Supplementary Crystallographic Tables

Table S1: Trehalose.

Dataset name	Trehalose anhydrous (RT)	Trehalose anhydrous (100K)	Trehalose anhydrous (100K, high dose)	Trehalose dihydrate (100K)	Trehalose anhydrous (monoclinic, RT)
Crystal data					
Chemical formula	$C_{12}H_{22}O_{11}$	$C_{12}H_{22}O_{11}$	$C_{12}H_{22}O_{11}$	$C_{12}H_{22}O_{11} \cdot 2(H_2O)$	$C_{12}H_{22}O_{11}$
M_r	342.30	342.30	342.30	378.33	342.30
Crystal system, space group	Orthorhombic, $P2_12_12_1$	Orthorhombic, $P2_12_12_1$	Orthorhombic, $P2_12_12_1$	Orthorhombic, $P2_12_12_1$	Monoclinic, $P2_1$
Collection temperature (K)	293	100	100	100	293
Transfer temperature (K)	293	293	293	100	293
a, b, c (Å)	6.8 (4), 11.6 (4), 18.5 (3)	6.7 (5), 11.6 (4), 18.5 (3)	6.8 (3), 11.6 (2), 18.5 (2)	7.50 (6), 12.08 (10), 17.67 (7)	6.75 (6), 8.19 (5), 12.94 (9)
α, β, γ (°)	90, 90, 90	90, 90, 90	90, 90, 90	90, 90, 90	90, 98.3 (2), 90
V (Å³)	1457 (103)	1442 (128)	1447 (79)	1602 (19)	708 (9)
Z	4	4	4	4	2
Radiation type	Electrons, $\lambda = 0.0251$ Å	Electrons, $\lambda = 0.0251$ Å	Electrons, $\lambda = 0.0251$ Å	Electrons, $\lambda = 0.0251$ Å	Electrons, $\lambda = 0.0251$ Å
Data collection and processing					
Diffractometer	Rigaku XtaLAB Synergy-ED	Rigaku XtaLAB Synergy-ED	Rigaku XtaLAB Synergy-ED	Rigaku XtaLAB Synergy-ED	Rigaku XtaLAB Synergy-ED
measured, independent, observed	6114, 2595, 980	5994, 2324, 985	6043, 2327, 1302	8500, 2835, 1758	3714, 2251, 1280
Resolution (Å)	0.80	0.80	0.80	0.80	0.80
Completeness (%)	86.7	79.1	78.7	84.6	75.6
Redundancy	4.0	4.4	4.4	5.3	3.2
R_{int}	0.189	0.193	0.126	0.227	0.132
R_{pim}	0.116	0.113	0.075	0.114	0.104
$CC_{1/2}$	0.992	0.993	0.997	0.970	0.977
$I/\sigma(I)$ [inf - 0.80 Å]	3.86	4.45	6.11	5.18	5.08
Total electron dose (e^-/Å²)	0.18	0.18	0.54	0.18	0.18
Min, Max collection angle (°)	-50, +50	-50, +50	-50, +50	-60, +60	-60, +60

$(\sin\theta/\lambda)_{max}$ (Å^{-1})	0.625	0.624	0.625	0.625	0.624
Detector distance (mm)	653	653	653	653	653
Refinement					
R_1, wR_2 [$F^2 > 2\sigma(F^2)$]	0.117, 0.258	0.117, 0.294	0.106, 0.255	0.124, 0.280	0.129, 0.316
R_1, wR_2 [all]	0.237, 0.319	0.216, 0,351	0.169, 0.285	0.174, 0.312	0.170, 0.346
S	1.01	1.04	1.19	1.09	1.22
No. of reflections	2595	2324	2327	2835	2251
No. of parameters	217	239	216	269	232
No. of restraints	177	332	178	335	189
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.11, -0.12	0.12, -0.15	0.13, -0.12	0.13, -0.15	0.15, -0.14
CCDC number	-	-	2267656	2267657	2267654

Table S2: Tyrosine.

Dataset name	Tyrosine (initial)	Tyrosine (full kinematical)	Tyrosine (L, CAP)	Tyrosine (D, CAP)	Tyrosine (L, PETS2)	Tyrosine (D, PETS2)
Crystal data						
Chemical formula	$C_9H_{11}NO_3$	$C_9H_{11}NO_3$	$C_9H_{11}NO_3$	$C_9H_{11}NO_3$	$C_9H_{11}NO_3$	$C_9H_{11}NO_3$
M_r	181.2	181.2	181.2	181.2	181.2	181.2
Crystal system, space group	Orthorhombic, $P2_12_12_1$	Orthorhombic, $P2_12_12_1$	Orthorhombic, $P2_12_12_1$	Orthorhombic, $P2_12_12_1$	Orthorhombic, $P2_12_12_1$	Orthorhombic, $P2_12_12_1$
Temperature (K)	293	293	293	293	293	293
a, b, c (Å)	5.85 (10), 6.97 (18), 21.24 (10)	5.85 (10), 6.97 (18), 21.24 (10)	5.85 (10), 6.97 (18), 21.24 (10)	5.85 (10), 6.97 (18), 21.24 (10)	5.85 (10), 6.97 (18), 21.24 (10)	5.85 (10), 6.97 (18), 21.24 (10)
V (Å^3)	866 (27)	866 (27)	866 (27)	866 (27)	866 (27)	866 (27)
Z	4	4	4	4	4	4
Radiation type	Electrons, $\lambda = 0.0251$ Å	Electrons, $\lambda = 0.0251$ Å	Electrons, $\lambda = 0.0251$ Å	Electrons, $\lambda = 0.0251$ Å	Electrons, $\lambda = 0.0251$ Å	Electrons, $\lambda = 0.0251$ Å
Data collection and processing						
Diffractometer	Rigaku XtaLAB Synergy-ED	Rigaku XtaLAB Synergy-ED	Rigaku XtaLAB Synergy-ED	Rigaku XtaLAB Synergy-ED	Rigaku XtaLAB Synergy-ED	Rigaku XtaLAB Synergy-ED
Processing program	CrysAlis^{Pro}	CrysAlis^{Pro}	CrysAlis^{Pro}	CrysAlis^{Pro}	PETS2	PETS2
Processed data type	Merged intensities	Merged intensities	Virtual frame intensities	Virtual frame intensities	Virtual frame intensities	Virtual frame intensities
measured, independent, observed	4026, 1550, 1102	4026, 1550, 1102	11915, 2680, 1337	11915, 2680, 1337	11488, 2593, 1690	11488, 2593, 1690
R_{int}	0.084	0.084	-	-	-	-
$CC_{1/2}$	0.994	0.994	-	-	-	-
Total electron dose (e$^-$/Å^2)	10	10	10	10	10	10
$(\sin \theta/\lambda)_{max}$ (Å^{-1})	0.625	0.625	0.625	0.625	0.625	0.625
Detector distance (mm)	645	645	645	645	645	645
Refinement						
Refinement type	kinematical	kinematical	dynamical	dynamical	dynamical	dynamical
R_1,	0.144,	0.102,	0.076,	0.097,	0.097,	0.122,
wR_2 [$F^2 > 2\sigma(F^2)$]	0.342	0.236	0.189	0.241	0.179	0.230
R_1, wR_2 [all]	0.170, 0.354	0.128, 0.249	0.113, 0.221	0.134, 0.268	0.126, 0.187	0.150, 0.237

S	1.84	1.29	1.19	1.44	2.85	3.62
No. of reflections	1550	1550	2680	2680	2593	2593
No. of parameters	54	121	156	156	181	181
No. of restraints	0	0	0	0	0	0
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (eÅ^{-3})	0.23, -0.14	0.12, -0.11	0.09, -0.09	0.12, -0.12	0.13, -0.12	0.19, -0.16

Table S3: Clarithromycin.

Dataset name	Clarithromycin (original)	Clarithromycin (inverted)
Crystal data		
Chemical formula	$C_{38}NO_{13}$ (H atoms excluded)	$C_{38}NO_{13}$ (H atoms excluded)
M_r	678.4	678.4
Crystal system, space group	Orthorhombic, $P2_12_12_1$	Orthorhombic, $P2_12_12_1$
Temperature (K)	293	293
a, b, c (Å)	8.8 (2), 20.1 (3), 23.91 (17)	8.8 (2), 20.1 (3), 23.91 (17)
V (Å^3)	4230 (120)	4230 (120)
Z	4	4
Radiation type	Electrons, λ = 0.0251 Å	Electrons, λ = 0.0251 Å
Data collection and processing		
Diffractometer	Rigaku XtaLAB Synergy-ED	Rigaku XtaLAB Synergy-ED
Processing program	CrysAlis^{Pro}	CrysAlis^{Pro}
Processed data type	Virtual frame intensities	Virtual frame intensities
measured, independent, observed	20812, 6151, 1678	20812, 6151, 1678
Total electron dose (e$^-$/Å^2)	10	10
$(\sin \theta/\lambda)_{max}$ (Å^{-1})	0.625	0.625
Detector distance (mm)	645	645
Refinement		
Refinement type	dynamical	dynamical
R_1, wR_2 [$F^2 > 2\sigma(F^2)$]	0.130, 0.220	0.167, 0.275
R_1, wR_2 [all]	0.271, 0.257	0.311, 0.313
S	1.95	2.37
No. of reflections	6151	6151
No. of parameters	241	241
No. of restraints	0	0
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.17, -0.17	0.25, -0.18

Table S4: Thaumatin.

Dataset name	Thaumatin
Crystal data	
Crystal system, space group	Tetragonal, $P4_12_12$
Temperature (K)	100
a, b, c (Å)	58.40(15), 58.40(15), 151.2(2)
α, β, γ (°)	90, 90, 90
Data collection and processing	
Radiation type	Electrons, $\lambda = 0.0251$ Å
Diffractometer	Rigaku XtaLAB Synergy-ED
Detector distance (mm)	1800
Total electron dose ($e^-/(Å^2 s)$)	10
Resolution range (Å)	16.14-2.15 (2.22-2.15)
# unique reflections	12870 (1081)
I/σ_I	3.5 (1.2)
$CC_{1/2}$	0.972 (0.603)
Completeness (%)	86.2 (86.0)
Multiplicity	6.4 (6.1)
R_{int}	0.43 (1.90)
R_{pim}	0.17 (0.74)
Refinement	
R_{work}, R_{free} (%)	19.5, 22.6
# atoms (protein, ligand, water)	1558, 10, 23
B-factors (protein, ligand, water) ($Å^2$)	23.8, 7.2, 15.0
RMS bonds, angles	0.01, 1.86
Ramachandran outliers, favored (%)	0.0, 96.1
Rotamer outliers (%)	3.57
Cβ deviations	3
Clahscore	2.62
MolProbity score	1.73

Table S5: Cystine.

Dataset name	Cystine (1, 653mm)	Cystine (1, 1029mm)	Cystine (1, 1289mm)	Cystine (2, 777mm)	Cystine (2, 1029mm)	Cystine (2, 1289mm)
Crystal data						
Chemical formula	$C_6H_{12}N_2O_4S_2$	$C_6H_{12}N_2O_4S_2$	$C_6H_{12}N_2O_4S_2$	$C_6H_{12}N_2O_4S_2$	$C_6H_{12}N_2O_4S_2$	$C_6H_{12}N_2O_4S_2$
M_r	240.30	240.30	240.30	240.30	240.30	240.30
Crystal system, space group	Hexagonal, $P6_122$	Hexagonal, $P6_122$	Hexagonal, $P6_122$	Hexagonal, $P6_122$	Hexagonal, $P6_122$	Hexagonal, $P6_122$
Temperature (K)	293	293	293	293	293	293
a, b, c (Å)	5.44 (8), 5.44 (8), 56.60 (13)	5.42 (10), 5.42 (10), 56.41 (14)	5.46 (10), 5.46 (10), 56.91 (13)	5.5 (12), 5.5 (12), 58.5 (10)	5.4 (9), 5.4 (9), 56.6 (7)	5.5 (8), 5.5 (8), 57.2 (7)
α, β, γ (°)	90, 90, 120	90, 90, 120	90, 90, 120	90, 90, 120	90, 90, 120	90, 90, 120
V (Å^3)	1449 (44)	1436 (52)	1470 (56)	1532 (659)	1451 (501)	1501 (462)
Z	6	6	6	6	6	6
Radiation type	Electrons, λ = 0.0251 Å	Electrons, λ = 0.0251 Å	Electrons, λ = 0.0251 Å	Electrons, λ = 0.0251 Å	Electrons, λ = 0.0251 Å	Electrons, λ = 0.0251 Å
Data collection and processing						
Diffractometer	Rigaku XtaLAB Synergy-ED	Rigaku XtaLAB Synergy-ED	Rigaku XtaLAB Synergy-ED	Rigaku XtaLAB Synergy-ED	Rigaku XtaLAB Synergy-ED	Rigaku XtaLAB Synergy-ED
measured, inde-pendent, observed	7866, 880, 818	6143, 882, 669	4983, 877, 571	2731, 393, 251	2448, 375, 261	2211, 365, 148
Resolution (Å)	0.80	0.80	0.80	1.10	1.10	1.10
Completeness (%)	79.2	79.6	77.7	99.5	99.5	92.3
Redundancy	12.6	9.9	8.1	3.5	3.3	3.1
R_{int}	0.133	0.162	0.121	0.505	0.286	0.462
R_{pim}	0.040	0.055	0.044	0.307	0.146	0.174
$CC_{1/2}$	0.998	0.995	0.998	0.472	0.952	0.940
$I/\sigma(I)$ [inf - 0.80 Å]	13.96	10.25	11.29	2.45	3.69	2.73
Total electron dose ($e^-/Å^2$)	0.8	0.8	0.8	0.8	0.8	0.8
Min, Max collec-tion angle (°)	-55, +70	-55, +70	-55, +70	-55, +55	-55, +55	-55, +55
$(\sin\theta/\lambda)_{max}$ (Å^{-1})	0.624	0.624	0.624	0.454	0.454	0.454
Detector distance (mm)	653	1029	1289	777	1029	1289
Refinement						

R_1, wR$_2$ [F^2 > 2σ(F^2)]	0.164, 0.403	0.140, 0.362	0.122, 0.343	0.288, 0.603	0.227, 0.433	0.233, 0.481
R_1, wR$_2$ [all]	0.170, 0.406	0.160, 0,374	0.154, 0.365	0.308, 0.621	0.250, 0.443	0.292, 0.515
S	1.19	1.18	1.15	1.03	1.87	1.22
No. of reflections	880	882	877	393	375	365
No. of parameters	66	66	66	66	66	66
No. of restraints	75	39	0	75	75	75
Δρmax, Δρmin (e Å^{-3})	0.22, -0.18	0.20, -0.17	0.12, -0.15	0.14, -0.10	0.16, -0.17	0.15, -0.11
CCDC number	-	-	2267655	-	-	-