



wwPDB EM Map/Model Validation Report ⓘ

Apr 10, 2016 – 02:06 PM BST

PDB ID : 3ZQ1
EMDB ID: : EMD-2327
Title : Visualizing GroEL-ES in the Act of Encapsulating a Non-Native Substrate Protein
Authors : Chen, D.-H.; Madan, D.; Weaver, J.; Lin, Z.; Schroder, G.F.; Chiu, W.; Rye, H.S.
Deposited on : 2013-03-04
Resolution : 15.90 Å(reported)
Based on PDB ID : 1AON

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 : 1.7.1 (RC1), CSD as537be (2016)
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

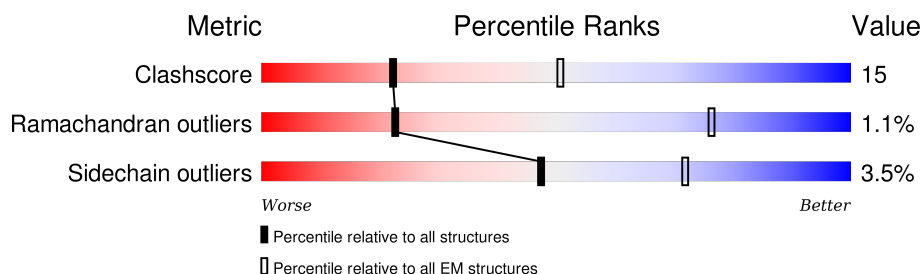
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 15.90 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	526	71% 26% .
1	B	526	71% 27% .
1	C	526	68% 29% .
1	D	526	68% 29% .
1	E	526	68% 30% .
1	F	526	69% 29% .
1	G	526	70% 28% .
1	H	526	70% 29% .
1	I	526	69% 29% .

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Mol	Chain	Length	Quality of chain
1	J	526	 67% 31% .
1	K	526	 67% 32% .
1	L	526	 69% 29% .
1	M	526	 66% 33% .
1	N	526	 68% 30% .
2	O	97	 64% 29% 7% .
2	P	97	 63% 28% 9% .
2	Q	97	 71% 27% .
2	R	97	 66% 28% 6% .
2	S	97	 67% 29% .
2	T	97	 69% 25% 6% .
2	U	97	 71% 26% .

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 59276 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	525	Total	C	N	O	S	0	1
			3856	2397	666	773	20		
1	B	525	Total	C	N	O	S	0	1
			3856	2397	666	773	20		
1	C	525	Total	C	N	O	S	0	1
			3856	2397	666	773	20		
1	D	525	Total	C	N	O	S	0	1
			3856	2397	666	773	20		
1	E	525	Total	C	N	O	S	0	1
			3856	2397	666	773	20		
1	F	525	Total	C	N	O	S	0	1
			3856	2397	666	773	20		
1	G	525	Total	C	N	O	S	0	1
			3856	2397	666	773	20		
1	H	525	Total	C	N	O	S	0	1
			3856	2397	666	773	20		
1	I	525	Total	C	N	O	S	0	1
			3856	2397	666	773	20		
1	J	525	Total	C	N	O	S	0	1
			3856	2397	666	773	20		
1	K	525	Total	C	N	O	S	0	1
			3856	2397	666	773	20		
1	L	525	Total	C	N	O	S	0	1
			3856	2397	666	773	20		
1	M	525	Total	C	N	O	S	0	1
			3856	2397	666	773	20		
1	N	525	Total	C	N	O	S	0	1
			3856	2397	666	773	20		

- Molecule 2 is a protein called 10 KDA CHAPERONIN.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	O	97	Total	C	N	O	S	0	0
			728	454	127	145	2		

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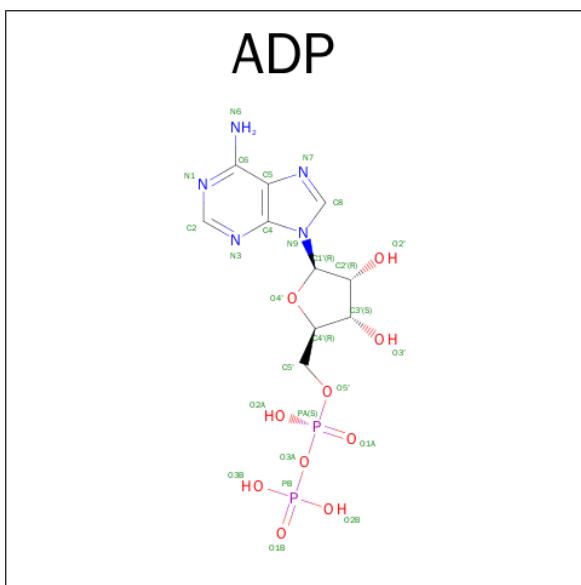
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Mol	Chain	Residues	Atoms					AltConf	Trace
2	P	97	Total	C	N	O	S	0	0
			728	454	127	145	2		
2	Q	97	Total	C	N	O	S	0	0
			728	454	127	145	2		
2	R	97	Total	C	N	O	S	0	0
			728	454	127	145	2		
2	S	97	Total	C	N	O	S	0	0
			728	454	127	145	2		
2	T	97	Total	C	N	O	S	0	0
			728	454	127	145	2		
2	U	97	Total	C	N	O	S	0	0
			728	454	127	145	2		

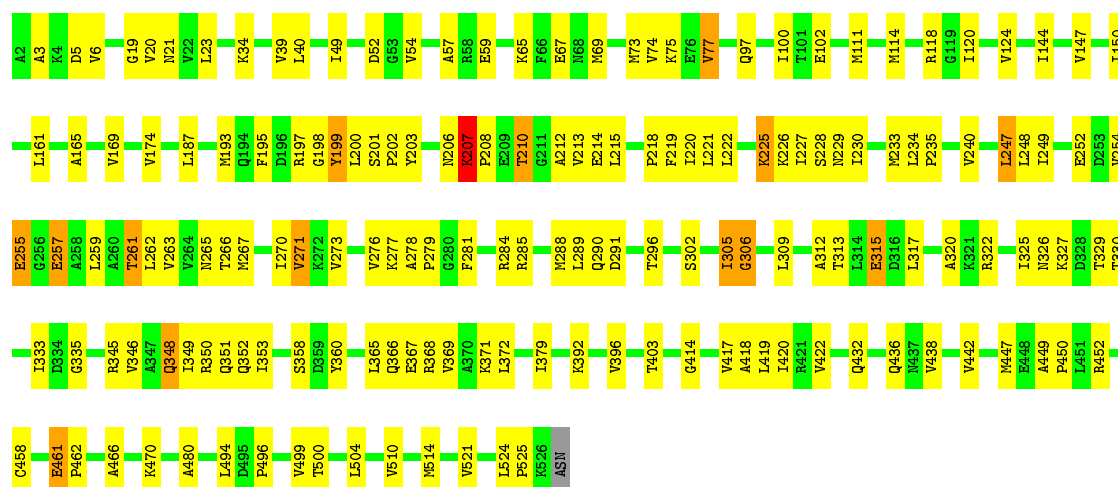
- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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'-DIPHOSPHATE (three-letter code: ADP) (formula: C₁₀H₁₅N₅O₁₀P₂).

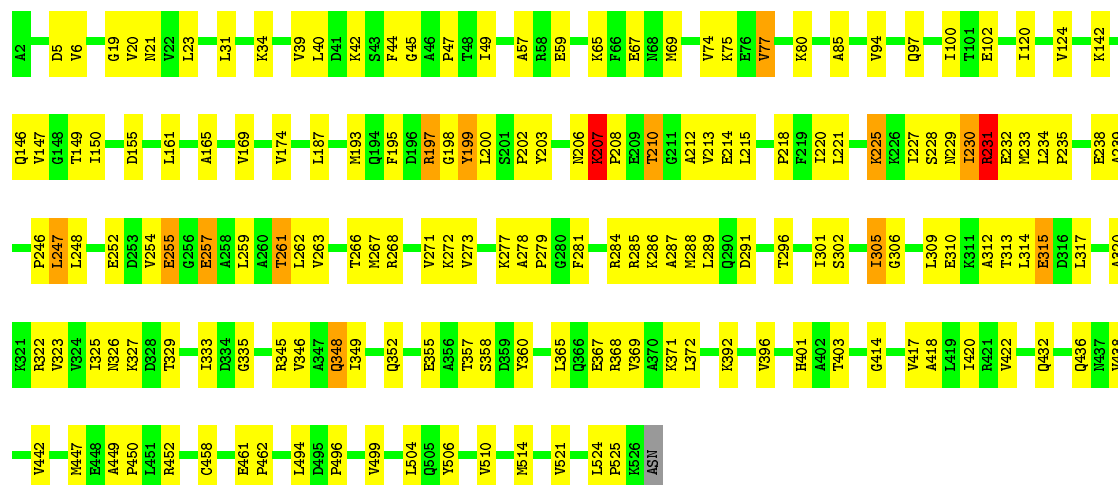


Mol	Chain	Residues	Atoms					AltConf
4	A	1	Total 27	C 10	N 5	O 10	P 2	0
4	B	1	Total 27	C 10	N 5	O 10	P 2	0
4	C	1	Total 27	C 10	N 5	O 10	P 2	0
4	D	1	Total 27	C 10	N 5	O 10	P 2	0
4	E	1	Total 27	C 10	N 5	O 10	P 2	0
4	F	1	Total 27	C 10	N 5	O 10	P 2	0
4	G	1	Total 27	C 10	N 5	O 10	P 2	0



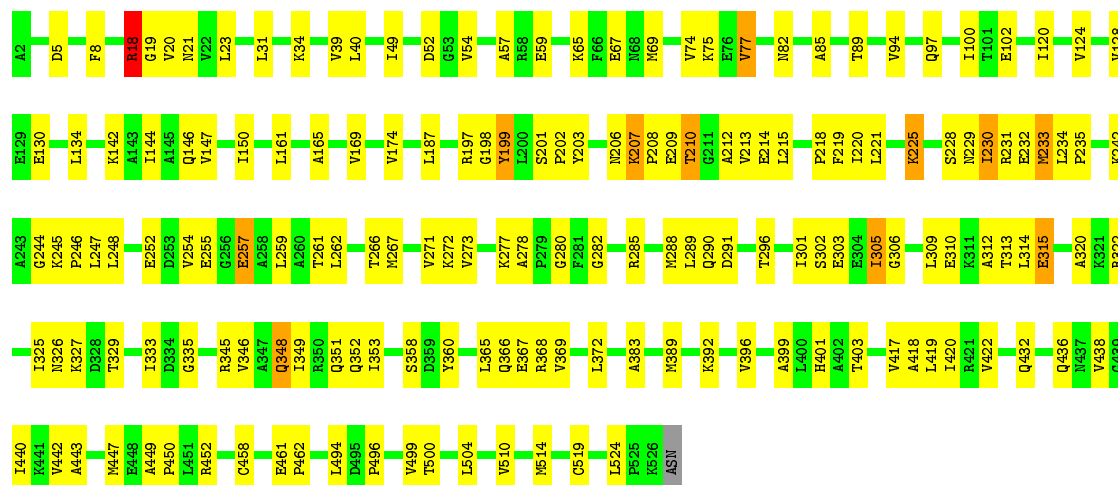
• Molecule 1: 60 KDA CHAPERONIN

Chain D: 68% 29% .

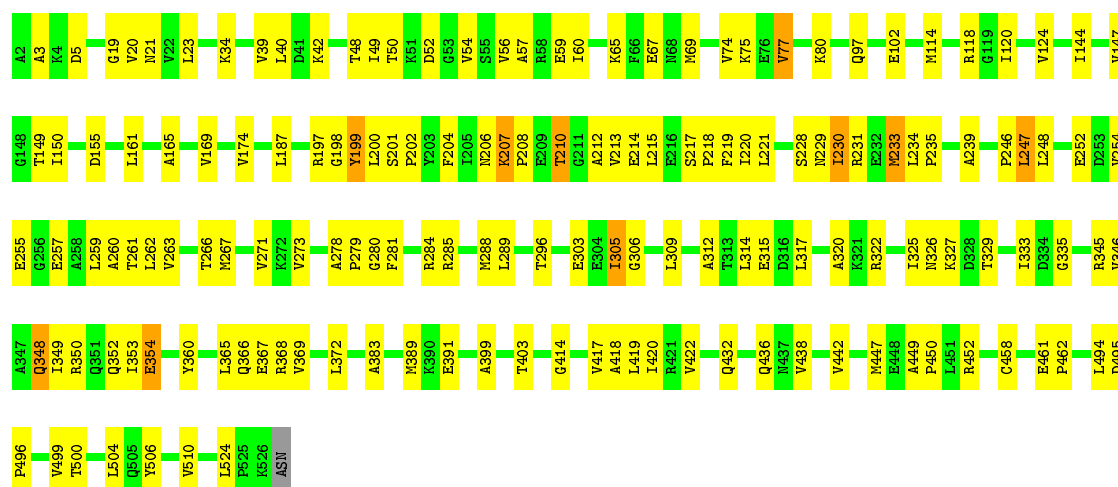


• Molecule 1: 60 KDA CHAPERONIN

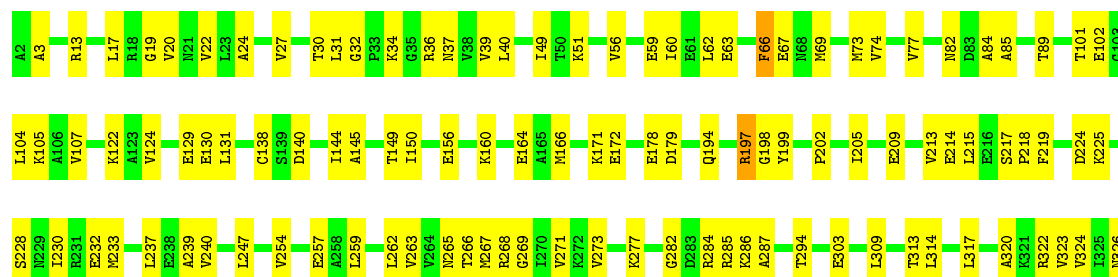
Chain E: 68% 30% .

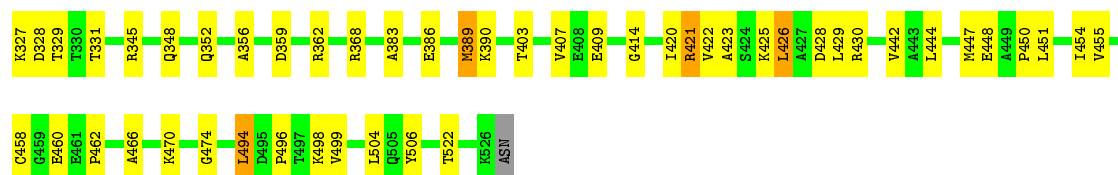


Chain F: 69% 29%

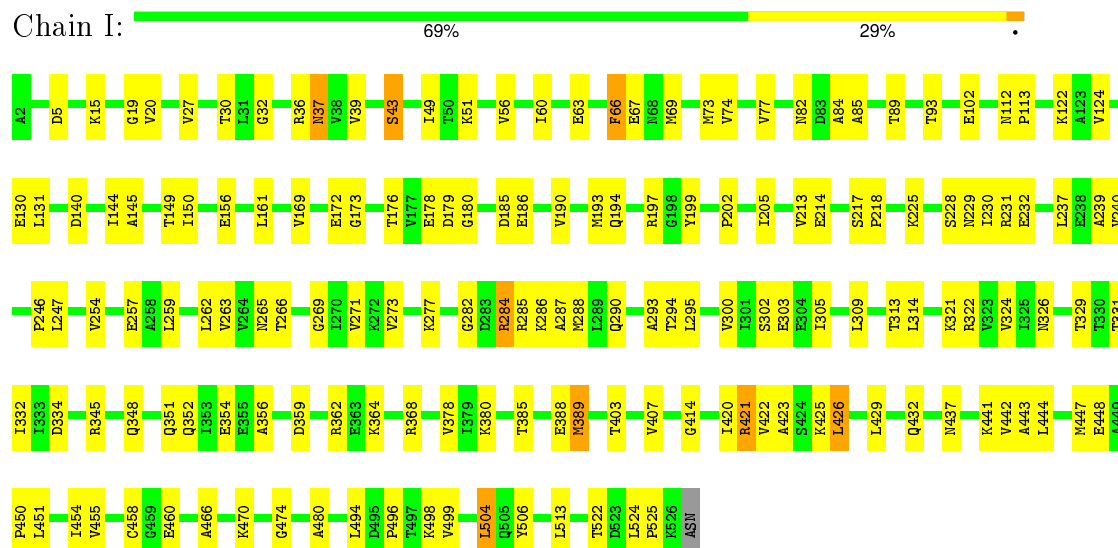


Chain H: 70% 29%

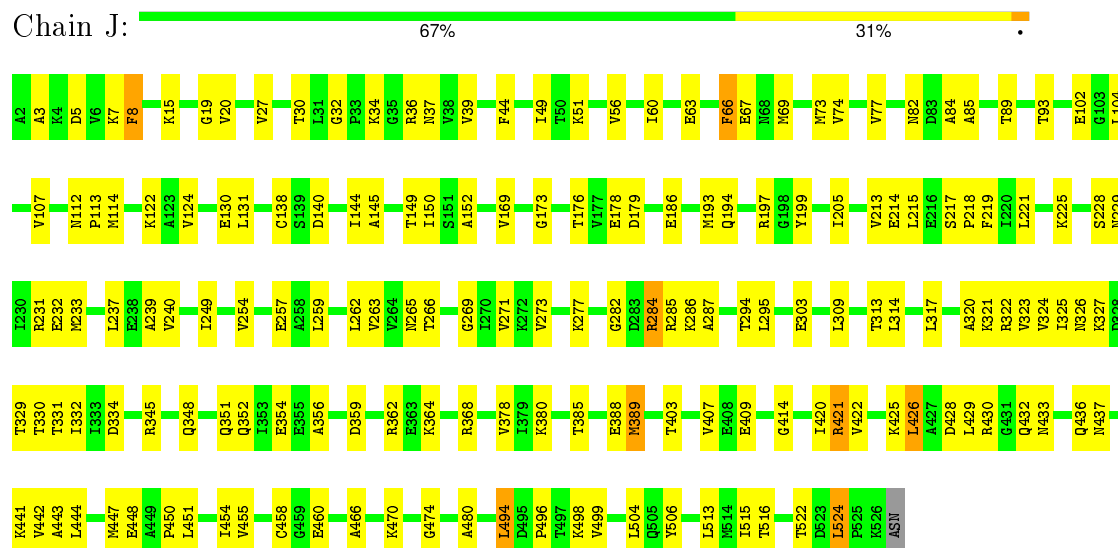




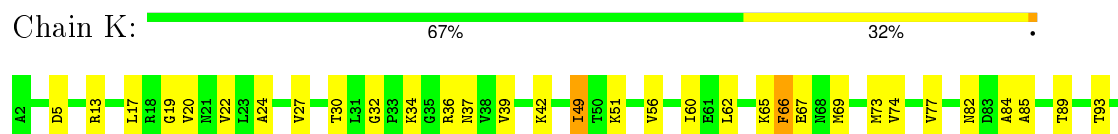
• Molecule 1: 60 KDA CHAPERONIN

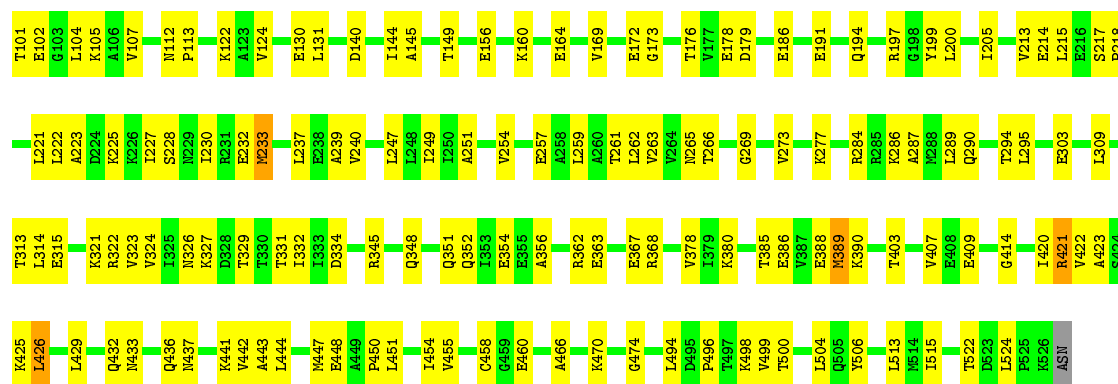


• Molecule 1: 60 KDA CHAPERONIN



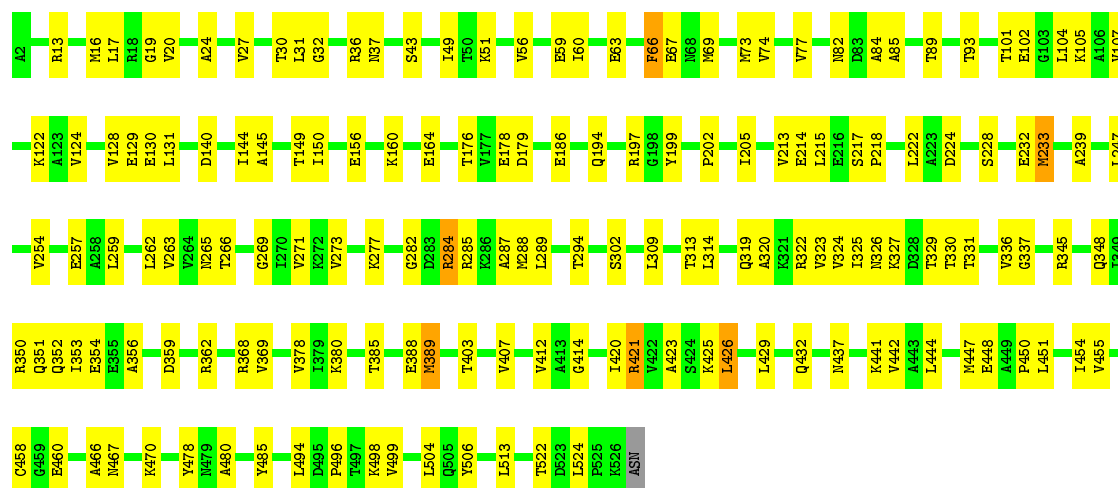
• Molecule 1: 60 KDA CHAPERONIN





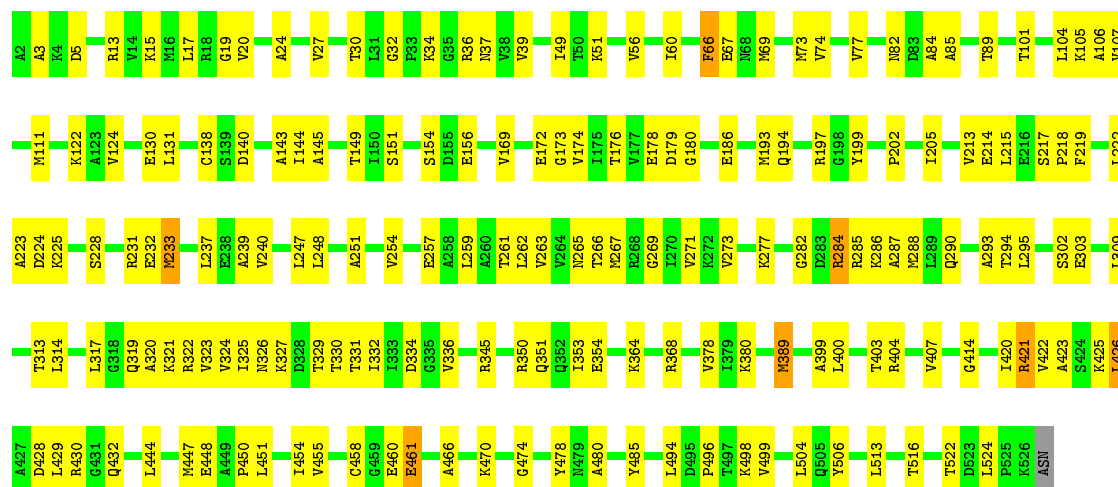
• Molecule 1: 60 KDA CHAPERONIN

Chain L: 69% 29% .

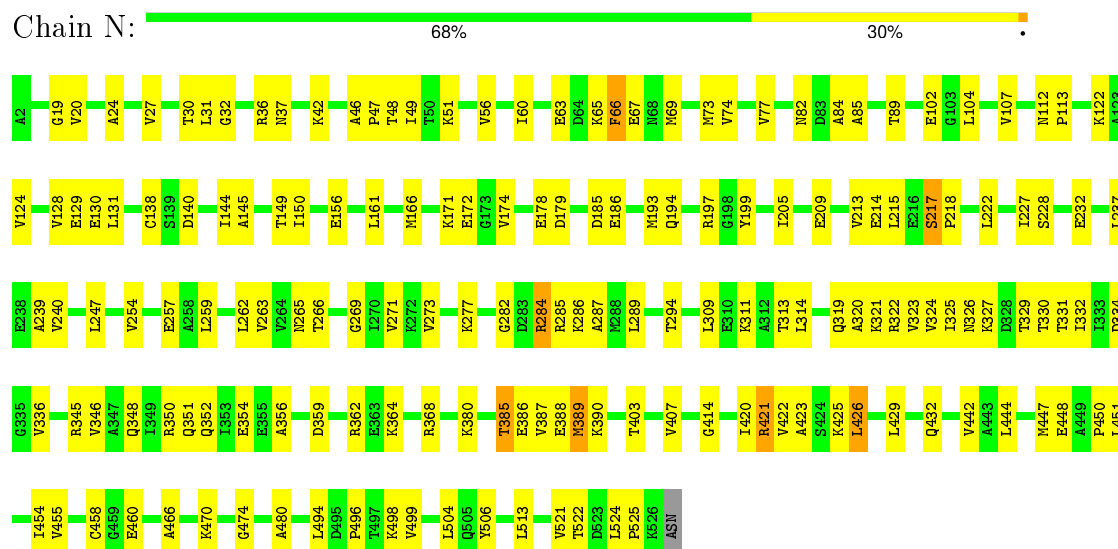


• Molecule 1: 60 KDA CHAPERONIN

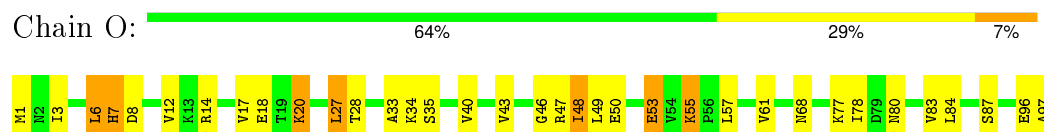
Chain M: 66% 33% .



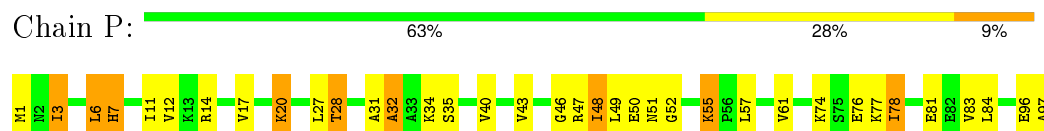
• Molecule 1: 60 KDA CHAPERONIN



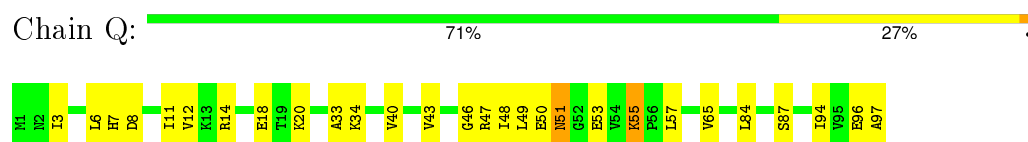
• Molecule 2: 10 KDA CHAPERONIN



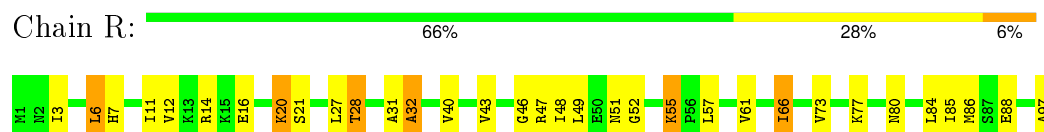
• Molecule 2: 10 KDA CHAPERONIN



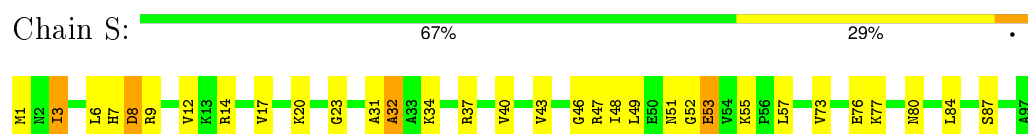
• Molecule 2: 10 KDA CHAPERONIN



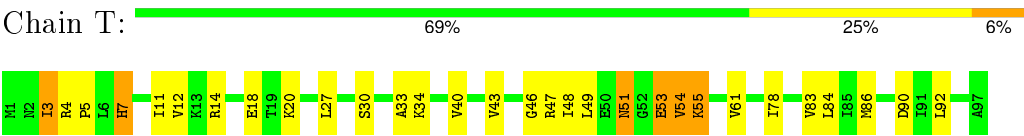
• Molecule 2: 10 KDA CHAPERONIN



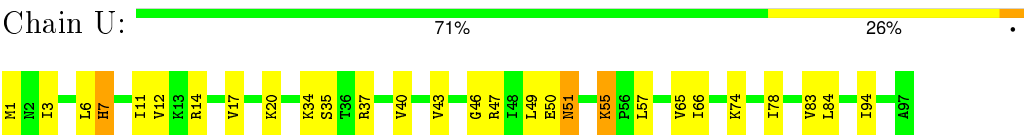
• Molecule 2: 10 KDA CHAPERONIN



● Molecule 2: 10 KDA CHAPERONIN



● Molecule 2: 10 KDA CHAPERONIN



4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of images	Not provided	Depositor
Resolution determination method	Not provided	Depositor
CTF correction method	EACH FRAME, Not provided	Depositor
Microscope	OTHER	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	20	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	5000	Depositor
Magnification	50000	Depositor
Image detector	GATAN CCD	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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	0.35	0/3884	0.55	0/5245
1	B	0.35	0/3884	0.57	0/5245
1	C	0.35	0/3884	0.57	0/5245
1	D	0.36	0/3884	0.56	0/5245
1	E	0.36	0/3884	0.57	1/5245 (0.0%)
1	F	0.35	0/3884	0.56	0/5245
1	G	0.35	0/3884	0.56	0/5245
1	H	0.35	0/3884	0.55	0/5245
1	I	0.35	0/3884	0.56	0/5245
1	J	0.35	0/3884	0.55	0/5245
1	K	0.35	0/3884	0.55	0/5245
1	L	0.34	0/3884	0.55	0/5245
1	M	0.35	0/3884	0.56	0/5245
1	N	0.35	0/3884	0.55	0/5245
2	O	0.40	0/732	0.62	0/983
2	P	0.39	0/732	0.63	0/983
2	Q	0.39	0/732	0.63	0/983
2	R	0.37	0/732	0.63	0/983
2	S	0.41	0/732	0.63	0/983
2	T	0.43	0/732	0.67	0/983
2	U	0.40	0/732	0.63	0/983
All	All	0.36	0/59500	0.57	1/80311 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	18	ARG	NE-CZ-NH1	5.12	122.86	120.30

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	3856	0	3976	118	0
1	B	3856	0	3976	125	0
1	C	3856	0	3976	134	0
1	D	3856	0	3976	124	0
1	E	3856	0	3976	133	0
1	F	3856	0	3976	124	0
1	G	3856	0	3976	131	0
1	H	3856	0	3976	106	0
1	I	3856	0	3976	113	0
1	J	3856	0	3976	117	0
1	K	3856	0	3976	116	0
1	L	3856	0	3976	110	0
1	M	3856	0	3976	128	0
1	N	3856	0	3976	114	0
2	O	728	0	762	25	0
2	P	728	0	762	25	0
2	Q	728	0	762	17	0
2	R	728	0	762	23	0
2	S	728	0	762	18	0
2	T	728	0	762	23	0
2	U	728	0	762	19	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	27	0	12	1	0
4	B	27	0	12	2	0
4	C	27	0	12	0	0
4	D	27	0	12	0	0
4	E	27	0	12	2	0
4	F	27	0	12	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	G	27	0	12	0	0
All	All	59276	0	61082	1800	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 15.

The worst 5 of 1800 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:352:GLN:HB3	1:E:365:LEU:HD11	1.33	1.02
1:E:161:LEU:HD11	1:E:187:LEU:HB2	1.40	1.02
1:D:161:LEU:HD11	1:D:187:LEU:HB2	1.42	1.01
1:F:161:LEU:HD11	1:F:187:LEU:HB2	1.44	1.00
1:D:352:GLN:HB3	1:D:365:LEU:HD11	1.41	0.99

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	523/526 (99%)	504 (96%)	12 (2%)	7 (1%)	15	60
1	B	523/526 (99%)	505 (97%)	10 (2%)	8 (2%)	13	57
1	C	523/526 (99%)	502 (96%)	14 (3%)	7 (1%)	15	60
1	D	523/526 (99%)	502 (96%)	12 (2%)	9 (2%)	11	55
1	E	523/526 (99%)	507 (97%)	7 (1%)	9 (2%)	11	55
1	F	523/526 (99%)	504 (96%)	13 (2%)	6 (1%)	17	63
1	G	523/526 (99%)	505 (97%)	12 (2%)	6 (1%)	17	63
1	H	523/526 (99%)	514 (98%)	7 (1%)	2 (0%)	39	80

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	I	523/526 (99%)	511 (98%)	9 (2%)	3 (1%)	30	74
1	J	523/526 (99%)	514 (98%)	7 (1%)	2 (0%)	39	80
1	K	523/526 (99%)	516 (99%)	6 (1%)	1 (0%)	52	86
1	L	523/526 (99%)	512 (98%)	8 (2%)	3 (1%)	30	74
1	M	523/526 (99%)	512 (98%)	9 (2%)	2 (0%)	39	80
1	N	523/526 (99%)	513 (98%)	9 (2%)	1 (0%)	52	86
2	O	95/97 (98%)	89 (94%)	4 (4%)	2 (2%)	9	50
2	P	95/97 (98%)	88 (93%)	3 (3%)	4 (4%)	3	34
2	Q	95/97 (98%)	91 (96%)	1 (1%)	3 (3%)	5	41
2	R	95/97 (98%)	87 (92%)	4 (4%)	4 (4%)	3	34
2	S	95/97 (98%)	89 (94%)	2 (2%)	4 (4%)	3	34
2	T	95/97 (98%)	90 (95%)	1 (1%)	4 (4%)	3	34
2	U	95/97 (98%)	86 (90%)	7 (7%)	2 (2%)	9	50
All	All	7987/8043 (99%)	7741 (97%)	157 (2%)	89 (1%)	23	63

5 of 89 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	210	THR
1	A	233	MET
1	B	233	MET
1	B	312	ALA
1	B	358	SER

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	404/406 (100%)	392 (97%)	12 (3%)	48	77
1	B	404/406 (100%)	394 (98%)	10 (2%)	55	81
1	C	404/406 (100%)	388 (96%)	16 (4%)	38	71

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	404/406 (100%)	386 (96%)	18 (4%)	34	69
1	E	404/406 (100%)	388 (96%)	16 (4%)	38	71
1	F	404/406 (100%)	387 (96%)	17 (4%)	36	70
1	G	404/406 (100%)	392 (97%)	12 (3%)	48	77
1	H	404/406 (100%)	392 (97%)	12 (3%)	48	77
1	I	404/406 (100%)	393 (97%)	11 (3%)	52	79
1	J	404/406 (100%)	394 (98%)	10 (2%)	55	81
1	K	404/406 (100%)	394 (98%)	10 (2%)	55	81
1	L	404/406 (100%)	393 (97%)	11 (3%)	52	79
1	M	404/406 (100%)	392 (97%)	12 (3%)	48	77
1	N	404/406 (100%)	392 (97%)	12 (3%)	48	77
2	O	80/80 (100%)	73 (91%)	7 (9%)	12	45
2	P	80/80 (100%)	72 (90%)	8 (10%)	9	38
2	Q	80/80 (100%)	77 (96%)	3 (4%)	40	73
2	R	80/80 (100%)	73 (91%)	7 (9%)	12	45
2	S	80/80 (100%)	75 (94%)	5 (6%)	22	59
2	T	80/80 (100%)	77 (96%)	3 (4%)	40	73
2	U	80/80 (100%)	76 (95%)	4 (5%)	30	66
All	All	6216/6244 (100%)	6000 (96%)	216 (4%)	47	74

5 of 216 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	G	348	GLN
1	I	421	ARG
2	R	28	THR
1	G	461	GLU
1	H	389	MET

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 121 such sidechains are listed below:

Mol	Chain	Res	Type
1	F	112	ASN
1	G	352	GLN
1	N	21	ASN

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Mol	Chain	Res	Type
1	F	153	ASN
1	G	21	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 14 ligands modelled in this entry, 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	ADP	A	1526	3	24,29,29	1.29	3 (12%)	23,45,45	3.22	5 (21%)
4	ADP	B	1526	3	24,29,29	1.29	3 (12%)	23,45,45	3.24	5 (21%)
4	ADP	C	1526	3	24,29,29	1.29	3 (12%)	23,45,45	3.22	6 (26%)
4	ADP	D	1526	3	24,29,29	1.29	3 (12%)	23,45,45	3.18	5 (21%)
4	ADP	E	1526	3	24,29,29	1.28	3 (12%)	23,45,45	3.23	6 (26%)
4	ADP	F	1526	3	24,29,29	1.28	3 (12%)	23,45,45	3.23	6 (26%)
4	ADP	G	1526	3	24,29,29	1.29	3 (12%)	23,45,45	3.22	5 (21%)

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	ADP	A	1526	3	-	0/12/32/32	0/3/3/3
4	ADP	B	1526	3	-	0/12/32/32	0/3/3/3
4	ADP	C	1526	3	-	0/12/32/32	0/3/3/3
4	ADP	D	1526	3	-	0/12/32/32	0/3/3/3
4	ADP	E	1526	3	-	0/12/32/32	0/3/3/3
4	ADP	F	1526	3	-	0/12/32/32	0/3/3/3
4	ADP	G	1526	3	-	0/12/32/32	0/3/3/3

The worst 5 of 21 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	1526	ADP	C5-N7	-2.18	1.31	1.39
4	C	1526	ADP	C5-N7	-2.18	1.31	1.39
4	F	1526	ADP	C5-N7	-2.17	1.31	1.39
4	B	1526	ADP	C5-N7	-2.17	1.31	1.39
4	E	1526	ADP	C5-N7	-2.16	1.31	1.39

The worst 5 of 38 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	E	1526	ADP	N3-C2-N1	-13.12	118.57	128.87
4	A	1526	ADP	N3-C2-N1	-13.11	118.57	128.87
4	B	1526	ADP	N3-C2-N1	-13.10	118.58	128.87
4	G	1526	ADP	N3-C2-N1	-13.10	118.58	128.87
4	C	1526	ADP	N3-C2-N1	-13.09	118.59	128.87

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1526	ADP	1	0
4	B	1526	ADP	2	0
4	E	1526	ADP	2	0

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.