Supplementary Information

Table S1 | Jensen–Shannon divergence ($\times 10^{-3}$) between the bond length

Bond	Pocket2Mol	TargetDiff	Lingo3DMol	3DSMILES-GPT
C-C	0.4422	**0.3035**	0.4062	0.4285
C=C	0.3091	**0.2014**	0.5038	0.3994
C#C	0.7276	0.6726	0.7048	**0.577**
C:C	0.4273	**0.199**	0.411	0.4711
C-N	0.3251	**0.2419**	0.4	0.4183
C=N	0.3776	**0.1597**	0.6044	0.4086
C#N	0.7487	0.6514	0.5625	**0.4789**
C:N	0.4186	**0.1315**	0.4128	0.4596
N-O	0.3743	**0.3997**	0.6086	0.4234
N=O	0.5625	0.6684	0.7832	**0.5534**
C-O	0.3272	**0.2997**	0.4084	0.409
C=O	0.4604	**0.4006**	0.4992	0.4796
C:O	0.5066	**0.4483**	0.486	0.4805
C-F	0.4775	**0.3141**	0.4882	0.4769
C-S	0.5076	0.3349	0.2188	**0.2164**
C=S	0.5684	0.5845	0.8325	**0.5128**
C:S	0.4105	0.388	0.3368	**0.3084**

O-S	0.8054	**0.3567**	0.7434	0.6134
O=S	0.6534	0.6987	0.7126	**0.4556**
C-Cl	0.3652	0.3433	**0.1766**	0.2284

Table S2 | The performance in PoseBusters benchmark.

Metrics	All atoms connected	Bond lengths	Bond angles	Internal steric clash	Aromatic ring flatness	Double bond flatness	Internal energy	Overall pass Rate
Ref.	≈1.00	1	1	0.95	1.00	≈1.00	1	0.95
Pocket2Mol	1	0.92	**0.99**	**0.99**	0.99	0.99	**0.97**	**0.86**
TargetDiff	1	0.99	0.75	0.92	1	**1**	0.74	0.50
Lingo3DMol	1	0.91	0.55	0.59	0.99	≈1.00	0.58	0.17
3DSMILES-GPT	1	**0.98**	0.98	0.97	**≈1.00**	**1**	0.92	**0.86**

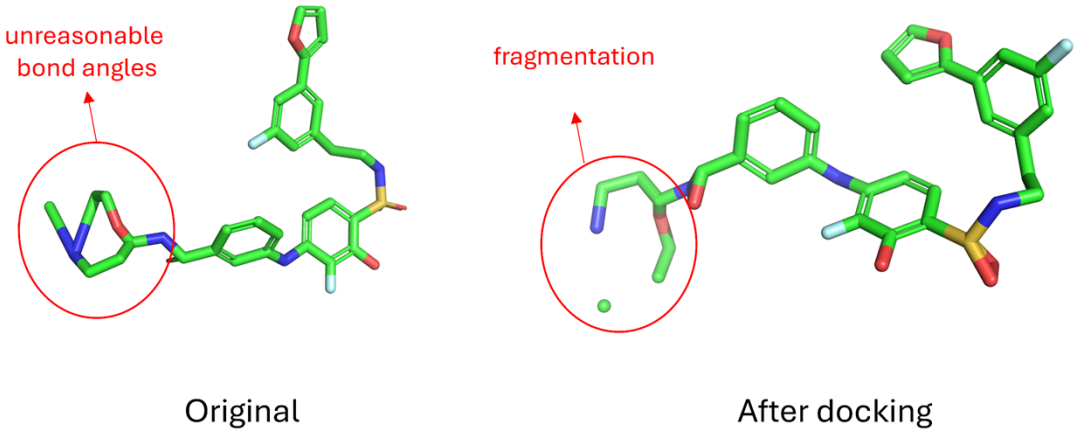

Fig S1. Comparison of the conformations of a generated molecule before and after docking.