



wwPDB EM Map/Model Validation Report ⓘ

Apr 10, 2016 – 01:52 PM BST

PDB ID : 3J1B
EMDB ID: : EMD-5391
Title : Cryo-EM structure of 8-fold symmetric rATcpn-alpha in apo state
Authors : Zhang, K.; Wang, L.; Liu, Y.X.; Wang, X.; Gao, B.; Hu, Z.J.; Ji, G.; Chan, K.Y.; Schulten, K.; Dong, Z.Y.; Sun, F.
Deposited on : 2012-02-06
Resolution : 4.90 Å(reported)
Based on PDB ID : 3KO1

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>

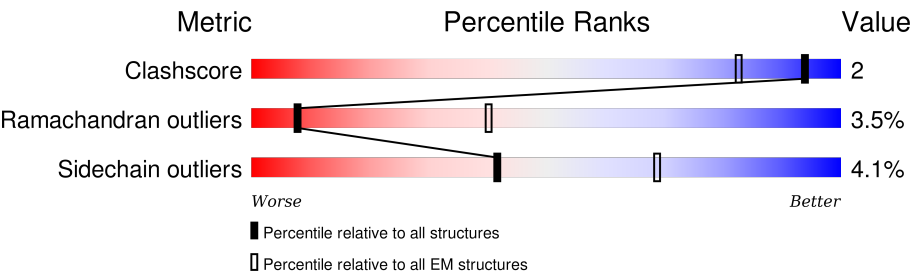
MolProbity : 4.02b-467
Mogul : unknown
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : trunk27241

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 4.90 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 ≥ 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	563	<div><div>68%</div><div>20%</div><div>• • 8%</div></div>
1	B	563	<div><div>70%</div><div>18%</div><div>• • 8%</div></div>
1	C	563	<div><div>70%</div><div>17%</div><div>• • 8%</div></div>
1	D	563	<div><div>66%</div><div>22%</div><div>• • 8%</div></div>
1	E	563	<div><div>68%</div><div>19%</div><div>• • 8%</div></div>
1	F	563	<div><div>71%</div><div>18%</div><div>• • 8%</div></div>
1	G	563	<div><div>65%</div><div>22%</div><div>• 8%</div></div>
1	H	563	<div><div>69%</div><div>19%</div><div>• • 8%</div></div>
1	I	563	<div><div>70%</div><div>18%</div><div>• • 8%</div></div>

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Mol	Chain	Length	Quality of chain
1	J	563	<div><div></div><div>67%</div><div>20%</div><div>5%</div><div>8%</div></div>
1	K	563	<div><div></div><div>67%</div><div>21%</div><div>•</div><div>8%</div></div>
1	L	563	<div><div></div><div>68%</div><div>20%</div><div>• •</div><div>8%</div></div>
1	M	563	<div><div></div><div>67%</div><div>20%</div><div>5%</div><div>•</div><div>8%</div></div>
1	N	563	<div><div></div><div>68%</div><div>19%</div><div>• •</div><div>8%</div></div>
1	O	563	<div><div></div><div>69%</div><div>17%</div><div>5%</div><div>•</div><div>8%</div></div>
1	P	563	<div><div></div><div>69%</div><div>20%</div><div>• •</div><div>8%</div></div>

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 62992 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.

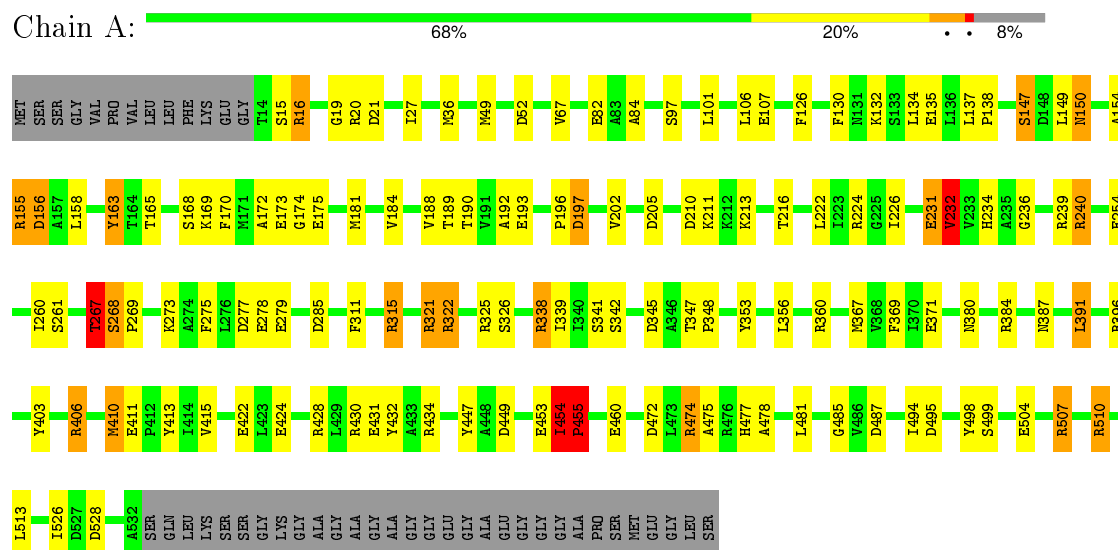
- Molecule 1 is a protein called Chaperonin alpha subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	519	Total	C	N	O	S	0	0
			3937	2475	673	773	16		
1	B	519	Total	C	N	O	S	0	0
			3937	2475	673	773	16		
1	C	519	Total	C	N	O	S	0	0
			3937	2475	673	773	16		
1	D	519	Total	C	N	O	S	0	0
			3937	2475	673	773	16		
1	E	519	Total	C	N	O	S	0	0
			3937	2475	673	773	16		
1	F	519	Total	C	N	O	S	0	0
			3937	2475	673	773	16		
1	G	519	Total	C	N	O	S	0	0
			3937	2475	673	773	16		
1	H	519	Total	C	N	O	S	0	0
			3937	2475	673	773	16		
1	I	519	Total	C	N	O	S	0	0
			3937	2475	673	773	16		
1	J	519	Total	C	N	O	S	0	0
			3937	2475	673	773	16		
1	K	519	Total	C	N	O	S	0	0
			3937	2475	673	773	16		
1	L	519	Total	C	N	O	S	0	0
			3937	2475	673	773	16		
1	M	519	Total	C	N	O	S	0	0
			3937	2475	673	773	16		
1	N	519	Total	C	N	O	S	0	0
			3937	2475	673	773	16		
1	O	519	Total	C	N	O	S	0	0
			3937	2475	673	773	16		
1	P	519	Total	C	N	O	S	0	0
			3937	2475	673	773	16		

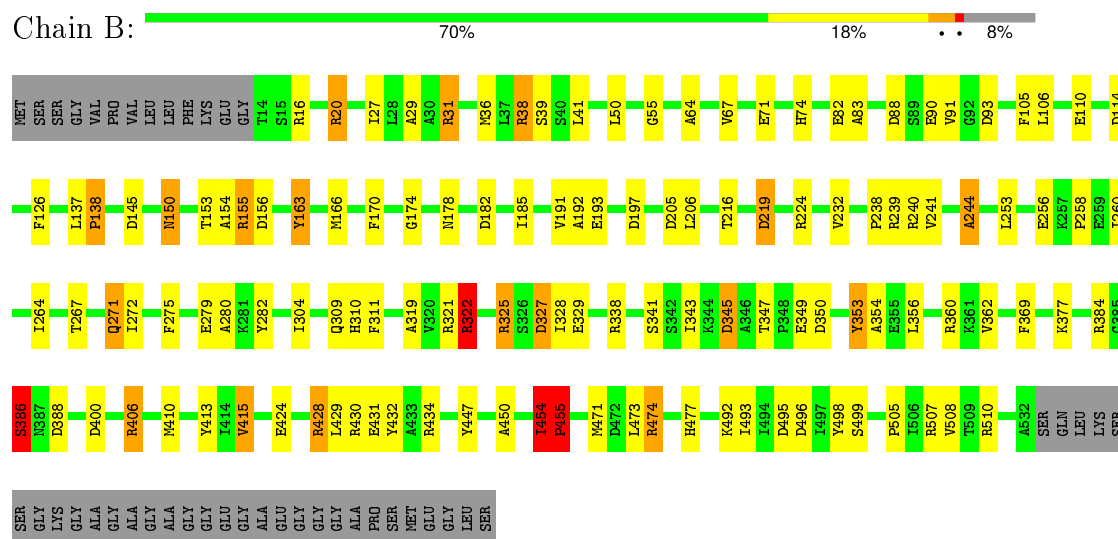
3 Residue-property plots

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 alpha subunit

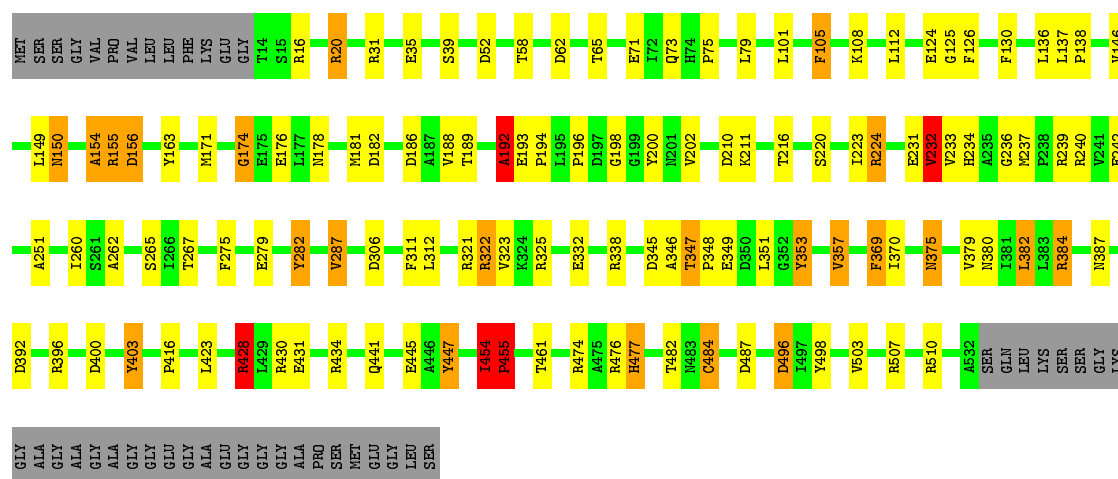


• Molecule 1: Chaperonin alpha subunit



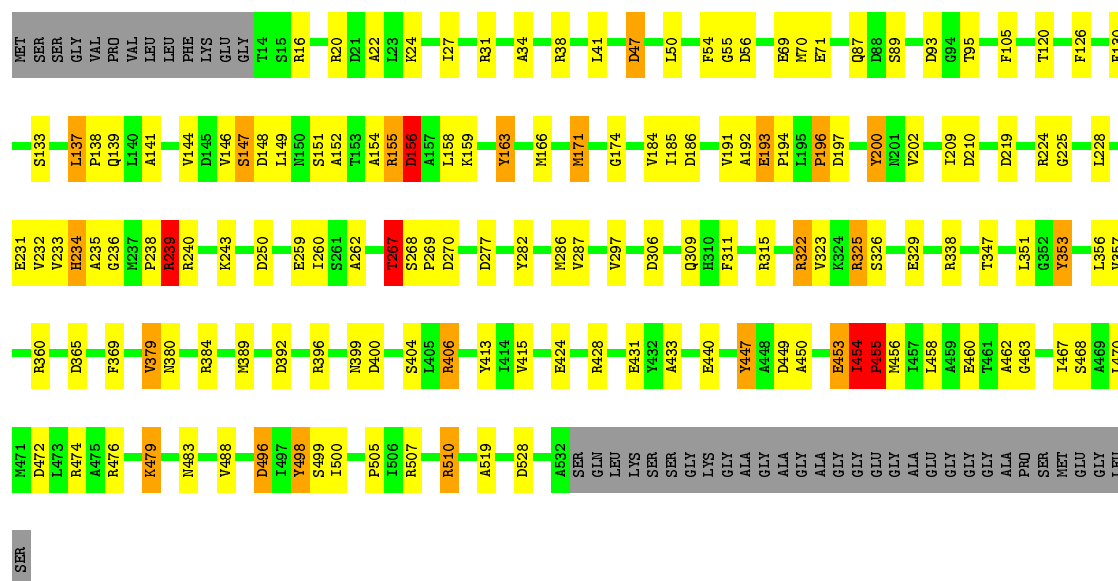
• Molecule 1: Chaperonin alpha subunit





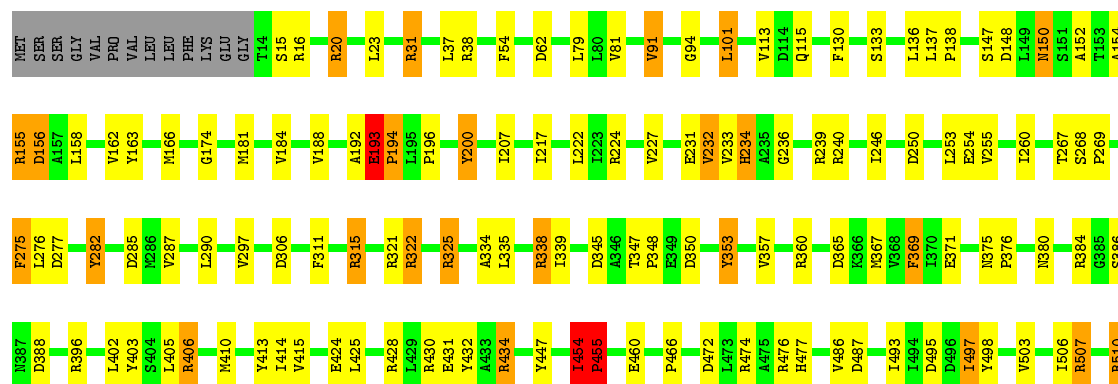
• Molecule 1: Chaperonin alpha subunit

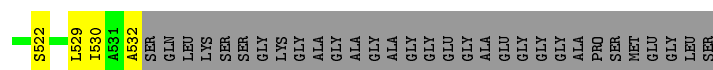
Chain D: 66% 22% 8%



• Molecule 1: Chaperonin alpha subunit

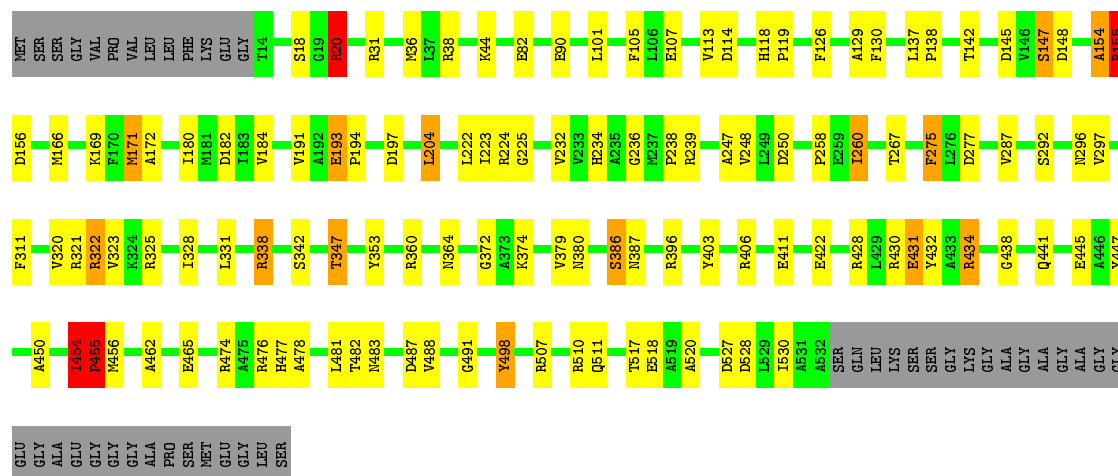
Chain E: 68% 19% 8%





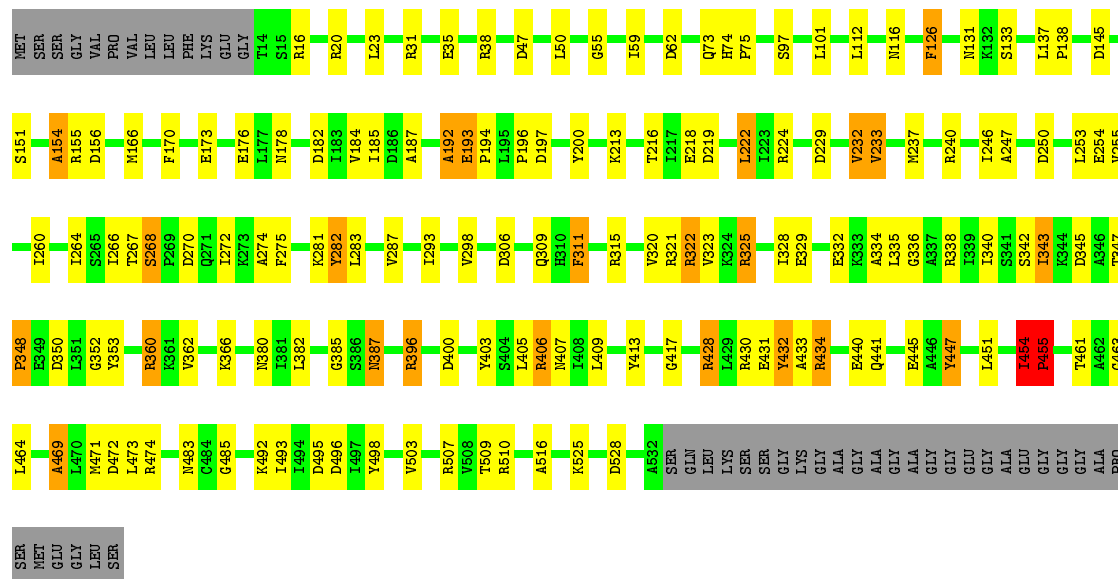
• Molecule 1: Chaperonin alpha subunit

Chain F: 71% 18% 8%



• Molecule 1: Chaperonin alpha subunit

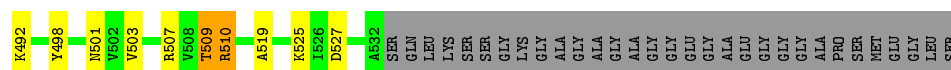
Chain G: 65% 22% 8%



• Molecule 1: Chaperonin alpha subunit

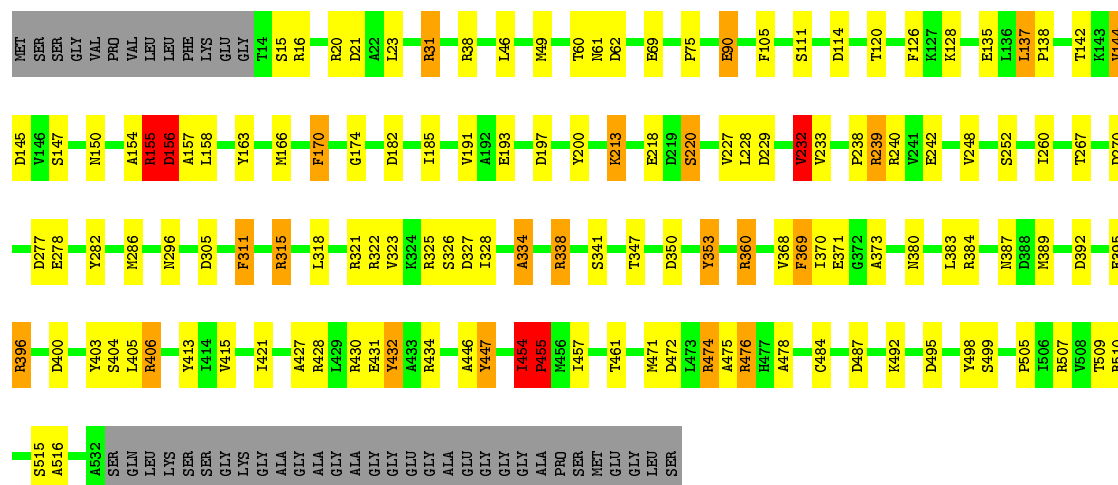
Chain H: 69% 19% 8%





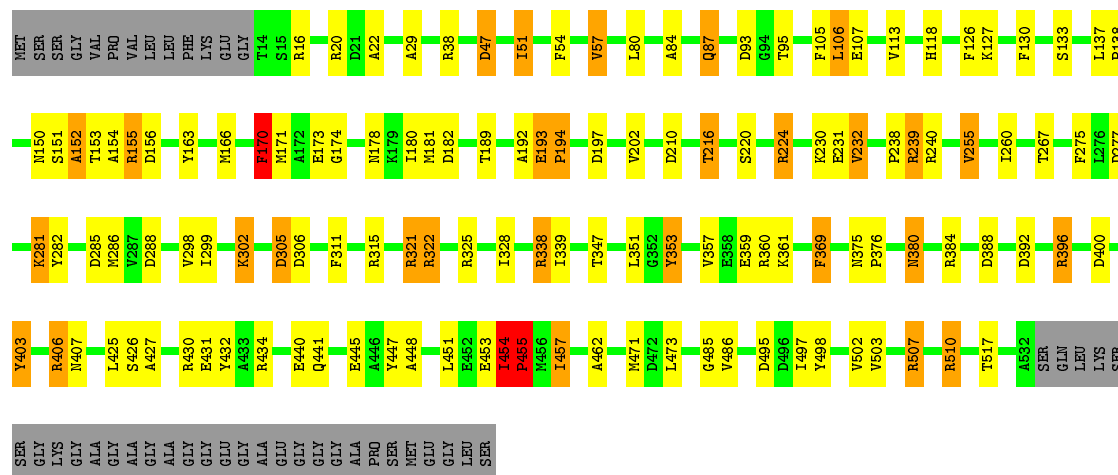
• Molecule 1: Chaperonin alpha subunit

Chain N: 68% 19% 8%



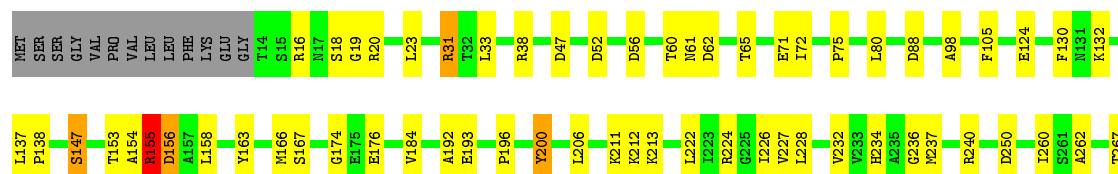
• Molecule 1: Chaperonin alpha subunit

Chain O: 69% 17% 5% 8%



• Molecule 1: Chaperonin alpha subunit

Chain P: 69% 20% 8%



GLN	P412	D270
LEU	Y413	D277
LYS	L423	E278
SER		E279
SER		R280
GLY	R428	R281
LYS	L429	Y282
GLY	R430	
ALA	E431	D288
GLY		K289
ALA	E440	V297
GLY	L441	F311
GLY	L442	
GLY	Y447	R315
GLY	A448	R321
GLU	D449	R322
GLY		E332
ALA	T454	R338
GLU	P455	I343
GLY	N456	T347
GLY		F348
GLY	A459	L356
ALA	E460	R360
PRO		K361
SER	G463	V362
SER		D365
NET	P466	F369
GLU		I370
LEU	L470	A373
GLY	Y471	V379
SER	D472	N380
GLY	L473	L383
ALA	R474	R384
ALA	A475	G385
ALA	R476	S386
		K389
	L494	E393
	D495	Y403
	D496	
	L497	R406
	Y498	
	S499	
	I500	
	V503	
	R507	
	R510	
	E518	
	A519	
	K525	
	I526	
	D627	
	A532	
	S532	

4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of images	55460	Depositor
Resolution determination method	Not provided	Depositor
CTF correction method	The whole micrograph	Depositor
Microscope	FEI Titan Krios	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	20	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	3500	Depositor
Magnification	96000	Depositor
Image detector	Gatan Ultrascan 4000 Model 895	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	1.60	20/3974 (0.5%)	1.93	83/5360 (1.5%)
1	B	1.59	17/3974 (0.4%)	1.98	94/5360 (1.8%)
1	C	1.55	16/3974 (0.4%)	1.93	90/5360 (1.7%)
1	D	1.57	21/3974 (0.5%)	2.00	116/5360 (2.2%)
1	E	1.53	12/3974 (0.3%)	2.05	103/5360 (1.9%)
1	F	1.57	17/3974 (0.4%)	1.99	95/5360 (1.8%)
1	G	1.57	20/3974 (0.5%)	2.01	101/5360 (1.9%)
1	H	1.58	19/3974 (0.5%)	1.97	95/5360 (1.8%)
1	I	1.56	22/3974 (0.6%)	1.94	80/5360 (1.5%)
1	J	1.58	21/3974 (0.5%)	2.00	112/5360 (2.1%)
1	K	1.56	23/3974 (0.6%)	1.95	84/5360 (1.6%)
1	L	1.53	19/3974 (0.5%)	1.99	99/5360 (1.8%)
1	M	1.56	20/3974 (0.5%)	2.01	120/5360 (2.2%)
1	N	1.59	20/3974 (0.5%)	1.97	101/5360 (1.9%)
1	O	1.58	13/3974 (0.3%)	2.01	116/5360 (2.2%)
1	P	1.60	26/3974 (0.7%)	1.97	92/5360 (1.7%)
All	All	1.57	306/63584 (0.5%)	1.98	1581/85760 (1.8%)

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	20
1	B	0	21
1	C	0	21
1	D	0	19
1	E	0	24
1	F	0	15
1	G	0	25
1	H	0	19
1	I	0	23

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Mol	Chain	#Chirality outliers	#Planarity outliers
1	J	0	23
1	K	0	20
1	L	0	17
1	M	0	17
1	N	0	26
1	O	0	19
1	P	0	20
All	All	0	329

The worst 5 of 306 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	N	447	TYR	CE1-CZ	9.27	1.50	1.38
1	O	353	TYR	CG-CD1	8.65	1.50	1.39
1	D	326	SER	CA-CB	8.46	1.65	1.52
1	B	386	SER	CA-CB	8.39	1.65	1.52
1	F	491	GLY	CA-C	-8.08	1.39	1.51

The worst 5 of 1581 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	406	ARG	NE-CZ-NH1	-19.65	110.47	120.30
1	I	507	ARG	NE-CZ-NH2	19.50	130.05	120.30
1	L	430	ARG	NE-CZ-NH2	18.88	129.74	120.30
1	I	507	ARG	NE-CZ-NH1	-17.58	111.51	120.30
1	J	240	ARG	NE-CZ-NH2	17.26	128.93	120.30

There are no chirality outliers.

5 of 329 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	154	ALA	Peptide
1	A	16	ARG	Sidechain
1	A	163	TYR	Sidechain
1	A	193	GLU	Peptide
1	A	213	LYS	Peptide

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	3937	0	4104	12	0
1	B	3937	0	4104	14	0
1	C	3937	0	4104	12	0
1	D	3937	0	4104	8	0
1	E	3937	0	4104	18	0
1	F	3937	0	4104	13	0
1	G	3937	0	4104	20	0
1	H	3937	0	4104	11	0
1	I	3937	0	4104	8	0
1	J	3937	0	4104	13	0
1	K	3937	0	4104	14	0
1	L	3937	0	4104	15	0
1	M	3937	0	4104	15	0
1	N	3937	0	4104	13	0
1	O	3937	0	4104	15	0
1	P	3937	0	4104	10	0
All	All	62992	0	65664	207	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 207 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:454:ILE:HG22	1:K:455:PRO:HD2	1.67	0.77
1:K:232:VAL:HG11	1:K:368:VAL:HG21	1.72	0.72
1:L:343:ILE:HD12	1:L:343:ILE:H	1.56	0.69
1:J:87:GLN:HE21	1:J:91:VAL:HG22	1.60	0.66
1:F:454:ILE:HB	1:F:455:PRO:HD2	1.79	0.65

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	517/563 (92%)	468 (90%)	30 (6%)	19 (4%)	4	39
1	B	517/563 (92%)	468 (90%)	37 (7%)	12 (2%)	8	49
1	C	517/563 (92%)	470 (91%)	27 (5%)	20 (4%)	4	37
1	D	517/563 (92%)	455 (88%)	38 (7%)	24 (5%)	3	33
1	E	517/563 (92%)	472 (91%)	28 (5%)	17 (3%)	5	42
1	F	517/563 (92%)	466 (90%)	28 (5%)	23 (4%)	3	34
1	G	517/563 (92%)	470 (91%)	31 (6%)	16 (3%)	5	43
1	H	517/563 (92%)	459 (89%)	38 (7%)	20 (4%)	4	37
1	I	517/563 (92%)	462 (89%)	33 (6%)	22 (4%)	3	34
1	J	517/563 (92%)	464 (90%)	33 (6%)	20 (4%)	4	37
1	K	517/563 (92%)	467 (90%)	35 (7%)	15 (3%)	6	44
1	L	517/563 (92%)	471 (91%)	29 (6%)	17 (3%)	5	42
1	M	517/563 (92%)	460 (89%)	37 (7%)	20 (4%)	4	37
1	N	517/563 (92%)	470 (91%)	32 (6%)	15 (3%)	6	44
1	O	517/563 (92%)	465 (90%)	36 (7%)	16 (3%)	5	43
1	P	517/563 (92%)	464 (90%)	41 (8%)	12 (2%)	8	49
All	All	8272/9008 (92%)	7451 (90%)	533 (6%)	288 (4%)	8	40

5 of 288 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	150	ASN
1	A	155	ARG
1	A	322	ARG
1	A	387	ASN
1	A	455	PRO

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	427/453 (94%)	406 (95%)	21 (5%)	31	68
1	B	427/453 (94%)	405 (95%)	22 (5%)	29	67
1	C	427/453 (94%)	414 (97%)	13 (3%)	48	78
1	D	427/453 (94%)	401 (94%)	26 (6%)	23	62
1	E	427/453 (94%)	412 (96%)	15 (4%)	43	76
1	F	427/453 (94%)	417 (98%)	10 (2%)	58	83
1	G	427/453 (94%)	410 (96%)	17 (4%)	38	72
1	H	427/453 (94%)	411 (96%)	16 (4%)	41	74
1	I	427/453 (94%)	411 (96%)	16 (4%)	41	74
1	J	427/453 (94%)	412 (96%)	15 (4%)	43	76
1	K	427/453 (94%)	401 (94%)	26 (6%)	23	62
1	L	427/453 (94%)	406 (95%)	21 (5%)	31	68
1	M	427/453 (94%)	409 (96%)	18 (4%)	36	71
1	N	427/453 (94%)	413 (97%)	14 (3%)	45	77
1	O	427/453 (94%)	412 (96%)	15 (4%)	43	76
1	P	427/453 (94%)	414 (97%)	13 (3%)	48	78
All	All	6832/7248 (94%)	6554 (96%)	278 (4%)	42	72

5 of 278 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	H	39	SER
1	I	495	ASP
1	O	281	LYS
1	H	275	PHE
1	I	170	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 38 such sidechains are listed below:

Mol	Chain	Res	Type
1	E	477	HIS
1	G	477	HIS
1	O	477	HIS
1	F	234	HIS
1	H	234	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 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.