7.3 Crystallographic Data

Table 5: Crystal data and structure refinement for **95a**, **95b** and **95d**.

	95a	**95b**	**95d**
Empirical formula	$C_{117}H_{121}N_3O_5$	$C_{117}H_{115}N_3O_5$	$C_{135}H_{149}N_3O_4$
Formula weight	1649.17	1643.12	1877.57
Temperature	100(2) K	143(2) K	100(2) K
Wavelength	0.71073 Å	0.71073 Å	0.71073 Å
Crystal system	Triclinic	Triclinic	Triclinic
Space group	P-1	P-1	P-1
Unit cell dimensions a	14.493(4) Å	14.661(2) Å	9.287(3) Å
b	17.862(5) Å	14.909(2) Å	22.591(7) Å
c	20.589(6) Å	23.734(3) Å	27.042(8) Å
α	97.097(7)°	107.173(2)°	101.705(7)°
β	100.914(7)°	105.122(2)°	93.268(8)°
γ	112.715(5)°	93.121(3)°	99.724(7)°
V	4712.13 $Å^3$	4735.9(9) $Å^3$	5451.02 $Å^3$
Z	2	2	2
Density (calculated)	1.162 Mg/m^3	1.152 Mg/m^3	1.144 Mg/m^3
Absorption coefficient μ	0.07 mm^{-1}	0.07 mm^{-1}	0.07 mm^{-1}
F(000)	1768	1756	2024
Crystal size	0.52×0.41×0.13 mm	0.33×0.12×0.10 mm	0.5×0. 2×0.05 mm
Theta range for data collection	$2\theta_{max}$ = 45°	$2\theta_{max}$ = 45°	$2\theta_{max}$ = 45°
Index ranges	-15≤h≤15, -19≤k≤19, -22≤l≤22	-15≤h≤15, -16≤k≤15, -25≤l≤25	-9≤h≤9, -24≤k≤23, -29≤l≤29
Reflections collected	31122	36482	43770
Independent reflections	12331 [R_{int} = 0.171]	12205 [R_{int} = 0.10]	14211 [R_{int} = 0.17]
Completeness to Θ_{max}	99.9 %	98.7 %	99.9 %
Absorption correction	none	none	none
Max. and min. transmission	-	-	-
Refinement method	Full-matrix least-squares on F^2	Full-matrix least-squares on F^2	Full-matrix least-squares on F^2
Data / restraints / parameters	12331 / 981 / 343	12205 / 1164 / 1084	14211 / 1306/1210
Goodness-of-fit on F^2	1.452	1.072	1.20
Final R indices [I>2sigma(I)]	R_1 = 0.127, wR_2 = 0.246	R_1 = 0.0839, wR_2 = 0.2465	R_1 = 0.113, wR_2 = 0.271
R indices (all data)	R_1 = 0.314, wR_2 = 0.275	R_1 = 0.1617, wR_2 = 0.2869	R_1 = 0.262, wR_2 = 0.317
Largest diff. peak and hole	0.33 and –0.28 e.$Å^{-3}$	0.86 and –0.48 e.$Å^{-3}$	0.68 and –0.51 e.$Å^{-3}$