wwPDB EM Map/Model Validation Report (i)

Apr 10, 2016 – 02:04 PM BST

PDB ID	:	2C7E
EMDB ID:	:	EMD-1047
Title	:	REVISED ATOMIC STRUCTURE FITTING INTO A GROEL(D398A)-ATP7 CRYO-EM MAP (EMD 1047)
Authors	:	Ranson, N.A.; Farr, G.W.; Roseman, A.M.; Gowen, B.; Fenton, W.A.; Horwich, A.L.; Saibil, H.R.
Deposited on	:	2005-11-22
Resolution	:	9.70 Å(reported)

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

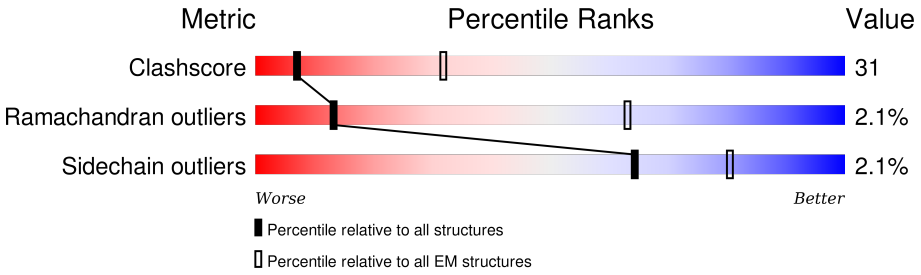
MolProbity	:	4.02b-467
Mogul	:	1.7.1 (RC1), CSD as537be (2016)
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk27241

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 9.70 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	547	59% 35%
1	B	547	60% 34%
1	C	547	59% 34%
1	D	547	59% 34%
1	E	547	60% 34%
1	F	547	60% 33%
1	G	547	60% 34%
1	H	547	63% 30%
1	I	547	64% 29%

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Mol	Chain	Length	Quality of chain
1	J	547	63% 30%
1	K	547	63% 31%
1	L	547	63% 30%
1	M	547	63% 30%
1	N	547	63% 30%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 54243 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	0
			3855	2399	664	772	20		
1	B	525	Total	C	N	O	S	0	0
			3855	2399	664	772	20		
1	C	525	Total	C	N	O	S	0	0
			3855	2399	664	772	20		
1	D	525	Total	C	N	O	S	0	0
			3855	2399	664	772	20		
1	E	525	Total	C	N	O	S	0	0
			3855	2399	664	772	20		
1	F	525	Total	C	N	O	S	0	0
			3855	2399	664	772	20		
1	G	525	Total	C	N	O	S	0	0
			3855	2399	664	772	20		
1	H	525	Total	C	N	O	S	0	0
			3855	2399	664	772	20		
1	I	525	Total	C	N	O	S	0	0
			3855	2399	664	772	20		
1	J	525	Total	C	N	O	S	0	0
			3855	2399	664	772	20		
1	K	525	Total	C	N	O	S	0	0
			3855	2399	664	772	20		
1	L	525	Total	C	N	O	S	0	0
			3855	2399	664	772	20		
1	M	525	Total	C	N	O	S	0	0
			3855	2399	664	772	20		
1	N	525	Total	C	N	O	S	0	0
			3855	2399	664	772	20		

There are 28 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	13	GLY	ARG	ENGINEERED MUTATION	UNP P06139
A	126	VAL	ALA	ENGINEERED MUTATION	UNP P06139

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Chain	Residue	Modelled	Actual	Comment	Reference
B	13	GLY	ARG	ENGINEERED MUTATION	UNP P06139
B	126	VAL	ALA	ENGINEERED MUTATION	UNP P06139
C	13	GLY	ARG	ENGINEERED MUTATION	UNP P06139
C	126	VAL	ALA	ENGINEERED MUTATION	UNP P06139
D	13	GLY	ARG	ENGINEERED MUTATION	UNP P06139
D	126	VAL	ALA	ENGINEERED MUTATION	UNP P06139
E	13	GLY	ARG	ENGINEERED MUTATION	UNP P06139
E	126	VAL	ALA	ENGINEERED MUTATION	UNP P06139
F	13	GLY	ARG	ENGINEERED MUTATION	UNP P06139
F	126	VAL	ALA	ENGINEERED MUTATION	UNP P06139
G	13	GLY	ARG	ENGINEERED MUTATION	UNP P06139
G	126	VAL	ALA	ENGINEERED MUTATION	UNP P06139
H	13	GLY	ARG	ENGINEERED MUTATION	UNP P06139
H	126	VAL	ALA	ENGINEERED MUTATION	UNP P06139
I	13	GLY	ARG	ENGINEERED MUTATION	UNP P06139
I	126	VAL	ALA	ENGINEERED MUTATION	UNP P06139
J	13	GLY	ARG	ENGINEERED MUTATION	UNP P06139
J	126	VAL	ALA	ENGINEERED MUTATION	UNP P06139
K	13	GLY	ARG	ENGINEERED MUTATION	UNP P06139
K	126	VAL	ALA	ENGINEERED MUTATION	UNP P06139
L	13	GLY	ARG	ENGINEERED MUTATION	UNP P06139
L	126	VAL	ALA	ENGINEERED MUTATION	UNP P06139
M	13	GLY	ARG	ENGINEERED MUTATION	UNP P06139
M	126	VAL	ALA	ENGINEERED MUTATION	UNP P06139
N	13	GLY	ARG	ENGINEERED MUTATION	UNP P06139
N	126	VAL	ALA	ENGINEERED MUTATION	UNP P06139

- Molecule 2 is POTASSIUM ION (three-letter code: K) (formula: K).

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

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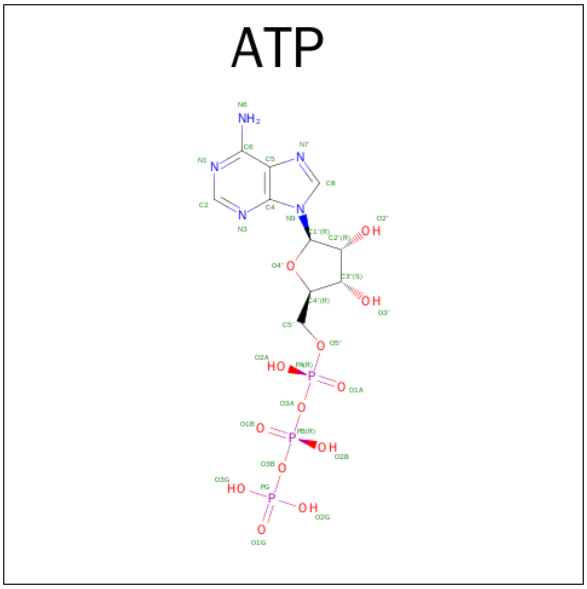
Mol	Chain	Residues	Atoms	AltConf
2	F	1	Total K 1 1	0

- 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	D	1	Total Mg 1 1	0
3	E	1	Total Mg 1 1	0
3	B	1	Total Mg 1 1	0
3	C	1	Total Mg 1 1	0
3	A	1	Total Mg 1 1	0
3	F	1	Total Mg 1 1	0

- 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 C N O P 31 10 5 13 3	0

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Mol	Chain	Residues	Atoms					AltConf
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	

- Molecule 5 is water.

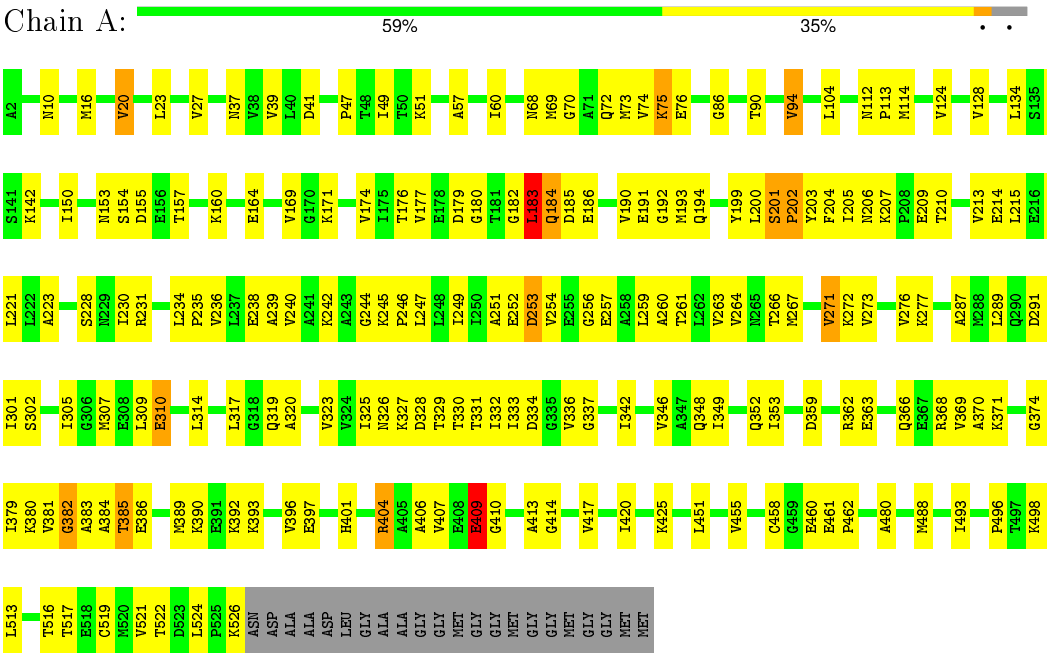
Mol	Chain	Residues	Atoms		AltConf
5	A	42	Total	O	0
			42	42	

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.

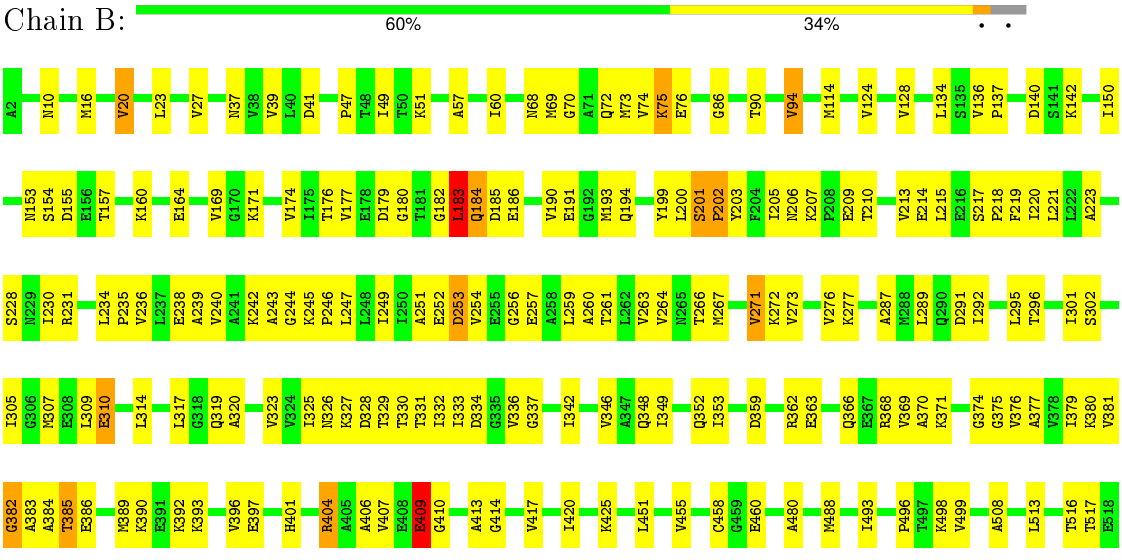
- Molecule 1: 60 KDA CHAPERONIN

Chain A:



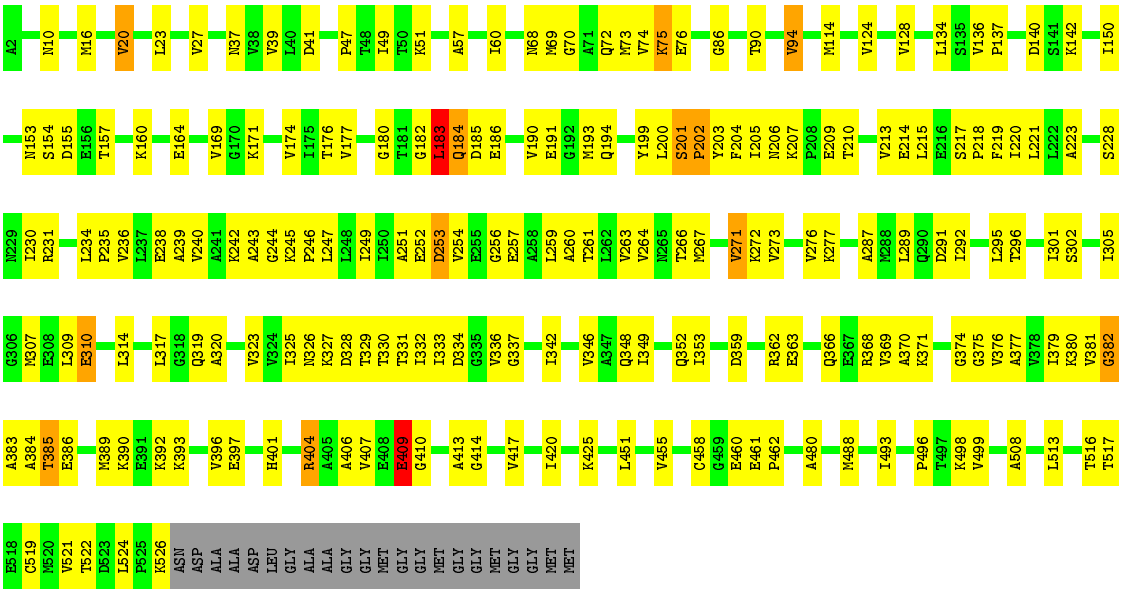
- Molecule 1: 60 KDA CHAPERONIN

Chain B:



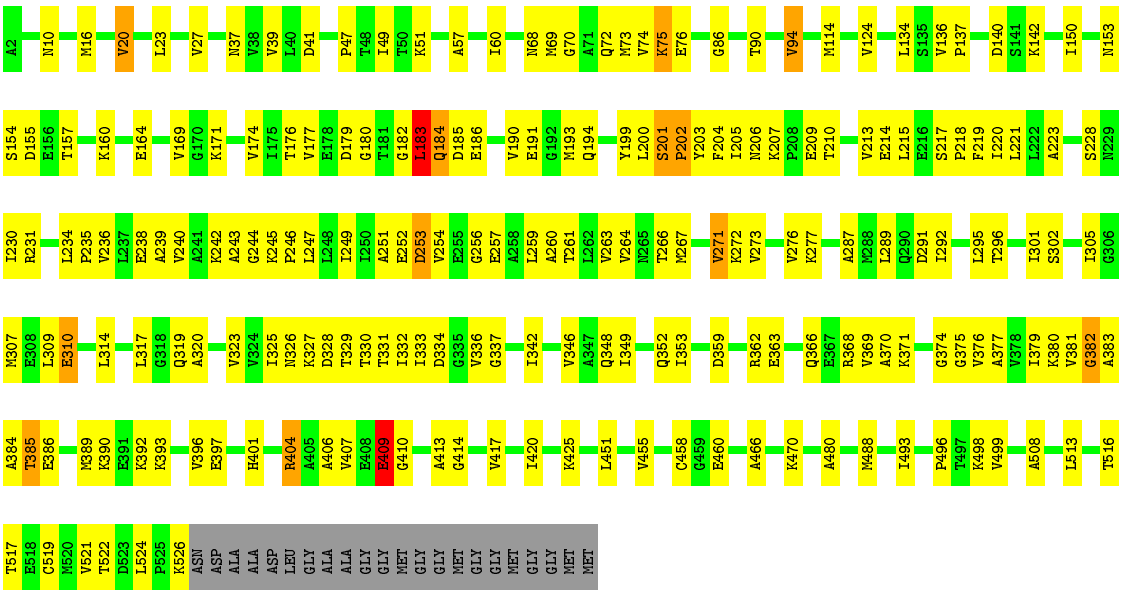
- Molecule 1: 60 KDA CHAPERONIN

Chain C:



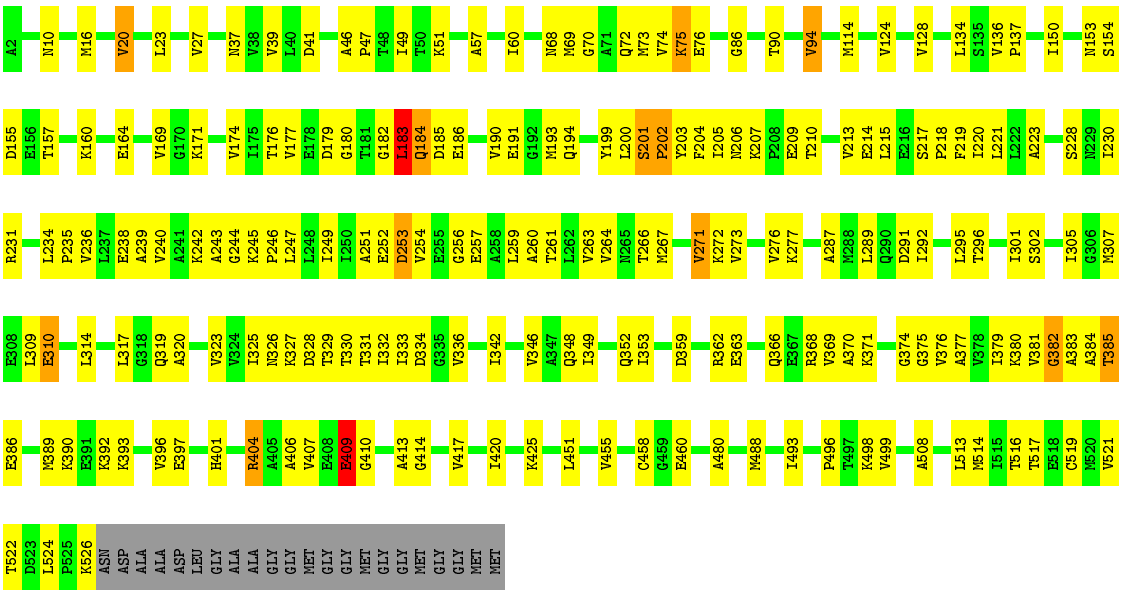
- Molecule 1: 60 KDA CHAPERONIN

Chain D:



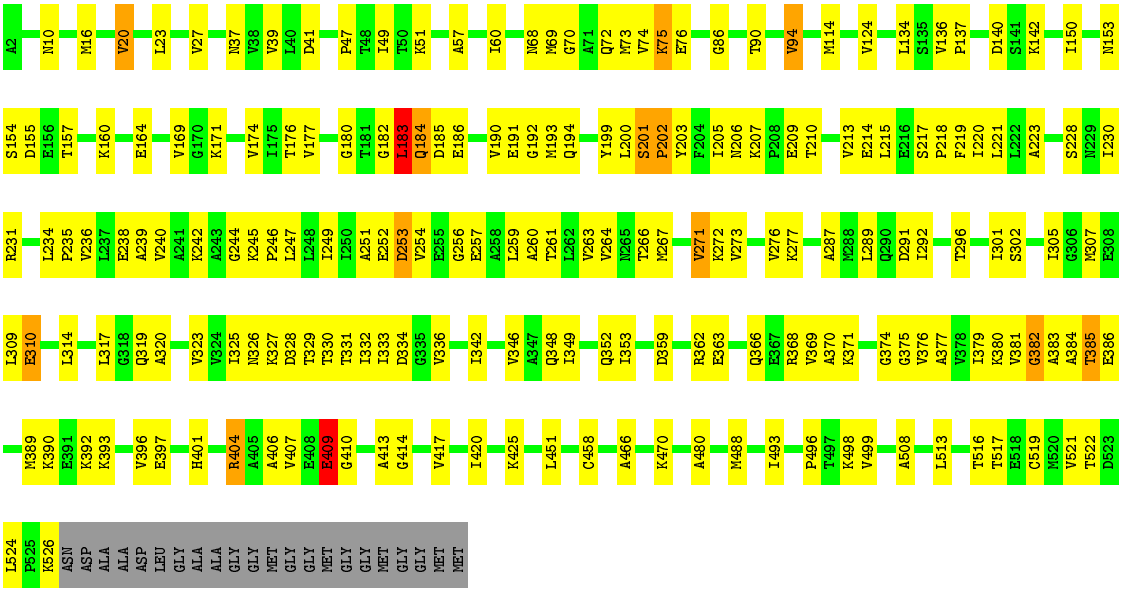
- Molecule 1: 60 KDA CHAPERONIN

Chain E:



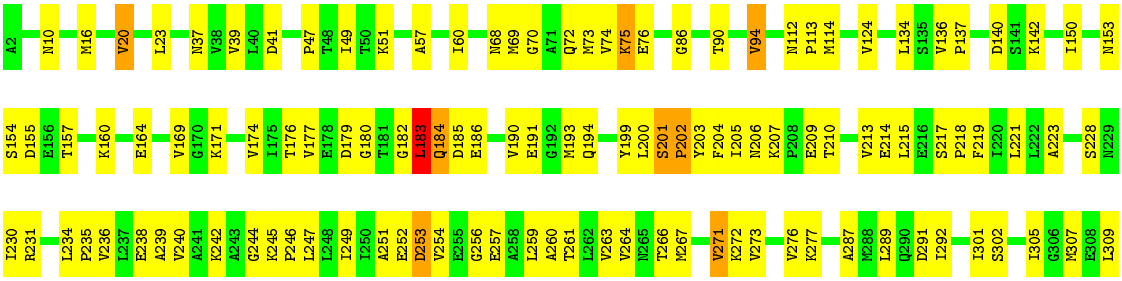
- Molecule 1: 60 KDA CHAPERONIN

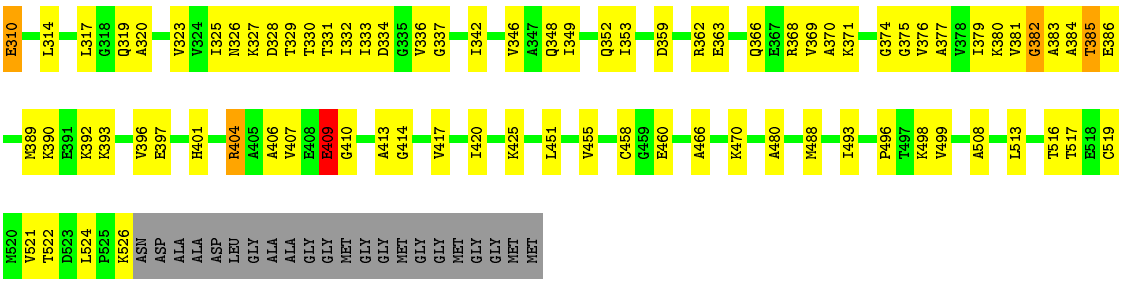
Chain F:



- Molecule 1: 60 KDA CHAPERONIN

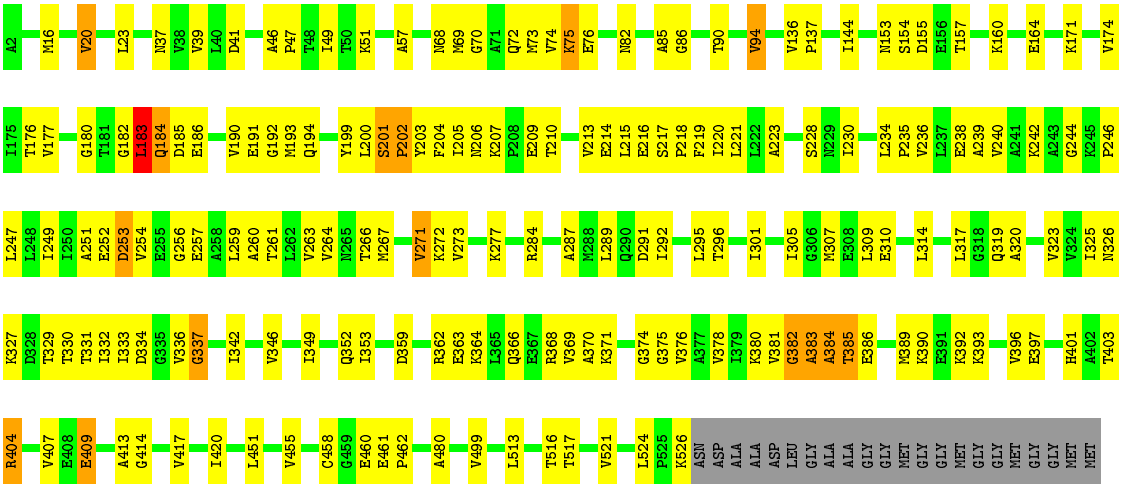
Chain G:





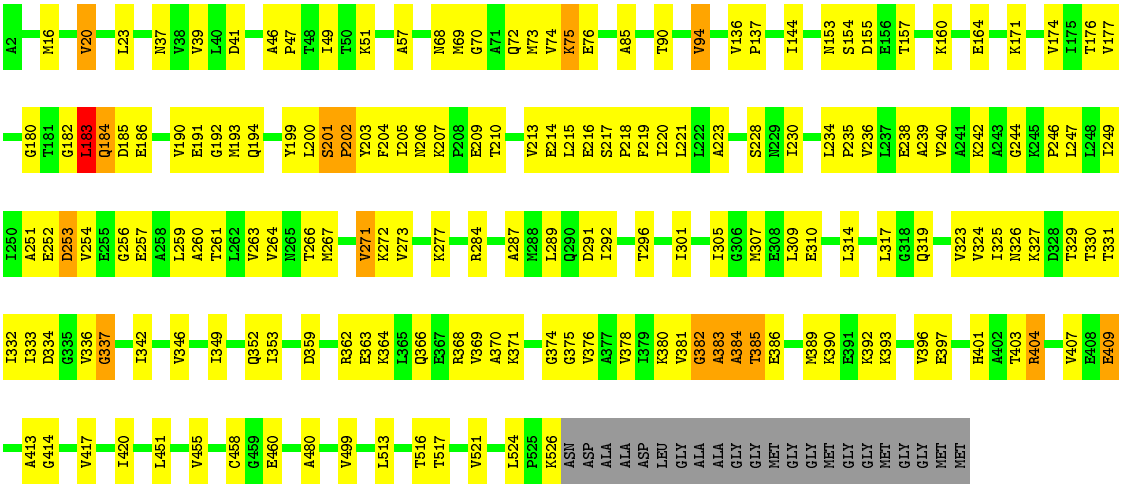
• Molecule 1: 60 KDA CHAPERONIN

Chain H:



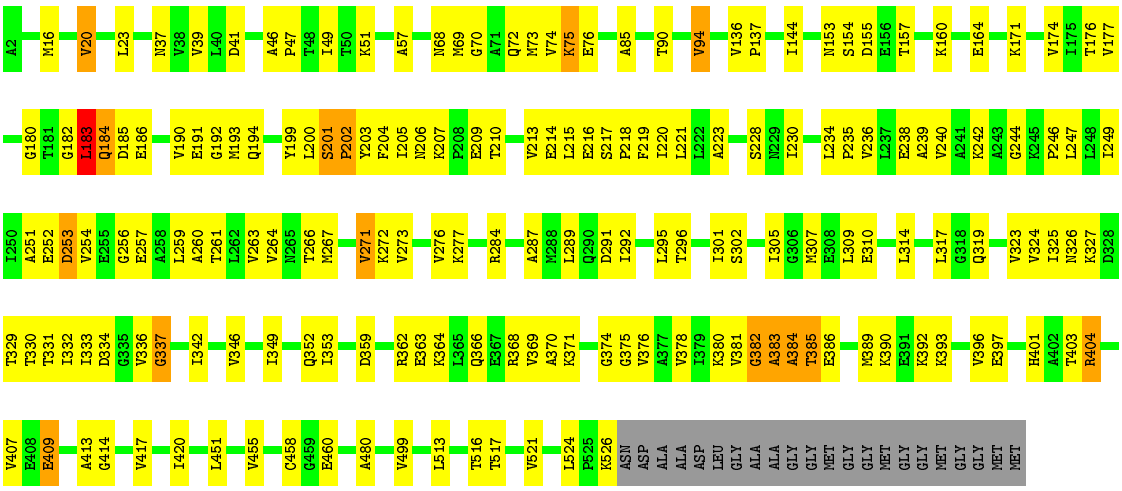
• Molecule 1: 60 KDA CHAPERONIN

Chain I:



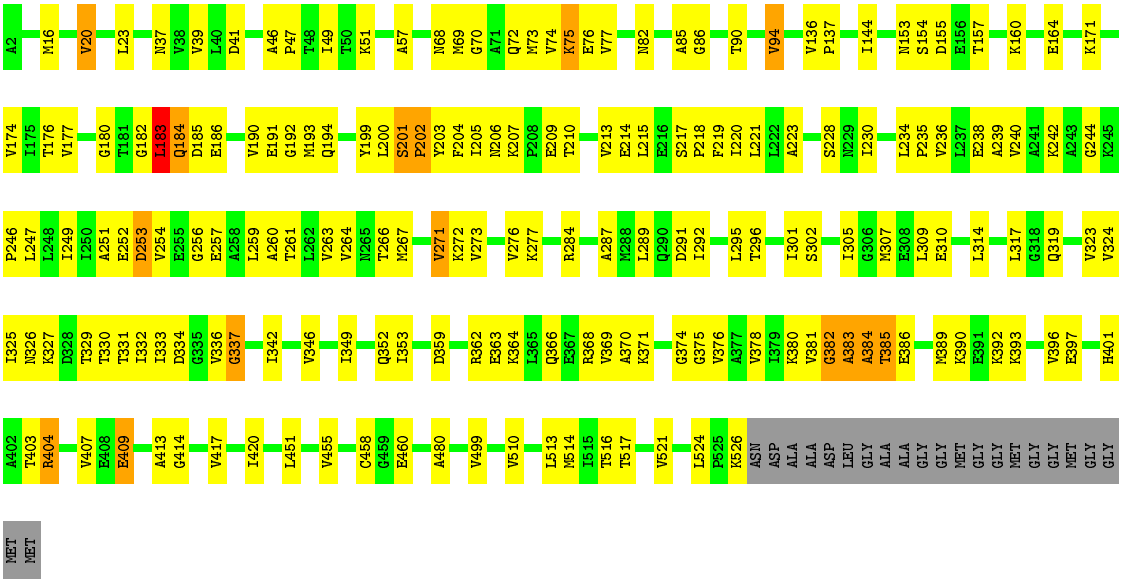
• Molecule 1: 60 KDA CHAPERONIN

Chain J:



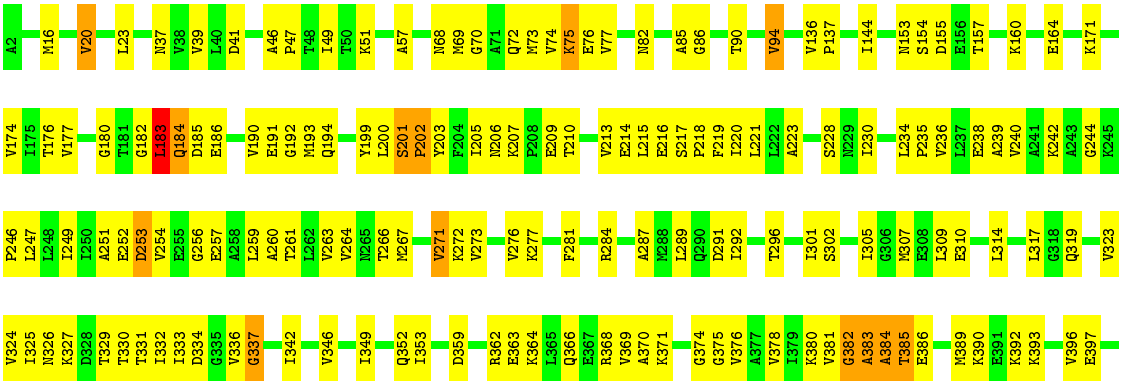
• Molecule 1: 60 KDA CHAPERONIN

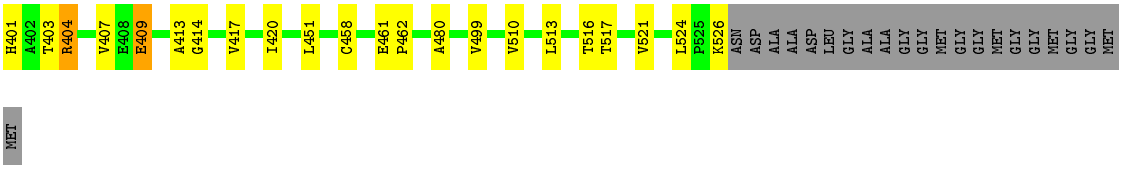
Chain K:



• Molecule 1: 60 KDA CHAPERONIN

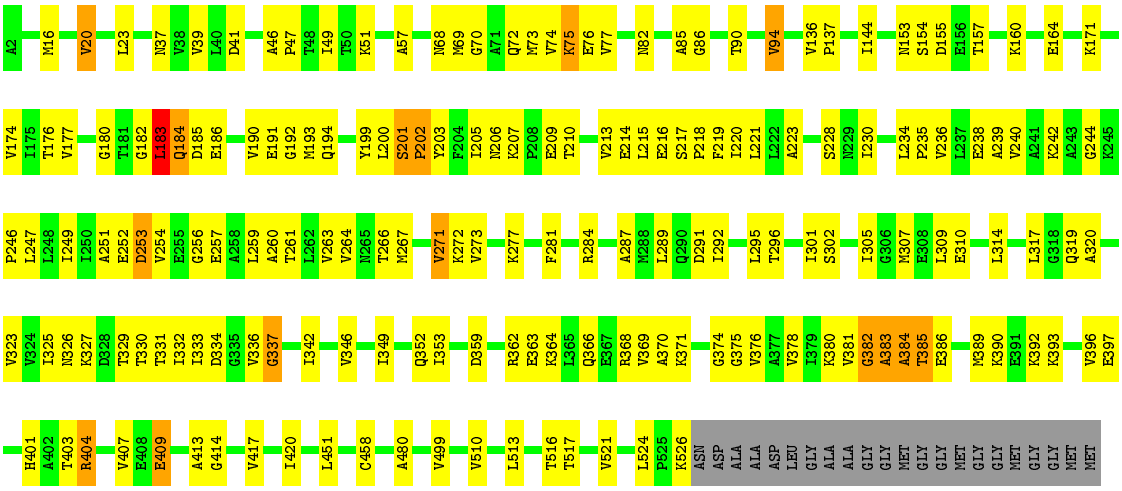
Chain L:





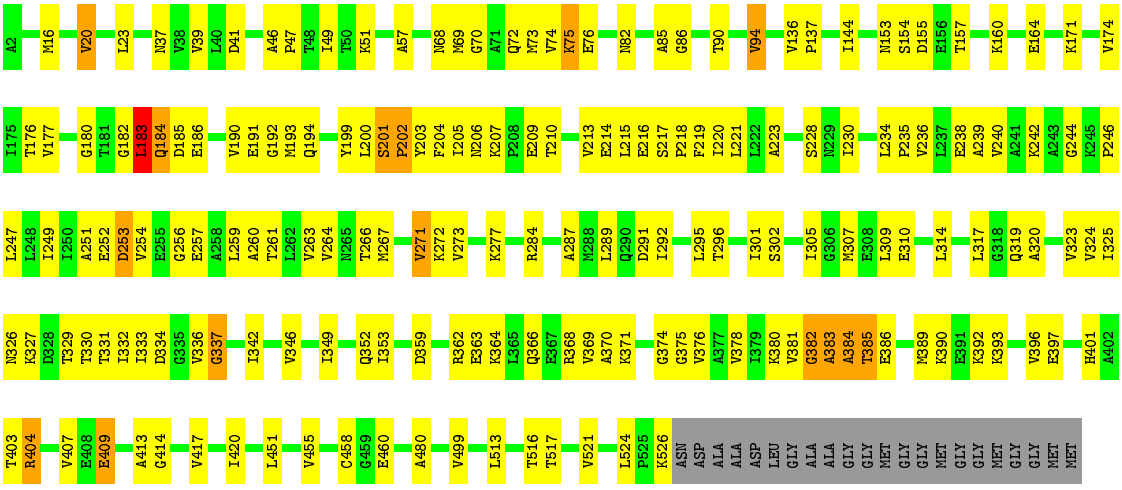
• Molecule 1: 60 KDA CHAPERONIN

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	FULL CORRECTION ON 2D CLASS AVERAGES	Depositor
Microscope	FEI CM200 FEG	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/Å^2$)	Not provided	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	5000	Depositor
Magnification	38000	Depositor
Image detector	KODAK SO163 FILM	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, K, 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	0.34	1/3880 (0.0%)	0.85	2/5233 (0.0%)
1	B	0.34	1/3880 (0.0%)	0.85	2/5233 (0.0%)
1	C	0.34	1/3880 (0.0%)	0.85	2/5233 (0.0%)
1	D	0.34	1/3880 (0.0%)	0.85	2/5233 (0.0%)
1	E	0.34	1/3880 (0.0%)	0.85	2/5233 (0.0%)
1	F	0.34	1/3880 (0.0%)	0.85	2/5233 (0.0%)
1	G	0.34	1/3880 (0.0%)	0.85	2/5233 (0.0%)
1	H	0.77	1/3880 (0.0%)	0.81	3/5233 (0.1%)
1	I	0.77	1/3880 (0.0%)	0.81	3/5233 (0.1%)
1	J	0.77	1/3880 (0.0%)	0.81	3/5233 (0.1%)
1	K	0.77	1/3880 (0.0%)	0.81	3/5233 (0.1%)
1	L	0.77	1/3880 (0.0%)	0.81	3/5233 (0.1%)
1	M	0.77	1/3880 (0.0%)	0.81	3/5233 (0.1%)
1	N	0.77	1/3880 (0.0%)	0.81	3/5233 (0.1%)
All	All	0.60	14/54320 (0.0%)	0.83	35/73262 (0.0%)

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

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Mol	Chain	#Chirality outliers	#Planarity outliers
1	J	0	1
1	K	0	1
1	L	0	1
1	M	0	1
1	N	0	1
All	All	0	14

The worst 5 of 14 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	J	409	GLU	C-N	-43.70	0.54	1.33
1	K	409	GLU	C-N	-43.68	0.54	1.33
1	M	409	GLU	C-N	-43.66	0.54	1.33
1	H	409	GLU	C-N	-43.65	0.54	1.33
1	N	409	GLU	C-N	-43.65	0.54	1.33

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

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	F	409	GLU	O-C-N	-45.43	45.96	123.20
1	A	409	GLU	O-C-N	-45.43	45.97	123.20
1	C	409	GLU	O-C-N	-45.43	45.97	123.20
1	E	409	GLU	O-C-N	-45.43	45.98	123.20
1	D	409	GLU	O-C-N	-45.42	45.99	123.20

There are no chirality outliers.

5 of 14 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	409	GLU	Mainchain
1	B	409	GLU	Mainchain
1	C	409	GLU	Mainchain
1	D	409	GLU	Mainchain
1	E	409	GLU	Mainchain

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	3855	0	3976	329	0
1	B	3855	0	3976	331	0
1	C	3855	0	3976	334	0
1	D	3855	0	3976	331	0
1	E	3855	0	3976	324	0
1	F	3855	0	3976	318	0
1	G	3855	0	3976	325	0
1	H	3855	0	3970	243	0
1	I	3855	0	3970	238	0
1	J	3855	0	3970	241	0
1	K	3855	0	3970	248	0
1	L	3855	0	3970	240	0
1	M	3855	0	3970	239	0
1	N	3855	0	3970	242	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
2	E	1	0	0	0	0
2	F	1	0	0	0	0
2	G	1	0	0	0	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	0	0
4	B	31	0	12	0	0
4	C	31	0	12	0	0
4	D	31	0	12	0	0
4	E	31	0	12	0	0
4	F	31	0	12	0	0
4	G	31	0	12	0	0
5	A	42	0	0	0	0
All	All	54243	0	55706	3419	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 31.

The worst 5 of 3419 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:190:VAL:HG11	1:J:333:ILE:CG2	1.30	1.61
1:J:190:VAL:CG1	1:J:333:ILE:HG22	1.20	1.60
1:N:190:VAL:HG11	1:N:333:ILE:CG2	1.30	1.60
1:K:190:VAL:HG11	1:K:333:ILE:CG2	1.30	1.59
1:M:190:VAL:CG1	1:M:333:ILE:HG22	1.20	1.59

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	517/547 (94%)	480 (93%)	27 (5%)	10 (2%)	10	52
1	B	517/547 (94%)	480 (93%)	27 (5%)	10 (2%)	10	52
1	C	517/547 (94%)	480 (93%)	27 (5%)	10 (2%)	10	52
1	D	517/547 (94%)	480 (93%)	27 (5%)	10 (2%)	10	52
1	E	517/547 (94%)	480 (93%)	27 (5%)	10 (2%)	10	52
1	F	517/547 (94%)	480 (93%)	27 (5%)	10 (2%)	10	52
1	G	517/547 (94%)	480 (93%)	27 (5%)	10 (2%)	10	52
1	H	517/547 (94%)	480 (93%)	25 (5%)	12 (2%)	8	48
1	I	517/547 (94%)	480 (93%)	25 (5%)	12 (2%)	8	48
1	J	517/547 (94%)	480 (93%)	25 (5%)	12 (2%)	8	48
1	K	517/547 (94%)	480 (93%)	25 (5%)	12 (2%)	8	48
1	L	517/547 (94%)	480 (93%)	25 (5%)	12 (2%)	8	48
1	M	517/547 (94%)	480 (93%)	25 (5%)	12 (2%)	8	48
1	N	517/547 (94%)	480 (93%)	25 (5%)	12 (2%)	8	48
All	All	7238/7658 (94%)	6720 (93%)	364 (5%)	154 (2%)	13	50

5 of 154 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	410	GLY
1	B	410	GLY
1	C	410	GLY
1	D	410	GLY
1	E	410	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	404/414 (98%)	394 (98%)	10 (2%)	55	81
1	B	404/414 (98%)	394 (98%)	10 (2%)	55	81
1	C	404/414 (98%)	394 (98%)	10 (2%)	55	81
1	D	404/414 (98%)	394 (98%)	10 (2%)	55	81
1	E	404/414 (98%)	394 (98%)	10 (2%)	55	81
1	F	404/414 (98%)	394 (98%)	10 (2%)	55	81
1	G	404/414 (98%)	394 (98%)	10 (2%)	55	81
1	H	404/414 (98%)	397 (98%)	7 (2%)	68	87
1	I	404/414 (98%)	397 (98%)	7 (2%)	68	87
1	J	404/414 (98%)	397 (98%)	7 (2%)	68	87
1	K	404/414 (98%)	397 (98%)	7 (2%)	68	87
1	L	404/414 (98%)	397 (98%)	7 (2%)	68	87
1	M	404/414 (98%)	397 (98%)	7 (2%)	68	87
1	N	404/414 (98%)	397 (98%)	7 (2%)	68	87
All	All	5656/5796 (98%)	5537 (98%)	119 (2%)	64	84

5 of 119 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	F	94	VAL
1	G	310	GLU
1	M	289	LEU

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Mol	Chain	Res	Type
1	F	289	LEU
1	G	10	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 119 such sidechains are listed below:

Mol	Chain	Res	Type
1	G	351	GLN
1	I	146	GLN
1	M	453	GLN
1	G	453	GLN
1	H	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, 14 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	551	3,2	26,33,33	0.92	0	26,52,52	1.34	4 (15%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
4	ATP	B	551	3,2	26,33,33	0.92	0	26,52,52	1.34	4 (15%)
4	ATP	C	551	3,2	26,33,33	0.92	0	26,52,52	1.34	4 (15%)
4	ATP	D	551	3,2	26,33,33	0.92	0	26,52,52	1.34	4 (15%)
4	ATP	E	551	3,2	26,33,33	0.92	0	26,52,52	1.34	4 (15%)
4	ATP	F	551	3,2	26,33,33	0.92	0	26,52,52	1.34	4 (15%)
4	ATP	G	551	3,2	26,33,33	0.92	0	26,52,52	1.34	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
4	ATP	A	551	3,2	-	0/18/38/38	0/3/3/3
4	ATP	B	551	3,2	-	0/18/38/38	0/3/3/3
4	ATP	C	551	3,2	-	0/18/38/38	0/3/3/3
4	ATP	D	551	3,2	-	0/18/38/38	0/3/3/3
4	ATP	E	551	3,2	-	0/18/38/38	0/3/3/3
4	ATP	F	551	3,2	-	0/18/38/38	0/3/3/3
4	ATP	G	551	3,2	-	0/18/38/38	0/3/3/3

There are no bond length outliers.

The worst 5 of 28 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	C	551	ATP	C1'-N9-C4	-2.88	123.59	126.81
4	A	551	ATP	C1'-N9-C4	-2.86	123.61	126.81
4	G	551	ATP	C1'-N9-C4	-2.86	123.61	126.81
4	B	551	ATP	C1'-N9-C4	-2.86	123.61	126.81
4	E	551	ATP	C1'-N9-C4	-2.86	123.62	126.81

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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.