Bin. Crossentropy on generated structures ■ ■ 150k 709 N test 150k 709 N train ■ 150k 300N test 150k 300N train ■ ■ 150k 100N test ■ ■ 150k 100N train 150k 50N test 150k 50N train 0.70 Test bin. crossentropy on generated structures 0.7075 0.7050 0.69 0.7025 0.7000 0.6975 0.68 0.6950 0.6925 100 200 300 400 500 600 700 0.67 200 600 800 1200 400 1000 0