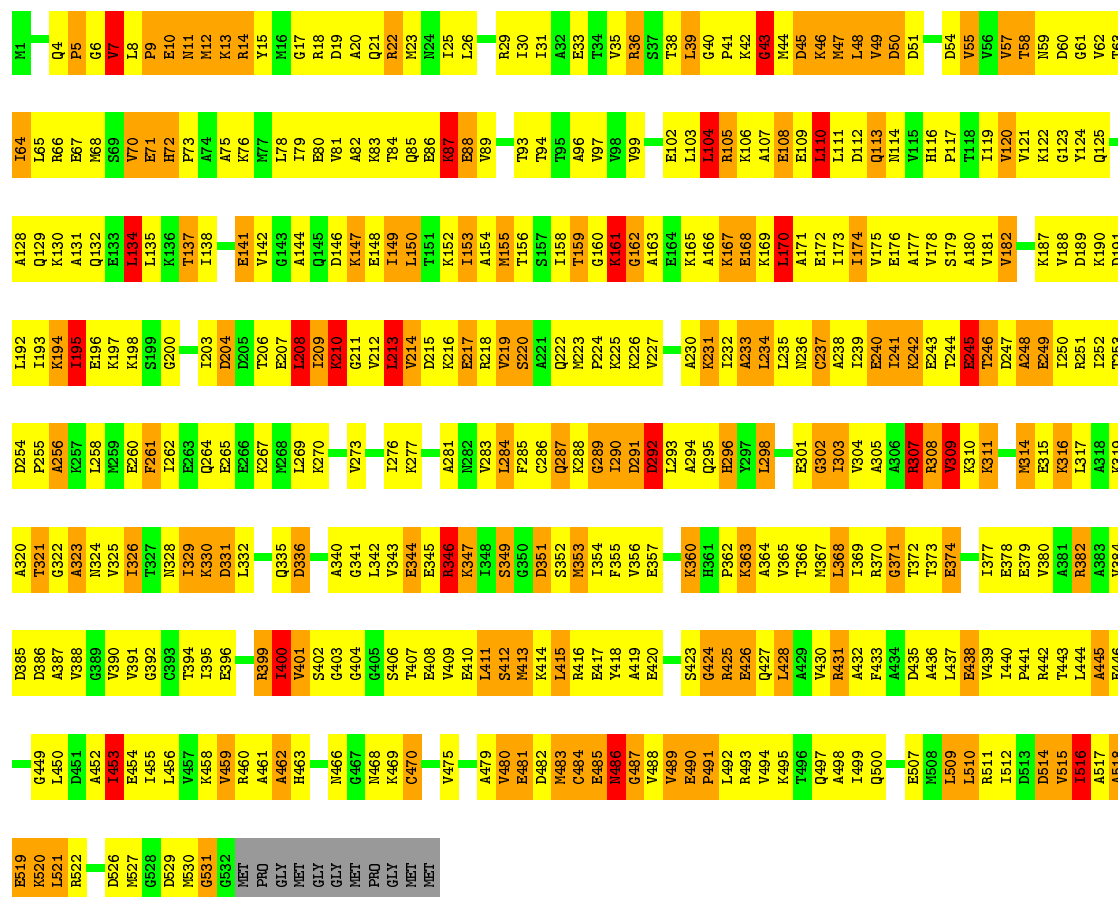
Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	532	Total	C	N	O	S	0	0
			3982	2468	689	797	28		
1	B	532	Total	C	N	O	S	0	0
			3982	2468	689	797	28		
1	C	532	Total	C	N	O	S	0	0
			3982	2468	689	797	28		
1	D	532	Total	C	N	O	S	0	0
			3982	2468	689	797	28		
1	E	532	Total	C	N	O	S	0	0
			3982	2468	689	797	28		
1	F	532	Total	C	N	O	S	0	0
			3982	2468	689	797	28		
1	G	532	Total	C	N	O	S	0	0
			3982	2468	689	797	28		
1	H	532	Total	C	N	O	S	0	0
			3982	2468	689	797	28		
1	I	532	Total	C	N	O	S	0	0
			3982	2468	689	797	28		
1	J	532	Total	C	N	O	S	0	0
			3982	2468	689	797	28		
1	K	532	Total	C	N	O	S	0	0
			3982	2468	689	797	28		
1	L	532	Total	C	N	O	S	0	0
			3982	2468	689	797	28		
1	M	532	Total	C	N	O	S	0	0
			3982	2468	689	797	28		
1	N	532	Total	C	N	O	S	0	0
			3982	2468	689	797	28		
1	O	532	Total	C	N	O	S	0	0
			3982	2468	689	797	28		
1	P	532	Total	C	N	O	S	0	0
			3982	2468	689	797	28		

3 Residue-property plots

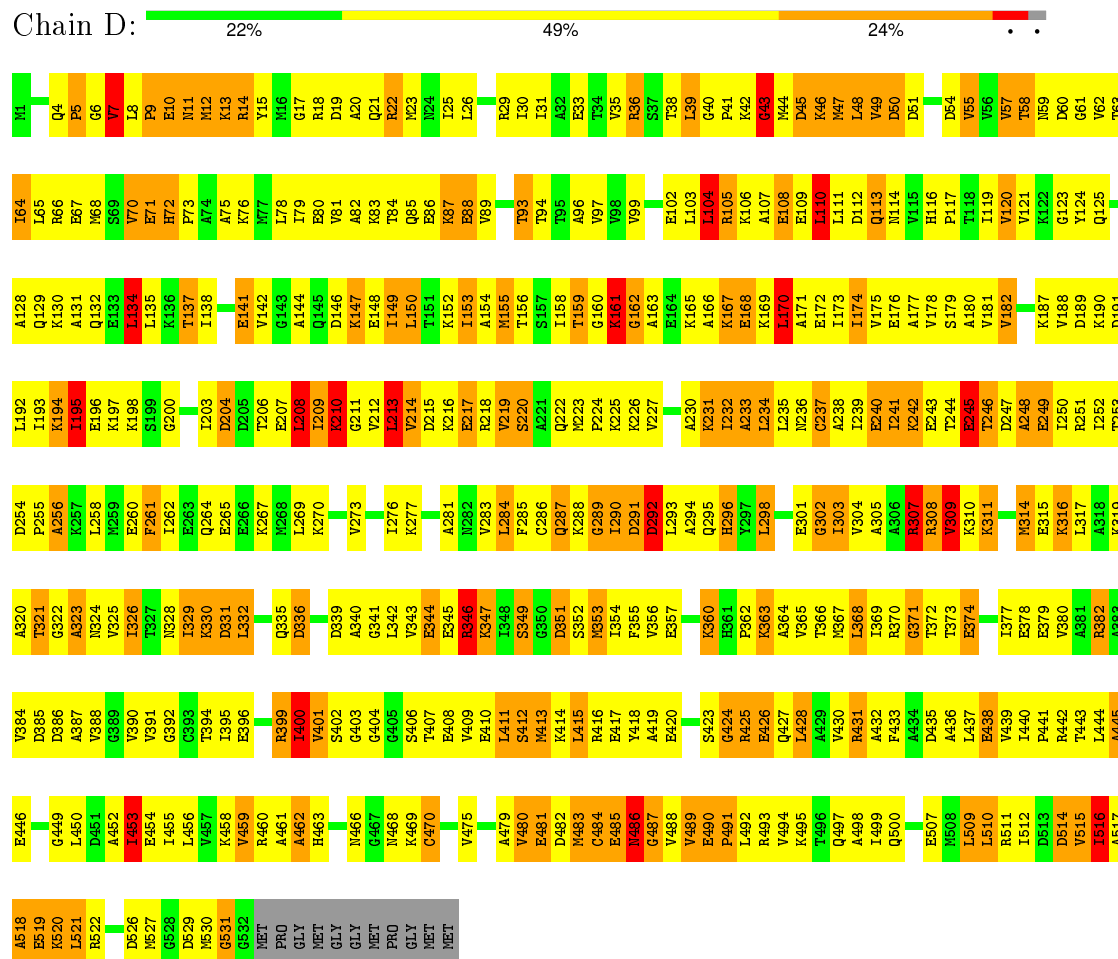
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according to the number of geometric 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.

• Molecule 1: Chaperonin

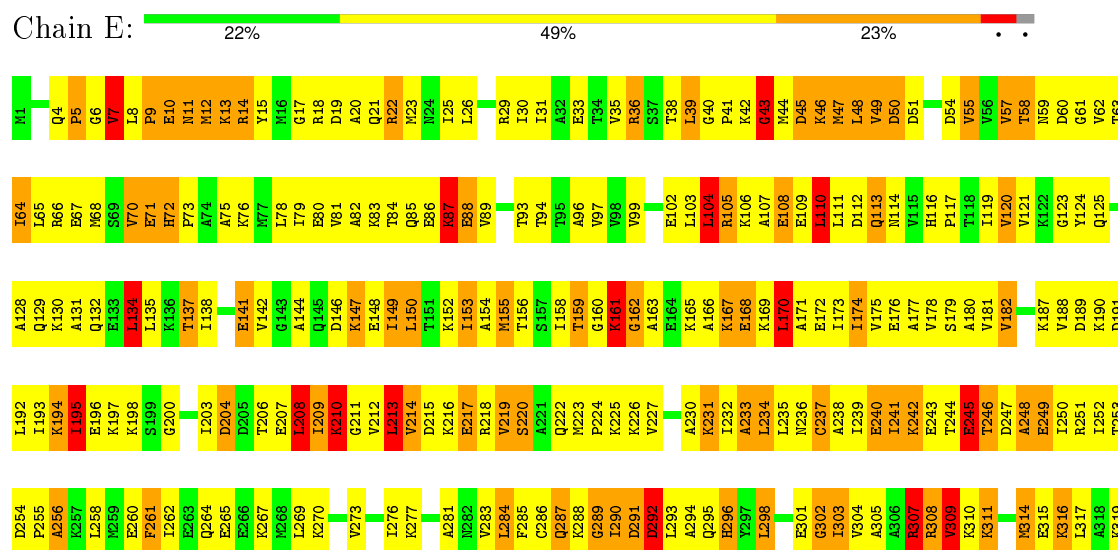


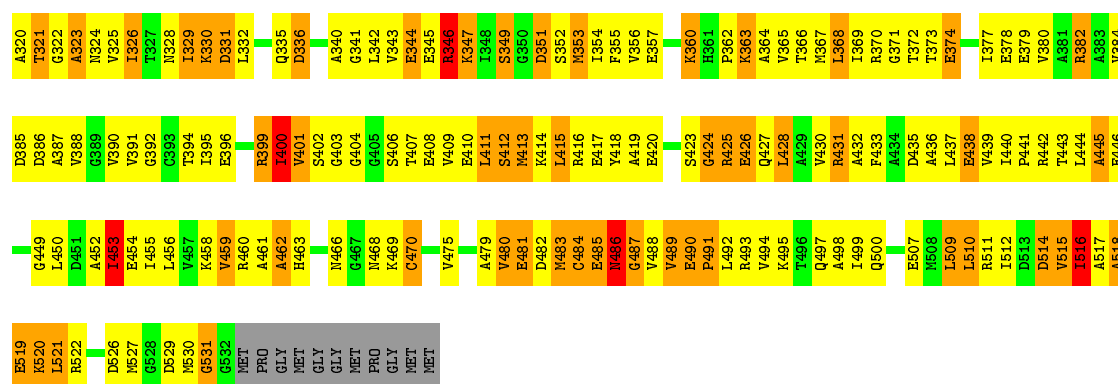


- Molecule 1: Chaperonin



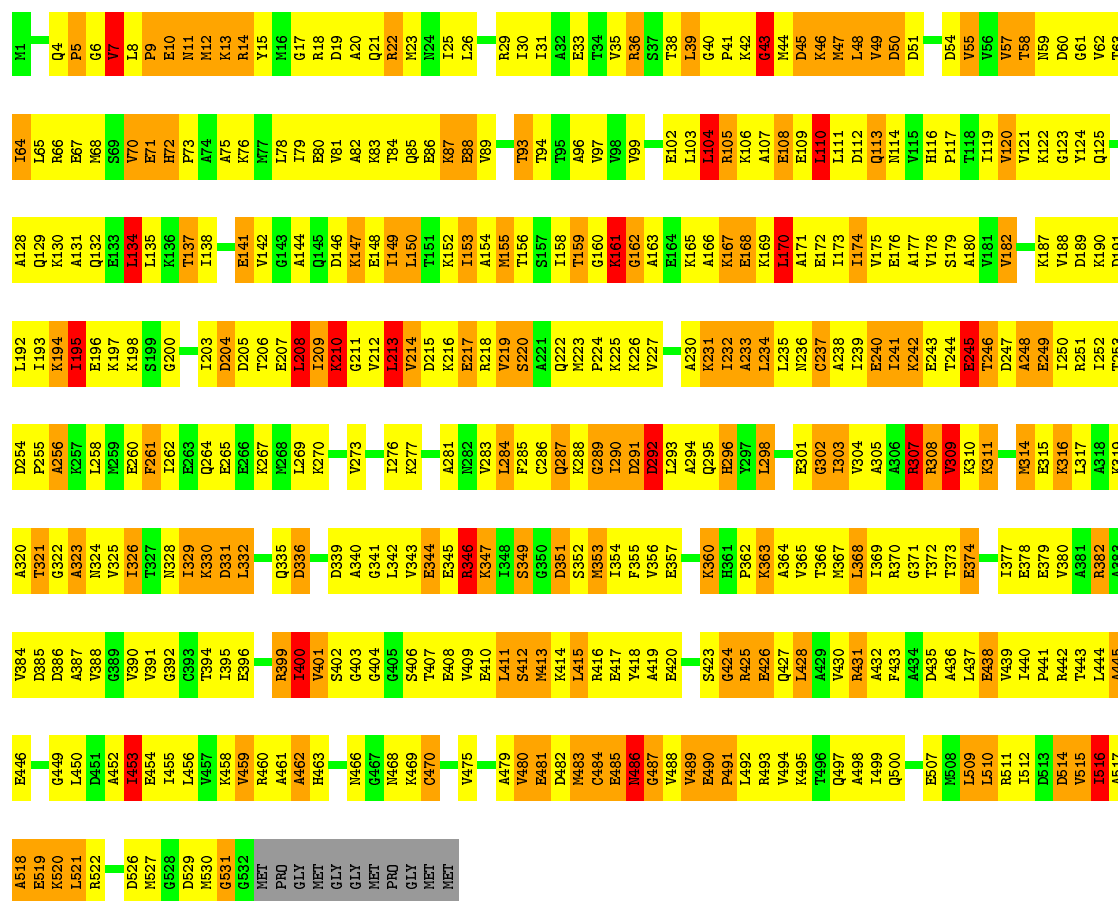
- Molecule 1: Chaperonin





• Molecule 1: Chaperonin

Chain F: 22% 49% 24%



• Molecule 1: Chaperonin

Chain G: 22% 49% 23%



A517	A518	A519	A520	A521	A522	D526	D527	D528	D529	D530	D531	D532	MET	PRO	GLY	MET	GLY	GLY	MET	GLY	MET	GLY	MET	MET
------	------	------	------	------	------	------	------	------	------	------	------	------	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

• Molecule 1: Chaperonin

Chain I: 22% 49% 23%

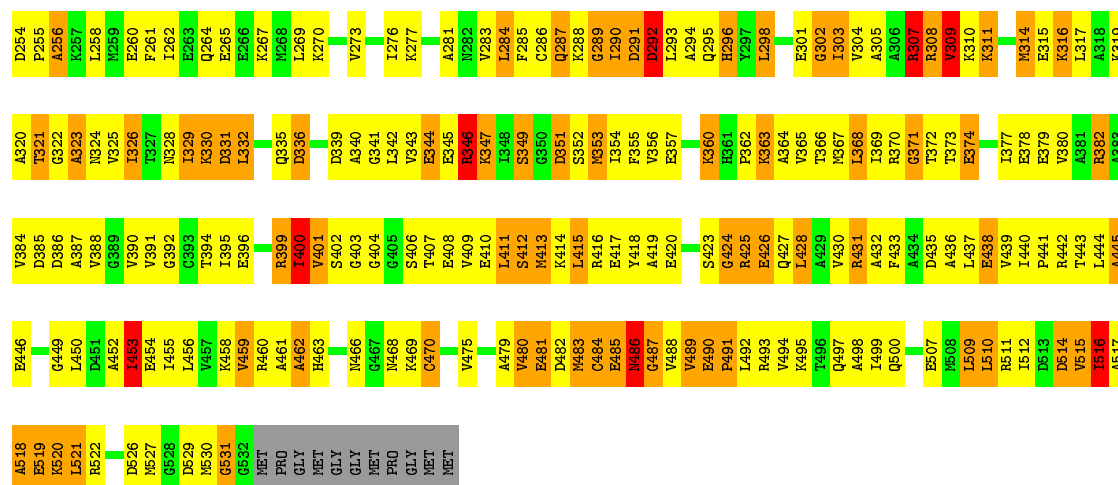
A445	A383	K319	D254	L192	A128	H1
E446	V384	A320	P255	I193	Q129	I64
G449	D385	T321	A256	K194	K130	Q4
L450	D386	G322	K257	L195	A131	P5
D451	V388	A323	L258	E196	Q132	G6
A452	G389	K324	M259	K197	E133	V7
L453	V390	V325	E260	K198	L134	L8
E454	V391	T327	T262	G200	L135	P9
L455	G392	N328	L263		K136	E10
L456	C393	K329	Q264	I203	T137	N11
A457	T394	K330	E265	D204	L138	M12
K458	L395	D331	E266	D205	E141	K13
V459	E396	L332	K267	T206	V142	R14
R460			M268	E207	G143	Y15
A461	R399	Q335	L269	L208	L144	M16
A462	L400	D336	K270	I209	Q145	R17
H463	V401			K210	D146	D19
	S402	D339	V273	G211	K147	A18
M466	G403	A340		V212	E148	A20
G467	G404	G341	T276	L213	L149	K83
N468	G405	L342	K277	V214	T150	R22
K469	S406	V343		D215	T151	M23
C470	T407	E344	A281	K216	K152	N24
	E408	E345	N282	E217	L153	L25
V475	V409	R346	L284	R218	A154	L26
	E410	K347	F285	V219	M155	
A479	L411	L348	C286	S220	T156	R29
V480	S412	S349	Q287	A221	A157	I30
E481	K414	D351	K288	M223	L158	I31
M483	L415	S352	C289	K223	T159	A32
C484	R416	M353	D290	P224	G160	E33
E485	E417	L354	D291	K225	K161	T34
M486	Y418	F355	K226	K226	G162	V35
	A419	V356	D342	V227	V99	R36
A487			L293		A163	S37
V488	E420	E357	A294	A230	E164	T38
V489			Q295	K231	K165	S38
E490	S423	K360	E296	L232	L103	L39
P491	G424	E361	H296	A233	R105	R40
L492	R425	P362	T297	E233	K106	P41
R493	E426	K363	A299	L234	A107	K42
V494	Q427	A364	E301	L235	E108	G43
K495	L428	V365	G302	M236	E109	M44
T496	A429	T366	L303	A238	L110	D45
Q497	V430	M367	V304	L239	L111	M47
A498	R431	L368	A305	E240	D112	L48
L499	A432	L369	A306	K241	Q113	V49
Q500	F433	R370	R307	E242	N114	D50
	A434	G371	K308	K243	V115	D51
E507	D435	T372	R308	T244	H116	
M508	A436	T373	V309	E245	P117	D54
L509	L437	E374	K310	R246	L118	V55
L510	E438		K311	D247	V181	V56
R511	V439	I377		A248	V182	V57
I512	L440	E378	M314	E249		T58
D513	P441	E379	E315	A248	K187	N59
D514	R442	V380	K316	L250	V188	D60
V515	T443	A381	L317	R251	G123	G61
	L444	E382	E316	K252	I124	V62
				T252	Q125	T63

A517	A518	A519	A520	A521	A522	D526	D527	D528	D529	D530	D531	D532	MET	PRO	GLY	MET	GLY	GLY	MET	GLY	MET	GLY	MET	MET
------	------	------	------	------	------	------	------	------	------	------	------	------	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

• Molecule 1: Chaperonin

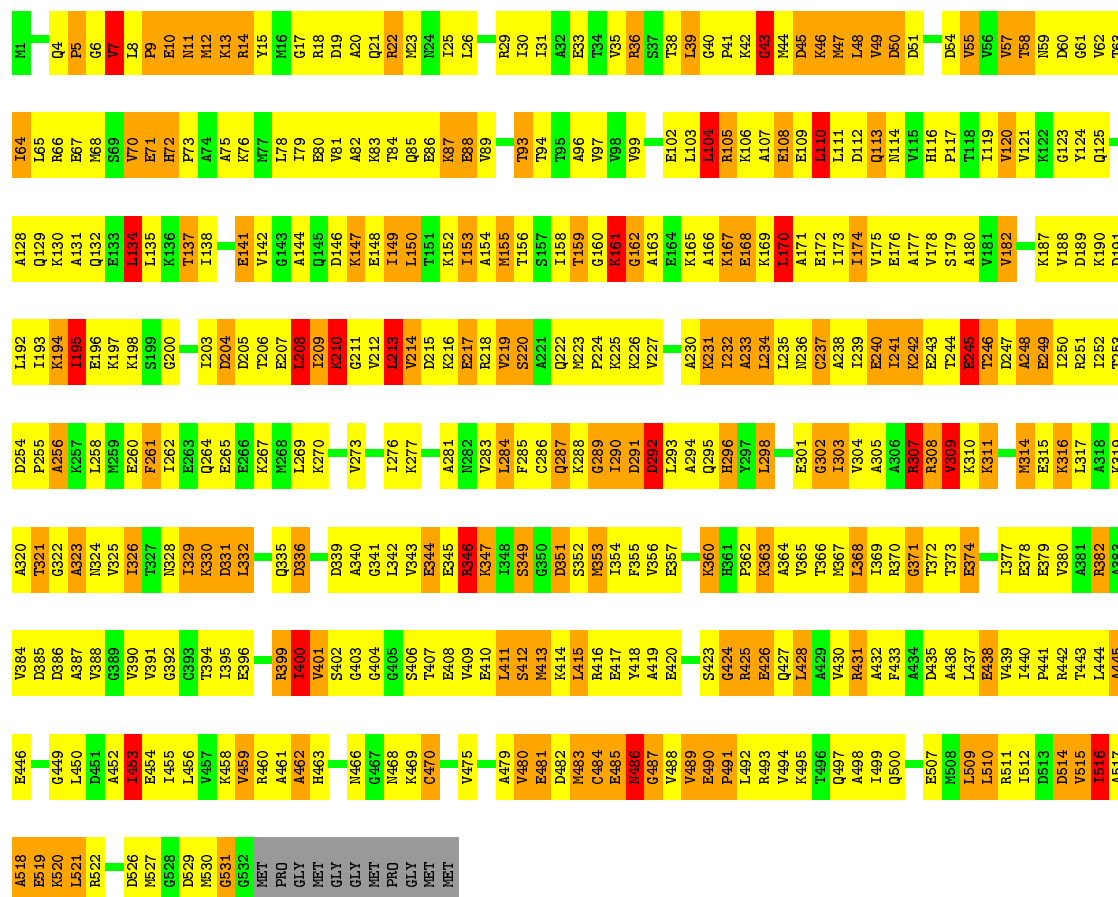
Chain J: 22% 49% 23%

L192	I193	K194	L195	E196	K197	K198	S199	G200	L203	D204	D205	T206	E207	L208	L209	K210	G211	V212	L213	L214	D215	L216	E217	R218	V219	S220	Q221	Q222	M223	P224	K225	K226	V227	L230	A230	R231	L232	L233	A234	L235	M236	C237	E238	L239	D240	L241	Q242	T243	T244	L245	E246	D247	A248	E249	L250	R251	L252	T253
A128	Q129	K130	A131	Q132	E133	L134	L135	K136	T137	L138	E141	V142	G143	A144	Q145	D146	K147	E148	T149	L150	T151	K152	L153	A154	M155	T156	A157	L158	T159	G160	K161	G162	A163	E164	K165	A166	K167	E168	K169	L170	A171	E172	L173	T174	V175	E176	A177	V178	S179	A180	V181	V182	K187	V188	D189	K190	T191	
I64	L65	R66	E67	M68	S69	V70	E71	H72	P73	A74	A75	K76	H77	L78	I79	E80	V81	A82	K83	T84	Q85	E86	K87	E88	V89	T93	T94	T95	A96	V97	V98	V99	E102	L103	L104	R105	K106	A107	E108	E109	L110	L111	D112	Q113	N114	D115	H116	P117	T118	L119	V120	V121	K122	G123	Y124	Q125	T126	
M1	Q4	P5	G6	V7	L8	P9	E10	M11	M12	K13	K14	Y15	M16	R17	R18	D19	A20	Q21	R22	M23	K24	L25	L26	R29	T30	T31	A32	E33	T34	V35	R36	S37	T38	L39	G40	F41	K42	G43	M44	D45	K46	M47	L48	V49	D50	D51	L54	V55	V56	V57	T58	N59	D60	G61	Y62	T63		



• Molecule 1: Chaperonin

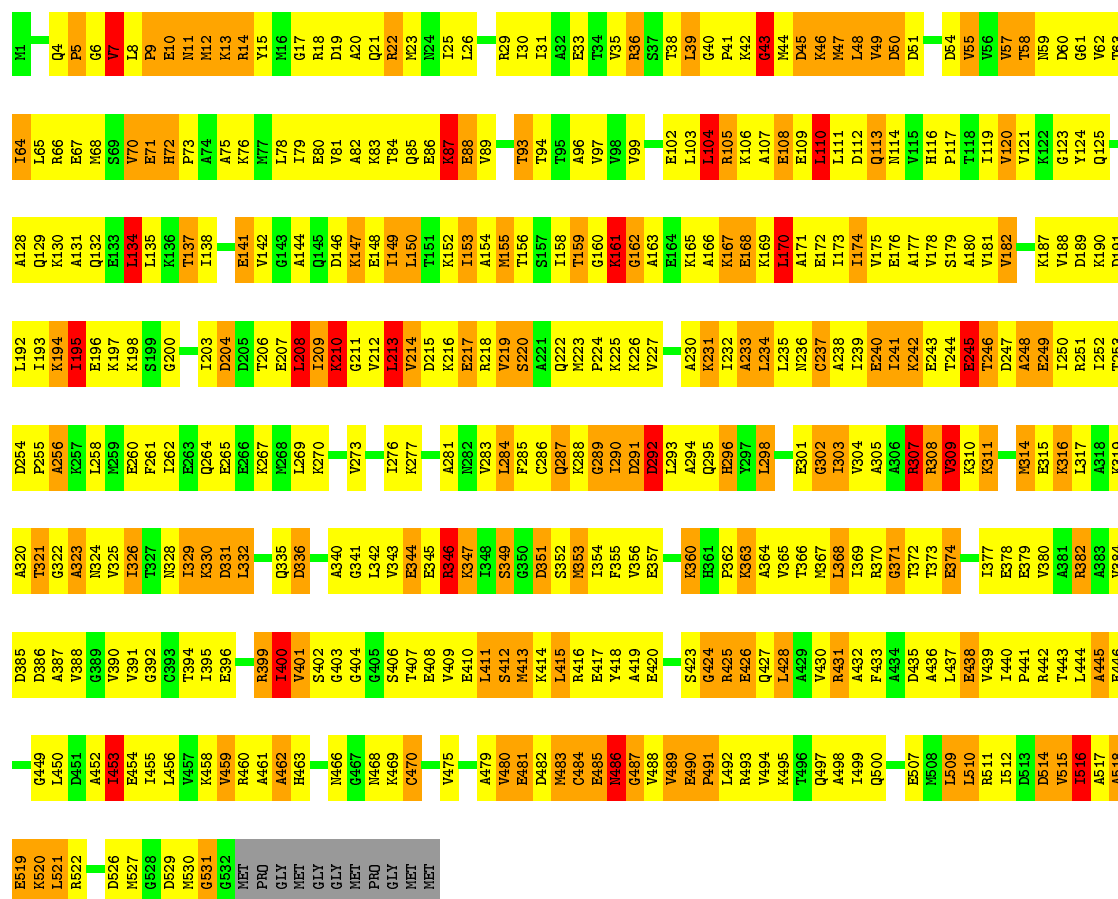
Chain K: 22% 49% 24%



• Molecule 1: Chaperonin

Chain L: 22% 49% 23%





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	Each micrograph	Depositor
Microscope	JEM3200FSC	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	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	0.34	0/4007	0.98	26/5390 (0.5%)
1	B	0.34	0/4007	0.98	27/5390 (0.5%)
1	C	0.34	0/4007	0.98	26/5390 (0.5%)
1	D	0.34	0/4007	0.98	26/5390 (0.5%)
1	E	0.34	0/4007	0.98	26/5390 (0.5%)
1	F	0.34	0/4007	0.98	26/5390 (0.5%)
1	G	0.34	0/4007	0.98	26/5390 (0.5%)
1	H	0.34	0/4007	0.98	26/5390 (0.5%)
1	I	0.34	0/4007	0.98	26/5390 (0.5%)
1	J	0.34	0/4007	0.98	26/5390 (0.5%)
1	K	0.34	0/4007	0.98	26/5390 (0.5%)
1	L	0.34	0/4007	0.98	26/5390 (0.5%)
1	M	0.34	0/4007	0.98	26/5390 (0.5%)
1	N	0.34	0/4007	0.98	26/5390 (0.5%)
1	O	0.34	0/4007	0.98	26/5390 (0.5%)
1	P	0.34	0/4007	0.98	26/5390 (0.5%)
All	All	0.34	0/64112	0.98	417/86240 (0.5%)

There are no bond length outliers.

The worst 5 of 417 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	424	GLY	N-CA-C	-9.72	88.81	113.10
1	C	424	GLY	N-CA-C	-9.72	88.81	113.10
1	E	424	GLY	N-CA-C	-9.72	88.81	113.10
1	G	424	GLY	N-CA-C	-9.72	88.81	113.10
1	J	424	GLY	N-CA-C	-9.72	88.81	113.10

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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	3982	0	4119	772	0
1	B	3982	0	4119	774	0
1	C	3982	0	4119	773	0
1	D	3982	0	4119	775	0
1	E	3982	0	4119	770	0
1	F	3982	0	4119	774	0
1	G	3982	0	4119	772	0
1	H	3982	0	4119	786	0
1	I	3982	0	4119	782	0
1	J	3982	0	4119	768	0
1	K	3982	0	4119	774	0
1	L	3982	0	4119	773	0
1	M	3982	0	4119	775	0
1	N	3982	0	4119	769	0
1	O	3982	0	4119	775	0
1	P	3982	0	4119	770	0
All	All	63712	0	65904	11149	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 86.

The worst 5 of 11149 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:A:144:ALA:HB2	1:A:400:ILE:HG13	1.30	1.14
1:P:144:ALA:HB2	1:P:400:ILE:HG13	1.30	1.14
1:C:144:ALA:HB2	1:C:400:ILE:HG13	1.30	1.14
1:N:144:ALA:HB2	1:N:400:ILE:HG13	1.30	1.13
1:C:277:LYS:HG3	1:C:301:GLU:HB3	1.31	1.13

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	530/543 (98%)	365 (69%)	91 (17%)	74 (14%)	0	6
1	B	530/543 (98%)	364 (69%)	93 (18%)	73 (14%)	0	6
1	C	530/543 (98%)	365 (69%)	92 (17%)	73 (14%)	0	6
1	D	530/543 (98%)	365 (69%)	92 (17%)	73 (14%)	0	6
1	E	530/543 (98%)	365 (69%)	92 (17%)	73 (14%)	0	6
1	F	530/543 (98%)	365 (69%)	92 (17%)	73 (14%)	0	6
1	G	530/543 (98%)	365 (69%)	92 (17%)	73 (14%)	0	6
1	H	530/543 (98%)	365 (69%)	92 (17%)	73 (14%)	0	6
1	I	530/543 (98%)	365 (69%)	92 (17%)	73 (14%)	0	6
1	J	530/543 (98%)	365 (69%)	92 (17%)	73 (14%)	0	6
1	K	530/543 (98%)	365 (69%)	92 (17%)	73 (14%)	0	6
1	L	530/543 (98%)	365 (69%)	92 (17%)	73 (14%)	0	6
1	M	530/543 (98%)	365 (69%)	92 (17%)	73 (14%)	0	6
1	N	530/543 (98%)	365 (69%)	92 (17%)	73 (14%)	0	6
1	O	530/543 (98%)	365 (69%)	92 (17%)	73 (14%)	0	6
1	P	530/543 (98%)	365 (69%)	92 (17%)	73 (14%)	0	6
All	All	8480/8688 (98%)	5839 (69%)	1472 (17%)	1169 (14%)	1	6

5 of 1169 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	5	PRO
1	A	7	VAL
1	A	9	PRO
1	A	12	MET
1	A	45	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	427/434 (98%)	333 (78%)	94 (22%)	1	10
1	B	427/434 (98%)	331 (78%)	96 (22%)	1	10
1	C	427/434 (98%)	332 (78%)	95 (22%)	1	10
1	D	427/434 (98%)	332 (78%)	95 (22%)	1	10
1	E	427/434 (98%)	332 (78%)	95 (22%)	1	10
1	F	427/434 (98%)	332 (78%)	95 (22%)	1	10
1	G	427/434 (98%)	332 (78%)	95 (22%)	1	10
1	H	427/434 (98%)	332 (78%)	95 (22%)	1	10
1	I	427/434 (98%)	332 (78%)	95 (22%)	1	10
1	J	427/434 (98%)	333 (78%)	94 (22%)	1	10
1	K	427/434 (98%)	332 (78%)	95 (22%)	1	10
1	L	427/434 (98%)	333 (78%)	94 (22%)	1	10
1	M	427/434 (98%)	332 (78%)	95 (22%)	1	10
1	N	427/434 (98%)	333 (78%)	94 (22%)	1	10
1	O	427/434 (98%)	332 (78%)	95 (22%)	1	10
1	P	427/434 (98%)	333 (78%)	94 (22%)	1	10
All	All	6832/6944 (98%)	5316 (78%)	1516 (22%)	4	10

5 of 1516 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	H	110	LEU
1	I	514	ASP
1	O	412	SER
1	H	213	LEU
1	I	47	MET

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 191 such sidechains are listed below:

Mol	Chain	Res	Type
1	H	85	GLN
1	I	497	GLN
1	O	468	ASN
1	H	222	GLN
1	I	4	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.