Table S14.

Data collection and refinement statistics for drug-MELK cocrystals (molecular replacement).

	MELK Nintedanib (5MAF)	*MELK PF-3758309 (5MAG)*	*MELK K-252a (5M5A)*	*MELK Defactinib (5MAH)*	*MELK BI-847325 (5MAI)*
Data collection					
Space group	$P2_12_12_1$	$P2_12_12_1$	$P2_12_12_1$	$P2_12_12_1$	$I4_132$
Cell dimensions					
a, b, c *(Å)*	59.91, 63.71, 91.29	61.18, 62.81, 94.11	63.28, 91.21, 59.65	59.67, 63.70, 90.94	169.13, 169.13, 169.13
α, β, γ (°)	90, 90, 90	90, 90, 90	90, 90, 90	90, 90, 90	90, 90, 90
Resolution (Å)	52.25 - 2.80 (2.95 - 2.80)[a]	94.11 - 2.35 (2.48 - 2.35)[a]	49.93 - 1.90 (2.00 - 1.90)[a]	43.55 - 2.00 (2.11 - 2.00)[a]	53.48 - 2.15 (2.27 - 2.15)[a]
R_{merge}	0.129 (0.733)[a]	0.131 (0.369)[a]	0.032 (0.224)[a]	0.068 (0.735)[a]	0.063 (0.793)[a]
$I/\sigma(I)$	10.5 (2.6)[a]	7.7 (3.9)[a]	21.3 (5.6)[a]	15.4 (2.5)[a]	18.1 (3.1)[a]
$CC_{1/2}$	0.993 (0.774)[a]	0.981 (0.885)[a]	1.000 (0.974)[a]	0.999 (0.824)[a]	0.999 (0.798)[a]
Completeness (%)	99.8 (99.8)[a]	95.9 (99.9)[a]	94.7 (84.2)[a]	98.3 (98.6)[a]	100.0 (100.0)[a]
Redundancy	6.0 (6.2)[a]	4.6 (4.8)[a]	4.5 (4.6)[a]	5.1 (4.9)[a]	8.6 (8.5)[a]
Refinement					
Resolution (Å)	52.25 - 2.80	52.24 - 2.35	49.93 - 1.90	43.55 - 2.00	53.49 - 2.15
No. reflections	8550	14303	19461	22356	21616
R_{work} / R_{free}	0.223 / 0.257	0.194 / 0.251	0.185 / 0.214	18.3 / 23.8	19.2 / 23.7
No. atoms					
Protein	2578	2586	2587	2604	2563
Ligand	40	35	35	35	35
Water	34	92	109	105	69
B *factors*					
Protein	57.01	36.42	43.85	38.46	54.60
Ligand	51.42	32.19	36.74	35.66	65.12
Water	46.57	35.72	47.23	42.52	55.01
R.m.s. deviations					
Bond lengths (Å)	0.0076	0.0091	0.0116	0.0107	0.0120
Bond angles (°)	1.2854	1.4091	1.8555	1.4383	1.5352

[a] Values in parentheses are for highest-resolution shell.