wwPDB EM Map/Model Validation Report (i)

Apr 10, 2016 – 01:51 PM BST

PDB ID	:	3J1C
EMDB ID:	:	EMD-5392
Title	:	Cryo-EM structure of 9-fold symmetric rATcpn-alpha in apo state
Authors	:	Zhang, K.; Wang, L.; Liu, Y.X.; Wang, X.; Gao, B.; Hu, Z.J.; Ji, G.; Chan, K.Y.; Schulten, K.; Dong, Z.Y.; Sun, F.
Deposited on	:	2012-02-06
Resolution	:	9.10 Å(reported)
Based on PDB ID	:	3KO1

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

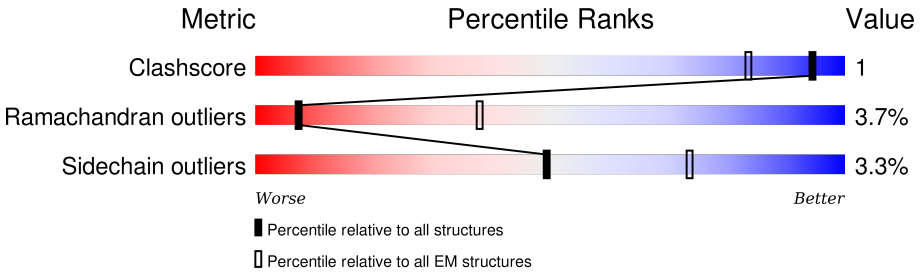
MolProbity	:	4.02b-467
Mogul	:	unknown
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk27241

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 9.10 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	563	66% 22% • 8%
1	B	563	68% 19% • • 8%
1	C	563	67% 21% • • 8%
1	D	563	69% 19% • 8%
1	E	563	66% 22% • • 8%
1	F	563	70% 19% • • 8%
1	G	563	69% 18% • • 8%
1	H	563	67% 20% • • 8%
1	I	563	65% 23% • 8%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	J	563	67% 21% 8%
1	K	563	72% 17% 8%
1	L	563	71% 18% 8%
1	M	563	68% 19% 5% 8%
1	N	563	67% 20% 8%
1	O	563	68% 19% 8%
1	P	563	71% 17% 8%
1	Q	563	71% 18% 8%
1	R	563	69% 19% 8%

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 70866 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 Chaperonin alpha subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	519	Total	C	N	O	S	0	0
			3937	2475	673	773	16		
1	B	519	Total	C	N	O	S	0	0
			3937	2475	673	773	16		
1	C	519	Total	C	N	O	S	0	0
			3937	2475	673	773	16		
1	D	519	Total	C	N	O	S	0	0
			3937	2475	673	773	16		
1	E	519	Total	C	N	O	S	0	0
			3937	2475	673	773	16		
1	F	519	Total	C	N	O	S	0	0
			3937	2475	673	773	16		
1	G	519	Total	C	N	O	S	0	0
			3937	2475	673	773	16		
1	H	519	Total	C	N	O	S	0	0
			3937	2475	673	773	16		
1	I	519	Total	C	N	O	S	0	0
			3937	2475	673	773	16		
1	J	519	Total	C	N	O	S	0	0
			3937	2475	673	773	16		
1	K	519	Total	C	N	O	S	0	0
			3937	2475	673	773	16		
1	L	519	Total	C	N	O	S	0	0
			3937	2475	673	773	16		
1	M	519	Total	C	N	O	S	0	0
			3937	2475	673	773	16		
1	N	519	Total	C	N	O	S	0	0
			3937	2475	673	773	16		
1	O	519	Total	C	N	O	S	0	0
			3937	2475	673	773	16		
1	P	519	Total	C	N	O	S	0	0
			3937	2475	673	773	16		
1	Q	519	Total	C	N	O	S	0	0
			3937	2475	673	773	16		

Continued on next page...

Continued from previous page...

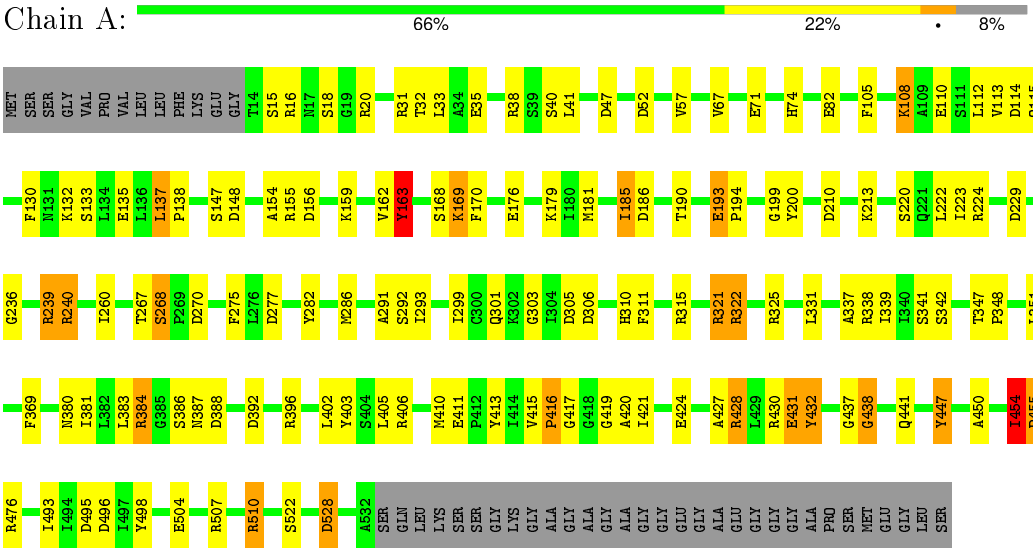
Mol	Chain	Residues	Atoms					AltConf	Trace
1	R	519	Total	C	N	O	S	0	0
			3937	2475	673	773	16		

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.

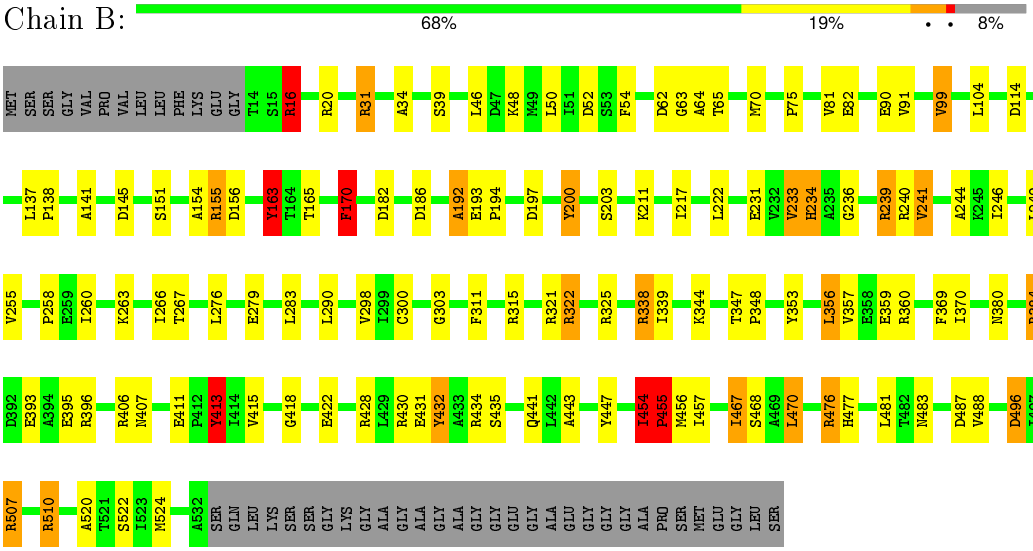
- Molecule 1: Chaperonin alpha subunit

Chain A:



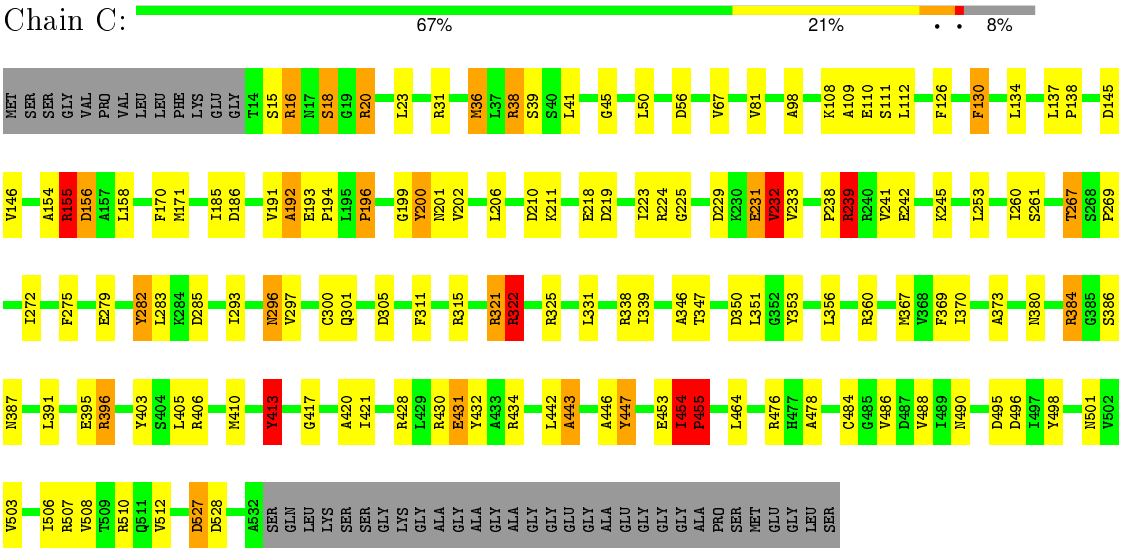
- Molecule 1: Chaperonin alpha subunit

Chain B:



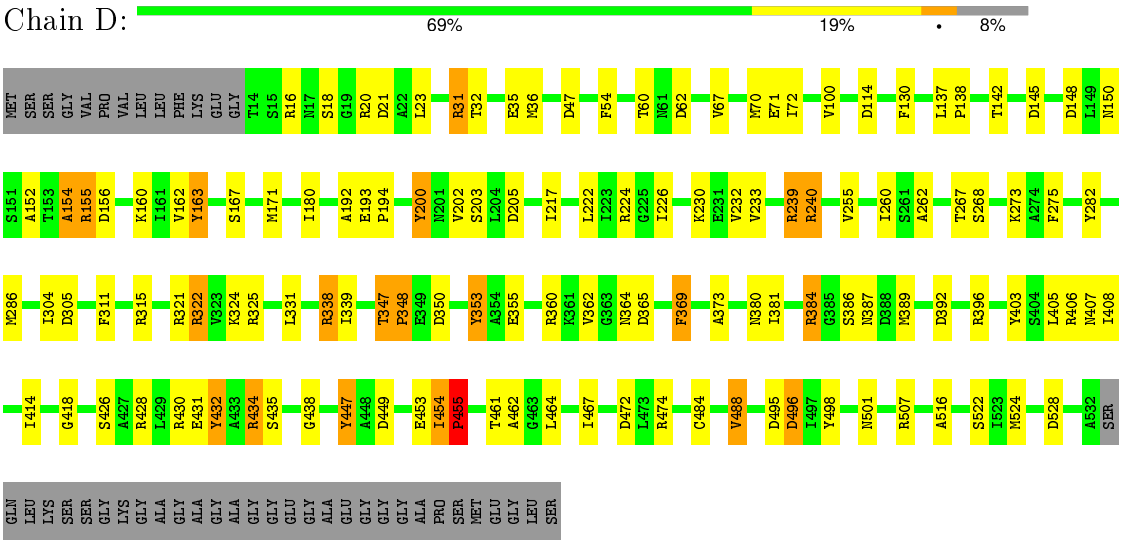
- Molecule 1: Chaperonin alpha subunit

Chain C:



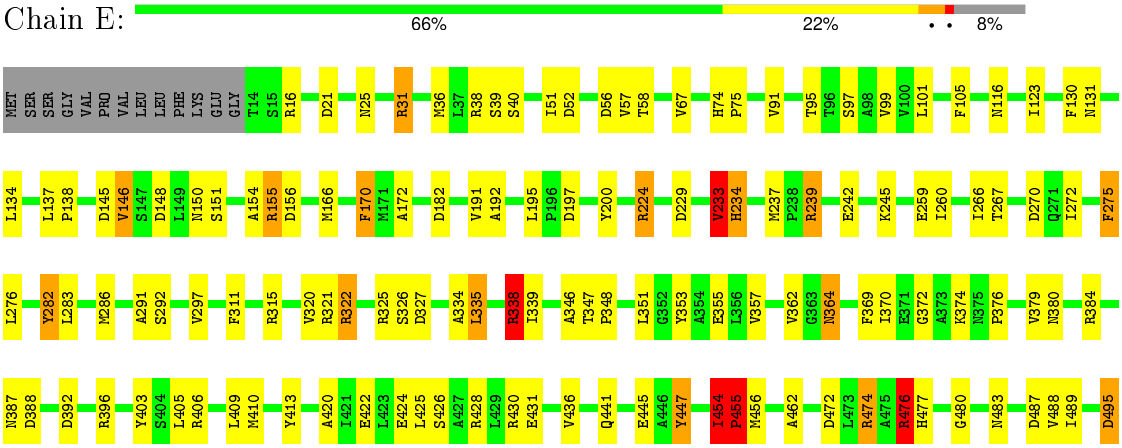
• Molecule 1: Chaperonin alpha subunit

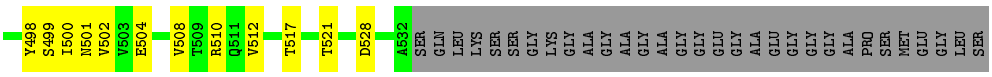
Chain D:



• Molecule 1: Chaperonin alpha subunit

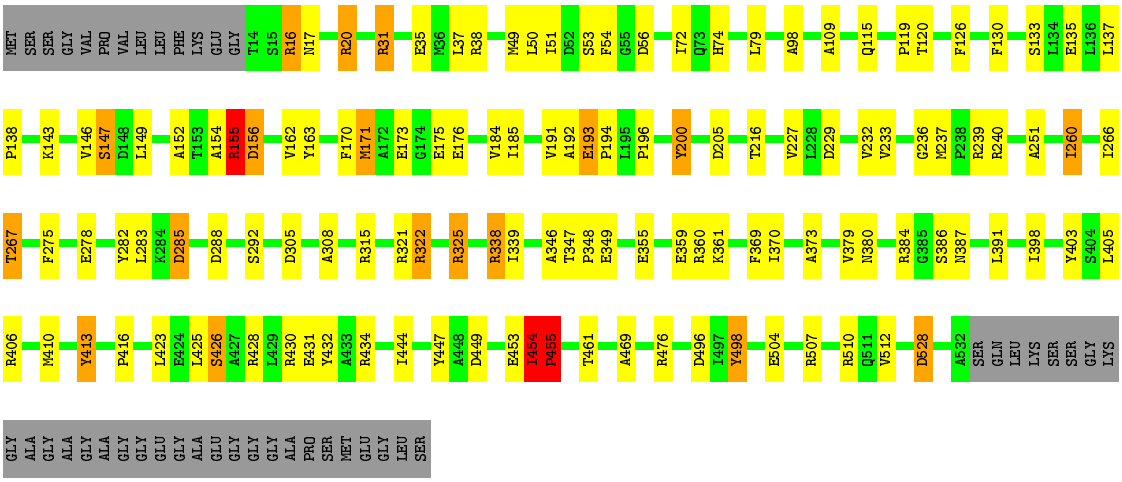
Chain E:





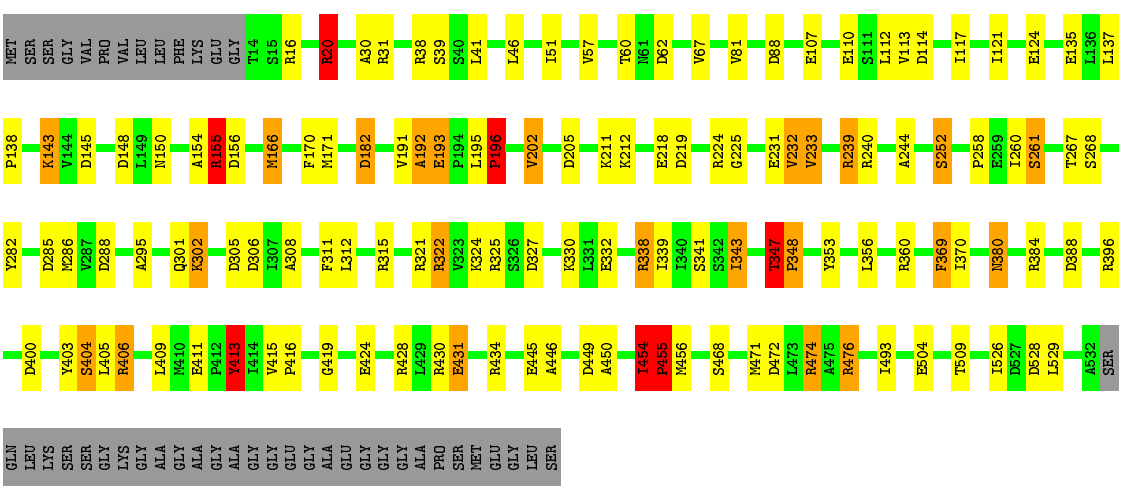
- Molecule 1: Chaperonin alpha subunit

Chain F:



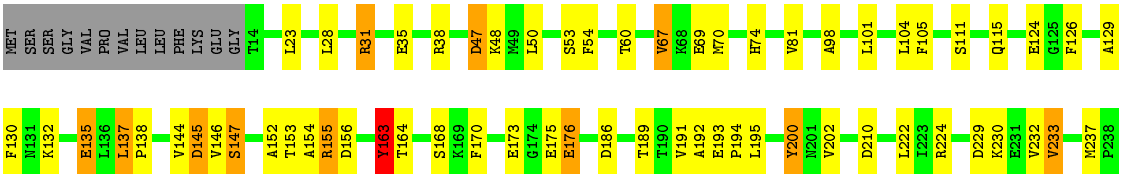
- Molecule 1: Chaperonin alpha subunit

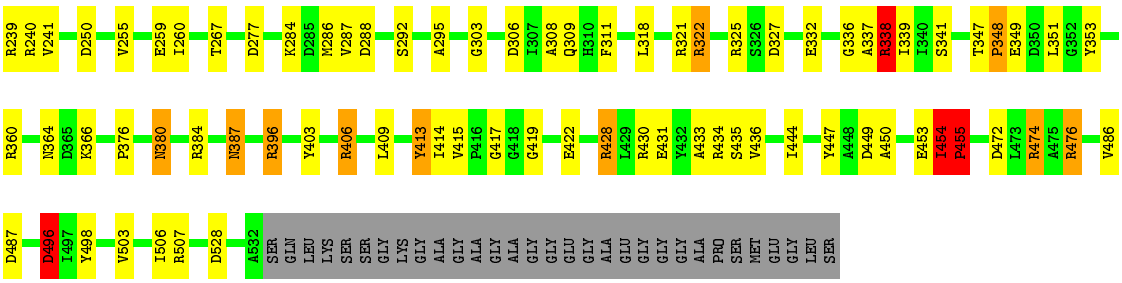
Chain G:



- Molecule 1: Chaperonin alpha subunit

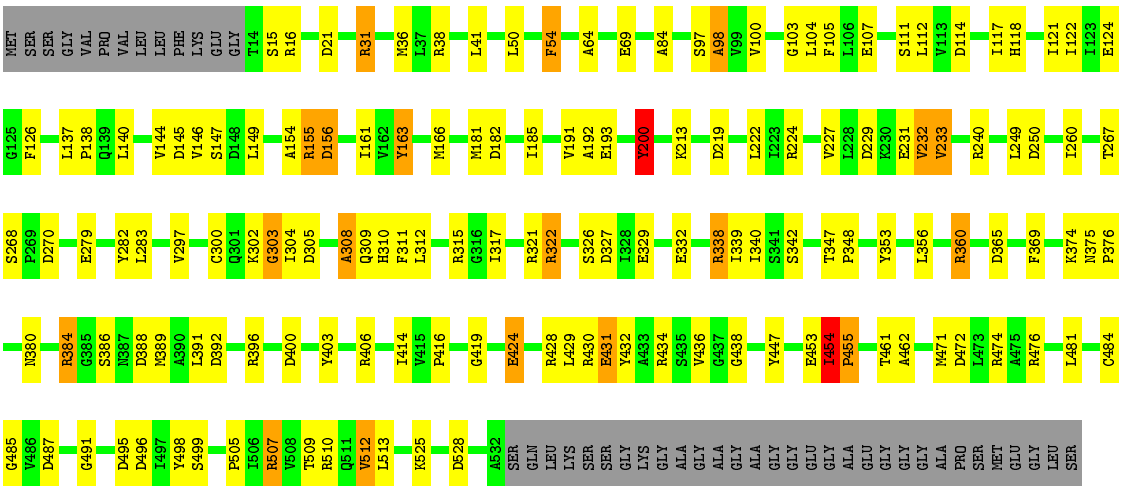
Chain H:





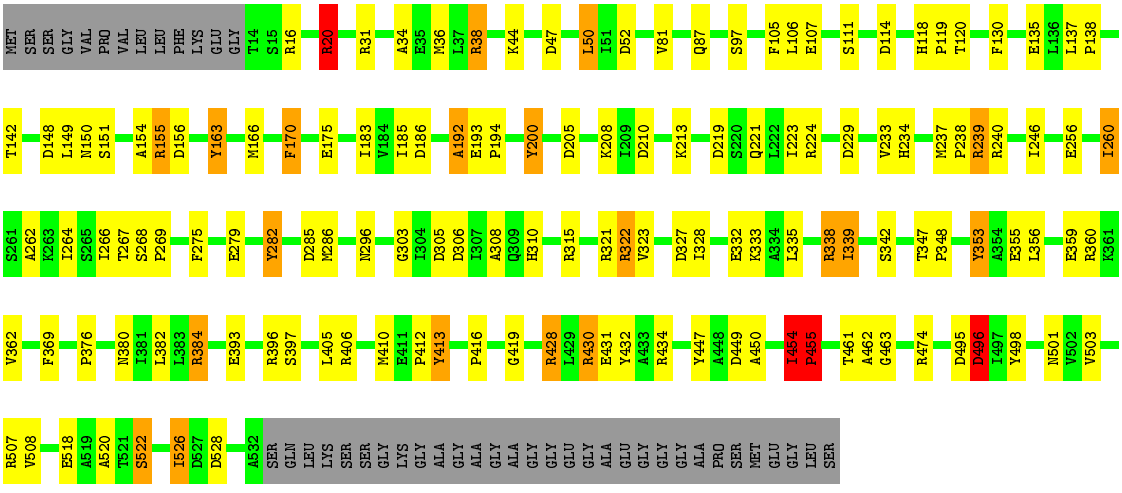
• Molecule 1: Chaperonin alpha subunit

Chain I:



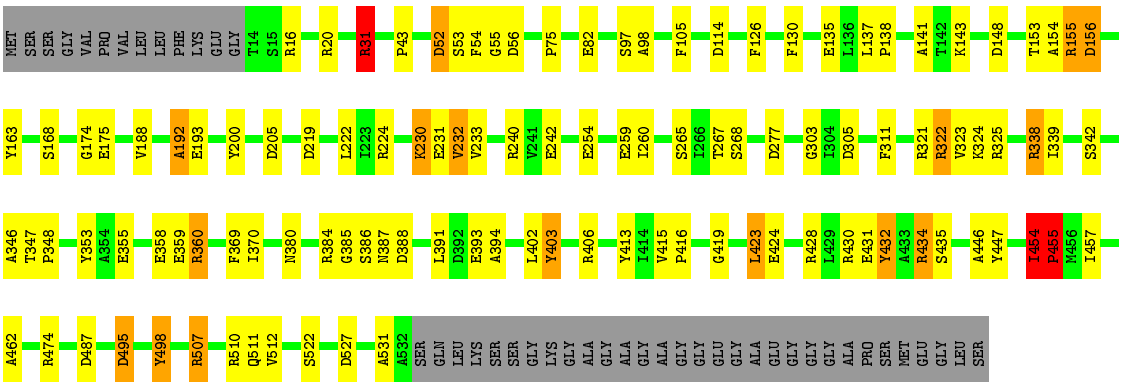
• Molecule 1: Chaperonin alpha subunit

Chain J:



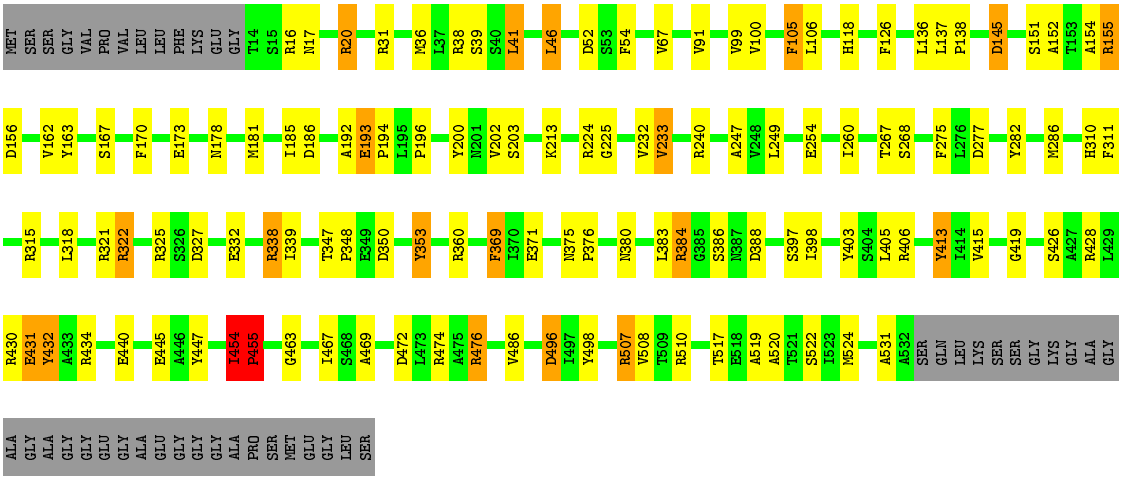
• Molecule 1: Chaperonin alpha subunit

Chain K:



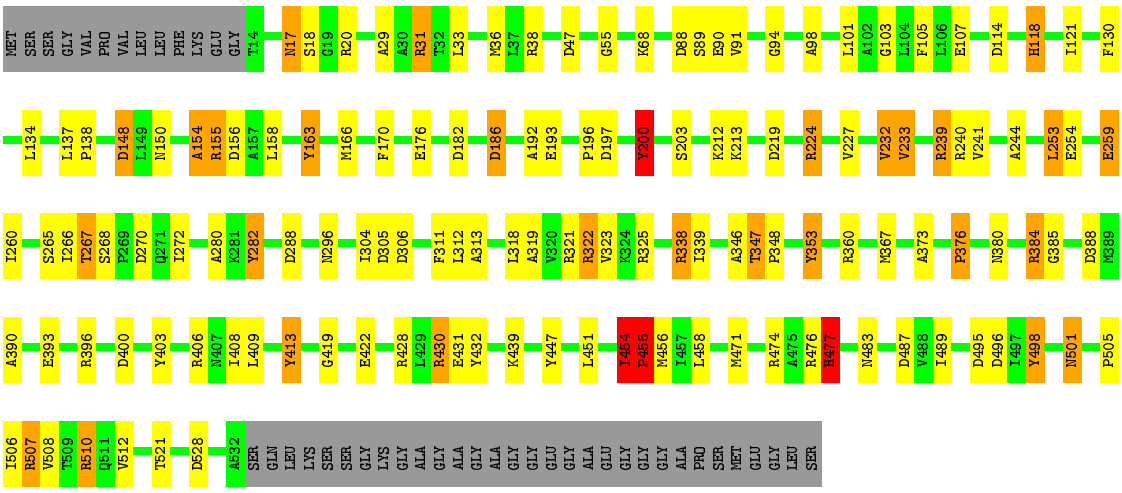
• Molecule 1: Chaperonin alpha subunit

Chain L:



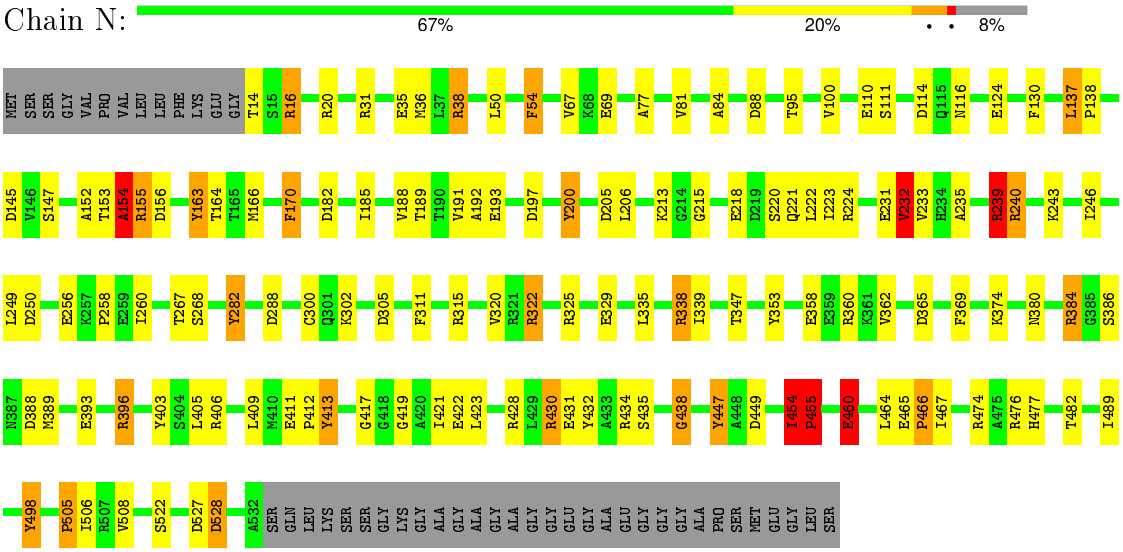
• Molecule 1: Chaperonin alpha subunit

Chain M:



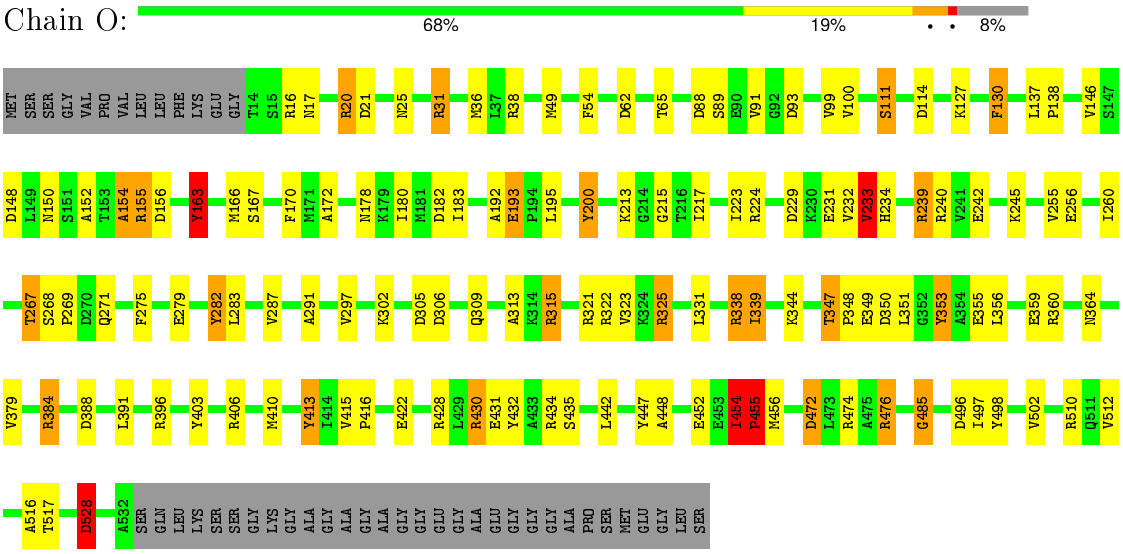
• Molecule 1: Chaperonin alpha subunit

Chain N:



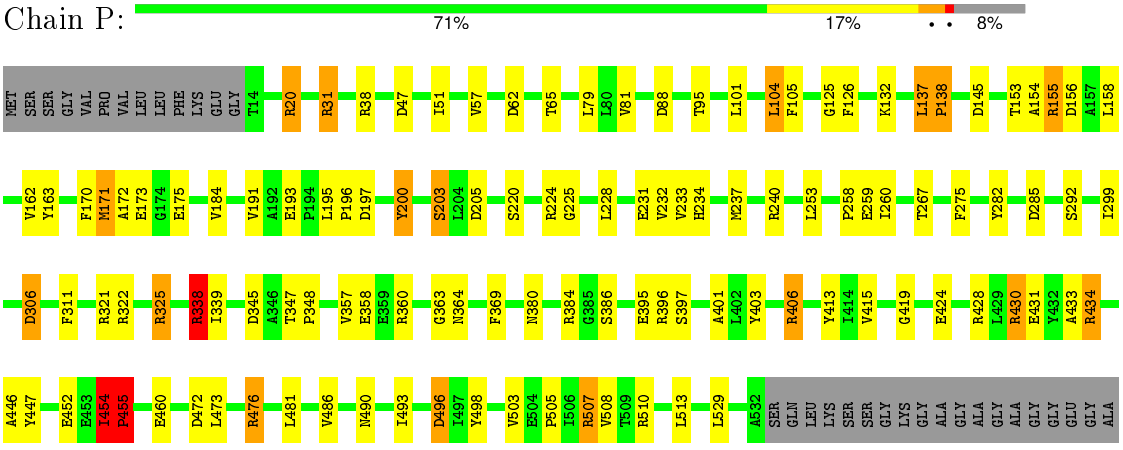
- Molecule 1: Chaperonin alpha subunit

Chain O:



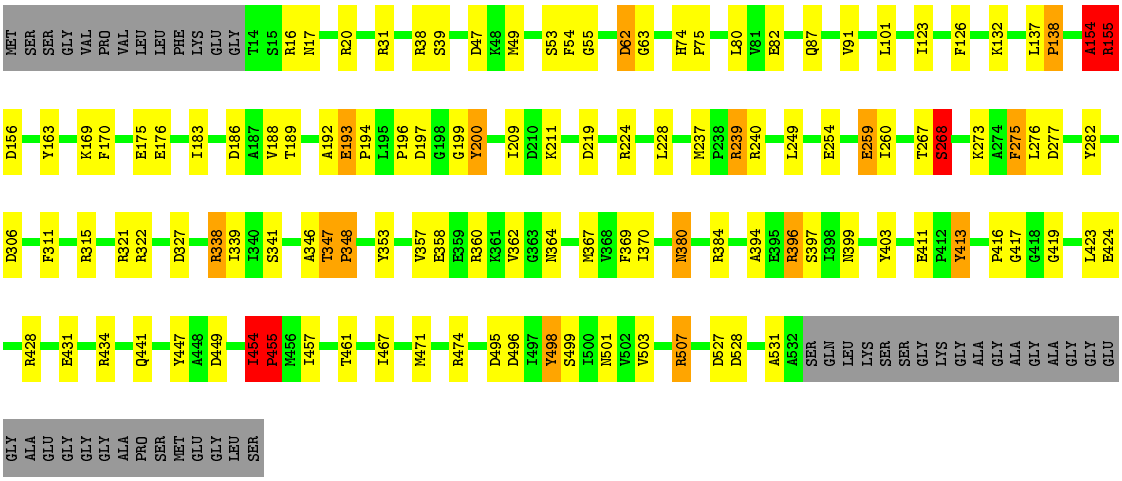
- Molecule 1: Chaperonin alpha subunit

Chain P:



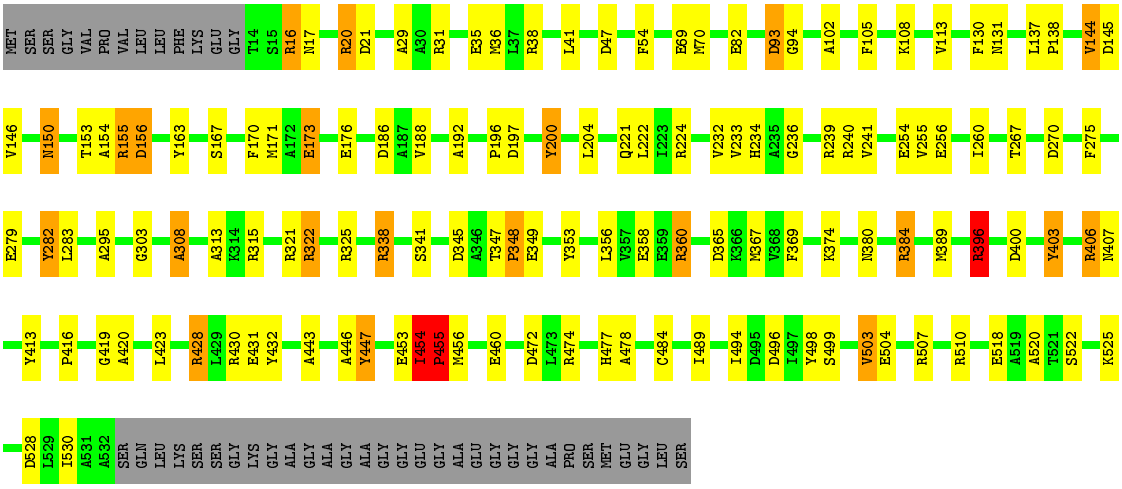
• Molecule 1: Chaperonin alpha subunit

Chain Q:



• Molecule 1: Chaperonin alpha subunit

Chain R:



4 Experimental information (i)

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of images	9596	Depositor
Resolution determination method	Not provided	Depositor
CTF correction method	The whole micrograph	Depositor
Microscope	Titan Krios	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	Not provided	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	3500	Depositor
Magnification	96000	Depositor
Image detector	Gatan Ultrascan 4000 Model 895	Depositor

5 Model quality

5.1 Standard geometry

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	1.58	25/3974 (0.6%)	2.04	116/5360 (2.2%)
1	B	1.61	19/3974 (0.5%)	2.00	94/5360 (1.8%)
1	C	1.56	17/3974 (0.4%)	1.98	106/5360 (2.0%)
1	D	1.56	17/3974 (0.4%)	1.97	105/5360 (2.0%)
1	E	1.58	24/3974 (0.6%)	1.92	91/5360 (1.7%)
1	F	1.60	21/3974 (0.5%)	1.96	95/5360 (1.8%)
1	G	1.56	13/3974 (0.3%)	1.98	103/5360 (1.9%)
1	H	1.58	17/3974 (0.4%)	2.08	121/5360 (2.3%)
1	I	1.62	20/3974 (0.5%)	1.98	102/5360 (1.9%)
1	J	1.63	23/3974 (0.6%)	2.02	100/5360 (1.9%)
1	K	1.61	26/3974 (0.7%)	1.92	85/5360 (1.6%)
1	L	1.58	15/3974 (0.4%)	1.98	99/5360 (1.8%)
1	M	1.57	22/3974 (0.6%)	1.98	110/5360 (2.1%)
1	N	1.60	18/3974 (0.5%)	2.03	114/5360 (2.1%)
1	O	1.59	21/3974 (0.5%)	2.04	106/5360 (2.0%)
1	P	1.57	15/3974 (0.4%)	2.05	98/5360 (1.8%)
1	Q	1.59	17/3974 (0.4%)	1.94	88/5360 (1.6%)
1	R	1.62	28/3974 (0.7%)	1.97	110/5360 (2.1%)
All	All	1.59	358/71532 (0.5%)	1.99	1843/96480 (1.9%)

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	21
1	B	0	19
1	C	0	23
1	D	0	21
1	E	0	19
1	F	0	15
1	G	0	20

Continued on next page...

Continued from previous page...

Mol	Chain	#Chirality outliers	#Planarity outliers
1	H	0	16
1	I	0	19
1	J	0	20
1	K	0	18
1	L	0	22
1	M	0	22
1	N	0	21
1	O	0	22
1	P	0	18
1	Q	0	18
1	R	0	21
All	All	0	355

The worst 5 of 358 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	Q	397	SER	CA-CB	10.83	1.69	1.52
1	Q	413	TYR	CE2-CZ	9.00	1.50	1.38
1	F	413	TYR	CG-CD2	8.70	1.50	1.39
1	A	15	SER	CA-CB	8.59	1.65	1.52
1	A	268	SER	CA-CB	8.57	1.65	1.52

The worst 5 of 1843 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	H	384	ARG	NE-CZ-NH2	22.41	131.51	120.30
1	P	224	ARG	NE-CZ-NH2	20.40	130.50	120.30
1	D	406	ARG	NE-CZ-NH2	20.01	130.31	120.30
1	P	325	ARG	NE-CZ-NH1	-19.55	110.52	120.30
1	O	510	ARG	NE-CZ-NH2	19.31	129.96	120.30

There are no chirality outliers.

5 of 355 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	126	PHE	Sidechain
1	A	147	SER	Peptide
1	A	154	ALA	Peptide
1	A	163	TYR	Sidechain
1	A	74	HIS	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	3937	0	4104	11	0
1	B	3937	0	4104	18	0
1	C	3937	0	4104	17	0
1	D	3937	0	4104	5	0
1	E	3937	0	4104	19	0
1	F	3937	0	4104	8	0
1	G	3937	0	4104	15	0
1	H	3937	0	4104	11	0
1	I	3937	0	4104	16	0
1	J	3937	0	4104	13	0
1	K	3937	0	4104	9	0
1	L	3937	0	4104	9	0
1	M	3937	0	4104	17	0
1	N	3937	0	4104	14	0
1	O	3937	0	4104	13	0
1	P	3937	0	4104	8	0
1	Q	3937	0	4104	9	0
1	R	3937	0	4104	8	0
All	All	70866	0	73872	214	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 1.

The worst 5 of 214 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:454:ILE:HG22	1:J:455:PRO:HD2	1.66	0.78
1:D:454:ILE:HB	1:D:455:PRO:HD2	1.75	0.69
1:O:255:VAL:HG21	1:O:279:GLU:HG3	1.74	0.69
1:E:233:VAL:HG13	1:E:234:HIS:H	1.60	0.66
1:J:362:VAL:HG11	1:J:382:LEU:HD21	1.77	0.66

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	517/563 (92%)	456 (88%)	40 (8%)	21 (4%)	3	35
1	B	517/563 (92%)	455 (88%)	40 (8%)	22 (4%)	3	34
1	C	517/563 (92%)	459 (89%)	38 (7%)	20 (4%)	4	36
1	D	517/563 (92%)	461 (89%)	36 (7%)	20 (4%)	4	36
1	E	517/563 (92%)	456 (88%)	42 (8%)	19 (4%)	4	38
1	F	517/563 (92%)	456 (88%)	40 (8%)	21 (4%)	3	35
1	G	517/563 (92%)	461 (89%)	37 (7%)	19 (4%)	4	38
1	H	517/563 (92%)	460 (89%)	37 (7%)	20 (4%)	4	36
1	I	517/563 (92%)	463 (90%)	33 (6%)	21 (4%)	3	35
1	J	517/563 (92%)	468 (90%)	29 (6%)	20 (4%)	4	36
1	K	517/563 (92%)	464 (90%)	35 (7%)	18 (4%)	4	39
1	L	517/563 (92%)	459 (89%)	39 (8%)	19 (4%)	4	38
1	M	517/563 (92%)	468 (90%)	33 (6%)	16 (3%)	5	42
1	N	517/563 (92%)	454 (88%)	44 (8%)	19 (4%)	4	38
1	O	517/563 (92%)	461 (89%)	37 (7%)	19 (4%)	4	38
1	P	517/563 (92%)	465 (90%)	34 (7%)	18 (4%)	4	39
1	Q	517/563 (92%)	464 (90%)	33 (6%)	20 (4%)	4	36
1	R	517/563 (92%)	463 (90%)	38 (7%)	16 (3%)	5	42
All	All	9306/10134 (92%)	8293 (89%)	665 (7%)	348 (4%)	7	38

5 of 348 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	233	VAL
1	A	322	ARG
1	A	455	PRO
1	B	145	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	155	ARG

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	427/453 (94%)	416 (97%)	11 (3%)	54	80
1	B	427/453 (94%)	406 (95%)	21 (5%)	31	67
1	C	427/453 (94%)	408 (96%)	19 (4%)	35	69
1	D	427/453 (94%)	420 (98%)	7 (2%)	70	88
1	E	427/453 (94%)	416 (97%)	11 (3%)	54	80
1	F	427/453 (94%)	410 (96%)	17 (4%)	38	71
1	G	427/453 (94%)	412 (96%)	15 (4%)	43	74
1	H	427/453 (94%)	412 (96%)	15 (4%)	43	74
1	I	427/453 (94%)	411 (96%)	16 (4%)	41	73
1	J	427/453 (94%)	410 (96%)	17 (4%)	38	71
1	K	427/453 (94%)	415 (97%)	12 (3%)	51	78
1	L	427/453 (94%)	417 (98%)	10 (2%)	58	83
1	M	427/453 (94%)	415 (97%)	12 (3%)	51	78
1	N	427/453 (94%)	407 (95%)	20 (5%)	32	68
1	O	427/453 (94%)	413 (97%)	14 (3%)	45	76
1	P	427/453 (94%)	416 (97%)	11 (3%)	54	80
1	Q	427/453 (94%)	412 (96%)	15 (4%)	43	74
1	R	427/453 (94%)	416 (97%)	11 (3%)	54	80
All	All	7686/8154 (94%)	7432 (97%)	254 (3%)	49	76

5 of 254 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	H	454	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	J	356	LEU
1	Q	211	LYS
1	I	104	LEU
1	I	380	ASN

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	J	118	HIS
1	K	477	HIS
1	M	490	ASN
1	I	309	GLN
1	O	309	GLN

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)

There are no ligands in this entry.

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.