



wwPDB/EMDataBank EM Map/Model Validation Summary Report ⓘ

Feb 16, 2018 – 06:36 am GMT

PDB ID : 4AB3
EMDB ID: : EMD-2003
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 : 2011-12-06
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

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

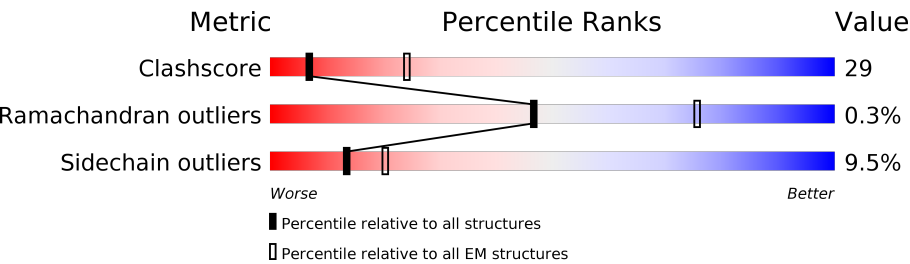
MolProbity : 4.02b-467
Mogul : 1.7.3 (157068), CSD as539be (2018)
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : trunk30686

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 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	136279	1886
Ramachandran outliers	132675	1663
Sidechain outliers	132484	1531

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	57% 29% 7% . .
1	B	548	56% 30% 7% . .
1	C	548	56% 29% 7% . .
1	D	548	56% 30% 7% . .
1	E	548	57% 29% 7% . .
1	F	548	57% 29% 7% . .
1	G	548	57% 29% 7% . .
1	H	548	52% 34% 9% . .
1	I	548	52% 34% 8% . .

Continued on next page...

Continued from previous page...

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	PO4	H	1525	-	-	X	-
2	PO4	I	1525	-	-	X	-
2	PO4	J	1525	-	-	X	-
2	PO4	K	1525	-	-	X	-
2	PO4	L	1525	-	-	X	-
2	PO4	M	1525	-	-	X	-
2	PO4	N	1525	-	-	X	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 54293 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:

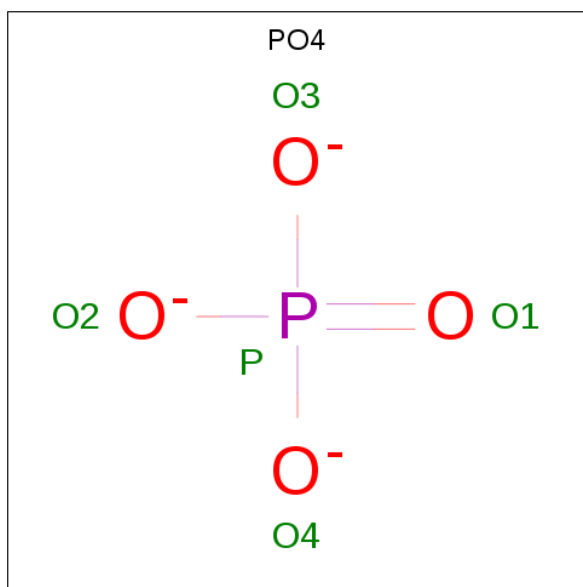
Chain	Residue	Modelled	Actual	Comment	Reference
A	398	ALA	ASP	engineered mutation	UNP P0A6F5
B	398	ALA	ASP	engineered mutation	UNP P0A6F5

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	AltConf
2	F	1	Total P 1 1	0
2	G	1	Total P 1 1	0
2	H	1	Total P 1 1	0
2	I	1	Total P 1 1	0
2	J	1	Total P 1 1	0
2	K	1	Total P 1 1	0
2	L	1	Total P 1 1	0
2	M	1	Total P 1 1	0
2	N	1	Total P 1 1	0

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

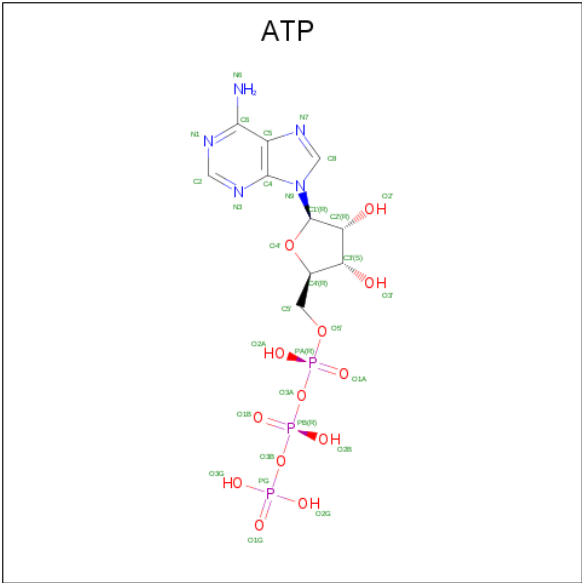
Mol	Chain	Residues	Atoms	AltConf
3	G	1	Total Mg 1 1	0
3	J	1	Total Mg 1 1	0
3	D	1	Total Mg 1 1	0
3	K	1	Total Mg 1 1	0
3	E	1	Total Mg 1 1	0
3	H	1	Total Mg 1 1	0
3	B	1	Total Mg 1 1	0
3	I	1	Total Mg 1 1	0
3	C	1	Total Mg 1 1	0
3	A	1	Total Mg 1 1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		AltConf
3	N	1	Total	Mg	0
			1	1	
3	L	1	Total	Mg	0
			1	1	
3	F	1	Total	Mg	0
			1	1	
3	M	1	Total	Mg	0
			1	1	

- Molecule 4 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: C₁₀H₁₆N₅O₁₃P₃).

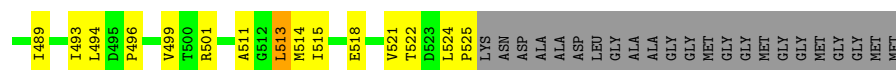


Mol	Chain	Residues	Atoms					AltConf
4	A	1	Total	C	N	O	P	0
			31	10	5	13	3	
4	B	1	Total	C	N	O	P	0
			31	10	5	13	3	
4	C	1	Total	C	N	O	P	0
			31	10	5	13	3	
4	D	1	Total	C	N	O	P	0
			31	10	5	13	3	
4	E	1	Total	C	N	O	P	0
			31	10	5	13	3	
4	F	1	Total	C	N	O	P	0
			31	10	5	13	3	
4	G	1	Total	C	N	O	P	0
			31	10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

Continued on next page...

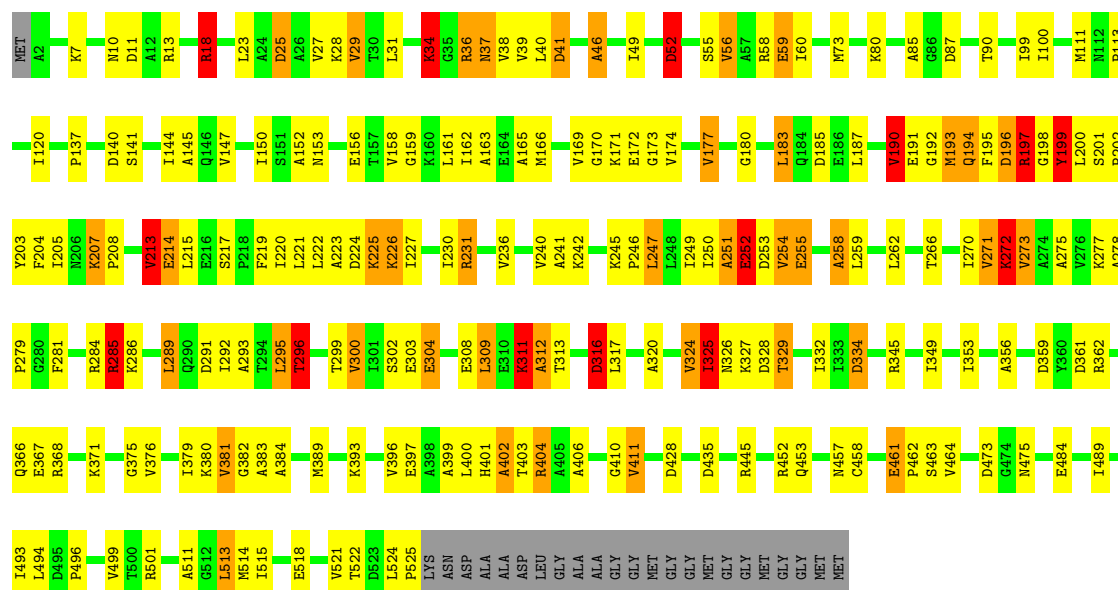
Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
4	H	1	Total	C	N	O	P	0
			31	10	5	13	3	
4	I	1	Total	C	N	O	P	0
			31	10	5	13	3	
4	J	1	Total	C	N	O	P	0
			31	10	5	13	3	
4	K	1	Total	C	N	O	P	0
			31	10	5	13	3	
4	L	1	Total	C	N	O	P	0
			31	10	5	13	3	
4	M	1	Total	C	N	O	P	0
			31	10	5	13	3	
4	N	1	Total	C	N	O	P	0
			31	10	5	13	3	



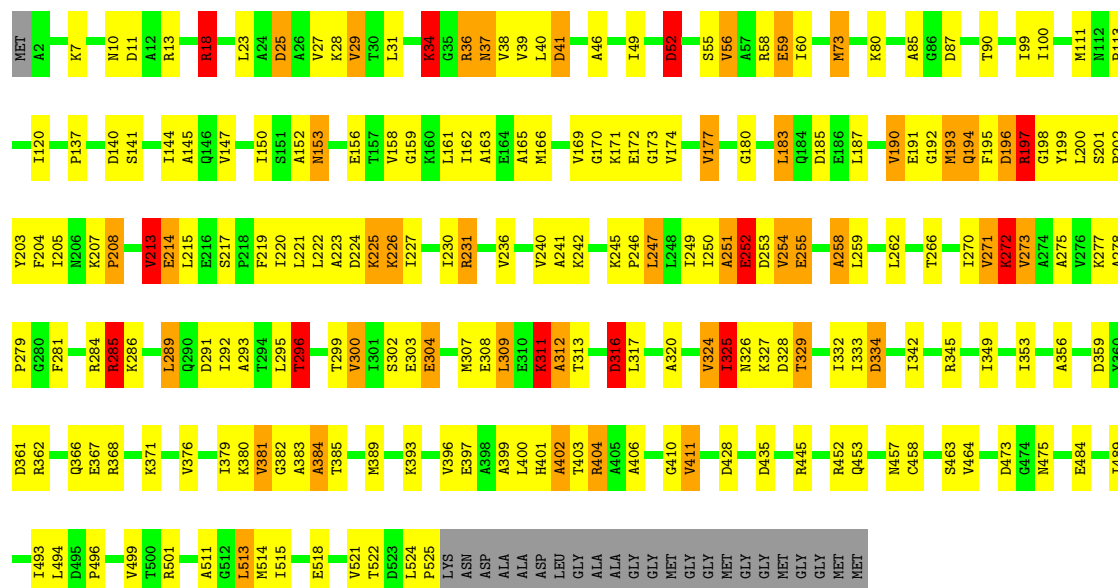
• Molecule 1: 60 KDA CHAPERONIN

Chain C: 56% 29% 7%



• Molecule 1: 60 KDA CHAPERONIN

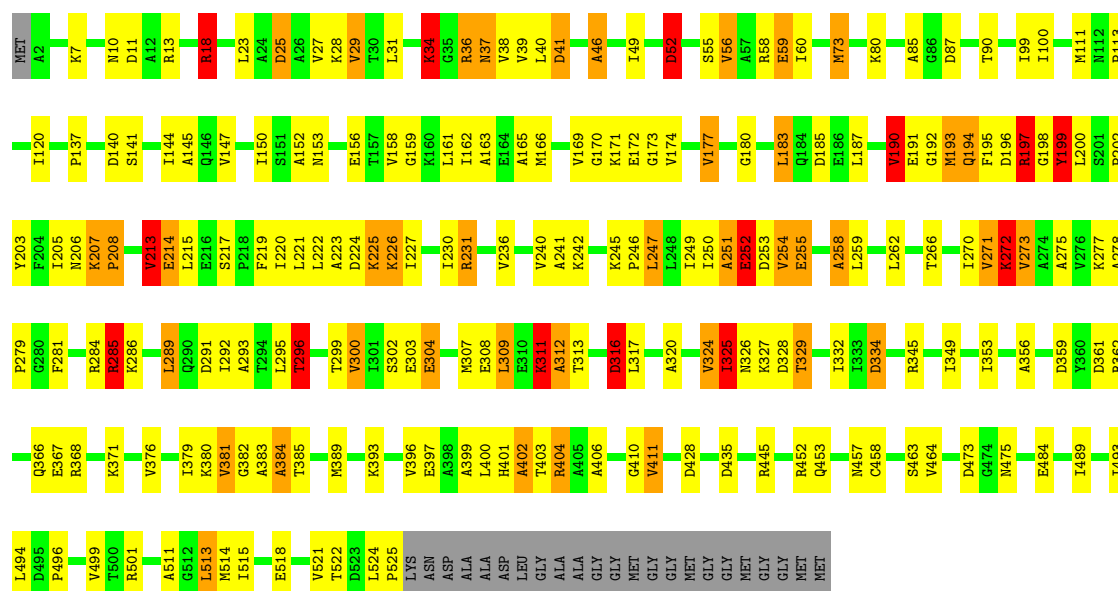
Chain D: 56% 30% 7%



• Molecule 1: 60 KDA CHAPERONIN

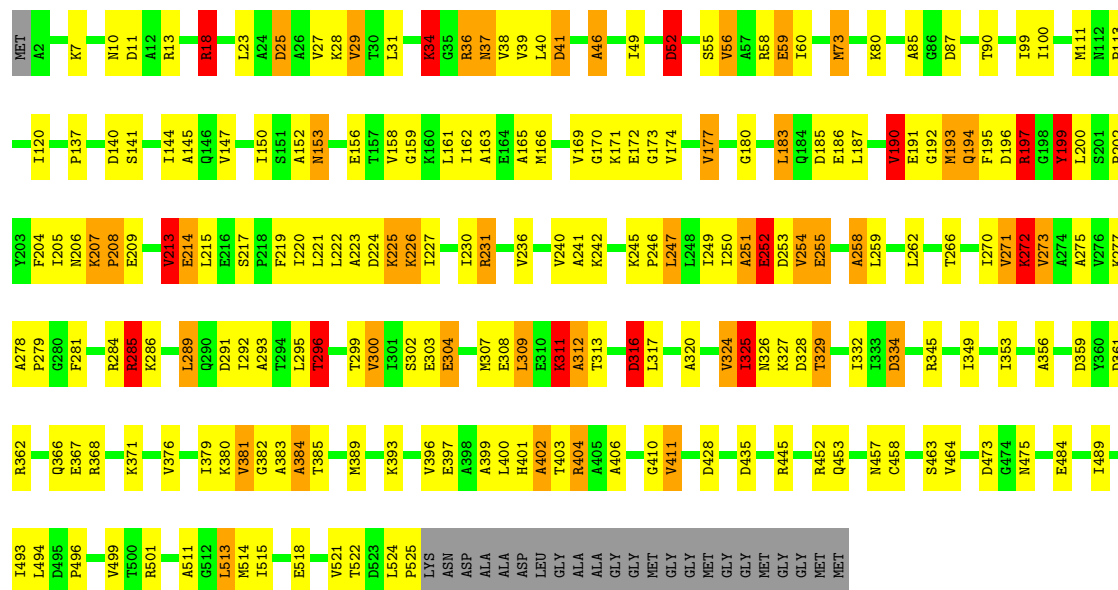
Chain E: 57% 29% 7%





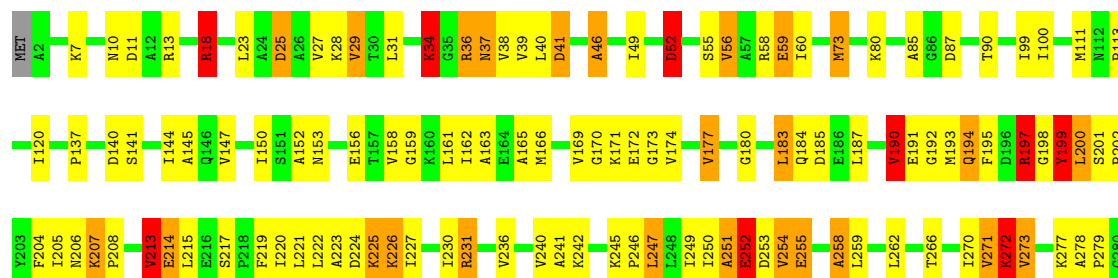
- Molecule 1: 60 KDA CHAPERONIN

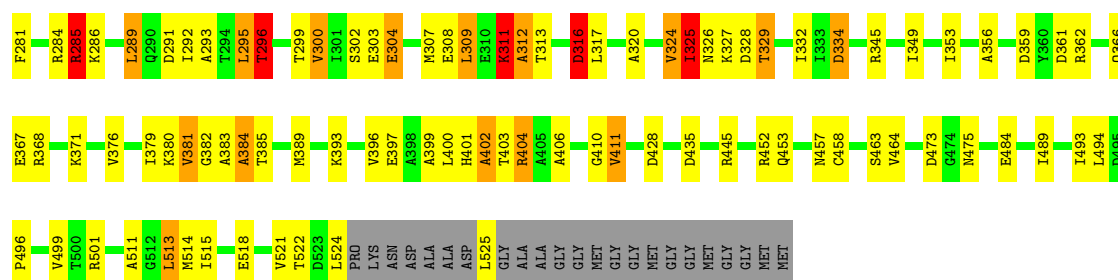
Chain F:  57% 29% 7% . .



- Molecule 1: 60 KDA CHAPERONIN

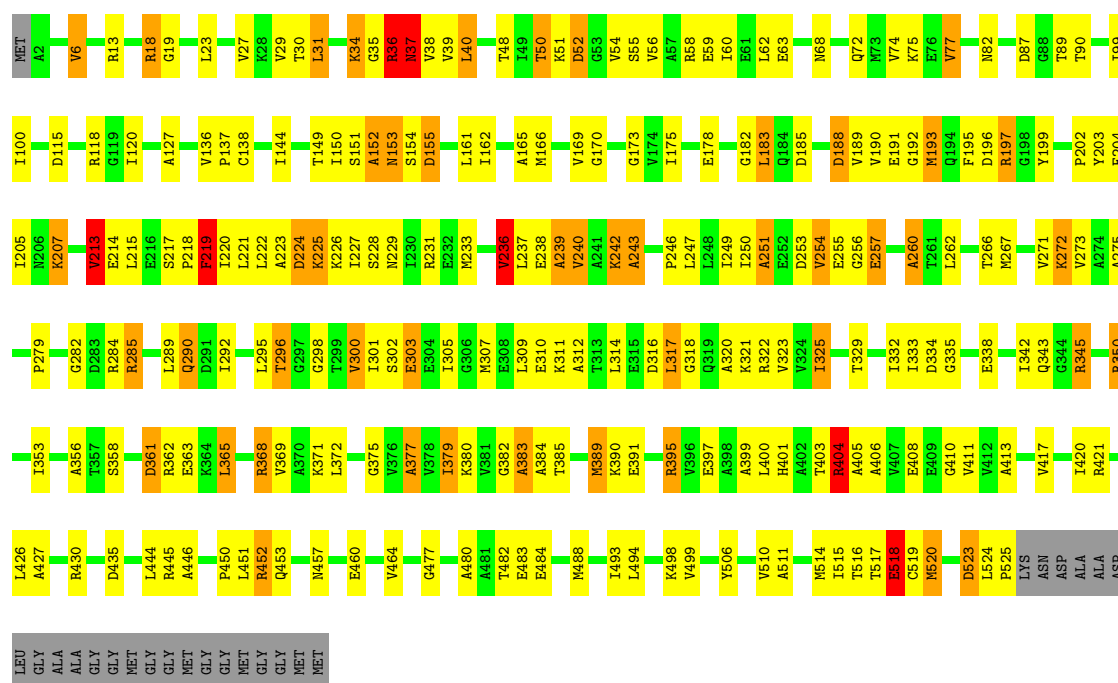
Chain G: 57% 29% 7% • •





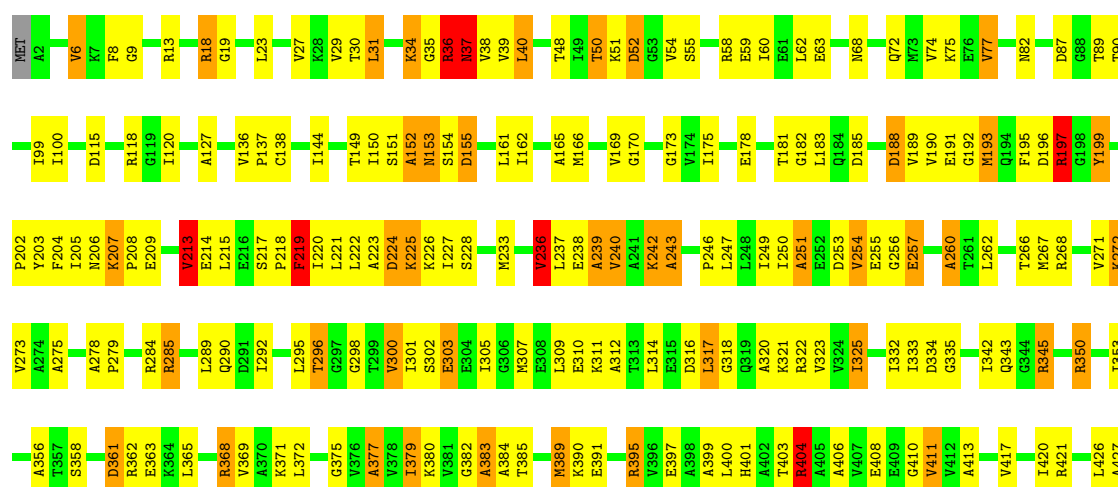
• Molecule 1: 60 KDA CHAPERONIN

Chain H: 



• Molecule 1: 60 KDA CHAPERONIN

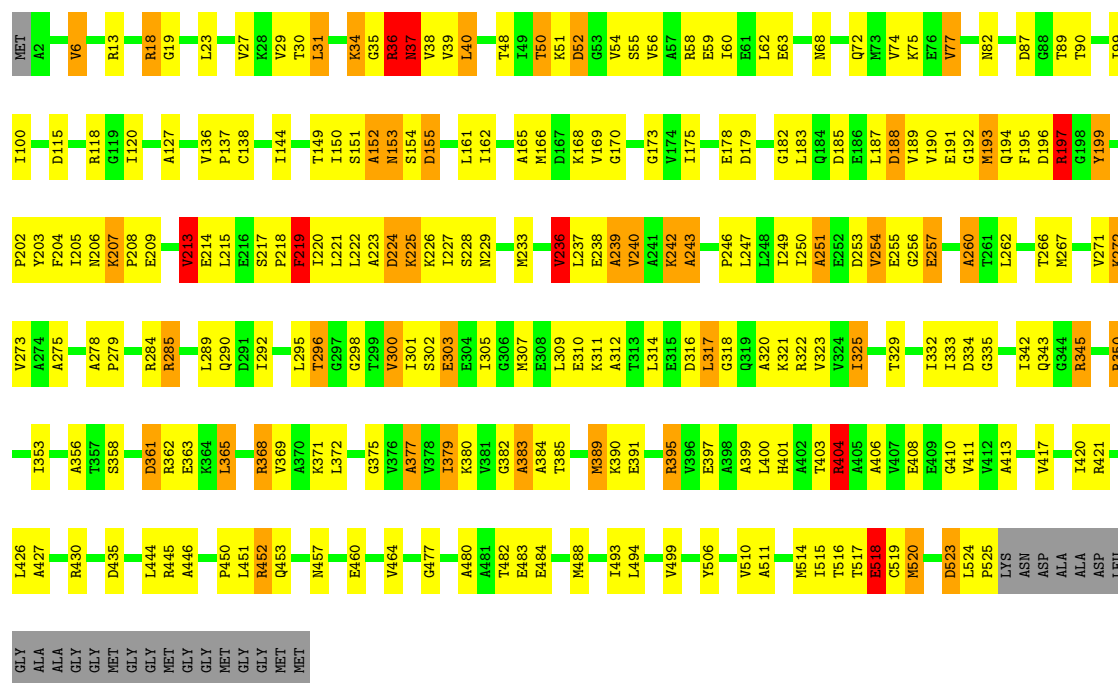
Chain I: 





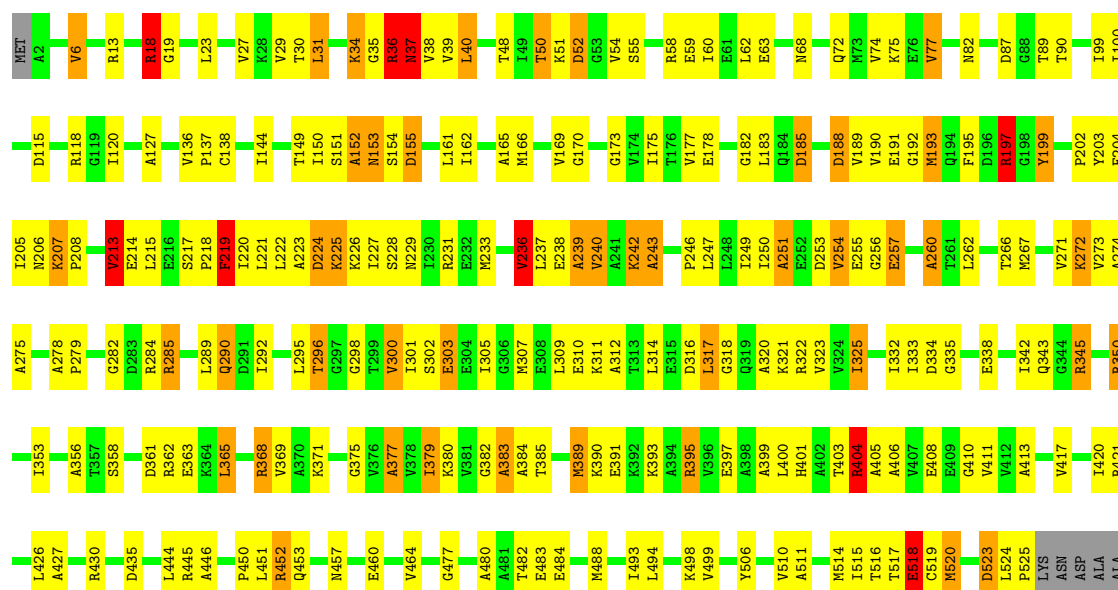
• Molecule 1: 60 KDA CHAPERONIN

Chain J: 52% 34% 8% . .



• Molecule 1: 60 KDA CHAPERONIN

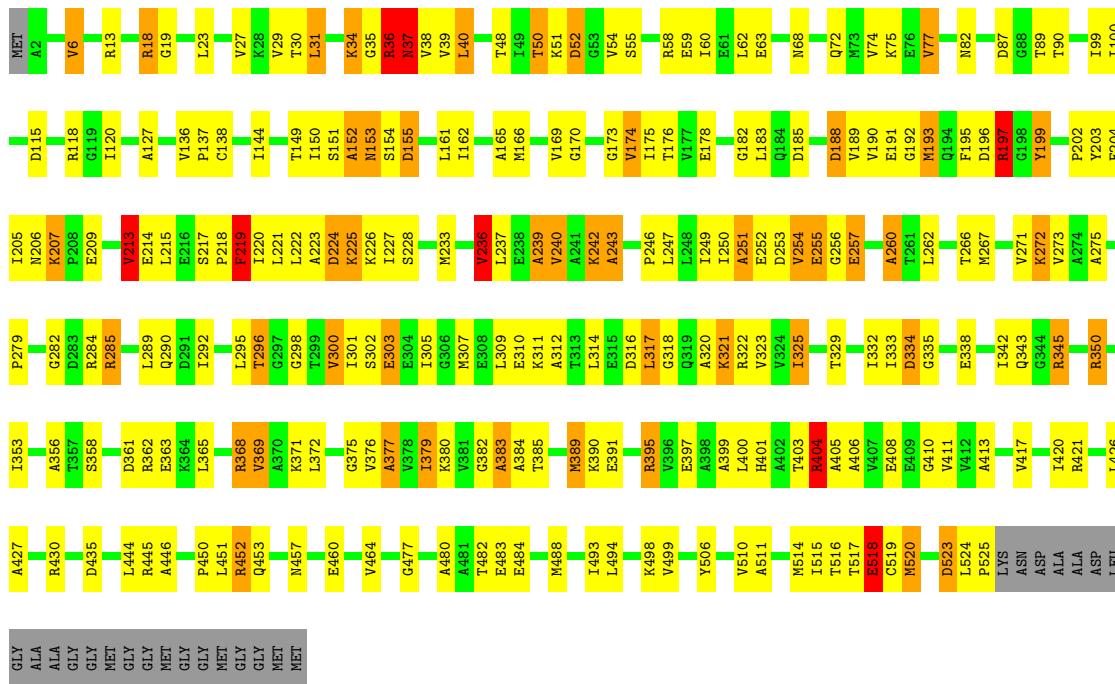
Chain K: 52% 34% 8% . .



ASP
LEU
GLY
ALA
ALA
GLY
GLY
MET
GLY
GLY
MET
GLY
GLY
MET
GLY
GLY
MET
MET

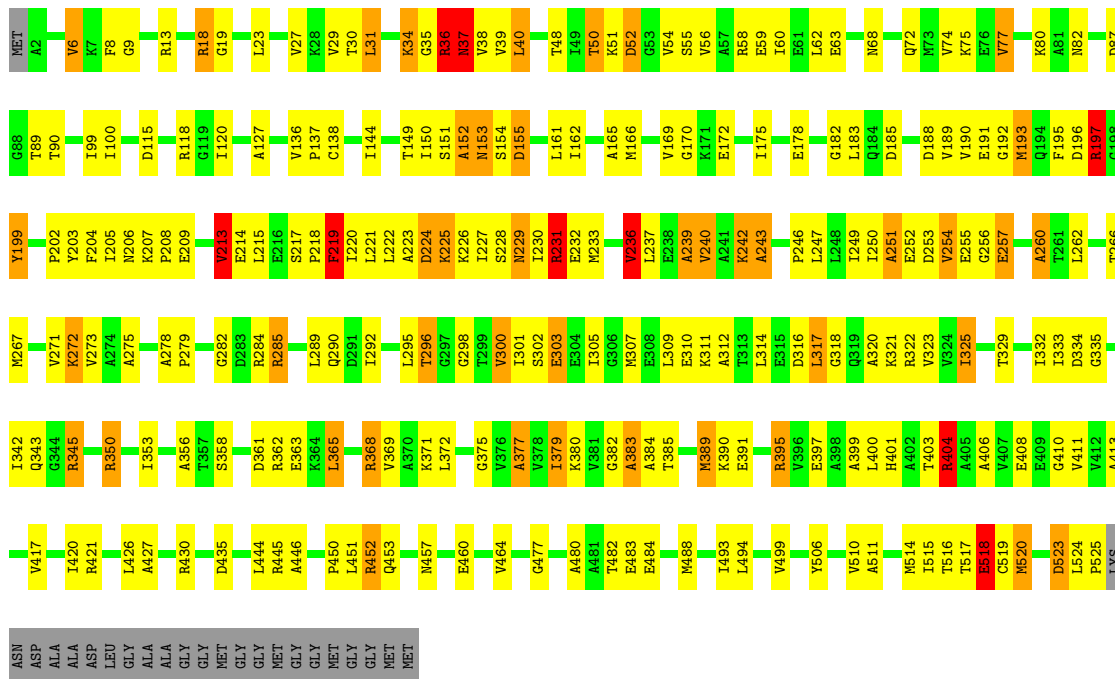
- Molecule 1: 60 KDA CHAPERONIN

Chain L:  52% 34% 9% ..



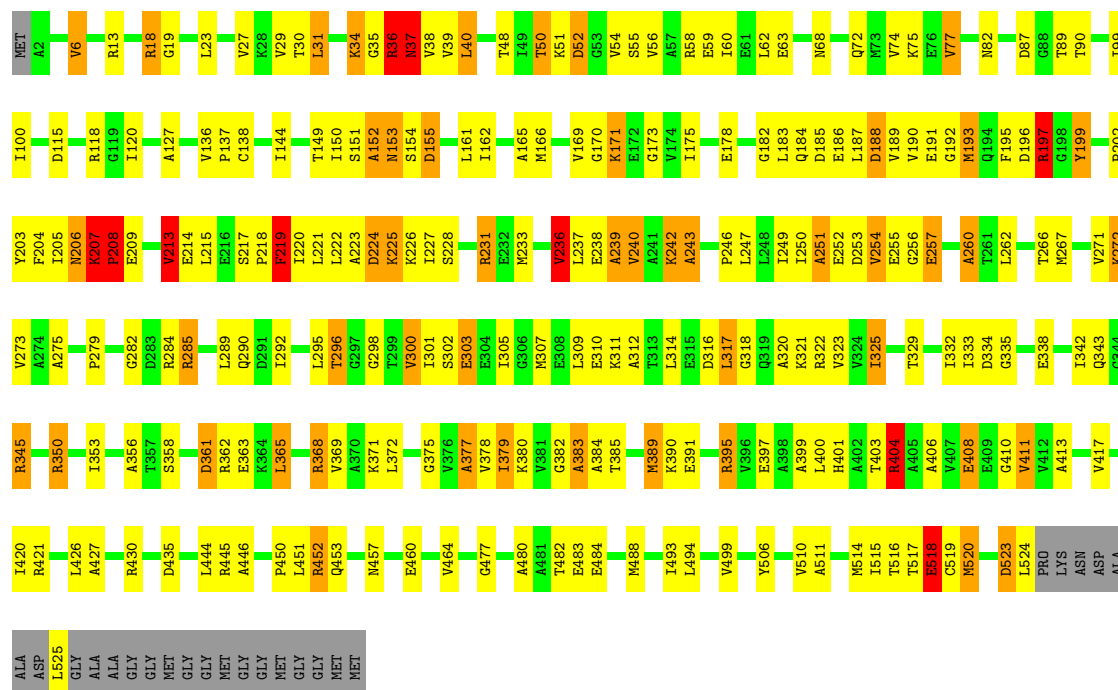
- Molecule 1: 60 KDA CHAPERONIN

Chain M: 51% 35% 8% 6%



- Molecule 1: 60 KDA CHAPERONIN

Chain N:  51% 34% 9% . .



4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, D7	Depositor
Number of particles used	15000	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	0.84	6/3873 (0.2%)	1.48	78/5229 (1.5%)
1	B	0.86	7/3872 (0.2%)	1.49	81/5227 (1.5%)
1	C	0.86	7/3872 (0.2%)	1.49	82/5227 (1.6%)
1	D	0.86	7/3872 (0.2%)	1.49	81/5227 (1.5%)
1	E	0.86	7/3872 (0.2%)	1.49	81/5227 (1.5%)
1	F	0.86	7/3872 (0.2%)	1.50	81/5227 (1.5%)
1	G	0.86	7/3872 (0.2%)	1.50	85/5227 (1.6%)
1	H	1.01	3/3872 (0.1%)	1.62	80/5227 (1.5%)
1	I	1.01	2/3872 (0.1%)	1.61	82/5227 (1.6%)
1	J	1.01	2/3872 (0.1%)	1.61	80/5227 (1.5%)
1	K	1.02	3/3872 (0.1%)	1.61	78/5227 (1.5%)
1	L	1.01	2/3872 (0.1%)	1.62	83/5227 (1.6%)
1	M	1.01	2/3872 (0.1%)	1.60	78/5227 (1.5%)
1	N	1.08	11/3872 (0.3%)	1.67	94/5227 (1.8%)
All	All	0.94	73/54209 (0.1%)	1.56	1144/73180 (1.6%)

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	19
1	B	0	18
1	C	0	18
1	D	0	18
1	E	0	19
1	F	0	19
1	G	0	18
1	H	1	13
1	I	1	14

Continued on next page...

Continued from previous page...

Mol	Chain	#Chirality outliers	#Planarity outliers
1	J	1	14
1	K	1	15
1	L	1	14
1	M	1	14
1	N	1	18
All	All	7	231

The worst 5 of 73 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	L	518	GLU	CA-CB	13.48	1.83	1.53
1	M	518	GLU	CA-CB	13.48	1.83	1.53
1	H	518	GLU	CA-CB	13.48	1.83	1.53
1	J	518	GLU	CA-CB	13.48	1.83	1.53
1	K	518	GLU	CA-CB	13.47	1.83	1.53

The worst 5 of 1144 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	243	ALA	CB-CA-C	-22.85	75.83	110.10
1	L	243	ALA	CB-CA-C	-22.84	75.83	110.10
1	N	243	ALA	CB-CA-C	-22.84	75.84	110.10
1	J	243	ALA	CB-CA-C	-22.84	75.85	110.10
1	H	243	ALA	CB-CA-C	-22.82	75.86	110.10

5 of 7 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	H	37	ASN	CA
1	I	37	ASN	CA
1	J	37	ASN	CA
1	K	37	ASN	CA
1	L	37	ASN	CA

5 of 231 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	13	ARG	Sidechain
1	A	18	ARG	Sidechain
1	A	190	VAL	Peptide
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	219	0
1	B	3845	0	3962	231	0
1	C	3845	0	3962	229	0
1	D	3845	0	3962	233	0
1	E	3845	0	3962	222	0
1	F	3845	0	3962	232	0
1	G	3845	0	3962	228	0
1	H	3845	0	3965	254	0
1	I	3845	0	3965	251	0
1	J	3845	0	3965	259	0
1	K	3845	0	3965	264	0
1	L	3845	0	3965	262	0
1	M	3845	0	3965	258	0
1	N	3845	0	3965	272	0
2	A	1	0	0	3	0
2	B	1	0	0	3	0
2	C	1	0	0	4	0
2	D	1	0	0	3	0
2	E	1	0	0	4	0
2	F	1	0	0	3	0
2	G	1	0	0	3	0
2	H	1	0	0	5	0
2	I	1	0	0	5	0
2	J	1	0	0	5	0
2	K	1	0	0	5	0
2	L	1	0	0	5	0
2	M	1	0	0	5	0
2	N	1	0	0	5	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
3	H	1	0	0	0	0
3	I	1	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	J	1	0	0	0	0
3	K	1	0	0	0	0
3	L	1	0	0	0	0
3	M	1	0	0	0	0
3	N	1	0	0	0	0
4	A	31	0	12	2	0
4	B	31	0	12	2	0
4	C	31	0	12	3	0
4	D	31	0	12	2	0
4	E	31	0	12	3	0
4	F	31	0	12	2	0
4	G	31	0	12	2	0
4	H	31	0	12	4	0
4	I	31	0	12	4	0
4	J	31	0	12	5	0
4	K	31	0	12	4	0
4	L	31	0	12	5	0
4	M	31	0	12	5	0
4	N	31	0	12	5	0
All	All	54293	0	55662	3207	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 29.

The worst 5 of 3207 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:D:249:ILE:HD12	1:D:262:LEU:CD1	1.30	1.62
1:C:249:ILE:HD12	1:C:262:LEU:CD1	1.30	1.61
1:E:249:ILE:HD12	1:E:262:LEU:CD1	1.30	1.60
1:B:249:ILE:HD12	1:B:262:LEU:CD1	1.30	1.59
1:A:249:ILE:HD12	1:A:262:LEU:CD1	1.29	1.57

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	522/548 (95%)	498 (95%)	21 (4%)	3 (1%)	27	70
1	B	522/548 (95%)	497 (95%)	23 (4%)	2 (0%)	36	77
1	C	522/548 (95%)	497 (95%)	22 (4%)	3 (1%)	27	70
1	D	522/548 (95%)	497 (95%)	22 (4%)	3 (1%)	27	70
1	E	522/548 (95%)	497 (95%)	21 (4%)	4 (1%)	21	65
1	F	522/548 (95%)	497 (95%)	21 (4%)	4 (1%)	21	65
1	G	522/548 (95%)	495 (95%)	24 (5%)	3 (1%)	27	70
1	H	522/548 (95%)	516 (99%)	6 (1%)	0	100	100
1	I	522/548 (95%)	516 (99%)	6 (1%)	0	100	100
1	J	522/548 (95%)	517 (99%)	5 (1%)	0	100	100
1	K	522/548 (95%)	517 (99%)	5 (1%)	0	100	100
1	L	522/548 (95%)	513 (98%)	9 (2%)	0	100	100
1	M	522/548 (95%)	515 (99%)	7 (1%)	0	100	100
1	N	522/548 (95%)	515 (99%)	5 (1%)	2 (0%)	36	77
All	All	7308/7672 (95%)	7087 (97%)	197 (3%)	24 (0%)	47	81

5 of 24 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	G	199	TYR
1	N	207	LYS
1	N	208	PRO
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%)	11	37
1	B	402/414 (97%)	366 (91%)	36 (9%)	10	36
1	C	402/414 (97%)	367 (91%)	35 (9%)	11	37
1	D	402/414 (97%)	369 (92%)	33 (8%)	12	41
1	E	402/414 (97%)	368 (92%)	34 (8%)	12	40
1	F	402/414 (97%)	367 (91%)	35 (9%)	11	37
1	G	402/414 (97%)	367 (91%)	35 (9%)	11	37
1	H	402/414 (97%)	359 (89%)	43 (11%)	7	28
1	I	402/414 (97%)	361 (90%)	41 (10%)	8	30
1	J	402/414 (97%)	361 (90%)	41 (10%)	8	30
1	K	402/414 (97%)	358 (89%)	44 (11%)	7	28
1	L	402/414 (97%)	364 (90%)	38 (10%)	9	33
1	M	402/414 (97%)	358 (89%)	44 (11%)	7	28
1	N	402/414 (97%)	360 (90%)	42 (10%)	8	30
All	All	5628/5796 (97%)	5092 (90%)	536 (10%)	13	33

5 of 536 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	G	522	THR
1	I	197	ARG
1	N	31	LEU
1	H	63	GLU
1	H	325	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 18 such sidechains are listed below:

Mol	Chain	Res	Type
1	F	475	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	G	351	GLN
1	K	401	HIS
1	D	475	ASN
1	E	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 42 ligands modelled in this entry, 14 are monoatomic and 14 are modelled with single atom - leaving 14 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	0.72	0	27,52,52	1.77	3 (11%)
4	ATP	B	1527	3	27,33,33	0.66	0	27,52,52	1.65	3 (11%)
4	ATP	C	1527	3	27,33,33	0.72	0	27,52,52	1.77	3 (11%)
4	ATP	D	1527	3	27,33,33	0.67	0	27,52,52	1.61	3 (11%)
4	ATP	E	1527	3	27,33,33	0.72	0	27,52,52	1.77	3 (11%)
4	ATP	F	1527	3	27,33,33	0.67	0	27,52,52	1.61	3 (11%)
4	ATP	G	1527	3	27,33,33	0.72	0	27,52,52	1.77	3 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	ATP	H	1527	3	27,33,33	0.76	0	27,52,52	1.70	3 (11%)
4	ATP	I	1527	3	27,33,33	0.77	0	27,52,52	1.70	4 (14%)
4	ATP	J	1527	3	27,33,33	0.77	0	27,52,52	1.70	3 (11%)
4	ATP	K	1527	3	27,33,33	0.76	0	27,52,52	1.70	3 (11%)
4	ATP	L	1527	3	27,33,33	0.76	0	27,52,52	1.70	3 (11%)
4	ATP	M	1527	3	27,33,33	0.77	0	27,52,52	1.70	4 (14%)
4	ATP	N	1527	3	27,33,33	0.76	0	27,52,52	1.69	3 (11%)

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
4	ATP	H	1527	3	-	0/18/38/38	0/3/3/3
4	ATP	I	1527	3	-	0/18/38/38	0/3/3/3
4	ATP	J	1527	3	-	0/18/38/38	0/3/3/3
4	ATP	K	1527	3	-	0/18/38/38	0/3/3/3
4	ATP	L	1527	3	-	0/18/38/38	0/3/3/3
4	ATP	M	1527	3	-	0/18/38/38	0/3/3/3
4	ATP	N	1527	3	-	0/18/38/38	0/3/3/3

There are no bond length outliers.

The worst 5 of 44 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	E	1527	ATP	PB-O3B-PG	-5.86	112.94	132.63
4	C	1527	ATP	PB-O3B-PG	-5.85	112.95	132.63
4	A	1527	ATP	PB-O3B-PG	-5.85	112.96	132.63
4	G	1527	ATP	PB-O3B-PG	-5.85	112.96	132.63
4	M	1527	ATP	PA-O3A-PB	-5.47	114.23	132.63

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

14 monomers are involved in 48 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1527	ATP	2	0
4	B	1527	ATP	2	0
4	C	1527	ATP	3	0
4	D	1527	ATP	2	0
4	E	1527	ATP	3	0
4	F	1527	ATP	2	0
4	G	1527	ATP	2	0
4	H	1527	ATP	4	0
4	I	1527	ATP	4	0
4	J	1527	ATP	5	0
4	K	1527	ATP	4	0
4	L	1527	ATP	5	0
4	M	1527	ATP	5	0
4	N	1527	ATP	5	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

Continued on next page...

Continued from previous page...

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
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