



wwPDB EM Map/Model Validation Report ⓘ

Apr 10, 2016 – 01:56 PM BST

PDB ID : 3J1F
EMDB ID: : EMD-5396
Title : Cryo-EM structure of 9-fold symmetric rATcpn-beta in ATP-binding 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 : 6.20 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 : 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

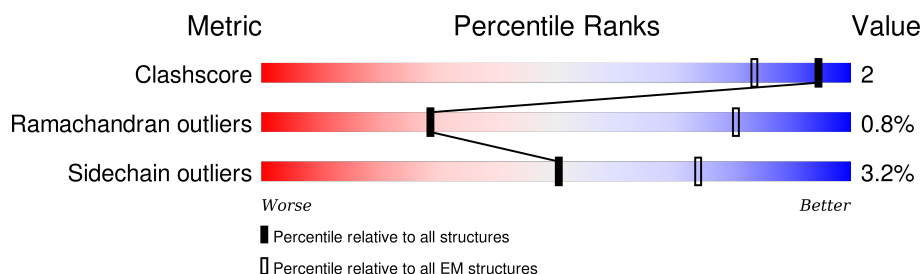
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 6.20 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	553	73% 15% • 9%
1	B	553	70% 17% • • 9%
1	C	553	73% 15% • 9%
1	D	553	72% 16% • 9%
1	E	553	69% 20% • 9%
1	F	553	73% 16% • 9%
1	G	553	70% 17% • • 9%
1	H	553	73% 17% • 9%
1	I	553	72% 16% • 9%

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Mol	Chain	Length	Quality of chain
1	K	553	 72%15%••9%
1	L	553	 73%16%•9%
1	M	553	 70%19%•9%
1	N	553	 68%21%•9%
1	O	553	 70%17%•9%
1	P	553	 72%16%•9%
1	Q	553	 72%16%•9%
1	R	553	 71%17%•9%
1	S	553	 71%18%•9%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 69858 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 beta subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	505	Total	C	N	O	S	0	0
			3849	2423	658	757	11		
1	B	505	Total	C	N	O	S	0	0
			3849	2423	658	757	11		
1	C	505	Total	C	N	O	S	0	0
			3849	2423	658	757	11		
1	D	505	Total	C	N	O	S	0	0
			3849	2423	658	757	11		
1	E	505	Total	C	N	O	S	0	0
			3849	2423	658	757	11		
1	F	505	Total	C	N	O	S	0	0
			3849	2423	658	757	11		
1	G	505	Total	C	N	O	S	0	0
			3849	2423	658	757	11		
1	H	505	Total	C	N	O	S	0	0
			3849	2423	658	757	11		
1	I	505	Total	C	N	O	S	0	0
			3849	2423	658	757	11		
1	K	505	Total	C	N	O	S	0	0
			3849	2423	658	757	11		
1	L	505	Total	C	N	O	S	0	0
			3849	2423	658	757	11		
1	M	505	Total	C	N	O	S	0	0
			3849	2423	658	757	11		
1	N	505	Total	C	N	O	S	0	0
			3849	2423	658	757	11		
1	O	505	Total	C	N	O	S	0	0
			3849	2423	658	757	11		
1	P	505	Total	C	N	O	S	0	0
			3849	2423	658	757	11		
1	Q	505	Total	C	N	O	S	0	0
			3849	2423	658	757	11		
1	R	505	Total	C	N	O	S	0	0
			3849	2423	658	757	11		

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	S	505	Total	C	N	O	S	0	0
			3849	2423	658	757	11		

- # ATP
-
- The diagram illustrates the chemical structure of Adenosine Triphosphate (ATP). It consists of an adenine base (a purine ring system) attached to a ribose sugar, which is in turn attached to a chain of three phosphate groups. The adenine base is shown with atoms N1, N3, N7, C2, C4, C6, and C8. The ribose sugar is shown with atoms C1', C2', C3', C4', and C5'. The three phosphate groups are shown with atoms P1, P2, and P3, and their respective oxygen atoms (O1, O2, O3, O4, O5, O6, O7, O8, O9, O10, O11, O12, O13, O14, O15, O16, O17, O18, O19, O20, O21, O22, O23, O24, O25, O26, O27, O28, O29, O30, O31, O32, O33, O34, O35, O36, O37, O38, O39, O40, O41, O42, O43, O44, O45, O46, O47, O48, O49, O50, O51, O52, O53, O54, O55, O56, O57, O58, O59, O60, O61, O62, O63, O64, O65, O66, O67, O68, O69, O70, O71, O72, O73, O74, O75, O76, O77, O78, O79, O80, O81, O82, O83, O84, O85, O86, O87, O88, O89, O90, O91, O92, O93, O94, O95, O96, O97, O98, O99, O100). The structure is color-coded: adenine is blue, ribose is green, and the phosphate chain is red. The adenine base is connected to the ribose sugar via a glycosidic bond at the C1' position. The ribose sugar is connected to the first phosphate group (P1) via an ester bond at the C5' position. The three phosphate groups are connected in a chain (P1-P2-P3) via phosphoanhydride bonds. The terminal phosphate group (P3) is shown with a negative charge on one of its oxygen atoms (O33).

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Mol	Chain	Residues	Atoms					AltConf
2	L	1	Total	C	N	O	P	0
			31	10	5	13	3	
2	M	1	Total	C	N	O	P	0
			31	10	5	13	3	
2	N	1	Total	C	N	O	P	0
			31	10	5	13	3	
2	O	1	Total	C	N	O	P	0
			31	10	5	13	3	
2	P	1	Total	C	N	O	P	0
			31	10	5	13	3	
2	Q	1	Total	C	N	O	P	0
			31	10	5	13	3	
2	R	1	Total	C	N	O	P	0
			31	10	5	13	3	
2	S	1	Total	C	N	O	P	0
			31	10	5	13	3	

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

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

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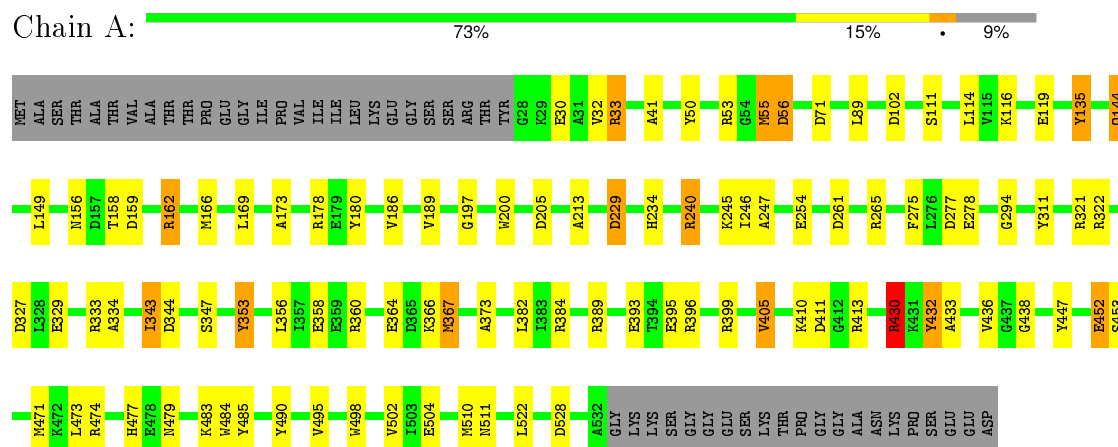
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Mol	Chain	Residues	Atoms		AltConf
3	N	1	Total 1	Mg 1	0
3	O	1	Total 1	Mg 1	0
3	R	1	Total 1	Mg 1	0
3	L	1	Total 1	Mg 1	0
3	S	1	Total 1	Mg 1	0
3	F	1	Total 1	Mg 1	0
3	M	1	Total 1	Mg 1	0

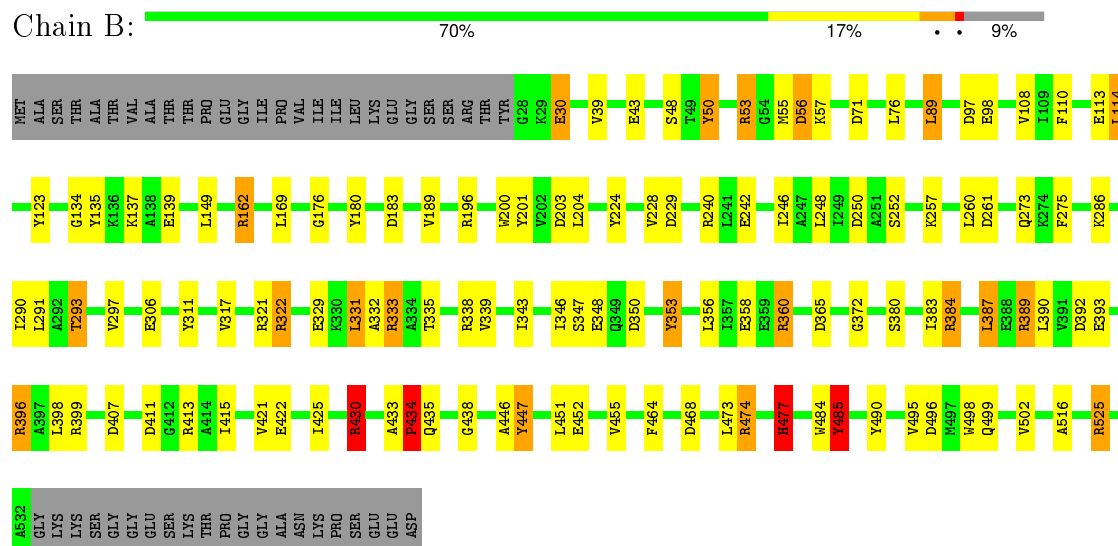
3 Residue-property plots

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 beta subunit

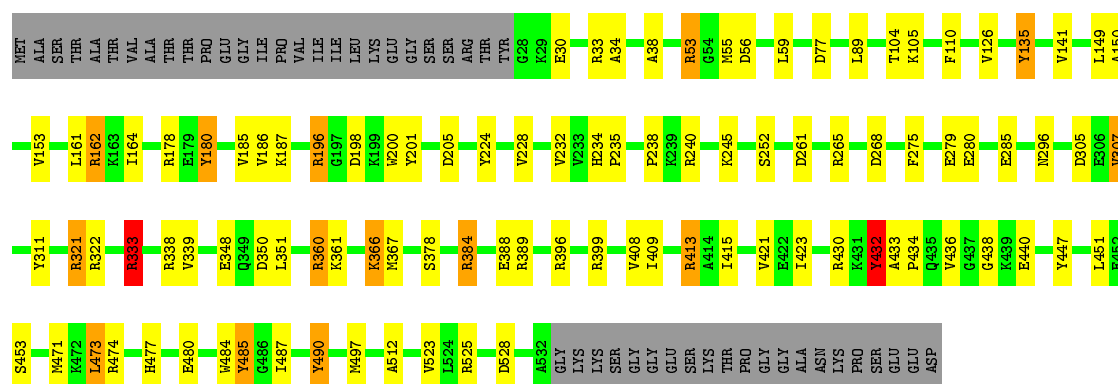


- Molecule 1: Chaperonin beta subunit

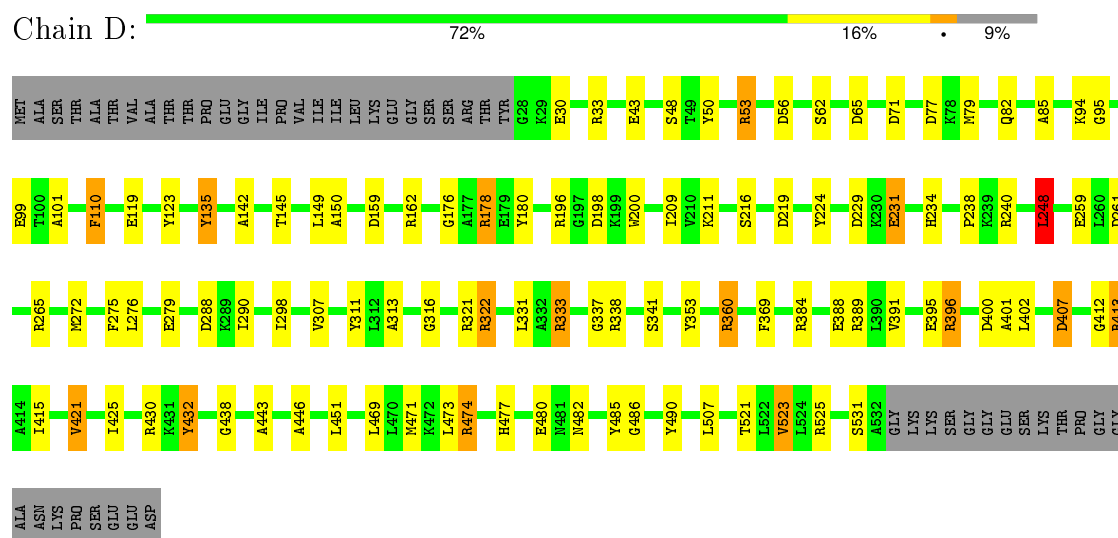


- Molecule 1: Chaperonin beta subunit

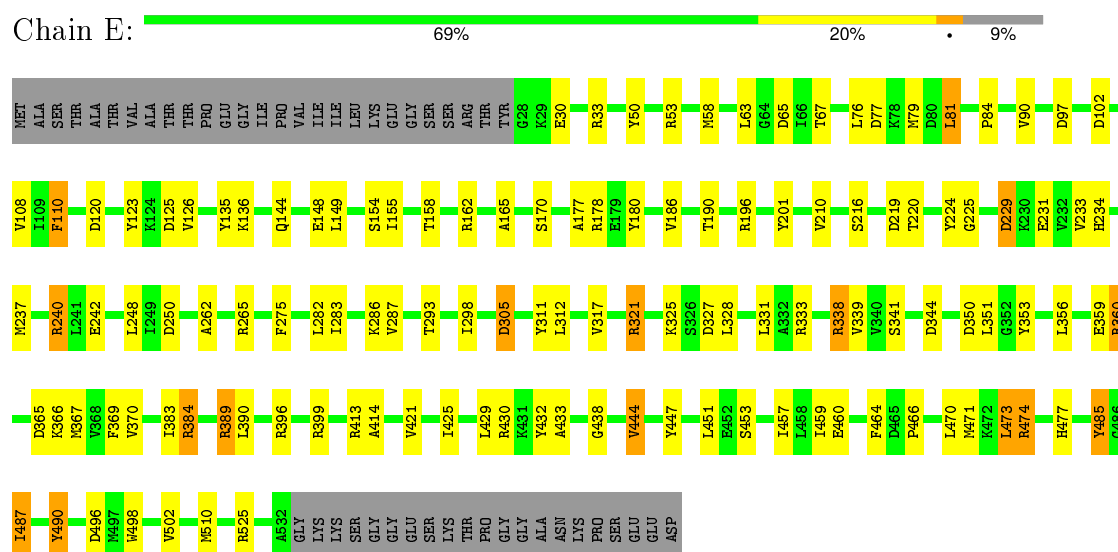




• Molecule 1: Chaperonin beta subunit

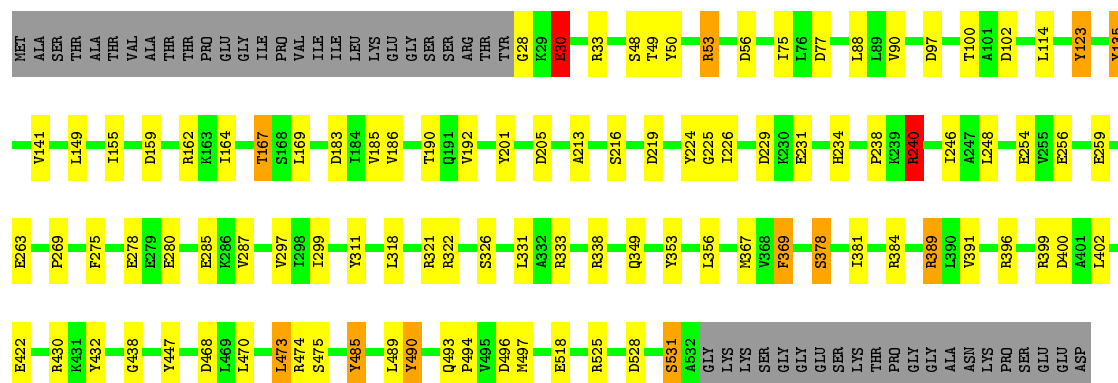


• Molecule 1: Chaperonin beta subunit



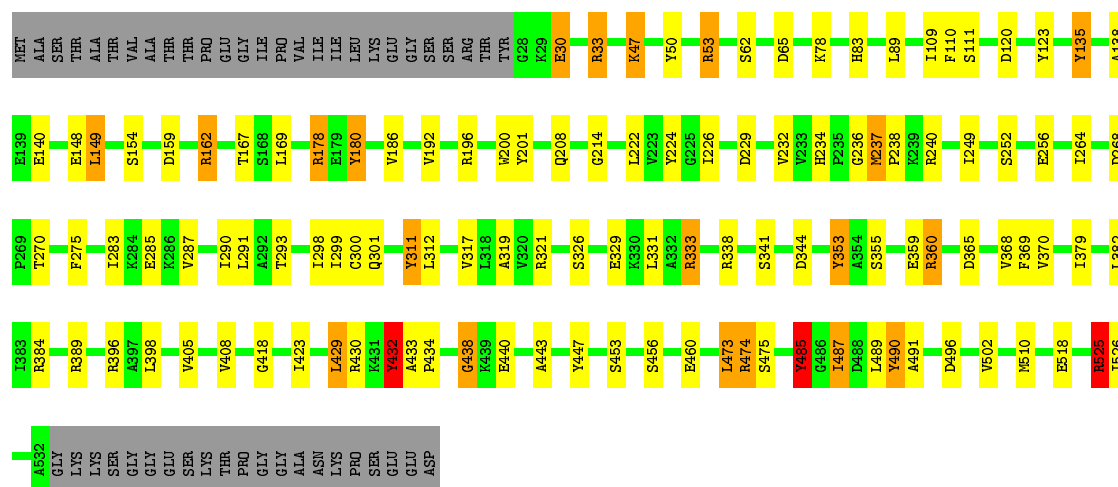
• Molecule 1: Chaperonin beta subunit

Chain F:  73% 16% 9%



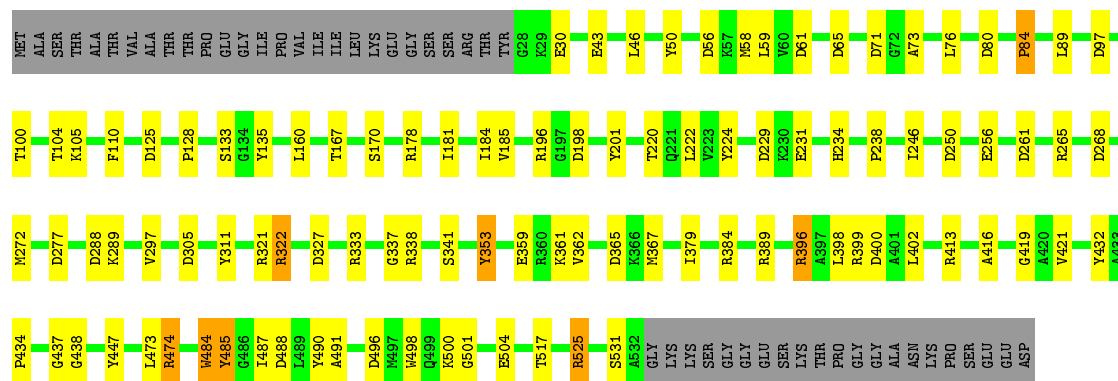
- Molecule 1: Chaperonin beta subunit

Chain G:  70% 17% 9%



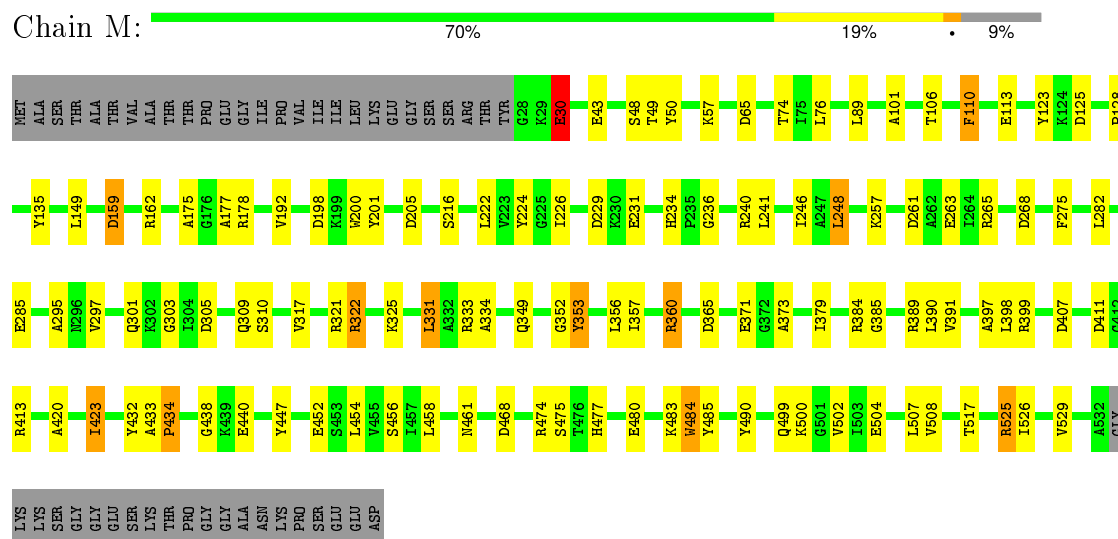
- Molecule 1: Chaperonin beta subunit

Chain H:  73% 17% 9%

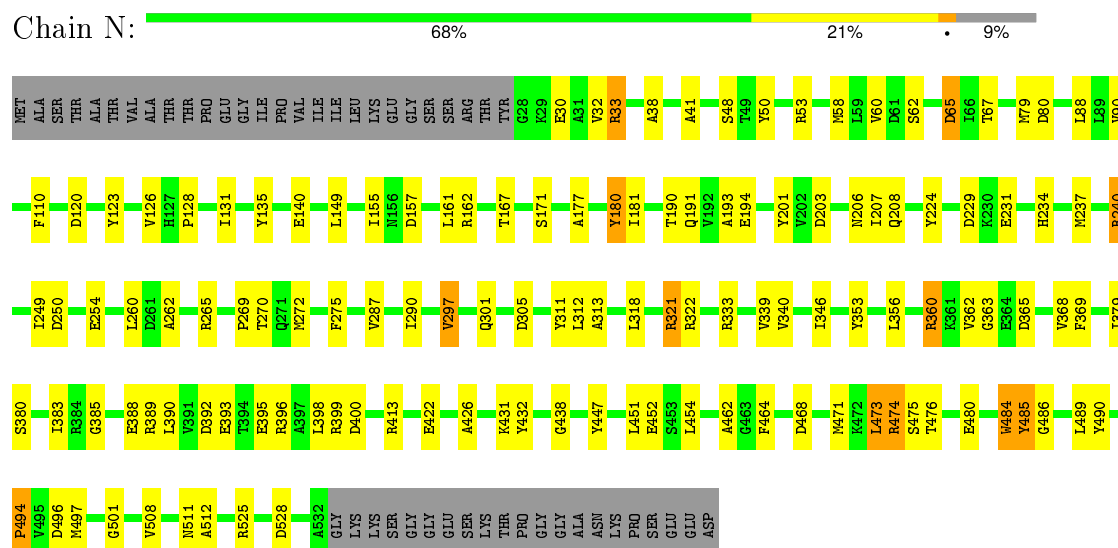


- Molecule 1: Chaperonin beta subunit

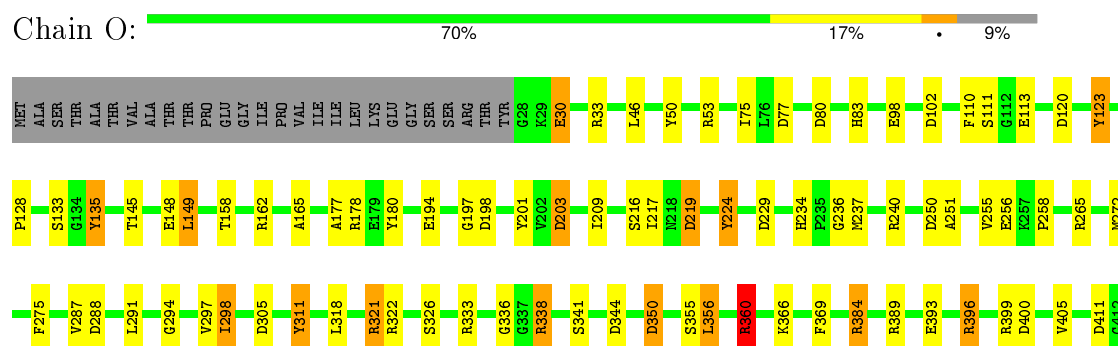
- Molecule 1: Chaperonin beta subunit



- Molecule 1: Chaperonin beta subunit



- Molecule 1: Chaperonin beta subunit



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	The whole micrograph	Depositor
Microscope	FEI Titan Krios	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	20	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 ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: 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	1.59	16/3886 (0.4%)	1.94	81/5245 (1.5%)
1	B	1.59	20/3886 (0.5%)	1.94	87/5245 (1.7%)
1	C	1.59	15/3886 (0.4%)	1.94	82/5245 (1.6%)
1	D	1.57	21/3886 (0.5%)	1.94	81/5245 (1.5%)
1	E	1.58	19/3886 (0.5%)	1.97	97/5245 (1.8%)
1	F	1.63	25/3886 (0.6%)	1.92	74/5245 (1.4%)
1	G	1.59	25/3886 (0.6%)	1.91	83/5245 (1.6%)
1	H	1.57	13/3886 (0.3%)	1.91	79/5245 (1.5%)
1	I	1.63	19/3886 (0.5%)	1.90	81/5245 (1.5%)
1	K	1.60	18/3886 (0.5%)	1.90	78/5245 (1.5%)
1	L	1.58	21/3886 (0.5%)	1.99	88/5245 (1.7%)
1	M	1.57	18/3886 (0.5%)	1.92	79/5245 (1.5%)
1	N	1.59	15/3886 (0.4%)	1.96	104/5245 (2.0%)
1	O	1.57	16/3886 (0.4%)	1.95	106/5245 (2.0%)
1	P	1.54	13/3886 (0.3%)	1.91	80/5245 (1.5%)
1	Q	1.57	20/3886 (0.5%)	1.97	93/5245 (1.8%)
1	R	1.58	20/3886 (0.5%)	1.98	101/5245 (1.9%)
1	S	1.58	18/3886 (0.5%)	1.95	89/5245 (1.7%)
All	All	1.58	332/69948 (0.5%)	1.94	1563/94410 (1.7%)

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	16
1	C	0	15
1	D	0	12
1	E	0	7

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Mol	Chain	#Chirality outliers	#Planarity outliers
1	F	0	9
1	G	0	14
1	H	0	13
1	I	0	12
1	K	0	14
1	L	0	13
1	M	0	8
1	N	0	6
1	O	0	13
1	P	0	10
1	Q	0	17
1	R	0	12
1	S	0	7
All	All	0	207

The worst 5 of 332 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	S	135	TYR	CG-CD2	9.30	1.51	1.39
1	N	494	PRO	N-CD	-8.56	1.35	1.47
1	K	113	GLU	CD-OE1	8.50	1.34	1.25
1	L	490	TYR	CZ-OH	8.11	1.51	1.37
1	A	432	TYR	CG-CD1	7.84	1.49	1.39

The worst 5 of 1563 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	196	ARG	NE-CZ-NH1	-24.99	107.81	120.30
1	L	33	ARG	NE-CZ-NH1	21.31	130.95	120.30
1	F	430	ARG	NE-CZ-NH1	19.66	130.13	120.30
1	Q	135	TYR	CB-CG-CD1	-18.98	109.61	121.00
1	Q	178	ARG	NE-CZ-NH2	18.75	129.67	120.30

There are no chirality outliers.

5 of 207 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	135	TYR	Sidechain
1	A	178	ARG	Sidechain
1	A	234	HIS	Sidechain
1	A	240	ARG	Sidechain

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Mol	Chain	Res	Type	Group
1	A	33	ARG	Sidechain

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	3849	0	3995	8	0
1	B	3849	0	3995	17	0
1	C	3849	0	3995	12	0
1	D	3849	0	3995	13	0
1	E	3849	0	3995	19	0
1	F	3849	0	3995	10	0
1	G	3849	0	3995	18	0
1	H	3849	0	3995	9	0
1	I	3849	0	3995	14	0
1	K	3849	0	3995	15	0
1	L	3849	0	3995	6	0
1	M	3849	0	3995	12	0
1	N	3849	0	3995	14	0
1	O	3849	0	3995	11	0
1	P	3849	0	3995	16	0
1	Q	3849	0	3995	12	0
1	R	3849	0	3995	7	0
1	S	3849	0	3995	10	0
2	A	31	0	12	0	0
2	B	31	0	12	0	0
2	C	31	0	12	0	0
2	D	31	0	12	0	0
2	E	31	0	12	0	0
2	F	31	0	12	0	0
2	G	31	0	12	0	0
2	H	31	0	12	0	0
2	I	31	0	12	0	0
2	K	31	0	12	0	0
2	L	31	0	12	0	0
2	M	31	0	12	0	0
2	N	31	0	12	0	0
2	O	31	0	12	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	P	31	0	12	0	0
2	Q	31	0	12	0	0
2	R	31	0	12	0	0
2	S	31	0	12	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
3	H	1	0	0	0	0
3	I	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
3	O	1	0	0	0	0
3	P	1	0	0	0	0
3	Q	1	0	0	0	0
3	R	1	0	0	0	0
3	S	1	0	0	0	0
All	All	69858	0	72126	216	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 2.

The worst 5 of 216 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:F:246:ILE:HA	1:F:297:VAL:HG13	1.62	0.79
1:P:88:LEU:HD13	1:Q:68:ILE:HD11	1.73	0.71
1:K:189:VAL:HG11	1:K:405:VAL:HG12	1.76	0.67
1:E:331:LEU:HD11	1:E:370:VAL:HG11	1.76	0.66
1:K:473:LEU:HD12	1:K:487:ILE:HG23	1.79	0.64

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	503/553 (91%)	453 (90%)	46 (9%)	4 (1%)	24	69
1	B	503/553 (91%)	451 (90%)	44 (9%)	8 (2%)	12	56
1	C	503/553 (91%)	456 (91%)	44 (9%)	3 (1%)	30	74
1	D	503/553 (91%)	459 (91%)	41 (8%)	3 (1%)	30	74
1	E	503/553 (91%)	449 (89%)	50 (10%)	4 (1%)	24	69
1	F	503/553 (91%)	457 (91%)	42 (8%)	4 (1%)	24	69
1	G	503/553 (91%)	449 (89%)	50 (10%)	4 (1%)	24	69
1	H	503/553 (91%)	459 (91%)	42 (8%)	2 (0%)	39	79
1	I	503/553 (91%)	456 (91%)	44 (9%)	3 (1%)	30	74
1	K	503/553 (91%)	457 (91%)	44 (9%)	2 (0%)	39	79
1	L	503/553 (91%)	451 (90%)	46 (9%)	6 (1%)	16	61
1	M	503/553 (91%)	456 (91%)	42 (8%)	5 (1%)	19	64
1	N	503/553 (91%)	454 (90%)	43 (8%)	6 (1%)	16	61
1	O	503/553 (91%)	452 (90%)	46 (9%)	5 (1%)	19	64
1	P	503/553 (91%)	455 (90%)	43 (8%)	5 (1%)	19	64
1	Q	503/553 (91%)	450 (90%)	50 (10%)	3 (1%)	30	74
1	R	503/553 (91%)	455 (90%)	43 (8%)	5 (1%)	19	64
1	S	503/553 (91%)	451 (90%)	49 (10%)	3 (1%)	30	74
All	All	9054/9954 (91%)	8170 (90%)	809 (9%)	75 (1%)	29	69

5 of 75 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	L	213	ALA
1	B	30	GLU
1	C	30	GLU
1	D	30	GLU

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Mol	Chain	Res	Type
1	F	30	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	410/447 (92%)	396 (97%)	14 (3%)	44	75
1	B	410/447 (92%)	397 (97%)	13 (3%)	46	76
1	C	410/447 (92%)	398 (97%)	12 (3%)	50	78
1	D	410/447 (92%)	399 (97%)	11 (3%)	52	79
1	E	410/447 (92%)	396 (97%)	14 (3%)	44	75
1	F	410/447 (92%)	397 (97%)	13 (3%)	46	76
1	G	410/447 (92%)	396 (97%)	14 (3%)	44	75
1	H	410/447 (92%)	398 (97%)	12 (3%)	50	78
1	I	410/447 (92%)	394 (96%)	16 (4%)	39	72
1	K	410/447 (92%)	397 (97%)	13 (3%)	46	76
1	L	410/447 (92%)	403 (98%)	7 (2%)	68	87
1	M	410/447 (92%)	389 (95%)	21 (5%)	29	66
1	N	410/447 (92%)	391 (95%)	19 (5%)	33	68
1	O	410/447 (92%)	395 (96%)	15 (4%)	41	73
1	P	410/447 (92%)	400 (98%)	10 (2%)	57	82
1	Q	410/447 (92%)	402 (98%)	8 (2%)	63	85
1	R	410/447 (92%)	401 (98%)	9 (2%)	60	83
1	S	410/447 (92%)	398 (97%)	12 (3%)	50	78
All	All	7380/8046 (92%)	7147 (97%)	233 (3%)	50	76

5 of 233 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	I	89	LEU

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Mol	Chain	Res	Type
1	K	453	SER
1	R	102	ASP
1	I	205	ASP
1	I	485	TYR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 26 such sidechains are listed below:

Mol	Chain	Res	Type
1	L	441	GLN
1	M	234	HIS
1	S	234	HIS
1	M	144	GLN
1	M	206	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 36 ligands modelled in this entry, 18 are monoatomic - leaving 18 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	800	3	26,33,33	1.03	1 (3%)	26,52,52	1.70	5 (19%)
2	ATP	B	800	3	26,33,33	1.32	3 (11%)	26,52,52	1.69	4 (15%)
2	ATP	C	800	3	26,33,33	1.27	2 (7%)	26,52,52	1.55	4 (15%)
2	ATP	D	800	3	26,33,33	1.43	4 (15%)	26,52,52	1.86	4 (15%)
2	ATP	E	800	3	26,33,33	1.24	4 (15%)	26,52,52	1.74	6 (23%)
2	ATP	F	800	3	26,33,33	1.24	3 (11%)	26,52,52	1.54	5 (19%)
2	ATP	G	800	3	26,33,33	1.30	2 (7%)	26,52,52	1.94	5 (19%)
2	ATP	H	800	3	26,33,33	1.15	2 (7%)	26,52,52	1.69	5 (19%)
2	ATP	I	800	3	26,33,33	1.37	3 (11%)	26,52,52	1.55	5 (19%)
2	ATP	K	800	3	26,33,33	1.51	4 (15%)	26,52,52	1.55	4 (15%)
2	ATP	L	800	3	26,33,33	1.55	3 (11%)	26,52,52	1.59	5 (19%)
2	ATP	M	800	3	26,33,33	1.85	6 (23%)	26,52,52	1.62	2 (7%)
2	ATP	N	800	3	26,33,33	1.21	2 (7%)	26,52,52	1.74	3 (11%)
2	ATP	O	800	3	26,33,33	1.19	2 (7%)	26,52,52	1.59	7 (26%)
2	ATP	P	800	3	26,33,33	1.35	4 (15%)	26,52,52	1.27	1 (3%)
2	ATP	Q	800	3	26,33,33	1.96	4 (15%)	26,52,52	1.59	3 (11%)
2	ATP	R	800	3	26,33,33	1.08	2 (7%)	26,52,52	1.55	3 (11%)
2	ATP	S	800	3	26,33,33	1.49	4 (15%)	26,52,52	1.30	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
2	ATP	A	800	3	-	0/18/38/38	0/3/3/3
2	ATP	B	800	3	-	0/18/38/38	0/3/3/3
2	ATP	C	800	3	-	0/18/38/38	0/3/3/3
2	ATP	D	800	3	-	0/18/38/38	0/3/3/3
2	ATP	E	800	3	-	0/18/38/38	0/3/3/3
2	ATP	F	800	3	-	0/18/38/38	0/3/3/3
2	ATP	G	800	3	-	0/18/38/38	0/3/3/3
2	ATP	H	800	3	-	0/18/38/38	0/3/3/3
2	ATP	I	800	3	-	0/18/38/38	0/3/3/3
2	ATP	K	800	3	-	0/18/38/38	0/3/3/3
2	ATP	L	800	3	-	0/18/38/38	0/3/3/3
2	ATP	M	800	3	-	0/18/38/38	0/3/3/3
2	ATP	N	800	3	-	0/18/38/38	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	ATP	O	800	3	-	0/18/38/38	0/3/3/3
2	ATP	P	800	3	-	0/18/38/38	0/3/3/3
2	ATP	Q	800	3	-	0/18/38/38	0/3/3/3
2	ATP	R	800	3	-	0/18/38/38	0/3/3/3
2	ATP	S	800	3	-	0/18/38/38	0/3/3/3

The worst 5 of 55 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	Q	800	ATP	O4'-C1'	-7.69	1.30	1.41
2	M	800	ATP	C2'-C1'	-5.44	1.45	1.53
2	L	800	ATP	C8-N7	-4.37	1.26	1.34
2	I	800	ATP	C2'-C1'	-4.23	1.46	1.53
2	M	800	ATP	C8-N7	-3.51	1.27	1.34

The worst 5 of 74 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	M	800	ATP	C4'-O4'-C1'	-6.27	103.00	109.64
2	N	800	ATP	C4'-O4'-C1'	-6.15	103.12	109.64
2	B	800	ATP	C4'-O4'-C1'	-6.13	103.14	109.64
2	K	800	ATP	C4'-O4'-C1'	-5.26	104.06	109.64
2	C	800	ATP	C4'-O4'-C1'	-5.03	104.31	109.64

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 [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.