



wwPDB/EMDatabank EM Map/Model Validation Summary Report ⓘ

Aug 17, 2017 – 07:04 PM EDT

PDB ID : 4AAS
EMDB ID: : EMD-2000
Title : ATP-triggered molecular mechanics of the chaperonin GroEL
Authors : Clare, D.K.; Vasishtan, D.; Stagg, S.; Quispe, J.; Farr, G.W.; Topf, M.; Horwich, A.L.; Saibil, H.R.
Deposited on : unknown
Resolution : 8.50 Å(reported)
Based on PDB ID : 1OEL

This is a wwPDB/EMDatabank EM Map/Model Validation Summary Report
for a publicly released PDB/EMDB entry.

We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

MolProbity : 4.02b-467
Mogul : 1.7.2 (RC1), CSD as538be (2017)
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20029824

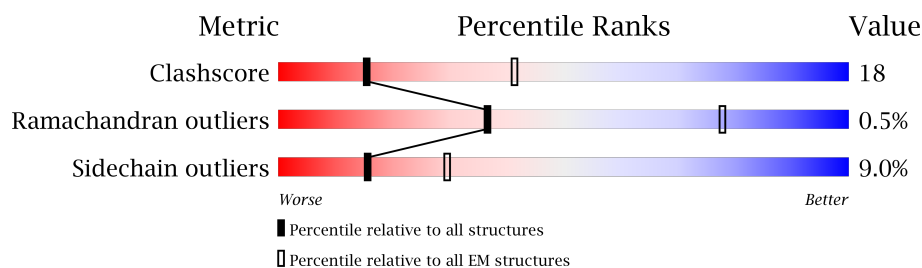
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 8.50 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	125131	1336
Ramachandran outliers	121729	1120
Sidechain outliers	121581	1026

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	548	
1	B	548	
1	C	548	
1	D	548	
1	E	548	
1	F	548	
1	G	548	
1	H	548	
1	I	548	

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Mol	Chain	Length	Quality of chain
1	J	548	
1	K	548	
1	L	548	
1	M	548	
1	N	548	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	PO4	A	1525	-	-	X	-
2	PO4	B	1525	-	-	X	-
2	PO4	C	1525	-	-	X	-
2	PO4	D	1525	-	-	X	-
2	PO4	E	1525	-	-	X	-
2	PO4	F	1525	-	-	X	-
2	PO4	G	1525	-	-	X	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 54062 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 60 KDA CHAPERONIN.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	524	Total	C	N	O	S	0	1
			3846	2391	665	770	20		
1	B	524	Total	C	N	O	S	0	1
			3845	2391	664	770	20		
1	C	524	Total	C	N	O	S	0	1
			3845	2391	664	770	20		
1	D	524	Total	C	N	O	S	0	1
			3845	2391	664	770	20		
1	E	524	Total	C	N	O	S	0	1
			3845	2391	664	770	20		
1	F	524	Total	C	N	O	S	0	1
			3845	2391	664	770	20		
1	G	524	Total	C	N	O	S	0	1
			3845	2391	664	770	20		
1	H	524	Total	C	N	O	S	0	1
			3845	2391	664	770	20		
1	I	524	Total	C	N	O	S	0	1
			3845	2391	664	770	20		
1	J	524	Total	C	N	O	S	0	1
			3845	2391	664	770	20		
1	K	524	Total	C	N	O	S	0	1
			3845	2391	664	770	20		
1	L	524	Total	C	N	O	S	0	1
			3845	2391	664	770	20		
1	M	524	Total	C	N	O	S	0	1
			3845	2391	664	770	20		
1	N	524	Total	C	N	O	S	0	1
			3845	2391	664	770	20		

There are 14 discrepancies between the modelled and reference sequences:

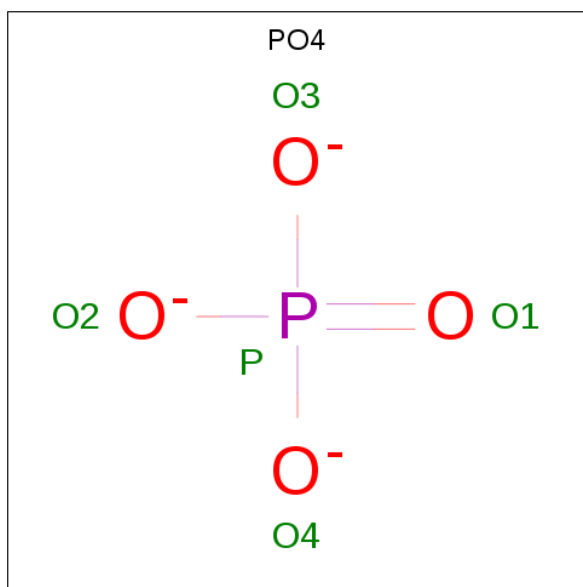
Chain	Residue	Modelled	Actual	Comment	Reference
A	398	ALA	ASP	engineered mutation	UNP P0A6F5
B	398	ALA	ASP	engineered mutation	UNP P0A6F5

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Chain	Residue	Modelled	Actual	Comment	Reference
C	398	ALA	ASP	engineered mutation	UNP P0A6F5
D	398	ALA	ASP	engineered mutation	UNP P0A6F5
E	398	ALA	ASP	engineered mutation	UNP P0A6F5
F	398	ALA	ASP	engineered mutation	UNP P0A6F5
G	398	ALA	ASP	engineered mutation	UNP P0A6F5
H	398	ALA	ASP	engineered mutation	UNP P0A6F5
I	398	ALA	ASP	engineered mutation	UNP P0A6F5
J	398	ALA	ASP	engineered mutation	UNP P0A6F5
K	398	ALA	ASP	engineered mutation	UNP P0A6F5
L	398	ALA	ASP	engineered mutation	UNP P0A6F5
M	398	ALA	ASP	engineered mutation	UNP P0A6F5
N	398	ALA	ASP	engineered mutation	UNP P0A6F5

- Molecule 2 is PHOSPHATE ION (three-letter code: PO4) (formula: O₄P).



Mol	Chain	Residues	Atoms	AltConf
2	A	1	Total P 1 1	0
2	B	1	Total P 1 1	0
2	C	1	Total P 1 1	0
2	D	1	Total P 1 1	0
2	E	1	Total P 1 1	0

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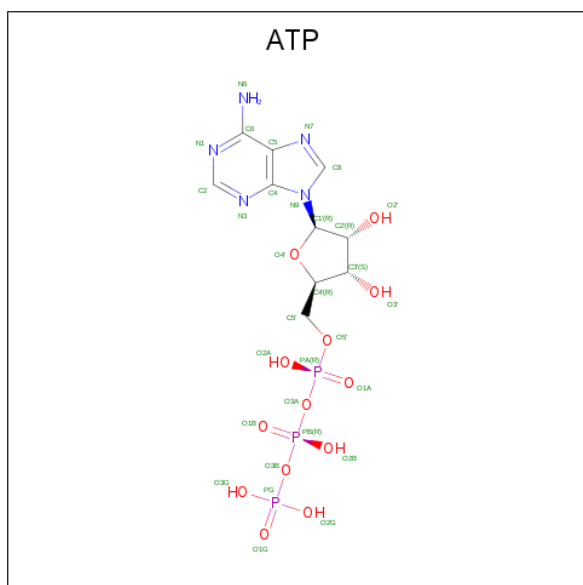
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Mol	Chain	Residues	Atoms		AltConf
2	F	1	Total	P	0
			1	1	
2	G	1	Total	P	0
			1	1	

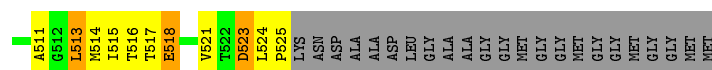
- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
3	G	1	Total	Mg	0
			1	1	
3	D	1	Total	Mg	0
			1	1	
3	E	1	Total	Mg	0
			1	1	
3	B	1	Total	Mg	0
			1	1	
3	C	1	Total	Mg	0
			1	1	
3	A	1	Total	Mg	0
			1	1	
3	F	1	Total	Mg	0
			1	1	

- Molecule 4 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).

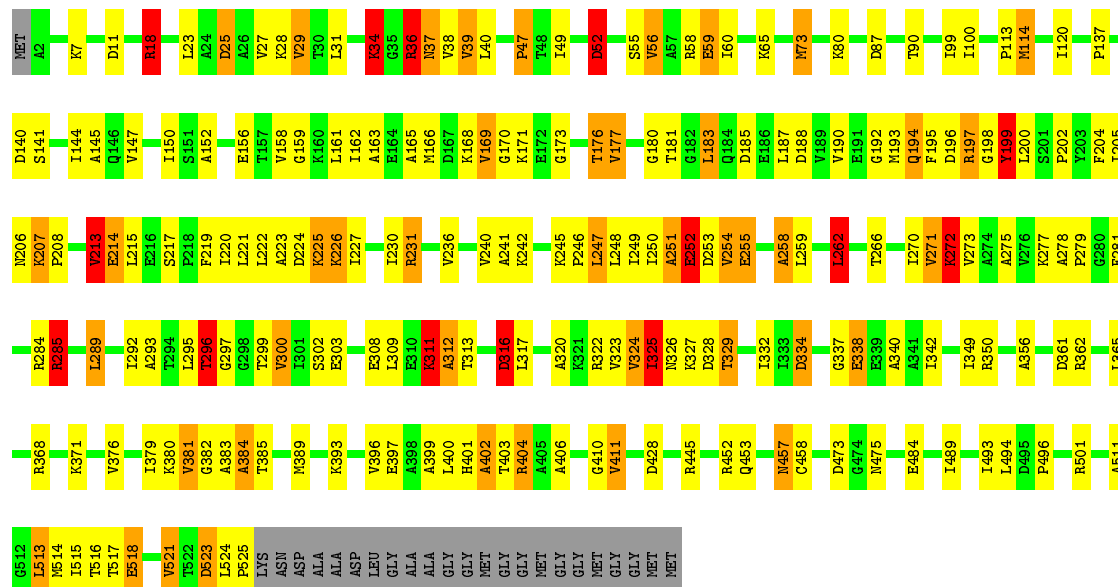


Mol	Chain	Residues	Atoms					AltConf
4	A	1	Total 31	C 10	N 5	O 13	P 3	0
4	B	1	Total 31	C 10	N 5	O 13	P 3	0
4	C	1	Total 31	C 10	N 5	O 13	P 3	0
4	D	1	Total 31	C 10	N 5	O 13	P 3	0
4	E	1	Total 31	C 10	N 5	O 13	P 3	0
4	F	1	Total 31	C 10	N 5	O 13	P 3	0
4	G	1	Total 31	C 10	N 5	O 13	P 3	0



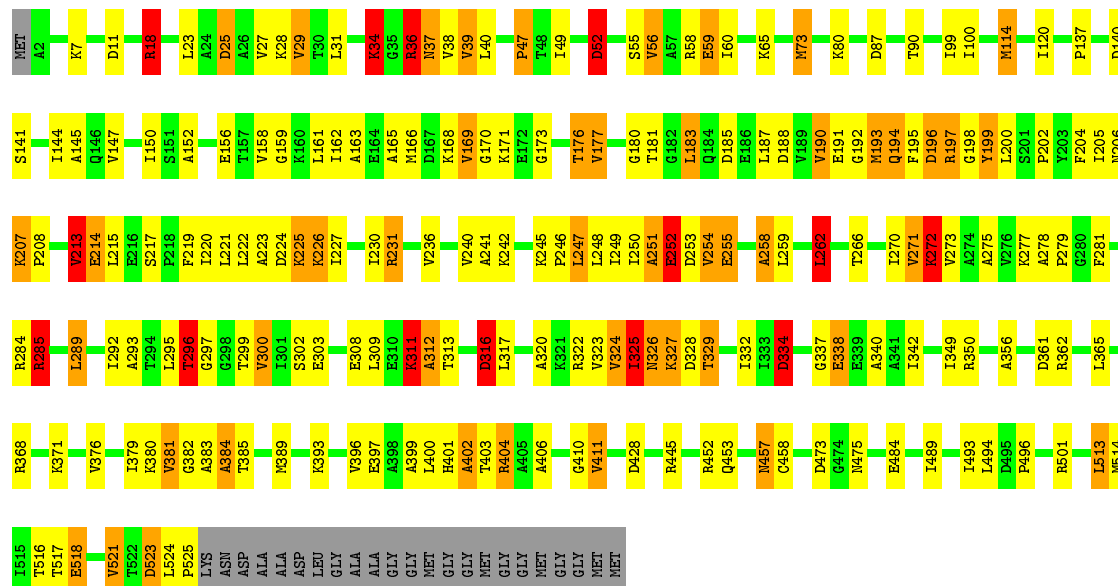
● Molecule 1: 60 KDA CHAPERONIN

Chain C:  57% 28% 8% . .



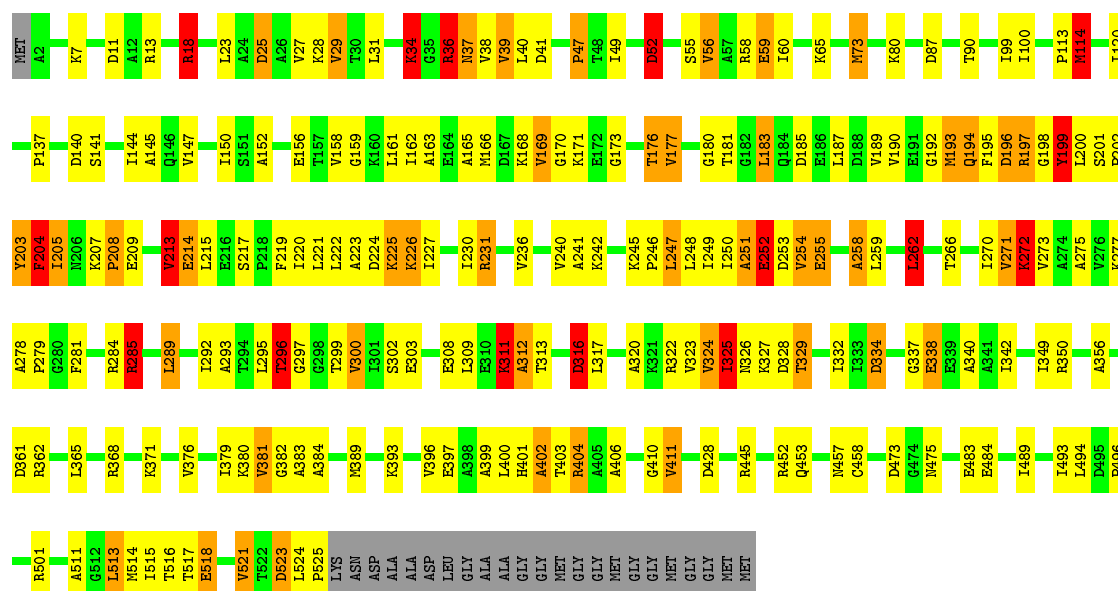
- Molecule 1: 60 KDA CHAPERONIN

Chain D: 58% 26% 9% . .



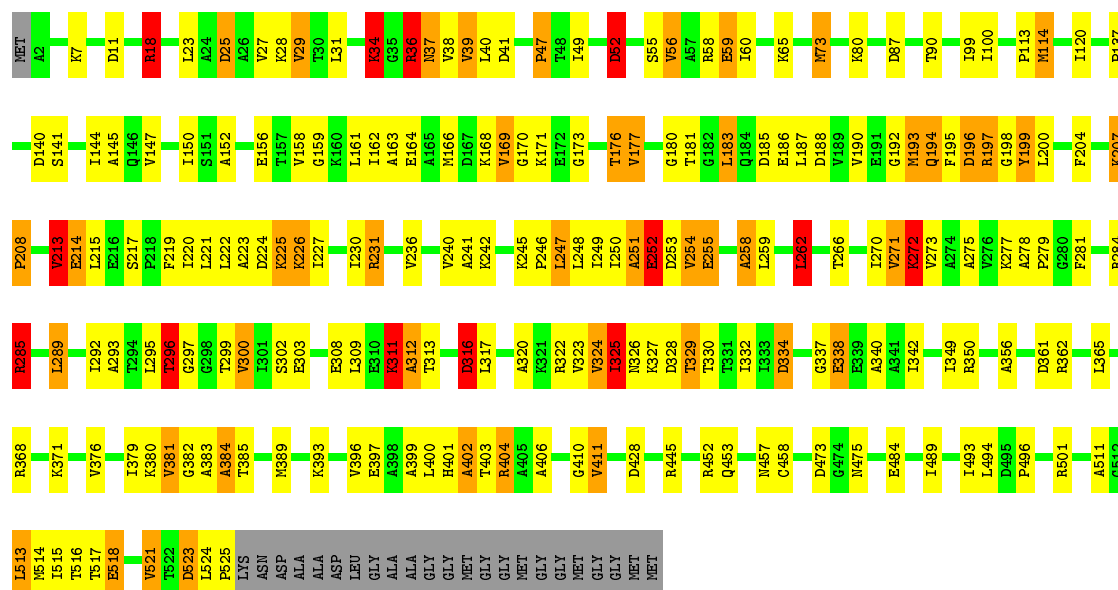
- Molecule 1: 60 KDA CHAPERONIN

Chain E: 57% 28% 8% . .



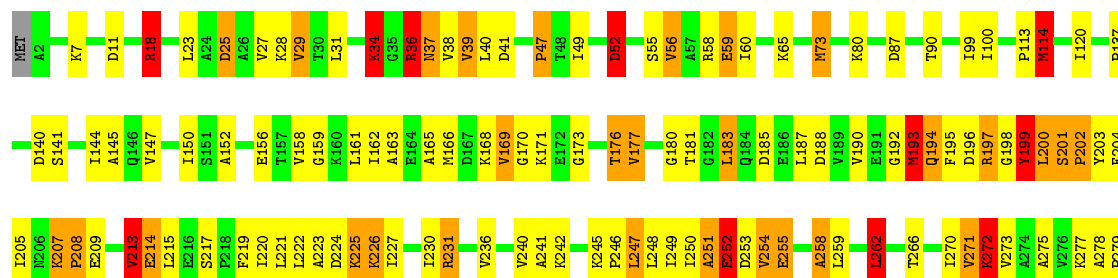
• Molecule 1: 60 KDA CHAPERONIN

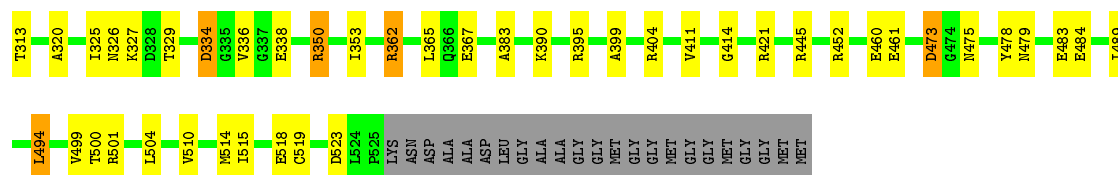
Chain F: 57% 27% 8%



• Molecule 1: 60 KDA CHAPERONIN

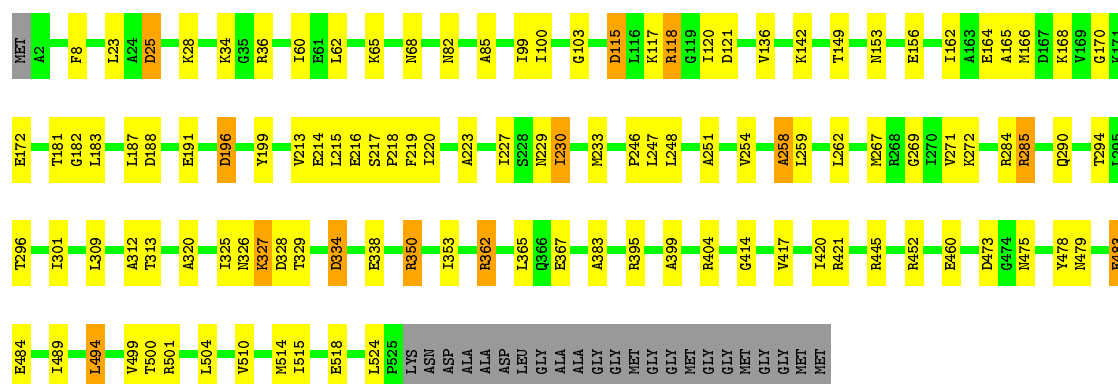
Chain G: 57% 28% 8%





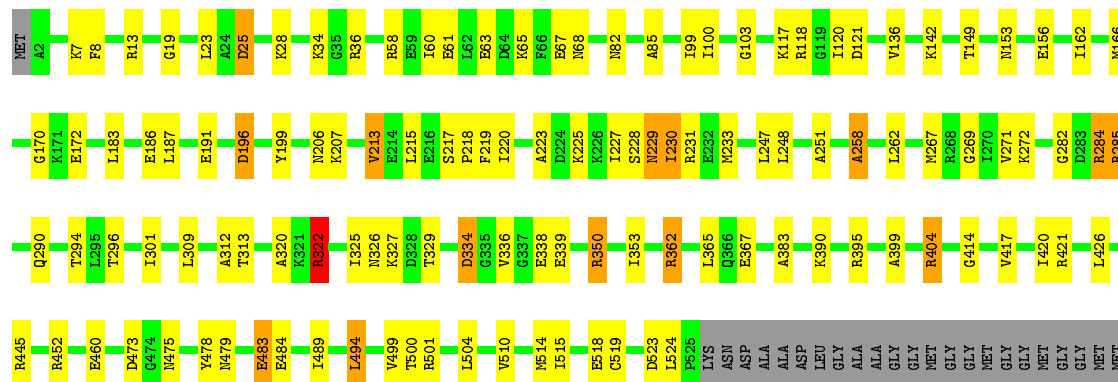
• Molecule 1: 60 KDA CHAPERONIN

Chain K: 75% 19%



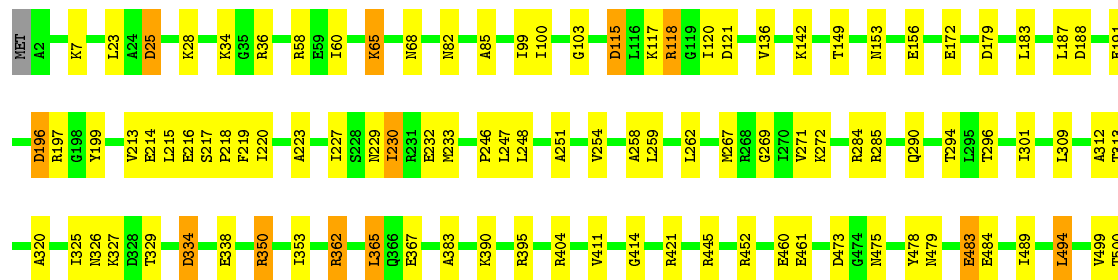
• Molecule 1: 60 KDA CHAPERONIN

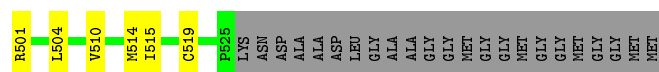
Chain L: 73% 20%



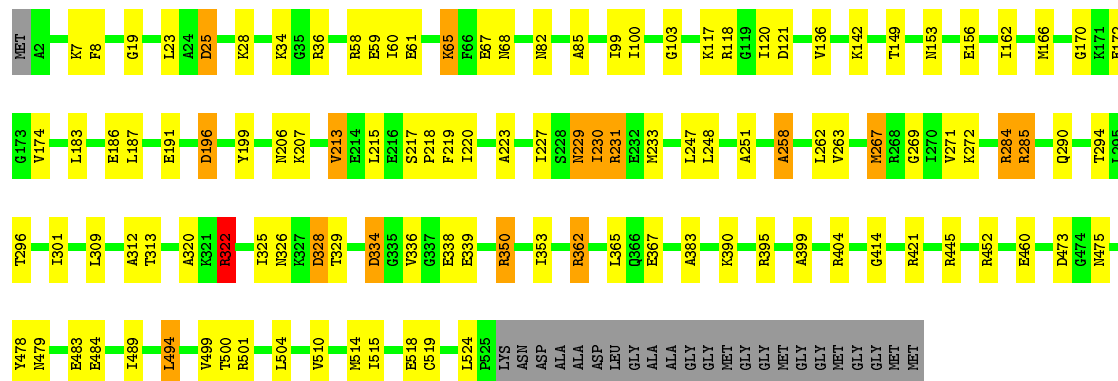
• Molecule 1: 60 KDA CHAPERONIN

Chain M: 76% 18%





- Molecule 1: 60 KDA CHAPERONIN



4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C7	Depositor
Number of particles used	5500	Depositor
Resolution determination method	Not provided	Depositor
CTF correction method	EACH PARTICLE WAS PHASE FLIPPED	Depositor
Microscope	FEI TECNAI F20	Depositor
Voltage (kV)	120	Depositor
Electron dose ($e^-/\text{\AA}^2$)	15	Depositor
Minimum defocus (nm)	700	Depositor
Maximum defocus (nm)	3500	Depositor
Magnification	148500	Depositor
Image detector	GATAN ULTRASCAN 4000 (4k x 4k)	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: PO4, MG, ATP

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	0.85	6/3873 (0.2%)	1.48	76/5229 (1.5%)
1	B	0.86	7/3872 (0.2%)	1.49	78/5227 (1.5%)
1	C	0.86	7/3872 (0.2%)	1.49	78/5227 (1.5%)
1	D	0.86	7/3872 (0.2%)	1.50	78/5227 (1.5%)
1	E	0.86	7/3872 (0.2%)	1.50	81/5227 (1.5%)
1	F	0.86	7/3872 (0.2%)	1.49	79/5227 (1.5%)
1	G	0.86	7/3872 (0.2%)	1.50	84/5227 (1.6%)
1	H	0.66	0/3872	1.08	21/5227 (0.4%)
1	I	0.67	0/3872	1.07	19/5227 (0.4%)
1	J	0.66	0/3872	1.09	26/5227 (0.5%)
1	K	0.66	0/3872	1.08	19/5227 (0.4%)
1	L	0.67	0/3872	1.11	28/5227 (0.5%)
1	M	0.66	0/3872	1.09	21/5227 (0.4%)
1	N	0.67	0/3872	1.09	25/5227 (0.5%)
All	All	0.77	48/54209 (0.1%)	1.30	713/73180 (1.0%)

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	18
1	B	0	16
1	C	0	15
1	D	0	17
1	E	0	18
1	F	0	17
1	G	0	16
1	H	0	5
1	I	0	7

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Mol	Chain	#Chirality outliers	#Planarity outliers
1	J	0	8
1	K	0	6
1	L	0	6
1	M	0	6
1	N	0	9
All	All	0	164

The worst 5 of 48 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	7	LYS	C-N	-11.63	1.07	1.34
1	C	7	LYS	C-N	-11.63	1.07	1.34
1	A	7	LYS	C-N	-11.63	1.07	1.34
1	G	7	LYS	C-N	-11.62	1.07	1.34
1	E	7	LYS	C-N	-11.62	1.07	1.34

The worst 5 of 713 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	M	267	MET	CG-SD-CE	12.87	120.79	100.20
1	I	267	MET	CG-SD-CE	12.81	120.70	100.20
1	N	267	MET	CG-SD-CE	12.80	120.68	100.20
1	L	267	MET	CG-SD-CE	12.78	120.65	100.20
1	H	267	MET	CG-SD-CE	12.74	120.59	100.20

There are no chirality outliers.

5 of 164 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	13	ARG	Sidechain
1	A	18	ARG	Sidechain
1	A	193	MET	Mainchain
1	A	29	VAL	Mainchain
1	A	52	ASP	Mainchain

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	3846	0	3967	230	0
1	B	3845	0	3962	237	0
1	C	3845	0	3962	239	0
1	D	3845	0	3962	233	0
1	E	3845	0	3962	240	0
1	F	3845	0	3962	238	0
1	G	3845	0	3962	243	0
1	H	3845	0	3966	70	0
1	I	3845	0	3966	67	0
1	J	3845	0	3966	60	0
1	K	3845	0	3966	80	0
1	L	3845	0	3966	72	0
1	M	3845	0	3966	70	0
1	N	3845	0	3966	61	0
2	A	1	0	0	3	0
2	B	1	0	0	3	0
2	C	1	0	0	3	0
2	D	1	0	0	3	0
2	E	1	0	0	3	0
2	F	1	0	0	3	0
2	G	1	0	0	3	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
3	E	1	0	0	0	0
3	F	1	0	0	0	0
3	G	1	0	0	0	0
4	A	31	0	12	3	0
4	B	31	0	12	3	0
4	C	31	0	12	3	0
4	D	31	0	12	3	0
4	E	31	0	12	3	0
4	F	31	0	12	3	0
4	G	31	0	12	3	0
All	All	54062	0	55585	2024	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 18.

The worst 5 of 2024 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:E:200:LEU:CD2	1:E:254:VAL:HG21	1.33	1.39
1:A:200:LEU:CD2	1:A:254:VAL:HG21	1.33	1.39
1:F:200:LEU:CD2	1:F:254:VAL:HG21	1.33	1.38
1:B:200:LEU:CD2	1:B:254:VAL:HG21	1.33	1.38
1:C:200:LEU:CD2	1:C:254:VAL:HG21	1.33	1.37

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	522/548 (95%)	496 (95%)	23 (4%)	3 (1%)	28	71
1	B	522/548 (95%)	495 (95%)	23 (4%)	4 (1%)	22	67
1	C	522/548 (95%)	497 (95%)	22 (4%)	3 (1%)	28	71
1	D	522/548 (95%)	498 (95%)	22 (4%)	2 (0%)	38	77
1	E	522/548 (95%)	494 (95%)	23 (4%)	5 (1%)	18	61
1	F	522/548 (95%)	495 (95%)	24 (5%)	3 (1%)	28	71
1	G	522/548 (95%)	494 (95%)	23 (4%)	5 (1%)	18	61
1	H	522/548 (95%)	496 (95%)	24 (5%)	2 (0%)	38	77
1	I	522/548 (95%)	498 (95%)	22 (4%)	2 (0%)	38	77
1	J	522/548 (95%)	497 (95%)	23 (4%)	2 (0%)	38	77
1	K	522/548 (95%)	497 (95%)	24 (5%)	1 (0%)	51	84
1	L	522/548 (95%)	497 (95%)	22 (4%)	3 (1%)	28	71
1	M	522/548 (95%)	497 (95%)	24 (5%)	1 (0%)	51	84
1	N	522/548 (95%)	498 (95%)	22 (4%)	2 (0%)	38	77
All	All	7308/7672 (95%)	6949 (95%)	321 (4%)	38 (0%)	37	74

5 of 38 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	199	TYR
1	E	205	ILE
1	G	199	TYR
1	A	384	ALA
1	B	384	ALA

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	402/414 (97%)	367 (91%)	35 (9%)	12	40
1	B	402/414 (97%)	364 (90%)	38 (10%)	10	36
1	C	402/414 (97%)	366 (91%)	36 (9%)	11	38
1	D	402/414 (97%)	365 (91%)	37 (9%)	11	37
1	E	402/414 (97%)	366 (91%)	36 (9%)	11	38
1	F	402/414 (97%)	366 (91%)	36 (9%)	11	38
1	G	402/414 (97%)	363 (90%)	39 (10%)	9	35
1	H	402/414 (97%)	369 (92%)	33 (8%)	13	43
1	I	402/414 (97%)	362 (90%)	40 (10%)	9	33
1	J	402/414 (97%)	365 (91%)	37 (9%)	11	37
1	K	402/414 (97%)	373 (93%)	29 (7%)	17	49
1	L	402/414 (97%)	365 (91%)	37 (9%)	11	37
1	M	402/414 (97%)	363 (90%)	39 (10%)	9	35
1	N	402/414 (97%)	367 (91%)	35 (9%)	12	40
All	All	5628/5796 (97%)	5121 (91%)	507 (9%)	16	38

5 of 507 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	G	183	LEU
1	H	460	GLU
1	M	494	LEU

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Mol	Chain	Res	Type
1	G	207	LYS
1	H	25	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 42 such sidechains are listed below:

Mol	Chain	Res	Type
1	F	37	ASN
1	G	194	GLN
1	M	326	ASN
1	F	194	GLN
1	F	475	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 ⓘ

Of 21 ligands modelled in this entry, 7 are modelled with single atom and 7 are monoatomic - leaving 7 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
4	ATP	A	1527	3	27,33,33	0.82	0	25,52,52	1.05	2 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	ATP	B	1527	3	27,33,33	0.82	0	25,52,52	1.06	2 (8%)
4	ATP	C	1527	3	27,33,33	0.82	0	25,52,52	1.06	2 (8%)
4	ATP	D	1527	3	27,33,33	0.83	0	25,52,52	1.06	1 (4%)
4	ATP	E	1527	3	27,33,33	0.83	0	25,52,52	1.05	2 (8%)
4	ATP	F	1527	3	27,33,33	0.82	0	25,52,52	1.06	2 (8%)
4	ATP	G	1527	3	27,33,33	0.82	0	25,52,52	1.06	2 (8%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	ATP	A	1527	3	-	0/18/38/38	0/3/3/3
4	ATP	B	1527	3	-	0/18/38/38	0/3/3/3
4	ATP	C	1527	3	-	0/18/38/38	0/3/3/3
4	ATP	D	1527	3	-	0/18/38/38	0/3/3/3
4	ATP	E	1527	3	-	0/18/38/38	0/3/3/3
4	ATP	F	1527	3	-	0/18/38/38	0/3/3/3
4	ATP	G	1527	3	-	0/18/38/38	0/3/3/3

There are no bond length outliers.

The worst 5 of 13 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	1527	ATP	C5-C6-N6	2.00	124.55	120.47
4	G	1527	ATP	C5-C6-N6	2.00	124.56	120.47
4	E	1527	ATP	C5-C6-N6	2.01	124.56	120.47
4	F	1527	ATP	C5-C6-N6	2.02	124.59	120.47
4	A	1527	ATP	C5-C6-N6	2.03	124.61	120.47

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

7 monomers are involved in 21 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1527	ATP	3	0
4	B	1527	ATP	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	1527	ATP	3	0
4	D	1527	ATP	3	0
4	E	1527	ATP	3	0
4	F	1527	ATP	3	0
4	G	1527	ATP	3	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	G	5
1	D	5
1	E	5
1	B	5
1	C	5
1	F	5
1	A	4

The worst 5 of 34 chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	52:ASP	C	53:GLY	N	1.20
1	B	52:ASP	C	53:GLY	N	1.20
1	C	52:ASP	C	53:GLY	N	1.20
1	D	52:ASP	C	53:GLY	N	1.20
1	E	52:ASP	C	53:GLY	N	1.20