



wwPDB X-ray Structure Validation Summary Report

Mar 31, 2014 – 05:40 PM BST

PDB ID : 1WE3
Title : Crystal Structure of the Chaperonin Complex Cpn60/Cpn10/(ADP)7 from Thermus Thermophilus
Authors : Shimamura, T.; Koike-Takeshita, A.; Yokoyama, K.; Masui, R.; Murai, N.; Yoshida, M.; Taguchi, H.; Iwata, S.
Deposited on : 2004-05-23
Resolution : 2.80 Å(reported)

This is a wwPDB validation summary report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

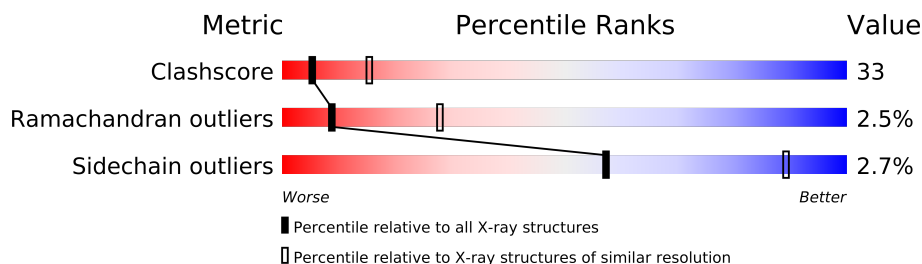
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : **NOT EXECUTED**
Percentile statistics : 21963
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable23004

1 Overall quality at a glance

The reported resolution of this entry is 2.80 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)	Similar resolution (#Entries, resolution range(Å))
Clashscore	79885	2295 (2.80-2.80)
Ramachandran outliers	78287	2252 (2.80-2.80)
Sidechain outliers	78261	2254 (2.80-2.80)


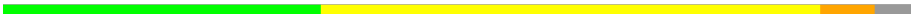
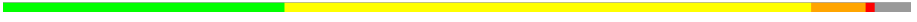

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	543	
1	B	543	
1	C	543	
1	D	543	
1	E	543	
1	F	543	
1	G	543	
1	H	543	
1	I	543	
1	J	543	
1	K	543	
1	L	543	
1	M	543	
1	N	543	
2	O	100	
2	P	100	
2	Q	100	

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Mol	Chain	Length	Quality of chain
2	R	100	
2	S	100	
2	T	100	
2	U	100	

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 60639 atoms, of which 0 are hydrogen and 0 are deuterium.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, 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 cpn60(GroEL).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	527	Total	C	N	O	S	0	0	0
			3956	2484	686	781	5			
1	B	527	Total	C	N	O	S	0	0	0
			3956	2484	686	781	5			
1	C	526	Total	C	N	O	S	0	0	0
			3947	2478	684	780	5			
1	D	526	Total	C	N	O	S	0	0	0
			3947	2478	684	780	5			
1	E	526	Total	C	N	O	S	0	0	0
			3947	2478	684	780	5			
1	F	529	Total	C	N	O	S	0	0	0
			3974	2495	689	785	5			
1	G	525	Total	C	N	O	S	0	0	0
			3938	2473	683	777	5			
1	H	526	Total	C	N	O	S	0	0	0
			3947	2478	684	780	5			
1	I	525	Total	C	N	O	S	0	0	0
			3938	2473	683	777	5			
1	J	525	Total	C	N	O	S	0	0	0
			3938	2473	683	777	5			
1	K	525	Total	C	N	O	S	0	0	0
			3938	2473	683	777	5			
1	L	526	Total	C	N	O	S	0	0	0
			3947	2478	684	780	5			
1	M	525	Total	C	N	O	S	0	0	0
			3938	2473	683	777	5			
1	N	526	Total	C	N	O	S	0	0	0
			3947	2478	684	780	5			

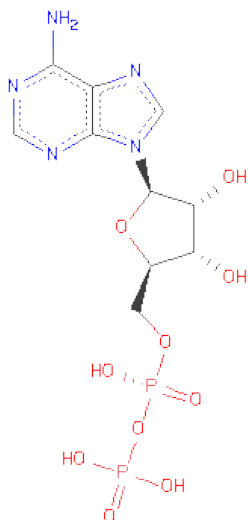
- Molecule 2 is a protein called cpn10(GroES).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	O	96	Total	C	N	O	0	0	0
			739	470	126	143			
2	P	94	Total	C	N	O	0	0	0
			723	460	123	140			
2	Q	96	Total	C	N	O	0	0	0
			739	470	126	143			
2	R	96	Total	C	N	O	0	0	0
			739	470	126	143			
2	S	96	Total	C	N	O	0	0	0
			739	470	126	143			
2	T	96	Total	C	N	O	0	0	0
			739	470	126	143			
2	U	96	Total	C	N	O	0	0	0
			739	470	126	143			

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

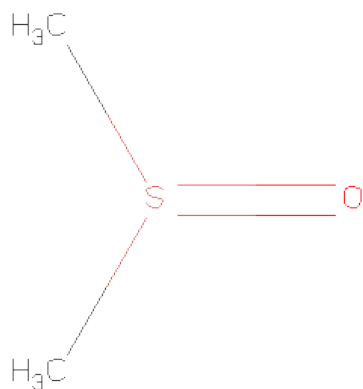
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	G	1	Total	Mg	0	0
			1	1		
3	D	1	Total	Mg	0	0
			1	1		
3	E	1	Total	Mg	0	0
			1	1		
3	B	1	Total	Mg	0	0
			1	1		
3	C	1	Total	Mg	0	0
			1	1		
3	A	1	Total	Mg	0	0
			1	1		
3	F	1	Total	Mg	0	0
			1	1		

- Molecule 4 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
4	B	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
4	C	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
4	D	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
4	E	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
4	F	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
4	G	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

- Molecule 5 is DIMETHYL SULFOXIDE (three-letter code: DMS) (formula: C₂H₆OS).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	H	1	Total	C	O	S	0	0
			4	2	1	1		
5	I	1	Total	C	O	S	0	0
			4	2	1	1		
5	J	1	Total	C	O	S	0	0
			4	2	1	1		
5	K	1	Total	C	O	S	0	0
			4	2	1	1		
5	L	1	Total	C	O	S	0	0
			4	2	1	1		
5	M	1	Total	C	O	S	0	0
			4	2	1	1		
5	N	1	Total	C	O	S	0	0
			4	2	1	1		

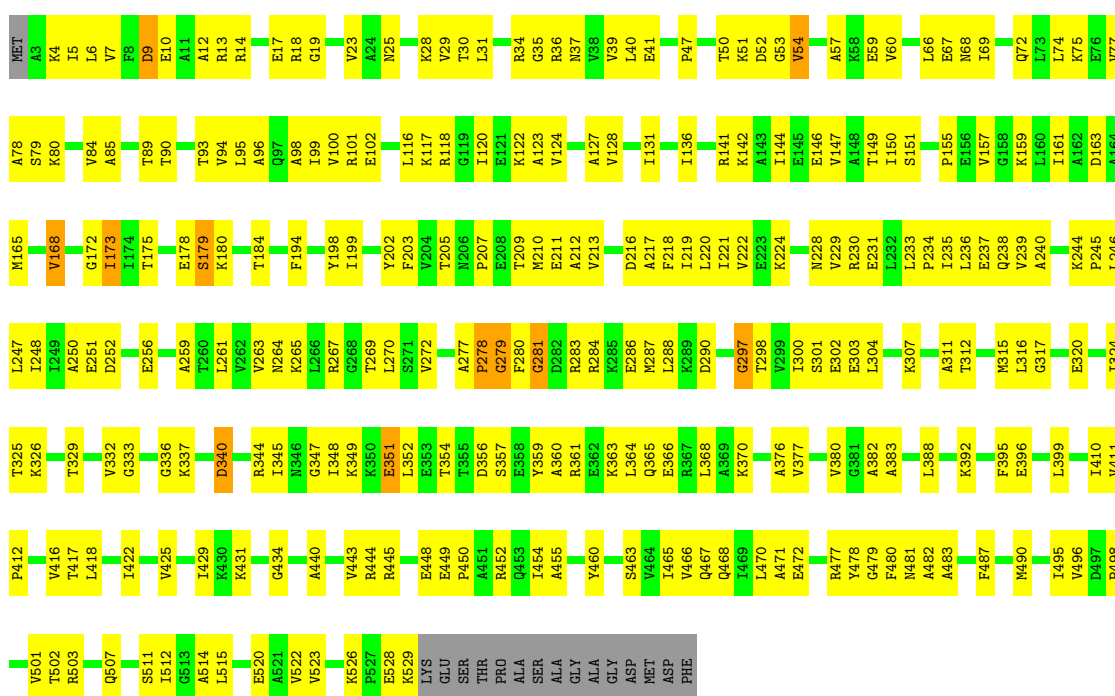
3 Residue-property plots

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 and electron density. 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. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). 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.

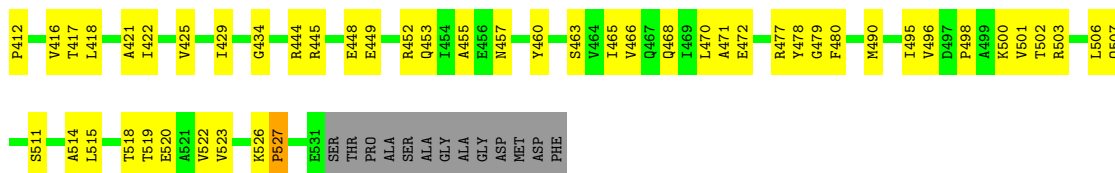
Note EDS was not executed.

- Molecule 1: cpn60(GroEL)

Chain A:

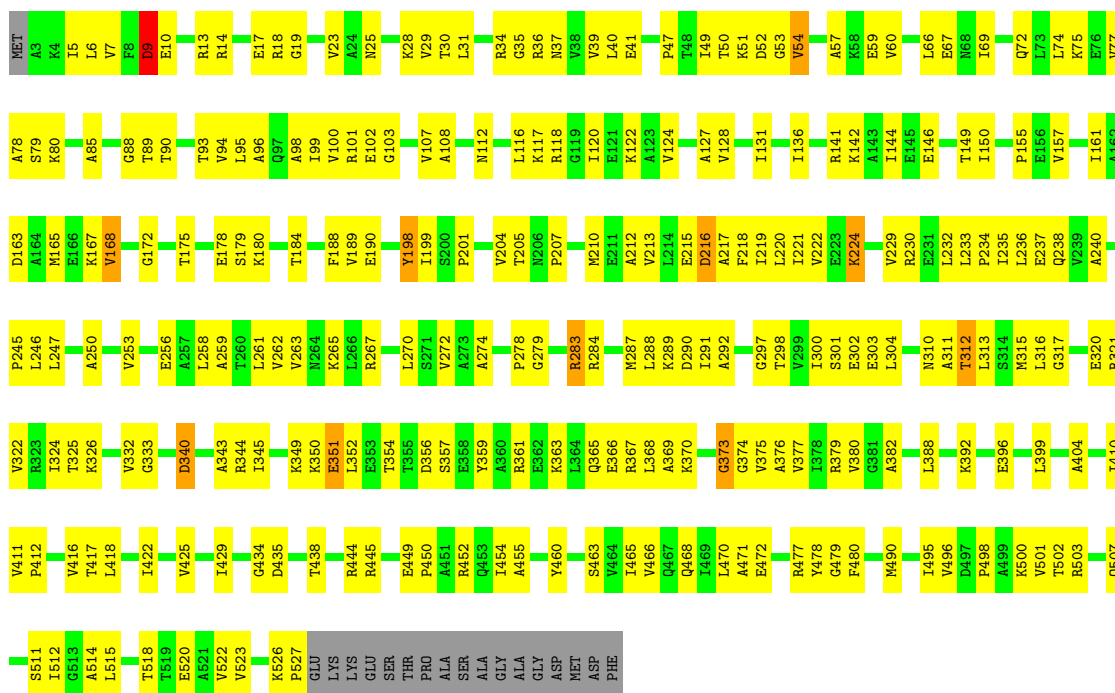






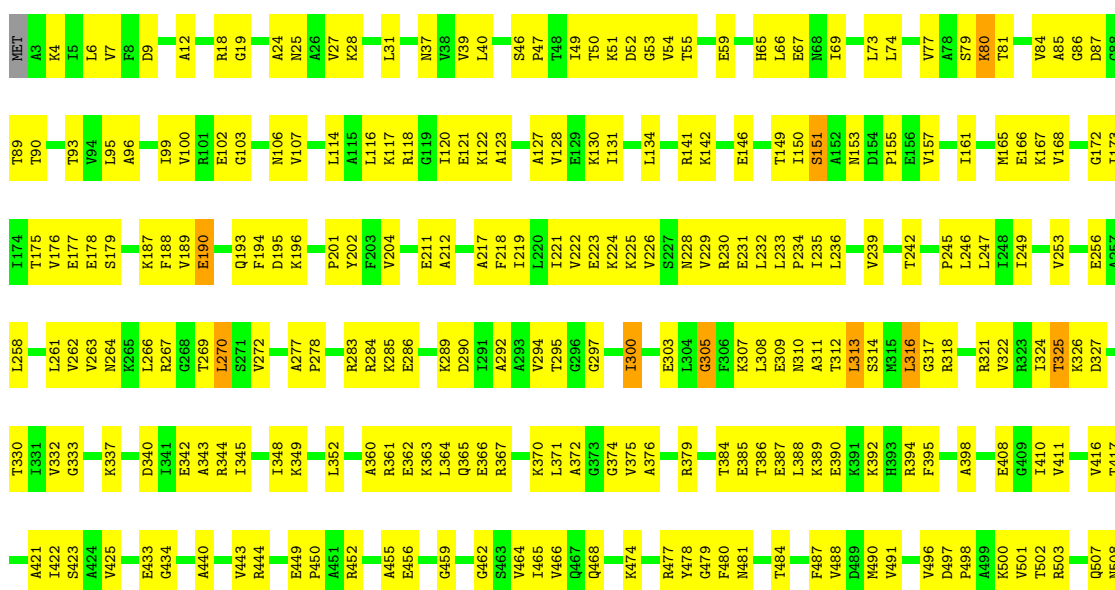
• Molecule 1: cpn60(GroEL)

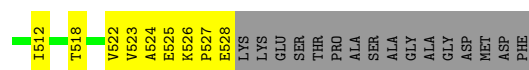
Chain G:



• Molecule 1: cpn60(GroEL)

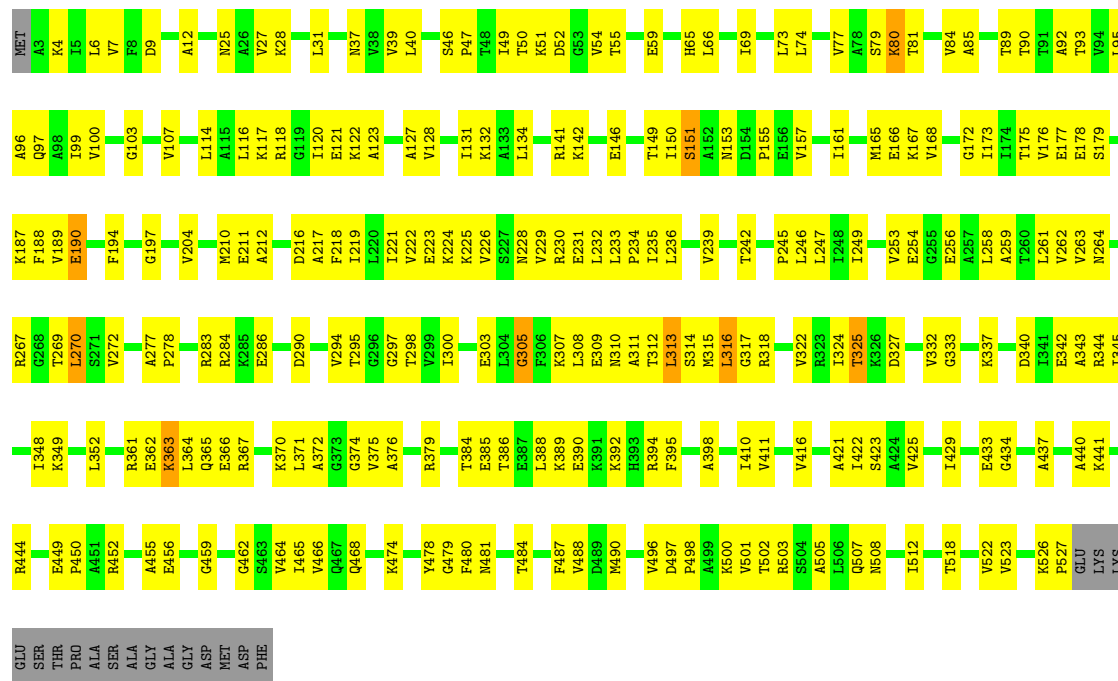
Chain H:





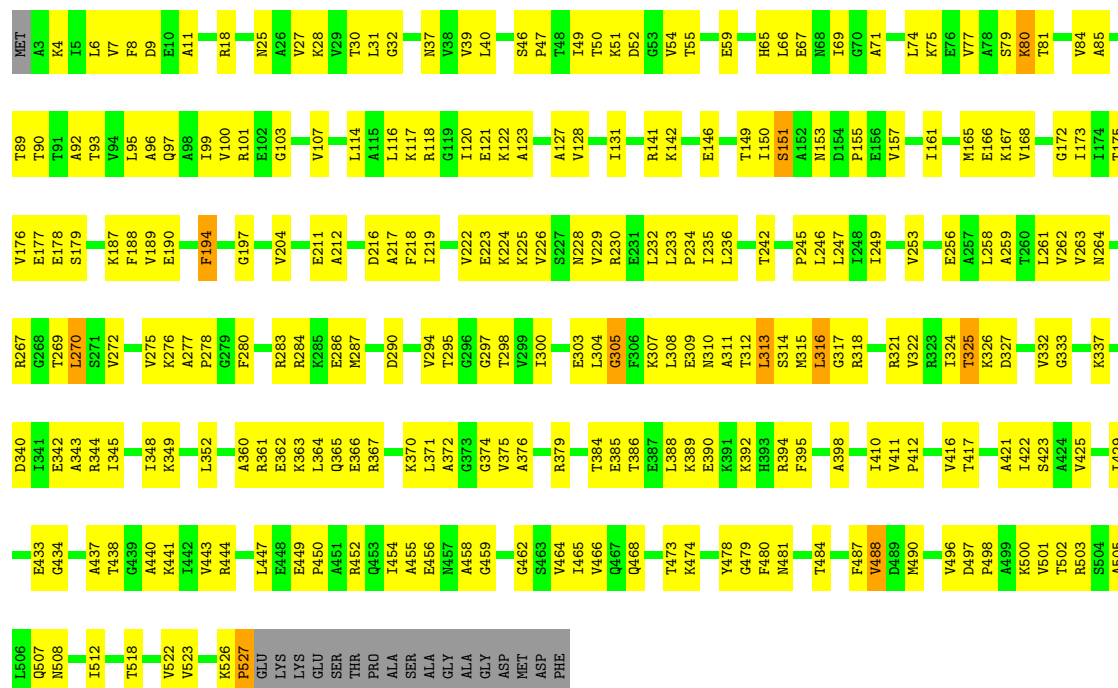
• Molecule 1: cpn60(GroEL)

Chain I:

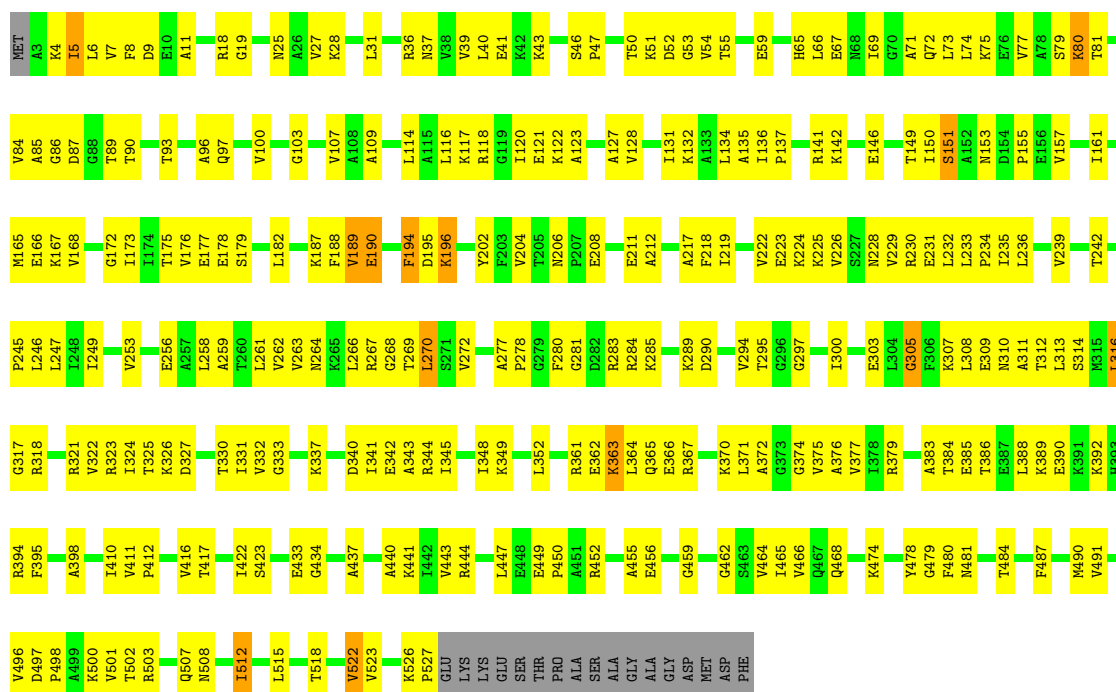


• Molecule 1: cpn60(GroEL)

Chain J:







• Molecule 1: cpn60(GroEL)

Chain N:

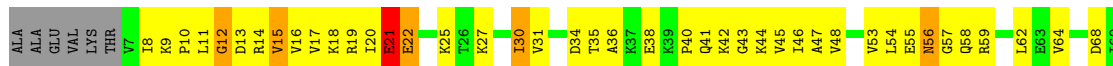
• Molecule 2: cpn10(GroES)

Chain O:



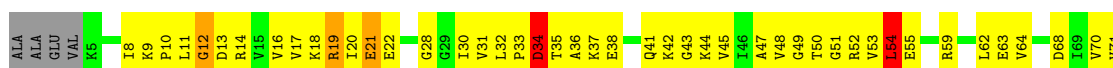
• Molecule 2: cpn10(GroES)

Chain P:



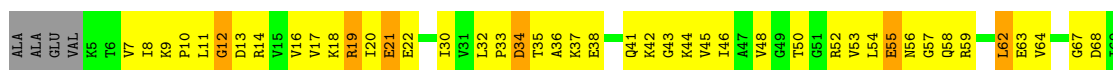
• Molecule 2: cpn10(GroES)

Chain Q:



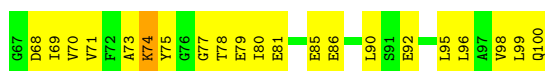
• Molecule 2: cpn10(GroES)

Chain R:



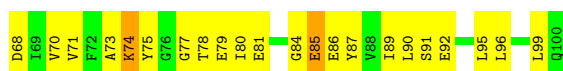
• Molecule 2: cpn10(GroES)

Chain S:



• Molecule 2: cpn10(GroES)

Chain T:



• Molecule 2: cpn10(GroES)

Chain U: 



4 Data and refinement statistics

EDS was not executed - this section will therefore be incomplete.

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	140.38Å 156.42Å 273.15Å 82.88° 85.35° 68.52°	Depositor
Resolution (Å)	39.98 – 2.80	Depositor
% Data completeness (in resolution range)	81.3 (39.98-2.80)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.35 (at 2.81Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.239 , 0.279	Depositor
Wilson B-factor (Å ²)	55.6	Xtriage
Anisotropy	0.047	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 429625 reflections	Xtriage
Total number of atoms	60639	wwPDB-VP
Average B, all atoms (Å ²)	71.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.53% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: MG, DMS, ADP

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 >5	RMSZ	# Z >5
1	A	0.44	0/3989	0.65	0/5383
1	B	0.43	1/3989 (0.0%)	0.65	1/5383 (0.0%)
1	C	0.45	0/3980	0.67	0/5372
1	D	0.42	0/3980	0.65	1/5372 (0.0%)
1	E	0.43	0/3980	0.64	0/5372
1	F	0.39	0/4007	0.63	0/5406
1	G	0.41	0/3971	0.64	0/5360
1	H	0.36	0/3980	0.60	0/5372
1	I	0.37	0/3971	0.60	0/5360
1	J	0.40	0/3971	0.62	0/5360
1	K	0.39	1/3971 (0.0%)	0.62	0/5360
1	L	0.38	0/3980	0.60	0/5372
1	M	0.39	1/3971 (0.0%)	0.62	1/5360 (0.0%)
1	N	0.38	0/3980	0.63	1/5372 (0.0%)
2	O	0.40	0/746	0.68	0/1003
2	P	0.54	0/730	0.77	0/982
2	Q	0.39	0/746	0.70	2/1003 (0.2%)
2	R	0.42	0/746	0.69	0/1003
2	S	0.42	0/746	0.72	1/1003 (0.1%)
2	T	0.39	0/746	0.67	0/1003
2	U	0.46	0/746	0.72	0/1003
All	All	0.41	3/60926 (0.0%)	0.64	7/82204 (0.0%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	K	237	GLU	CD-OE1	-5.26	1.19	1.25
1	M	512	ILE	CB-CG2	5.16	1.68	1.52
1	B	410	ILE	CB-CG2	5.08	1.68	1.52

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	N	444	ARG	NE-CZ-NH1	7.31	123.96	120.30
2	Q	51	GLY	N-CA-C	-5.32	99.81	113.10
1	M	512	ILE	CG1-CB-CG2	5.29	123.03	111.40
2	Q	54	LEU	CA-CB-CG	5.18	127.20	115.30
2	S	58	GLN	CA-CB-CG	5.13	124.69	113.40

There are no chirality outliers.

There are no planarity outliers.

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3956	0	4129	242	0
1	B	3956	0	4129	237	0
1	C	3947	0	4116	244	1
1	D	3947	0	4116	264	0
1	E	3947	0	4116	290	3
1	F	3974	0	4148	248	0
1	G	3938	0	4110	225	0
1	H	3947	0	4116	259	0
1	I	3938	0	4110	246	0
1	J	3938	0	4110	264	0
1	K	3938	0	4110	259	1
1	L	3947	0	4116	315	1
1	M	3938	0	4110	375	0
1	N	3947	0	4116	298	4
2	O	739	0	786	104	0
2	P	723	0	766	104	0
2	Q	739	0	786	94	0
2	R	739	0	786	87	0
2	S	739	0	786	83	0
2	T	739	0	786	79	0
2	U	739	0	786	84	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	27	0	12	0	0
4	B	27	0	12	0	0
4	C	27	0	12	0	0
4	D	27	0	12	1	0
4	E	27	0	12	2	0
4	F	27	0	12	0	0
4	G	27	0	12	1	0
5	H	4	0	6	3	0
5	I	4	0	6	0	0
5	J	4	0	6	0	0
5	K	4	0	6	0	0
5	L	4	0	6	0	0
5	M	4	0	6	0	0
5	N	4	0	6	0	0
All	All	60639	0	63260	4051	5

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 33.

The worst 5 of 4051 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:150:ILE:HD11	1:D:495:ILE:HA	1.22	1.21
1:N:235:ILE:HD11	1:N:311:ALA:HB3	1.29	1.14
1:D:173:ILE:HD11	1:D:365:GLN:HG3	1.16	1.14
1:M:182:LEU:HD11	1:N:363:LYS:NZ	1.62	1.13
1:L:189:VAL:HG12	1:L:190:GLU:H	1.13	1.12

All (5) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:E:474:LYS:CE	1:N:472:GLU:OE1[1_455]	1.85	0.35
1:K:474:LYS:NZ	1:N:493:ALA:O[1_455]	1.93	0.27
1:C:141:ARG:NH2	1:L:353:GLU:OE1[1_565]	2.11	0.09
1:E:473:THR:OG1	1:N:474:LYS:CE[1_455]	2.17	0.03
1:E:474:LYS:NZ	1:N:472:GLU:OE1[1_455]	2.18	0.02

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 X-ray entries followed by that with respect to entries of similar resolution. 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	525/543 (97%)	456 (87%)	56 (11%)	13 (2%)	9	28
1	B	525/543 (97%)	458 (87%)	55 (10%)	12 (2%)	10	31
1	C	524/543 (96%)	451 (86%)	58 (11%)	15 (3%)	7	23
1	D	524/543 (96%)	441 (84%)	67 (13%)	16 (3%)	7	21
1	E	524/543 (96%)	440 (84%)	65 (12%)	19 (4%)	5	17
1	F	527/543 (97%)	453 (86%)	60 (11%)	14 (3%)	8	25
1	G	523/543 (96%)	447 (86%)	65 (12%)	11 (2%)	11	33
1	H	524/543 (96%)	457 (87%)	60 (12%)	7 (1%)	18	51
1	I	523/543 (96%)	457 (87%)	61 (12%)	5 (1%)	22	60
1	J	523/543 (96%)	456 (87%)	58 (11%)	9 (2%)	14	42
1	K	523/543 (96%)	458 (88%)	57 (11%)	8 (2%)	15	46
1	L	524/543 (96%)	454 (87%)	63 (12%)	7 (1%)	18	51
1	M	523/543 (96%)	455 (87%)	61 (12%)	7 (1%)	18	51
1	N	524/543 (96%)	457 (87%)	61 (12%)	6 (1%)	21	57
2	O	94/100 (94%)	74 (79%)	13 (14%)	7 (7%)	2	3
2	P	92/100 (92%)	72 (78%)	13 (14%)	7 (8%)	2	3
2	Q	94/100 (94%)	75 (80%)	12 (13%)	7 (7%)	2	3
2	R	94/100 (94%)	75 (80%)	11 (12%)	8 (8%)	1	2
2	S	94/100 (94%)	72 (77%)	17 (18%)	5 (5%)	3	9
2	T	94/100 (94%)	72 (77%)	15 (16%)	7 (7%)	2	3
2	U	94/100 (94%)	77 (82%)	10 (11%)	7 (7%)	2	3
All	All	7992/8302 (96%)	6857 (86%)	938 (12%)	197 (2%)	9	28

5 of 197 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	9	ASP

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Mol	Chain	Res	Type
1	A	278	PRO
1	B	9	ASP
1	B	278	PRO
1	C	9	ASP

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 X-ray entries followed by that with respect to entries of similar resolution. 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	412/423 (97%)	402 (98%)	10 (2%)	61	91
1	B	412/423 (97%)	399 (97%)	13 (3%)	51	85
1	C	411/423 (97%)	399 (97%)	12 (3%)	55	88
1	D	411/423 (97%)	401 (98%)	10 (2%)	61	91
1	E	411/423 (97%)	395 (96%)	16 (4%)	43	80
1	F	414/423 (98%)	405 (98%)	9 (2%)	64	92
1	G	410/423 (97%)	400 (98%)	10 (2%)	61	91
1	H	411/423 (97%)	403 (98%)	8 (2%)	69	94
1	I	410/423 (97%)	400 (98%)	10 (2%)	61	91
1	J	410/423 (97%)	400 (98%)	10 (2%)	61	91
1	K	410/423 (97%)	401 (98%)	9 (2%)	64	92
1	L	411/423 (97%)	401 (98%)	10 (2%)	61	91
1	M	410/423 (97%)	399 (97%)	11 (3%)	57	89
1	N	411/423 (97%)	401 (98%)	10 (2%)	61	91
2	O	81/83 (98%)	76 (94%)	5 (6%)	26	60
2	P	79/83 (95%)	76 (96%)	3 (4%)	44	80
2	Q	81/83 (98%)	78 (96%)	3 (4%)	45	81
2	R	81/83 (98%)	78 (96%)	3 (4%)	45	81
2	S	81/83 (98%)	78 (96%)	3 (4%)	45	81
2	T	81/83 (98%)	77 (95%)	4 (5%)	35	71
2	U	81/83 (98%)	78 (96%)	3 (4%)	45	81

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	6319/6503 (97%)	6147 (97%)	172 (3%)	57 89

5 of 172 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	G	312	THR
1	I	423	SER
2	Q	48	VAL
1	H	151	SER
1	H	456	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 132 such sidechains are listed below:

Mol	Chain	Res	Type
1	I	400	ASN
1	J	468	GLN
1	N	228	ASN
1	I	481	ASN
1	J	193	GLN

5.3.3 RNA ⓘ

There are no RNA chains 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 21 ligands modelled in this entry, 7 are monoatomic - 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
4	ADP	A	1551	3	29,29,29	1.33	4 (13%)	45,45,45	2.29	8 (17%)
4	ADP	B	2551	3	29,29,29	1.44	5 (17%)	45,45,45	2.44	8 (17%)
4	ADP	C	3551	3	29,29,29	1.56	5 (17%)	45,45,45	2.42	7 (15%)
4	ADP	D	4551	3	29,29,29	1.56	6 (20%)	45,45,45	2.30	9 (20%)
4	ADP	E	5551	3	29,29,29	1.42	5 (17%)	45,45,45	2.41	8 (17%)
4	ADP	F	6551	3	29,29,29	1.63	5 (17%)	45,45,45	2.44	8 (17%)
4	ADP	G	7551	3	29,29,29	1.50	6 (20%)	45,45,45	2.38	8 (17%)
5	DMS	H	545	-	3,3,3	0.22	0	3,3,3	0.61	0
5	DMS	I	545	-	3,3,3	0.26	0	3,3,3	0.61	0
5	DMS	J	545	-	3,3,3	0.36	0	3,3,3	0.68	0
5	DMS	K	545	-	3,3,3	0.28	0	3,3,3	0.62	0
5	DMS	L	545	-	3,3,3	0.30	0	3,3,3	0.63	0
5	DMS	M	601	-	3,3,3	0.27	0	3,3,3	0.58	0
5	DMS	N	701	-	3,3,3	0.25	0	3,3,3	0.59	0

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	ADP	A	1551	3	-	0/16/32/32	0/1/3/3
4	ADP	B	2551	3	-	0/16/32/32	0/1/3/3
4	ADP	C	3551	3	-	0/16/32/32	0/1/3/3
4	ADP	D	4551	3	-	0/16/32/32	0/1/3/3
4	ADP	E	5551	3	-	0/16/32/32	0/1/3/3
4	ADP	F	6551	3	-	0/16/32/32	0/1/3/3
4	ADP	G	7551	3	-	0/16/32/32	0/1/3/3
5	DMS	H	545	-	-	0/0/0/0	0/0/0/0
5	DMS	I	545	-	-	0/0/0/0	0/0/0/0
5	DMS	J	545	-	-	0/0/0/0	0/0/0/0
5	DMS	K	545	-	-	0/0/0/0	0/0/0/0
5	DMS	L	545	-	-	0/0/0/0	0/0/0/0
5	DMS	M	601	-	-	0/0/0/0	0/0/0/0
5	DMS	N	701	-	-	0/0/0/0	0/0/0/0

The worst 5 of 36 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	F	6551	ADP	C4-N9	-4.40	1.31	1.37
4	C	3551	ADP	C2'-C1'	-4.40	1.47	1.53
4	F	6551	ADP	C2'-C1'	-4.33	1.47	1.53
4	G	7551	ADP	C4-N9	-4.09	1.31	1.37
4	E	5551	ADP	C4-N9	-3.83	1.32	1.37

The worst 5 of 56 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	3551	ADP	N3-C2-N1	-12.97	117.86	128.71
4	G	7551	ADP	N3-C2-N1	-12.91	117.91	128.71
4	E	5551	ADP	N3-C2-N1	-12.74	118.06	128.71
4	D	4551	ADP	N3-C2-N1	-12.51	118.25	128.71
4	A	1551	ADP	N3-C2-N1	-12.43	118.32	128.71

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

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.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

EDS was not executed - this section will therefore be empty.

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates ⓘ

EDS was not executed - this section will therefore be empty.

6.4 Ligands ⓘ

EDS was not executed - this section will therefore be empty.

6.5 Other polymers ⓘ

EDS was not executed - this section will therefore be empty.