

SUPPORTING INFORMATION

New In Silico Insights into the Application of (Hydroxy)Chloroquine with Macrolide Antibiotic Co-Crystals Against the SARS-CoV-2 Virus

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Table S1. Cartesian coordinates (in Å) for co-crystals computed at PM6.

Figure S1. Intermolecular interactions of single-crystals in the viral M^{pro} active site.

Table S1. Cartesian coordinates (in Å) for co-crystals computed at PM6.

Co-crystal CQ/AZ			
O	6.26250000	-1.23120000	-0.99040000
O	4.49360000	-2.62720000	-0.78790000
O	5.47030000	-2.61420000	2.28260000
H	4.94010000	-3.06690000	1.58250000
O	8.02220000	-2.04270000	2.11070000
H	7.49580000	-2.74000000	2.59080000
O	1.86860000	-0.71780000	-2.22610000
O	1.26480000	3.22180000	-0.77910000
O	1.56710000	0.05640000	0.94640000
H	0.85250000	-0.49360000	0.53230000
O	0.90640000	6.13430000	-2.38820000
H	0.91080000	7.07890000	-2.10510000
O	-0.55570000	3.15800000	-2.24820000
O	-0.71140000	-1.58510000	-4.42280000
O	-2.66510000	-1.88070000	-2.77860000
H	-2.47380000	-1.29880000	-3.57530000
O	0.42970000	-1.84530000	-0.80720000
N	4.09690000	0.09460000	3.02630000
N	-1.18970000	6.77760000	0.05020000
C	4.97350000	-1.60810000	-1.24120000
C	4.31740000	-0.54420000	-2.10490000
H	4.99540000	0.35330000	-2.12430000
C	2.95910000	-0.12130000	-1.47330000
H	2.89700000	-0.47540000	-0.40520000
C	2.73230000	1.40850000	-1.51840000
H	3.57250000	1.89280000	-0.95520000
C	1.41030000	1.78270000	-0.79670000
H	0.54390000	1.32510000	-1.32190000
C	1.36560000	1.46590000	0.75060000
C	2.54230000	2.12570000	1.49230000
H	2.58990000	3.19010000	1.18870000
H	3.47880000	1.65290000	1.12440000
C	2.48600000	1.98780000	3.02800000
H	1.67540000	1.25740000	3.28690000
C	3.81840000	1.44020000	3.61200000
H	4.65050000	2.12630000	3.34960000
H	3.75700000	1.42420000	4.72090000
C	5.52640000	-0.32890000	3.11840000
H	6.16300000	0.58910000	2.96200000
C	5.72070000	-1.24910000	1.87870000
H	4.97600000	-0.95200000	1.10320000
C	7.15330000	-1.27730000	1.26540000
C	7.09960000	-2.05400000	-0.09500000
H	6.61510000	-3.04610000	0.04250000
C	3.12900000	-0.93340000	3.49870000
H	3.48320000	-1.94460000	3.23880000
H	2.18140000	-0.76550000	2.94480000
H	2.92670000	-0.91010000	4.57750000
C	4.20240000	-1.09290000	-3.52540000
H	3.58440000	-0.42820000	-4.14530000
H	3.72060000	-2.07900000	-3.54470000
H	5.18610000	-1.18480000	-4.00080000
C	5.96510000	-1.00100000	4.41820000
H	5.70000000	-0.40010000	5.29220000
H	7.05050000	-1.16170000	4.42560000
H	5.49640000	-1.98860000	4.53550000
C	7.79700000	0.09270000	1.12280000
H	7.60220000	0.72650000	2.00080000
H	7.42870000	0.61520000	0.23140000
H	8.88910000	-0.00220000	1.04360000
C	8.44830000	-2.16590000	-0.79760000
H	9.23040000	-2.34590000	-0.02530000

H	8.70090000	-1.19630000	-1.27400000
C	8.46690000	-3.27940000	-1.83860000
H	9.43210000	-3.31680000	-2.35720000
H	7.69010000	-3.13080000	-2.59820000
H	8.30270000	-4.26420000	-1.38520000
C	2.76060000	1.92220000	-2.95830000
H	2.59750000	3.01110000	-3.00140000
H	1.98180000	1.44360000	-3.56440000
H	3.72520000	1.73120000	-3.43980000
C	-0.01120000	1.84530000	1.29460000
H	-0.81820000	1.25530000	0.82570000
H	-0.22800000	2.91150000	1.10330000
H	-0.07400000	1.67300000	2.37660000
C	2.16020000	3.33010000	3.69560000
H	2.03850000	3.22120000	4.77860000
H	1.22360000	3.74330000	3.30420000
H	2.94390000	4.07470000	3.52390000
C	0.58860000	3.87780000	-1.87010000
H	1.22700000	3.83910000	-2.78860000
C	0.42190000	5.30890000	-1.31030000
H	1.10360000	5.43700000	-0.43350000
C	-1.03980000	5.68820000	-0.96000000
H	-1.53480000	6.05850000	-1.90170000
C	-1.76260000	4.41790000	-0.48530000
H	-2.77360000	4.66520000	-0.09520000
H	-1.22130000	3.95060000	0.37120000
C	-1.86210000	3.43630000	-1.64890000
H	-2.42520000	3.87570000	-2.50670000
C	-2.43070000	2.08330000	-1.25780000
H	-2.43490000	1.39550000	-2.10930000
H	-3.46220000	2.18170000	-0.88720000
H	-1.84420000	1.61120000	-0.45310000
C	-0.72810000	8.08560000	-0.50220000
H	-1.42240000	8.38930000	-1.30480000
H	0.29880000	8.08480000	-0.90790000
H	-0.78850000	8.86070000	0.27870000
C	-0.52630000	6.48440000	1.35230000
H	-0.97900000	5.57830000	1.79000000
H	-0.73400000	7.30850000	2.05440000
H	0.56280000	6.33720000	1.29970000
C	1.45310000	-2.01860000	-1.78250000
H	2.25330000	-2.53510000	-1.19700000
C	1.00790000	-2.78050000	-3.03380000
H	1.23920000	-3.85500000	-2.86960000
H	1.65610000	-2.47090000	-3.88600000
C	-0.45630000	-2.64190000	-3.45950000
C	-1.41600000	-2.36970000	-2.26270000
H	-1.68190000	-3.30950000	-1.73390000
C	-0.84120000	-1.32530000	-1.28030000
H	-0.64460000	-0.35230000	-1.80200000
C	-0.92220000	-3.87030000	-4.24930000
H	-0.32010000	-3.99890000	-5.15890000
H	-1.96170000	-3.74430000	-4.58040000
H	-0.85760000	-4.79010000	-3.66170000
C	0.00080000	-0.33940000	-4.28490000
H	-0.42570000	0.26980000	-5.08870000
H	1.07600000	-0.49720000	-4.42960000
H	-0.17700000	0.11100000	-3.29530000
C	-1.67290000	-1.15050000	-0.03040000
H	-1.24710000	-0.39290000	0.65100000
H	-1.75850000	-2.07610000	0.57340000
H	-2.70290000	-0.82490000	-0.26780000
Cl	-5.18370000	3.48380000	0.85650000
N	-3.69690000	-2.69190000	3.33790000
H	-3.53790000	-2.67710000	4.35300000
N	-7.46770000	-0.91110000	2.22320000
H	-8.26060000	-0.32780000	2.52290000

N	-5.80000000	-2.83480000	-1.41910000
H	-6.62550000	-3.42300000	-1.14260000
C	-4.97070000	-0.74720000	2.54200000
C	-4.97160000	-2.05700000	3.05670000
C	-3.59050000	-4.10430000	2.83500000
H	-4.50610000	-4.70910000	3.06520000
C	-4.72350000	-3.94230000	0.56240000
H	-5.29670000	-4.88330000	0.63510000
H	-5.32700000	-3.16830000	1.11720000
C	-5.99480000	-1.45980000	-0.76060000
H	-7.05610000	-1.15100000	-0.88600000
C	-6.22490000	-2.67440000	3.38850000
H	-6.20620000	-3.61300000	3.93840000
C	-7.40580000	-2.11610000	3.03120000
H	-8.37170000	-2.53780000	3.27550000
C	-4.53290000	-3.51750000	-0.89220000
H	-3.68120000	-2.79300000	-0.98900000
H	-4.28260000	-4.38650000	-1.53480000
C	-3.80380000	0.03620000	2.35090000
H	-2.85040000	-0.39250000	2.64520000
C	-5.09900000	1.87310000	1.51530000
C	-6.24200000	-0.13070000	2.18380000
C	-3.38460000	-4.08070000	1.29660000
H	-2.85820000	-4.99250000	0.96810000
H	-2.71320000	-3.22030000	1.05560000
C	-6.30320000	1.16410000	1.69850000
H	-7.24860000	1.64140000	1.45940000
C	-5.04840000	-0.39750000	-1.26640000
H	-5.12360000	0.49440000	-0.60480000
H	-3.98460000	-0.70810000	-1.21690000
C	-3.86600000	1.33770000	1.85340000
H	-2.95910000	1.92750000	1.74710000
C	-5.75010000	-2.76960000	-2.94410000
H	-5.51230000	-3.78450000	-3.33820000
H	-4.89150000	-2.11400000	-3.24710000
C	-2.38450000	-4.77460000	3.51340000
H	-2.52300000	-4.84610000	4.59770000
H	-1.46490000	-4.19890000	3.34530000
H	-2.22050000	-5.78760000	3.13670000
C	-7.06040000	-2.26870000	-3.52220000
H	-7.01900000	-2.26780000	-4.62320000
H	-7.28650000	-1.23320000	-3.22500000
H	-7.92230000	-2.88800000	-3.24270000
H	-5.26110000	-0.05890000	-2.28360000
H	-5.96042880	-2.39417720	-1.30111629
H	-5.93451473	-1.65495708	0.29990903

Co-crystal CQ/CL

O	5.14400000	-2.10000000	-1.46080000
O	3.39030000	-2.98090000	-2.60270000
O	3.69710000	-3.24630000	1.29790000
H	2.86240000	-2.88790000	1.68270000
O	6.43050000	-4.07670000	1.29250000
H	5.67500000	-4.58600000	1.68310000
O	1.52160000	0.11150000	-2.74300000
O	1.69990000	3.28440000	-0.35990000
O	2.44500000	0.06780000	1.16400000
O	0.79930000	6.00540000	-2.25180000
H	0.97910000	6.96440000	-2.19000000
O	-0.50150000	3.29990000	-1.12420000
O	-1.50210000	0.94980000	-4.51140000
O	-3.29880000	0.11690000	-2.83160000
H	-3.08640000	0.99430000	-3.27160000
O	-0.06630000	-1.23480000	-1.73200000
N	0.39100000	6.99570000	0.97520000
C	4.07300000	-2.02770000	-2.30010000

C	3.89810000	-0.57220000	-2.71380000
H	4.82880000	-0.01280000	-2.42320000
C	2.70320000	0.01280000	-1.90920000
H	2.46510000	-0.65450000	-1.04270000
C	2.98520000	1.43790000	-1.38240000
H	3.94090000	1.37780000	-0.78350000
C	1.84260000	1.84470000	-0.41340000
H	0.87400000	1.39790000	-0.73720000
C	2.15330000	1.48850000	1.08580000
C	3.47910000	2.14100000	1.53240000
H	3.34280000	3.24170000	1.47650000
H	4.27600000	1.91360000	0.78460000
C	3.95640000	1.72400000	2.93130000
H	3.06600000	1.49100000	3.56690000
C	4.84960000	0.48060000	2.80080000
C	5.08310000	-2.04080000	2.94120000
H	6.18600000	-1.83140000	3.01640000
C	4.75660000	-2.27310000	1.44210000
H	4.42780000	-1.33070000	0.93940000
C	5.93770000	-2.89480000	0.63620000
C	5.44020000	-3.36980000	-0.76850000
H	4.49120000	-3.94880000	-0.67840000
C	4.49890000	-0.61770000	4.98640000
H	4.02190000	-1.43930000	5.53550000
H	4.04050000	0.31110000	5.34490000
H	5.55690000	-0.60320000	5.27750000
C	3.72960000	-0.49290000	-4.22720000
H	3.28000000	0.46690000	-4.51740000
H	3.06610000	-1.28260000	-4.60550000
H	4.69070000	-0.59240000	-4.74430000
C	4.77560000	-3.29320000	3.76420000
H	5.23300000	-3.24560000	4.75800000
H	5.17900000	-4.18920000	3.26440000
H	3.70030000	-3.45450000	3.89110000
C	7.12540000	-1.94800000	0.55230000
H	7.16530000	-1.24780000	1.40420000
H	7.08630000	-1.33470000	-0.35750000
H	8.06740000	-2.51230000	0.55060000
C	6.50600000	-4.10650000	-1.57430000
H	7.15450000	-4.67820000	-0.87240000
H	7.17110000	-3.36890000	-2.06660000
C	5.89670000	-5.04570000	-2.60860000
H	6.65960000	-5.43840000	-3.28830000
H	5.13420000	-4.53620000	-3.21580000
H	5.40300000	-5.90250000	-2.13480000
C	3.21120000	2.44200000	-2.50750000
H	3.39060000	3.44740000	-2.10290000
H	2.34370000	2.49110000	-3.17970000
H	4.08260000	2.17550000	-3.11590000
C	0.98610000	1.89620000	1.97570000
H	0.02420000	1.47570000	1.63900000
H	0.85640000	2.99580000	1.94890000
H	1.14220000	1.59610000	3.01750000
C	4.76780000	2.83330000	3.60360000
H	5.09960000	2.53980000	4.60620000
H	4.18200000	3.75280000	3.70630000
H	5.66960000	3.07340000	3.02180000
C	0.76970000	3.88470000	-1.28310000
H	1.02540000	3.63020000	-2.33740000
C	0.93600000	5.38690000	-0.95730000
H	1.97720000	5.55930000	-0.59060000
C	-0.11820000	5.96250000	0.02490000
H	-0.91890000	6.46220000	-0.59080000
C	-0.76060000	4.80800000	0.81270000
H	-1.47950000	5.20500000	1.55700000
H	0.01030000	4.25300000	1.40040000
C	-1.45340000	3.85830000	-0.16110000

H	-2.18080000	4.39850000	-0.81170000
C	-2.09540000	2.65630000	0.50470000
H	-2.60560000	2.02140000	-0.22920000
H	-2.83730000	2.95530000	1.25940000
H	-1.35030000	2.02050000	1.01180000
C	0.77660000	8.25100000	0.26500000
H	-0.07720000	8.61460000	-0.32910000
H	1.65830000	8.16900000	-0.38620000
H	0.98560000	9.02880000	1.02030000
C	1.51170000	6.51840000	1.83510000
H	1.16760000	5.65870000	2.43400000
H	1.78120000	7.31560000	2.54700000
H	2.41990000	6.21620000	1.29130000
C	0.76390000	-1.10670000	-2.87570000
H	1.41770000	-2.01060000	-2.78670000
C	0.04890000	-0.99640000	-4.22320000
H	0.07200000	-2.00060000	-4.69800000
H	0.66250000	-0.34920000	-4.89430000
C	-1.38770000	-0.46720000	-4.22380000
C	-2.12250000	-0.70840000	-2.87380000
H	-2.51230000	-1.74730000	-2.80970000
C	-1.23640000	-0.38090000	-1.65030000
H	-0.89620000	0.68740000	-1.66670000
C	-2.19630000	-1.05900000	-5.38490000
H	-1.74690000	-0.78430000	-6.34880000
H	-3.21630000	-0.65240000	-5.39080000
H	-2.25890000	-2.14910000	-5.33300000
C	-0.56640000	1.85570000	-3.89320000
H	-0.84050000	2.81860000	-4.33800000
H	0.46670000	1.58130000	-4.13790000
H	-0.70550000	1.86760000	-2.79840000
C	-1.89360000	-0.76010000	-0.34040000
H	-1.29120000	-0.46580000	0.52770000
H	-2.05310000	-1.85330000	-0.23900000
H	-2.88090000	-0.27660000	-0.22730000
Cl	-4.56990000	2.68450000	3.34270000
N	-3.58660000	-3.94570000	2.06810000
H	-3.31190000	-4.54130000	2.85870000
N	-7.19200000	-1.70080000	2.83610000
H	-7.83090000	-1.33280000	3.55370000
N	-6.34660000	-1.24510000	-1.52000000
H	-7.19840000	-1.84890000	-1.40080000
C	-4.67790000	-1.82170000	2.65390000
C	-4.78000000	-3.20510000	2.43320000
C	-3.75970000	-4.79550000	0.83890000
H	-4.71200000	-5.38660000	0.86250000
C	-5.17070000	-3.29720000	-0.66100000
H	-5.86720000	-4.09620000	-0.97180000
H	-5.55620000	-2.92250000	0.32840000
C	-6.22430000	-0.39430000	-0.24600000
H	-5.91550000	-1.09170000	0.59270000
H	-7.23590000	-0.02330000	0.03120000
C	-6.04210000	-3.85820000	2.65280000
H	-6.06910000	-4.94520000	2.62780000
C	-7.17260000	-3.15130000	2.88530000
H	-8.13880000	-3.60160000	3.07280000
C	-5.13210000	-2.16450000	-1.68480000
H	-4.20530000	-1.54380000	-1.56020000
H	-5.10510000	-2.56440000	-2.71990000
C	-3.45870000	-1.09430000	2.62750000
H	-2.54230000	-1.65120000	2.46060000
C	-4.60240000	0.95920000	3.09910000
C	-5.89100000	-1.06010000	2.92810000
C	-3.77390000	-3.88030000	-0.41400000
H	-3.42940000	-4.44150000	-1.29900000
H	-3.03220000	-3.06020000	-0.24730000
C	-5.84720000	0.30180000	3.16870000

H	-6.74150000	0.86980000	3.40630000
C	-5.23430000	0.74070000	-0.35860000
H	-5.05960000	1.16950000	0.65340000
H	-4.23740000	0.40660000	-0.71390000
C	-3.41860000	0.28040000	2.85390000
H	-2.46960000	0.80890000	2.84840000
C	-6.52620000	-0.40830000	-2.78540000
H	-6.51400000	-1.08840000	-3.66830000
H	-5.63350000	0.26180000	-2.90240000
C	-2.58090000	-5.77890000	0.75600000
H	-2.56870000	-6.46410000	1.61050000
H	-1.62040000	-5.24750000	0.75660000
H	-2.62610000	-6.38760000	-0.15100000
C	-7.81700000	0.38800000	-2.74750000
H	-7.94820000	0.95100000	-3.68560000
H	-7.83120000	1.13520000	-1.93940000
H	-8.71000000	-0.23970000	-2.63270000
H	-5.56890000	1.56180000	-0.99800000
O	5.90330000	0.51730000	2.20320000
C	4.33350000	-0.79430000	3.47490000
H	3.24420000	-0.89470000	3.23130000
C	1.33490000	-0.84950000	1.18350000
H	0.72610000	-0.75040000	0.27220000
H	1.83400000	-1.83310000	1.18980000
H	0.73590000	-0.71810000	2.08820000
H	-6.45924618	-1.05578147	-1.06675731

Co-crystal CQ/ER

O	5.57140000	-1.61570000	-1.20060000
O	3.93010000	-2.37420000	-2.55980000
O	4.72540000	-3.88960000	2.14640000
H	4.60130000	-4.60700000	1.48270000
O	6.80780000	-4.19570000	0.96540000
H	6.75600000	-4.35070000	1.94580000
O	1.91740000	0.53380000	-2.71850000
O	1.41000000	3.46140000	0.07930000
O	1.55220000	-0.06950000	0.82050000
O	1.14270000	6.70750000	-0.72760000
H	1.23320000	7.53040000	-0.19450000
O	-0.39330000	3.83460000	-1.35660000
O	-1.06690000	1.46470000	-4.32280000
O	-2.78610000	0.25120000	-2.89760000
H	-2.57180000	1.22800000	-3.07310000
O	0.48760000	-1.17640000	-2.07410000
N	-0.87890000	6.68630000	1.88600000
C	4.52680000	-1.44330000	-2.06600000
C	4.29390000	0.04880000	-2.25020000
H	5.08660000	0.60080000	-1.67520000
C	2.90830000	0.43620000	-1.66410000
H	2.56390000	-0.34580000	-0.93540000
C	2.91920000	1.81750000	-0.96210000
H	3.67050000	1.75670000	-0.12670000
C	1.52770000	2.08170000	-0.32820000
H	0.71620000	1.83380000	-1.06330000
C	1.30660000	1.33660000	1.04050000
C	2.36290000	1.75440000	2.07990000
H	2.26850000	2.84990000	2.24150000
H	3.37370000	1.62380000	1.63640000
C	2.24920000	0.99440000	3.41510000
H	1.40180000	0.26230000	3.35080000
C	3.55000000	0.20650000	3.63270000
C	5.03990000	-1.55820000	2.57340000
H	5.51360000	-0.64420000	2.12640000
C	5.00920000	-2.64530000	1.47400000
H	4.16970000	-2.43650000	0.76940000

C	6.33550000	-2.86870000	0.66000000
C	6.00600000	-2.98480000	-0.86100000
H	5.15650000	-3.68310000	-1.03400000
C	2.90030000	-2.17770000	3.86810000
H	3.07370000	-3.20040000	3.49220000
H	1.81820000	-2.01910000	3.91350000
H	3.29330000	-2.14680000	4.89080000
C	4.45000000	0.36880000	-3.73530000
H	4.07300000	1.37660000	-3.95790000
H	3.87430000	-0.32280000	-4.36490000
H	5.49840000	0.31890000	-4.05050000
C	5.87120000	-1.98970000	3.78100000
H	5.77890000	-1.25090000	4.59210000
H	6.93560000	-2.07240000	3.52640000
H	5.54090000	-2.96200000	4.16810000
C	7.45440000	-1.87520000	0.92870000
H	7.65070000	-1.75630000	2.00610000
H	7.22250000	-0.88850000	0.50820000
H	8.39580000	-2.21730000	0.47910000
C	7.20550000	-3.32610000	-1.74120000
H	7.86160000	-4.03510000	-1.18620000
H	7.81140000	-2.41380000	-1.91310000
C	6.78500000	-3.93980000	-3.07160000
H	7.63980000	-4.04250000	-3.74880000
H	6.02630000	-3.32910000	-3.57950000
H	6.35180000	-4.93880000	-2.93670000
C	3.34720000	2.94030000	-1.90250000
H	3.31290000	3.91360000	-1.39300000
H	2.69880000	2.98770000	-2.78650000
H	4.37600000	2.80470000	-2.25390000
C	-0.11930000	1.55170000	1.52380000
H	-0.87950000	1.34280000	0.75290000
H	-0.28050000	2.60570000	1.82050000
H	-0.36650000	0.93090000	2.39910000
C	1.99200000	1.92990000	4.59410000
H	1.83510000	1.36540000	5.52170000
H	1.10370000	2.54840000	4.42960000
H	2.84970000	2.59360000	4.77150000
C	0.77410000	4.40200000	-0.80970000
H	1.40820000	4.57910000	-1.70780000
C	0.65280000	5.64030000	0.10750000
H	1.35150000	5.51450000	0.97220000
C	-0.78780000	5.96260000	0.58320000
H	-1.25760000	6.63790000	-0.18690000
C	-1.58750000	4.65220000	0.64750000
H	-2.58850000	4.82630000	1.09260000
H	-1.09320000	3.91490000	1.32630000
C	-1.70680000	4.07840000	-0.76030000
H	-2.16400000	4.81370000	-1.46480000
C	-2.43090000	2.74420000	-0.81790000
H	-2.46080000	2.34270000	-1.84160000
H	-3.45880000	2.83870000	-0.44370000
H	-1.93910000	1.98510000	-0.18030000
C	-0.32550000	8.06820000	1.76840000
H	-0.97610000	8.65050000	1.09370000
H	0.71070000	8.12640000	1.39570000
H	-0.36390000	8.56550000	2.75150000
C	-0.25040000	5.95570000	3.02300000
H	-0.76770000	4.99070000	3.16260000
H	-0.40660000	6.53100000	3.95050000
H	0.82670000	5.75850000	2.91420000
C	1.32290000	-0.71200000	-3.12450000
H	2.08380000	-1.52920000	-3.19060000
C	0.60850000	-0.40770000	-4.44190000
H	0.68530000	-1.31210000	-5.08230000
H	1.18530000	0.37880000	-4.98290000
C	-0.85760000	0.02980000	-4.35970000

C	-1.59580000	-0.52160000	-3.10040000
H	-1.96000000	-1.55670000	-3.25960000
C	-0.72480000	-0.42250000	-1.82960000
H	-0.43390000	0.64410000	-1.62790000
C	-1.62180000	-0.35210000	-5.63240000
H	-1.17090000	0.12550000	-6.51280000
H	-2.65680000	0.01220000	-5.58080000
H	-1.64080000	-1.43180000	-5.79910000
C	-0.08630000	2.29010000	-3.66440000
H	-0.56580000	3.27770000	-3.65580000
H	0.84490000	2.29840000	-4.23690000
H	0.10460000	1.94700000	-2.62940000
C	-1.34120000	-1.10110000	-0.62290000
H	-0.71340000	-0.98120000	0.27820000
H	-1.44230000	-2.18600000	-0.76550000
H	-2.33970000	-0.68650000	-0.38440000
Cl	-3.13930000	2.17740000	2.42320000
N	-4.18480000	-4.55680000	2.28870000
H	-4.29290000	-5.14460000	3.12280000
N	-6.96710000	-1.24560000	2.33410000
H	-7.48890000	-0.62610000	2.96880000
N	-5.76630000	-1.71260000	-2.01400000
H	-6.66360000	-2.25860000	-2.05740000
C	-4.60640000	-2.14070000	2.40780000
C	-5.11630000	-3.44900000	2.36380000
C	-4.35210000	-5.39830000	1.05340000
H	-5.41170000	-5.73420000	0.91030000
C	-5.09920000	-3.77110000	-0.75130000
H	-5.82530000	-4.45890000	-1.22000000
H	-5.62790000	-3.29350000	0.11860000
C	-5.91250000	-0.70810000	-0.86030000
H	-5.93420000	-1.29610000	0.10750000
H	-6.90750000	-0.21910000	-0.94260000
C	-6.53230000	-3.65750000	2.48690000
H	-6.89620000	-4.67980000	2.56060000
C	-7.40060000	-2.61930000	2.51470000
H	-8.47160000	-2.73080000	2.62610000
C	-4.62870000	-2.70160000	-1.73690000
H	-3.75510000	-2.13880000	-1.31920000
H	-4.28660000	-3.16050000	-2.68780000
C	-3.22140000	-1.82500000	2.41350000
H	-2.51400000	-2.64980000	2.43180000
C	-3.69720000	0.52230000	2.46840000
C	-5.53620000	-1.02010000	2.45580000
C	-3.91620000	-4.56570000	-0.18230000
H	-3.48380000	-5.22170000	-0.95590000
H	-3.10700000	-3.87590000	0.14270000
C	-5.08570000	0.28780000	2.51370000
H	-5.77160000	1.12540000	2.59370000
C	-4.80300000	0.31550000	-0.81410000
H	-4.88090000	0.90830000	0.12000000
H	-3.79170000	-0.14010000	-0.77190000
C	-2.77010000	-0.50820000	2.45350000
H	-1.70230000	-0.29550000	2.48920000
C	-5.56240000	-1.04010000	-3.36970000
H	-5.33500000	-1.82300000	-4.12800000
H	-4.64600000	-0.38140000	-3.31970000
C	-3.46300000	-6.64390000	1.19570000
H	-3.77820000	-7.26730000	2.03930000
H	-2.41820000	-6.36180000	1.38150000
H	-3.49100000	-7.26590000	0.29760000
C	-6.78470000	-0.24110000	-3.78060000
H	-6.63160000	0.20480000	-4.77700000
H	-6.98860000	0.60010000	-3.10120000
H	-7.69770000	-0.84600000	-3.84690000
H	-4.81230000	1.01500000	-1.65620000
O	4.47270000	0.65600000	4.27470000

C	3.58830000	-1.16380000	2.95430000
H	2.98650000	-1.08990000	2.00200000
H	0.78430000	-0.51720000	0.38070000
H	-5.98866452	-1.46695471	-1.62498195

Co-crystal HQ/AZ

O	6.31880000	-1.29690000	-0.99920000
O	4.53930000	-2.68090000	-0.80590000
O	5.52360000	-2.63550000	2.28660000
H	4.97690000	-3.08370000	1.59650000
O	8.08470000	-2.12520000	2.09210000
H	7.54530000	-2.80770000	2.57890000
O	1.92680000	-0.69750000	-2.26740000
O	1.32080000	3.18990000	-0.84430000
O	1.64290000	0.07640000	0.98090000
H	0.91360000	-0.46610000	0.58440000
O	0.86570000	5.96610000	-2.65530000
H	0.89870000	6.92930000	-2.44800000
O	-0.59170000	3.01350000	-2.17440000
O	-0.85860000	-1.30800000	-4.30250000
O	-2.68020000	-1.77980000	-2.55230000
H	-2.55220000	-1.11840000	-3.30150000
O	0.57130000	-1.92070000	-0.84420000
N	4.21130000	0.10290000	3.01580000
N	-1.05040000	6.81550000	-0.12620000
C	5.02610000	-1.66270000	-1.25240000
C	4.38120000	-0.59060000	-2.11320000
H	5.06770000	0.30070000	-2.12790000
C	3.02410000	-0.15430000	-1.48770000
H	2.93480000	-0.53060000	-0.43050000
C	2.82950000	1.38120000	-1.51040000
H	3.67050000	1.84110000	-0.92880000
C	1.50160000	1.75590000	-0.80040000
H	0.64450000	1.25390000	-1.30330000
C	1.47150000	1.48690000	0.75460000
C	2.67180000	2.13440000	1.46850000
H	2.73690000	3.19180000	1.14610000
H	3.59360000	1.63530000	1.09720000
C	2.63250000	2.02310000	3.00710000
H	1.81310000	1.31120000	3.28820000
C	3.96260000	1.46190000	3.58380000
H	4.80280000	2.12960000	3.30080000
H	3.91430000	1.46390000	4.69340000
C	5.63450000	-0.34310000	3.09690000
H	6.28450000	0.56230000	2.92290000
C	5.80060000	-1.28050000	1.86610000
H	5.05790000	-0.97600000	1.09160000
C	7.22900000	-1.34630000	1.24560000
C	7.14860000	-2.13120000	-0.10870000
H	6.64650000	-3.11290000	0.04010000
C	3.23270000	-0.90160000	3.51550000
H	3.56550000	-1.92190000	3.26190000
H	2.28010000	-0.72420000	2.97380000
H	3.04790000	-0.86210000	4.59690000
C	4.26670000	-1.13260000	-3.53680000
H	3.59880000	-0.49740000	-4.13650000
H	3.84280000	-2.14430000	-3.55880000
H	5.24380000	-1.16440000	-4.03290000
C	6.07680000	-1.00750000	4.39950000
H	5.83360000	-0.39150000	5.26930000
H	7.15920000	-1.18810000	4.39530000
H	5.59190000	-1.98500000	4.53410000
C	7.90370000	0.00720000	1.08910000
H	7.73140000	0.65090000	1.96440000
H	7.54020000	0.53240000	0.19730000

H	8.99250000	-0.11410000	1.00150000
C	8.48850000	-2.27480000	-0.82240000
H	9.27360000	-2.46700000	-0.05620000
H	8.75680000	-1.31320000	-1.30650000
C	8.47440000	-3.39390000	-1.85740000
H	9.43360000	-3.45430000	-2.38470000
H	7.69360000	-3.23320000	-2.61050000
H	8.29360000	-4.37270000	-1.39710000
C	2.88830000	1.91420000	-2.94230000
H	2.69700000	2.99760000	-2.97720000
H	2.14380000	1.41800000	-3.57870000
H	3.87260000	1.75440000	-3.39440000
C	0.11440000	1.91680000	1.30890000
H	-0.72250000	1.40610000	0.80650000
H	-0.04020000	3.00010000	1.16080000
H	0.03570000	1.70060000	2.38120000
C	2.33850000	3.38150000	3.65630000
H	2.23310000	3.29340000	4.74280000
H	1.40200000	3.80260000	3.27310000
H	3.13060000	4.11080000	3.45900000
C	0.57480000	3.76120000	-1.93860000
H	1.14720000	3.64640000	-2.89170000
C	0.45080000	5.23350000	-1.48510000
H	1.19180000	5.42300000	-0.66920000
C	-0.98000000	5.65850000	-1.06780000
H	-1.53100000	5.97380000	-1.99850000
C	-1.68570000	4.43450000	-0.46400000
H	-2.66740000	4.72320000	-0.03110000
H	-1.09860000	4.01670000	0.38700000
C	-1.86570000	3.38030000	-1.55250000
H	-2.44750000	3.78140000	-2.41660000
C	-2.46540000	2.07970000	-1.04800000
H	-2.63140000	1.37370000	-1.86920000
H	-3.43240000	2.25900000	-0.55400000
H	-1.80870000	1.58800000	-0.30960000
C	-0.60740000	8.07500000	-0.79460000
H	-1.34820000	8.33710000	-1.56980000
H	0.39060000	8.02810000	-1.26410000
H	-0.60580000	8.90150000	-0.06590000
C	-0.30810000	6.59810000	1.14780000
H	-0.74240000	5.73030000	1.67300000
H	-0.45940000	7.47030000	1.80470000
H	0.77350000	6.42930000	1.03570000
C	1.50610000	-2.02300000	-1.90820000
H	2.33470000	-2.60580000	-1.43510000
C	0.95220000	-2.64540000	-3.19220000
H	1.18530000	-3.73100000	-3.16730000
H	1.52630000	-2.24310000	-4.05870000
C	-0.54070000	-2.45710000	-3.47460000
C	-1.39800000	-2.31020000	-2.18080000
H	-1.62710000	-3.29940000	-1.73060000
C	-0.73910000	-1.37070000	-1.14950000
H	-0.59270000	-0.34580000	-1.58160000
C	-1.08580000	-3.59520000	-4.34570000
H	-0.56870000	-3.62480000	-5.31410000
H	-2.14990000	-3.43520000	-4.56670000
H	-0.97760000	-4.57200000	-3.86690000
C	-0.16100000	-0.06690000	-4.07320000
H	-0.60210000	0.59400000	-4.82770000
H	0.91710000	-0.19210000	-4.23120000
H	-0.34620000	0.30970000	-3.05480000
C	-1.42220000	-1.33140000	0.20080000
H	-0.71580000	-1.00970000	0.98810000
H	-1.80130000	-2.31540000	0.54100000
H	-2.27760000	-0.64340000	0.22530000
Cl	-4.89540000	3.67800000	1.41250000
N	-3.56880000	-2.78290000	3.10430000

H	-3.27240000	-2.72030000	4.08760000
N	-7.30930000	-0.74550000	2.39860000
H	-8.06790000	-0.17600000	2.79700000
N	-5.87290000	-2.68040000	-1.28470000
H	-6.75270000	-3.20660000	-1.05840000
O	-5.51350000	0.40010000	-1.91660000
H	-6.02890000	1.14950000	-1.54300000
C	-4.79800000	-0.71070000	2.63890000
C	-4.83370000	-2.08220000	2.96100000
C	-3.58440000	-4.22160000	2.67540000
H	-4.53050000	-4.74700000	2.97140000
C	-4.80050000	-4.18740000	0.42990000
H	-5.28280000	-5.18080000	0.39870000
H	-5.46300000	-3.54770000	1.07110000
C	-5.84850000	-1.44690000	-0.38860000
H	-6.88310000	-1.04500000	-0.27240000
C	-6.09670000	-2.68720000	3.27330000
H	-6.09580000	-3.68780000	3.70290000
C	-7.26670000	-2.04410000	3.04480000
H	-8.23870000	-2.45610000	3.28240000
C	-4.68250000	-3.59310000	-0.97590000
H	-3.74330000	-2.98570000	-1.07690000
H	-4.62180000	-4.38860000	-1.74690000
C	-3.61030000	0.05250000	2.51770000
H	-2.66420000	-0.43070000	2.74100000
C	-4.85490000	2.01250000	1.91500000
C	-6.05580000	-0.01130000	2.39960000
C	-3.43920000	-4.28250000	1.13060000
H	-2.92030000	-5.20840000	0.83020000
H	-2.77410000	-3.43750000	0.82070000
C	-6.08090000	1.32860000	2.05760000
H	-7.01330000	1.86280000	1.90260000
C	-4.89890000	-0.35150000	-0.85920000
H	-4.63840000	0.31850000	-0.00860000
H	-3.96120000	-0.74490000	-1.31270000
C	-3.63690000	1.40510000	2.16950000
H	-2.71090000	1.97190000	2.10770000
C	-5.89810000	-2.30970000	-2.76760000
H	-4.84820000	-2.13540000	-3.12000000
H	-6.40300000	-1.31260000	-2.88490000
C	-2.40440000	-4.94850000	3.34070000
H	-2.50030000	-4.95460000	4.43230000
H	-1.45000000	-4.46010000	3.10460000
H	-2.33670000	-5.99000000	3.01420000
C	-6.59300000	-3.38080000	-3.58480000
H	-6.59110000	-3.10040000	-4.65190000
H	-7.64740000	-3.51580000	-3.30930000
H	-6.09860000	-4.35900000	-3.52560000
H	-5.75638776	-1.66901342	0.66429171
H	-5.77351762	-2.39305966	-1.69805318

Co-crystal HQ/CL

O	5.31360000	-2.14700000	-1.29460000
O	3.55950000	-3.24390000	-2.22920000
O	4.03410000	-2.98900000	1.65240000
H	3.18920000	-2.61190000	1.99230000
O	6.80180000	-3.69080000	1.62860000
H	6.08750000	-4.18070000	2.11010000
O	1.54470000	-0.28120000	-2.73230000
O	1.65390000	3.18380000	-0.75840000
O	2.60050000	0.21150000	1.10040000
O	0.58170000	5.63440000	-2.90130000
H	0.69640000	6.60440000	-2.94690000
O	-0.56960000	3.01460000	-1.43240000
O	-1.54530000	0.22870000	-4.46460000

O	-3.24470000	-0.42160000	-2.63410000
H	-3.06520000	0.40190000	-3.18400000
O	0.06250000	-1.57120000	-1.50950000
N	0.18520000	6.97090000	0.19420000
C	4.20690000	-2.23080000	-2.08600000
C	3.94970000	-0.85250000	-2.68000000
H	4.85850000	-0.21750000	-2.49340000
C	2.74650000	-0.21950000	-1.92500000
H	2.55670000	-0.77560000	-0.97250000
C	2.97650000	1.27390000	-1.59960000
H	3.95510000	1.33650000	-1.03970000
C	1.85200000	1.75440000	-0.64370000
H	0.89220000	1.23560000	-0.87180000
C	2.23100000	1.59900000	0.87420000
C	3.53520000	2.36410000	1.18370000
H	3.34100000	3.44120000	0.99410000
H	4.31750000	2.08060000	0.43960000
C	4.07940000	2.15280000	2.60410000
H	3.22440000	1.95760000	3.29810000
C	5.03630000	0.95080000	2.59640000
C	5.41890000	-1.51360000	3.05750000
H	6.51060000	-1.24140000	3.05380000
C	5.04760000	-1.95830000	1.61800000
H	4.65280000	-1.10710000	1.01070000
C	6.22680000	-2.62740000	0.84820000
C	5.69960000	-3.30190000	-0.46070000
H	4.78520000	-3.90640000	-0.25480000
C	4.84350000	0.14110000	4.92270000
H	4.44290000	-0.62400000	5.59960000
H	4.34580000	1.08340000	5.17880000
H	5.91060000	0.25270000	5.15390000
C	3.74270000	-0.98210000	-4.18530000
H	3.23910000	-0.09070000	-4.58500000
H	3.11040000	-1.84410000	-4.43780000
H	4.69530000	-1.10410000	-4.71300000
C	5.21320000	-2.65980000	4.04960000
H	5.69540000	-2.45380000	5.01070000
H	5.65630000	-3.58990000	3.65740000
H	4.15380000	-2.86370000	4.23490000
C	7.36230000	-1.64820000	0.59150000
H	7.39950000	-0.84170000	1.34350000
H	7.25840000	-1.16120000	-0.38720000
H	8.33030000	-2.16580000	0.62090000
C	6.76870000	-4.08830000	-1.21330000
H	7.47190000	-4.53520000	-0.47460000
H	7.37630000	-3.39150000	-1.82500000
C	6.16710000	-5.17930000	-2.09140000
H	6.92130000	-5.62150000	-2.75010000
H	5.35660000	-4.78670000	-2.72300000
H	5.73610000	-5.98920000	-1.49100000
C	3.11030000	2.12900000	-2.85510000
H	3.25040000	3.18670000	-2.59420000
H	2.21900000	2.04560000	-3.49200000
H	3.97310000	1.82550000	-3.45850000
C	1.07460000	2.05520000	1.75380000
H	0.12570000	1.54920000	1.51040000
H	0.88380000	3.13520000	1.59440000
H	1.28180000	1.90030000	2.81790000
C	4.84920000	3.37870000	3.10010000
H	5.23060000	3.23220000	4.11710000
H	4.21620000	4.27220000	3.11080000
H	5.71570000	3.58990000	2.45660000
C	0.66340000	3.63660000	-1.70380000
H	0.89670000	3.28020000	-2.73330000
C	0.76830000	5.17150000	-1.54950000
H	1.80770000	5.42780000	-1.22920000
C	-0.29140000	5.80760000	-0.61190000

H	-1.13180000	6.18990000	-1.25800000
C	-0.85340000	4.72500000	0.32510000
H	-1.57280000	5.17240000	1.04020000
H	-0.04090000	4.28070000	0.94910000
C	-1.52250000	3.63590000	-0.50910000
H	-2.29520000	4.05950000	-1.19350000
C	-2.08260000	2.48960000	0.31140000
H	-2.58360000	1.75560000	-0.33220000
H	-2.81610000	2.84060000	1.05210000
H	-1.29200000	1.95000000	0.85890000
C	0.48590000	8.15030000	-0.67020000
H	-0.40210000	8.39960000	-1.27320000
H	1.35190000	8.03390000	-1.33700000
H	0.67570000	9.02130000	-0.01870000
C	1.35030000	6.65570000	1.06970000
H	1.06580000	5.85930000	1.77730000
H	1.59600000	7.54520000	1.67260000
H	2.25890000	6.33430000	0.53780000
C	0.84480000	-1.54030000	-2.69100000
H	1.54690000	-2.39560000	-2.52460000
C	0.07550000	-1.62360000	-4.00970000
H	0.11240000	-2.67930000	-4.35360000
H	0.63920000	-1.05010000	-4.78330000
C	-1.37650000	-1.13900000	-4.01270000
C	-2.05800000	-1.23240000	-2.61580000
H	-2.43370000	-2.26040000	-2.41920000
C	-1.13860000	-0.75660000	-1.46990000
H	-0.84020000	0.31580000	-1.60820000
C	-2.20880000	-1.88880000	-5.06050000
H	-1.80450000	-1.72080000	-6.06790000
H	-3.24050000	-1.51260000	-5.07340000
H	-2.23530000	-2.96570000	-4.87540000
C	-0.62540000	1.23040000	-3.98560000
H	-0.95760000	2.12880000	-4.51750000
H	0.40780000	0.96970000	-4.24440000
H	-0.72220000	1.35540000	-2.89360000
C	-1.70810000	-1.02620000	-0.09240000
H	-0.92780000	-0.93060000	0.67890000
H	-2.11320000	-2.05150000	0.02510000
H	-2.51570000	-0.33160000	0.16910000
Cl	-4.29320000	3.16380000	3.37480000
N	-3.59880000	-3.54560000	2.42110000
H	-3.25930000	-3.94330000	3.30690000
N	-7.11650000	-1.10900000	3.01710000
H	-7.74970000	-0.68160000	3.70640000
N	-6.35090000	-1.53300000	-1.26840000
H	-7.25180000	-2.04650000	-1.10310000
O	-5.82150000	1.55200000	-0.77350000
H	-6.20200000	2.10890000	-0.05820000
C	-4.60860000	-1.35730000	2.88670000
C	-4.77680000	-2.74300000	2.70010000
C	-3.80930000	-4.65130000	1.42610000
H	-4.76720000	-5.20750000	1.60200000
C	-5.25640000	-3.64280000	-0.41850000
H	-5.82220000	-4.53460000	-0.74380000
H	-5.78170000	-3.27010000	0.49970000
C	-6.05960000	-0.72990000	-0.00520000
H	-7.01980000	-0.37760000	0.44410000
C	-6.06830000	-3.32370000	2.93510000
H	-6.14730000	-4.40910000	2.96030000
C	-7.16780000	-2.55560000	3.12210000
H	-8.15530000	-2.95230000	3.31910000
C	-5.25320000	-2.57210000	-1.51250000
H	-4.26730000	-2.03620000	-1.54700000
H	-5.39460000	-3.02290000	-2.51690000
C	-3.35620000	-0.69400000	2.86730000
H	-2.46150000	-1.29670000	2.74910000

C	-4.40530000	1.43430000	3.21590000
C	-5.78840000	-0.52710000	3.10430000
C	-3.83540000	-4.04280000	-0.00130000
H	-3.41000000	-4.75320000	-0.73030000
H	-3.15710000	-3.15210000	-0.00140000
C	-5.68340000	0.84050000	3.28200000
H	-6.55320000	1.46130000	3.47410000
C	-5.10700000	0.44310000	-0.20800000
H	-4.65060000	0.73430000	0.76560000
H	-4.30010000	0.23390000	-0.94690000
C	-3.25230000	0.68780000	3.03930000
H	-2.27640000	1.16590000	3.04210000
C	-6.52400000	-0.63520000	-2.49370000
H	-5.51380000	-0.39440000	-2.91720000
H	-6.93630000	0.35660000	-2.16250000
C	-2.64610000	-5.64870000	1.55140000
H	-2.62380000	-6.11900000	2.54060000
H	-1.67780000	-5.15140000	1.40950000
H	-2.72140000	-6.45020000	0.81110000
C	-7.42250000	-1.28880000	-3.52490000
H	-7.52730000	-0.62980000	-4.40360000
H	-8.44160000	-1.46690000	-3.15680000
H	-7.02670000	-2.24020000	-3.90310000
C	4.62290000	-0.24630000	3.45830000
H	3.53240000	-0.43490000	3.28610000
O	6.06140000	0.96040000	1.95020000
C	1.54940000	-0.73390000	1.36700000
H	0.79320000	-0.73560000	0.56510000
H	2.08590000	-1.69800000	1.37100000
H	1.09650000	-0.53790000	2.34270000
H	-5.80787841	-1.33810786	0.85102394
H	-5.95373861	-1.75140482	-1.55838099

Co-crystal HQ/ER

O	6.07640000	-0.96530000	-1.07530000
O	4.33100000	-2.18730000	-1.81740000
O	4.35910000	-3.03240000	1.06990000
H	4.08450000	-2.96080000	0.12110000
O	7.11160000	-2.99010000	1.77830000
H	6.43700000	-3.70230000	1.94820000
O	1.99710000	0.22970000	-2.70100000
O	1.03340000	3.46650000	-0.40980000
O	1.80310000	0.16690000	0.89680000
H	1.12090000	-0.41710000	0.46370000
O	0.06290000	6.29090000	-2.03880000
H	0.04980000	7.23980000	-1.80320000
O	-0.95330000	3.22890000	-1.60010000
O	-1.10750000	0.20920000	-4.51950000
O	-2.67300000	-0.93300000	-2.81560000
H	-2.67090000	-0.05760000	-3.31540000
O	0.76670000	-1.41060000	-1.62280000
N	-1.29750000	6.67330000	1.03530000
C	4.89880000	-1.11270000	-1.73670000
C	4.42730000	0.23310000	-2.26230000
H	5.12500000	1.02670000	-1.87910000
C	3.00530000	0.50330000	-1.69570000
H	2.81190000	-0.17080000	-0.81640000
C	2.78830000	1.97070000	-1.26100000
H	3.57410000	2.21430000	-0.49120000
C	1.40060000	2.07950000	-0.57380000
H	0.62320000	1.55410000	-1.18260000
C	1.39230000	1.55130000	0.90720000
C	2.44200000	2.27090000	1.77210000
H	2.12500000	3.32920000	1.87990000
H	3.41340000	2.32120000	1.22760000

C	2.65080000	1.62040000	3.14920000
H	1.71350000	1.08310000	3.44340000
C	3.81650000	0.62480000	3.05810000
C	4.72760000	-1.74030000	3.05100000
H	5.63000000	-1.25650000	3.51660000
C	4.96610000	-1.80540000	1.51680000
H	4.49290000	-0.94400000	0.99640000
C	6.48260000	-1.86690000	1.13750000
C	6.65780000	-2.14310000	-0.39120000
H	6.09240000	-3.05480000	-0.69040000
C	3.05420000	-0.95010000	4.82000000
H	2.69090000	-1.96140000	5.04520000
H	2.22940000	-0.26470000	5.04910000
H	3.87510000	-0.73400000	5.51390000
C	4.49320000	0.21450000	-3.78640000
H	3.97990000	1.09190000	-4.20500000
H	3.99210000	-0.66720000	-4.20670000
H	5.52880000	0.22100000	-4.14530000
C	4.58590000	-3.15240000	3.62210000
H	4.58340000	-3.15620000	4.71520000
H	5.42340000	-3.78640000	3.28910000
H	3.66600000	-3.63490000	3.26460000
C	7.24320000	-0.63230000	1.59220000
H	6.81320000	-0.19670000	2.51220000
H	7.21570000	0.16070000	0.83430000
H	8.29000000	-0.87740000	1.81030000
C	8.11230000	-2.19580000	-0.84570000
H	8.70270000	-2.72490000	-0.06290000
H	8.52410000	-1.16680000	-0.89710000
C	8.27230000	-2.89250000	-2.19200000
H	9.31980000	-2.88850000	-2.51480000
H	7.68430000	-2.39600000	-2.97300000
H	7.94810000	-3.93930000	-2.14970000
C	2.94890000	2.94360000	-2.42470000
H	2.76110000	3.97680000	-2.10230000
H	2.25930000	2.70260000	-3.24390000
H	3.96530000	2.91760000	-2.83340000
C	-0.01050000	1.65860000	1.49470000
H	-0.77570000	1.17050000	0.87000000
H	-0.31700000	2.71940000	1.57390000
H	-0.06280000	1.21220000	2.49540000
C	2.98590000	2.65790000	4.22230000
H	3.12790000	2.19110000	5.20390000
H	2.18660000	3.39990000	4.32410000
H	3.91390000	3.19500000	3.98000000
C	0.17340000	4.05170000	-1.41180000
H	0.66250000	4.03680000	-2.41160000
C	-0.01920000	5.47920000	-0.85020000
H	0.85250000	5.72270000	-0.19380000
C	-1.36630000	5.73370000	-0.12300000
H	-2.07090000	6.20110000	-0.86820000
C	-1.95900000	4.38990000	0.33050000
H	-2.89980000	4.55140000	0.89870000
H	-1.27110000	3.87000000	1.03970000
C	-2.20560000	3.51500000	-0.89430000
H	-2.81650000	4.04600000	-1.66190000
C	-2.79010000	2.15330000	-0.56940000
H	-3.06380000	1.60760000	-1.48030000
H	-3.69510000	2.24780000	0.05010000
H	-2.07650000	1.52720000	-0.00710000
C	-0.95780000	8.05970000	0.59850000
H	-1.67860000	8.39100000	-0.16620000
H	0.06300000	8.19310000	0.21310000
H	-1.08450000	8.73730000	1.46120000
C	-0.37510000	6.22500000	2.11730000
H	-0.74250000	5.26940000	2.52860000
H	-0.40430000	6.95540000	2.94220000

H	0.67290000	6.08880000	1.80960000
C	1.56310000	-1.14150000	-2.76570000
H	2.41910000	-1.84780000	-2.61530000
C	0.86920000	-1.27590000	-4.12020000
H	1.14560000	-2.26390000	-4.54530000
H	1.31420000	-0.52840000	-4.82000000
C	-0.65350000	-1.11720000	-4.14980000
C	-1.33610000	-1.45400000	-2.78950000
H	-1.46880000	-2.55010000	-2.66560000
C	-0.57420000	-0.85560000	-1.58840000
H	-0.49160000	0.26230000	-1.67330000
C	-1.27540000	-1.95450000	-5.27440000
H	-0.89460000	-1.63180000	-6.25290000
H	-2.36410000	-1.81200000	-5.30350000
H	-1.06980000	-3.02180000	-5.15910000
C	-0.43480000	1.35770000	-3.96440000
H	-0.91450000	2.18910000	-4.49360000
H	0.64190000	1.32300000	-4.16670000
H	-0.61690000	1.42940000	-2.87910000
C	-1.09790000	-1.29170000	-0.23640000
H	-0.36070000	-1.08440000	0.56040000
H	-1.29460000	-2.38030000	-0.16680000
H	-2.03680000	-0.78970000	0.03760000
Cl	-4.99530000	2.97510000	2.44850000
N	-2.79910000	-3.47040000	2.37850000
H	-2.36890000	-3.54600000	3.31050000
N	-6.79060000	-1.83810000	2.54970000
H	-7.55880000	-1.47680000	3.13020000
N	-5.53210000	-2.70330000	-1.66240000
H	-6.30090000	-3.41050000	-1.56230000
O	-5.67050000	0.45310000	-1.52550000
H	-6.25190000	1.01980000	-0.97190000
C	-4.28850000	-1.52770000	2.55160000
C	-4.13890000	-2.92790000	2.53740000
C	-2.72390000	-4.79830000	1.68220000
H	-3.58530000	-5.46850000	1.94320000
C	-4.15100000	-4.38550000	-0.39530000
H	-4.58550000	-5.37020000	-0.64250000
H	-4.78130000	-3.97010000	0.43640000
C	-5.65830000	-1.73370000	-0.49070000
H	-6.73430000	-1.53360000	-0.28080000
C	-5.28230000	-3.74860000	2.81920000
H	-5.12150000	-4.81100000	2.99690000
C	-6.53270000	-3.23020000	2.86560000
H	-7.41850000	-3.80890000	3.09300000
C	-4.19370000	-3.44560000	-1.60210000
H	-3.37350000	-2.68100000	-1.54090000
H	-4.03730000	-3.99860000	-2.55120000
C	-3.21230000	-0.60620000	2.51030000
H	-2.20040000	-0.99680000	2.51650000
C	-4.72270000	1.25850000	2.53150000
C	-5.63370000	-0.96330000	2.61330000
C	-2.72680000	-4.55720000	0.14810000
H	-2.21920000	-5.38890000	-0.36970000
H	-2.11180000	-3.64510000	-0.05200000
C	-5.84300000	0.40350000	2.61800000
H	-6.83830000	0.83130000	2.68950000
C	-4.90010000	-0.42650000	-0.69270000
H	-4.68920000	0.05360000	0.28930000
H	-3.94050000	-0.55570000	-1.24280000
C	-3.42640000	0.77450000	2.51340000
H	-2.58240000	1.45950000	2.50900000
C	-5.69630000	-1.99680000	-3.00850000
H	-4.70620000	-1.56960000	-3.32240000
H	-6.35640000	-1.09860000	-2.87100000
C	-1.42340000	-5.50640000	2.09430000
H	-1.40790000	-5.72590000	3.16780000

H	-0.54300000	-4.88700000	1.87910000
H	-1.29730000	-6.45660000	1.56720000
C	-6.25610000	-2.94130000	-4.05340000
H	-6.35420000	-2.41730000	-5.01950000
H	-7.26010000	-3.31070000	-3.80650000
H	-5.61140000	-3.80940000	-4.24180000
C	3.50200000	-0.84170000	3.36130000
H	2.65220000	-1.14850000	2.69040000
O	4.93080000	0.99730000	2.75360000
H	-5.49866404	-2.18169715	0.47894680
H	-5.04528065	-2.83713715	-1.86852703

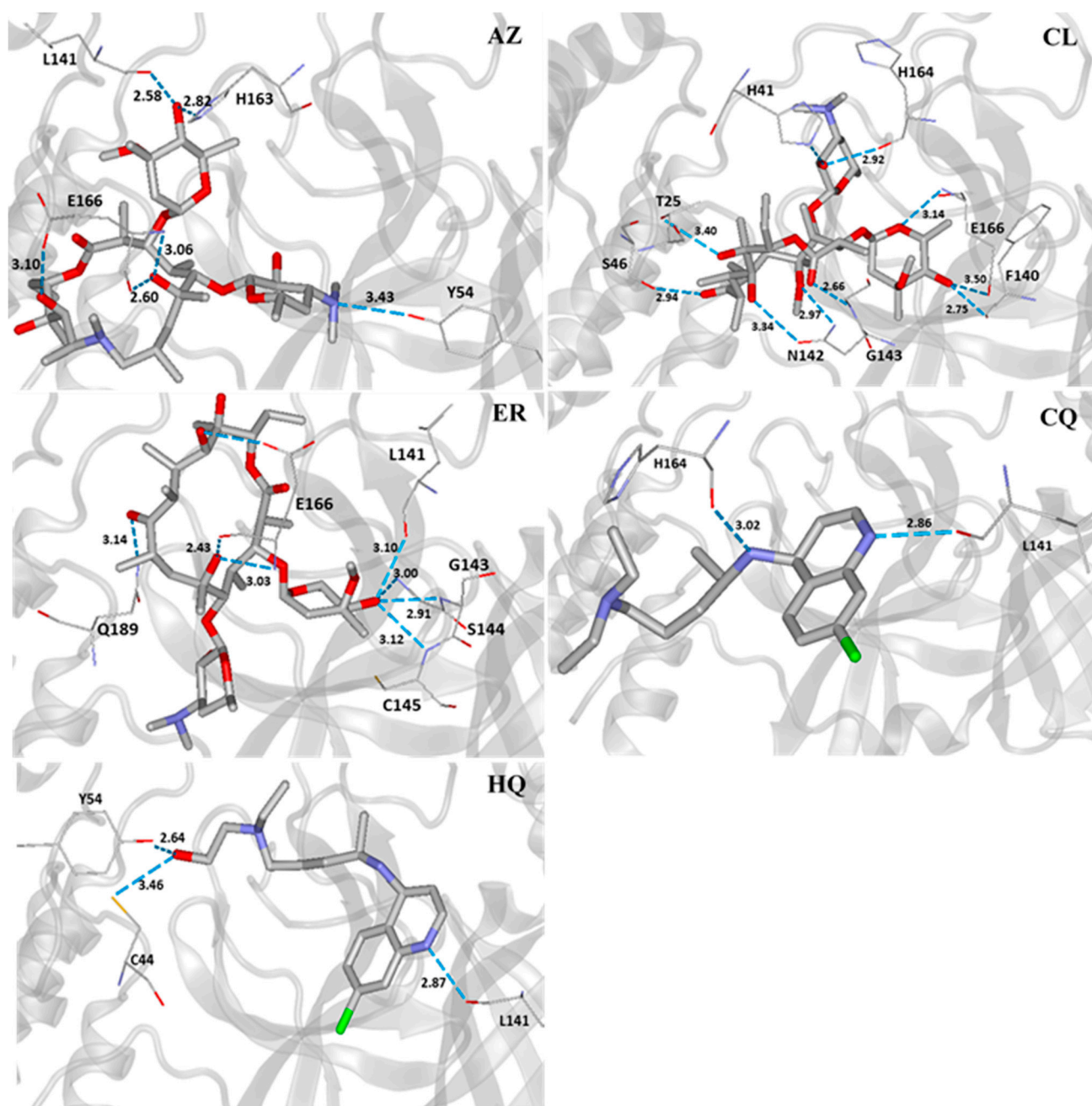


Figure S1. Intermolecular interactions of single-crystals in the viral M^{pro} active site.