



wwPDB X-ray Structure Validation Summary Report i

Mar 11, 2014 – 12:55 PM GMT

PDB ID : 2XSM
Title : Crystal structure of the mammalian cytosolic chaperonin CCT in complex with tubulin
Authors : Munoz, I.G.; Yebenes, H.; Zhou, M.; Mesa, P.; Serna, M.; Bragado-Nilsson, E.; Beloso, A.; Robinson, C.V.; Valpuesta, J.M.; Montoya, G.
Deposited on : 2010-10-29
Resolution : 5.50 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>

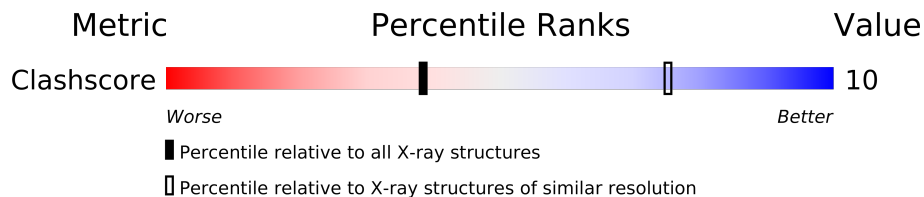
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.16 November 2013
Xtriage (Phenix) : dev-1323
EDS : trunk22699
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : trunk22699

1 Overall quality at a glance

















The reported resolution of this entry is 5.50 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	1008 (7.40-3.52)

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.

Mol	Chain	Length	Quality of chain
1	A	489	
2	B	478	
3	C	455	
4	D	471	
5	E	472	
6	F	466	
7	G	485	
8	H	474	
9	I	293	
10	J	299	
11	K	394	
12	L	297	
12	O	297	
13	M	298	
14	N	289	
15	P	481	

2 Entry composition

There are 15 unique types of molecules in this entry. The entry contains 6438 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 CCT.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf	Trace
1	A	489	Total	C	0	0	489
			489	489			

- Molecule 2 is a protein called CCT.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf	Trace
2	B	478	Total	C	0	0	478
			478	478			

- Molecule 3 is a protein called CCT.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf	Trace
3	C	455	Total	C	0	0	455
			455	455			

- Molecule 4 is a protein called CCT.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf	Trace
4	D	471	Total	C	0	0	471
			471	471			

- Molecule 5 is a protein called CCT.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf	Trace
5	E	472	Total	C	0	0	472
			472	472			

- Molecule 6 is a protein called CCT.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf	Trace
6	F	466	Total	C	0	0	466
			466	466			

- Molecule 7 is a protein called CCT.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
7	G	485	Total C 485 485	0	0	485

- Molecule 8 is a protein called CCT.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
8	H	474	Total C 474 474	0	0	474

- Molecule 9 is a protein called CCT.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
9	I	293	Total C 293 293	0	0	293

- Molecule 10 is a protein called CCT.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
10	J	299	Total C 299 299	0	0	299

- Molecule 11 is a protein called CCT.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
11	K	394	Total C 394 394	0	0	394

- Molecule 12 is a protein called CCT.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
12	L	297	Total C 297 297	0	0	297
12	O	297	Total C 297 297	0	0	297

- Molecule 13 is a protein called CCT.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
13	M	298	Total C 298 298	0	0	298

- Molecule 14 is a protein called CCT.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf	Trace
14	N	289	Total	C	0	0	289
			289	289			

- Molecule 15 is a protein called CCT.

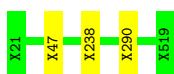
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf	Trace
15	P	481	Total	C	0	0	481
			481	481			

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.

- Molecule 1: CCT

Chain A: 



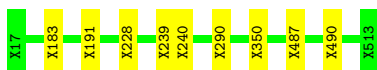
- Molecule 2: CCT

Chain B: 



- Molecule 3: CCT

Chain C: 



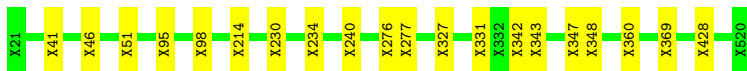
- Molecule 4: CCT

Chain D: 



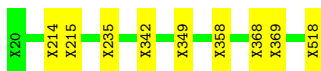
- Molecule 5: CCT

Chain E: 



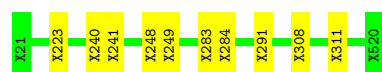
- Molecule 6: CCT

Chain F: 



- Molecule 7: CCT

Chain G: 



- Molecule 8: CCT

Chain H: 



- Molecule 9: CCT

Chain I: 



- Molecule 10: CCT

Chain J: 



- Molecule 11: CCT

Chain K: 



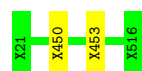
- Molecule 12: CCT

Chain L: 



- Molecule 12: CCT

Chain O: 



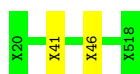
- Molecule 13: CCT

Chain M: 



- Molecule 14: CCT

Chain N: 



- Molecule 15: CCT

Chain P: 



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	272.70Å 313.50Å 158.30Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	100.00 – 5.50 97.58 – 5.44	Depositor EDS
% Data completeness (in resolution range)	(Not available) (100.00-5.50) 98.3 (97.58-5.44)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.37 (at 5.41Å)	Xtriage
Refinement program	REFMAC 5.5.0099	Depositor
R, R_{free}	(Not available) , (Not available) 0.955 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å ²)	257.8	Xtriage
Anisotropy	0.400	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	58.05 , 838.3	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.32$, $\langle L^2 \rangle = 0.16$	Xtriage
Outliers	0 of 45495 reflections	Xtriage
F_o, F_c correlation	0.64	EDS
Total number of atoms	6438	wwPDB-VP
Average B, all atoms (Å ²)	26.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.63% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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).

There are no protein, RNA or DNA chains available to summarize Z scores of covalent bonds and angles.

There are no bond length outliers.

There are no bond angle outliers.

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	489	0	0	2	0
2	B	478	0	0	5	0
3	C	455	0	0	5	0
4	D	471	0	0	4	0
5	E	472	0	0	11	0
6	F	466	0	0	5	0
7	G	485	0	0	5	0
8	H	474	0	0	2	0
9	I	293	0	0	6	0
10	J	299	0	0	4	0
11	K	394	0	0	8	0
12	L	297	0	0	2	0
12	O	297	0	0	1	0
13	M	298	0	0	3	0
14	N	289	0	0	1	0
15	P	481	0	0	4	0
All	All	6438	0	0	63	0

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 10.

The worst 5 of 63 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
11:K:171:UNK:C	11:K:172:UNK:CA	2.24	1.15
7:G:283:UNK:CA	7:G:284:UNK:CA	2.25	1.13
4:D:448:UNK:CA	4:D:449:UNK:CA	2.27	1.13
3:C:239:UNK:CA	3:C:290:UNK:CA	2.30	1.10
2:B:232:UNK:CA	2:B:346:UNK:CA	2.34	1.06

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone ⓘ

There are no protein backbone outliers to report in this entry.

5.3.2 Protein sidechains ⓘ

There are no protein residues with a non-rotameric sidechain to report in this entry.

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 ⓘ

There are no ligands in this entry.

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 ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	0/489	-	-	-	-
2	B	0/478	-	-	-	-
3	C	0/455	-	-	-	-
4	D	0/471	-	-	-	-
5	E	0/472	-	-	-	-
6	F	0/466	-	-	-	-
7	G	0/485	-	-	-	-
8	H	0/474	-	-	-	-
9	I	0/293	-	-	-	-
10	J	0/299	-	-	-	-
11	K	0/394	-	-	-	-
12	L	0/297	-	-	-	-
12	O	0/297	-	-	-	-
13	M	0/298	-	-	-	-
14	N	0/289	-	-	-	-
15	P	0/481	-	-	-	-
All	All	0/6438	-	-	-	-

There are no RSRZ outliers to report.

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

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands

There are no ligands in this entry.

6.5 Other polymers

There are no such residues in this entry.