Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 06:39 AM 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 Full wwPDB X-ray Structure Validation 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/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

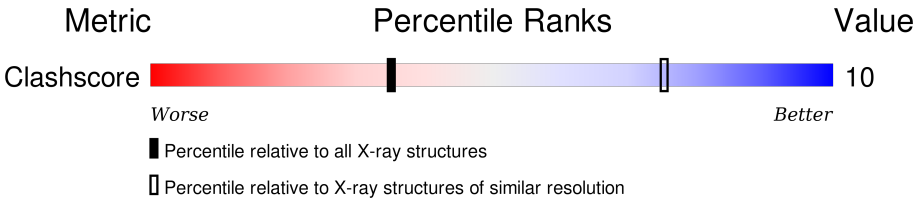
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

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	102246	1020 (7.10-3.70)

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. 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% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	489	99% .
2	B	478	98% .
3	C	455	98% .
4	D	471	99% .
5	E	472	96% .
6	F	466	98% .
7	G	485	98% .
8	H	474	99% .
9	I	293	96% .
10	J	299	97% .

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Mol	Chain	Length	Quality of chain
11	K	394	96%
12	L	297	99%
12	O	297	99%
13	M	298	98%
14	N	289	99%
15	P	481	99%

2 Entry composition

There are 15 unique types of molecules in this entry. The entry contains 6438 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 489 489	0	0	489

- Molecule 2 is a protein called CCT.

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

- Molecule 3 is a protein called CCT.

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

- Molecule 4 is a protein called CCT.

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

- Molecule 5 is a protein called CCT.

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

- Molecule 6 is a protein called CCT.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
6	F	466	Total C 466 466	0	0	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 289 289	0	0	289

- Molecule 15 is a protein called CCT.

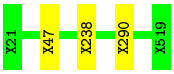
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
15	P	481	Total C 481 481	0	0	481

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 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.

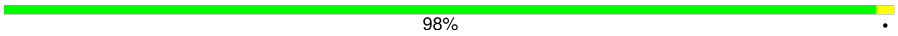
- Molecule 1: CCT

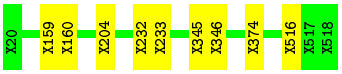
Chain A:



- Molecule 2: CCT

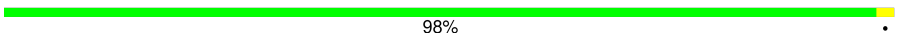
Chain B:

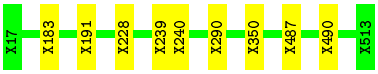




- Molecule 3: CCT

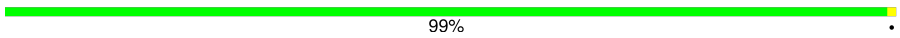
Chain C:





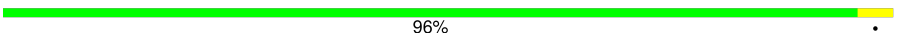
- Molecule 4: CCT

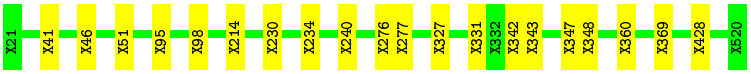
Chain D:



- Molecule 5: CCT

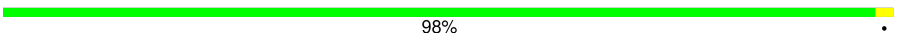
Chain E:





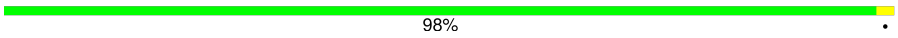
- Molecule 6: CCT

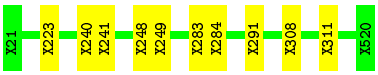
Chain F:



- Molecule 7: CCT

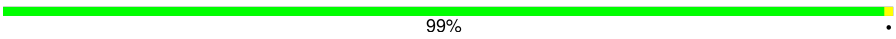
Chain G:





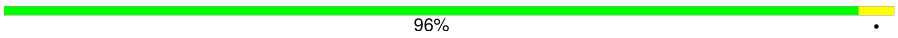
- Molecule 8: CCT

Chain H:



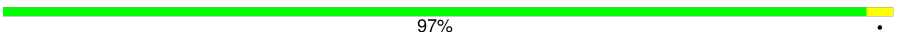
- Molecule 9: CCT

Chain I:



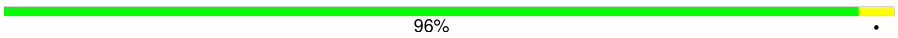
- Molecule 10: CCT

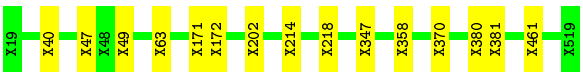
Chain J:



- Molecule 11: CCT

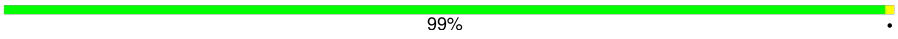
Chain K:

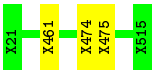




- Molecule 12: CCT

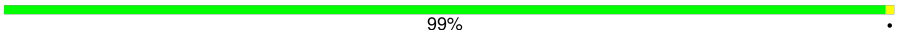
Chain L:





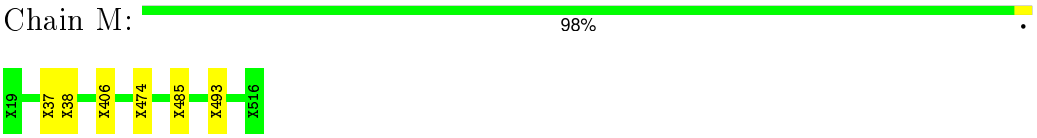
- Molecule 12: CCT

Chain O:



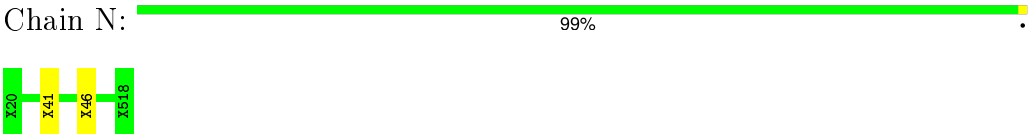
- Molecule 13: CCT

Chain M:



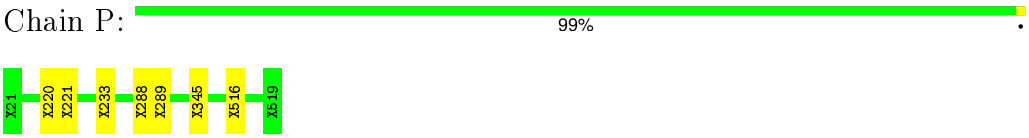
• Molecule 14: CCT

Chain N:



• Molecule 15: CCT

Chain P:



4 Data and refinement statistics (i)

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) 98.4 (97.58-5.44)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.37 (at 5.41Å)	Xtriage
Refinement program	REFMAC 5.5.0099	Depositor
R, R_{free}	(Not available) , (Not available) 0.490 , (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)	0.52 , 11.1	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.32$, $< L^2 > = 0.16$	Xtriage
Outliers	0 of 45495 reflections	Xtriage
F_o,F_c correlation	0.76	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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

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 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	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

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 10.

All (63) 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)
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
9:I:99:UNK:CA	9:I:100:UNK:CA	2.35	1.03
9:I:474:UNK:CA	9:I:485:UNK:CA	2.37	1.02
7:G:240:UNK:CA	7:G:241:UNK:CA	2.44	0.95
10:J:144:UNK:CA	10:J:145:UNK:CA	2.48	0.92
11:K:347:UNK:CA	11:K:358:UNK:CA	2.48	0.91
2:B:233:UNK:CA	2:B:345:UNK:CA	2.49	0.89
11:K:380:UNK:CA	11:K:381:UNK:CA	2.52	0.87
7:G:248:UNK:CA	7:G:249:UNK:CA	2.52	0.87
15:P:220:UNK:CA	15:P:221:UNK:CA	2.56	0.83
13:M:474:UNK:CA	13:M:485:UNK:CA	2.59	0.80
6:F:214:UNK:CA	6:F:369:UNK:CA	2.61	0.79
13:M:406:UNK:CA	13:M:493:UNK:CA	2.61	0.79
2:B:159:UNK:CA	2:B:160:UNK:CA	2.61	0.78
3:C:487:UNK:CA	3:C:490:UNK:CA	2.61	0.78
14:N:41:UNK:CA	14:N:46:UNK:CA	2.61	0.78
5:E:214:UNK:CA	5:E:369:UNK:CA	2.61	0.78
5:E:276:UNK:CA	5:E:277:UNK:CA	2.63	0.77
5:E:230:UNK:CA	5:E:348:UNK:CA	2.63	0.76
9:I:480:UNK:CA	9:I:481:UNK:CA	2.65	0.75
3:C:228:UNK:CA	3:C:350:UNK:CA	2.65	0.75
9:I:148:UNK:CA	9:I:151:UNK:CA	2.66	0.73
6:F:349:UNK:CA	6:F:358:UNK:CA	2.67	0.72
9:I:48:UNK:CA	15:P:516:UNK:CA	2.73	0.67
5:E:41:UNK:CA	5:E:46:UNK:CA	2.73	0.66
11:K:40:UNK:CA	11:K:47:UNK:CA	2.73	0.66
11:K:202:UNK:CA	11:K:218:UNK:CA	2.76	0.63
7:G:223:UNK:CA	7:G:308:UNK:CA	2.77	0.63
8:H:474:UNK:CA	8:H:484:UNK:CA	2.78	0.62
7:G:291:UNK:CA	7:G:311:UNK:CA	2.79	0.60
8:H:287:UNK:CA	8:H:308:UNK:CA	2.81	0.59
3:C:239:UNK:CA	3:C:240:UNK:CA	2.81	0.58
15:P:233:UNK:CA	15:P:345:UNK:CA	2.82	0.57
12:L:474:UNK:CA	12:L:475:UNK:CA	2.83	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:327:UNK:CA	5:E:342:UNK:CA	2.83	0.56
13:M:37:UNK:CA	13:M:38:UNK:CA	2.86	0.53
9:I:142:UNK:CA	9:I:143:UNK:CA	2.88	0.52
5:E:347:UNK:CA	5:E:360:UNK:CA	2.87	0.52
4:D:348:UNK:CA	4:D:358:UNK:CA	2.89	0.50
5:E:234:UNK:CA	5:E:343:UNK:CA	2.91	0.49
10:J:476:UNK:CA	10:J:483:UNK:CA	2.91	0.49
6:F:235:UNK:CA	6:F:342:UNK:CA	2.90	0.48
12:O:450:UNK:CA	12:O:453:UNK:CA	2.92	0.48
10:J:164:UNK:CA	10:J:167:UNK:CA	2.91	0.48
5:E:428:UNK:CA	12:L:461:UNK:CA	2.92	0.47
10:J:405:UNK:CA	10:J:493:UNK:CA	2.92	0.47
5:E:51:UNK:CA	6:F:518:UNK:CA	2.93	0.47
4:D:428:UNK:CA	11:K:461:UNK:CA	2.93	0.47
11:K:214:UNK:CA	11:K:370:UNK:CA	2.93	0.46
11:K:49:UNK:CA	11:K:63:UNK:CA	2.93	0.46
4:D:201:UNK:CA	4:D:373:UNK:CA	2.94	0.46
2:B:204:UNK:CA	2:B:374:UNK:CA	2.94	0.46
1:A:47:UNK:CA	2:B:516:UNK:CA	2.95	0.45
1:A:238:UNK:CA	1:A:290:UNK:CA	2.96	0.44
6:F:215:UNK:CA	6:F:368:UNK:CA	2.97	0.42
15:P:288:UNK:CA	15:P:289:UNK:CA	2.97	0.42
3:C:183:UNK:CA	3:C:191:UNK:CA	2.97	0.42
5:E:240:UNK:CA	5:E:331:UNK:CA	2.99	0.41
5:E:95:UNK:CA	5:E:98:UNK:CA	2.99	0.41

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

5.3.2 Protein sidechains (i)

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

5.3.3 RNA

There are no RNA molecules 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, 95^{th} 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.