



wwPDB EM Map/Model Validation Report ⓘ

Apr 10, 2016 – 02:06 PM BST

PDB ID : 4AB2
EMDB ID: : EMD-1998
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 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

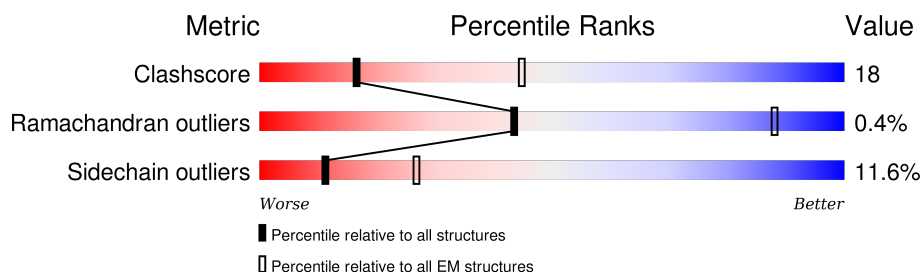
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 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	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	548	55% 29% 10% . .
1	B	548	55% 29% 10% . .
1	C	548	55% 29% 10% . .
1	D	548	56% 28% 10% . .
1	E	548	55% 29% 10% . .
1	F	548	55% 28% 10% . .
1	G	548	55% 29% 10% . .
1	H	548	57% 28% 9% . .
1	I	548	57% 28% 9% . .

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
4	PO4	A	1528	-	-	X	-
4	PO4	B	1528	-	-	X	-
4	PO4	C	1528	-	-	X	-
4	PO4	D	1528	-	-	X	-
4	PO4	E	1528	-	-	X	-
4	PO4	F	1528	-	-	X	-
4	PO4	G	1528	-	-	X	-
4	PO4	H	1528	-	-	X	-
4	PO4	I	1528	-	-	X	-
4	PO4	J	1528	-	-	X	-
4	PO4	K	1528	-	-	X	-
4	PO4	L	1528	-	-	X	-
4	PO4	M	1528	-	-	X	-
4	PO4	N	1528	-	-	X	-

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 54474 atoms, of which 168 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
			3846	2391	665	770	20		
1	C	524	Total	C	N	O	S	0	1
			3846	2391	665	770	20		
1	D	524	Total	C	N	O	S	0	1
			3846	2391	665	770	20		
1	E	524	Total	C	N	O	S	0	1
			3846	2391	665	770	20		
1	F	524	Total	C	N	O	S	0	1
			3846	2391	665	770	20		
1	G	524	Total	C	N	O	S	0	1
			3846	2391	665	770	20		
1	H	524	Total	C	N	O	S	0	1
			3846	2391	665	770	20		
1	I	524	Total	C	N	O	S	0	1
			3846	2391	665	770	20		
1	J	524	Total	C	N	O	S	0	1
			3846	2391	665	770	20		
1	K	524	Total	C	N	O	S	0	1
			3846	2391	665	770	20		
1	L	524	Total	C	N	O	S	0	1
			3846	2391	665	770	20		
1	M	524	Total	C	N	O	S	0	1
			3846	2391	665	770	20		
1	N	524	Total	C	N	O	S	0	1
			3846	2391	665	770	20		

There are 14 discrepancies between the modelled and reference sequences:

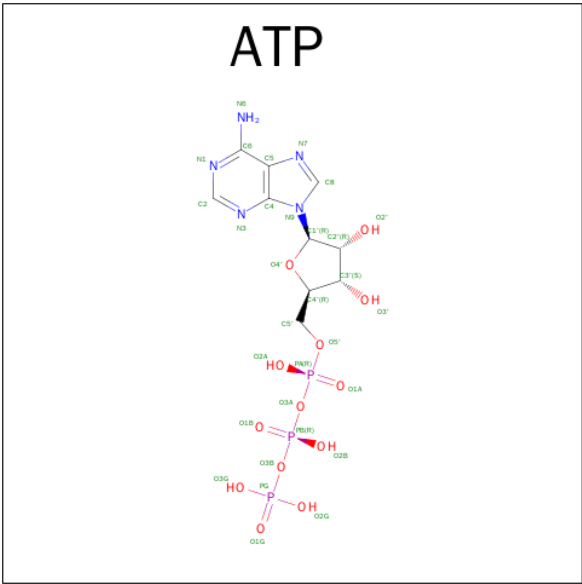
Chain	Residue	Modelled	Actual	Comment	Reference
A	398	ALA	ASP	ENGINEERED MUTATION	UNP P0A6F5
B	398	ALA	ASP	ENGINEERED MUTATION	UNP P0A6F5

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



Continued from previous page...

Mol	Chain	Residues	Atoms						AltConf
2	F	1	Total 43	C 10	H 12	N 5	O 13	P 3	0
2	G	1	Total 43	C 10	H 12	N 5	O 13	P 3	0
2	H	1	Total 43	C 10	H 12	N 5	O 13	P 3	0
2	I	1	Total 43	C 10	H 12	N 5	O 13	P 3	0
2	J	1	Total 43	C 10	H 12	N 5	O 13	P 3	0
2	K	1	Total 43	C 10	H 12	N 5	O 13	P 3	0
2	L	1	Total 43	C 10	H 12	N 5	O 13	P 3	0
2	M	1	Total 43	C 10	H 12	N 5	O 13	P 3	0
2	N	1	Total 43	C 10	H 12	N 5	O 13	P 3	0

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

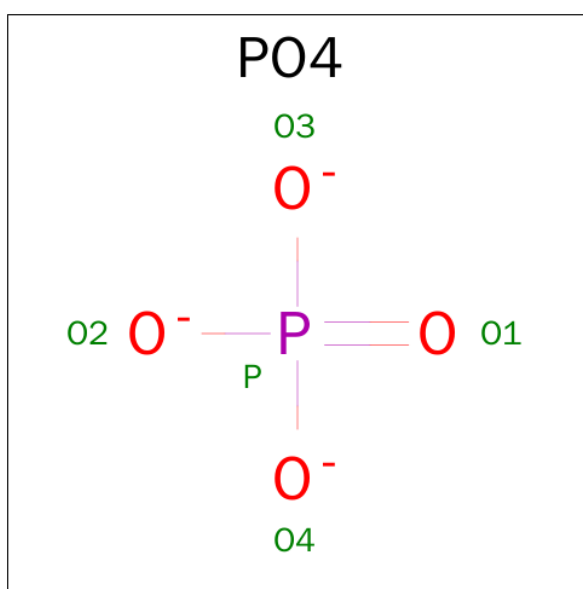
Mol	Chain	Residues	Atoms		AltConf
3	G	1	Total 1	Mg 1	0
3	J	1	Total 1	Mg 1	0
3	D	1	Total 1	Mg 1	0
3	K	1	Total 1	Mg 1	0
3	E	1	Total 1	Mg 1	0
3	H	1	Total 1	Mg 1	0
3	B	1	Total 1	Mg 1	0
3	I	1	Total 1	Mg 1	0
3	C	1	Total 1	Mg 1	0
3	A	1	Total 1	Mg 1	0

Continued on next page...

Continued from previous page...

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

- Molecule 4 is PHOSPHATE ION (three-letter code: PO4) (formula: O₄P).

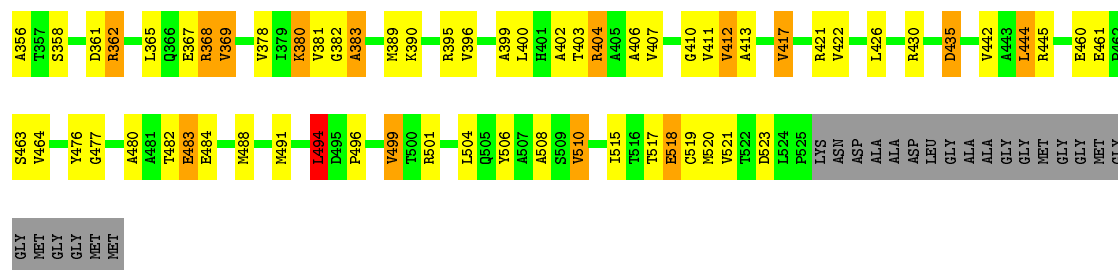


Mol	Chain	Residues	Atoms		AltConf
4	A	1	Total 1	P 1	0
4	B	1	Total 1	P 1	0
4	C	1	Total 1	P 1	0
4	D	1	Total 1	P 1	0
4	E	1	Total 1	P 1	0
4	F	1	Total 1	P 1	0
4	G	1	Total 1	P 1	0

Continued on next page...

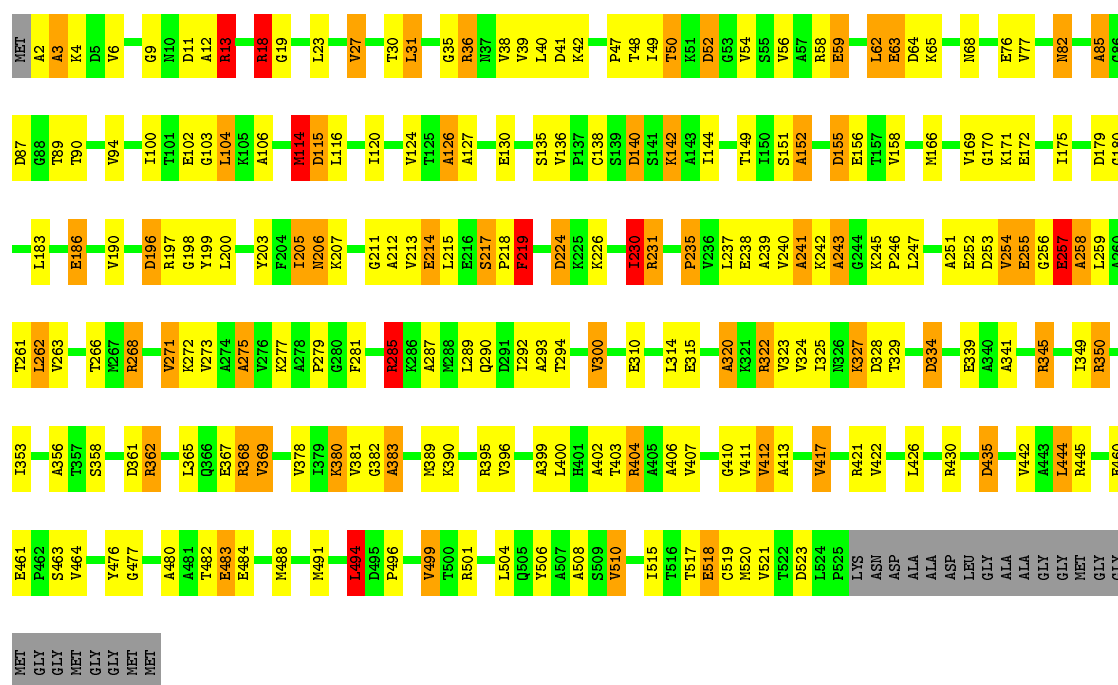
Continued from previous page...

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



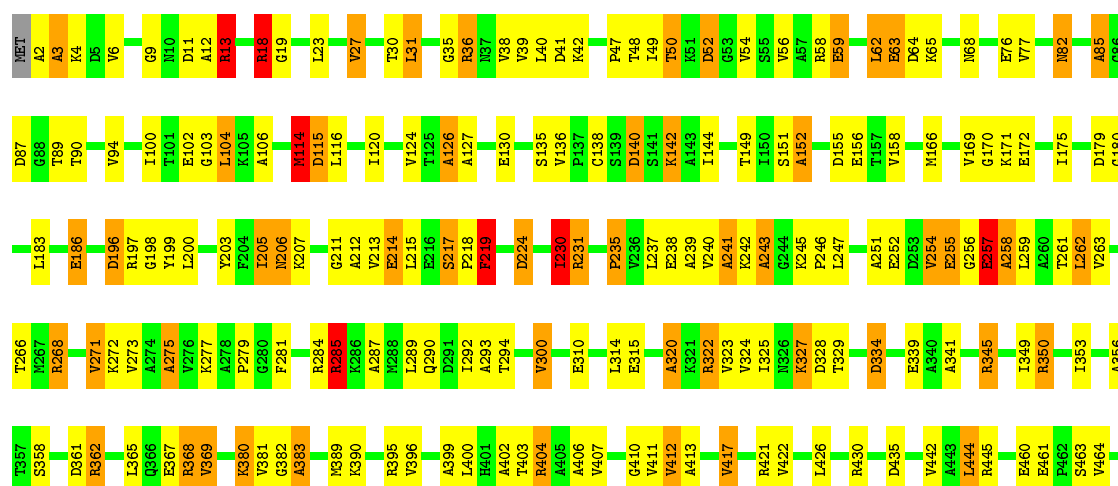
• Molecule 1: 60 KDA CHAPERONIN

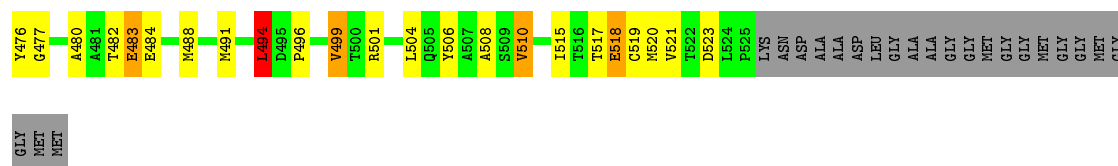
Chain C: 55% 29% 10%



• Molecule 1: 60 KDA CHAPERONIN

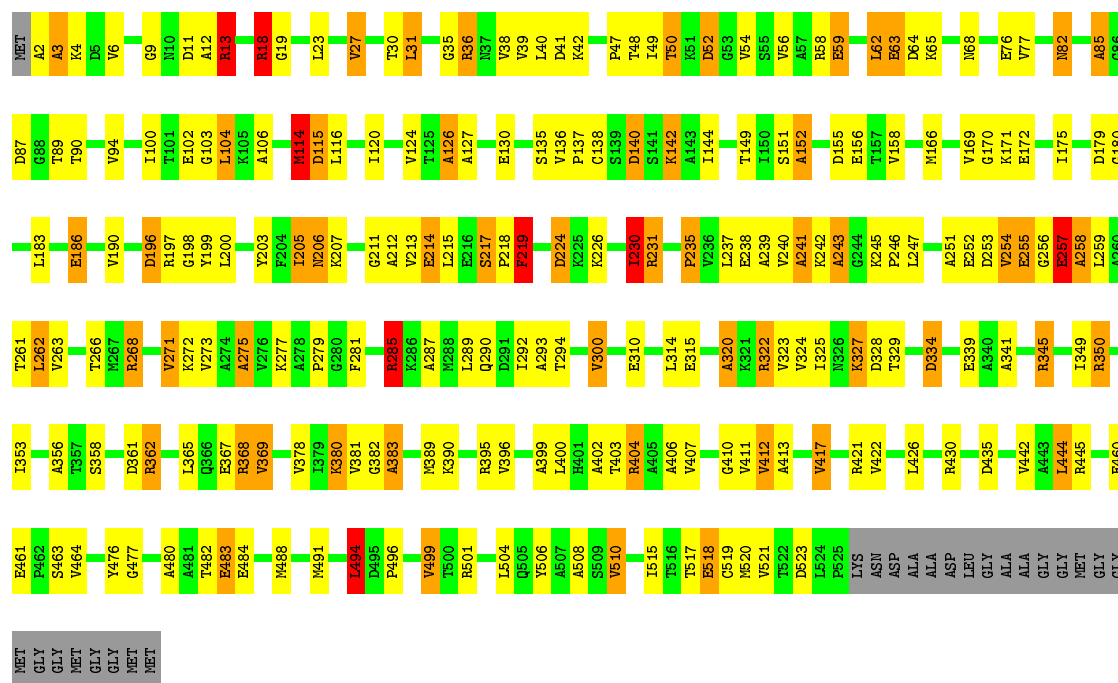
Chain D: 56% 28% 10%





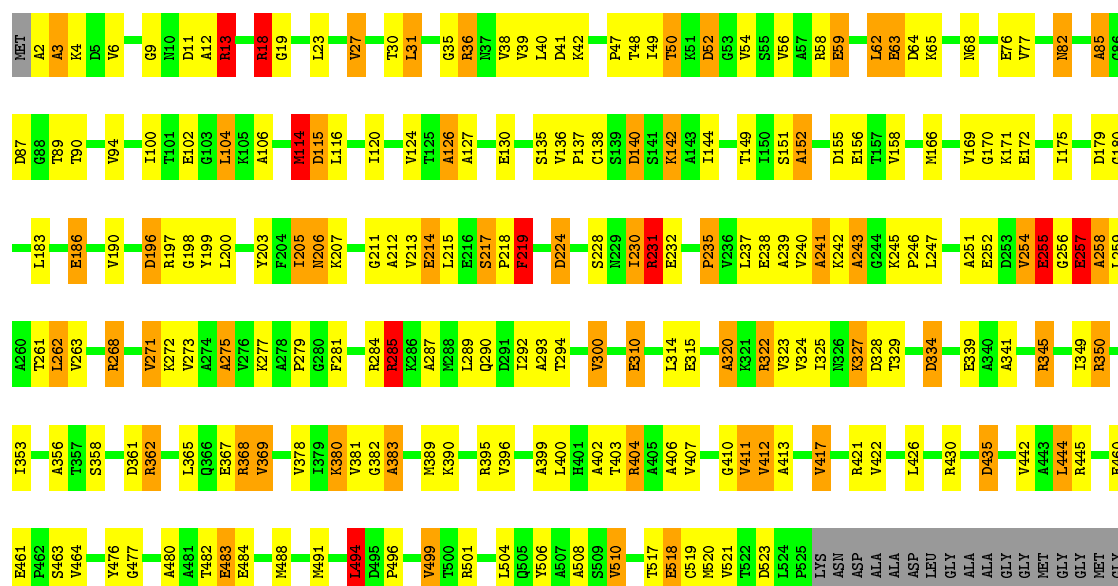
• Molecule 1: 60 KDA CHAPERONIN

Chain E: 55% 29% 10% . .



• Molecule 1: 60 KDA CHAPERONIN

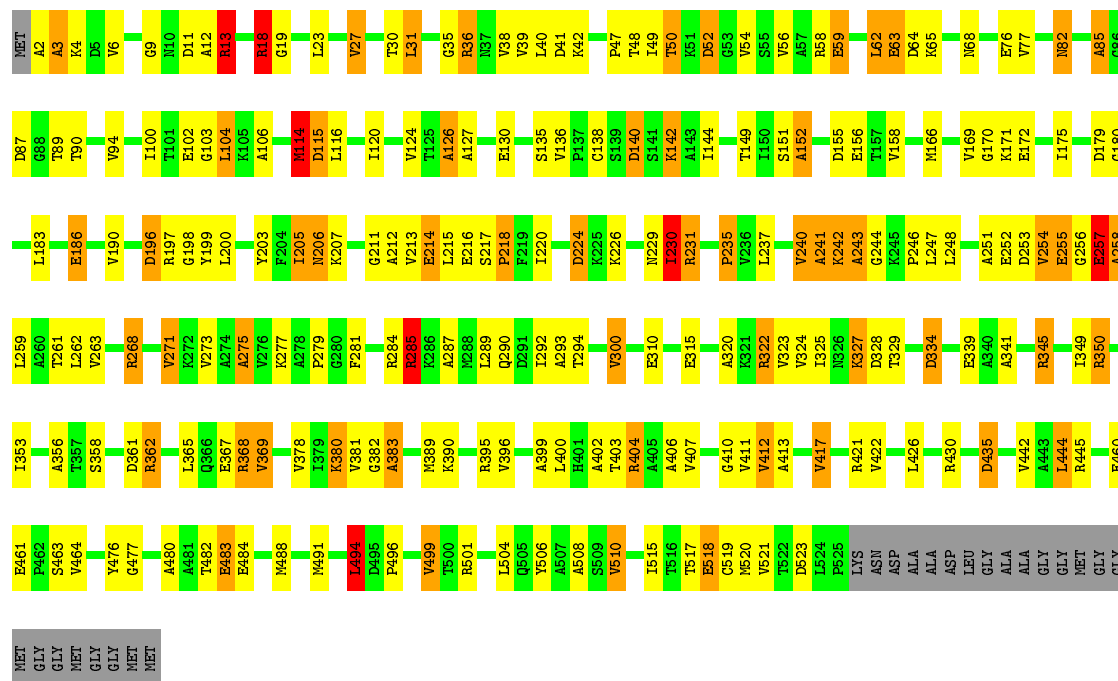
Chain F: 55% 28% 10% . .



GLY
MET
GLY
GLY
MET
MET

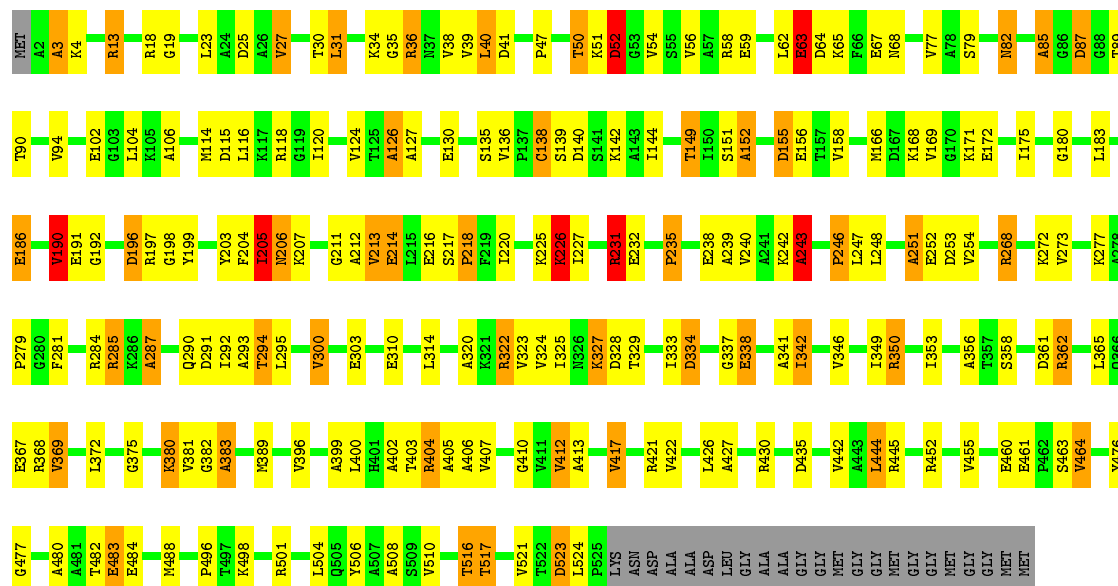
• Molecule 1: 60 KDA CHAPERONIN

Chain G: 55% 29% 10% . .

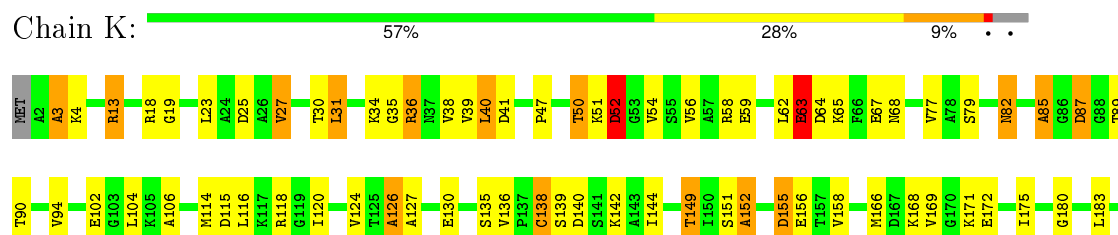


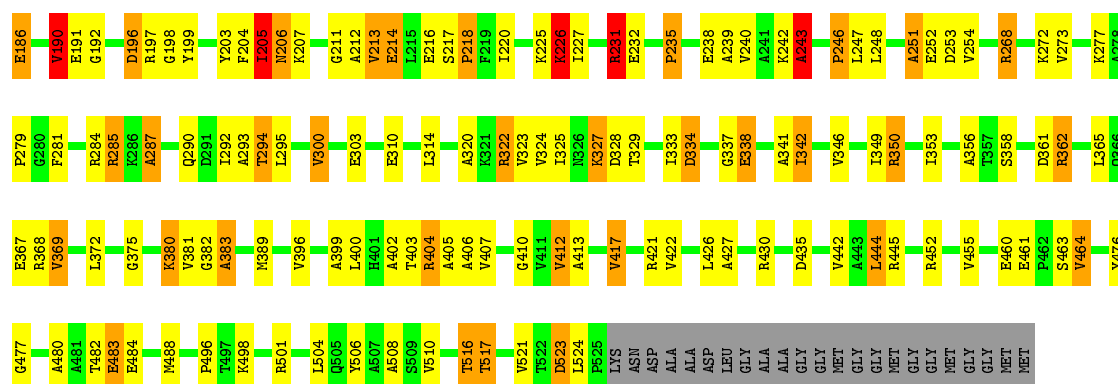
• Molecule 1: 60 KDA CHAPERONIN

Chain H: 57% 28% 9% . .



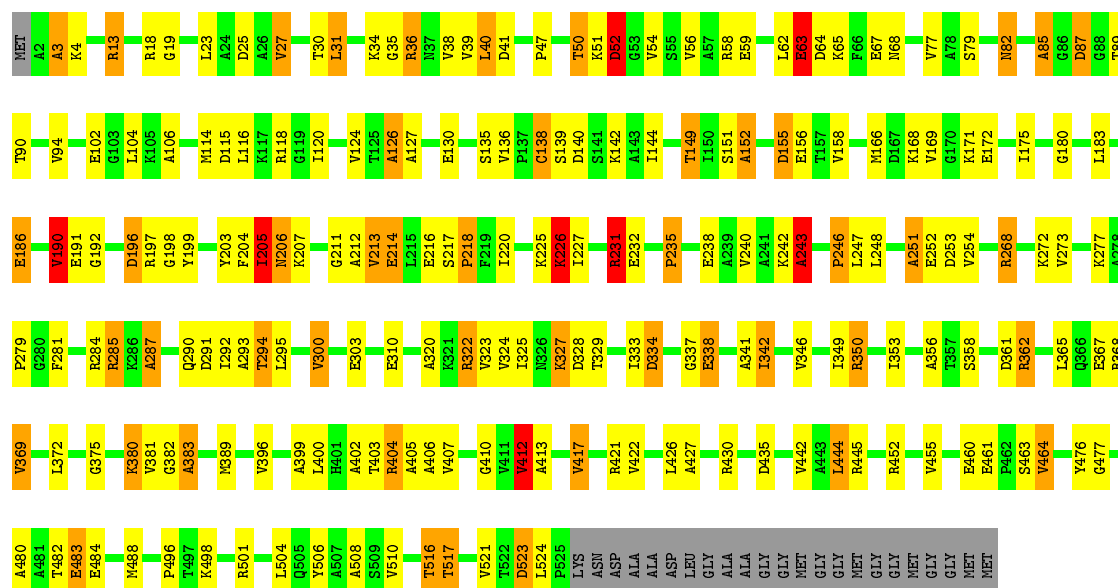
• Molecule 1: 60 KDA CHAPERONIN





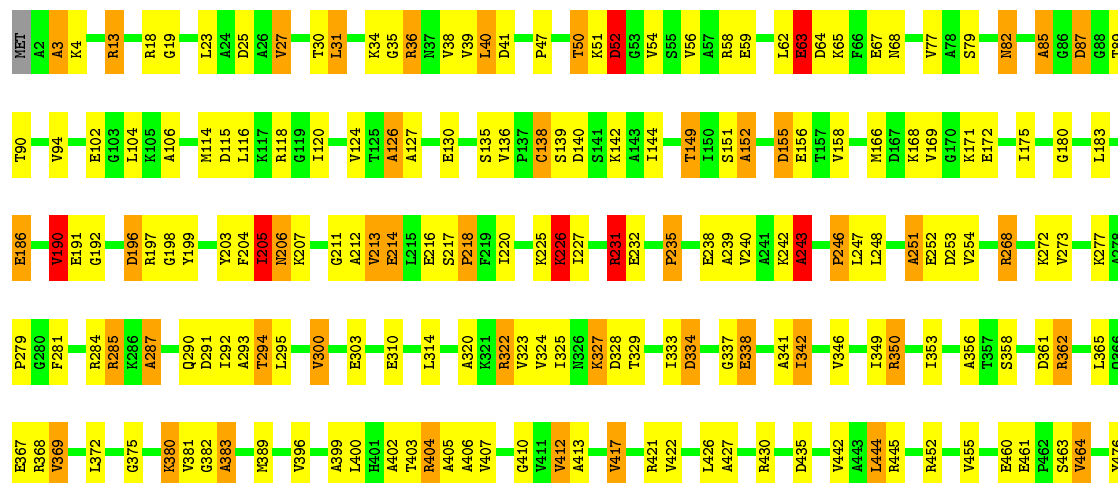
• Molecule 1: 60 KDA CHAPERONIN

Chain L: 58% 28% 9% . .

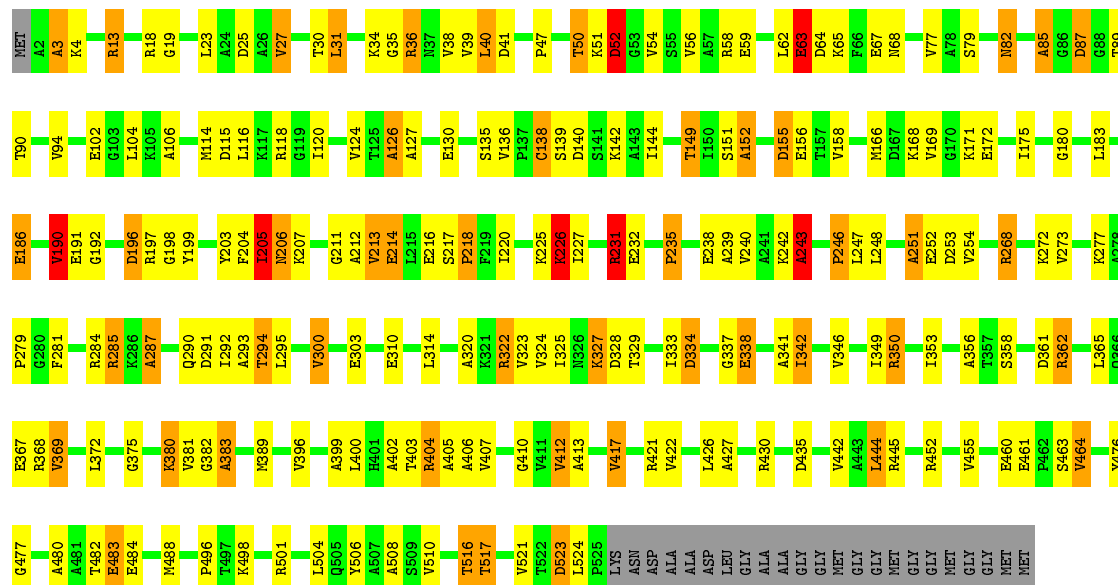


• Molecule 1: 60 KDA CHAPERONIN

Chain M: 57% 28% 9% . .



● Molecule 1: 60 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 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	Not provided	Depositor
Image detector	GATAN ULTRASCAN 4000 4K CCD CAM-ERA	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	1.02	1/3873 (0.0%)	1.53	78/5229 (1.5%)
1	B	1.02	1/3873 (0.0%)	1.53	78/5229 (1.5%)
1	C	1.02	1/3873 (0.0%)	1.53	78/5229 (1.5%)
1	D	1.02	1/3873 (0.0%)	1.53	78/5229 (1.5%)
1	E	1.02	1/3873 (0.0%)	1.53	77/5229 (1.5%)
1	F	1.01	1/3873 (0.0%)	1.51	76/5229 (1.5%)
1	G	1.02	1/3873 (0.0%)	1.52	72/5229 (1.4%)
1	H	1.00	0/3873	1.45	72/5229 (1.4%)
1	I	1.00	0/3873	1.44	71/5229 (1.4%)
1	J	1.00	0/3873	1.45	74/5229 (1.4%)
1	K	1.00	0/3873	1.45	72/5229 (1.4%)
1	L	1.00	0/3873	1.45	74/5229 (1.4%)
1	M	1.00	0/3873	1.45	73/5229 (1.4%)
1	N	1.00	0/3873	1.45	73/5229 (1.4%)
All	All	1.01	7/54222 (0.0%)	1.49	1046/73206 (1.4%)

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	11
1	B	0	11
1	C	0	11
1	D	0	11
1	E	0	11
1	F	1	12
1	G	0	12
1	H	0	8
1	I	0	8

Continued on next page...

Continued from previous page...

Mol	Chain	#Chirality outliers	#Planarity outliers
1	J	0	8
1	K	0	8
1	L	0	8
1	M	0	8
1	N	0	8
All	All	1	135

The worst 5 of 7 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	63	GLU	CA-CB	6.48	1.68	1.53
1	F	63	GLU	CA-CB	6.45	1.68	1.53
1	G	63	GLU	CA-CB	6.45	1.68	1.53
1	B	63	GLU	CA-CB	6.44	1.68	1.53
1	A	63	GLU	CA-CB	6.44	1.68	1.53

The worst 5 of 1046 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	63	GLU	N-CA-CB	-18.59	77.15	110.60
1	F	63	GLU	N-CA-CB	-18.58	77.16	110.60
1	A	63	GLU	N-CA-CB	-18.58	77.16	110.60
1	C	63	GLU	N-CA-CB	-18.57	77.17	110.60
1	E	63	GLU	N-CA-CB	-18.57	77.17	110.60

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	F	257	GLU	CA

5 of 135 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	18	ARG	Sidechain
1	A	197	ARG	Sidechain
1	A	241	ALA	Peptide
1	A	245	LYS	Peptide
1	A	256	GLY	Peptide

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	3970	181	0
1	B	3846	0	3970	181	0
1	C	3846	0	3970	179	0
1	D	3846	0	3970	181	0
1	E	3846	0	3970	182	0
1	F	3846	0	3970	183	0
1	G	3846	0	3970	182	0
1	H	3846	0	3970	127	0
1	I	3846	0	3970	129	0
1	J	3846	0	3970	128	0
1	K	3846	0	3970	127	0
1	L	3846	0	3970	125	0
1	M	3846	0	3970	127	0
1	N	3846	0	3970	128	0
2	A	31	12	12	3	0
2	B	31	12	12	3	0
2	C	31	12	12	3	0
2	D	31	12	12	3	0
2	E	31	12	12	3	0
2	F	31	12	12	3	0
2	G	31	12	12	3	0
2	H	31	12	12	3	0
2	I	31	12	12	3	0
2	J	31	12	12	3	0
2	K	31	12	12	3	0
2	L	31	12	12	3	0
2	M	31	12	12	3	0
2	N	31	12	12	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
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	1	0	0	4	0
4	B	1	0	0	4	0
4	C	1	0	0	4	0
4	D	1	0	0	4	0
4	E	1	0	0	4	0
4	F	1	0	0	4	0
4	G	1	0	0	4	0
4	H	1	0	0	4	0
4	I	1	0	0	4	0
4	J	1	0	0	4	0
4	K	1	0	0	4	0
4	L	1	0	0	4	0
4	M	1	0	0	4	0
4	N	1	0	0	4	0
All	All	54306	168	55748	2023	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 2023 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:3:ALA:HA	1:F:63:GLU:CA	1.69	1.23
1:D:3:ALA:HA	1:E:63:GLU:CA	1.69	1.22
1:F:3:ALA:HA	1:G:63:GLU:CA	1.69	1.22
1:C:3:ALA:HA	1:D:63:GLU:CA	1.69	1.22
1:N:30:THR:HA	1:N:35:GLY:HA3	1.22	1.21

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%)	516 (99%)	4 (1%)	2 (0%)	39	80
1	B	522/548 (95%)	516 (99%)	3 (1%)	3 (1%)	30	74
1	C	522/548 (95%)	516 (99%)	3 (1%)	3 (1%)	30	74
1	D	522/548 (95%)	516 (99%)	3 (1%)	3 (1%)	30	74
1	E	522/548 (95%)	515 (99%)	4 (1%)	3 (1%)	30	74
1	F	522/548 (95%)	516 (99%)	3 (1%)	3 (1%)	30	74
1	G	522/548 (95%)	518 (99%)	3 (1%)	1 (0%)	52	86
1	H	522/548 (95%)	518 (99%)	2 (0%)	2 (0%)	39	80
1	I	522/548 (95%)	518 (99%)	2 (0%)	2 (0%)	39	80
1	J	522/548 (95%)	518 (99%)	2 (0%)	2 (0%)	39	80
1	K	522/548 (95%)	518 (99%)	2 (0%)	2 (0%)	39	80
1	L	522/548 (95%)	518 (99%)	2 (0%)	2 (0%)	39	80
1	M	522/548 (95%)	518 (99%)	2 (0%)	2 (0%)	39	80
1	N	522/548 (95%)	518 (99%)	2 (0%)	2 (0%)	39	80
All	All	7308/7672 (95%)	7239 (99%)	37 (0%)	32 (0%)	43	80

5 of 32 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	257	GLU
1	B	257	GLU
1	C	257	GLU
1	D	257	GLU
1	E	257	GLU

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%)	357 (89%)	45 (11%)	7	33
1	B	402/414 (97%)	356 (89%)	46 (11%)	7	33
1	C	402/414 (97%)	356 (89%)	46 (11%)	7	33
1	D	402/414 (97%)	357 (89%)	45 (11%)	7	33
1	E	402/414 (97%)	357 (89%)	45 (11%)	7	33
1	F	402/414 (97%)	356 (89%)	46 (11%)	7	33
1	G	402/414 (97%)	357 (89%)	45 (11%)	7	33
1	H	402/414 (97%)	354 (88%)	48 (12%)	6	31
1	I	402/414 (97%)	355 (88%)	47 (12%)	7	32
1	J	402/414 (97%)	354 (88%)	48 (12%)	6	31
1	K	402/414 (97%)	354 (88%)	48 (12%)	6	31
1	L	402/414 (97%)	354 (88%)	48 (12%)	6	31
1	M	402/414 (97%)	354 (88%)	48 (12%)	6	31
1	N	402/414 (97%)	354 (88%)	48 (12%)	6	31
All	All	5628/5796 (97%)	4975 (88%)	653 (12%)	11	32

5 of 653 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	G	240	VAL
1	H	504	LEU
1	M	484	GLU
1	G	334	ASP
1	H	171	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 19 such sidechains are listed below:

Mol	Chain	Res	Type
1	E	229	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	F	453	GLN
1	K	453	GLN
1	D	453	GLN
1	L	453	GLN

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	$\# Z > 2$
2	ATP	A	1525	3	26,33,33	0.72	0	26,52,52	1.14	3 (11%)
2	ATP	B	1525	3	26,33,33	0.72	0	26,52,52	1.14	3 (11%)
2	ATP	C	1526	3	26,33,33	0.73	0	26,52,52	1.14	3 (11%)
2	ATP	D	1525	3	26,33,33	0.73	0	26,52,52	1.14	3 (11%)
2	ATP	E	1525	3	26,33,33	0.72	0	26,52,52	1.14	3 (11%)
2	ATP	F	1525	3	26,33,33	0.72	0	26,52,52	1.14	3 (11%)
2	ATP	G	1525	3	26,33,33	0.73	0	26,52,52	1.14	3 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	ATP	H	1527	3	26,33,33	0.71	0	26,52,52	1.11	4 (15%)
2	ATP	I	1525	3	26,33,33	0.72	0	26,52,52	1.11	4 (15%)
2	ATP	J	1526	3	26,33,33	0.72	0	26,52,52	1.11	3 (11%)
2	ATP	K	1527	3	26,33,33	0.71	0	26,52,52	1.11	4 (15%)
2	ATP	L	1527	3	26,33,33	0.71	0	26,52,52	1.11	4 (15%)
2	ATP	M	1527	3	26,33,33	0.72	0	26,52,52	1.11	4 (15%)
2	ATP	N	1527	3	26,33,33	0.71	0	26,52,52	1.11	4 (15%)

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
2	ATP	A	1525	3	-	0/18/38/38	0/3/3/3
2	ATP	B	1525	3	-	0/18/38/38	0/3/3/3
2	ATP	C	1526	3	-	0/18/38/38	0/3/3/3
2	ATP	D	1525	3	-	0/18/38/38	0/3/3/3
2	ATP	E	1525	3	-	0/18/38/38	0/3/3/3
2	ATP	F	1525	3	-	0/18/38/38	0/3/3/3
2	ATP	G	1525	3	-	0/18/38/38	0/3/3/3
2	ATP	H	1527	3	-	0/18/38/38	0/3/3/3
2	ATP	I	1525	3	-	0/18/38/38	0/3/3/3
2	ATP	J	1526	3	-	0/18/38/38	0/3/3/3
2	ATP	K	1527	3	-	0/18/38/38	0/3/3/3
2	ATP	L	1527	3	-	0/18/38/38	0/3/3/3
2	ATP	M	1527	3	-	0/18/38/38	0/3/3/3
2	ATP	N	1527	3	-	0/18/38/38	0/3/3/3

There are no bond length outliers.

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1525	ATP	C5'-C4'-C3'	-2.53	105.40	115.20
2	F	1525	ATP	C5'-C4'-C3'	-2.53	105.43	115.20
2	D	1525	ATP	C5'-C4'-C3'	-2.52	105.45	115.20
2	G	1525	ATP	C5'-C4'-C3'	-2.52	105.46	115.20
2	C	1526	ATP	C5'-C4'-C3'	-2.52	105.47	115.20

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

14 monomers are involved in 42 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1525	ATP	3	0
2	B	1525	ATP	3	0
2	C	1526	ATP	3	0
2	D	1525	ATP	3	0
2	E	1525	ATP	3	0
2	F	1525	ATP	3	0
2	G	1525	ATP	3	0
2	H	1527	ATP	3	0
2	I	1525	ATP	3	0
2	J	1526	ATP	3	0
2	K	1527	ATP	3	0
2	L	1527	ATP	3	0
2	M	1527	ATP	3	0
2	N	1527	ATP	3	0

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.