

Supplemental Information

**Structural Basis for Mitotic
Centrosome Assembly in Flies**

Zhe Feng, Anna Caballe, Alan Wainman, Steven Johnson, Andreas F.M. Haensele, Matthew A. Cottee, Paul T. Conduit, Susan M. Lea, and Jordan W. Raff

Crystal form	CF-1	CF-2	CF-2	CF-3	CF-4	CF-5
Crystal contents	LZ:CM2 WT	LZ:CM2 WT	LZ:CM2 L535E	LZ:CM2 L535E	LZ:CM2 WT	CM2 WT
Construct boundaries	490-552:1082-1148	490-544:1082-1148	490-544:1082-1148	490-544:1082-1148	490-567:1082-1148	1082-1148
Crystallization condition	MD-Morpheus B6 30% EDO-PEG8K, 0.1M Buffer system 2 pH7.5, 0.09M Halogens	20%(w/v) PEG6K, 0.1M Tris pH8.0, 0.2M MgCl2	15%(w/v) PEG4K, 0.2M imidazole malate pH7.0	18%(w/v) PEG2KMME, 0.2M sodium cacodylate pH6.5	20% (w/v) PEG 3350, 0.2M potassium/sodium tartrate	14.4% (w/v) PEG8K, 80mM sodium cacodylate pH6.5, 160mM calcium acetate
PDB Code		PDB: 5MVW	PDB: 5MW0	PDB: 5MW9	PDB: 5MWE	PDB: 5I7C
Data collection statistics						
Beamline	ESRF ID23-1	Diamond I04	Petra III P13	Petra III P13	Diamond I03	Diamond I04
Wavelength (Å)	1.282	1.28229	0.97623	0.97623	0.9763	0.9793
Resolution limits (Å) ^a	61.20-2.27 (2.28-2.27)	69.07-1.82 (1.87-1.82)	31.19-2.00 (2.05-2.00)	31.36-2.20 (2.27-2.20)	36.10-2.02 (2.07-2.02)	70.4-2.8 (2.9-2.8)
Space group	P2 ₁ 2 ₁ 2 ₁	P2 ₁	P2 ₁	C2	C2	P6 ₁
Unit cell dimensions (Å, °)	33.9,85.6,87.5,90,90, 90	44.9,44.3,72.5,90, 107.8,90	45.8,43.9,68.6,90, 108.3,90	275.8,43.0,48.4,90, 96.6,90	196.0,36.5,43.8,90, 102.8,90	49.2,49.2,211.2,90, 90,120
Unique reflections	12380 (119)	24465 (1806)	17198 (1246)	27935 (2406)	19929 (1450)	7171 (548)
Multiplicity ^a	13.1 (14.1)	16.9 (17.0)	3.0 (3.1)	2.9 (2.9)	3.3 (3.3)	10.4 (10.1)
Completeness (%) ^a	100.0 (100.0)	99.5 (99.8)	97.2 (97.6)	96.4 (96.7)	98.8 (98.7)	99.9 (100.0)
$\ /\sigma(\)$ ^a	13.1 (2.0)	22.9 (1.1)	6.1 (1.8)	6.7 (1.5)	18.2 (2.1)	19.7 (1.4)
$R_{\text{merge}} (\%)^{\text{a},\text{b}}$	0.13 (1.25)	0.08 (3.05)	0.07 (0.32)	0.07 (0.75)	0.03 (0.62)	0.07 (1.67)
$R_{\text{pim}} (\%)$	0.04 (0.34)	0.02 (0.76)	0.05 (0.22)	0.05 (0.53)	0.02 (0.40)	0.02 (0.55)
Processing programs	autoPROC	Xia2	Mosflm/Aimless	Mosflm/Aimless	Xia2	Xia2
Refinement statistics						

Resolution limits (Å)		42.74-1.82 (1.89-1.82)	31.19-2.00 (2.13-2.00)	31.35-2.20 (2.29-2.20)	36.10-2.02 (2.13-2.02)	42.6-2.8 (3.2-2.8)
Number of reflections in working set		23200 (2568)	16220 (2656)	26625 (2895)	18985 (2696)	7100 (2235)
Number of reflections in test set		1247 (133)	883 (146)	1240 (167)	941 (132)	369 (137)
R factor of working set ^{a,c}		0.223 (0.374)	0.237 (0.298)	0.258 (0.374)	0.228 (0.356)	0.243 (0.306)
$R_{\text{free}}^{\text{a,d}}$		0.246 (0.378)	0.264 (0.336)	0.302 (0.404)	0.269 (0.458)	0.268 (0.392)
Number of atoms (protein/water/other)		1697/208/14	1797/142/1	3651/77/2	1420/26/52	1953/0/2
Residues in Ramachandran favoured region (%)		100	99.1	98.6	98.8	99.6
Ramachandran outliers (%)		0	0.47	0.46	0.59	0
r.m.s.d. bond lengths (Å)		0.005	0.005	0.002	0.005	0.003
r.m.s.d. bond angles (°)		0.559	0.574	0.311	0.568	0.60

^aNumbers in parentheses refer to the appropriate outer shell.

^b $R_{\text{merge}} = 100 \times (\sum_{\text{hkl}} \sum_i |I(\text{hkl}; i) - \langle I(\text{hkl}) \rangle| / \sum_{\text{hkl}} \sum_i |I(\text{hkl}; i)|)$, where $I(\text{hkl}; i)$ is the intensity of an individual measurement of a reflection and $\langle I(\text{hkl}) \rangle$ is the average intensity of that reflection.

^c $R_{\text{factor}} = (\sum_{\text{hkl}} ||F_{\text{obs}}| - |F_{\text{calc}}|| / \sum_{\text{hkl}} |F_{\text{obs}}|)$, where $|F_{\text{obs}}$ and $|F_{\text{calc}}$ are the observed and calculated structure factor amplitudes.

^d R_{free} equals the R-factor of test set (5% of the data removed prior to refinement).

r.m.s.d.: root mean square deviation from ideal geometry.

Table S1.

Related to Figures 2, 4, S1 and S3: Crystallographic data collection and refinement statistics.