wwPDB EM Map/Model Validation Report (i)

Apr 10, 2016 – 02:04 PM BST

PDB ID	:	4AAQ
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	:	2011-12-05
Resolution	:	8.00 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

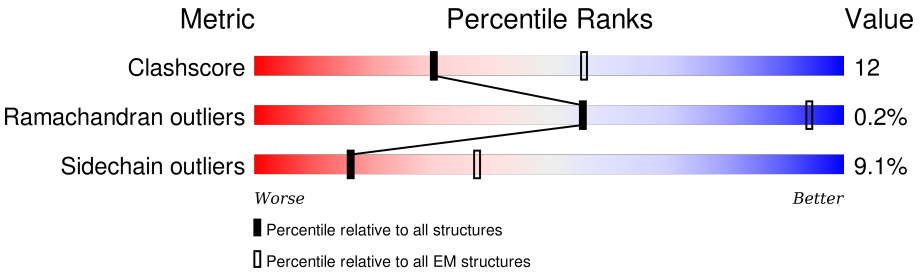
MolProbity	:	4.02b-467
Mogul	:	1.7.1 (RC1), CSD as537be (2016)
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk27241

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 8.00 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 <=5%

Mol	Chain	Length	Quality of chain
1	A	548	61% 27% 7%
1	B	548	60% 27% 7%
1	C	548	61% 26% 7%
1	D	548	60% 27% 8%
1	E	548	61% 27% 7%
1	F	548	61% 27% 7%
1	G	548	60% 27% 8%
1	H	548	78% 14%
1	I	548	78% 14%

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Mol	Chain	Length	Quality of chain
1	J	548	78% 14%
1	K	548	79% 14%
1	L	548	78% 14%
1	M	548	78% 14%
1	N	548	78% 14%

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
3	PO4	A	1526	-	-	X	-
3	PO4	B	1526	-	-	X	-
3	PO4	C	1527	-	-	X	-
3	PO4	D	1526	-	-	X	-
3	PO4	E	1526	-	-	X	-
3	PO4	F	1525	-	-	X	-
3	PO4	G	1525	-	-	X	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 54159 atoms, of which 84 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

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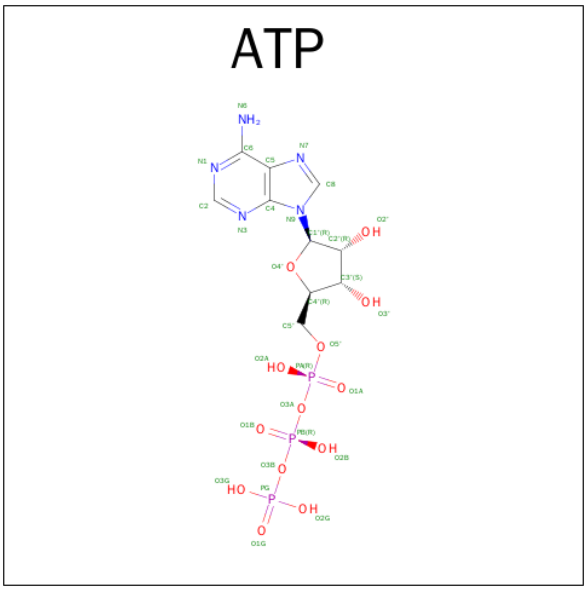
Chain	Residue	Modelled	Actual	Comment	Reference
C	398	ALA	ASP	ENGINEERED MUTATION	UNP P0A6F5
D	398	ALA	ASP	ENGINEERED MUTATION	UNP P0A6F5
E	398	ALA	ASP	ENGINEERED MUTATION	UNP P0A6F5
F	398	ALA	ASP	ENGINEERED MUTATION	UNP P0A6F5
G	398	ALA	ASP	ENGINEERED MUTATION	UNP P0A6F5
H	398	ALA	ASP	ENGINEERED MUTATION	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 ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).



Mol	Chain	Residues	Atoms						AltConf
2	A	1	Total	C	H	N	O	P	0
			43	10	12	5	13	3	
2	B	1	Total	C	H	N	O	P	0
			43	10	12	5	13	3	
2	C	1	Total	C	H	N	O	P	0
			43	10	12	5	13	3	
2	D	1	Total	C	H	N	O	P	0
			43	10	12	5	13	3	
2	E	1	Total	C	H	N	O	P	0
			43	10	12	5	13	3	

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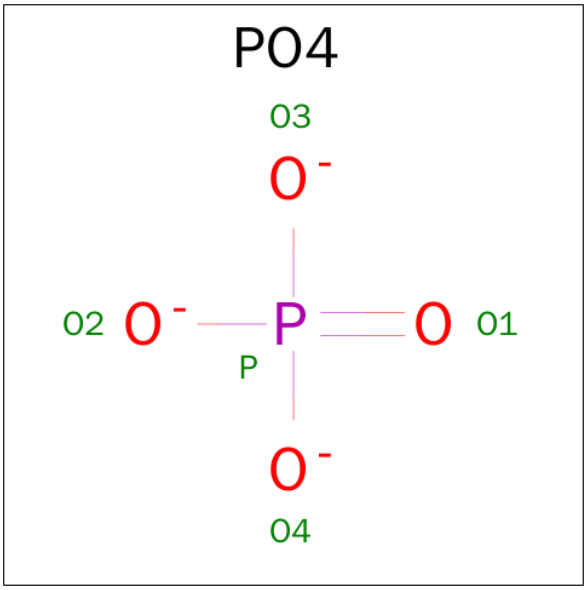
Mol	Chain	Residues	Atoms						AltConf
2	F	1	Total	C	H	N	O	P	0
			43	10	12	5	13	3	
2	G	1	Total	C	H	N	O	P	0
			43	10	12	5	13	3	

- Molecule 3 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).



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

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

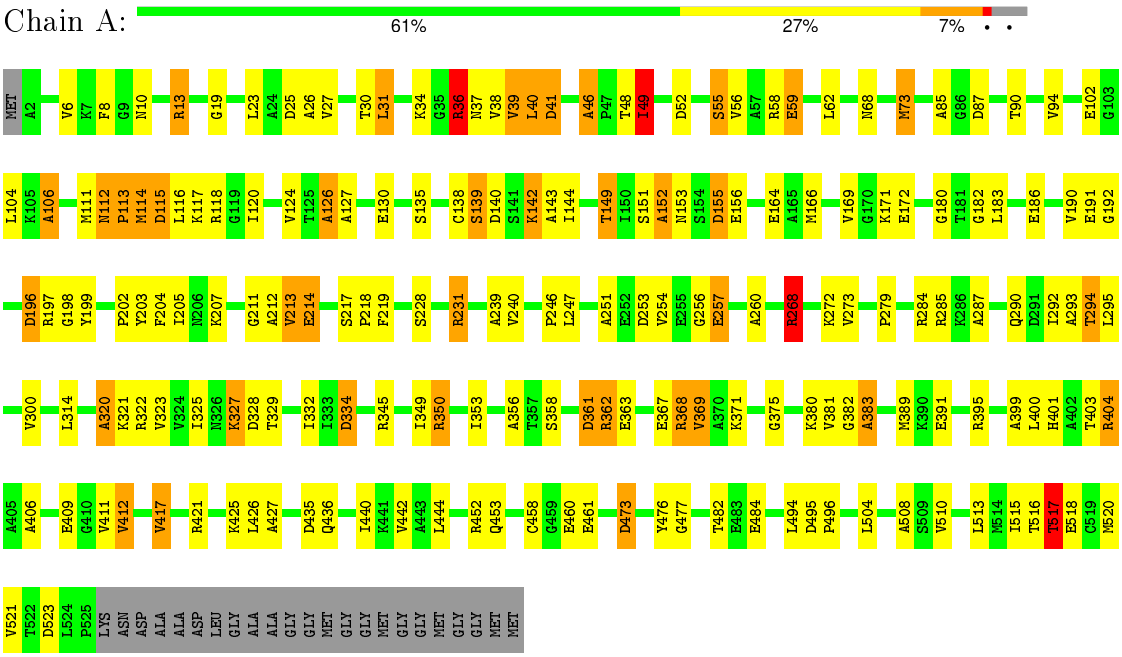
Mol	Chain	Residues	Atoms	AltConf
4	G	1	Total Mg 1 1	0
4	D	1	Total Mg 1 1	0
4	E	1	Total Mg 1 1	0
4	B	1	Total Mg 1 1	0
4	C	1	Total Mg 1 1	0
4	A	1	Total Mg 1 1	0
4	F	1	Total Mg 1 1	0

3 Residue-property plots (i)

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.

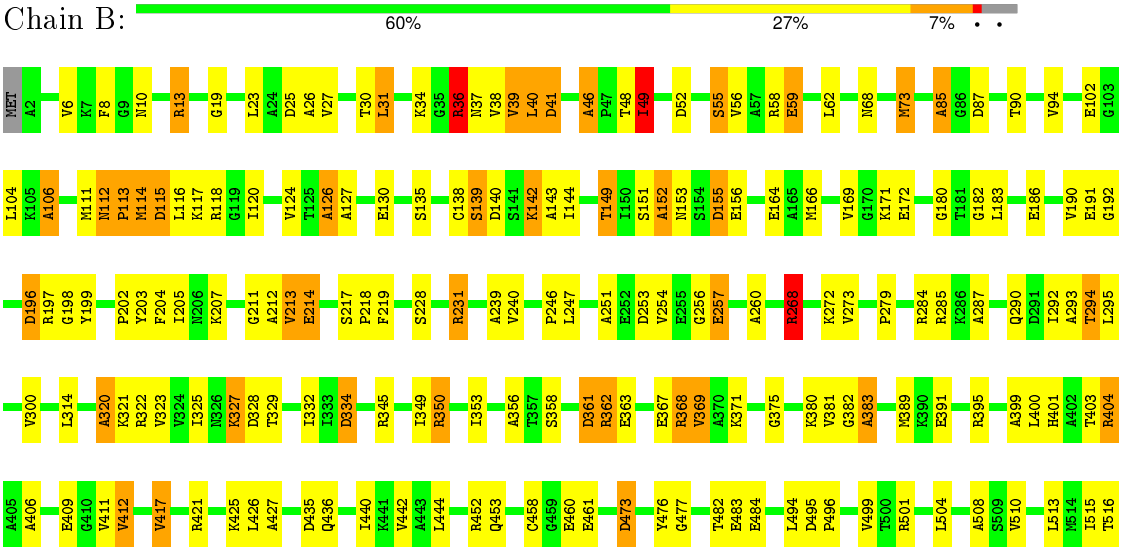
- Molecule 1: 60 KDA CHAPERONIN

Chain A:



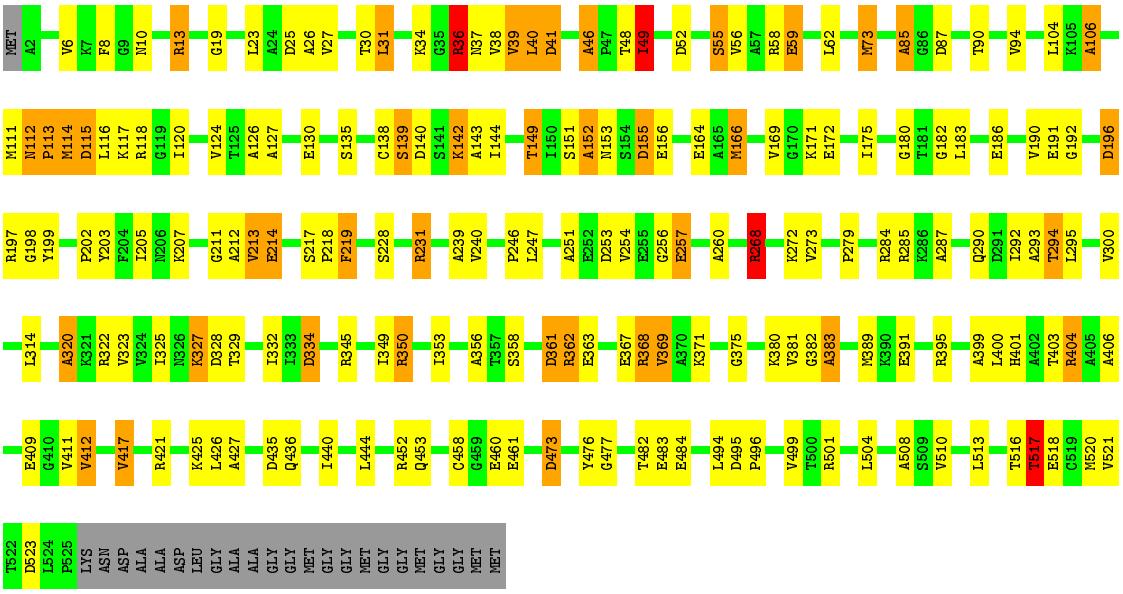
- Molecule 1: 60 KDA CHAPERONIN

Chain B:



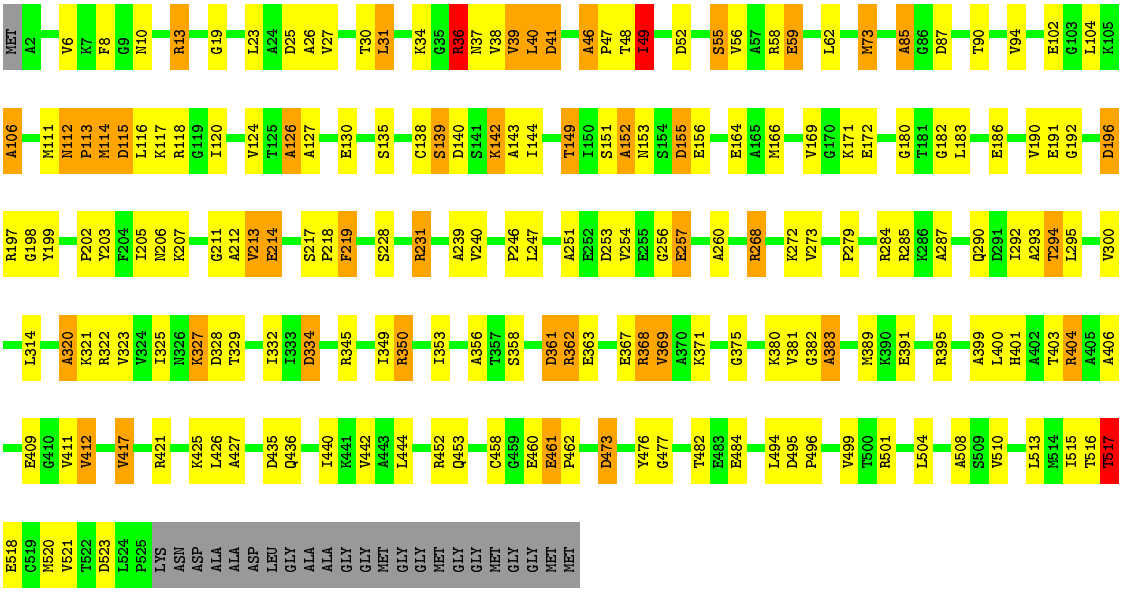
• Molecule 1: 60 KDA CHAPERONIN

Chain C:



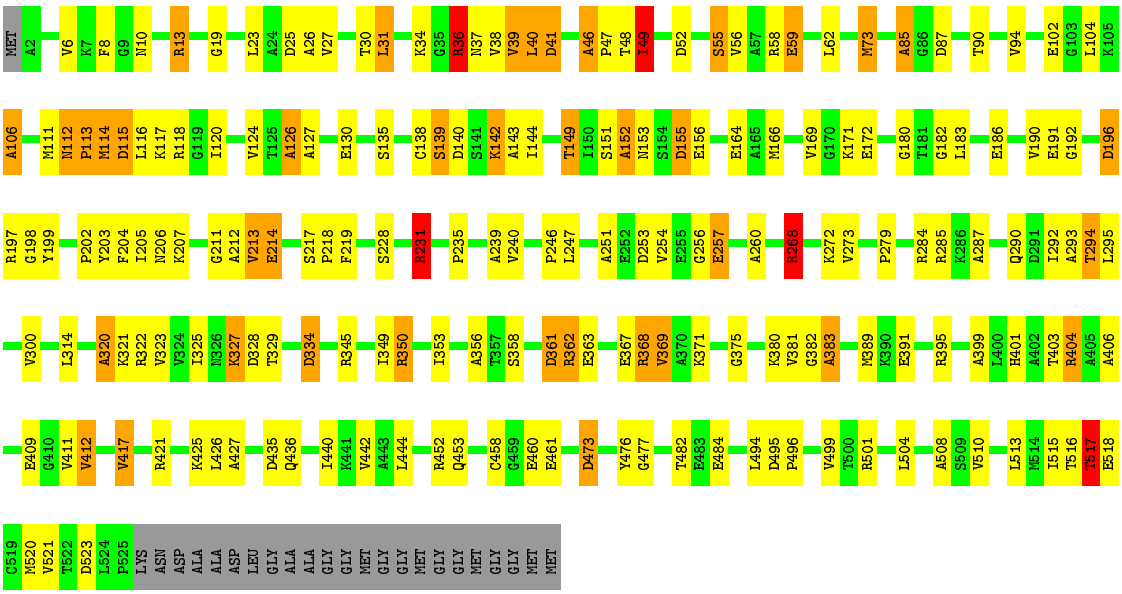
• Molecule 1: 60 KDA CHAPERONIN

Chain D:



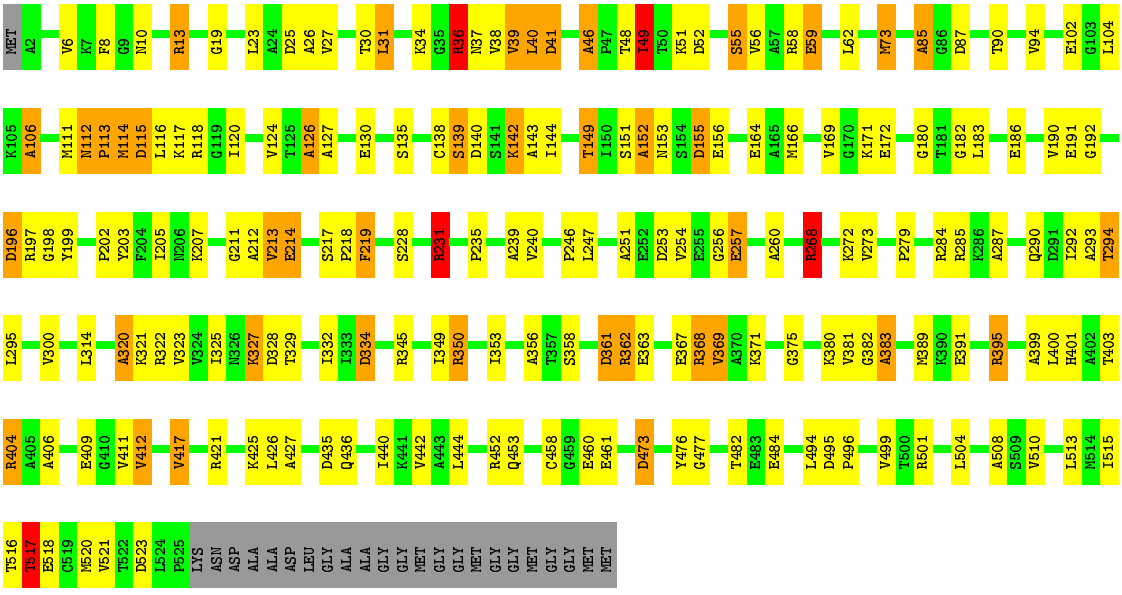
• Molecule 1: 60 KDA CHAPERONIN

Chain E:



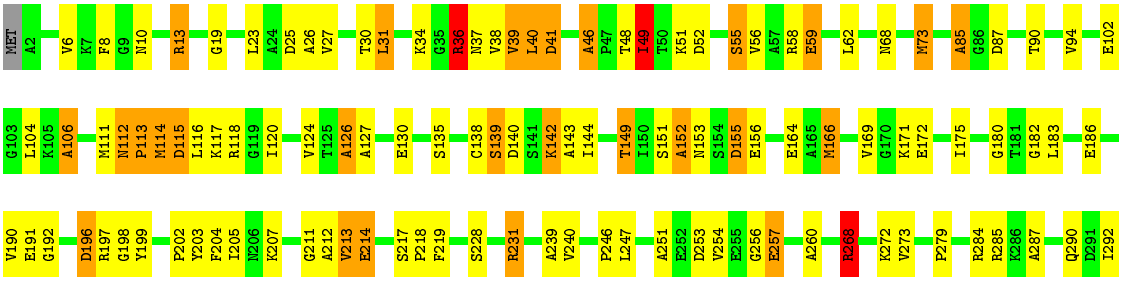
• Molecule 1: 60 KDA CHAPERONIN

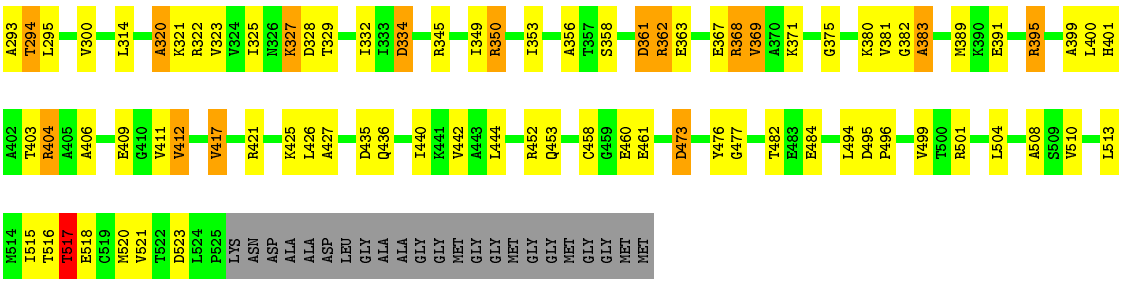
Chain F:



• Molecule 1: 60 KDA CHAPERONIN

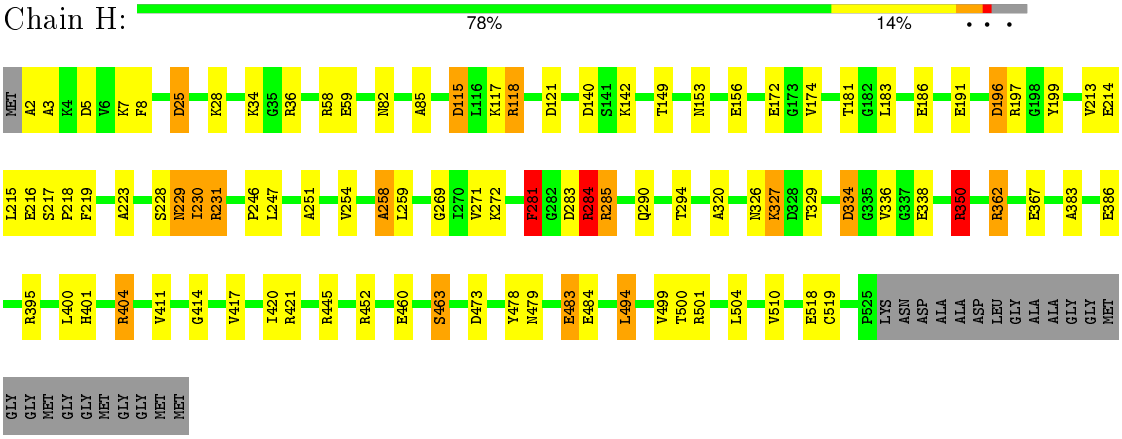
Chain G:





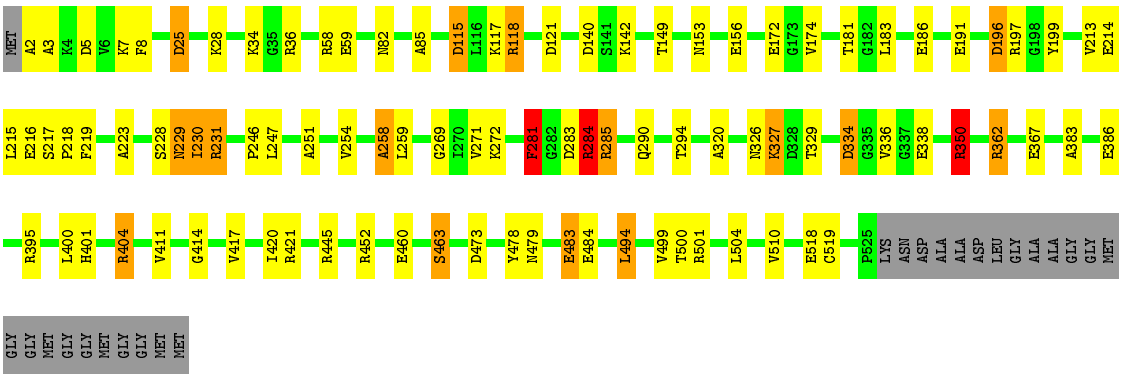
• Molecule 1: 60 KDA CHAPERONIN

Chain H:



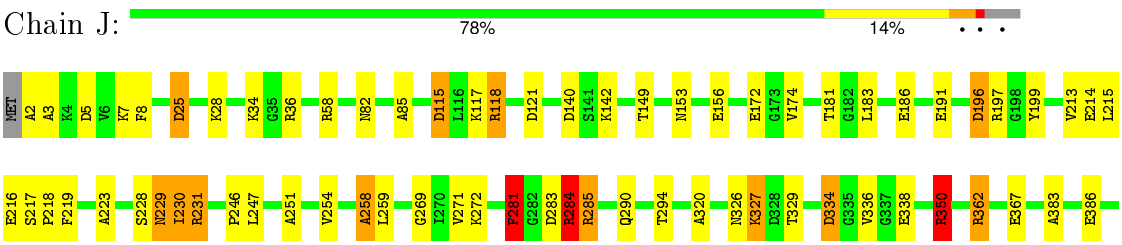
• Molecule 1: 60 KDA CHAPERONIN

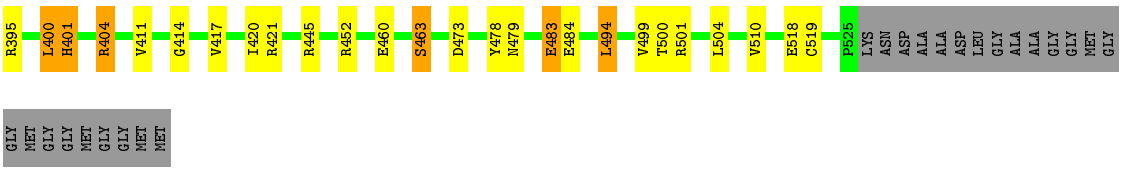
Chain I:



• Molecule 1: 60 KDA CHAPERONIN

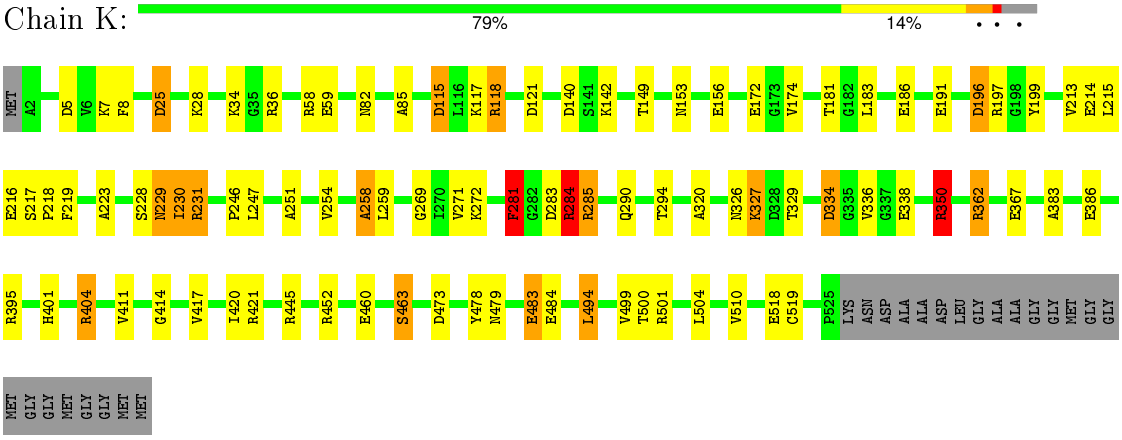
Chain J:





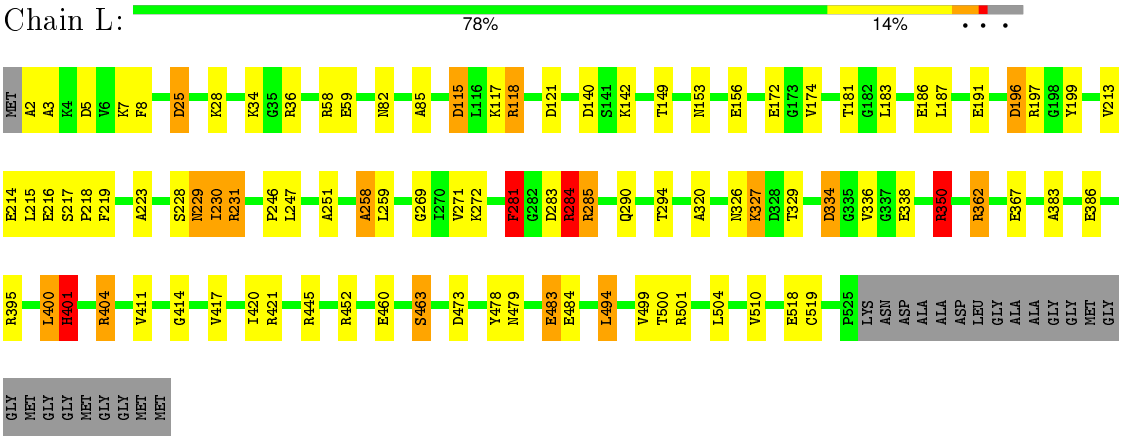
• Molecule 1: 60 KDA CHAPERONIN

Chain K:



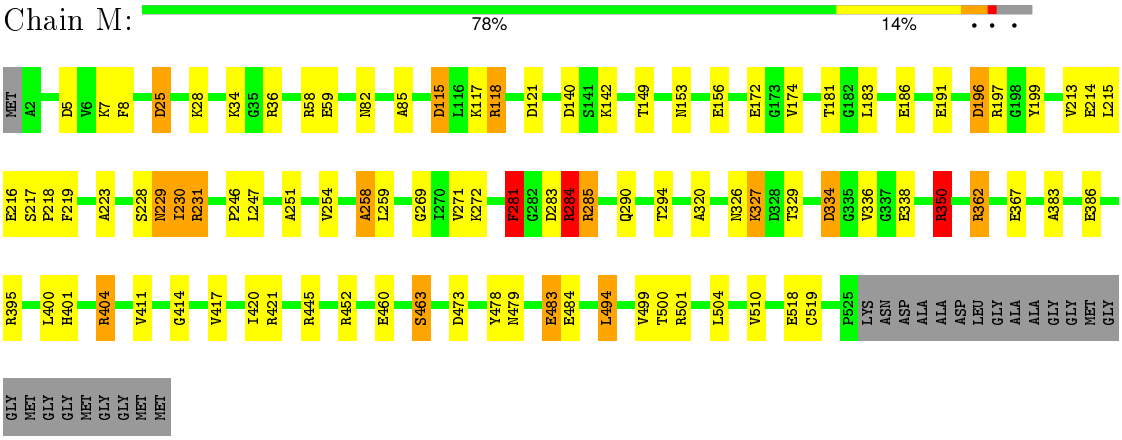
• Molecule 1: 60 KDA CHAPERONIN

Chain L:



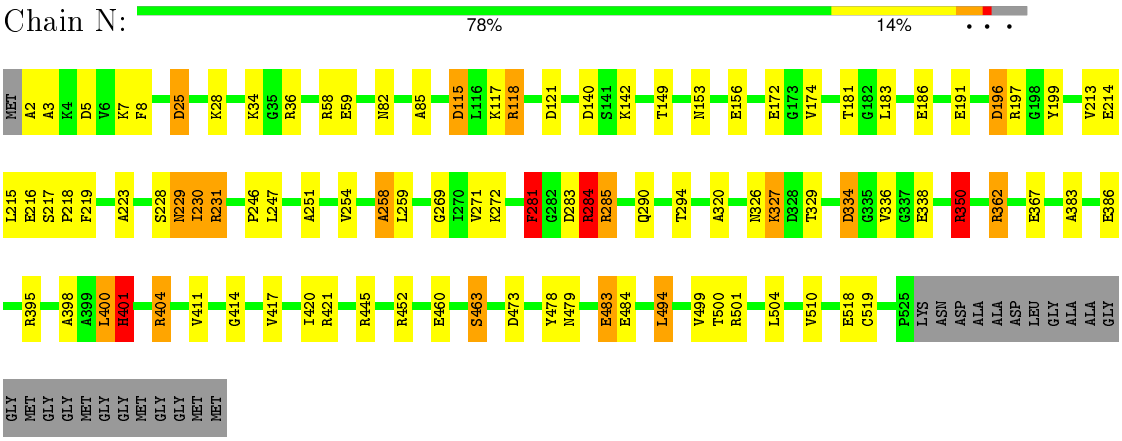
• Molecule 1: 60 KDA CHAPERONIN

Chain M:



- Molecule 1: 60 KDA CHAPERONIN

Chain N:



4 Experimental information (i)

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 ($e^-/Å^2$)	15	Depositor
Minimum defocus (nm)	700	Depositor
Maximum defocus (nm)	3500	Depositor
Magnification	Not provided	Depositor
Image detector	GATAN ULTRASCAN 4000 4K CCD CAMERA	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	1.79	4/3873 (0.1%)	1.57	89/5229 (1.7%)
1	B	1.79	4/3873 (0.1%)	1.57	90/5229 (1.7%)
1	C	1.79	4/3873 (0.1%)	1.57	87/5229 (1.7%)
1	D	1.79	4/3873 (0.1%)	1.57	89/5229 (1.7%)
1	E	1.80	4/3873 (0.1%)	1.57	89/5229 (1.7%)
1	F	1.79	4/3873 (0.1%)	1.57	89/5229 (1.7%)
1	G	1.79	4/3873 (0.1%)	1.57	89/5229 (1.7%)
1	H	0.70	2/3873 (0.1%)	1.09	22/5229 (0.4%)
1	I	0.68	2/3873 (0.1%)	1.09	22/5229 (0.4%)
1	J	0.74	2/3873 (0.1%)	1.11	24/5229 (0.5%)
1	K	0.69	1/3873 (0.0%)	1.10	23/5229 (0.4%)
1	L	0.74	1/3873 (0.0%)	1.12	28/5229 (0.5%)
1	M	0.68	1/3873 (0.0%)	1.12	27/5229 (0.5%)
1	N	0.81	2/3873 (0.1%)	1.10	23/5229 (0.4%)
All	All	1.37	39/54222 (0.1%)	1.36	791/73206 (1.1%)

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	9
1	B	0	9
1	C	0	10
1	D	0	10
1	E	0	9
1	F	0	10
1	G	0	9
1	H	0	10
1	I	0	10

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Mol	Chain	#Chirality outliers	#Planarity outliers
1	J	0	10
1	K	0	10
1	L	0	11
1	M	0	10
1	N	0	11
All	All	0	138

The worst 5 of 39 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	36	ARG	CZ-NH1	91.40	2.51	1.33
1	G	36	ARG	CZ-NH1	91.28	2.51	1.33
1	B	36	ARG	CZ-NH1	91.26	2.51	1.33
1	F	36	ARG	CZ-NH1	91.25	2.51	1.33
1	D	36	ARG	CZ-NH1	91.20	2.51	1.33

The worst 5 of 791 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	F	36	ARG	NE-CZ-NH1	22.64	131.62	120.30
1	D	36	ARG	NE-CZ-NH1	22.58	131.59	120.30
1	G	36	ARG	NE-CZ-NH1	22.57	131.58	120.30
1	C	36	ARG	NE-CZ-NH1	22.51	131.56	120.30
1	A	36	ARG	NE-CZ-NH1	22.48	131.54	120.30

There are no chirality outliers.

5 of 138 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	13	ARG	Sidechain
1	A	197	ARG	Sidechain
1	A	231	ARG	Sidechain
1	A	268	ARG	Sidechain
1	A	36	ARG	Sidechain

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	3846	0	3970	203	0
1	B	3846	0	3970	205	0
1	C	3846	0	3970	205	0
1	D	3846	0	3970	210	0
1	E	3846	0	3970	209	0
1	F	3846	0	3970	208	0
1	G	3846	0	3970	207	0
1	H	3846	0	3970	28	0
1	I	3846	0	3970	28	0
1	J	3846	0	3968	29	0
1	K	3846	0	3969	27	0
1	L	3846	0	3969	30	0
1	M	3846	0	3970	27	0
1	N	3846	0	3968	32	0
2	A	31	12	12	4	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	4	0
2	G	31	12	12	4	0
3	A	1	0	0	5	0
3	B	1	0	0	4	0
3	C	1	0	0	4	0
3	D	1	0	0	4	0
3	E	1	0	0	4	0
3	F	1	0	0	5	0
3	G	1	0	0	5	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
4	E	1	0	0	0	0
4	F	1	0	0	0	0
4	G	1	0	0	0	0
All	All	54075	84	55658	1291	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 12.

The worst 5 of 1291 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:J:400:LEU:C	1:J:401:HIS:N	1.72	1.43
1:A:115:ASP:H	1:B:36:ARG:CZ	1.37	1.37
1:C:115:ASP:H	1:D:36:ARG:CZ	1.37	1.37
1:D:115:ASP:H	1:E:36:ARG:CZ	1.37	1.36
1:A:116:LEU:H	1:B:36:ARG:NH1	1.24	1.36

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%)	517 (99%)	5 (1%)	0	100	100
1	B	522/548 (95%)	517 (99%)	5 (1%)	0	100	100
1	C	522/548 (95%)	517 (99%)	5 (1%)	0	100	100
1	D	522/548 (95%)	517 (99%)	5 (1%)	0	100	100
1	E	522/548 (95%)	517 (99%)	5 (1%)	0	100	100
1	F	522/548 (95%)	517 (99%)	5 (1%)	0	100	100
1	G	522/548 (95%)	517 (99%)	5 (1%)	0	100	100
1	H	522/548 (95%)	498 (95%)	22 (4%)	2 (0%)	39	80
1	I	522/548 (95%)	498 (95%)	22 (4%)	2 (0%)	39	80
1	J	522/548 (95%)	498 (95%)	22 (4%)	2 (0%)	39	80
1	K	522/548 (95%)	498 (95%)	22 (4%)	2 (0%)	39	80
1	L	522/548 (95%)	498 (95%)	22 (4%)	2 (0%)	39	80
1	M	522/548 (95%)	498 (95%)	22 (4%)	2 (0%)	39	80
1	N	522/548 (95%)	498 (95%)	22 (4%)	2 (0%)	39	80
All	All	7308/7672 (95%)	7105 (97%)	189 (3%)	14 (0%)	56	86

5 of 14 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	H	269	GLY
1	I	269	GLY
1	J	269	GLY
1	K	269	GLY
1	L	269	GLY

5.3.2 Protein sidechains (i)

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%)	364 (90%)	38 (10%)	11	41
1	B	402/414 (97%)	364 (90%)	38 (10%)	11	41
1	C	402/414 (97%)	364 (90%)	38 (10%)	11	41
1	D	402/414 (97%)	364 (90%)	38 (10%)	11	41
1	E	402/414 (97%)	364 (90%)	38 (10%)	11	41
1	F	402/414 (97%)	364 (90%)	38 (10%)	11	41
1	G	402/414 (97%)	364 (90%)	38 (10%)	11	41
1	H	402/414 (97%)	367 (91%)	35 (9%)	13	45
1	I	402/414 (97%)	367 (91%)	35 (9%)	13	45
1	J	402/414 (97%)	367 (91%)	35 (9%)	13	45
1	K	402/414 (97%)	367 (91%)	35 (9%)	13	45
1	L	402/414 (97%)	366 (91%)	36 (9%)	12	44
1	M	402/414 (97%)	367 (91%)	35 (9%)	13	45
1	N	402/414 (97%)	367 (91%)	35 (9%)	13	45
All	All	5628/5796 (97%)	5116 (91%)	512 (9%)	16	43

5 of 512 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	G	37	ASN
1	H	327	LYS
1	M	494	LEU

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Mol	Chain	Res	Type
1	G	164	GLU
1	G	473	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 21 such sidechains are listed below:

Mol	Chain	Res	Type
1	I	68	ASN
1	J	68	ASN
1	M	68	ASN
1	H	326	ASN
1	M	326	ASN

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)

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	$\#\|Z\| > 2$
2	ATP	A	1525	4	26,33,33	0.96	1 (3%)	26,52,52	1.34	5 (19%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	ATP	B	1525	4	26,33,33	0.97	1 (3%)	26,52,52	1.35	5 (19%)
2	ATP	C	1526	4	26,33,33	0.98	1 (3%)	26,52,52	1.34	5 (19%)
2	ATP	D	1525	4	26,33,33	0.98	1 (3%)	26,52,52	1.35	5 (19%)
2	ATP	E	1527	4	26,33,33	0.99	1 (3%)	26,52,52	1.35	5 (19%)
2	ATP	F	1527	4	26,33,33	0.98	1 (3%)	26,52,52	1.35	5 (19%)
2	ATP	G	1527	4	26,33,33	0.97	1 (3%)	26,52,52	1.35	5 (19%)

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	4	-	0/18/38/38	0/3/3/3
2	ATP	B	1525	4	-	0/18/38/38	0/3/3/3
2	ATP	C	1526	4	-	0/18/38/38	0/3/3/3
2	ATP	D	1525	4	-	0/18/38/38	0/3/3/3
2	ATP	E	1527	4	-	0/18/38/38	0/3/3/3
2	ATP	F	1527	4	-	0/18/38/38	0/3/3/3
2	ATP	G	1527	4	-	0/18/38/38	0/3/3/3

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	1527	ATP	C2'-C1'	-3.34	1.48	1.53
2	C	1526	ATP	C2'-C1'	-3.33	1.48	1.53
2	D	1525	ATP	C2'-C1'	-3.32	1.48	1.53
2	G	1527	ATP	C2'-C1'	-3.29	1.48	1.53
2	B	1525	ATP	C2'-C1'	-3.29	1.48	1.53

The worst 5 of 35 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	E	1527	ATP	C4'-O4'-C1'	-2.51	106.98	109.64
2	D	1525	ATP	C4'-O4'-C1'	-2.50	106.99	109.64
2	B	1525	ATP	C4'-O4'-C1'	-2.48	107.02	109.64
2	C	1526	ATP	C4'-O4'-C1'	-2.48	107.02	109.64
2	F	1527	ATP	C4'-O4'-C1'	-2.48	107.02	109.64

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

7 monomers are involved in 24 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1525	ATP	4	0
2	B	1525	ATP	3	0
2	C	1526	ATP	3	0
2	D	1525	ATP	3	0
2	E	1527	ATP	3	0
2	F	1527	ATP	4	0
2	G	1527	ATP	4	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.