

## *qFit-ligand* Reveals Widespread Conformational Heterogeneity of Drug-Like Molecules in X-Ray Electron Density Maps

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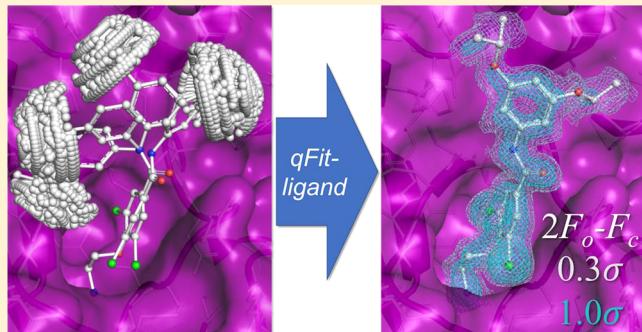
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### Supporting Information

**ABSTRACT:** Proteins and ligands sample a conformational ensemble that governs molecular recognition, activity, and dissociation. In structure-based drug design, access to this conformational ensemble is critical to understand the balance between entropy and enthalpy in lead optimization. However, ligand conformational heterogeneity is currently severely underreported in crystal structures in the Protein Data Bank, owing in part to a lack of automated and unbiased procedures to model an ensemble of protein–ligand states into X-ray data. Here, we designed a computational method, *qFit-ligand*, to automatically resolve conformationally averaged ligand heterogeneity in crystal structures, and applied it to a large set of protein receptor–ligand complexes. In an analysis of the cancer related BRD4 domain, we found that up to 29% of protein crystal structures bound with drug-like molecules present evidence of unmodeled, averaged, relatively isoenergetic conformations in ligand–receptor interactions. In many retrospective cases, these alternate conformations were adventitiously exploited to guide compound design, resulting in improved potency or selectivity. Combining *qFit-ligand* with high-throughput screening or multitemperature crystallography could therefore augment the structure-based drug design toolbox.



### INTRODUCTION

Ligands and their protein receptors sample an ensemble of conformations in solution. The energetic contribution of conformational entropy plays a critical role in receptor–ligand molecular recognition,<sup>1,2</sup> but the ensemble of conformations that determines the free energy of binding, activity, and dissociation often remains poorly characterized. The majority of three-dimensional protein structures are single, static models obtained from X-ray crystallography by averaging over the unique conformations in the unit cells. Crystallographic atomic displacement parameters (ADP) quantify harmonic displacements from average atomic positions but are adversely affected when unmodeled discrete alternate conformations overlap. By their nature, such static, harmonic models cannot rationalize molecular attributes that rely on dynamic, anharmonic displacements of atoms.<sup>3,4</sup> Revealing discrete conformations<sup>5–7</sup> that are more fully representative of the receptor–ligand conformational ensemble from X-ray electron density maps would overcome this limitation and create new opportunities to address open questions in chemical and structural biology.

For example, such models might help to provide a structural basis for on-pathway conformational intermediates in substrate binding or release detected by NMR.<sup>8,9</sup>

Additionally, an incomplete picture of receptor–ligand structural dynamics impedes structure-based drug design. While overall binding affinities measured in solution report on a receptor–ligand ensemble, the structure–activity relationships are often informed by static models for further optimization, with some exceptions that incorporate flexibility.<sup>10</sup> During small-molecule optimization, even minor chemical changes can lead to apparently altered binding modes that are unforeseen due to the limitations of conventional X-ray structural models, frustrating design<sup>11,12</sup> (Figure 1A). One hypothesis to explain how subtle modifications cause a switch to a second binding pose is that the unmodified ligand samples the second pose at low, but potentially detectable, occupancy (Figure 1B). Examples where

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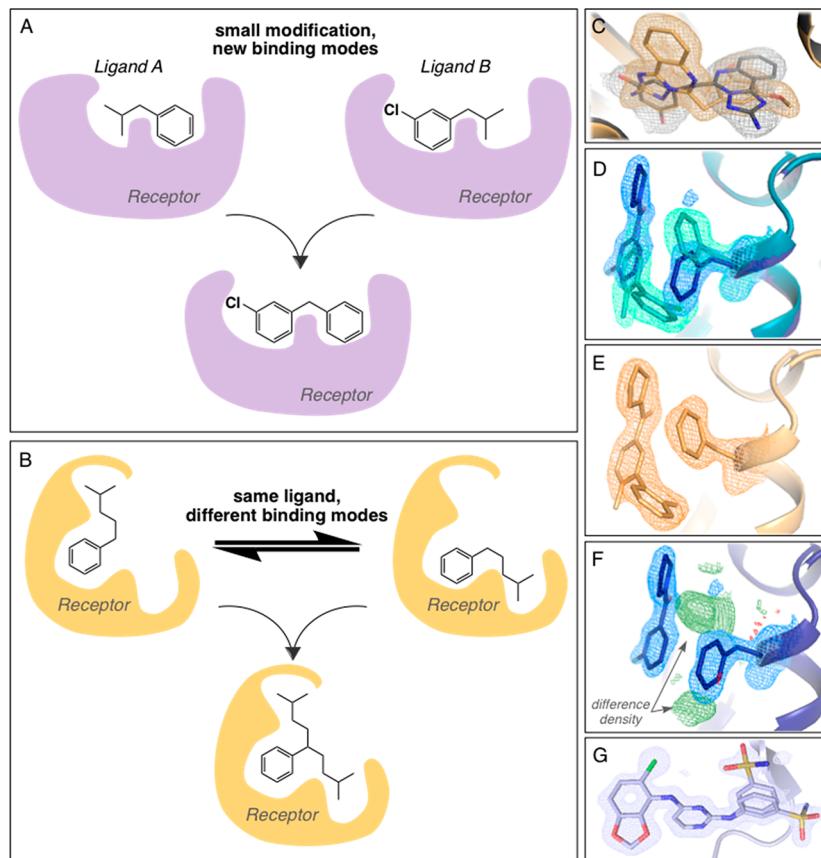


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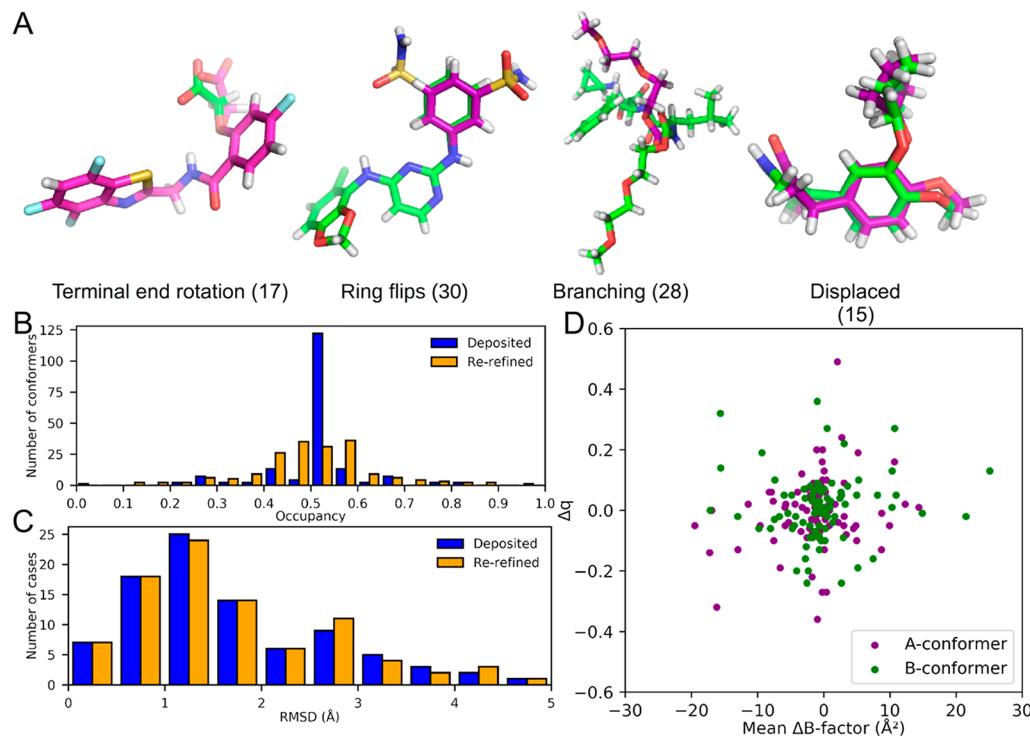


**Figure 1.** Ligand structural dynamics and minor changes during fragment optimization lead to new binding modes and drive drug design. (A) Subtle changes in chemical structure of ligands can impose new binding modes. (B) Near isoenergetic receptor–ligand conformations exchange in dynamic equilibrium in crystal structures. These conformations can inform the design of a ligand with higher affinity. (C) Hsp90 inhibitors in gray (PDB 4CWO) and gold (PDB 4CWN). (D) Subtle changes in chemical structures lead to changes in binding pose for Lp-PLA2, changing the course of design (PDBs 5JAL, 5JAO). (E) New Lp-PLA2 inhibitor designed as a result of observed alternate binding poses of fragments (PDB 5JAP). (F) Evidence of difference density in X-ray crystal structure of Lp-PLA2 fragment shows alternate binding poses pre-exist at low occupancy (PDB 5JAL). (G) Alternate conformations exploited in the design of EphB4-binding ligands (PDB 2VWX). Electron densities are shown at  $1.5\sigma$ . Positive (green) and negative (red) difference densities in part F are shown at  $+3.0\sigma$  and  $-3.0\sigma$ , respectively.

subtle changes in chemical structure of the ligand led to different binding modes are abundant. Fragment optimization of CDK8 inhibitors revealed that small modifications led to a new binding mode, which was exploited to develop potent and selective inhibitors.<sup>13</sup> Dramatically different binding modes as a result of minor changes in the chemical structure of the ligand are also illustrated by Hsp90 and PTR1 inhibitors. In the course of structure-based optimization of Hsp90 inhibitors, Casale and co-workers observed a flipped binding mode of the ligand in the crystal structure, leading them to change the direction of design toward a low nanomolar compound (Figure 1C).<sup>14</sup> In PTR1, compounds that presumably could not be accommodated by the binding site ultimately led to a boost in affinity, owing to altered binding modes.<sup>14,15</sup> In human lipoprotein-associated phospholipase A2, two related ligands (Figure 1D) that explored distinct subpockets were merged into a more potent ligand (Figure 1E).<sup>16</sup> These selected examples highlight both the perils of design based solely on an initial ligand pose but also how the fortuitous discovery of alternate poses can create new opportunities for design. It is possible that some of these “new” binding poses pre-exist as alternative conformations at slightly higher energies than the conformation modeled into the conventional X-ray structure. Many of those are infrequently sampled due to high energy

differences and fall below the detection level in the maps. However, some of these conformations may be evident in electron density maps but at levels that are frequently ignored in modeling.

Indeed, in the phospholipase example above, the presence of difference electron density suggested that multiple conformations might have been sampled in at least one of the smaller ligands (Figure 1F). This view posits that degeneracies in ligand binding modes can also be accessed by small modifications of the ligand chemical structure that shift the receptor–ligand equilibrium ensemble. This hypothesis is supported by additional anecdotal examples, such as long time-scale molecular dynamics (MD) simulations of trypsin, in which both the ligand and receptor adopt many stable configurations.<sup>17</sup> Experimentally, multiple conformations can be present in X-ray electron density, as in HDAC6, where many related ligands were modeled in multiple conformations in concert with distinct conformations of the receptor.<sup>18</sup> In other cases where the alternate conformations have been experimentally revealed, they have been exploited to improve affinity. For example, X-ray crystallography revealed alternate conformations for singly substituted EphB4 ligands that inspired the creation of bis-substituted ligands with increased potency (Figure 1G).<sup>19</sup> NMR measurements of conforma-



**Figure 2.** Benchmark statistics. (A) Categories of alternate conformations present in the benchmark. (B) Conformer occupancies pre- (blue) and post- (orange) rerefinement. (C) Ligand A to B conformer RMSD, pre (blue) and post (orange) rerefinement. (D) Occupancy shift versus mean B-factor difference after rerefinement.

tional heterogeneity for ligands generated against the antibacterial target LpxC uncovered a larger cryptic envelope that was filled by larger, more potent ligands.<sup>20</sup> Collectively, these examples suggest that multiple ligand poses are likely energetically accessible for many proteins. Fully realizing the potential of this phenomenon in structure-based design, exemplified by EphB4 and LpxC inhibitors, requires reliable characterization of pre-existing conformational heterogeneity (Figure 1B) of ligand–receptor complexes.

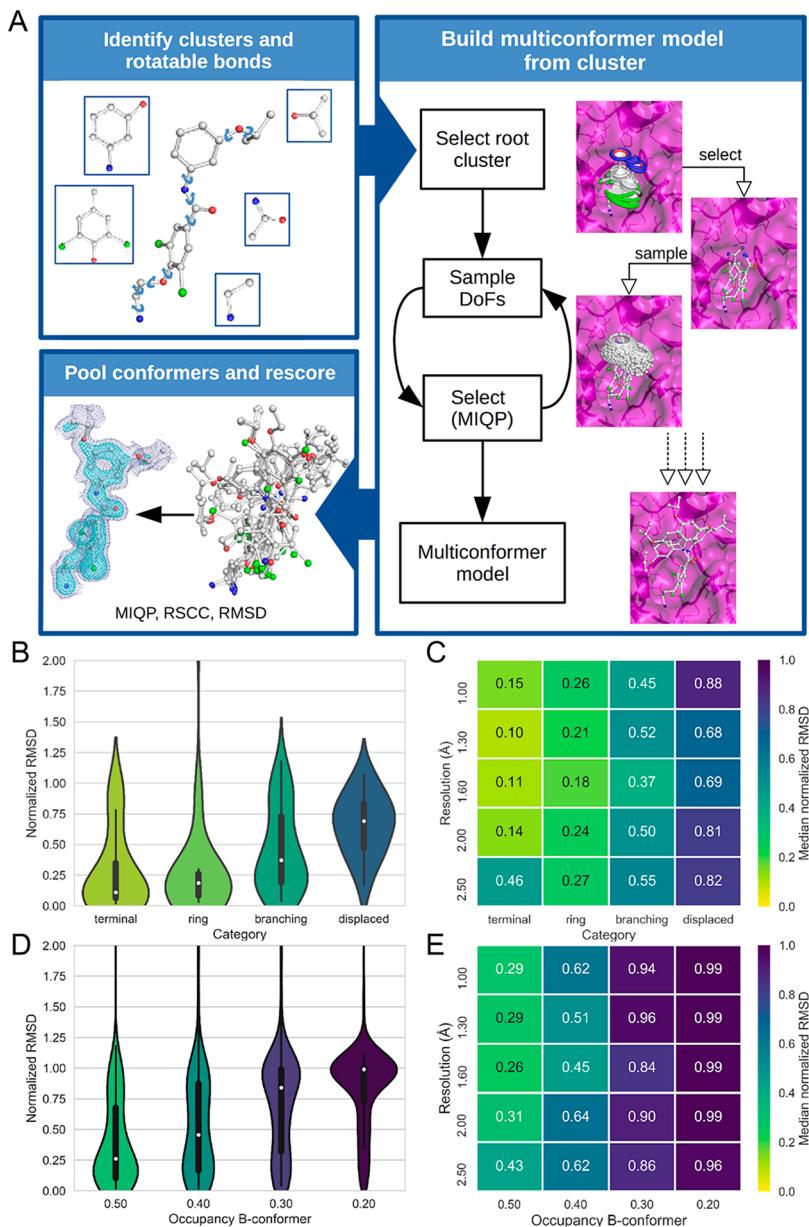
While protein conformational heterogeneity has been automatically and systematically characterized in X-ray crystallography data,<sup>7,21–24</sup> ligand conformational heterogeneity is less explored. Various software algorithms can identify and build ligands into electron density maps without human intervention;<sup>25–30</sup> however, these approaches typically provide several top scoring ligand conformations at unit occupancy. While in principle the user can select multiple candidate conformations for the final model, none of these approaches consider an ensemble of alternate conformations from the outset. Moreover, they may build unrealistic conformations that incorrectly fit into the ensemble-averaged electron density.<sup>31</sup> Despite the importance of low occupancy alternative conformations in biochemical function and ligand design, statistical measures for monitoring the fit of ensemble models to data are less developed than for single conformer models.

Here, we present a new, automated approach based on *qFit*,<sup>22,23</sup> called *qFit-ligand*, to create parsimonious multiconformer ligand models in crystallographic electron densities. We first surveyed the PDB to investigate ligand heterogeneity in current crystal structures and selected a diverse, curated benchmark set of pharmaceutically relevant protein targets with alternate ligand conformations across a wide range of resolution and occupancy (Supporting Information, Table S1).

We found that *qFit-ligand* can detect alternate conformations at occupancies down to 20%, even at relatively modest resolutions of 2.0 Å. We then applied our method prospectively to all cases of the *Drug Design Data Resource* (D3R, [drugdesigndata.org](http://drugdesigndata.org)), a subset of the *Twilight Database*,<sup>32</sup> and all PDB entries for the bromodomain-containing protein 4 (BRD4), revealing unmodeled alternate conformations in 29% of the cases for the latter. To evaluate the quality of our multiconformer ligands, we calculated *R*-factors and ligand energies relative to a single conformer ligand model. Our results indicate that *qFit-ligand* is a powerful, efficient, and user-friendly tool to model and discover alternate ligand conformations.

## RESULTS

**Creating a Benchmark Set of True Positive Ligand Alternative Conformations from the PDB.** To estimate the prevalence of multiconformer ligands in crystal structures, we surveyed all 130054 PDB entries as of June 2017 that contained noncovalently bound ligands with more than 15 non-hydrogen atoms in their X-ray crystal structure. This resulted in 44620 PDB entries totaling 133724 ligands. Of those, 2611 ligands, or less than 2% (1078 unique ligand codes), distributed over 1845 PDB entries, consisted of two or more alternate conformations (Supporting Information, Materials and Methods, Figure S1). Many of these molecules are common crystallographic additives (PEG, cholesterol, etc.) or metabolites (ATP, NADPH, etc.). We therefore manually curated a true positive benchmark set of receptors of pharmaceutical interest containing multiconformer, drug-like molecules. Cases where ligands adopted entirely different binding modes, such as flipped ligands, were discarded. This resulted in 90 crystal structures that could be stably refined

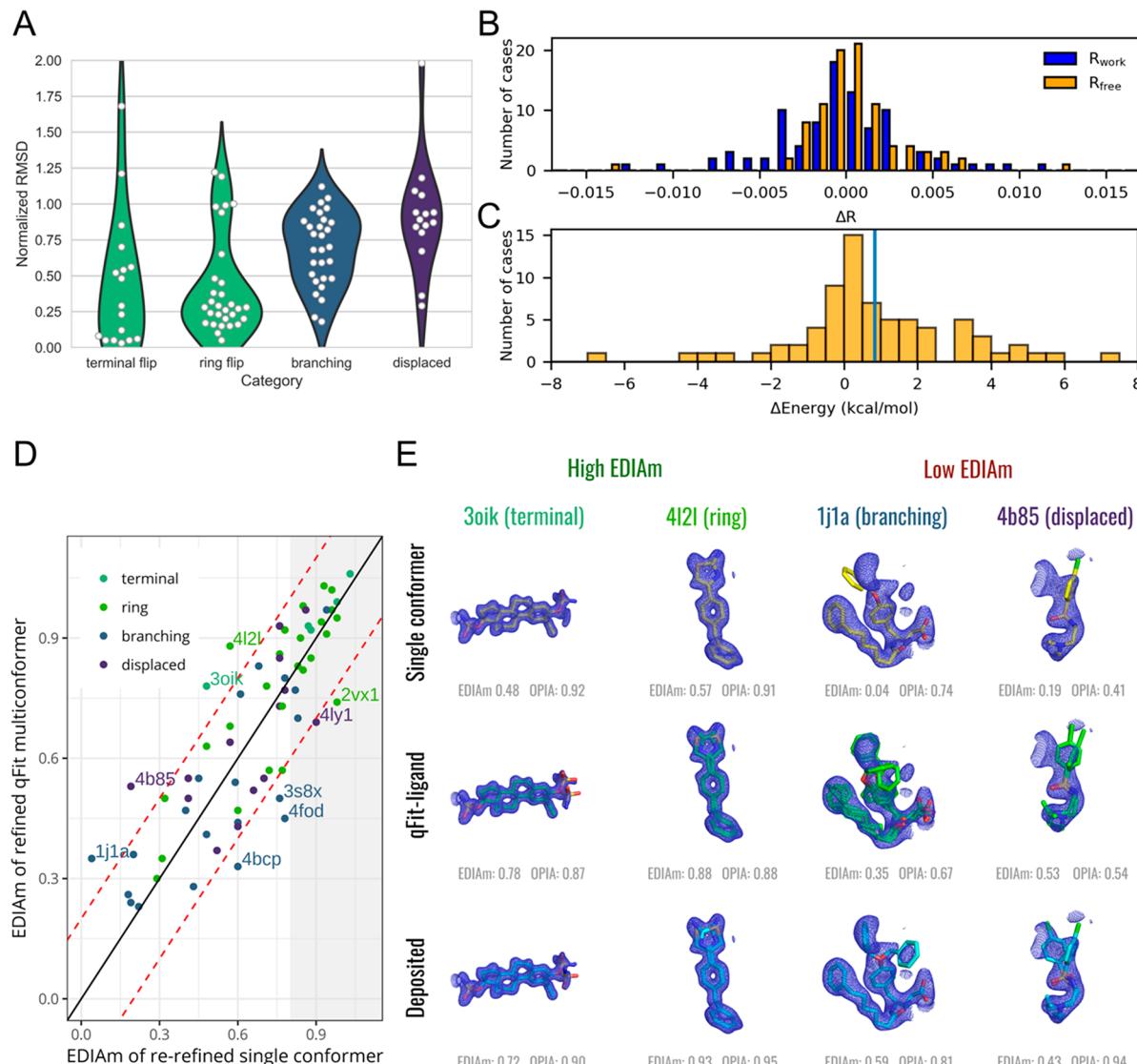


**Figure 3.** *qFit-ligand* workflow and statistics on synthetic data. (A) Rigid clusters are defined as rings or terminal ends, and rotatable bonds as any bond that is not part of a ring. The local search finds possible positions and orientations of each cluster in the binding site, avoiding steric clashes with the protein. As clusters are joined, torsions and degrees of freedom are sampled. Up to five ligand conformations that best match the ligand density are selected and combined with the protein model to give a final ligand multiconformer model. (B) Violin plot of categories at 1.60 Å resolution and occupancy 0.50 across 90 test cases. The white dot represents the median, the bold center line represent the interquartile range (IQR), and the thin center line represents the percentile range 25th – 1.5 IQR to 75th + 1.5 IQR. Lower nRMSD is better. (C) Heatmap of category vs resolution at 0.50 occupancy. Lower nRMSD is better. (D) Violin plot for representative resolution 1.60 Å and 0.50/0.50 occupancy at optimal parameters. (E) Heatmap of normalized RMSD at optimal parameters (resolution vs occupancy).

against the deposited structure factors and CIF restraints files (Supporting Information, Table S1).

We apportioned the conformational heterogeneity of ligands in our benchmark set into four categories (Figure 2A): terminal end flips, where only terminal atoms are flipped/rotated, ring flips where a ring system is flipped, usually by 180°, branching ligands, where a side chain or branch of a ligand has an alternate conformation, and displaced ligands, where all atoms are at least slightly displaced in combination with differences in their internal degrees of freedom. The benchmark set heavily overrepresented 50/50 occupancy splits (Figure 2B), reflecting a historical tendency against refining (Figure 2B), reflecting a historical tendency against refining

occupancies in favor of refining ADPs only. Inaccurate 50/50 occupancy splits do not inform on which conformation represents the dominant binding mode, which is often critical information for design decisions in lead optimization. Rerefinement with PHENIX<sup>33</sup> substantially broadened the distribution (Figure 2B). Unlike the occupancies, the RMSD between alternate conformations was similar after rerefinement (Figure 2C). Interestingly, we observed no correlation between occupancy shift and difference in mean *B*-factor (Figure 2D). This result is in contrast to earlier reports,<sup>34,35</sup> likely owing to improvements in refinement software.



**Figure 4.** Electron density support measures and energetics of *qFit-ligand* multiconformers are similar to those of single-conformer models for the benchmark set while reporting on conformational heterogeneity. (A) nRMSD distributions by category of conformational heterogeneity. The nRMSD of terminal end flips was determined from only atoms affected by the dihedral changes. Lower nRMSD is better. (B) Histogram of  $R_{\text{work}}$  and  $R_{\text{free}}$  differences between refined *qFit-ligand* models and single conformer structures. Negative values indicate a lower  $R$  for refined *qFit-ligand* models. (C) The distribution of occupancy-weighted, ligand internal energies of *qFit-ligand* multiconformer ligands relative to single “A” conformation. Negative values indicate that the multiconformer ensemble has lower internal energy than the single benchmark “A” conformation. Positive values indicate the multiconformer ensemble has higher internal ligand energies. (D) Ligand EDIAM scores for rerefined single conformer models against automatically refined *qFit-ligand* multiconformer models. Higher EDIAM scores are better, with scores greater than 0.8 indicating that the model is well-supported by the density (shaded area for single conformer models). (E) Examples where the ligand EDIAM was improved by modeling alternate conformations with *qFit-ligand*. The  $2mF_o - DF_c$  maps are shown in blue at a contour level of  $1\sigma$ .

**Developing the *qFit-ligand* Algorithm and Calibration against Synthetic Data.** We designed the *qFit-ligand* algorithm to iteratively explore a vast conformational space to determine a parsimonious ensemble of up to five occupancy-weighted conformations that, collectively, optimally fit the electron density (Figure 3A and Supporting Information, Materials and Methods, Figure S2). Briefly, *qFit-ligand* takes as input a refined, single conformation receptor–ligand structure in PDB format, and a  $2mF_o - DF_c$  density map. It first determines rotatable bonds and rigid groups of atoms within the ligand (Supporting Information, Materials and Methods, Figure S2). Starting from each rigid group, *qFit-ligand* performs a local, six-dimensional translational and rotational search in the rigid group’s neighborhood, selecting up to five occupancy-

weighted candidate positions that, collectively, minimize the real-space density residual of the rigid group. In subsequent steps, *qFit-ligand* iteratively grows the rigid group by exhaustively sampling increments of several torsion angles simultaneously while avoiding collisions with the receptor. At each step, it selects up to five occupancy-weighted conformations by again minimizing the density residual. This is repeated until all torsion angles are determined and the full ligand is built up. The maximum number of conformations generated by *qFit-ligand* at this stage is five times the number of rigid groups. The final occupancy-weighted, multiconformer ensemble is selected from this pool by combining cross-correlation, geometric, and density residual measures. The

ligand multiconformer ensemble is then combined with the receptor and refined with *phenix.refine*.

We calibrated *qFit-ligand* on synthetic data calculated from the benchmark set at varying resolutions and occupancies (Supporting Information, Materials and Methods, Figure S3). To create starting models we deleted the alternate “B” conformation of the ligand, set the occupancy of the “A” conformation to 1.0, and rerefined against the deposited structure factors to reposition the “A” conformation as the only modeled conformation.

We first determined optimal sampling parameters for *qFit-ligand*, balancing accuracy of the results and computational demands, measured by the minimum normalized RMSD (nRMSD, Supporting Information, Materials and Methods, Figure S3) between *qFit-ligand* generated conformations and the benchmark B conformation. RMSDs between the A and B conformers range from 0.22 to 4.86 Å across the benchmark set. nRMSD controls for this large variation by normalizing the RMSD between *qFit-ligand* generated conformations and the B conformer by the RMSD between A and B. nRMSD values range from 0 to 1, with values closer to 0 indicating better performance. To compare performance, we report the median nRMSD of the benchmark set for different resolutions and occupancies. Our analysis suggested that sampling two torsion angles simultaneously at 6° intervals gave the best result across resolutions and occupancies while limiting computational costs (Supporting Information, Figure S4).

Benchmarking *qFit-ligand* showed performance differences across category, resolution, and true occupancy. We evaluated the performance of *qFit-ligand* for each category of conformational heterogeneity (Figure 3B,C). At a resolution of 1.60 Å and equal occupancies for the A and B conformer, the median nRMSD is 0.11 for terminal end flips, 0.18 for ring flips, 0.37 for branched ligands, and 0.69 for displaced ligands (Figure 3B). Unsurprisingly, *qFit-ligand* performance decreased with increasing complexity of conformational heterogeneity.

The resolution dependence is more complex, however, with better performance of *qFit-ligand* at an intermediate resolution of 1.60 Å (Figure 3C,E). We attribute this to more sharply defined density peaks at high resolutions relative to intermediate resolutions. Undersampling of conformations during ligand building can result in failure to accurately hit the density peaks at high resolution, thereby leading to suboptimal scores of electron density-based measures.

The performance of *qFit-ligand* is sensitive to the occupancy of the alternate conformation, indicated by an increasing median nRMSD for lower occupancies of the B conformation (Figure 3D,E). At occupancies of 0.2 and below, the alternate conformer was rarely detected at any resolution. While *qFit-ligand* samples conformations close to the alternate conformer, evidenced by favorable (low) nRMDS before final rescoring (Supporting Information, Figure S4), selecting them at low occupancies would increase the false positive rate (data not shown).

Finally, note that the *qFit-ligand* multiconformer ensemble *collectively* explains the density best. In virtually all cases, density profile contributions from all ligand conformers are required to match the experimental profile. Overlapping ensemble members evaluated in isolation generally return suboptimal density fitting statistics.

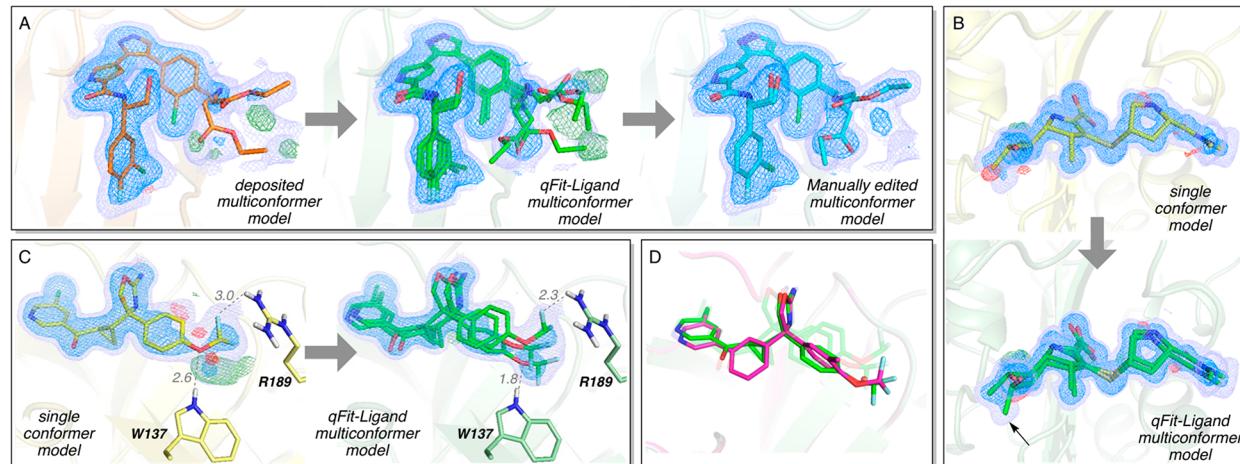
***qFit-ligand* Reidentifies Low Energy Alternative Conformations in Experimental Data.** Next, we applied our method to the experimental benchmark data set for cases

with resolution better than 2.20 Å (73 cases), with only the “A” conformation retained in the rerefined starting model (Figure 4). *qFit-ligand* performance with real data followed the trend we observed with simulated data: localized conformational disorder like terminal end flips and ring flips were determined with higher accuracy than branched or displaced disorder. In the case of terminal ends, only one or two atoms report on the distance between alternate conformations, but the nRMSD is dominated by small coordinate shifts distributed over the entire ligand. Despite a median nRMSD of 0.56 for terminal ends, the median nRMSD for only the “reporting” atoms is less than 0.30 (Figure 4A; all RMSDs reported in Supporting Information, Figure S5). Consequently, 13 out of 17 terminal end flip *qFit-ligand* results were sufficiently accurate to recognize the benchmark alternate conformer. Similarly, *qFit-ligand* determined ring rotations to within a median nRMSD of 0.27. However, the median nRMSD for branched cases is 0.78 and for displaced cases is 0.87. If we conservatively designate a *qFit-ligand* result with more than one conformation and nRMSD > 0.6 as a false positive (Supporting Information, Figure S6), the false positive rates for each category are 29% (terminal flip), 14% (ring flip), 67% (branching), and 85% (displaced) (see Discussion section regarding false positives).

The distribution of  $R_{\text{free}}$  values of fully automated refined *qFit-ligand* models were nearly identical to that of the single conformer ligand models (*qFit-ligand*  $\bar{x} = 0.2043$ , single conformer  $\bar{x} = 0.2048$ ,  $p$ -value = 0.46, two-sided  $t$  test) and statistically indistinguishable from the deposited, manually curated multiconformers ( $\bar{x} = 0.2038$ ,  $p$ -value = 0.51) (Figure 4B, Supporting Information, Figure S7, Table S2). The *qFit-ligand* multiconformer models improved (worsen)  $R_{\text{free}}$  in 53% (47%) of cases compared to single conformer ligand models.

The  $R_{\text{free}}$  value alone is generally not sufficiently sensitive to detect if a multiconformer model is, collectively, supported by the electron density. Therefore, as an independent validation in addition to the RSCC in the *qFit-ligand* algorithm, we calculated the electron density support for individual atoms (EDIAM) score.<sup>36</sup> The EDIAM score quantifies how well a group of atoms is supported by the electron density (Materials and Methods). EDIAM scores indicated that the *qFit-ligand* models improve agreement with the electron density in 63% of cases compared to a single conformer model (Figure 4D) and overall were within 0.2 of those of single conformer models. In cases where deposited models were well-supported by the electron density (EDIAM > ~0.8), *qFit-ligand* models generally increased EDIAM compared to single conformer models, in some cases even improving the deposited model (Figure 4D,E, 3oik). Unsurprisingly, EDIAM scores correlated with the categories of conformational disorder; branched or displaced ligands had lower EDIAM scores. Nonetheless, even in those challenging cases, automated *qFit-ligand* multiconformers EDIAM scores are on par with those of single-conformer models while alerting to the presence of conformational heterogeneity (Figure 4E, right-hand panels; Supporting Information, Figure S15). We emphasize that  $R_{\text{free}}$  and EDIAM values from fully automated modeling generally improve with manual refinement.

To further evaluate the quality of *qFit-ligand* multiconformer models, we examined internal ligand energies, ignoring interactions with the receptor. Although *qFit-ligand* does not observe restraints in modeling, the quality of *qFit-ligand* multiconformer models as measured by their internal energy was excellent. We found a median conformationally averaged



**Figure 5.** Prospective discovery of additional conformations and recovered conformations from the D3R and *Twilight* data set. (A) The deposited multiconformer model, *qFit-ligand* multiconformer model, and manually edited multiconformer model of ERK2 (PDB 4FV3; new PDB 6DMG). (B) Single conformer and *qFit-ligand* multiconformer models of *Serratia fonticola* carbapenemase E166A mutant with the acylenzyme intermediate of meropenem (PDB 4EV4; new PDB 6DMH). (C) Prospective application of *qFit-ligand* to inhibitor ST5 of BACE-1 (PDB 5EZZ; new PDB 6DMI). Single conformer and *qFit-ligand* multiconformer models shown. (D) Overlay of multiconformer model of inhibitor ST5 (green) with inhibitor ST6 (magenta) (PDB 5EZZ). Electron densities are shown at  $1.5\sigma$  (blue) and  $0.3\sigma$  (purple). Positive (green) and negative (red) difference densities are shown at  $+3.0\sigma$  and  $-3.0\sigma$ , respectively. All structures shown have been refined using Phenix.

excess energy of only 0.35 kcal/mol (Supporting Information, Figure S16, Table S2), i.e., *qFit-ligand* multiconformer models were, on average, nearly indistinguishable from that of the rerefined single “A” conformation in our benchmark set. Interestingly, automatically building a *qFit-ligand* multiconformer model in some cases substantially reduced the ligand energy compared to the single “A” conformation. For example, for acyliminobenzimidazole inhibitor 36 in complex with human anaplastic lymphoma kinase,<sup>37</sup> a series of concerted dihedral angle changes resulted in conformations that better fit the density and reduced the energy by nearly 7 kcal/mol (Supporting Information, Figure S8). This suggests that a ligand can accumulate strain energy when it is forced into an averaged conformation to fit the density. On the other hand, the distribution of ligand excess energies suggests that ligands also access higher energy conformations, within a few kcal/mol from the single conformation (Figure 4D). Indeed, ligands generally may not bind in the lowest energy conformation or even adopt a local minimum.<sup>38</sup> Favorable noncovalent interactions with the receptor, buried hydrophobic surfaces, or desolvation of ordered waters in the binding pocket can overcome penalties of strained conformations.<sup>39,40</sup> Thus, alternate conformations, even at elevated ligand energies, may reduce the free energy of the receptor–ligand complex.

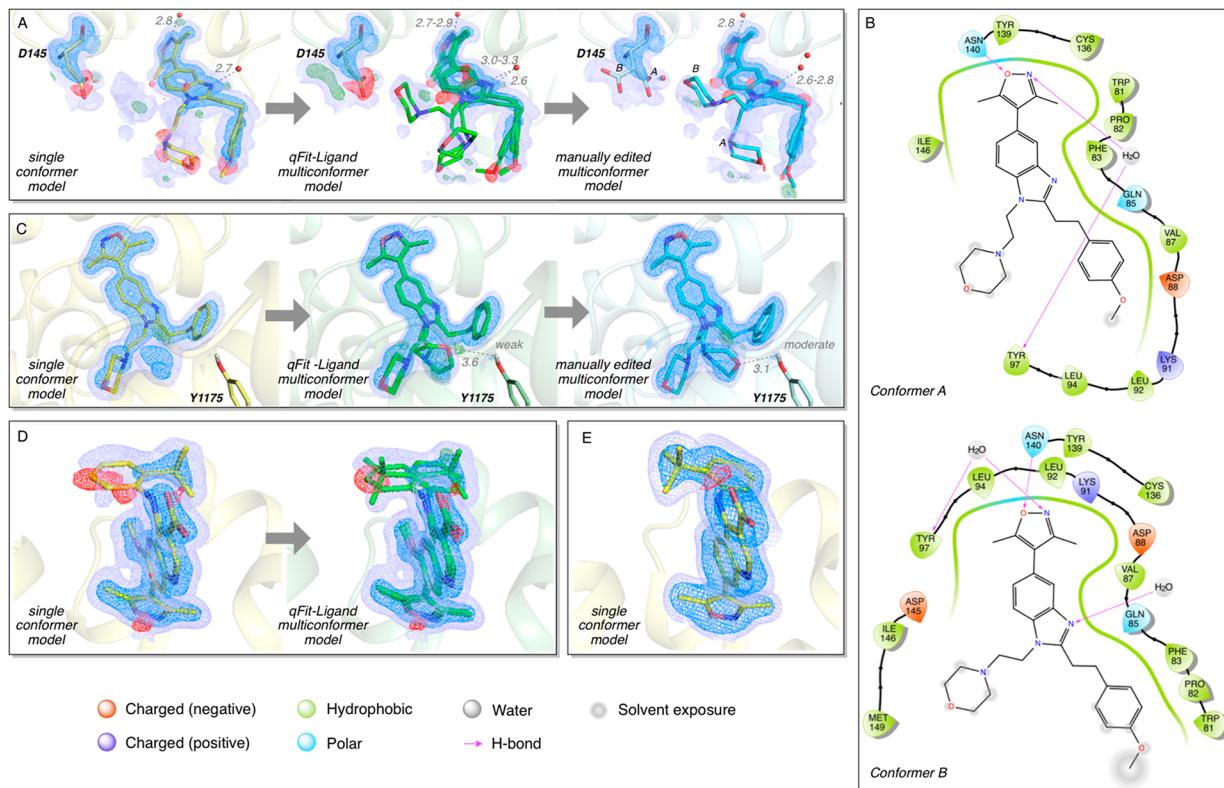
***qFit-ligand* Discovers New Alternate Conformations in the D3R and the *Twilight* Databases.** For prospective discovery, we first applied *qFit-ligand* to the 145 crystal structures in the D3R data set, a high-quality collection of manually curated protein–ligand crystal structures ranging in resolution from 1.26 to 2.75 Å, designed for validation and improvement of methods in computer-aided drug design. Of the 10 crystal structures in the D3R data set with alternate ligand conformations, *qFit-ligand* recovered seven to within a median nRMSD of 0.24. Four of these overlap with our benchmark (PDB 4FV3, Figure 5A, and PDBs 4EK6, 4EK8, 4Y6D). We ranked all *qFit-ligand* multiconformer ligands using the Fisher *z*-transformation, a cross-correlation based metric which measures if alternate conformations are supported by the electron density (Materials and Methods). Three of the top

four ranked ligands already had a modeled alternate conformation, and six out of seven recovered multiconformer ligands ranked within the top 20, indicating that the Fisher-*z* transformation is an effective ranking measure. A new alternate ligand conformation was uncovered by *qFit-ligand* in the crystal structure of the E166A mutant of *Serratia fonticola* carbapenemase (PDB 4EV4; new PDB 6DMH) from the D3R data set (Figure 5B). The terminal propanol functional group of a bound meropenem intermediate adopts a previously undetected conformation. Thus, *qFit-ligand* recovered 70% of ligand alternate conformations and even revealed a new alternate conformation in highly scrutinized experimental data (*qFit-ligand* multiconformer models of prospective cases can be found in Zenodo; DOI: 10.5281/zenodo.1256262).

We also applied *qFit-ligand* to a subset of the *Twilight* data set. The *Twilight* data set represents ligand structures in the PDB poorly supported by the electron density map, potentially indicating conformational disorder in the map, or incorrectly modeled ligands. We applied *qFit-ligand* to ligands in the *Twilight* database with 15–36 non-hydrogen atoms, resolutions better than 2.0 Å, and a correlation coefficient higher than 0.6, resulting in 2379 cases over 1168 PDB entries, which we ranked by Fisher *z*-score to identify “hits” of unmodeled, alternate conformations (Supporting Information, Table S3). We proceeded by manually inspecting the top 10% of cases.

In many cases, the electron density near the ligand was severely disordered, consistent with the intent of the *Twilight* database to flag questionable models of ligands. While *qFit-ligand* suggested alternate conformations, their validity could not unambiguously be confirmed using electron density measures. Nonetheless, in some instances, significantly improved receptor–ligand interactions signified plausible alternate ligand conformations (Supporting Information, Figures S9, S10, S11).

However, for several crystal structures, *qFit-ligand* unambiguously detected alternate ligand binding conformations. For example, in the crystal structure of BACE-1, *qFit-ligand* finds three conformations (occupancies of 0.32/0.36/0.32) of inhibitor ST5 (PDB 5EZZ; new PDB 6DMI) (Figure 5C).



**Figure 6.** Prospective application of *qFit-ligand* to BRD compounds (A) Single conformer crystal structure, *qFit-ligand* multiconformer and manually edited multiconformer models including alternate conformations of Asp145 and compound BDOIA383 bound to BRD4 (PDB 5CFW; new PDB 6DMJ). (B) Protein–ligand interactions of the major, crystal-contact stabilized “A” and minor “B” BDOIA383 conformations of the final *qFit-ligand* model (A). (C) Single conformer crystal structure, *qFit-ligand* multiconformer and manually edited multiconformer models of a isoxazolyl-benzimidazole ligand bound to CBP BRD (PDB 4NRS; new PDB 6DMK). (D) Single conformer and *qFit-ligand* multiconformer models of ligand 9BM bound to BRD4 (PDB 4BW3; new PDB 6DML). Viewing orientation differs from parts A and C to clearly show ligand conformations. (E) Ligand SSB’s single binding conformation in BRD2 (PDB 4AKN). Electron densities are shown at  $1.5\sigma$  (blue) and  $0.3\sigma$  (purple). Positive (green) and negative (red) difference densities are shown at  $\pm 3.0\sigma$ . Distances in Ångstroms.

These conformations show the potential to engineer a ligand that can accommodate strong hydrogen bonding interactions to R189 and W137. In the single conformer model, one of the difluoromethoxy fluorines of the ligand and the amino group of R189 interact weakly through a 3.0 Å hydrogen bond.<sup>41</sup> Our multiconformer model shows that the ligand can adopt a position where strong hydrogen bonding between these groups occur (i.e., shorter contact distances), although at the expense of sacrificing a favorable hydrogen bonding interaction to W137. In addition, one of the *qFit-ligand* conformations turns a nonideal hydrogen bond geometry in the crystal structure between the difluoromethoxy oxygen and amino group of W137 into an ideal geometry. Strikingly, the difluoromethoxy group of BACE-1 inhibitor ST6 (PDB 5EZZ) has a binding conformation that exploits this same hydrogen bonding interaction with W137 sampled by ST5 at low occupancy (Figure 5D).<sup>42</sup> These insights could be used to create a new ligand with branching substituents that can simultaneously form strong hydrogen bonding interactions with R189 and W137 in hopes of increasing binding affinity.

***qFit-ligand* Identifies Widespread Conformational Heterogeneity in BRD4 Ligand.** In another notable example from the *Twilight* data set, *qFit-ligand* identified a minor, unmodeled population of inhibitor compound BDOIA383 bound to bromodomain-containing protein 4 (BRD4), a BET (bromodomain and extra terminal domain) and BRD (Figure 6A, PDB 5CFW; new PDB 6DMJ). BRDs

are small, epigenetic “readers”, which recognize and bind histone acetylated lysine (AcK).<sup>43</sup> BRDs can thereby epigenetically control gene transcription and have recently emerged as important drug targets.<sup>44</sup> The human genome contains 61 BRDs, distributed over 46 diverse proteins.<sup>43</sup> Several potent small-molecule inhibitors for BRD4 have been structurally characterized, but designing modulators selective between BRD4 and CREB binding protein (CBP) has proved challenging.<sup>45–47</sup>

The BRD4-BDOIA383 example highlights how alternate conformations can expose molecular surfaces away from the primary recognition site that could be exploited for selectivity. Inspection of the major population of BDOIA383 bound to BRD4 revealed that it is stabilized by a crystal contact between the BDOIA383 morpholine oxygen and the K91 carbonyl (Figure 6A). By contrast, the minor conformation does not engage in crystal contacts and buries nearly 6% more ligand solvent accessible surface area ( $3115 \text{ \AA}^2$ ) than the major conformation ( $3302 \text{ \AA}^2$ ) (Figure 6B). Additionally, the minor conformation interacts with D145 at the N-terminus of helix δC (Figure 6A,B). Interestingly, compound BDOIA383 in complex with CBP BRD revealed a rotation of the isoxazole-benzimidazole bond by  $180^\circ$ , exposing the phenethyl group to substituted R1173 at the δC N-terminus<sup>46</sup> (PDB ID 5CGP), occupying the space of the *qFit-ligand* minor morpholine conformation in BRD4. Subsequent ligand modifications

strengthened these interactions, leading to increasingly selective CBP modulators.

Flipped binding modes between BRD4 and CBP had been observed earlier with a bound isoxazolyl-benzimidazole ligand, also leading to improved selectivity.<sup>47</sup> Strikingly, in this case too, *qFit-ligand* identified a minor conformation in the CBP complex structurally close to the BRD4 bound conformation (Figure 6C). Because selectivity is often achieved by leveraging unique structural ligand–receptor interactions, identifying alternate ligand conformations may help profile auspicious ligand–receptor secondary molecular recognition sites.

Application of *qFit-ligand* to all 126 BRD2–4 crystal structures in the PDB (deposited in Zenodo; DOI: 10.5281/zenodo.1256262) suggests that differential binding modes and ligand heterogeneity are remarkably ubiquitous (Materials and Methods). Visual inspection and manual curation revealed 12 new binding conformations detected with high confidence (Supporting Information, Figure S12) and an additional 24 with possible alternate conformations (Supporting Information, Table S5, Figure S13). The alternate conformation detected by *qFit-ligand* in the crystal structure of BRD4 with ligand 9BM<sup>48</sup> (phenyl ring flip) is the same conformation observed in the crystal structure of BRD2 with ligand S5B,<sup>49</sup> further supporting the idea that ligands can sample a second, minor pose which becomes dominant after small chemical modifications to their structure. These observations and the pervasiveness of ligand heterogeneity in BRDs suggest that the potential of alternate ligand conformations for structure-based drug design is significantly undervalued.

## ■ DISCUSSION

Ligand conformational heterogeneity is widespread in X-ray data deposited in the PDB but underreported in the absence of automated and reliable computational methods. *qFit-ligand* is a new method to model a parsimonious multiconformer ligand in crystallographic electron densities. We formulated the challenge of identifying an ensemble that collectively best agrees with the electron density, from up to tens of thousands of candidate conformations, as a stepwise combinatorial optimization problem. *qFit-ligand* relies on exhaustive sampling, iteratively restrained by the electron density, to fully cover the conformational space of each ligand. Our method was designed to provide a measure of statistical confidence for model selection in cases of ligand conformational heterogeneity, separating the contributions between harmonic displacement and multiple conformations.

We highlighted three examples of previously unmodeled alternate ligand conformations obtained from prospective application of *qFit-ligand* to the D3R and *Twilight* data sets (Supporting Information, Table S4 lists all prospective discoveries). Strikingly, even the highly curated D3R data set revealed a previously unmodeled alternate conformation. Targeted application to a single bromodomain receptor suggests that as many as 29% of receptor–ligand crystal structures could have alternate ligand conformations. This is a likely conservative estimate of the accessible ligand conformational landscape in protein crystal structures. The portrait of rigid receptors and ligands is exacerbated by the common practice of collecting X-ray crystallographic data at cryogenic temperature (100 K). Although cryocooling increases the precision of structure determination by reducing thermal motions, cooling affects the conformational distribution of more than 35% of side chains in proteins<sup>50</sup> and has been found

to alter ligand binding and abolish transient binding sites observed at room temperature.<sup>51</sup> Applying *qFit-ligand* to room temperature X-ray crystallography data, which can shift the equilibrium of receptor–ligand conformational ensembles, may reveal additional minor ligand binding poses that are typically masked in cryogenic data.

*qFit-ligand* conformational strain energies after refinement were nearly indistinguishable from those of the manually curated benchmark set, signifying that its multiconformer models are chemically accurate. Our analysis showed that *qFit-ligand* conformations were nearly isoenergetic. Less often we identified a ligand for which the *qFit-ligand* multiconformer model significantly reduced strain energy, suggesting that conformational averaging of the single conformer model had led to a poorly modeled ligand to fit the density. Changes in the free energy of the ligand–receptor complex will give a more complete picture of the effect of multiconformer ligands but require a model of the receptor response to binding, which is beyond the scope of the current study. Ironically, multiconformer ligands are commonly filtered out of major test sets for development of docking and conformational sampling approaches but may be a more “trustworthy” representation of the underlying data.<sup>52</sup> Multiconformer ligand models can therefore address important challenges in ligand validation and deposition in the Protein Data Bank (PDB).<sup>53,54</sup>

Several aspects of *qFit-ligand* could be improved in the future. First and foremost, modeling the *joint* conformational ensemble of the binding site residues and ligand will be a major step forward toward a better understanding of receptor response to ligand binding. The potential of this approach is underlined by our finding that 12% of structures in the *Twilight* data set already present alternate receptor conformations within 5 Å of the ligand. While ultimately an accurate thermodynamic distribution for receptor–ligand conformations is desired, our approach determines a parsimonious ensemble of conformations that is supported by the data alone. These conformations can provide a starting point for MD simulation to obtain a better estimation for a thermodynamic distribution. Second, while in principle our conformational sampling approach could be combined with a sophisticated force field,<sup>55</sup> relying on energy restraints in the discovery stage can result in increased computational cost and can risk excluding promising candidate conformations owing to imperfect sampling and steep potential energy gradients. Rather, we advocate including energy restraints in refinement.<sup>31</sup> Other conformational search methods with force fields, such as Schrödinger’s ConfGen<sup>56</sup> and MacroModel,<sup>57</sup> OpenEye’s Omega,<sup>58</sup> MOE,<sup>59</sup> and many other freely available tools,<sup>60</sup> could independently validate results in the absence of data.

Third, the false-positive rates can likely be decreased. Several techniques are available to guard against overfitting. For example, the BIC criteria weighs increased model complexity (number of conformations) to a better statistical fit. Terminal ends and ring flips had low false positive rates, whereas those for the branched and displaced categories were elevated. *qFit-ligand* recovered terminal end and ring flips to within an nRMSD of 0.27. Disordered parts of branched ligands were often solvent-exposed and therefore more difficult to recover. Accounting for partial occupancy of ligand, receptor conformers, and solvent will be required to reveal details at the solvent interface. Displaced ligands are not “anchored” in the binding pocket and are among the most challenging to recover.

An nRMSD of 0.5 or below often sufficed for further refinement, but even nRMSDs up to 0.75 sometimes required only minor manual adjustments, depending on the absolute RMSD between states. For example, ring flips involving rotationally symmetric atom species cannot be uniquely assigned based on the electron density alone, leading to inflated RMSD measures, which are easily adjusted (Supporting Information, Materials and Methods, PDB 3P4V). All benchmark *qFit-ligand* results were obtained with the same parameters. In practice, specific problems will dictate tailored settings. For example, selecting finer sampling steps or larger volumes for rigid body searches could give better results at the expense of increased computational time (Supporting Information, Figure S17). Nonetheless, on our benchmark set, the fully automated *qFit-ligand* multiconformer models were supported by real-space validation measures, and their  $R_{\text{free}}$  values were statistically indistinguishable from the manually curated set. While these measures cannot perfectly distinguish false positives, structural models consistent with the reflection data create a pool of testable hypothesis, which can be evaluated in drug discovery using ligand structure activity relationships or protein residue mutations.

Fourth, the partial occupancy of an “unbound”/apo state could be explicitly considered. Weak, overlapping densities originating from partially occupied receptor and ligand conformations in the binding pocket are often difficult to tease apart, owing to a vast number of possible ligand conformations to be evaluated, even in sterically constrained binding cavities. Partially occupied water molecules and crystallographic additives often further confound modeling efforts. In these challenging cases, difference densities from alternate states are often incorrectly resolved by waters. Promising new approaches such as PanDDa<sup>61</sup> can reveal the electron density of partially occupied states; however, it requires a large number of “ground state” crystal structures to reliably compute their contribution to the partially occupied state. Our method is highly complementary, and PanDDa maps could even be used as input to *qFit-ligand*. Synergy of these approaches holds the promise to enable efficient, accurate, and unbiased discovery of alternate fragment and ligand binding poses. This is increasingly important in view of the ability to structurally screen hundreds of candidate ligands within hours on modern synchrotrons. The combination of these methods may help remove temptation to fill all difference density with waters while avoiding the overly optimistic modeling of partial occupancy ligands that are highlighted by the *Twilight Database*.

Even with these improvements, it is important to be sensitive to concerns of overfitting when fitting additional conformations into electron density maps. We have guarded against this possibility in multiple ways: (1) we identify conformations similar to “expert” manual modeling in experimental test sets, (2) in synthetic data sets, the Fisher  $z$  score identifies a statistically significant parsimonious set that correspond in number to the underlying “true” number of conformations, and (3) traditional global metrics ( $R_{\text{free}}$ ) and new local metrics (EDIA) do not identify major concerns. Furthermore, on the prospective set (1), new interactions are identified that make biochemical sense, (2) we identified similar conformations in ligands that differ by only a few atoms, and (3) visual inspection confirms that  $F_o - F_c$  difference density is reduced. This last point underscores how visual inspection is important for eliminating false

positives and, as shown here, for manually improving the fit. Furthermore, these checks are especially important for verifying the correct stereochemistry. Ultimately, biochemical tests with mutations or altered ligands are the best forward validation.

Finally, as the particle size and resolution limitations of single-particle cryoelectron microscopy (cryo-EM) continue to improve, that technology will have a major impact on drug discovery.<sup>62</sup> High-throughput and automation approaches, combined with the size of the complexes in cryo-EM structure determination, will soon turn careful modeling of protein and ligand structural heterogeneity into a major bottleneck. *qFit-ligand* can provide an efficient, automated modeling approach at the amino acid length scale, as EM maps are immutable during modeling and refinement. Beyond applications to drug discovery, as time-resolved serial crystallography is rapidly becoming routine at X-ray free electron lasers and even synchrotrons,<sup>64</sup> *qFit-ligand* can help resolve minor populations of structural protein–ligand intermediates in light-driven pump–probe<sup>65</sup> or structural enzymology “mix-and-inject” experiments.<sup>66,67</sup>

## ■ CONCLUSIONS

Revealing the full receptor–ligand conformational ensemble can help drug design by exploiting the balance between entropy and enthalpy in compound design<sup>68,69</sup> and by characterizing the effect of prerigidifying ligands on affinity.<sup>70</sup> Equally important, it can help the rational design of ligand selectivity by exposing accessible molecular surfaces unique to their intended targets.<sup>71</sup> In the future, full integration of *qFit-ligand* with *qFit* could reveal the structural reorganization of binding pockets and allosteric signal propagation in the receptor upon ligand binding.<sup>21,72</sup> Our *qFit-ligand* open source software, available from [https://github.com/ExcitedStates/qfit\\_ligand](https://github.com/ExcitedStates/qfit_ligand), provides promising, new starting points for ligand optimization and structure-based drug discovery. However, communication between structural biologists, computational chemists, and medicinal chemists remains a requisite for successful, rational design.

## ■ MATERIALS AND METHODS

**Survey of the Protein Data Bank and benchmark creation.** All structure coordinate files were downloaded from the PDB. Structures determined by X-ray crystallography were checked for HETATM entries (ligands) containing at least two different altloc identifiers with identical chemical composition. We aim to characterize conformational heterogeneity of ligands that are (1) drug-like and (2) have multiple internal degrees of freedom. Ligands with fewer than 15 non-hydrogen atoms were therefore discarded as were covalently linked ligands. This resulted in a list of 2611 ligands divided over 1845 PDB files. The list was further pruned to exclude ligand flips, i.e., alternate conformations that do not have a common cluster of atoms in space, and alternate conformations consisting exclusively of ring puckers as our algorithm was not designed to sample these types of conformational changes. We then selected receptors and ligands of pharmaceutical interest, resulting in a final benchmark set of 90 cases that refined against the deposited structure factors and CIF files. As the quality of X-ray data affects model building and refinement, we verified that low-resolution X-ray data cutoff and data completeness were within acceptable ranges (Supporting Information, Table S1). Each case was rerefined using phenix.refine v1.11 with the following parameters

For PDBs Better than 1.5 Å. optimize\_xyd\_weight = true  
optimize\_adp\_weight = true optimize\_mask=True main.number\_

of\_macro\_cycles=10 adp.individual.anisotropic='not water and not element H' adp.individual.isotropic='water or element H'

For PDBs Worse than 1.5 Å, optimize\_xyz\_weight=true  
optimize\_adp\_weight=true optimize\_mask=True main.number\_of\_macro\_cycles=10 adp.individual.isotropic=all

Single conformer ligand models were created by removing the ligand's "B" conformation from the original deposited PDB model and resetting the occupancy of the "A" conformation to 1. The single conformer models were re-refined as above.

**The qFit-ligand Approach.** The *qFit-ligand* algorithm takes as input the initial structure of a refined single conformer ligand modeled in the electron density, a real-space map ( $2mF_o - DF_c$ ) in *ccp4* format and its resolution and, optionally, the receptor and other ligand and solvent atoms for clash avoidance. The *qFit-ligand* algorithm starts by scaling the map electron density values to approximate absolute scale, using only the density under the footprint of the receptor. Next, the algorithm calculates an  $F_c$  map corresponding to the receptor and any other atoms in the crystal not part of the ligand. This map is subtracted from the experimental density. Map values below the mean are set to zero to prevent building into spurious density. We call the resulting map the *target map*.

Next, *qFit-ligand* determines rotatable covalent bonds of the ligand and rigid groups of atoms. Covalent bonds are determined based on proximity; i.e., if the distance between two atoms is smaller than their combined covalent radius plus 0.5 Å, the atoms are considered covalently bonded. It partitions the ligand into rigid groups of atoms (i.e., groups of atoms without internal DoFs) as follows: It constructs a graph  $G = (V_m, E_m)$  such that the vertices  $V_m$  represent atoms, and edges  $E_m$  represent covalent bonds. Next, members of  $E_m$  that (1) are in a ring system, and (2) edges  $(u, v)$  in  $E_m$  where  $u$  or  $v$  has degree one are edge-contracted. Hybridization states (partial double bonds) are ignored in the current implementation. A covalent bond is rotatable if it is not part of the same ring system. After edge contraction, each edge  $E_m$  ultimately corresponds to a rotating bond (one degree of freedom) and each vertex  $V_m$  corresponds to a collection of atoms that form a rigid body. Thus, rigid groups of atoms do not have internal, rotatable covalent bonds (Supporting Information, Figure S2).

Analogous to existing crystallographic model building procedures,<sup>73</sup> *qFit-ligand* iteratively generates and ranks a large number of candidate ensembles by scoring against the electron density and retaining a small ensemble (Figure 3A and Supporting Information, Figure S2). It uses modern statistical routines for subset selection in regression models by MIQP.<sup>74,75</sup> *qFit-ligand* builds up candidate ligand conformers starting from each rigid group of atoms in turn, similar to the approach implemented in FlexX/S<sup>76</sup> (Supporting Information, Figure S2). To prevent a combinatorial explosion, *qFit-ligand* iteratively samples and selects candidate conformers for successive rigid groups. The first sampling iteration consists of a local rigid body search of the starting group within a box with an edge size of 0.4 Å at a 0.1 Å interval and 10 randomly generated orientations at a maximum rotation angle of 10° (1250 conformations). An MIQP step (details below) selects up to five occupancy-weighted candidate positions that, collectively, minimize the real-space density residual of the rigid group. For each selected conformation, subsequent iterations each sample N (user-defined, default 2) torsion angles with a user-defined (default 6°) step size to add N successive rigid groups simultaneously. Clash detection is divided into internal clashes, i.e., clashes within a single ligand conformer, and external clashes, i.e., clashes between a ligand conformer and the receptor. Clashing conformations, both internal and with the receptor (using an efficient, O(1), spatial hashing algorithm), are detected and removed from the set before selection with MIQP. Bond lengths and angles are kept fixed during the whole procedure.

After each sampling iteration, the optimal occupancies of generated conformations are determined as follows. Each conformation is transformed into a density given by

$$\rho(r) = 8/r \int_{s_{\min}}^{s_{\max}} f(s) \exp(-Bs^2) \sin(4\pi rs) ds$$

where  $r$  is the position compared to the atom position,  $f(s)$  is the atomic scattering factor as a function of the momentum vector of the atom,  $B$  is the isotropic  $B$ -factor, and  $s_{\min}$  and  $s_{\max}$  are the minimum and maximum momentum vector length. For computational efficiency, a lookup table is created for each atom at an interval of 0.01 Å.

A combined mask is calculated by forming the union of all individual conformation masks, using a resolution dependent radius, where  $r = 0.5 + R/3$ . Density values under the footprint of the resulting mask are extracted and used as input for Quadratic Programming (QP) and Mixed Integer Quadratic Programming (MIQP) to select up to five conformations that best represent the density data locally. QP and MIQP solvers guarantee the global optimal occupancy of each conformation by minimizing the real-space residual given by

$$\begin{aligned} \min_w & \| \rho^o - \sum_i w_i \rho_i^c \|_2 \\ \text{s.t. } & w_i \geq t_{d_{\min}}, \quad i = 1, \dots, n \\ & 0 \leq \sum_i w_i \leq 1 \end{aligned} \quad (1)$$

where  $\rho^o$  is the target map,  $\rho_i$  is the calculated density of conformer  $i$ ,  $w_i$  is the weight, or occupancy, of conformer  $i$ , and  $0 \leq t \leq 1$  is a threshold on the occupancy. If  $t = 0$ , the constraints enforce non-negativity for the occupancies, and the program is a QP. The combined occupancy cannot exceed unity. Selecting  $t > 0$  introduces sparsity or threshold constraints, which turns the program (1) into a MIQP. To reduce computational complexity, relevant conformations are preselected using QP and used as input for a subsequent round of MIQP.<sup>23</sup>

After the ligand has been fully built up starting from each cluster, all resulting conformations are pooled together for a final round of rescoring. The individual Pearson product-moment cross-correlation (RSCC) is calculated for each individual conformation. Conformations with RSCC score less than 0.9 times the highest correlation, and redundant conformations for which all pairwise atom distances are within those of previously accepted conformations, are discarded. Finally, a parsimonious multiconformer model is created as follows. An MIQP step at an occupancy threshold of 0.20 is performed on the remaining pool of conformations. Visual inspection of conformers at minimum occupancy of 0.2 generally indicated density contours exceeded noise levels.<sup>77</sup> For very high resolution data sets, this threshold can be reduced. The resulting selected conformations are ranked by RSCC value, and starting from the conformation carrying the highest RSCC, additional conformations are added if the RSCC increases under the combined footprint and else discarded. This is performed iteratively until self-consistent, i.e., all conformations increase the RSCC under the combined footprint. The output of *qFit-ligand* consists of all conformations before the final rescoring round and the sparse, occupancy-weighted multiconformer ligand model.

*qFit-ligand* is implemented in Python 2.7 and relies on the open-source NumPy, SciPy, and CVXOPT<sup>78</sup> packages and the freely available Community Edition of IBM ILOG CPLEX, with added modules from the mmLib Python toolkit.<sup>79</sup> *qFit-ligand* is released under the MIT license and can be downloaded free of charge from [https://github.com/ExcitedStates/qfit\\_ligand](https://github.com/ExcitedStates/qfit_ligand), where additional documentation and installation instructions can be found.

**Benchmarking qFit-ligand.** Simulated structure factors were generated from the rerefined benchmark set using *phenix.fmodel* at 1.0, 1.3, 1.6, 2.0, and 2.5 Å resolution. Occupancy of the B-conformer was varied from 0.5 to 0.0 occupancy in 0.1 decrements, requiring that the combined occupancy of the multiconformer ligand summed up to unity. A random error of 10% was added to the amplitudes, a fraction of 0.1 was used for  $R_{\text{free}}$  flags, and we selected  $k_{\text{sol}} = 0.4$  and  $b_{\text{sol}} = 45 \text{ \AA}^2$ . The B-factor of each ligand atom was adjusted by 10 times the difference in real and simulated resolution, i.e., the B-factor was inflated for lower resolution simulated data and sharpened for high resolution data. The resulting *mtz* files were converted into *ccp4* density files using *phenix.mtz2map*.

For each resolution and occupancy combination, *qFit-ligand* was run on the full benchmark set using different sampling parameters: sampling 1 degree of freedom (DoF) using a torsion sampling interval of 1 degree, and sampling 2 DoFs simultaneously using a torsion sampling interval of 6 degrees. To obtain a uniform metric for evaluating the performance of *qFit-ligand*, we therefore analyzed the results by calculating a normalized RMSD, calculated in the receptor frame of reference:<sup>80,81</sup>

$$\text{nRMSD} = \min C_i \frac{\text{RMSD}(B, C_i)}{\text{RMSD}(A, B)}$$

between the output structures  $C_i$  of *qFit-ligand* and the ligand  $B$  conformer used during the structure factor generation, normalized by the RMSD between the A and B conformer. Conformers  $C_i$  for which  $\text{nRMSD} < 0.5$  are more similar to the B conformer than the A conformer. The nRMSD measure puts equal weight on each benchmark case by normalization while providing uniform thresholds for determining success (Figure S14). We note that the RMSD (and therefore also the nRMSD) measure has important limitations, affecting the results. For example, because RMSD is typically calculated between unique points, it fails to account for symmetric transformations within a ligand, e.g., a 180° flipped acidic group or aromatic ring, thus introducing additional error. Unfortunately, to our knowledge, there is no readily available method that addresses this issue. While a low nRMSD guarantees a good solution, a relatively high nRMSD can still suggest an alternate conformation that requires some manual adjustments, including symmetric transformations.

We subsequently evaluated the performance of *qFit-ligand* for each category in the benchmark set, at simulated resolutions and occupancies, after refinement with PHENIX v1.11 using the same protocol as stated above for refinement. The final selection stage was optimized heuristically by finding a balance between maximizing sensitivity and minimizing false-positives against the benchmark.

**D3R and Twilight Database Investigation.** We downloaded the D3R (<https://drugdesigndata.org/about/datasets>) and Twilight (<http://www.ruppweb.org/twilight/newligands-2016.tsv.bz2>) databases deposited in 2016. For all cases, structure coordinates and  $2\text{mF}_o - \text{DF}_c$  maps were downloaded from the PDB. For the *Twilight* cases, we discarded structures with a reported resolution worse than 2.0 Å and ligands consisting of less than 15 and more than 35 non-hydrogen atoms and a cross-correlation score less than 0.6. The resulting *qFit-ligand* multiconformer models were ranked on the Fisher  $z$ -transformation score. The Fisher  $z$ -transformation is a mapping of the RSCC  $r$  so that its distribution is approximately normal. It was previously applied to significance testing for cryo-EM rigid body fitting<sup>82–84</sup> and is given by

$$z = \frac{1}{2} \ln \left( \frac{1+r}{1-r} \right)$$

where  $r$  is the RSCC. The standard error of  $z$  is given by

$$\sigma = \frac{1}{\sqrt{N-3}}$$

where  $N$  represents the number of independent observations, approximated by  $N = MV/(c \times R)$ , where  $MV$  represents the molecular volume of the ligand in Å<sup>3</sup>,  $R$  the resolution in Å, and  $c = 1$  Å<sup>2</sup>, a constant.<sup>83</sup> Starting with the conformer with the highest RSCC, additional conformations are added. Our approach is based on hypothesis testing of the normally distributed, random variable. For each additional conformer, the  $z$ -score is recalculated for both the starting conformation and the combined multiconformer under the footprint of the latter. The resulting difference in  $z$ -score is divided by its standard error to provide a resolution and size corrected measure of significance for the increase in cross-correlation, where higher is better. The test statistic is

$$\xi_i = \frac{z_i^\Sigma - z_{\text{best}}}{\sigma_z}$$

where  $Z_{\text{best}}$  is the recalculated  $z$ -score of the single conformer with the highest RSCC, and  $z_i^\Sigma$  is the  $z$ -score of the  $i$ th combined multiconformer. The highest  $z$ -score increase found during this iterative process is reported in Supporting Information, Table S3.

#### EDIAm and OPIA Calculation.

$$\text{EDIA}_m(U) = \sum_{U_x \in U} \left( \text{occ}(U_x) \times \left[ \left( \frac{1}{|U_x|} \sum_{a \in U_x} (\text{EDIA}(a) - 0.1)^{-1/2} \right)^{-2} + 0.1 \right] \right)$$

where  $U_x$  is a conformer of the ligand  $U$ ,  $a$  is an atom in  $U_x$  with an EDIA score of  $\text{EDIA}(a)$ , and  $\text{occ}(U_x)$  is the occupancy of that conformer. The OPIA of multiconformer mode was calculated as an occupancy-weighted average of the OPIA of each conformer.

**Ligand Energy.** To assess ligand conformational energies, we carried out constrained minimizations (flat bottom width of 0.2 Å) of all ligands (from single conformer and *qFit-ligand* multiconformer models) using Jaguar<sup>85</sup> with the M06-2X functional<sup>86,87</sup> and 6-31G(d,p) basis set, except for bromine atoms, which used the LAV2P basis set. Gas-phase energies of ligand conformations generated by *qFit-ligand* (which were subsequently refined) were compared to ligand conformations in the single conformer model (i.e., 0 kcal/mol). The relative energies of each alternative conformation in the *qFit-ligand* multiconformer model were multiplied by their respective occupancies, then summed to arrive at the occupancy-weighted ligand energy.

## ASSOCIATED CONTENT

### S Supporting Information

The Supporting Information is available free of charge on the ACS Publications website at DOI: [10.1021/acs.jmedchem.8b01292](https://doi.org/10.1021/acs.jmedchem.8b01292).

Additional statistics for our data sets and results, detailed flowchart of the *qFit-ligand* algorithm, and molecular visualizations of its multiconformer models ([PDF](#))

Overview of benchmark cases and categorization of conformational change between alternate conformers ([PDF](#))

Performance of *qFit-ligand* on the benchmark using refined deposited data, showing quality metrics of refined single conformer structures, re-refined multiconformer deposited structures, and refined *qfit-ligand* generated structures ([PDF](#))

Results of applying *qFit-ligand* on a subset of the *Twilight Database* ([PDF](#))

Overview of prospective cases with an unmodeled alternate conformer found by *qFit-ligand* ([PDF](#))

BRD4 structures subjected to *qFit-ligand* approach, ordered by the Fisher  $z$ -score ([PDF](#))

### Accession Codes

6DMG (remodeled 4FV3); 6DMH (remodeled 4EV4); 6DMI (remodeled SEZX); 6DMJ (remodeled 5CFW); 6DMK (remodeled 4NR5); 6DML (remodeled 4BW3).

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**Author Contributions**

G.C.P.v.Z. and B.M.H. contributed equally. G.C.P.v.Z., R.F., A.H., and H.v.d.B. developed and implemented core algorithms; G.C.P.v.Z., B.M.H., S.H.P.d.O., K.B., T.D., J.S.F., and H.v.d.B. analyzed data; D.A.K. and P.S. contributed code and data analysis. J.S.F. and H.v.d.B. conceived the study. G.C.P.v.Z., B.M.H., J.S.F., and H.v.d.B. wrote the manuscript. All authors edited the manuscript.

**Notes**

The authors declare the following competing financial interest(s): J.S.F. is a paid consultant and has a financial stake in Relay Therapeutics. G.C.P.v.Z., K.B., and T.D. are employees of Schrödinger.

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**ABBREVIATIONS USED**

BRD4, bromodomain-containing protein 4; CBP, CREB binding protein; D3R, Drug Design Data Resource; EDIAm, Electron Density Support for Individual Atoms; RSCC, Pearson product-moment cross-correlation

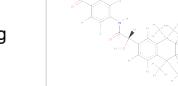
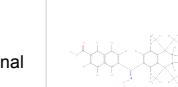
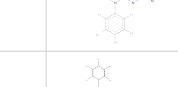
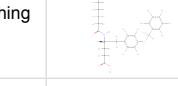
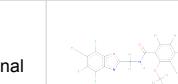
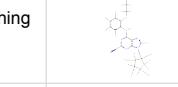
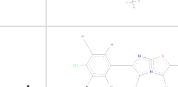
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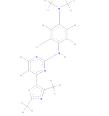
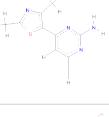
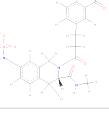
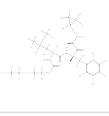
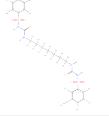
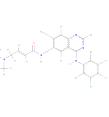
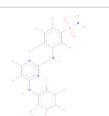
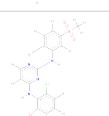
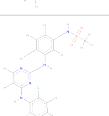
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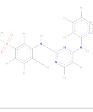
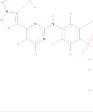
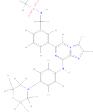
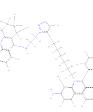
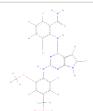
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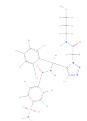
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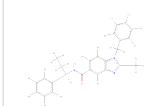
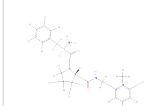
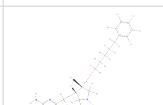
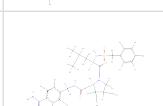
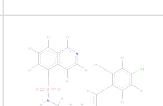
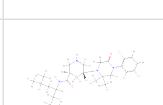
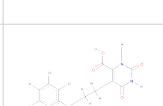
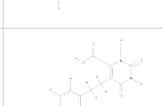
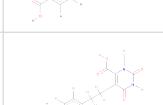
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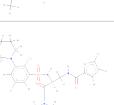
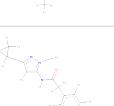
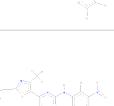
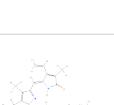
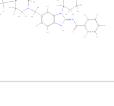
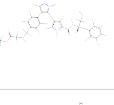
PDBID	Ligand	Receptor	Ligand Code	Resolution (Å)	SMILES	Occupancies	RMSD vs A conformer (Å)	Category	Structural formula
1exx	A-450	RETINOIC ACID RECEPTOR GAMMA-2;	961	1.67	CC1(CCC(c2c1ccc(c2)[C@@H](C(=O)Nc3ccc(cc3F)C(=O)O)O)(C)C)C	0.40 / 0.60	2.98	ring	
1fd0	A-450	RETINOIC ACID RECEPTOR GAMMA-1;	254	1.38	CC1(CCC(c2c1ccc(c2)/C(=N/O)/c3ccc4cc(ccc4c3)C(=O)O)(C)C)C	0.54 / 0.46	0.58	terminal	
1h1r	A-1298	CELL DIVISION PROTEIN KINASE 2;	6CP	2.00	c1cc(cc(c1)Cl)Nc2nc3c(c(n2)OCC4CCCC4)[nH]cn3	0.50 / 0.50	2.52	ring	
1j1a	A-1301	PHOSPHOLIPASE A2;	BHP	2.20	c1ccc(cc1)CCCCCCC(=O)N[C@@H](CCC(=O)O)Cc2ccc(cc2)OCc3cccc3	0.50 / 0.50	4.64	branching	
1q2o	A-790	NITRIC-OXIDE SYNTHASE, ENDOTHELIAL;	DP1	1.74	C([C@H](C(=O)N[C@H](CCNC(=O)N)N)CNC(=N)N[N+](=O)[O-])	0.50 / 0.50	1.89	displaced	
1t41	A-320	ALDOSE REDUCTASE;	ID5	1.05	c1cc(c(cc1F)OCC(=O)O)C(=O)NCC2nc3c(c(cc(c3s2)F)F)F	0.62 / 0.38	1.53	terminal	
1tbb	A-501	CAMP-SPECIFIC 3',5'-CYCLIC PHOSPHODIESTERASE 4D;	ROL	1.60	COc1ccc(cc1OC2CCCC2)[C@H]3CC(=O)NC3	0.50 / 0.50	1.24	displaced	
1u9x	A-300	CATHEPSIN K;	IHJ	2.10	CN1CCN(CC1)CCCOc2cccc2Nc3c4c(nc(n3)C#N)N(cn4)C5CCCC5	0.50 / 0.50	1.80	branching	
1xdd	A-401	INTEGRIN ALPHA-L;	AAV	2.20	CC[C@H](C(=O)O)[C@H]1C[C@H](C=C2[C@H]1[C@H](C[C@H](C=C2)C)CC[C@H]3C[C@H](C(=O)N3Cc4cccc5c(c4)ccc(c5CO)OC)O)C	0.50 / 0.50	2.66	ring	
1xvp	D-1003	RETINOIC ACID RECEPTOR RXR-ALPHA;	CID	2.60	c1cc(ccc1c2c(n3ccsc32)\C=NOCC4ccc(c(c4)Cl)Cl)Cl	0.50 / 0.50	1.03	displaced	
1zsk	A-301	COAGULATION FACTOR XI;	421	1.90	[H]/N=C(c1ccc2cc(cc(c21)NC(=O)c3cccc(c3)O)C(=O)OC)/N	0.50 / 0.50	2.71	terminal	
1zzq	A-799	NITRIC-OXIDE SYNTHASE, BRAIN;	DP9	1.90	C1[C@H](CN[C@H]1C(=O)N)NC(=O)[C@H](CCCNc2n[n+]([O-])n2)N	0.50 / 0.50	2.75	displaced	

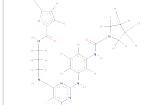
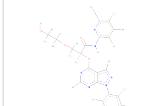
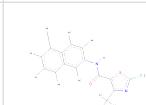
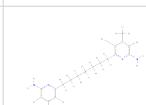
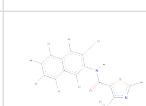
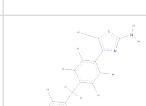
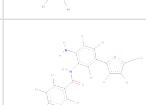
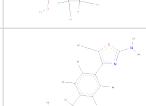
PDBID	Ligand	Receptor	Ligand Code	Resolution (Å)	SMILES	Occupancies	RMSD vs A conformer (Å)	Category	Structural formula
2c5n	A-1297	CELL DIVISION PROTEIN KINASE 2;	CK8	2.10	Cc1c(sc(n1)C)c2ccnc(n2)Nc3ccc(cc3)N(C)C	0.60 / 0.40	1.58	ring	
2c5o	A-1297	CELL DIVISION PROTEIN KINASE 2;	CK2	2.10	Cc1c(sc(n1)C)c2ccnc(n2)N	0.40 / 0.60	1.94	ring	
2f71	A-608	TYROSINE-PROTEIN PHOSPHATASE, NON-RECEPTOR TYPE 1;	UN7	1.55	CNC(=O)[C@H](C)c1Cc2ccc(cc2CN1C(=O)OCCc3cccc(c3)C(=O)O)NS(=O)(=O)O	0.50 / 0.50	0.81	terminal	
2g8j	A-400	CALPAIN-1 CATALYTIC SUBUNIT;	D7G	1.61	CC(C)C[C@H](C(=O)N[C@H](C)c1cccccc1C(=O)OC2CC2)NC(=O)OCCOCCOC	0.65 / 0.35	8.21	branching	
2jjk	A-1336	FRUCTOSE-1,6-BISPHOSPHATASE 1;	R15	2.00	c1cc(cc(c1)Cl)S(=O)(=O)NC(=O)NCCCCCCCNC(=O)NS(=O)(=O)c2cccc(c2)Cl	0.50 / 0.50	1.50	displaced	
2qlq	A-1345	PROTO-ONCOGENE TYROSINE-PROTEIN KINASE SRC;	SR2	2.33	CN(C)CC=CC(=O)Nc1ccc2c(c1)c(ncn2)Nc3cccc(c3)Br	0.70 / 0.30	1.36	ring	
2r3i	A-501	CELL DIVISION PROTEIN KINASE 2;	SCF	1.28	c1ccc(c(c1)c2cc(n3c(n2)cn3)NCc4ccncc4)F	0.60 / 0.40	1.43	ring	
2r3p	A-501	CELL DIVISION PROTEIN KINASE 2;	3SC	1.66	c1cc(c(c(c1)Cl)Cl)c2cc(n3c(n2)cn3)SC#N)NCc4ccncc4	0.50 / 0.50	1.72	ring	
2vip	A-1247	UROKINASE-TYPE PLASMINOGEN ACTIVATOR CHAIN B;	L1R	1.72	CC(C)Oc1cccc(c1)NC(=O)c2cc(c(c(c2)Cl)OCCN)Cl	0.50 / 0.50	2.85	ring	
2vwx	A-1889	EPHRIN TYPE-B RECEPTOR 4;	7X4	1.65	c1cc(cc(c1)S(=O)(=O)N)Nc2nccc(n2)Nc3c(ccc4c3OCO4)Cl	0.50 / 0.50	4.35	ring	
2vwy	A-1889	EPHRIN TYPE-B RECEPTOR 4;	7X5	1.65	CS(=O)(=O)c1cccc(c1)Nc2nccc(n2)Nc3c(ccc4c3OCO4)Cl	0.30 / 0.70	4.61	ring	
2vwz	A-1889	EPHRIN TYPE-B RECEPTOR 4;	7X6	1.65	CS(=O)(=O)Nc1cccc(c1)Nc2nccc(n2)Nc3c(ccc4c3OCO4)Cl	0.80 / 0.20	5.47	ring	

PDBID	Ligand	Receptor	Ligand Code	Resolution (Å)	SMILES	Occupancies	RMSD vs A conformer (Å)	Category	Structural formula
2vx1	A-1889	EPHRIN TYPE-B RECEPTOR 4;	7X8	1.65	c1cc(cc(c1)Nc2nccc(n2)Nc3c(ccc4c3OCO4)Cl)C(=O)N	0.80 / 0.20	4.02	ring	
2w9h	A-1160	DIHYDROFOLATE REDUCTASE;	TOP	1.48	COc1cc(cc(c1OC)OC)Cc2cnc(nc2N)N	0.50 / 0.50	0.74	terminal	
2x9f	A-1889	EPHRIN TYPE-B RECEPTOR 4;	X9F	1.75	CS(=O)(=O)c1cccc(c1)Nc2nccc(n2)Nc3cccc4c3cn[nH]4	0.70 / 0.30	4.15	ring	
2xmy	A-500	CELL DIVISION PROTEIN KINASE 2;	CDK	1.90	CC1=C(SC(=O)N1C)c2ccnc(n2)Nc3ccc(cc3)S(=O)(=O)NCCOC	0.50 / 0.50	1.68	branching	
2xnb	A-1299	CELL DIVISION PROTEIN KINASE 2;	Y8L	1.85	CC1=C(SC(=O)N1C)c2ccnc(n2)N=c3cc=C(C=C3)N4CCNC4	0.50 / 0.50	1.47	ring	
2xng	A-1391	SERINE/THREONINE-PROTEIN KINASE 6;	A0H	2.60	CS(=O)(=O)NCc1cccc(c1)c2cn3c(cnc3c(n2)Nc4ccc(cc4)N5CCOCC5)Cl	0.50 / 0.50	1.65	terminal	
2xup	A-1548	ACETYLCHOLINESTERASE;	TZ5	2.70	c1ccc(cc1)c2c3cc(ccc3c4cccc4c[nH]2CCCCCCC5cnnn5CNC6c7cccc7nc8c6CCCC8)N)N	0.50 / 0.50	3.62	branching	
2yoh	B-211	THYMIDYLATE KINASE;	WMJ	1.60	CC1=CN(C(=O)NC1=O)[C@H]2[C@H](C([O])CNC(=O)Nc3cccc(cc3)[N+](=O)[O-])O	0.50 / 0.50	4.64	branching	
3elj	A-365	MITOGEN-ACTIVATED PROTEIN KINASE 8;	GS7	1.80	COc1cc(ccc1Nc2nc3c(cc[nH]3)c(n2)Nc4cccc(c4)C(=O)F)CS(=O)(=O)C	0.50 / 0.50	1.28	ring	
3i95	A-1130	PHYCOCYANOBILIN: FERREDOXIN OXIDOREDUCTASE;	BLA	1.40	Cc1cc(c([nH]c1C=C2C=C(C(=O)N2)C(=C)C)\C=C3C=C(C=C(N3)C=C4C=C(C(=O)N4)C=C)C)CCC(=O)O)CCC(=O)O	0.50 / 0.50	2.19	terminal	
3jt7	A-800	NITRIC OXIDE SYNTHASE, BRAIN;	JM5	2.10	[H]/N=C(/CSCCC)\NCCCC[C@@H](C(=O)O)N	0.70 / 0.30	1.69	branching	
3jt8	A-800	NITRIC OXIDE SYNTHASE, BRAIN;	JM4	1.95	[H]/N=C(/CCSC(C)C)\NCCCC[C@@H](C(=O)O)N	0.50 / 0.50	1.41	branching	

PDBID	Ligand	Receptor	Ligand Code	Resolution (Å)	SMILES	Occupancies	RMSD vs A conformer (Å)	Category	Structural formula
3kne	A-502	CARBONIC ANHYDRASE 2;	DAW	1.35	c1ccc(cc1)[C@@@H](c2ccnnn2CC(=O)NCCCS)NC(=O)c3ccc(cc3)S(=O)(=O)N	0.50 / 0.50	1.42	displaced	
3lff	A-362	MITOGEN-ACTIVATED PROTEIN KINASE 14;	Z83	1.50	CC(C)(C)c1cc(n(n1)c2ccc(cc2)CC(=O)O)NC(=O)Nc3ncs3	0.50 / 0.50	0.50	terminal	
3n0n	A-263	CARBONIC ANHYDRASE 2;	P9B	1.50	c1cc(ccc1NC(=O)Nc2c(c(c(c2F)F)F)F)S(=O)(=O)N	0.60 / 0.40	2.58	displaced	
3nlx	A-800	NITRIC OXIDE SYNTHASE, BRAIN;	3XB	1.87	Cc1cc(nc(c1)N)C[C@@H]2CNC[C@@H]2OCCNCC(c3cccc(c3)F)(F)F	0.70 / 0.30	1.89	branching	
3nlz	A-800	NITRIC OXIDE SYNTHASE, BRAIN;	3XD	1.92	Cc1cc(nc(c1)N)C[C@@H]2CNC[C@@H]2OCCNCC(c3cccc(c3)F)(F)F	0.60 / 0.40	2.24	branching	
3nm0	A-800	NITRIC OXIDE SYNTHASE, BRAIN;	3XE	1.81	C[C@H]1C[C@H](N=C(C1)N)C[C@@H]2CNC[C@@H]2OCCNCC(c3cccc(c3)F)F	0.60 / 0.40	2.20	branching	
3o57	A-506	CAMP-SPECIFIC 3',5'-CYCLIC PHOSPHODIESTERASE 4B;	ZG2	2.00	CCn1c2c(cn1)cc(c2)Cn3nc(c(o3)Cc4cccc4)CC(=O)N5CCCC5)NC6CCOCOC6	0.50 / 0.50	2.28	branching	
3oiK	A-300	CARBONIC ANHYDRASE 2;	WZB	1.50	CCc1cc2c(cc1OS(=O)(=O)N)CC[C@@H]3C[C@H]2CC[C@H]4[C@H]3CC[C@H]4OOS(=O)(=O)N)C	0.50 / 0.50	3.73	terminal	
3p0m	A-351	CAMP-DEPENDENT PROTEIN KINASE CATALYTIC SUBUNIT ALPHA;	4SB	2.03	c1ccc(cc1)[C@@H](CCN)C(=O)N/N=C/C/c2ccc(c(c2)Br)O	0.54 / 0.46	2.13	terminal	
3p4v	A-300	CARBONIC ANHYDRASE 2;	PMX	2.00	COC(=O)/C=C/C(=O)N[C@@H](Cc1ccc(c(c1)Cl)O)C(=O)O	0.35 / 0.65	3.23	ring	
3pne	A-800	NITRIC OXIDE SYNTHASE, BRAIN;	8AX	1.97	Cc1cc(nc(c1)N)C[C@@H]2CNC[C@@H]2OCCNCC(c3cccc(c3)Cl)(F)F	0.60 / 0.40	1.83	branching	
3s7a	A-192	DIHYDROFOLATE REDUCTASE;	684	1.80	c1ccc2c(c1)C=Cc3cc(c3N2Cc4ccnc5c(n4)cc(c5)N)OCCCC(=O)O	0.50 / 0.50	0.74	branching	

PDBID	Ligand	Receptor	Ligand Code	Resolution (Å)	SMILES	Occupancies	RMSD vs A conformer (Å)	Category	Structural formula
3s8x	A-266	CARBONIC ANHYDRASE 2;	E59	1.30	CC1=CC(=O)NC(=N1)SCC(=O)c2ccc(cc2)S(=O)(=O)N	0.50 / 0.50	1.76	branching	
3s9s	A-1	PEROXISOME-PROLIFERATOR-ACTIVATED RECEPTOR GAMMA;	M0T	2.55	CC[C@H](c1ccccc1)NC(=O)c2cc3c(c2)nc(n3Cc4ccc(c(c4)Cl)Cl)C	0.50 / 0.50	2.41	ring	
3si4	H-1	THROMBIN LIGHT CHAIN;	B04	1.27	C[n+]1cccc1CNC(=O)[C@@H]2CCCN2C(=O)[C@@H](Cc3cccc3)N	0.59 / 0.41	2.03	ring	
3t5f	H-1	THROMBIN LIGHT CHAIN;	M34	1.45	CC(C)C[C@H](C(=O)N1CCCC[C@H]1C(=O)Ncc2cc(cc2CN)Cl)NS(=O)(=O)Cc3cccc3	0.42 / 0.58	2.00	terminal	
3ufo	B-800	NITRIC OXIDE SYNTHASE, BRAIN;	HW4	2.17	Cc1cc(nc(c1)N)C[C@H]2NC[C@H]2OCCCCCC3cccc(c3)F	0.50 / 0.50	5.09	branching	
3uwj	H-302	THROMBIN LIGHT CHAIN;	TIF	1.50	[H]/N=C(/c1ccc(cc1)CNC(=O)[C@@H]2CCCN2C(=O)[C@@H](CC(C)C)NS(=O)(=O)Cc3cccc3)N	0.62 / 0.38	3.10	terminal	
3vqh	A-401	CAMP-DEPENDENT PROTEIN KINASE CATALYTIC SUBUNIT ALPHA;	IQB	1.95	c1cc2cnccc2c(c1)S(=O)(=O)NCCNC(C=C)c3ccc(cc3)Br	0.50 / 0.50	1.08	branching	
3vyf	A-402	RENIN;	VYF	2.80	CC(C)CC(CC(C)C)NC(=O)[C@H]1C[C@H](CNC1)N2CC(=O)N(CC2(C)Cc3cccc3Cl)	0.50 / 0.50	0.89	displaced	
3w72	B-401	DIHYDROOROTATE DEHYDROGENASE (FUMARATE);	W7B	1.55	c1ccc2c(c1)cccc2CC3=C(NC(=O)NC3=O)C(=O)O	0.50 / 0.50	2.54	branching	
3w7j	B-401	DIHYDROOROTATE DEHYDROGENASE (FUMARATE);	W7J	1.58	c1cc2cc(cc2)ccc1CC3=C(NC(=O)NC3=O)C(=O)C(=O)O	0.50 / 0.50	3.37	branching	
3w7r	A-408	DIHYDROOROTATE DEHYDROGENASE (QUINONE), MITOCHONDRIAL;	W7A	1.68	c1ccc(cc1)c2ccc(cc2)CCC3=C(NC(=O)NC3=O)C(=O)O	0.50 / 0.50	2.52	branching	
4a9s	A-1515	SERINE/THREONINE-PROTEIN KINASE CHK2;	RU9	2.66	c1cc(cc(c1)Oc2ccc(cc2)c3[nH]c4cc(cc4n3)C(=O)N)O	0.50 / 0.50	3.04	branching	

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4anw	A-1189	PHOSPHATIDYLINOSITOL-4,5-BISPHOSPHATE 3-KINASE CATALYTIC	O92	2.31	CNC(=O)c1c(ncc(n1)c2ccc(c(c2)S(=O)(=O)Nc3cccc(c3F)Cl)N)Cl	0.50 / 0.50	1.64	ring	
4b0o	A-1307	CHOLINESTERASE;	15F	2.35	[H]/N=C(/C(Cl)(Cl)Cl)\OCc1cc[n+](cc1)Cc2cccc2	0.56 / 0.44	4.95	branching	
4b85	A-600	ACETYLCHOLINESTERASE;	B3W	2.10	CCN(CC)CCNS(=O)(=O)c1ccc(cc1)Cl	0.50 / 0.50	2.41	displaced	
4bcp	A-1299	CYCLIN-DEPENDENT KINASE 2;	T3C	2.26	Cc1c(sc(n1)NC)c2c(cnc(n2)Nc3cccc(c3)N4CCCNCC4)C#N	0.50 / 0.50	3.92	branching	
4btu	B-1246	COAGULATION FACTOR X HEAVY CHAIN;	6XS	2.37	CN1CCN(CC1)C(=O)[C@H](CNC(=O)c2ccc(s2)C)NS(=O)(=O)c3cc(cc(c3Cl)N4CCCC4=O)F	0.50 / 0.50	2.36	branching	
4ek6	A-301	CYCLIN-DEPENDENT KINASE 2;	10K	1.52	c1cc(sc1)c2ccc(cc2)CC(=O)Nc3cc(c[nH]3)C4CC4	0.60 / 0.40	1.81	ring	
4ek8	A-301	CYCLIN-DEPENDENT KINASE 2;	16K	1.70	Cc1c(sc(n1)C)c2ccn(c(n2)Nc3cccc(c3)[N+]([O-])=O)F	0.51 / 0.49	3.97	ring	
4eoc	A-1001	PHYCOCYANOBILIN: FERREDOXIN OXIDOREDUCTASE;	BLA	1.49	Cc1c(c([nH]c1 C=C/2 C(=C(C(=O)N2)C(=C)C) C=C/3 C(=C(C(=N3)C=C/4 C(=C(C(=O)N4)C)=C)C)CCC(=O)O)CCC(=O)O	0.41 / 0.59	1.49	terminal	
4fod	A-1501	ALK TYROSINE KINASE RECEPTOR;	0UV	2.00	CC(C)NC(=O)C1CCC(CC1)N2c3cc(cc3N/C2=N\ C(=O)c4ccc(cc4)F)CN5CCC(CC5)C(C)(C)O	0.50 / 0.50	4.07	branching	
4ftt	A-301	SERINE/THREONINE-PROTEIN KINASE CHK1;	6HK	2.30	Cn1cncc1c2ccc3c(c2)Nc4ccc(cc4NC3=O)CC(=O)OC	0.50 / 0.50	3.68	ring	
4fv3	A-401	MITOGEN-ACTIVATED PROTEIN KINASE 1;	EK6	2.20	CCOC(=O)CNCC1ccc(cc1Cl)c2cn[nH]c2c3cc([nH]c3)C(=O)N[C@H](CO)c4ccc(c(c4)Cl)F	0.50 / 0.50	2.66	branching	
4g95	A-201	DIHYDROFOLATE REDUCTASE;	OAG	1.35	c1cc(c(cc1Cl)NCc2cc3c(nc(nc3nc2)N)N)Cl	0.50 / 0.50	2.44	displaced	

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4im2	A-701	SERINE/THREONINE-PROTEIN KINASE TBK1;	BX7	2.50	c1cc(cc(c1)NC(=O)N2CCCC2)Nc3ncc(c(n3)NCCCN(=O)c4cccs4)l	0.51 / 0.49	3.59	branching	
4iwf	A-601	ESTROGEN RECEPTOR;	15Q	1.93	c1cc(c(cc1c2ccc(c(c2Cl)/C=N/O)O)F)O	0.25 / 0.75	3.29	displaced	
4iwv	A-503	GLUCOKINASE ISOFORM 3;	1J9	2.10	c1ccc(c(c1)n2c3c(cn2)c(ncn3)O[C@H](COCCO)C(=O)Nc4ccc(cn4)Cl)Cl	0.50 / 0.50	1.32	ring	
4js3	A-403	DIHYDROOROTATE DEHYDROGENASE (QUINONE), MITOCHONDRIAL;	JS3	2.00	Cc1c(sc(n1)Cl)C(=O)Nc2ccc3cccc3c2	0.50 / 0.50	1.73	ring	
4jsf	A-803	NITRIC OXIDE SYNTHASE, BRAIN;	QJ4	2.05	Cc1cc(nc(c1)N)CCCCCCCc2cc(cc(n2)N)C	0.50 / 0.50	2.17	branching	
4jts	A-412	DIHYDROOROTATE DEHYDROGENASE (QUINONE), MITOCHONDRIAL;	JTS	2.21	Cc1c(scn1)C(=O)Nc2ccc3cccc3c2	0.50 / 0.50	1.59	ring	
4l2l	A-702	LEUKOTRIENE A-4 HYDROLASE;	1V6	1.65	c1ccc(cc1)Cc2ccc(cc2)c3scs(n3)N	0.50 / 0.50	1.49	ring	
4ly1	A-407	HISTONE DEACETYLASE 2;	20Y	1.57	CC(=O)Nc1ccc(cc1)C(=O)Nc2cc(ccc2N)c3cccs3	0.50 / 0.50	0.93	displaced	
4mkt	A-702	LEUKOTRIENE A-4 HYDROLASE;	28T	1.62	C1C[C@H](NC1)C(=O)CCC(=O)N2CCC[C@H]2C(=O)O	0.50 / 0.50	0.88	displaced	
4mkt	A-703	LEUKOTRIENE A-4 HYDROLASE;	1V6	1.62	c1ccc(cc1)Cc2ccc(cc2)c3scs(n3)N	0.50 / 0.50	1.26	displaced	
4ms6	A-702	LEUKOTRIENE A-4 HYDROLASE;	28T	1.72	C1C[C@H](NC1)C(=O)CCC(=O)N2CCC[C@H]2C(=O)O	0.50 / 0.50	0.85	displaced	
4o1z	A-807	PROSTAGLANDIN G/H SYNTHASE 1;	MXM	2.40	Cc1ncn(s1)NC(=O)C2=C(c3cccc3S(=O)(=O)N2C)O	0.04 / 0.96	0.93	ring	

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4pqn	A-701	TYROSINE-PROTEIN KINASE ITK/TSK;	2W6	1.71	CC1(CCc2c([nH]nc2C(=O)Nc3ccn(c3)[C@@@H](CCN(C)Cc4cccc4)C1)C	0.50 / 0.50	0.75	terminal	
4qj0	D-305	CARBONIC ANHYDRASE 12;	WWX	1.55	c1ccc(cc1)[C@H]([C@H](c2ccccc2)O)Nc3c(c(c(c3S(=O)(=O)CCOF)F)S(=O)(=O)N)F	0.50 / 0.50	0.33	terminal	
4qsj	B-302	CARBONIC ANHYDRASE 13;	EWW	1.70	CC1=CC(=O)NC(=N1)SCC(=O)c2ccc(c(c2)Cl)S(=O)(=O)N	0.50 / 0.50	3.83	branching	
4y6d	A-301	COAGULATION FACTOR X;	48U	1.55	CN(C)C(=O)c1ccc(c(c1)F)N2CC[C@H](C2=O)NS(=O)(=O)/C=C/c3ccc(s3)Cl	0.50 / 0.50	1.22	ring	
4yl3	A-201	PROSTAGLANDIN E SYNTHASE;	4U9	1.41	c1cc(c(c(c1)Cl)c2[nH]c(c(n2)Br)c3ccc(nc3)C#Cc4ccc(cc4)C(F)(F)F)F	0.50 / 0.50	1.12	terminal	
4ys1	A-402	ALDOSE REDUCTASE;	4G7	1.07	c1cc(cc(c1)C(=O)O)CNC(=O)c2ccc(cc2OCC(=O)O)F	0.28 / 0.49	1.03	terminal	
5agk	A-801	NITRIC OXIDE SYNTHASE, BRAIN;	RGE	2.00	[H]/N=C(\CS(=O)C)/NCCC[C@@H](C(=O)O)N	0.50 / 0.50	1.81	terminal	

PDBID	Ligand	Receptor	Ligand Code	Resolution (Å)	Occupancies (deposited re-refined)	Occupancies (qFit refined)	RMSD vs A conformer (Å) (deposited re-refined)	RMSD vs A conformer (Å) (qFit refined)	R-work (single refined)	R-work (deposited re-refined)	R-work (qFit refined)	R-free (single refined)	R-free (deposited re-refined)	R-free (qFit refined)	Ligand Energy (kcal/mol) qFit confs relative to single conf
1t41	A-320	ALDOSE REDUCTASE;	ID5	1.05	0.63 / 0.37	0.66 / 0.09 / 0.24	0.58	1.24 / 0.83	0.1224	0.1207	0.1172	0.1336	0.1315	0.1304	-1.740
4ys1	A-402	ALDOSE REDUCTASE;	4G7	1.07	0.41 / 0.59	0.72	0.48		0.1317	0.1283	0.1288	0.1469	0.1409	0.1468	0.010
3si4	H-1	THROMBIN LIGHT CHAIN;	B04	1.27	0.60 / 0.40	0.72 / 0.28	1.34	1.43	0.1306	0.1309	0.1286	0.1552	0.1543	0.1530	0.310
2r31	A-501	PROTO-ONCOGENE TYROSINE-PROTEIN KINASE SRC;	SCF	1.28	0.84 / 0.16	0.00 / 0.38 / 0.62	1.38	3.41 / 1.18	0.1429	0.1410	0.2033	0.1703	0.1694	0.1689	-1.130
3s8x	A-266	CARBONIC ANHYDRASE 2;	E59	1.38	0.40 / 0.60	0.58 / 0.42 / 0.00	1.89	2.63 / 1.88	0.1396	0.1403	0.1364	0.1644	0.1631	0.1631	0.200
3kne	A-502	CARBONIC ANHYDRASE 2;	DAW	1.35	0.44 / 0.56	0.37 / 0.00 / 0.22 / 0.41	0.66	0.84 / 3.53 / 3.42	0.1337	0.1343	0.1343	0.1551	0.1545	0.1674	3.310
4g95	A-201	DIHYDROFOLATE REDUCTASE;	OAG	1.35	0.50 / 0.50	0.43 / 0.01 / 0.37 / 0.19	2.33	2.04 / 2.37 / 4.06	0.1318	0.1357	0.1372	0.1601	0.1603	0.1597	-0.050
1fd0	A-450	RETINOIC ACID RECEPTOR GAMMA-1;	254	1.38	0.52 / 0.48	0.59 / 0.41	0.34	0.40	0.1394	0.1403	0.1384	0.1625	0.1599	0.1602	1.520
3i95	A-1130	PHYCOCYANOBILIN:FERREDOXIN OXIDOREDUCTASE;	BLA	1.40	0.56 / 0.44	0.00 / 0.70 / 0.30	0.22	0.35 / 0.47	0.1276	0.1257	0.1298	0.1559	0.1548	0.1556	1.120
4yl3	A-201	PROSTAGLANDIN E SYNTHASE;	4U9	1.41	0.45 / 0.55	0.64 / 0.36	0.4	0.95	0.1385	0.1325	0.1346	0.1534	0.1493	0.1508	0.010
3t5f	H-1	THROMBIN LIGHT CHAIN;	M34	1.45	0.42 / 0.58	0.00 / 0.34 / 0.66	0.77	2.26 / 0.67	0.1301	0.1288	0.1300	0.1591	0.1555	0.1572	1.650
2w9h	A-1160	EPHRIN TYPE-B RECEPTOR 4;	TOP	1.48	0.74 / 0.26	0.34 / 0.66	2.72	0.96	0.1525	0.1559	0.1611	0.1909	0.1944	0.1942	-1.230
4eoc	A-1001	PHYCOCYANOBILIN:FERREDOXIN OXIDOREDUCTASE;	BLA	1.49	0.32 / 0.68	0.05 / 0.95	0.29	0.30	0.1485	0.1512	0.1511	0.1878	0.1911	0.1895	-1.470
3lff	A-362	MITOGEN-ACTIVATED PROTEIN KINASE 14;	Z83	1.50	0.58 / 0.42	0.60 / 0.00 / 0.40	0.55	0.87 / 0.68	0.1551	0.1517	0.1539	0.1904	0.1892	0.1903	0.490
3n0n	A-263	CARBONIC ANHYDRASE 2;	P9B	1.50	0.59 / 0.41	0.91	2.9		0.1254	0.1351	0.1260	0.1680	0.1625	0.1688	0.700
3oik	A-300	CARBONIC ANHYDRASE 2;	WZB	1.50	0.58 / 0.42	0.00 / 0.39 / 0.61	1.48	1.42 / 0.84	0.1151	0.1156	0.1179	0.1541	0.1527	0.1528	0.450
3uwj	H-302	THROMBIN LIGHT CHAIN;	TIF	1.50	0.53 / 0.47	0.77 / 0.05 / 0.18	1.07	3.60 / 2.13	0.1293	0.1294	0.1270	0.1601	0.1562	0.1597	6.100
4ek6	A-301	CYCLIN-DEPENDENT KINASE 2;	10K	1.52	0.62 / 0.38	0.69 / 0.18 / 0.13	0.83	0.91 / 0.89	0.1850	0.1815	0.1838	0.2011	0.2019	0.2011	-0.110
2f71	A-608	TYROSINE-PROTEIN PHOSPHATASE, NON-RECEPTOR TYPE 1;	UN7	1.55	0.53 / 0.47	0.49 / 0.29 / 0.22	0.47	0.60 / 0.74	0.1656	0.1606	0.1607	0.1832	0.1823	0.1831	2.290
3w72	B-401	DIHYDROORotate DEHYDROGENASE (FUMARATE);	W7B	1.55	0.50 / 0.50	0.60 / 0.40	2.56	2.44	0.1374	0.1361	0.1365	0.1664	0.1654	0.1658	0.890
4qj0	D-305	CARBONIC ANHYDRASE 12;	WWX	1.55	0.86 / 0.14	1.00 / 0.00	0.37	0.85	0.1731	0.1726	0.1721	0.2114	0.2114	0.2108	-0.060
4y6d	A-301	COAGULATION FACTOR X;	48U	1.55	0.41 / 0.59	0.43 / 0.25 / 0.31	1.31	1.37 / 1.36	0.1831	0.1827	0.1831	0.2222	0.2206	0.2209	0.860
4ly1	A-407	HISTONE DEACETYLASE 2;	20Y	1.57	0.53 / 0.47	0.27 / 0.33 / 0.15 / 0.25	0.98	0.85 / 1.41 / 0.87	0.1551	0.1558	0.1547	0.1777	0.1774	0.1771	1.250
3w7j	B-401	DEHYDROGENASE (FUMARATE);	W7J	1.58	0.53 / 0.47	0.48 / 0.52	3.35	0.92	0.1446	0.1443	0.1436	0.1794	0.1791	0.1794	0.020
1tbb	A-501	CAMP-SPECIFIC 3',5'-CYCLIC PHOSPHODIESTERASE 4D;	R0L	1.60	0.26 / 0.74	0.78 / 0.22 / 0.00	1.25	1.31 / 0.69	0.1913	0.1863	0.1860	0.2108	0.2088	0.2085	2.250
2yoh	B-211	THYMIDYLATE KINASE;	WMJ	1.60	0.57 / 0.43	0.54 / 0.00 / 0.28 / 0.18	4.86	1.96 / 5.11 / 5.09	0.1670	0.1648	0.1671	0.2080	0.2049	0.2067	1.730
2g8j	A-400	CALPAIN-1 CATALYTIC SUBUNIT;	D7G	1.61	0.59 / 0.41	0.29 / 0.17 / 0.54 / 0.00	4.39	2.01 / 2.02 / 1.56	0.1672	0.1705	0.1692	0.1931	0.1942	0.1928	3.890
4mkt	A-702	LEUKOTRIENE A4 HYDROLASE;	28T	1.62	0.49 / 0.51	0.55 / 0.45	0.83	1.19	0.1551	0.1539	0.1542	0.1870	0.1841	0.1847	5.820
4mkt	A-703	LEUKOTRIENE A4 HYDROLASE;	1V6	1.62	0.55 / 0.45	0.59	1.32		0.1530	0.1539	0.1548	0.1848	0.1841	0.1848	0.020
2vwx	A-1889	EPHRIN TYPE-B RECEPTOR 4;	7X4	1.65	0.57 / 0.43	0.60 / 0.40	2.77	2.77	0.1615	0.1616	0.1607	0.2090	0.2106	0.1607	0.290
2vwy	A-1889	EPHRIN TYPE-B RECEPTOR 4;	7X5	1.65	0.39 / 0.61	0.49 / 0.00 / 0.51	2.76	0.79 / 2.69	0.1915	0.1903	0.1933	0.2402	0.2395	0.2415	0.620
2vwz	A-1889	EPHRIN TYPE-B RECEPTOR 4;	7X6	1.65	0.64 / 0.36	0.97	3.41		0.1652	0.1626	0.1649	0.2015	0.2024	0.2014	0.040
2vx1	A-1889	EPHRIN TYPE-B RECEPTOR 4;	7X8	1.65	0.60 / 0.40	0.62 / 0.38	2.35	2.11	0.1677	0.1671	0.1689	0.2067	0.2063	0.2061	-0.050
4121	A-702	LEUKOTRIENE A4 HYDROLASE;	1V6	1.65	0.54 / 0.46	0.59 / 0.41	1.16	1.17	0.1374	0.1373	0.1366	0.1599	0.1587	0.1592	-0.730
2r3p	A-501	CELL DIVISION PROTEIN KINASE 2;	3SC	1.66	0.45 / 0.55	0.22 / 0.52 / 0.26	1.63	1.81 / 0.57	0.1760	0.1716	0.1787	0.2212	0.2204	0.2208	-3.490
1exx	A-450	RETINOIC ACID RECEPTOR GAMMA-2;	961	1.67	0.48 / 0.52	0.66 / 0.34	1.24	1.30	0.1681	0.1639	0.1615	0.2066	0.2066	0.2066	1.250
3w7r	A-408	DIHYDROORotate DEHYDROGENASE (QUINONE), MITOCHONDRIAL;	W7A	1.68	0.55 / 0.45	0.38 / 0.62	2.68	1.15	0.1451	0.1412	0.1417	0.1735	0.1684	0.1712	-0.380
4ek8	A-301	CYCLIN-DEPENDENT KINASE 2;	16K	1.70	0.49 / 0.51	0.47 / 0.00 / 0.53	2.5	2.25 / 2.53	0.1855	0.1784	0.1823	0.2200	0.2216	0.2208	0.550
4qsj	B-302	CARBONIC ANHYDRASE 13;	EWW	1.70	0.59 / 0.41	0.54 / 0.44 / 0.03	3.99	2.98 / 1.85	0.1569	0.1541	0.1534	0.1893	0.1884	0.1898	3.440
4pqn	A-701	TYROSINE-PROTEIN KINASE ITK/TSK;	2W6	1.71	0.53 / 0.47	0.50 / 0.21 / 0.00 / 0.29	0.71	0.68 / 0.55 / 0.97	0.1695	0.1627	0.1659	0.2026	0.2013	0.2015	1.130
2vip	A-1247	UROKINASE-TYPE PLASMINOGEN ACTIVATOR CHAIN B;	L1R	1.72	0.51 / 0.49	0.58 / 0.42	2.86	2.82	0.2238	0.2216	0.2238	0.2897	0.2861	0.2875	-0.620
4ms6	A-702	LEUKOTRIENE A4 HYDROLASE;	28T	1.72	0.43 / 0.57	0.42 / 0.00 / 0.58	0.78	1.33 / 1.05	0.1757	0.1747	0.1839	0.2137	0.2122	0.2166	4.810

PDBID	Ligand	Receptor	Ligand Code	Resolution (Å)	Occupancies (deposited re-refined)	Occupancies (qFit refined)	RMSD vs A conformer (Å) (deposited re-refined)	RMSD vs A conformer (Å) (qFit refined)	R-work (single refined)	R-work (deposited re-refined)	R-work (qFit refined)	R-free (single refined)	R-free (deposited re-refined)	R-free (qFit refined)	Ligand Energy (kcal/mol) qFit confs relative to single conf
1q2o	A-790	NITRIC-OXIDE SYNTHASE, ENDOTHELIAL;	DP1	1.74	0.43 / 0.57	0.65 / 0.35	2.07	1.29	0.1592	0.1581	0.1581	0.1898	0.1879	0.1884	-3.680
2x9f	A-1889	DIHYDROFOLATE REDUCTASE;	X9F	1.75	0.45 / 0.55	0.23 / 0.77	0.56	0.59	0.1607	0.1602	0.1547	0.2031	0.2016	0.2027	-0.780
3elj	A-365	MITOGEN-ACTIVATED PROTEIN KINASE 8;	GS7	1.80	0.57 / 0.43	0.05 / 0.31 / 0.30 / 0.34	0.72	0.81 / 0.58 / 0.71	0.1664	0.1649	0.1671	0.1990	0.1951	0.1967	2.270
3s7a	A-192	DIHYDROFOLATE REDUCTASE;	684	1.80	0.38 / 0.62	0.69 / 0.31	0.78	0.64	0.2239	0.2213	0.2259	0.2664	0.2685	0.2678	-2.310
3nm0	A-800	NITRIC OXIDE SYNTHASE, BRAIN;	3XE	1.81	0.62 / 0.38	0.40 / 0.60	1.56	0.72	0.1922	0.1940	0.1915	0.2223	0.2225	0.2217	2.330
2xnb	A-1299	CELL DIVISION PROTEIN KINASE 2;	Y8L	1.85	0.77 / 0.23	0.85 / 0.15	1.58	1.63	0.2592	0.2567	0.2637	0.3112	0.3085	0.3177	-0.250
3nlx	A-800	NITRIC OXIDE SYNTHASE, BRAIN;	3XB	1.87	0.64 / 0.36	0.70 / 0.30	1.33	1.08	0.1952	0.1924	0.1892	0.2253	0.2248	0.2257	0.270
1zsk	A-301	COAGULATION FACTOR XI;	421	1.90	0.77 / 0.23	0.66 / 0.34 / 0.00	0.9	1.08 / 0.42	0.1509	0.1489	0.1507	0.1925	0.1917	0.1932	4.570
1zzq	A-799	NITRIC-OXIDE SYNTHASE, BRAIN;	DP9	1.90	0.55 / 0.45	0.17 / 0.37 / 0.46	2.67	1.79 / 0.94	0.1866	0.1930	0.1894	0.2185	0.2184	0.2174	-1.390
2xmy	A-500	CELL DIVISION PROTEIN KINASE 2;	CDK	1.90	0.48 / 0.52	0.24 / 0.32 / 0.13 / 0.31	1.64	1.50 / 0.98 / 1.59	0.2591	0.2459	0.2489	0.3183	0.3085	0.3046	-0.460
3nlz	A-800	NITRIC OXIDE SYNTHASE, BRAIN;	3XD	1.92	0.65 / 0.35	0.28 / 0.33 / 0.12 / 0.28	1.58	2.08 / 1.65 / 1.95	0.1903	0.1880	0.1837	0.2220	0.2218	0.2203	-1.230
4iwf	A-601	ESTROGEN RECEPTOR;	15Q	1.93	0.25 / 0.75	0.00 / 0.45 / 0.55	2.81	1.02 / 1.61	0.1902	0.1868	0.1780	0.2226	0.2222	0.2230	3.750
3jt8	A-800	NITRIC OXIDE SYNTHASE, BRAIN;	JM4	1.95	0.63 / 0.37	0.30 / 0.46 / 0.24	1.19	1.09 / 0.86	0.2146	0.2130	0.2076	0.2382	0.2376	0.2386	1.720
		CAMP-DEPENDENT PROTEIN KINASE CATALYTIC SUBUNIT ALPHA;													
3vqh	A-401	IQB	1.95	0.51 / 0.49	0.64 / 0.36 / 0.00	1.1	0.80 / 0.64	0.1816	0.1787	0.1799	0.2149	0.2150	0.2155	0.800	
3pne	A-800	NITRIC OXIDE SYNTHASE, BRAIN;	8AX	1.97	0.58 / 0.42	0.67 / 0.33	1.28	0.65	0.2053	0.2024	0.1980	0.2369	0.2360	0.2382	-0.010
1h1r	A-1298	CELL DIVISION PROTEIN KINASE 2;	6CP	2.00	0.41 / 0.59	0.15 / 0.27 / 0.58	1.43	1.14 / 1.50	0.2218	0.2260	0.2231	0.2623	0.2634	0.2619	-1.690
2jjk	A-1336	FRUCTOSE-1,6-BISPHOSPHATASE 1;	R15	2.00	0.37 / 0.63	0.47 / 0.20 / 0.13 / 0.20	0.56	0.56 / 0.83 / 3.14	0.2159	0.2141	0.2178	0.2630	0.2625	0.2635	1.940
3o57	A-506	CAMP-SPECIFIC 3',5'-CYCLIC PHOSPHODIESTERASE 4B;	ZG2	2.00	0.50 / 0.50	0.03 / 0.52 / 0.45	0.99	1.22 / 1.24	0.1969	0.1950	0.1967	0.2432	0.2389	0.2438	5.040
3p4v	A-300	CARBONIC ANHYDRASE 2;	PMX	2.00	0.41 / 0.59	0.33 / 0.67	1.53	1.63	0.1569	0.1562	0.1583	0.1878	0.1880	0.1882	-0.070
4fod	A-1501	ALK TYROSINE KINASE RECEPTOR;	0UV	2.00	0.54 / 0.46	0.53 / 0.11 / 0.36	4.13	4.37 / 4.31	0.1734	0.1720	0.1722	0.2198	0.2214	0.2210	-6.860
		DIHYDROORotate DEHYDROGENASE (QUINONE), MITOCHONDRIAL;													
4js3	A-403	JS3	2.00	0.44 / 0.56	0.49 / 0.51	1.76	1.75	0.1498	0.1490	0.1500	0.1750	0.1745	0.1754	0.120	
5agk	A-801	NITRIC OXIDE SYNTHASE, BRAIN;	RGE	2.00	0.82 / 0.18	0.53 / 0.47	0.53	2.23	0.1972	0.1928	0.1939	0.2346	0.2318	0.2340	2.150
		CAMP-DEPENDENT PROTEIN KINASE CATALYTIC SUBUNIT ALPHA;													
3p0m	A-351	4SB	2.03	0.46 / 0.54	0.53 / 0.04 / 0.43	0.51	0.91 / 0.69	0.1784	0.1772	0.1785	0.2066	0.2066	0.2066	1.090	
4jsf	A-803	NITRIC OXIDE SYNTHASE, BRAIN;	QJ4	2.05	0.55 / 0.45	0.45 / 0.24 / 0.30	1.54	4.83 / 3.91	0.1926	0.1922	0.1932	0.2228	0.2238	0.2255	1.010
1u9x	A-300	CATHEPSIN K;	IHJ	2.10	0.48 / 0.52	0.34 / 0.05 / 0.30 / 0.31	1.49	2.15 / 2.02 / 3.78	0.1669	0.1529	0.1688	0.1974	0.1957	0.2040	4.250
2c5n	A-1297	CELL DIVISION PROTEIN KINASE 2;	CK8	2.10	0.41 / 0.59	0.23 / 0.28 / 0.30 / 0.19	1.6	1.68 / 0.61 / 1.52	0.1921	0.1895	0.1984	0.2511	0.2486	0.2570	0.350
2c5o	A-1297	CELL DIVISION PROTEIN KINASE 2;	CK2	2.10	0.53 / 0.47	0.51 / 0.49	1.98	2.00	0.1953	0.1971	0.1932	0.2391	0.2390	0.2408	0.030
3jt7	A-800	NITRIC OXIDE SYNTHASE, BRAIN;	JM5	2.10	0.54 / 0.46	0.52 / 0.29 / 0.20	1.14	1.52 / 0.76	0.1882	0.1898	0.1881	0.2248	0.2245	0.2261	-0.520
4b85	A-600	ACETYLCHOLINESTERASE;	B3W	2.10	0.56 / 0.44	0.45 / 0.00 / 0.55	2.37	1.15 / 1.21	0.1905	0.1906	0.1903	0.2107	0.2122	0.2114	3.340
4iwv	A-503	GLUCOKINASE ISOFORM 3;	1J9	2.10	0.46 / 0.54	0.41 / 0.10 / 0.49	1.3	0.97 / 1.25	0.2108	0.2113	0.2107	0.2531	0.2546	0.2560	0.620
3ufo	B-800	NITRIC OXIDE SYNTHASE, BRAIN;	HW4	2.17	0.55 / 0.45	0.00 / 0.33 / 0.35 / 0.32	3.23	2.40 / 3.45 / 2.92	0.2215	0.2228	0.2185	0.2540	0.2542	0.2580	4.460
1j1a	A-1301	BHP	2.20	0.26 / 0.74	0.17 / 0.34 / 0.08 / 0.42	2.4	1.36 / 2.22 / 1.96	0.2196	0.2242	0.2190	0.2502	0.2516	0.2551	3.180	
1xdd	A-401	INTEGRIN ALPHA-L;	AAV	2.20	0.46 / 0.54	0.56 / 0.32 / 0.00 / 0.12	1.61	1.77 / 1.53 / 1.18	0.1607	0.1581	0.1594	0.1940	0.1951	0.1974	3.070
		MITOGEN-ACTIVATED PROTEIN KINASE 1;	EK6	2.20	0.51 / 0.49	0.29 / 0.20 / 0.10 / 0.11 / 0.30	1.25	2.40 / 2.15 / 2.14 / 2.57	0.1828	0.1830	0.1878	0.2328	0.2318	0.2358	0.750
		DIHYDROORotate DEHYDROGENASE (QUINONE), MITOCHONDRIAL;													
4jts	A-412	JTS	2.21	0.47 / 0.53	0.62 / 0.38	1.58	1.53	0.1522	0.1503	0.1531	0.1796	0.1786	0.1799	0.310	
4bcg	A-1299	T3C	2.26	0.51 / 0.49	0.18 / 0.43 / 0.15 / 0.24	4.01	3.56 / 0.64 / 1.84	0.1851	0.1865	0.1923	0.2231	0.2224	0.2248	1.000	
4ftt	A-301	6HK	2.30	0.30 / 0.70	0.63 / 0.27 / 0.10	1.16	2.12 / 1.46	0.1655	0.1651	0.1609	0.2064	0.2048	0.2076	3.030	
		PHOSPHATIDYLINOSITOL-4,5-BISPHOSPHATE 3-KINASE CATALYTIC													
4anw	A-1189	092	2.31	0.69 / 0.31	0.56 / 0.26 / 0.18	1.39	1.67 / 1.62	0.2321	0.2288	0.2291	0.2829	0.2865	0.2799	7.150	
2qlq	A-1345	SR2	2.33	0.67 / 0.33	0.96	1.41		0.1990	0.1963	0.1412	0.2452	0.2496	0.2477	-0.010	
4b0o	A-1307	15F	2.35	0.55 / 0.45	0.19 / 0.35 / 0.46	3.17	1.56 / 3.37	0.1740	0.1760	0.1767	0.2165	0.2163	0.2169	0.270	
4btu	B-1246	6XS	2.37	0.72 / 0.28	0.57 / 0.16 / 0.27	2.37	1.37 / 1.04	0.2118	0.2112	0.2083	0.2745	0.2739	0.2788	3.550	

PDBID	Ligand	Receptor	Ligand Code	Resolution (Å)	Occupancies (deposited re-refined)	Occupancies (qFit refined)	RMSD vs A conformer (Å) (deposited re-refined)	RMSD vs A conformer (Å) (qFit refined)	R-work (single refined)	R-work (deposited re-refined)	R-work (qFit refined)	R-free (single refined)	R-free (deposited re-refined)	R-free (qFit refined)	Ligand Energy (kcal/mol) qFit confs relative to single conf
4o1z	A-807	PROSTAGLANDIN G/H SYNTHASE 1;	MXM	2.40	0.14 / 0.86	0.46 / 0.54	1.09	1.14	0.2619	0.2633	0.2619	0.2921	0.2904	0.2927	1.380
3s9s	A-1	PEROXISOME PROLIFERATOR-ACTIVATED RECEPTOR GAMMA; RETINOIC ACID RECEPTOR RXR-ALPHA;	M0T	2.55	0.60 / 0.40	0.67 / 0.33	1.23	0.88	0.2395	0.2365	0.2382	0.2792	0.2853	0.2847	0.110
1xvp	D-1003	SERINE/THREONINE-PROTEIN KINASE 6;	CID	2.60	0.65 / 0.35	0.27 / 0.73	1.1	1.57	0.2948	0.3022	0.2994	0.3341	0.3373	0.3355	0.720
2xng	A-1391	SERINE/THREONINE-PROTEIN KINASE CHK2;	A0H	2.60	0.49 / 0.51	0.52 / 0.48	1.69	1.9	0.2260	0.2260	0.2250	0.2682	0.2706	0.2733	1.650
4a9s	A-1515	ACETYLCHOLINESTERASE;	RU9	2.66	0.40 / 0.60	0.42 / 0.58	2.98	3.10	0.2035	0.2095	0.2059	0.2560	0.2541	0.2558	-0.380
2xup	A-1548	RENIN;	TZ5	2.70	0.48 / 0.52	0.39 / 0.61	3.59	3.73	0.2036	0.2073	0.2126	0.2347	0.2321	0.2361	0.810
3vyf	A-402		VYF	2.80	0.55 / 0.45	0.24 / 0.30 / 0.19 / 0.28	0.9	2.64 / 2.57 / 2.45	0.2108	0.2121	0.2115	0.2529	0.2513	0.2518	1.770
												mean	0.2048	0.2038	0.2043
												t_test	0.4577	0.5136	

PDB	Ligand	Resolution (Å)	Twilight score	Rwork	Rfree	Occupancy (deposited)	Occupancy (qFit)	RMSD A->B (Å) (deposited)	RMSD A->B (qFit)	Best Fisher z improvement
5a6h	A-1266	1.57	0.713	0.15	0.19	0.70	0.26 / 0.20 / 0.27		6.14 / 6.65	6.55
5ghn	B-201	1.39	0.855	0.15	0.19	1.00	0.38 / 0.20 / 0.20 / 0.22		1.99 / 2.53 / 3.68	4.60
5ih8	A-401	1.85	0.676	0.18	0.20	1.00	0.20 / 0.23 / 0.30 / 0.20		3.26 / 3.09 / 1.38	4.44
5kk4	C-101	1.70	0.718	0.18	0.21	1.00	0.35 / 0.20 / 0.44		2.97 / 3.69	4.38
5l4i	A-201	1.45	0.775	0.14	0.18	0.45	0.42 / 0.37		3.37	4.34
5jbb	S-302	1.56	0.710	0.16	0.19	1.00	0.34 / 0.20 / 0.36		2.50 / 2.56	4.34
5dlv	A-930	2.00	0.688	0.19	0.23	0.34 / 0.33 / 0.33	0.34 / 0.27 / 0.38	3.03 / 4.29	1.22 / 3.33	4.33
4z7m	B-302	1.43	0.763	0.25	0.31	1.00	0.47 / 0.53		0.61	4.18
5e1g	A-501	1.85	0.709	0.20	0.23	1.00	0.20 / 0.20 / 0.20 / 0.20		1.47 / 3.79 / 4.11	4.02
5jxq	A-405	1.20	0.797	0.14	0.16	0.84	0.57 / 0.21 / 0.22		4.00 / 3.87	3.92
5i9y	A-1001	1.23	0.782	0.16	0.18	0.45 / 0.55	0.30 / 0.20 / 0.47	1.53	0.92 / 1.54	3.87
5t77	A-522	2.00	0.705	0.19	0.21	1.00	0.25 / 0.48 / 0.20		3.35 / 0.41	3.81
5c8x	A-301	1.80	0.682	0.15	0.17	0.94	0.23 / 0.45 / 0.26		2.44 / 1.98	3.72
5ivj	A-601	1.57	0.723	0.16	0.19	0.50 / 0.50	0.33 / 0.20 / 0.20 / 0.21	3.24	3.47 / 3.12 / 2.77	3.70
5lia	A-908	1.92	0.649	0.16	0.20	1.00	0.41 / 0.27 / 0.26		1.60 / 1.29	3.50
5fok	A-1721	1.90	0.684	0.19	0.21	1.00	0.34 / 0.46 / 0.20		4.44 / 1.37	3.49
5ep7	A-1201	1.20	0.799	0.17	0.18	0.50 / 0.50	0.56 / 0.35	0.98	0.87	3.47
4uef	A-1419	1.69	0.689	0.16	0.19	1.00	0.20 / 0.25 / 0.31 / 0.20		4.08 / 1.36 / 3.75	3.46
5k2c	A-1225	1.90	0.722	0.17	0.21	1.00	0.20 / 0.26 / 0.54		2.91 / 4.74	3.46
5fw0	B-800	1.80	0.691	0.19	0.23	1.00	0.20 / 0.24 / 0.36 / 0.20		2.66 / 2.75 / 2.41	3.42
5jcu	C-112	1.93	0.701	0.18	0.24	0.57	0.20 / 0.80		2.12	3.27
5g28	A-1269	1.57	0.768	0.15	0.19	1.00	0.45 / 0.55		2.78	3.26
5kn7	B-415	1.99	0.725	0.21	0.27	1.00	0.26 / 0.20 / 0.29 / 0.25		5.04 / 4.80 / 5.71	3.26
5e4o	B-201	1.50	0.727	0.19	0.21	0.43	0.46 / 0.29 / 0.24		1.97 / 2.07	3.25
5da3	A-503	1.70	0.699	0.20	0.23	0.50 / 0.50	0.30 / 0.27 / 0.26	1.24	1.51 / 0.90	3.22
5hvs	C-202	1.75	0.710	0.17	0.21	1.00	0.50 / 0.20 / 0.27		2.53 / 3.66	3.22
5lf1	N-307	2.00	0.644	0.18	0.21	1.00	0.83			3.20
5c8x	B-301	1.80	0.680	0.15	0.17	0.87	0.37 / 0.28 / 0.29		5.78 / 2.27	3.16
5e4o	A-201	1.50	0.757	0.19	0.21	0.39	0.31 / 0.20 / 0.40		1.53 / 1.82	3.15
5k0f	B-302	1.81	0.667	0.17	0.21	0.58 / 0.42	0.20 / 0.20 / 0.20 / 0.40	2.26	0.79 / 0.54 / 2.10	3.14
5anv	A-1157	1.16	0.838	0.20	0.21	0.50 / 0.50	0.39 / 0.23 / 0.26	1.29	1.40 / 0.69	3.12
5fsk	A-1157	1.56	0.741	0.20	0.24	0.75	0.29 / 0.20 / 0.40		2.49 / 0.90	3.08
5cgq	B-401	1.18	0.785	0.14	0.16	1.00	0.49 / 0.47		1.16	3.00
5hfk	A-301	1.55	0.742	0.19	0.21	1.00	0.38 / 0.20 / 0.39		1.30 / 0.81	2.97
5eng	A-1201	1.30	0.785	0.16	0.17	1.00	0.29 / 0.20 / 0.24 / 0.20		3.19 / 0.84 / 3.17	2.93
4ywr	A-300	1.65	0.709	0.16	0.18	0.49 / 0.51	0.20 / 0.20 / 0.20 / 0.20 / 0.20	1.71	0.65 / 1.13 / 1.85 / 1.76	2.92
5jb8	S-302	1.45	0.742	0.15	0.19	1.00	0.26 / 0.20 / 0.20 / 0.20		3.06 / 2.96 / 0.80	2.89
5l4i	B-201	1.45	0.752	0.14	0.18	0.55	0.48 / 0.45		1.92	2.88
5u1h	A-201	1.50	0.739	0.17	0.20	1.00	0.25 / 0.21 / 0.27 / 0.20		3.28 / 3.23 / 1.34	2.87
5ehi	C-4000	1.30	0.765	0.19	0.21	0.50 / 0.50	0.41 / 0.39 / 0.20	0.57	0.77 / 4.08	2.87
5syt	A-505	2.00	0.690	0.22	0.25	1.00	0.22 / 0.78		1.14	2.86
5jyc	C-401	2.00	0.663	0.15	0.19	1.00	0.36 / 0.20 / 0.24 / 0.20		2.65 / 2.52 / 2.58	2.85
4xt8	A-302	1.95	0.655	0.18	0.22	1.00	0.30 / 0.20 / 0.30 / 0.20		0.34 / 2.85 / 3.78	2.83
5syt	A-508	2.00	0.680	0.22	0.25	1.00	0.40 / 0.40 / 0.20		2.72 / 2.55	2.78
5hbn	A-207	1.60	0.709	0.15	0.17	0.25 / 0.75	0.29 / 0.20 / 0.20 / 0.31	4.94	3.30 / 1.69 / 4.42	2.76
5ltr	A-59	1.21	0.782	0.16	0.18	1.00	0.50 / 0.49		1.18	2.75
5jr3	C-401	1.84	0.669	0.16	0.18	1.00	0.38 / 0.20 / 0.42		1.33 / 0.89	2.70
5lf1	K-306	2.00	0.643	0.18	0.21	1.00	0.33 / 0.23 / 0.44		1.15 / 2.40	2.70
5lf7	K-305	2.00	0.656	0.18	0.21	1.00	0.26 / 0.20 / 0.25 / 0.20		0.96 / 1.19 / 2.50	2.70
5c41	A-401	1.95	0.640	0.17	0.21	0.50 / 0.50	0.20 / 0.20 / 0.20 / 0.20 / 0.20	1.94	1.86 / 1.05 / 1.99 / 1.12	2.70
5ia3	A-1001	1.79	0.674	0.16	0.20	0.49 / 0.51	0.33 / 0.24 / 0.20 / 0.20	1.84	1.88 / 0.65 / 1.76	2.69
5er5	A-103	1.26	0.891	0.15	0.19	0.50	0.28 / 0.24 / 0.37		0.87 / 4.45	2.68
5c5o	A-401	1.50	0.843	0.25	0.27	1.00	0.20 / 0.20 / 0.20 / 0.20 / 0.20		2.49 / 2.26 / 4.56 / 4.87	2.68
4uef	B-1419	1.69	0.691	0.16	0.19	1.00	0.26 / 0.20 / 0.20 / 0.27		3.48 / 4.15 / 1.32	2.67
5c7y	B-301	1.75	0.733	0.15	0.18	0.85	0.35 / 0.20 / 0.20 / 0.21		2.81 / 2.34 / 2.84	2.62
5k2d	A-1203	1.90	0.655	0.17	0.21	1.00	0.20 / 0.80		1.08	2.62
5fag	B-502	1.51	0.716	0.20	0.23	1.00	0.52 / 0.37		1.35	2.61
5k9c	A-402	1.66	0.696	0.13	0.15	0.40 / 0.60	0.33 / 0.20 / 0.33	0.78	0.65 / 0.98	2.58
5c81	A-301	1.80	0.693	0.15	0.18	0.87	0.27 / 0.27 / 0.21		2.11 / 2.16	2.57
5kgj	A-407	1.90	0.672	0.17	0.22	0.50	0.35 / 0.33		1.44	2.55
4yyv	A-306	1.90	0.665	0.17	0.24	0.50	0.20 / 0.20 / 0.32 / 0.26		1.36 / 1.43 / 1.25	2.52

PDB	Ligand	Resolution (Å)	Twilight score	Rwork	Rfree	Occupancy (deposited)	Occupancy (qFit)	RMSD A->B (Å) (deposited)	RMSD A->B (qFit)	Best Fisher z improvement
5e28	A-302	1.30	0.780	0.18	0.20	1.00	0.53 / 0.47		1.21	2.48
4y1y	A-202	1.86	0.787	0.20	0.23	1.00	0.27 / 0.25 / 0.20 / 0.20		2.18 / 2.57 / 1.55	2.47
5lf1	b-306	2.00	0.640	0.18	0.21	1.00	0.34 / 0.20 / 0.24		2.04 / 0.45	2.46
5u20	A-184	1.50	0.716	0.14	0.18	1.00	0.31 / 0.29 / 0.20 / 0.20		1.17 / 0.95 / 0.71	2.46
5fra	C-201	2.00	0.633	0.18	0.21	1.00	0.34 / 0.25 / 0.20 / 0.20		1.10 / 1.06 / 0.94	2.45
5l9i	A-401	1.90	0.652	0.18	0.21	1.00	0.22 / 0.39 / 0.36		1.26 / 0.98	2.45
5htv	A-501	1.78	0.717	0.17	0.20	1.00	0.21 / 0.20 / 0.25 / 0.20		1.89 / 1.57 / 1.78	2.44
5k2c	A-1227	1.90	0.692	0.17	0.21	1.00	0.29 / 0.71		1.23	2.44
5fw0	A-800	1.80	0.683	0.19	0.23	1.00	0.35 / 0.20 / 0.45		3.09 / 3.24	2.43
5g10	B-1381	1.71	0.733	0.16	0.19	1.00	0.28 / 0.26 / 0.34		3.43 / 1.19	2.43
5fvn	D-405	1.45	0.815	0.16	0.18	1.00	0.24 / 0.76		1.08	2.42
4xjm	B-501	1.60	0.732	0.20	0.22	1.00	0.61 / 0.27		3.25	2.41
5ecm	B-301	1.60	0.708	0.23	0.25	1.00	0.65 / 0.35		0.90	2.40
5jf1	A-301	2.00	0.653	0.15	0.20	1.00	0.23 / 0.20 / 0.55		1.25 / 1.34	2.40
5lyi	A-404	1.64	0.690	0.17	0.21	1.00	0.51 / 0.48		0.63	2.40
5adw	A-312	1.90	0.665	0.23	0.26	1.00	0.20 / 0.76		0.65	2.40
5cu3	A-404	1.79	0.705	0.18	0.20	1.00	0.36 / 0.20 / 0.20 / 0.22		1.23 / 1.69 / 1.04	2.39
5a27	A-1002	1.37	0.746	0.15	0.18	1.00	0.60 / 0.20 / 0.20		1.68 / 3.56	2.37
5c5n	A-401	1.69	0.860	0.29	0.32	1.00	0.25 / 0.23 / 0.23		1.56 / 3.08	2.34
5l9o	A-301	1.84	0.694	0.22	0.25	1.00	0.33 / 0.20 / 0.27 / 0.20		1.64 / 1.53 / 1.30	2.33
5li7	A-502	1.58	0.711	0.17	0.20	1.00	0.33 / 0.67		0.94	2.32
5jsq	B-301	1.50	0.720	0.16	0.18	0.59 / 0.41	0.44 / 0.43	1.20	1.04	2.32
5csd	B-202	1.45	0.851	0.18	0.20	1.00	0.47 / 0.20 / 0.32		1.89 / 1.64	2.29
5exb	H-64	1.81	0.668	0.18	0.25	1.00	0.37 / 0.20 / 0.42		1.24 / 1.39	2.28
5exb	I-64	1.81	0.666	0.18	0.25	1.00	0.61 / 0.36		1.31	2.26
5cbu	A-205	1.40	0.759	0.17	0.20	0.50 / 0.50	0.43 / 0.36	1.64	0.76	2.26
5j7p	B-201	1.85	0.697	0.18	0.20	0.90	0.50 / 0.33		0.91	2.23
5c1u	B-201	1.49	0.746	0.18	0.21	1.00	0.20 / 0.36 / 0.32		2.95 / 2.67	2.23
5jcw	A-301	1.95	0.660	0.15	0.19	1.00	0.20 / 0.20 / 0.20 / 0.20 / 0.20		1.88 / 1.06 / 0.94 / 1.75	2.22
5ja7	B-301	1.61	0.770	0.18	0.22	1.00	0.20 / 0.25 / 0.38		2.12 / 1.40	2.22
5g4n	B-1293	1.35	0.848	0.15	0.17	0.53 / 0.47	0.30 / 0.35 / 0.22	0.69	1.39 / 0.68	2.21
5iu8	A-2425	2.00	0.690	0.18	0.20	1.00	0.56 / 0.44		2.18	2.21
5ee8	A-303	1.54	0.803	0.15	0.18	0.80	0.25 / 0.20 / 0.34		0.42 / 1.04	2.21
5ewy	A-301	1.40	0.764	0.15	0.17	1.00	0.52 / 0.39		0.91	2.19
5exb	G-64	1.81	0.666	0.18	0.25	1.00	0.45 / 0.22 / 0.34		1.32 / 1.11	2.19
5jcu	D-301	1.93	0.653	0.18	0.24	1.00	0.39 / 0.20 / 0.20 / 0.20		1.04 / 1.05 / 1.74	2.17
5b2f	B-302	1.90	0.652	0.22	0.27	1.00	0.31 / 0.59		1.39	2.16
4yqu	B-301	1.94	0.668	0.20	0.24	1.00	0.20 / 0.20 / 0.48		1.35 / 2.26	2.15
5c5o	B-401	1.50	0.852	0.25	0.27	1.00	0.41 / 0.39		4.23	2.15
5e0r	A-205	1.35	0.787	0.17	0.20	1.00	0.29 / 0.20 / 0.27		1.18 / 1.57	2.15
5e1c	B-901	1.98	0.639	0.18	0.21	1.00	0.64 / 0.31		1.10	2.14
5hbg	B-46	1.90	0.651	0.19	0.22	1.00	0.66 / 0.34		1.20	2.14
5ee8	A-301	1.54	0.716	0.15	0.18	0.50 / 0.50	0.38 / 0.22 / 0.36	0.89	2.46 / 0.89	2.14
5bqh	A-201	1.60	0.759	0.15	0.17	1.00	0.40 / 0.20 / 0.32		1.17 / 0.65	2.13
5lt8	A-1804	1.57	0.705	0.17	0.22	1.00	0.46 / 0.26 / 0.20		0.77 / 0.60	2.13
5lf7	G-161	2.00	0.641	0.18	0.21	1.00	0.31 / 0.56		0.68	2.13
5js3	E-411	1.16	0.791	0.10	0.12	0.36 / 0.64	0.49 / 0.20 / 0.31	0.39	0.98 / 1.25	2.13
5h9s	B-201	1.82	0.727	0.18	0.23	1.00	0.40 / 0.46		2.03	2.13
5kdo	A-401	1.90	0.645	0.18	0.21	1.00	0.70 / 0.30		0.93	2.12
5evz	B-503	1.85	0.653	0.17	0.21	1.00	0.53 / 0.45		0.93	2.12
5lf1	H-305	2.00	0.640	0.18	0.21	1.00	0.52 / 0.34		0.63	2.12
5ewk	A-301	1.60	0.715	0.15	0.18	1.00	0.41 / 0.29 / 0.26		3.00 / 3.17	2.10
5hvs	A-203	1.75	0.697	0.17	0.21	1.00	0.36 / 0.20 / 0.20 / 0.20		1.81 / 1.74 / 1.91	2.10
4zqc	A-302	1.54	0.726	0.14	0.19	0.80	0.49 / 0.26		1.70	2.10
5l2f	C-301	1.77	0.701	0.18	0.19	1.00	0.52 / 0.26 / 0.20		1.76 / 1.79	2.10
5tf5	A-263	1.81	0.728	0.22	0.25	1.00	0.30 / 0.20 / 0.27		1.64 / 1.35	2.09
5g4s	A-1739	1.60	0.727	0.19	0.19	0.50 / 0.50	0.48 / 0.20 / 0.28	1.70	2.02 / 1.67	2.09
4xjm	A-501	1.60	0.752	0.20	0.22	1.00	0.20 / 0.20 / 0.20 / 0.20		1.96 / 1.38 / 3.59	2.08
4d76	A-1247	1.77	0.678	0.18	0.21	1.00	0.55 / 0.20 / 0.22		0.94 / 1.11	2.07
4y0i	B-502	1.66	0.694	0.17	0.20	0.90	0.43 / 0.42		0.71	2.07
5tb6	A-1201	1.79	0.680	0.17	0.24	1.00	0.55 / 0.41		1.19	2.07

PDB	Ligand	Resolution (Å)	Twilight score	Rwork	Rfree	Occupancy (deposited)	Occupancy (qFit)	RMSD A->B (Å) (deposited)	RMSD A->B (qFit)	Best Fisher z improvement
5bqh	A-202	1.60	0.700	0.15	0.17	1.00	0.50 / 0.46		0.77	2.06
5e0r	A-201	1.35	0.760	0.17	0.20	1.00	0.48 / 0.35		0.88	2.05
5dtz	C-68	1.50	0.718	0.17	0.20	1.00	0.51 / 0.40		1.18	2.05
5i4f	A-302	1.55	0.776	0.17	0.19	0.50 / 0.50	0.50 / 0.38	6.19	1.26	2.04
5eck	B-301	1.54	0.708	0.16	0.18	1.00	0.51 / 0.43		0.79	2.03
5jxn	E-411	1.38	0.751	0.11	0.14	0.40 / 0.60	0.28 / 0.20 / 0.48	0.36	3.01 / 1.06	2.03
4yh2	C-301	1.72	0.692	0.16	0.19	1.00	0.42 / 0.20 / 0.27		1.04 / 0.87	2.03
5hbn	A-206	1.60	0.700	0.15	0.17	1.00	0.21 / 0.34 / 0.24 / 0.21		1.90 / 1.85 / 2.07	2.02
4z15	C-2	1.60	0.705	0.18	0.21	1.00	0.39 / 0.20 / 0.41		1.00 / 1.02	2.02
5e1i	A-502	2.00	0.682	0.19	0.23	1.00	0.22 / 0.24 / 0.32		0.97 / 1.31	2.02
4zu5	B-201	1.80	0.687	0.21	0.24	0.50	0.26 / 0.25 / 0.25 / 0.24		5.72 / 5.76 / 5.75	2.00
5iy5	J-101	2.00	0.676	0.17	0.21	1.00	0.25 / 0.21 / 0.45		0.51 / 2.71	2.00
4xcf	H-301	1.43	0.742	0.14	0.17	1.00	0.21 / 0.25 / 0.20 / 0.29		3.03 / 1.28 / 3.18	1.99
5l9o	B-301	1.84	0.682	0.22	0.25	1.00	0.46 / 0.24 / 0.30		1.20 / 1.52	1.98
5fvn	C-429	1.45	0.756	0.16	0.18	1.00	0.48 / 0.20 / 0.32		0.84 / 0.94	1.98
4zz0	A-1102	1.65	0.711	0.16	0.19	1.00	0.31 / 0.22 / 0.20 / 0.20		2.24 / 2.84 / 2.22	1.97
5i23	A-910	1.95	0.650	0.16	0.19	1.00	0.23 / 0.37 / 0.20 / 0.20		1.97 / 1.96 / 1.09	1.96
5mji	A-301	2.00	0.632	0.19	0.21	1.00	0.59 / 0.39		0.81	1.95
4ypm	A-801	1.85	0.659	0.18	0.20	1.00	0.61 / 0.36		0.81	1.95
5g44	A-1512	1.84	0.653	0.19	0.23	1.00	0.53 / 0.40		1.30	1.95
5ehe	A-306	1.50	0.749	0.18	0.21	1.00	0.23 / 0.30 / 0.23		1.79 / 1.09	1.95
5i19	A-601	1.79	0.674	0.19	0.23	1.00	0.49 / 0.39		0.93	1.95
5fafj	B-401	1.64	0.696	0.21	0.24	1.00	0.55 / 0.35		1.46	1.94
5g0o	A-800	1.85	0.675	0.19	0.23	1.00	0.30 / 0.28 / 0.20 / 0.23		3.78 / 3.78 / 2.26	1.94
5hmr	A-602	2.00	0.638	0.18	0.21	1.00	0.44 / 0.20 / 0.25		1.14 / 0.78	1.94
5syt	A-516	2.00	0.675	0.22	0.25	1.00	0.27 / 0.26 / 0.44		1.22 / 0.83	1.93
5csd	A-202	1.45	0.855	0.18	0.20	1.00	0.33 / 0.25 / 0.22 / 0.20		1.42 / 0.43 / 1.55	1.92
5b5t	D-600	1.70	0.693	0.18	0.19	1.00	0.34 / 0.21 / 0.25 / 0.20		1.09 / 2.37 / 2.92	1.92
4xcf	L-301	1.43	0.748	0.14	0.17	0.88	0.34 / 0.20 / 0.36		3.05 / 2.78	1.92
5hyk	A-501	1.83	0.692	0.21	0.26	1.00	0.40 / 0.33 / 0.20		2.59 / 0.65	1.90
5a6i	A-1124	1.86	0.699	0.20	0.27	0.50	0.28 / 0.24 / 0.26		2.93 / 2.81	1.89
5seyk	B-401	1.93	0.654	0.20	0.22	1.00	0.40 / 0.20 / 0.20 / 0.20		1.49 / 1.21 / 1.45	1.89
5cfw	A-201	1.15	0.863	0.19	0.21	1.00	0.24 / 0.20 / 0.24 / 0.32		1.15 / 0.84 / 2.31	1.89
5an1	C-1220	2.00	0.660	0.21	0.26	0.54 / 0.46	0.39 / 0.21 / 0.30	0.77	1.10 / 0.94	1.89
5jyc	D-401	2.00	0.657	0.15	0.19	1.00	0.35 / 0.34 / 0.31		1.10 / 2.19	1.89
5lgw	B-701	1.95	0.641	0.18	0.19	1.00	0.69 / 0.28		0.56	1.88
5fp1	A-1717	1.94	0.674	0.16	0.18	1.00	0.61 / 0.34		1.54	1.88
5syv	A-111	1.75	0.680	0.16	0.19	0.60 / 0.10	0.55 / 0.37	0.55	0.71	1.88
5j14	A-503	1.91	0.791	0.17	0.20	1.00	0.28 / 0.32 / 0.21		4.48 / 2.64	1.88
5ecx	A-202	1.95	0.696	0.22	0.27	1.00	0.27 / 0.21 / 0.37		1.35 / 1.08	1.87
5dj1	A-304	1.80	0.689	0.15	0.18	0.68	0.33 / 0.20 / 0.21		1.13 / 0.89	1.87
4xtp	A-304	1.97	0.670	0.20	0.25	1.00	0.32 / 0.33 / 0.35		1.38 / 0.80	1.86
5sz3	A-307	1.69	0.716	0.16	0.20	0.80	0.22 / 0.20 / 0.23		1.81 / 1.86	1.86
5dnk	B-601	1.90	0.652	0.20	0.25	1.00	0.54 / 0.26 / 0.20		4.14 / 1.27	1.86
5g6g	A-1367	1.98	0.647	0.17	0.22	1.00	0.49 / 0.26 / 0.23		2.61 / 1.09	1.85
5f05	D-302	1.70	0.682	0.14	0.18	1.00	0.61 / 0.29		0.72	1.84
5fag	C-401	1.51	0.716	0.20	0.23	1.00	0.20 / 0.25 / 0.49		1.49 / 1.23	1.84
5i7w	A-42	1.95	0.640	0.18	0.22	1.00	0.52 / 0.27 / 0.21		0.99 / 1.08	1.84
5f0z	A-402	1.75	0.830	0.15	0.19	1.00	0.45 / 0.28		1.75	1.83
5ieg	A-1003	1.82	0.664	0.18	0.20	0.61 / 0.39	0.33 / 0.38 / 0.20	3.58	2.76 / 0.43	1.83
5liw	X-403	1.75	0.672	0.18	0.21	1.00	0.38 / 0.20 / 0.20 / 0.20		3.55 / 3.62 / 4.24	1.83
5e1c	A-900	1.98	0.647	0.18	0.21	1.00	0.46 / 0.28 / 0.20		4.32 / 1.31	1.83
5i9l	A-401	1.80	0.679	0.21	0.24	1.00	0.35 / 0.24 / 0.20 / 0.20		0.87 / 0.92 / 0.69	1.83
5t77	A-530	2.00	0.731	0.19	0.21	1.00	0.27 / 0.20 / 0.24 / 0.28		1.45 / 1.28 / 2.95	1.83
5f8f	A-401	1.90	0.676	0.19	0.22	1.00	0.29 / 0.20 / 0.46		1.24 / 0.86	1.83
5ecr	B-301	1.72	0.696	0.26	0.28	1.00	0.52 / 0.47		1.16	1.83
5jt9	E-412	1.26	0.767	0.10	0.12		0.51 / 0.49		1.12	1.82
5f6b	A-201	1.31	0.863	0.20	0.24	1.00	0.23 / 0.22 / 0.20 / 0.36		1.67 / 1.87 / 1.64	1.82
5hkb	D-401	1.65	0.692	0.19	0.22	0.83	0.37 / 0.25 / 0.28		2.08 / 1.29	1.82
5ism	B-810	2.00	0.635	0.17	0.20	0.60 / 0.40	0.54 / 0.46	1.61	1.74	1.81
5d4n	A-201	1.60	0.703	0.21	0.24	0.50	0.55 / 0.33		1.04	1.81

PDB	Ligand	Resolution (Å)	Twilight score	Rwork	Rfree	Occupancy (deposited)	Occupancy (qFit)	RMSD A->B (Å) (deposited)	RMSD A->B (qFit)	Best Fisher z improvement
5eyk	A-401	1.93	0.649	0.20	0.22	1.00	0.20 / 0.20 / 0.20 / 0.20 / 0.20		1.29 / 1.12 / 1.75 / 0.48	1.81
5dl7	A-505	1.75	0.701	0.17	0.19	1.00	0.44 / 0.24 / 0.31		1.62 / 1.08	1.80
5syz	A-601	1.93	0.691	0.21	0.23	1.00	0.37 / 0.26 / 0.22		2.00 / 1.94	1.80
5f05	B-302	1.70	0.684	0.14	0.18	1.00	0.45 / 0.23 / 0.20		0.91 / 0.91	1.80
5i8b	A-1405	1.52	0.798	0.19	0.20	1.00	0.31 / 0.25 / 0.31		1.40 / 1.96	1.80
5ghm	B-201	1.50	0.881	0.17	0.20	1.00	0.21 / 0.24 / 0.20 / 0.26		1.24 / 2.55 / 2.39	1.79
5sxr	B-111	1.69	0.682	0.14	0.17	0.60 / 0.20	0.59 / 0.34	0.60	0.74	1.79
5exb	K-64	1.81	0.663	0.18	0.25	1.00	0.68 / 0.32		1.14	1.79
5lf4	N-307	1.99	0.640	0.18	0.22	1.00	0.59 / 0.29		0.56	1.79
5eaj	A-201	1.70	0.707	0.20	0.23	1.00	0.20 / 0.20 / 0.24 / 0.26		1.90 / 1.33 / 2.09	1.78
4zyz	A-1102	1.60	0.715	0.17	0.19	1.00	0.35 / 0.30 / 0.28		1.27 / 1.74	1.78
5hni	X-1401	1.71	0.783	0.23	0.25	1.00	0.22 / 0.24 / 0.20 / 0.20		1.15 / 1.19 / 1.34	1.78
5t6m	C-82	1.80	0.669	0.20	0.24	1.00	0.57 / 0.20 / 0.23		1.26 / 0.90	1.78
4z15	A-2	1.60	0.701	0.18	0.21	1.00	0.46 / 0.20 / 0.31		1.05 / 0.98	1.77
5hhw	A-1401	1.79	0.670	0.17	0.20	1.00	0.44 / 0.25 / 0.31		1.34 / 0.98	1.77
5syk	A-111	1.80	0.664	0.15	0.18	0.60 / 0.40	0.50 / 0.46	0.61	0.77	1.77
5tvc	C-302	1.93	0.697	0.19	0.23	1.00	0.48 / 0.41		1.02	1.76
5jcu	C-303	1.93	0.661	0.18	0.24	1.00	0.34 / 0.22 / 0.23 / 0.20		3.22 / 0.81 / 3.53	1.75
5dlw	A-905	1.80	0.707	0.19	0.22	1.00	0.20 / 0.32 / 0.28 / 0.20		1.68 / 0.97 / 1.01	1.74
5exz	A-305	1.90	0.656	0.15	0.20	0.65	0.29 / 0.20 / 0.20		0.67 / 2.52	1.74
5fij	G-301	1.82	0.682	0.16	0.21	0.84	0.29 / 0.52		1.44	1.74
5ltp	F-59	1.70	0.697	0.19	0.21	1.00	0.43 / 0.20 / 0.32		2.73 / 1.25	1.74
5eco	C-301	1.80	0.678	0.22	0.24	1.00	0.27 / 0.20 / 0.31 / 0.23		1.16 / 0.87 / 1.48	1.74
5exb	O-64	1.81	0.701	0.18	0.25	1.00	0.52 / 0.20 / 0.23		1.28 / 0.94	1.73
5euA	B-301	1.85	0.735	0.17	0.22	0.80	0.20 / 0.23 / 0.20 / 0.23		2.00 / 0.75 / 1.64	1.73
5ha0	A-201	1.44	0.760	0.16	0.19	1.00	0.34 / 0.20 / 0.23 / 0.23		0.80 / 0.71 / 3.23	1.73
5jvi	E-411	1.12	0.802	0.10	0.12	0.51 / 0.49	0.20 / 0.20 / 0.40 / 0.20	0.39	0.87 / 0.98 / 2.97	1.72
5lb5	D-504	2.00	0.645	0.24	0.28	1.00	0.28 / 0.44 / 0.28		1.06 / 0.60	1.72
5iy5	W-101	2.00	0.742	0.17	0.21	1.00	0.38 / 0.20 / 0.42		1.12 / 2.74	1.71
4yh2	A-301	1.72	0.685	0.16	0.19	1.00	0.46 / 0.23 / 0.24		1.05 / 0.88	1.71
5a8w	J-1556	1.80	0.662	0.17	0.20	1.00	0.30 / 0.20 / 0.23 / 0.26		0.86 / 0.53 / 1.11	1.71
5iu8	A-2431	2.00	0.683	0.18	0.20	1.00	0.24 / 0.20 / 0.36 / 0.20		1.06 / 1.27 / 0.80	1.71
5kee	A-202	1.50	0.717	0.18	0.20	0.50 / 0.50	0.52 / 0.46	0.79	0.61	1.70
5fmc	A-1001	1.84	0.703	0.16	0.18	1.00	0.25 / 0.23 / 0.22 / 0.20		1.03 / 1.89 / 0.92	1.70
5epo	D-302	2.00	0.679	0.18	0.22	1.00	0.57 / 0.21 / 0.20		2.90 / 2.49	1.70
5ecq	B-301	1.66	0.694	0.23	0.23	1.00	0.34 / 0.40 / 0.26		0.79 / 0.98	1.69
4zyx	A-1102	1.65	0.713	0.16	0.18	1.00	0.69 / 0.25		1.19	1.69
5ha7	A-402	1.65	0.720	0.17	0.20	0.60	0.42 / 0.26		2.29	1.69
5fck	A-301	1.86	0.659	0.19	0.24	1.00	0.63 / 0.33		0.64	1.69
5hgg	S-201	1.97	0.771	0.17	0.20	1.00	0.22 / 0.20 / 0.36 / 0.21		2.67 / 1.33 / 1.58	1.68
5an1	E-1220	2.00	0.650	0.21	0.26	1.00	0.46 / 0.20 / 0.30		0.72 / 0.95	1.68
5g4i	A-1445	1.50	0.739	0.15	0.18	1.00	0.48 / 0.20 / 0.20		1.92 / 1.91	1.67
4yq5	A-301	1.76	0.671	0.17	0.19	1.00	0.52 / 0.20 / 0.24		0.87 / 1.16	1.67
5lbu	A-306	1.65	0.790	0.18	0.21	0.70 / 0.30	0.20 / 0.20 / 0.20 / 0.20 / 0.20	3.27	0.89 / 1.67 / 2.65 / 1.60	1.67
5faj	A-401	1.64	0.699	0.21	0.24	1.00	0.53 / 0.32		0.81	1.67
5lqn	A-301	1.72	0.694	0.20	0.24	1.00	0.55 / 0.34		1.62	1.67
5g0i	B-1808	1.99	0.660	0.17	0.20	1.00	0.24 / 0.38 / 0.31		2.15 / 1.80	1.66
5u20	D-184	1.50	0.715	0.14	0.18	1.00	0.52 / 0.28 / 0.20		0.75 / 0.76	1.66
5iru	B-202	2.00	0.644	0.22	0.27	1.00	0.57 / 0.31		2.70	1.66
5fvn	B-417	1.45	0.905	0.16	0.18	1.00	0.24 / 0.76		1.06	1.65
5sx6	B-111	1.90	0.655	0.14	0.17	0.50 / 0.10	0.54 / 0.40	0.62	0.78	1.65
5g0o	B-800	1.85	0.692	0.19	0.23	1.00	0.22 / 0.42 / 0.32		2.72 / 1.56	1.65
5f05	C-301	1.70	0.685	0.14	0.18	1.00	0.20 / 0.31 / 0.20 / 0.20		0.69 / 1.09 / 0.84	1.64
5lf1	Y-306	2.00	0.636	0.18	0.21	1.00	0.27 / 0.39 / 0.33		2.68 / 1.19	1.64
5tvc	E-302	1.93	0.681	0.19	0.23	1.00	0.39 / 0.25 / 0.30		1.43 / 1.13	1.64
5fvn	D-420	1.45	0.823	0.16	0.18	1.00	0.41 / 0.46		1.11	1.64
5hkb	A-401	1.65	0.699	0.19	0.22	0.72	0.20 / 0.26 / 0.21		2.20 / 2.09	1.64
5f9e	A-1001	2.00	0.637	0.20	0.23	1.00	0.63 / 0.31		1.01	1.63
5lf7	b-304	2.00	0.652	0.18	0.21	1.00	0.62 / 0.20		0.46	1.63
5ehi	A-4002	1.30	0.774	0.19	0.21	0.71	0.37 / 0.20 / 0.20		0.56 / 1.18	1.63
5kk4	F-102	1.70	0.716	0.18	0.21	1.00	0.39 / 0.33 / 0.21		1.97 / 2.65	1.63

PDB	Ligand	Resolution (Å)	Twilight score	Rwork	Rfree	Occupancy (deposited)	Occupancy (qFit)	RMSD A->B (Å) (deposited)	RMSD A->B (qFit)	Best Fisher z improvement
5sym	B-301	1.55	0.764	0.18	0.20	1.00	0.40 / 0.41		0.79	1.63
5iu8	A-2408	2.00	0.679	0.18	0.20	1.00	0.35 / 0.27 / 0.38		1.18 / 1.30	1.62
5faj	C-401	1.64	0.695	0.21	0.24	1.00	0.40 / 0.28 / 0.26		0.96 / 0.96	1.61
5ej4	D-602	1.77	0.686	0.18	0.22	1.00	0.59 / 0.30		1.25	1.61
5ant	C-1157	2.00	0.688	0.21	0.25	1.00	0.38 / 0.50		0.94	1.61
5fmc	B-1001	1.84	0.707	0.16	0.18	1.00	0.37 / 0.20 / 0.33		0.67 / 2.12	1.61
5j0d	A-1201	1.05	0.863	0.18	0.20	1.00	0.30 / 0.23 / 0.27 / 0.20		1.55 / 0.41 / 2.91	1.61
5sx6	A-111	1.90	0.656	0.14	0.17	0.40 / 0.10	0.28 / 0.25 / 0.20 / 0.20	0.60	1.18 / 0.56 / 0.93	1.61
5kcd	A-601	1.82	0.669	0.18	0.21	0.90	0.45 / 0.29 / 0.23		1.10 / 0.97	1.60
5c41	D-401	1.95	0.650	0.17	0.21	1.00	0.30 / 0.26 / 0.36		1.14 / 0.51	1.60
5c3z	A-401	1.90	0.651	0.15	0.19	1.00	0.30 / 0.24 / 0.36		1.39 / 0.87	1.60
5fbe	A-302	1.43	0.819	0.17	0.19	1.00	0.54 / 0.31		0.86	1.60
5seen	B-804	1.86	0.679	0.18	0.22	1.00	0.72 / 0.28		1.05	1.60
5sxw	A-111	1.60	0.699	0.14	0.17	0.60 / 0.20	0.44 / 0.46	0.60	0.77	1.59
5evz	A-503	1.85	0.653	0.17	0.21	1.00	0.52 / 0.46		0.87	1.59
5m51	A-301	1.90	0.674	0.22	0.26	1.00	0.48 / 0.22 / 0.27		1.43 / 1.26	1.59
5g6g	A-1365	1.98	0.750	0.17	0.22	1.00	0.20 / 0.42 / 0.36		1.65 / 1.46	1.59
5d4v	B-307	1.60	0.740	0.17	0.21	1.00	0.31 / 0.34 / 0.23		1.96 / 1.56	1.59
5lf1	U-47	2.00	0.684	0.18	0.21	1.00	0.30 / 0.24 / 0.20 / 0.20		1.00 / 3.60 / 3.59	1.58
4zyy	A-1102	1.85	0.674	0.17	0.20	1.00	0.51 / 0.20 / 0.20		2.79 / 1.11	1.58
5jcu	B-301	1.93	0.655	0.18	0.24	1.00	0.20 / 0.20 / 0.20 / 0.20 / 0.20		0.91 / 1.24 / 1.02 / 1.37	1.57
5dc5	A-402	1.94	0.661	0.18	0.21	1.00	0.47 / 0.53		1.18	1.57
5jsq	A-301	1.50	0.722	0.16	0.18	0.44 / 0.56	0.41 / 0.30 / 0.20	1.05	0.84 / 0.97	1.56
5iu8	A-2404	2.00	0.660	0.18	0.20	1.00	0.26 / 0.30 / 0.44		2.78 / 0.75	1.56
5du4	A-301	1.70	0.692	0.19	0.22	1.00	0.44 / 0.32 / 0.20		3.07 / 1.05	1.56
5t77	A-548	2.00	0.707	0.19	0.21	1.00	0.20 / 0.22 / 0.58		2.50 / 1.26	1.56
5jc1	A-501	1.65	0.709	0.18	0.20	1.00	0.20 / 0.20 / 0.20 / 0.20 / 0.20		0.96 / 0.93 / 1.18 / 1.80	1.56
5sz4	A-304	1.60	0.701	0.18	0.22	1.00	0.62 / 0.38		1.48	1.56
5ar0	A-1384	1.90	0.654	0.17	0.21	1.00	0.63 / 0.32		0.72	1.55
5eph	B-302	1.79	0.671	0.16	0.20	1.00	0.20 / 0.33 / 0.26 / 0.20		2.30 / 0.96 / 0.87	1.55
5j1a	A-301	1.86	0.768	0.19	0.22	1.00	0.30 / 0.70		0.71	1.55
4z51	A-401	1.86	0.654	0.18	0.22	1.00	0.53 / 0.46		0.84	1.55
5syt	A-510	2.00	0.669	0.22	0.25	1.00	0.58 / 0.38		1.99	1.55
5ixj	A-82	1.54	0.710	0.18	0.20	1.00	0.48 / 0.21 / 0.30		0.94 / 0.99	1.55
5fag	A-401	1.51	0.719	0.20	0.23	1.00	0.44 / 0.24 / 0.22		1.56 / 1.36	1.54
5ley	X-91	1.90	0.675	0.19	0.23	1.00	0.20 / 0.20 / 0.30 / 0.20		0.67 / 0.91 / 1.61	1.53
5seyd	A-1401	1.85	0.665	0.19	0.25	1.00	0.47 / 0.32 / 0.20		0.92 / 0.80	1.53
5fvn	C-427	1.45	0.756	0.16	0.18	1.00	0.42 / 0.20 / 0.33		0.87 / 0.80	1.52
5exb	J-64	1.81	0.669	0.18	0.25	1.00	0.59 / 0.34		1.09	1.52
5eg7	A-501	1.40	0.759	0.16	0.18	1.00	0.20 / 0.20 / 0.29 / 0.20		2.49 / 1.49 / 1.07	1.52
5ep4	A-401	1.50	0.736	0.16	0.18	0.84	0.64 / 0.24		0.90	1.51
5jcw	B-301	1.95	0.657	0.15	0.19	1.00	0.42 / 0.25 / 0.28		1.86 / 1.14	1.51
4zyu	A-1102	1.95	0.658	0.18	0.21	1.00	0.27 / 0.35 / 0.32		1.26 / 0.94	1.51
4ys1	A-402	1.07	0.842	0.13	0.15	0.28 / 0.49	0.37 / 0.33	0.49	0.70	1.50
5l9i	B-401	1.90	0.654	0.18	0.21	1.00	0.41 / 0.26 / 0.30		0.98 / 0.83	1.50
5eco	B-301	1.80	0.679	0.22	0.24	1.00	0.54 / 0.22 / 0.24		0.86 / 0.70	1.50
5l4j	B-201	1.62	0.872	0.18	0.22	0.50	0.58 / 0.42		4.45	1.50
4zij	A-201	1.78	0.662	0.17	0.22	0.85	0.35 / 0.20 / 0.29		2.31 / 0.79	1.50
5jlb	A-1801	1.50	0.720	0.16	0.19	1.00	0.52 / 0.20 / 0.25		0.80 / 0.65	1.50
5lbu	B-307	1.65	0.733	0.18	0.21	1.00	0.31 / 0.31 / 0.36		2.00 / 0.79	1.49
5u20	C-184	1.50	0.716	0.14	0.18	1.00	0.39 / 0.20 / 0.20 / 0.21		0.86 / 0.93 / 0.74	1.49
5fas	A-301	1.74	0.678	0.16	0.18	1.00	0.20 / 0.20 / 0.20 / 0.20 / 0.20		1.48 / 0.86 / 1.06 / 0.86	1.48
5jmw	A-501	1.55	0.724	0.18	0.20	1.00	0.29 / 0.25 / 0.20 / 0.21		1.18 / 1.38 / 0.78	1.48
5g54	A-1275	2.00	0.692	0.18	0.23	1.00	0.20 / 0.32 / 0.48		3.64 / 0.69	1.48
5hat	F-500	2.00	0.641	0.21	0.25	1.00	0.41 / 0.20 / 0.25		1.31 / 0.71	1.48
5e8q	B-201	1.80	0.681	0.20	0.25	1.00	0.22 / 0.23 / 0.34 / 0.20		0.71 / 0.39 / 0.76	1.47
5eph	D-302	1.79	0.679	0.16	0.20	1.00	0.20 / 0.20 / 0.20 / 0.20 / 0.20		2.40 / 1.21 / 1.71 / 3.25	1.47
5tar	A-202	1.90	0.650	0.22	0.27	1.00	0.52 / 0.48		0.91	1.47
5exb	B-64	1.81	0.689	0.18	0.25	1.00	0.61 / 0.36		0.89	1.46
5g6d	A-904	1.82	0.676	0.16	0.19	1.00	0.33 / 0.20 / 0.25 / 0.20		1.76 / 0.90 / 1.36	1.46
5c7y	A-301	1.75	0.703	0.15	0.18	0.91	0.42 / 0.39		1.03	1.46

PDB	Ligand	Resolution (Å)	Twilight score	Rwork	Rfree	Occupancy (deposited)	Occupancy (qFit)	RMSD A->B (Å) (deposited)	RMSD A->B (qFit)	Best Fisher z improvement
5fjg	A-1275	2.00	0.677	0.17	0.22	1.00	0.44 / 0.50		1.05	1.46
4yav	A-302	1.40	0.774	0.14	0.16	1.00	0.24 / 0.32 / 0.20 / 0.24		2.96 / 1.18 / 1.70	1.46
4ysn	C-1001	1.94	0.639	0.15	0.19	1.00	0.39 / 0.20 / 0.21 / 0.20		0.93 / 2.16 / 1.24	1.46
5djl	B-307	1.80	0.688	0.15	0.18	0.67	0.23 / 0.20 / 0.30		3.08 / 0.89	1.46
5t77	A-533	2.00	0.729	0.19	0.21	1.00	0.31 / 0.28 / 0.41		1.43 / 2.20	1.46
5el2	B-202	1.75	0.750	0.18	0.22	1.00	0.36 / 0.20 / 0.37		3.00 / 1.47	1.46
5fvn	D-429	1.45	0.829	0.16	0.18	1.00	0.51 / 0.44		0.96	1.45
5ca6	A-307	1.90	0.711	0.16	0.20	1.00	0.38 / 0.20 / 0.22 / 0.20		0.96 / 0.87 / 0.76	1.45
5dlw	A-904	1.80	0.683	0.19	0.22	1.00	0.32 / 0.20 / 0.20 / 0.20		1.23 / 1.19 / 2.23	1.45
5csd	C-201	1.45	0.827	0.18	0.20	1.00	0.30 / 0.27 / 0.43		0.97 / 0.63	1.45
5fnr	A-1614	1.89	0.661	0.21	0.26	0.88	0.54 / 0.31		1.09	1.44
5aqt	A-1381	1.90	0.655	0.18	0.22	1.00	0.41 / 0.53		0.60	1.44
5k2c	A-1219	1.90	0.684	0.17	0.21	1.00	0.22 / 0.78		0.99	1.44
5jcu	A-301	1.93	0.654	0.18	0.24	1.00	0.20 / 0.20 / 0.20 / 0.20 / 0.20		1.34 / 1.10 / 0.82 / 0.87	1.44
5li7	B-502	1.58	0.716	0.17	0.20	1.00	0.34 / 0.33 / 0.28		1.12 / 1.81	1.44
5syv	B-111	1.85	0.665	0.15	0.19	0.90 / 0.10	0.58 / 0.42	0.60	0.79	1.44
5dq8	A-65	1.25	0.781	0.18	0.23	0.50 / 0.50	0.49 / 0.39	0.67	0.72	1.43
5d75	A-302	1.83	0.739	0.19	0.23	1.00	0.20 / 0.26 / 0.22 / 0.32		1.65 / 1.27 / 2.43	1.43
5kct	B-601	1.60	0.706	0.18	0.21	0.89	0.44 / 0.20 / 0.20		0.85 / 1.39	1.43
5lbu	B-306	1.65	0.737	0.18	0.21	1.00	0.53 / 0.20 / 0.26		1.56 / 1.78	1.43
5ezu	A-101	1.55	0.782	0.20	0.24	1.00	0.20 / 0.20 / 0.53		1.20 / 1.15	1.43
5sxr	A-111	1.69	0.683	0.14	0.17	0.50 / 0.10	0.50 / 0.40	0.61	0.68	1.42
5hfk	B-301	1.55	0.725	0.19	0.21	1.00	0.20 / 0.25 / 0.25 / 0.27		1.06 / 0.79 / 1.24	1.42
4xjp	B-501	1.60	0.697	0.16	0.19	1.00	0.54 / 0.46		1.17	1.42
5hux	A-501	1.96	0.654	0.17	0.23	1.00	0.47 / 0.24 / 0.29		1.35 / 0.87	1.42
5jmp	B-502	1.70	0.692	0.18	0.21	1.00	0.44 / 0.20 / 0.32		0.81 / 1.38	1.42
5ixj	B-82	1.54	0.709	0.18	0.20	1.00	0.45 / 0.29 / 0.24		0.66 / 0.97	1.42
5f9s	B-401	1.70	0.680	0.16	0.21	1.00	0.56 / 0.32		1.25	1.42
5edl	A-202	1.95	0.723	0.20	0.22	1.00	0.58 / 0.35		2.19	1.41
5hat	J-500	2.00	0.644	0.21	0.25	1.00	0.20 / 0.35 / 0.21 / 0.20		1.43 / 1.34 / 1.19	1.41
5g3l	H-200	1.72	0.685	0.17	0.20	1.00	0.52 / 0.42		0.53	1.41
4zof	A-402	1.80	0.663	0.19	0.22	1.00	0.39 / 0.23 / 0.38		1.29 / 0.93	1.40
5lf4	Y-306	1.99	0.638	0.18	0.22	1.00	0.38 / 0.20 / 0.20 / 0.20		0.73 / 0.52 / 0.81	1.40
5fas	B-304	1.74	0.685	0.16	0.18	1.00	0.22 / 0.29 / 0.23 / 0.20		1.07 / 0.81 / 0.64	1.39
5fra	B-201	2.00	0.638	0.18	0.21	1.00	0.30 / 0.41 / 0.20		0.91 / 0.56	1.39
4ykm	B-201	1.58	0.737	0.18	0.22	1.00	0.38 / 0.20 / 0.36		0.98 / 0.66	1.39
5le5	X-91	1.80	0.687	0.18	0.21	1.00	0.41 / 0.45		0.81	1.39
5csd	D-201	1.45	0.810	0.18	0.20	1.00	0.49 / 0.20 / 0.31		0.95 / 0.84	1.39
5jjs	A-1009	1.65	0.733	0.17	0.20	1.00	0.62 / 0.26		3.87	1.39
5dn8	A-403	1.95	0.687	0.21	0.23	1.00	0.30 / 0.20 / 0.23 / 0.20		0.68 / 0.68 / 1.03	1.38
5ley	J-91	1.90	0.670	0.19	0.23	1.00	0.54 / 0.34		0.97	1.38
5ep3	A-401	1.80	0.767	0.19	0.23	0.68	0.21 / 0.20 / 0.32		1.19 / 1.31	1.38
5dux	D-201	1.85	0.686	0.17	0.21	1.00	0.62 / 0.28		0.73	1.37
5exb	L-64	1.81	0.741	0.18	0.25	1.00	0.27 / 0.22 / 0.24 / 0.20		1.28 / 1.01 / 1.46	1.37
5lf1	X-91	2.00	0.657	0.18	0.21	1.00	0.41 / 0.24 / 0.32		1.29 / 3.31	1.37
5syt	A-506	2.00	0.686	0.22	0.25	1.00	0.45 / 0.31 / 0.20		1.01 / 1.13	1.37
5azp	A-505	1.69	0.860	0.16	0.18	1.00	0.37 / 0.39 / 0.20		0.94 / 0.49	1.37
5bqs	A-402	1.90	0.703	0.21	0.25	1.00	0.45 / 0.43		1.16	1.37
5e9q	A-301	1.79	0.668	0.17	0.20	1.00	0.48 / 0.49		0.65	1.37
5h9l	A-201	1.37	0.798	0.16	0.19	1.00	0.48 / 0.20 / 0.30		1.02 / 0.78	1.37
5l8j	A-501	1.68	0.709	0.20	0.23	1.00	0.56 / 0.41		0.74	1.36
5iu8	A-2416	2.00	0.725	0.18	0.20	1.00	0.63 / 0.37		0.94	1.36
5bzr	A-202	1.15	1.016	0.18	0.19	1.00	0.25 / 0.20 / 0.20		2.34 / 1.97	1.36
5ej4	H-602	1.77	0.684	0.18	0.22	1.00	0.20 / 0.22 / 0.22 / 0.34		1.15 / 0.62 / 0.79	1.36
4yb6	D-301	1.98	0.636	0.20	0.22	1.00	0.67 / 0.29		0.98	1.36
5g6h	A-904	1.91	0.661	0.16	0.19	1.00	0.46 / 0.21 / 0.32		2.30 / 0.75	1.36
5bqg	A-204	1.44	0.779	0.15	0.17	1.00	0.40 / 0.20 / 0.40		0.58 / 0.96	1.36
4zoj	B-402	1.96	0.642	0.22	0.26	1.00	0.29 / 0.21 / 0.24 / 0.20		0.93 / 1.01 / 1.45	1.35
5br2	A-301	1.80	0.706	0.19	0.24	1.00	0.72 / 0.26		0.67	1.35
5lsc	A-404	1.50	0.733	0.14	0.17	0.99	0.62 / 0.29		0.78	1.35
5g2d	A-1274	1.80	0.671	0.18	0.21	1.00	0.45 / 0.20 / 0.35		1.15 / 0.55	1.34

PDB	Ligand	Resolution (Å)	Twilight score	Rwork	Rfree	Occupancy (deposited)	Occupancy (qFit)	RMSD A->B (Å) (deposited)	RMSD A->B (qFit)	Best Fisher z improvement
5ecs	A-301	1.65	0.742	0.17	0.19	1.00	0.48 / 0.20 / 0.20		1.43 / 0.71	1.34
5lf7	Y-306	2.00	0.652	0.18	0.21	1.00	0.22 / 0.35 / 0.20 / 0.20		1.21 / 0.76 / 2.00	1.34
5iy5	M-101	2.00	0.640	0.17	0.21	1.00	0.63 / 0.35		0.71	1.33
5bqh	A-204	1.60	0.730	0.15	0.17	1.00	0.32 / 0.38 / 0.30		1.28 / 0.67	1.33
5ecl	F-301	1.85	0.657	0.21	0.22	1.00	0.24 / 0.27 / 0.50		0.93 / 0.87	1.33
5ef7	A-804	1.90	0.688	0.18	0.22	1.00	0.54 / 0.28		3.20	1.33
4zse	D-4001	1.97	0.640	0.19	0.21	1.00	0.48 / 0.42		0.83	1.32
5fsi	A-1157	1.63	0.733	0.20	0.23	0.50	0.42 / 0.29		1.02	1.32
5i4d	B-405	1.75	0.671	0.16	0.20	1.00	0.43 / 0.25 / 0.29		1.10 / 0.86	1.32
5jga	A-601	2.00	0.640	0.20	0.22	1.00	0.50 / 0.20 / 0.30		0.95 / 2.42	1.32
5cph	B-302	1.20	0.943	0.17	0.19	0.75	0.52 / 0.35		3.12	1.31
5e2k	A-302	1.40	0.749	0.17	0.19	1.00	0.55 / 0.20 / 0.25		1.33 / 1.87	1.31
4zen	B-501	1.93	0.660	0.16	0.20	1.00	0.66 / 0.26		1.32	1.31
4z8d	A-401	2.00	0.641	0.16	0.22	1.00	0.20 / 0.34 / 0.46		0.67 / 1.11	1.30
5e2n	B-306	1.53	0.747	0.18	0.21	1.00	0.45 / 0.30		2.78	1.30
5kk4	D-103	1.70	0.711	0.18	0.21	1.00	0.24 / 0.20 / 0.20 / 0.27		1.87 / 1.74 / 3.75	1.30
5iz4	A-300	1.75	0.687	0.15	0.18	1.00	0.20 / 0.24 / 0.21 / 0.20		2.74 / 1.08 / 1.00	1.29
5eph	C-302	1.79	0.673	0.16	0.20	1.00	0.21 / 0.31 / 0.20 / 0.28		1.40 / 1.07 / 0.92	1.29
5fvn	D-408	1.45	0.822	0.16	0.18	1.00	0.39 / 0.61		1.39	1.29
5itp	A-301	1.85	0.654	0.18	0.20	1.00	0.25 / 0.34 / 0.20 / 0.20		1.00 / 0.75 / 0.89	1.29
4ysn	B-1001	1.94	0.645	0.15	0.19	1.00	0.37 / 0.20 / 0.20 / 0.20		1.25 / 2.11 / 0.88	1.29
5e72	A-400	1.74	0.719	0.19	0.22	1.00	0.31 / 0.21 / 0.20 / 0.28		0.96 / 0.63 / 3.78	1.29
5sexy	A-305	1.55	0.713	0.13	0.17	0.62	0.42 / 0.28		0.83	1.29
5l99	A-2001	2.00	0.655	0.18	0.20	1.00	0.39 / 0.27 / 0.20		1.63 / 1.08	1.29
5d4u	A-301	2.00	0.643	0.20	0.23	1.00	0.55 / 0.20 / 0.24		1.16 / 0.82	1.28
5kvs	A-402	1.28	0.774	0.16	0.17	0.85	0.39 / 0.23 / 0.20		1.56 / 0.74	1.28
5u1h	B-201	1.50	0.752	0.17	0.20	1.00	0.33 / 0.20 / 0.20 / 0.20		2.02 / 0.73 / 1.12	1.28
5k9d	A-400	1.70	0.678	0.14	0.16	1.00	0.80 / 0.20		0.87	1.28
5fjg	A-1269	2.00	0.681	0.17	0.22	1.00	0.59 / 0.41		1.67	1.28
4zno	A-401	1.86	0.696	0.19	0.23	1.00	0.69 / 0.28		1.24	1.28
4zn7	B-600	1.93	0.686	0.20	0.23	1.00	0.47 / 0.24 / 0.20		1.01 / 1.08	1.28
5d85	A-402	1.92	0.654	0.17	0.21	1.00	0.23 / 0.29 / 0.28 / 0.20		0.81 / 1.26 / 1.01	1.27
5e8q	A-201	1.80	0.680	0.20	0.25	1.00	0.47 / 0.20 / 0.30		1.47 / 1.33	1.27
5drn	L-303	1.99	0.649	0.18	0.22	1.00	0.23 / 0.20 / 0.37 / 0.20		0.73 / 1.43 / 0.64	1.27
5i4d	A-404	1.75	0.673	0.16	0.20	1.00	0.45 / 0.35 / 0.20		1.08 / 0.77	1.26
5ecr	F-301	1.72	0.713	0.26	0.28	1.00	0.64 / 0.35		1.10	1.26
5ca6	B-305	1.90	0.697	0.16	0.20	1.00	0.52 / 0.20 / 0.24		1.05 / 0.81	1.26
5iru	D-202	2.00	0.658	0.22	0.27	1.00	0.37 / 0.32 / 0.20		2.63 / 0.70	1.25
5iu8	A-2430	2.00	0.774	0.18	0.20	1.00	0.34 / 0.23 / 0.23 / 0.20		1.89 / 1.41 / 1.64	1.25
5irc	D-201	1.72	0.683	0.17	0.21	1.00	0.37 / 0.22 / 0.38		0.82 / 0.89	1.24
5j8q	A-501	1.70	0.677	0.12	0.15	1.00	0.53 / 0.27 / 0.20		1.05 / 1.16	1.24
5iyz	B-501	1.80	0.660	0.17	0.20	1.00	0.74 / 0.25		0.83	1.24
5f7g	B-201	1.48	0.799	0.20	0.25	1.00	0.66 / 0.34		2.48	1.24
5eci	B-301	1.56	0.714	0.21	0.23	1.00	0.41 / 0.21 / 0.38		0.79 / 0.76	1.24
4ym9	A-1001	1.80	0.692	0.13	0.16	1.00	0.41 / 0.20 / 0.23		0.49 / 1.25	1.24
5iyt	B-201	1.73	0.752	0.19	0.22	1.00	0.34 / 0.20 / 0.29		1.59 / 1.87	1.24
5kva	A-301	1.83	0.659	0.16	0.19	1.00	0.65 / 0.35		0.65	1.24
5ecl	B-301	1.85	0.658	0.21	0.22	1.00	0.76 / 0.24		0.71	1.24
5etm	A-201	1.46	0.747	0.20	0.24	1.00	0.63 / 0.31		1.01	1.24
5fsx	A-1262	2.00	0.645	0.21	0.25	1.00	0.56 / 0.39		1.07	1.23
5jbi	B-501	1.70	0.689	0.18	0.21	1.00	0.48 / 0.27 / 0.20		1.27 / 1.15	1.23
4zcp	A-801	1.98	0.634	0.21	0.25	1.00	0.44 / 0.20 / 0.31		1.07 / 1.05	1.23
5f06	A-301	1.80	0.670	0.18	0.21	1.00	0.46 / 0.20 / 0.30		0.85 / 0.79	1.23
5el2	A-202	1.75	0.708	0.18	0.22	1.00	0.73 / 0.21		1.28	1.23
5fcf	A-516	1.55	0.732	0.16	0.19	1.00	0.33 / 0.53		1.15	1.23
5f58	B-201	1.54	0.757	0.19	0.23	1.00	0.60 / 0.32		0.99	1.23
4z1t	C-1	1.50	0.732	0.19	0.23	1.00	0.52 / 0.45		1.20	1.23
5euA	A-301	1.85	0.672	0.17	0.22	0.90	0.51 / 0.34		0.84	1.22
5jil	A-512	1.85	0.703	0.18	0.20	1.00	0.29 / 0.28 / 0.20 / 0.20		0.64 / 0.84 / 0.83	1.22
5u1h	D-201	1.50	0.740	0.17	0.20	1.00	0.43 / 0.27 / 0.20		1.60 / 0.77	1.22
5eph	A-303	1.79	0.673	0.16	0.20	1.00	0.20 / 0.20 / 0.20 / 0.20 / 0.20		1.91 / 0.92 / 3.22 / 1.97	1.22

PDB	Ligand	Resolution (Å)	Twilight score	Rwork	Rfree	Occupancy (deposited)	Occupancy (qFit)	RMSD A->B (Å) (deposited)	RMSD A->B (qFit)	Best Fisher z improvement
5il2	A-601	1.61	0.730	0.19	0.20	1.00	0.51 / 0.20 / 0.25		0.95 / 0.77	1.21
5cxw	A-702	1.75	0.685	0.15	0.19	1.00	0.27 / 0.20 / 0.46		1.08 / 0.40	1.21
5ioq	B-303	1.93	0.650	0.17	0.20	1.00	0.70 / 0.26		0.71	1.21
5epo	A-302	2.00	0.663	0.18	0.22	1.00	0.20 / 0.20 / 0.20 / 0.20 / 0.20		2.53 / 0.84 / 2.83 / 0.80	1.20
5efi	C-101	1.80	0.824	0.22	0.24	1.00	0.31 / 0.44 / 0.20		0.91 / 1.73	1.20
5g4j	B-1440	1.87	0.660	0.17	0.20	1.00	0.63 / 0.29		1.03	1.20
5k5p	A-201	1.83	0.669	0.19	0.24	1.00	0.48 / 0.20 / 0.28		1.82 / 0.88	1.20
5ey4	B-501	1.86	0.728	0.17	0.21	1.00	0.30 / 0.21 / 0.20 / 0.20		1.89 / 2.90 / 2.16	1.19
5cgq	A-301	1.18	0.794	0.14	0.16	0.77	0.21 / 0.20 / 0.35		1.00 / 1.06	1.19
5epo	B-302	2.00	0.655	0.18	0.22	1.00	0.45 / 0.24 / 0.31		1.53 / 2.38	1.19
5f0f	A-301	1.76	0.703	0.20	0.24	1.00	0.58 / 0.38		1.12	1.19
5g3l	E-200	1.72	0.712	0.17	0.20	1.00	0.48 / 0.31		0.99	1.19
5g68	A-904	1.63	0.715	0.16	0.19	1.00	0.56 / 0.38		1.28	1.19
5iu8	A-2401	2.00	0.640	0.18	0.20	1.00	0.78 / 0.21		1.02	1.19
5d15	A-301	1.50	0.723	0.20	0.21	0.97	0.32 / 0.20 / 0.20 / 0.20		4.44 / 0.82 / 1.04	1.18
5k2d	A-1206	1.90	0.686	0.17	0.21	1.00	0.20 / 0.20 / 0.60		1.37 / 0.64	1.18
5e5i	A-501	1.70	0.720	0.17	0.21	1.00	0.31 / 0.22 / 0.21 / 0.23		1.16 / 0.91 / 0.87	1.18
5g0n	A-800	1.94	0.653	0.18	0.22	1.00	0.30 / 0.23 / 0.25 / 0.23		2.57 / 0.93 / 2.52	1.18
5eci	F-301	1.56	0.719	0.21	0.23	1.00	0.27 / 0.26 / 0.27 / 0.20		1.59 / 1.37 / 1.47	1.18
5exb	N-64	1.81	0.667	0.18	0.25	1.00	0.45 / 0.29 / 0.22		1.04 / 1.23	1.17
5fdi	A-302	1.85	0.667	0.16	0.19	1.00	0.23 / 0.69		1.16	1.17
5g3w	C-373	1.60	0.811	0.13	0.17	0.60	0.34 / 0.28		1.30	1.17
5an1	D-1220	2.00	0.666	0.21	0.26	1.00	0.28 / 0.28 / 0.20 / 0.20		1.22 / 0.81 / 1.73	1.17
5g0o	B-760	1.85	0.687	0.19	0.23	1.00	0.58 / 0.25		1.08	1.17
5hq8	B-508	1.72	0.688	0.17	0.20	1.00	0.57 / 0.21 / 0.20		1.27 / 0.70	1.17
5kr0	A-101	1.80	0.682	0.18	0.21	1.00	0.34 / 0.25 / 0.35		0.91 / 0.54	1.17
5b5t	B-600	1.70	0.693	0.18	0.19	1.00	0.26 / 0.24 / 0.22 / 0.22		1.07 / 0.65 / 2.72	1.17
4zns	B-601	1.86	0.664	0.20	0.24	0.88	0.21 / 0.28 / 0.20 / 0.20		1.24 / 0.93 / 0.97	1.17
5azp	C-505	1.69	0.866	0.16	0.18	1.00	0.26 / 0.50 / 0.21		2.76 / 2.51	1.17
5hgg	S-202	1.97	0.728	0.17	0.20	1.00	0.26 / 0.32 / 0.42		1.04 / 1.56	1.16
5d24	A-201	1.65	0.706	0.17	0.20	1.00	0.39 / 0.20 / 0.33		0.70 / 0.69	1.16
4ysn	D-1001	1.94	0.641	0.15	0.19	1.00	0.71 / 0.28		2.07	1.16
5dxx	A-7401	1.45	0.757	0.13	0.16	1.00	0.42 / 0.33		0.86	1.16
5g18	A-301	1.10	0.810	0.12	0.14	1.00	0.33 / 0.20 / 0.20 / 0.20		1.48 / 1.66 / 4.33	1.16
5g28	A-1273	1.57	0.828	0.15	0.19	1.00	0.39 / 0.21 / 0.20 / 0.20		2.56 / 0.99 / 3.14	1.16
5g6k	A-904	1.95	0.711	0.17	0.22	1.00	0.30 / 0.27 / 0.33		1.55 / 3.11	1.16
4yqq	A-301	1.78	0.677	0.16	0.20	1.00	0.39 / 0.20 / 0.29		1.19 / 0.72	1.16
5enm	A-503	1.98	0.648	0.26	0.28	1.00	0.41 / 0.30 / 0.26		1.62 / 1.00	1.16
5hk9	B-401	1.80	0.685	0.17	0.20	0.89	0.20 / 0.26 / 0.42		1.98 / 1.35	1.16
5dwe	A-900	1.92	0.651	0.20	0.24	1.00	0.42 / 0.30 / 0.26		4.76 / 1.08	1.16
5cu4	A-404	1.56	0.778	0.17	0.20	0.90	0.31 / 0.24 / 0.30		1.17 / 0.91	1.15
5kct	A-601	1.60	0.723	0.18	0.21	0.89	0.25 / 0.20 / 0.20 / 0.20		0.71 / 1.14 / 0.98	1.15
5e5i	B-501	1.70	0.681	0.17	0.21	1.00	0.29 / 0.25 / 0.34		0.98 / 1.40	1.15
5er9	A-501	1.69	0.710	0.19	0.22	0.65	0.31 / 0.33		0.94	1.15
5fvn	C-421	1.45	0.746	0.16	0.18	1.00	0.36 / 0.49		1.00	1.15
5fvn	D-402	1.45	0.831	0.16	0.18	1.00	0.64 / 0.36		0.97	1.15
5l02	A-111	1.90	0.650	0.17	0.21	1.00	0.52 / 0.36		0.76	1.14
4zqc	B-401	1.54	0.706	0.14	0.19	1.00	0.50 / 0.49		1.17	1.14
5ezx	A-501	1.90	0.660	0.21	0.24	1.00	0.22 / 0.32 / 0.20 / 0.26		0.71 / 0.91 / 1.46	1.14
4wv8	C-303	1.83	0.760	0.16	0.20	1.00	0.53 / 0.26		0.78	1.14
4z7m	A-302	1.43	0.759	0.25	0.31	1.00	0.51 / 0.40		0.93	1.14
5g1c	B-373	1.81	0.823	0.17	0.22	0.70	0.26 / 0.27		2.12	1.14
4wi1	B-801	1.65	0.710	0.16	0.19	1.00	0.48 / 0.49		0.98	1.14
5a8w	D-1553	1.80	0.665	0.17	0.20	1.00	0.40 / 0.20 / 0.20 / 0.20		0.69 / 0.80 / 0.93	1.14
5an1	G-1220	2.00	0.648	0.21	0.26	1.00	0.35 / 0.20 / 0.20 / 0.25		1.05 / 0.88 / 0.84	1.14
5fvn	C-418	1.45	0.776	0.16	0.18	1.00	0.57 / 0.38		2.32	1.14
4xug	B-400	1.65	0.691	0.17	0.19	1.00	0.65 / 0.35		1.16	1.14
5csd	A-201	1.45	0.893	0.18	0.20	1.00	0.62 / 0.38		0.93	1.14
5etl	C-205	1.82	0.686	0.20	0.24	1.00	0.60 / 0.20 / 0.20		3.95 / 2.07	1.13
5sw4	A-111	1.90	0.656	0.14	0.17	0.90 / 0.10	0.58 / 0.34	0.59	0.78	1.13
5e93	B-401	1.41	0.762	0.15	0.17	1.00	0.45 / 0.20 / 0.20		1.30 / 0.78	1.13

PDB	Ligand	Resolution (Å)	Twilight score	Rwork	Rfree	Occupancy (deposited)	Occupancy (qFit)	RMSD A->B (Å) (deposited)	RMSD A->B (qFit)	Best Fisher z improvement
5fvn	D-423	1.45	0.764	0.16	0.18	1.00	0.23 / 0.20 / 0.20 / 0.20		1.40 / 1.40 / 1.31	1.12
5drn	B-301	1.99	0.661	0.18	0.22	1.00	0.49 / 0.20 / 0.30		1.34 / 0.80	1.12
5f7g	A-201	1.48	0.811	0.20	0.25	1.00	0.27 / 0.20 / 0.20 / 0.33		1.15 / 1.07 / 2.58	1.12
5fok	B-1721	1.90	0.675	0.19	0.21	1.00	0.67 / 0.33		1.25	1.12
5i9v	A-1001	1.46	0.748	0.16	0.19	1.00	0.27 / 0.26 / 0.22 / 0.20		1.64 / 1.01 / 1.45	1.12
5a1g	A-404	1.83	0.669	0.12	0.18	1.00	0.51 / 0.21 / 0.24		0.60 / 0.73	1.12
5jmp	A-501	1.70	0.695	0.18	0.21	1.00	0.38 / 0.39 / 0.20		0.86 / 1.38	1.12
5ccn	A-206	1.80	0.727	0.18	0.21	1.00	0.42 / 0.20 / 0.20		1.90 / 1.25	1.12
5bo3	A-400	1.75	0.699	0.21	0.24	1.00	0.55 / 0.20 / 0.20		0.53 / 0.91	1.11
5hat	E-500	2.00	0.652	0.21	0.25	1.00	0.20 / 0.20 / 0.48		1.40 / 0.83	1.11
5t77	A-525	2.00	0.663	0.19	0.21	1.00	0.66 / 0.25		0.88	1.11
5ecn	C-301	1.72	0.694	0.17	0.19	1.00	0.40 / 0.26 / 0.20		0.58 / 0.81	1.11
5fvn	F-415	1.45	0.792	0.16	0.18	1.00	0.52 / 0.43		1.15	1.11
5lf1	V-303	2.00	0.647	0.18	0.21	1.00	0.31 / 0.56		0.96	1.11
5a8w	A-1554	1.80	0.663	0.17	0.20	1.00	0.39 / 0.20 / 0.20 / 0.21		0.75 / 0.86 / 1.36	1.11
5ccr	A-207	1.90	0.658	0.16	0.19	1.00	0.44 / 0.30 / 0.20		1.51 / 1.07	1.11
5fvn	F-406	1.45	0.739	0.16	0.18	1.00	0.47 / 0.40		0.91	1.11
4ykt	A-301	1.85	0.664	0.18	0.21	1.00	0.38 / 0.27 / 0.25		2.91 / 0.88	1.10
5d9f	A-301	1.91	0.667	0.19	0.22	1.00	0.72 / 0.22		1.22	1.10
5iv3	A-507	1.86	0.665	0.18	0.22	1.00	0.43 / 0.29 / 0.20		0.85 / 0.56	1.10
5t77	A-528	2.00	0.734	0.19	0.21	1.00	0.37 / 0.30 / 0.33		1.88 / 1.32	1.10
5sxw	B-111	1.60	0.700	0.14	0.17	0.70 / 0.30	0.60 / 0.36	0.57	0.58	1.10
5fvn	F-412	1.45	0.751	0.16	0.18	1.00	0.20 / 0.22 / 0.38 / 0.20		3.28 / 0.65 / 4.77	1.09
5bqh	A-203	1.60	0.767	0.15	0.17	1.00	0.20 / 0.23 / 0.25 / 0.22		2.84 / 2.15 / 3.02	1.09
5k2d	A-1210	1.90	0.794	0.17	0.21	1.00	0.47 / 0.33 / 0.20		3.76 / 1.08	1.09
5bqi	A-201	1.88	0.718	0.17	0.18	1.00	0.45 / 0.20 / 0.24		0.59 / 0.82	1.09
5lbu	A-305	1.65	0.716	0.18	0.21	1.00	0.67 / 0.26		0.95	1.09
5ehi	A-4001	1.30	0.761	0.19	0.21	0.50 / 0.50	0.27 / 0.26 / 0.39	0.71	1.04 / 0.60	1.09
5ekd	A-402	1.82	0.663	0.17	0.21	1.00	0.59 / 0.20 / 0.20		1.16 / 0.84	1.09
5g09	C-1475	1.90	0.647	0.17	0.20	1.00	0.60 / 0.38		1.07	1.09
5f0x	A-503	1.60	0.716	0.17	0.20	1.00	0.48 / 0.20 / 0.20		1.11 / 0.75	1.08
5hdz	A-501	1.49	0.745	0.19	0.21	1.00	0.55 / 0.40		2.18	1.08
5dlv	B-927	2.00	0.660	0.19	0.23	0.34 / 0.33 / 0.33	0.29 / 0.26 / 0.20	3.82 / 2.85	0.78 / 0.85	1.08
5gzd	A-201	1.19	0.837	0.20	0.21	1.00	0.31 / 0.29 / 0.20 / 0.20		1.08 / 0.53 / 3.00	1.08
4yce	A-201	1.95	0.683	0.19	0.24	1.00	0.55 / 0.25		1.07	1.08
5l8k	A-501	1.79	0.673	0.19	0.24	1.00	0.38 / 0.21 / 0.32		1.02 / 0.75	1.08
4yfp	A-201	1.95	0.660	0.19	0.23	1.00	0.43 / 0.25 / 0.20		1.12 / 0.61	1.07
5dvz	D-82	1.69	0.683	0.20	0.23	1.00	0.29 / 0.20 / 0.29 / 0.20		0.57 / 0.99 / 0.58	1.07
5ef7	B-804	1.90	0.690	0.18	0.22	1.00	0.55 / 0.33		1.21	1.07
5hat	G-500	2.00	0.637	0.21	0.25	1.00	0.22 / 0.20 / 0.20 / 0.20		1.27 / 1.24 / 1.36	1.07
5ltp	C-59	1.70	0.685	0.19	0.21	1.00	0.56 / 0.38		1.16	1.07
5f8f	B-400	1.90	0.678	0.19	0.22	1.00	0.42 / 0.27 / 0.22		0.68 / 0.74	1.07
5jtt	A-902	1.85	0.654	0.16	0.19	1.00	0.52 / 0.45		1.06	1.07
5an1	F-1220	2.00	0.654	0.21	0.26	1.00	0.30 / 0.30 / 0.39		0.64 / 0.99	1.07
5k2c	A-1205	1.90	0.655	0.17	0.21	1.00	0.20 / 0.32 / 0.48		0.78 / 0.94	1.07
5b1s	B-501	1.58	0.706	0.19	0.23	1.00	0.34 / 0.48		2.21	1.06
5bnr	A-401	1.89	0.705	0.20	0.25	1.00	0.50 / 0.28 / 0.20		1.89 / 1.24	1.06
5k7w	A-601	1.65	0.714	0.16	0.18	1.00	0.58 / 0.37		0.71	1.06
5lkd	A-401	1.68	0.688	0.16	0.20	1.00	0.26 / 0.20 / 0.23 / 0.20		0.87 / 0.86 / 0.87	1.06
5eq3	A-501	2.00	0.664	0.20	0.24	1.00	0.28 / 0.34 / 0.23		1.32 / 0.78	1.06
5ecn	E-301	1.72	0.693	0.17	0.19	1.00	0.48 / 0.48		0.76	1.06
5li6	A-502	1.95	0.651	0.19	0.24	1.00	0.32 / 0.20 / 0.20 / 0.28		0.78 / 0.57 / 0.61	1.06
5ffh	A-202	1.68	0.724	0.22	0.27	1.00	0.20 / 0.20 / 0.20 / 0.20		2.32 / 0.67 / 1.05 / 0.93	1.06
5lf7	N-305	2.00	0.642	0.18	0.21	1.00	0.90			1.05
5k2d	A-1223	1.90	0.766	0.17	0.21	1.00	0.49 / 0.51		3.86	1.05
5kk4	D-102	1.70	0.791	0.18	0.21	1.00	0.24 / 0.56 / 0.20		2.66 / 1.59	1.05
5l9g	B-401	1.75	0.678	0.18	0.21	1.00	0.54 / 0.24 / 0.22		1.07 / 0.83	1.05
5dvz	C-82	1.69	0.688	0.20	0.23	1.00	0.30 / 0.20 / 0.21 / 0.20		0.97 / 1.06 / 0.69	1.05
5iu8	A-2407	2.00	0.766	0.18	0.20	1.00	0.54 / 0.46		1.12	1.05
5t0k	B-1304	1.70	0.680	0.17	0.19	1.00	0.54 / 0.44		0.62	1.05
5exb	P-64	1.81	0.673	0.18	0.25	1.00	0.60 / 0.30		1.05	1.05

PDB	Ligand	Resolution (Å)	Twilight score	Rwork	Rfree	Occupancy (deposited)	Occupancy (qFit)	RMSD A->B (Å) (deposited)	RMSD A->B (qFit)	Best Fisher z improvement
5fok	A-1722	1.90	0.670	0.19	0.21	1.00	0.61 / 0.39		2.29	1.05
5e2m	B-302	1.41	0.764	0.18	0.21	1.00	0.40 / 0.21 / 0.21		0.94 / 0.82	1.04
5t67	B-502	1.60	0.713	0.20	0.25	1.00	0.56 / 0.41		0.66	1.04
5syt	A-511	2.00	0.739	0.22	0.25	1.00	0.38 / 0.40		1.30	1.04
5adw	B-312	1.90	0.668	0.23	0.26	1.00	0.38 / 0.24 / 0.39		1.34 / 0.83	1.04
5ecn	B-301	1.72	0.695	0.17	0.19	1.00	0.68 / 0.20		1.08	1.04
5ca3	A-1004	1.80	0.684	0.15	0.19	1.00	0.74 / 0.22		1.42	1.04
5ley	G-161	1.90	0.655	0.19	0.23	1.00	0.20 / 0.20 / 0.20 / 0.27		0.81 / 0.81 / 0.82	1.03
5fvn	C-425	1.45	0.752	0.16	0.18	1.00	0.36 / 0.23 / 0.33		1.53 / 1.02	1.03
5lf4	K-305	1.99	0.644	0.18	0.22	1.00	0.29 / 0.21 / 0.26 / 0.20		0.84 / 0.97 / 1.40	1.03
5f06	B-301	1.80	0.672	0.18	0.21	1.00	0.22 / 0.20 / 0.27 / 0.24		0.79 / 0.54 / 1.23	1.03
4zi3	A-301	2.00	0.630	0.19	0.24	1.00	0.45 / 0.24 / 0.29		0.80 / 0.79	1.03
5lk4	A-67	1.47	0.738	0.14	0.17	1.00	0.59 / 0.24		1.07	1.03
5c8z	B-301	1.60	0.716	0.15	0.17	0.85	0.20 / 0.20 / 0.26 / 0.20		1.30 / 0.72 / 1.02	1.03
5k0n	A-304	1.99	0.644	0.18	0.23	1.00	0.62 / 0.36		1.21	1.03
5c3z	B-401	1.90	0.655	0.15	0.19	1.00	0.48 / 0.20 / 0.20		0.86 / 0.87	1.02
5g3m	A-1134	1.85	0.673	0.20	0.23	1.00	0.33 / 0.20 / 0.41		0.83 / 1.22	1.02
5ddx	B-301	1.95	0.652	0.20	0.26	1.00	0.36 / 0.24 / 0.20 / 0.20		0.88 / 0.69 / 0.41	1.02
5i3q	A-1003	1.88	0.653	0.18	0.20	1.00	0.74 / 0.20		0.96	1.02
5m53	A-301	1.90	0.656	0.20	0.24	1.00	0.20 / 0.20 / 0.20 / 0.20 / 0.20		1.03 / 0.69 / 1.59 / 1.24	1.02
5d4a	A-201	1.70	0.722	0.19	0.22	1.00	0.70 / 0.30		0.82	1.02
4yb6	E-301	1.98	0.639	0.20	0.22	1.00	0.66 / 0.31		1.10	1.01
5f4n	A-302	1.91	0.712	0.15	0.19	0.82	0.33 / 0.44		1.41	1.01
5ios	D-302	1.90	0.650	0.18	0.21	1.00	0.65 / 0.35		1.00	1.01
5d75	A-303	1.83	0.795	0.19	0.23	1.00	0.42 / 0.42		1.15	1.01
5ee8	A-302	1.54	0.723	0.15	0.18	1.00	0.48 / 0.20 / 0.31		0.67 / 0.89	1.01
4zv5	A-101	1.57	0.762	0.23	0.26	1.00	0.39 / 0.22 / 0.39		0.86 / 0.53	1.01
5fre	C-201	1.90	0.661	0.17	0.21	1.00	0.52 / 0.20 / 0.21		0.61 / 1.19	1.01
5ely	A-817	1.81	0.677	0.18	0.20	1.00	0.26 / 0.24 / 0.47		0.82 / 1.24	1.00
5buc	A-304	1.87	0.706	0.15	0.20	1.00	0.20 / 0.35 / 0.33		1.04 / 0.45	1.00
5lbc	A-503	1.82	0.670	0.16	0.18	1.00	0.61 / 0.35		0.86	1.00
4yqo	A-301	1.68	0.689	0.18	0.20	1.00	0.52 / 0.21 / 0.20		0.86 / 0.55	1.00
5f38	C-401	1.90	0.691	0.20	0.24	1.00	0.33 / 0.22 / 0.20		1.28 / 0.85	1.00
5f05	A-301	1.70	0.697	0.14	0.18	1.00	0.24 / 0.20 / 0.20 / 0.20		0.78 / 0.98 / 0.95	1.00
5edl	A-203	1.95	0.735	0.20	0.22	1.00	0.43 / 0.37		1.11	1.00
5fhm	A-304	1.55	0.721	0.14	0.16	1.00	0.55 / 0.20 / 0.20		0.70 / 0.62	1.00
5jin	B-1205	1.85	0.678	0.20	0.24	1.00	0.40 / 0.20 / 0.20 / 0.20		1.12 / 0.85 / 1.30	0.99
5f2l	A-3001	1.75	0.719	0.16	0.19	0.68 / 0.28	0.38 / 0.35	6.86	1.47	0.99
5fvn	C-432	1.45	0.803	0.16	0.18	1.00	0.34 / 0.28 / 0.39		0.99 / 0.87	0.99
4ych	A-201	1.96	0.679	0.21	0.25	1.00	0.39 / 0.20 / 0.26		0.62 / 0.67	0.99
5dlz	A-201	1.70	0.756	0.25	0.33	1.00	0.54 / 0.33		1.77	0.99
5syt	A-512	2.00	0.670	0.22	0.25	1.00	0.29 / 0.27 / 0.22 / 0.20		1.42 / 1.12 / 1.17	0.99
5kvs	B-402	1.28	0.800	0.16	0.17	0.70	0.27 / 0.25 / 0.26		1.66 / 1.52	0.98
5syt	A-504	2.00	0.711	0.22	0.25	1.00	0.49 / 0.33		1.11	0.98
5m0p	B-502	1.95	0.667	0.16	0.20	1.00	0.53 / 0.26 / 0.20		0.93 / 0.69	0.98
5aqu	A-1388	1.92	0.650	0.18	0.20	1.00	0.63 / 0.35		0.63	0.98
5cfs	A-203	1.70	0.705	0.17	0.19	1.00	0.59 / 0.41		0.69	0.98
5ecm	C-301	1.60	0.707	0.23	0.25	1.00	0.38 / 0.20 / 0.42		0.80 / 0.78	0.98
5g6d	A-902	1.82	0.713	0.16	0.19	1.00	0.20 / 0.37 / 0.30		1.07 / 1.46	0.98
5hfk	B-302	1.55	0.721	0.19	0.21	1.00	0.68 / 0.24		1.10	0.98
5m0o	A-502	1.80	0.694	0.18	0.22	1.00	0.45 / 0.48		1.03	0.98
5azp	C-503	1.69	0.777	0.16	0.18	1.00	0.29 / 0.27 / 0.44		4.55 / 0.51	0.98
5d0e	A-302	1.48	0.747	0.19	0.23	0.85	0.28 / 0.20 / 0.38		3.39 / 1.11	0.97
5ey1	A-302	2.00	0.633	0.19	0.23	1.00	0.57 / 0.20 / 0.23		1.15 / 0.63	0.97
5jcw	A-308	1.95	0.705	0.15	0.19	0.56	0.20 / 0.20 / 0.20		1.56 / 1.36	0.97
5jq2	A-502	2.00	0.653	0.17	0.22	1.00	0.28 / 0.26 / 0.20 / 0.24		0.80 / 0.57 / 0.81	0.97
5l2f	A-301	1.77	0.677	0.18	0.19	1.00	0.20 / 0.20 / 0.29 / 0.20		1.08 / 0.74 / 0.64	0.97
5bo2	A-400	2.00	0.664	0.19	0.23	1.00	0.47 / 0.20 / 0.29		1.05 / 0.80	0.97
5fl1	B-1716	1.95	0.648	0.19	0.22	1.00	0.51 / 0.23 / 0.20		0.71 / 0.45	0.97
5hjk	A-401	2.00	0.644	0.18	0.22	1.00	0.49 / 0.20 / 0.30		1.17 / 0.86	0.97
5lmd	A-302	1.70	0.708	0.17	0.20	1.00	0.26 / 0.20 / 0.39		1.95 / 0.48	0.97

PDB	Ligand	Resolution (Å)	Twilight score	Rwork	Rfree	Occupancy (deposited)	Occupancy (qFit)	RMSD A->B (Å) (deposited)	RMSD A->B (qFit)	Best Fisher z improvement
5kjk	A-501	1.93	0.648	0.18	0.20	1.00	0.66 / 0.28		0.61	0.96
5g6o	A-905	1.72	0.839	0.19	0.23	1.00	0.34 / 0.20 / 0.23 / 0.20		1.26 / 1.09 / 1.61	0.96
5hvs	B-203	1.75	0.689	0.17	0.21	1.00	0.74 / 0.20		1.10	0.96
5syh	B-111	1.65	0.687	0.14	0.17	1.00	0.64 / 0.30		0.74	0.96
5f3f	A-201	1.76	0.680	0.14	0.17	0.48 / 0.52	0.42 / 0.33 / 0.24	0.45	2.67 / 0.44	0.96
5aez	A-904	1.47	0.843	0.14	0.15	1.00	0.48 / 0.52		0.80	0.96
5ehv	A-301	1.21	0.816	0.15	0.18	0.83	0.33 / 0.28 / 0.27		1.51 / 0.71	0.96
4znt	A-601	1.90	0.654	0.20	0.21	1.00	0.47 / 0.22 / 0.22		1.05 / 0.82	0.95
5c81	B-301	1.80	0.704	0.15	0.18	0.88	0.33 / 0.23 / 0.23		1.14 / 1.08	0.95
5d3x	A-501	1.69	0.693	0.18	0.21	1.00	0.25 / 0.21 / 0.20 / 0.23		1.45 / 0.97 / 1.44	0.95
5iha	A-401	1.96	0.647	0.17	0.20	1.00	0.27 / 0.20 / 0.32 / 0.20		0.99 / 1.03 / 1.37	0.95
5egr	A-406	1.55	0.730	0.17	0.19	1.00	0.70 / 0.30		0.84	0.95
5cuq	A-301	1.70	0.846	0.20	0.22	1.00	0.41 / 0.34		1.00	0.95
4zoj	A-403	1.96	0.684	0.22	0.26	1.00	0.23 / 0.20 / 0.39		0.99 / 0.64	0.95
5e0r	A-202	1.35	0.761	0.17	0.20	1.00	0.20 / 0.20 / 0.28 / 0.20		0.84 / 0.99 / 1.20	0.95
5jhn	B-1205	1.67	0.697	0.21	0.24	1.00	0.58 / 0.37		0.71	0.95
5ej4	F-602	1.77	0.682	0.18	0.22	1.00	0.27 / 0.25 / 0.20 / 0.21		0.95 / 0.61 / 0.78	0.94
5c1u	A-201	1.49	0.762	0.18	0.21	1.00	0.48 / 0.20 / 0.20		1.91 / 3.05	0.94
5iu8	A-2417	2.00	0.718	0.18	0.20	1.00	0.65 / 0.35		2.58	0.94
5f3z	A-1003	2.00	0.637	0.18	0.22	1.00	0.49 / 0.22 / 0.20		1.10 / 0.57	0.94
5iui	A-1501	1.88	0.676	0.18	0.21	1.00	0.54 / 0.20 / 0.26		2.17 / 0.69	0.94
5jij	B-1205	1.48	0.732	0.21	0.23	1.00	0.56 / 0.20 / 0.20		0.85 / 0.70	0.94
5eru	A-810	1.60	0.702	0.15	0.18	0.45	0.62 / 0.20		1.08	0.94
5cu3	B-403	1.79	0.733	0.18	0.20	1.00	0.31 / 0.20 / 0.33		0.91 / 1.43	0.94
5lf7	V-303	2.00	0.684	0.18	0.21	1.00	0.37 / 0.51		0.94	0.94
4zj0	A-202	1.50	0.747	0.20	0.25	1.00	0.45 / 0.55		0.87	0.94
5eek	A-2004	1.59	0.762	0.13	0.16	1.00	0.68 / 0.22		0.82	0.93
5t67	B-503	1.60	0.715	0.20	0.25	1.00	0.55 / 0.20 / 0.21		1.45 / 0.46	0.93
5f25	B-201	1.68	0.700	0.19	0.21	1.00	0.40 / 0.32 / 0.20		1.32 / 0.74	0.93
5lf7	H-305	2.00	0.682	0.18	0.21	1.00	0.49 / 0.20 / 0.20		0.88 / 0.86	0.93
5etl	A-206	1.82	0.697	0.20	0.24	1.00	0.80 / 0.20		4.60	0.93
5drp	B-402	1.89	0.665	0.16	0.19	1.00	0.23 / 0.74		0.95	0.93
5jmw	B-501	1.55	0.728	0.18	0.20	1.00	0.31 / 0.20 / 0.20 / 0.24		0.64 / 1.16 / 0.90	0.92
4ykm	A-201	1.58	0.725	0.18	0.22	1.00	0.57 / 0.20 / 0.20		0.83 / 0.60	0.92
5e93	A-401	1.41	0.767	0.15	0.17	1.00	0.58 / 0.23		1.20	0.92
5k2d	A-1212	1.90	0.713	0.17	0.21	1.00	0.20 / 0.26 / 0.25 / 0.28		0.90 / 0.92 / 1.05	0.92
5t77	A-553	2.00	0.777	0.19	0.21	1.00	0.20 / 0.80		0.75	0.92
5hae	A-201	2.00	0.640	0.15	0.20	1.00	0.42 / 0.23 / 0.35		0.90 / 0.63	0.92
5g2d	A-1268	1.80	0.731	0.18	0.21	1.00	0.51 / 0.49		0.83	0.91
5k2d	A-1209	1.90	0.696	0.17	0.21	1.00	0.20 / 0.48 / 0.32		1.28 / 0.83	0.91
5bo3	B-400	1.75	0.784	0.21	0.24	0.75	0.24 / 0.20 / 0.25		1.01 / 0.90	0.91
5ja3	D-202	1.81	0.689	0.23	0.27	0.96	0.49 / 0.20 / 0.27		1.30 / 0.64	0.91
5khm	A-201	1.48	0.737	0.18	0.21	0.50 / 0.50	0.53 / 0.25	12.61	0.68	0.91
5byt	B-402	2.00	0.648	0.22	0.27	0.60 / 0.40	0.48 / 0.20 / 0.20	3.13	0.67 / 0.99	0.91
5bqi	A-203	1.88	0.683	0.17	0.18	1.00	0.21 / 0.54 / 0.20		1.72 / 0.99	0.91
5ea9	B-408	1.71	0.677	0.18	0.22	1.00	0.71 / 0.29		0.78	0.91
5i8g	A-1405	1.41	0.831	0.19	0.21	1.00	0.23 / 0.21 / 0.49		1.87 / 1.92	0.91
5in3	A-416	1.73	0.708	0.20	0.23	0.84	0.42 / 0.33		0.88	0.90
5exb	C-64	1.81	0.670	0.18	0.25	1.00	0.40 / 0.28 / 0.30		0.39 / 0.99	0.90
5lf4	b-304	1.99	0.645	0.18	0.22	1.00	0.78			0.90
5g67	A-1367	1.97	0.665	0.17	0.20	1.00	0.65 / 0.30		2.20	0.90
5gmd	A-1002	1.50	0.764	0.17	0.19	1.00	0.20 / 0.31 / 0.26		1.20 / 1.37	0.90
5ly3	A-501	1.60	0.702	0.18	0.20	1.00	0.74 / 0.20		0.62	0.89
5g28	A-1271	1.57	0.822	0.15	0.19	1.00	0.45 / 0.25 / 0.30		1.58 / 1.06	0.89
5l2f	D-301	1.77	0.684	0.18	0.19	1.00	0.49 / 0.20 / 0.20		0.74 / 0.85	0.89
4zrs	A-151	2.00	0.629	0.15	0.20	1.00	0.53 / 0.47		1.24	0.89
5f0h	A-301	1.99	0.657	0.20	0.23	1.00	0.31 / 0.20 / 0.20 / 0.20		1.19 / 0.64 / 1.22	0.89
5fa7	B-301	1.67	0.689	0.18	0.21	1.00	0.36 / 0.20 / 0.38		0.89 / 0.89	0.89
4z13	A-608	1.78	0.696	0.16	0.20	1.00	0.52 / 0.48		0.91	0.89
5faq	A-305	1.96	0.656	0.17	0.21	1.00	0.42 / 0.20 / 0.20		1.10 / 0.48	0.89
5a8w	J-1553	1.80	0.664	0.17	0.20	1.00	0.59 / 0.36		0.59	0.89

PDB	Ligand	Resolution (Å)	Twilight score	Rwork	Rfree	Occupancy (deposited)	Occupancy (qFit)	RMSD A->B (Å) (deposited)	RMSD A->B (qFit)	Best Fisher z improvement
4yh2	D-301	1.72	0.690	0.16	0.19	1.00	0.20 / 0.26 / 0.23 / 0.20		0.82 / 0.88 / 1.07	0.89
5fbg	A-702	1.97	0.684	0.16	0.19	1.00	0.36 / 0.48		0.58	0.89
5hat	C-500	2.00	0.643	0.21	0.25	1.00	0.23 / 0.20 / 0.29 / 0.20		1.32 / 1.04 / 0.94	0.89
5f6b	B-201	1.31	0.798	0.20	0.24	1.00	0.25 / 0.41 / 0.34		0.80 / 2.24	0.89
5ix0	A-404	1.72	0.701	0.18	0.20	1.00	0.55 / 0.44		1.31	0.89
5fub	A-409	2.00	0.643	0.18	0.22	1.00	0.39 / 0.23 / 0.30		1.23 / 0.61	0.88
5fvn	B-404	1.45	0.863	0.16	0.18	1.00	0.27 / 0.73		0.65	0.88
5jil	A-513	1.85	0.686	0.18	0.20	1.00	0.24 / 0.20 / 0.33 / 0.20		0.80 / 0.84 / 1.14	0.88
4yfr	A-201	1.95	0.667	0.20	0.27	1.00	0.24 / 0.25 / 0.20 / 0.25		0.69 / 0.49 / 1.14	0.88
5iuc	A-602	1.25	0.785	0.16	0.18	1.00	0.36 / 0.20 / 0.20 / 0.20		0.95 / 0.80 / 0.80	0.88
5t77	A-545	2.00	0.700	0.19	0.21	1.00	0.34 / 0.44 / 0.20		1.69 / 0.62	0.88
5j41	B-301	1.19	0.805	0.16	0.19	1.00	0.29 / 0.20 / 0.20 / 0.20		1.03 / 0.80 / 0.74	0.88
5apg	C-1185	1.60	0.699	0.19	0.20	1.00	0.46 / 0.45		0.61	0.88
5hat	B-500	2.00	0.648	0.21	0.25	1.00	0.46 / 0.20 / 0.23		1.55 / 1.37	0.87
5ecs	B-301	1.65	0.703	0.17	0.19	1.00	0.24 / 0.28 / 0.34		0.63 / 0.76	0.87
5g6o	A-904	1.72	0.708	0.19	0.23	1.00	0.35 / 0.34 / 0.28		0.92 / 0.80	0.87
5u1h	C-201	1.50	0.728	0.17	0.20	1.00	0.54 / 0.20 / 0.20		1.12 / 1.56	0.87
5g4j	A-1441	1.87	0.658	0.17	0.20	1.00	0.38 / 0.20 / 0.30		0.92 / 1.34	0.87
5csd	B-201	1.45	0.905	0.18	0.20	1.00	0.64 / 0.36		0.64	0.87
5sx5	B-809	1.89	0.657	0.16	0.19	1.00	0.57 / 0.27		0.55	0.87
5duv	B-201	1.90	0.662	0.16	0.20	1.00	0.59 / 0.35		0.51	0.87
5eaj	B-201	1.70	0.693	0.20	0.23	1.00	0.46 / 0.20 / 0.25		0.61 / 0.51	0.87
4yb6	F-301	1.98	0.641	0.20	0.22	1.00	0.66 / 0.31		0.99	0.86
4d7f	A-1245	1.62	0.707	0.18	0.21	1.00	0.36 / 0.20 / 0.20 / 0.20		0.71 / 0.63 / 0.79	0.86
5bo2	B-400	2.00	0.662	0.19	0.23	1.00	0.22 / 0.24 / 0.37		1.19 / 0.70	0.86
5fvn	A-416	1.45	0.785	0.16	0.18	1.00	0.33 / 0.20 / 0.31		1.03 / 0.69	0.86
5cft	A-203	1.50	0.719	0.15	0.17	1.00	0.61 / 0.34		0.86	0.86
5dw1	A-500	1.55	0.720	0.16	0.20	1.00	0.24 / 0.23 / 0.34 / 0.20		1.20 / 0.73 / 1.48	0.86
5hsj	A-701	1.90	0.661	0.17	0.21	1.00	0.61 / 0.34		1.19	0.86
5hya	A-423	1.90	0.696	0.18	0.21	1.00	0.36 / 0.22 / 0.20 / 0.22		1.85 / 2.71 / 0.85	0.86
5k2c	A-1221	1.90	0.755	0.17	0.21	1.00	0.53 / 0.47		1.29	0.86
5lgw	A-701	1.95	0.641	0.18	0.19	1.00	0.75 / 0.21		0.56	0.86
5hdx	A-501	1.60	0.720	0.18	0.19	1.00	0.25 / 0.33 / 0.37		2.41 / 0.59	0.86
5hdz	B-501	1.49	0.745	0.19	0.21	1.00	0.33 / 0.33 / 0.29		2.19 / 0.50	0.85
5kk4	E-102	1.70	0.723	0.18	0.21	1.00	0.22 / 0.20 / 0.29 / 0.26		2.52 / 2.57 / 2.29	0.85
5f04	A-301	1.84	0.730	0.19	0.22	1.00	0.57 / 0.26		0.88	0.85
5faq	B-306	1.96	0.658	0.17	0.21	1.00	0.33 / 0.20 / 0.20		1.00 / 0.42	0.85
5thu	B-404	1.95	0.673	0.18	0.20	0.93	0.23 / 0.20 / 0.20 / 0.28		1.18 / 0.73 / 1.45	0.85
5jba	S-302	1.40	0.741	0.15	0.18	1.00	0.48 / 0.20 / 0.24		0.54 / 0.92	0.85
5f2g	A-3001	1.92	0.658	0.16	0.20	0.80	0.34 / 0.27 / 0.20		1.17 / 0.92	0.85
5ej4	E-601	1.77	0.685	0.18	0.22	1.00	0.33 / 0.20 / 0.20 / 0.20		0.65 / 0.95 / 0.80	0.85
5fag	D-502	1.51	0.722	0.20	0.23	1.00	0.66 / 0.20		0.98	0.85
5ctj	A-97	1.93	0.645	0.14	0.17	1.00	0.76 / 0.24		0.56	0.84
5lom	A-301	1.50	0.724	0.19	0.22	1.00	0.41 / 0.26 / 0.32		0.74 / 0.71	0.84
5drb	A-501	1.65	0.699	0.20	0.24	1.00	0.29 / 0.24 / 0.45		0.77 / 0.79	0.84
5hht	A-703	1.50	0.719	0.13	0.16	1.00	0.41 / 0.24 / 0.31		0.71 / 0.87	0.84
5igc	A-202	1.80	0.663	0.19	0.23	1.00	0.65 / 0.35		0.92	0.84
5g3n	A-1129	1.80	0.678	0.20	0.23	1.00	0.46 / 0.22 / 0.25		1.01 / 0.62	0.84
5ecm	F-301	1.60	0.704	0.23	0.25	1.00	0.44 / 0.30 / 0.27		1.53 / 0.83	0.84
5faz	B-202	1.40	0.837	0.22	0.26	1.00	0.59 / 0.41		2.26	0.84
5ja3	A-202	1.81	0.676	0.23	0.27	1.00	0.48 / 0.29 / 0.23		0.80 / 0.43	0.84
5dj9	B-508	1.55	0.712	0.16	0.19	1.00	0.52 / 0.20 / 0.26		0.93 / 0.71	0.83
5ec8	A-302	1.71	0.700	0.17	0.20	0.79	0.55 / 0.25		0.80	0.83
5iu8	A-2410	2.00	0.765	0.18	0.20	1.00	0.56 / 0.44		1.14	0.83
5jbc	S-302	1.90	0.651	0.17	0.21	1.00	0.29 / 0.20 / 0.22 / 0.20		1.21 / 0.94 / 0.63	0.83
4xoc	B-501	1.42	0.741	0.15	0.18	0.47 / 0.53	0.57 / 0.39	4.00	1.26	0.83
5lf7	U-47	2.00	0.679	0.18	0.21	1.00	0.20 / 0.36 / 0.29		2.32 / 0.71	0.83
5d4u	C-301	2.00	0.645	0.20	0.23	1.00	0.33 / 0.21 / 0.23 / 0.21		0.55 / 0.68 / 1.33	0.82
5gzf	A-201	2.00	0.657	0.20	0.22	1.00	0.54 / 0.44		0.61	0.82
5g6n	A-904	1.91	0.672	0.18	0.22	1.00	0.45 / 0.25 / 0.21		1.77 / 1.26	0.82
5jf3	A-301	1.60	0.827	0.19	0.21	1.00	0.20 / 0.59		0.55	0.82

PDB	Ligand	Resolution (Å)	Twilight score	Rwork	Rfree	Occupancy (deposited)	Occupancy (qFit)	RMSD A->B (Å) (deposited)	RMSD A->B (qFit)	Best Fisher z improvement
5bwz	B-404	1.59	0.718	0.14	0.16	1.00	0.32 / 0.60		1.76	0.82
5ayt	A-201	1.40	0.799	0.19	0.21	0.50	0.34 / 0.20 / 0.26		1.16 / 1.21	0.82
5dtz	B-68	1.50	0.718	0.17	0.20	1.00	0.54 / 0.38		1.10	0.82
5ecl	C-301	1.85	0.665	0.21	0.22	1.00	0.50 / 0.26 / 0.23		0.79 / 1.07	0.82
5t3i	A-66	1.60	0.703	0.13	0.18	1.00	0.66 / 0.28		0.77	0.82
5hdx	B-501	1.60	0.720	0.18	0.19	1.00	0.38 / 0.37 / 0.20		2.48 / 0.66	0.81
5k2c	A-1204	1.90	0.671	0.17	0.21	1.00	0.29 / 0.29 / 0.41		2.60 / 0.51	0.81
5hkb	C-401	1.65	0.703	0.19	0.22	0.68	0.21 / 0.23 / 0.21		1.91 / 1.69	0.81
4yaw	B-701	2.00	0.647	0.20	0.25	1.00	0.56 / 0.24 / 0.20		0.94 / 1.00	0.81
5f07	A-301	1.50	0.717	0.16	0.19	1.00	0.80 / 0.20		0.55	0.81
5ltp	D-59	1.70	0.686	0.19	0.21	1.00	0.61 / 0.30		0.56	0.81
5hbg	A-46	1.90	0.662	0.19	0.22	1.00	0.61 / 0.37		0.60	0.81
5k0f	A-302	1.81	0.664	0.17	0.21	1.00	0.29 / 0.27 / 0.41		1.31 / 0.51	0.81
4y6g	B-402	1.65	0.699	0.16	0.18	0.90	0.39 / 0.20 / 0.21		1.03 / 1.43	0.80
5byt	A-402	2.00	0.636	0.22	0.27	1.00	0.33 / 0.23 / 0.24 / 0.20		0.98 / 0.95 / 0.70	0.80
5eko	A-401	2.00	0.640	0.20	0.24	1.00	0.20 / 0.23 / 0.24 / 0.26		1.35 / 1.02 / 1.43	0.80
5l8p	E-406	1.29	0.776	0.11	0.13	0.70 / 0.30	0.40 / 0.20 / 0.20 / 0.20	2.88	2.16 / 0.72 / 3.10	0.80
5t77	A-517	2.00	0.730	0.19	0.21	1.00	0.66 / 0.24		1.48	0.80
5ggl	A-301	1.27	0.835	0.15	0.16	1.00	0.36 / 0.21 / 0.20 / 0.23		0.70 / 1.18 / 1.76	0.80
4zof	A-403	1.80	0.692	0.19	0.22	1.00	0.51 / 0.20 / 0.20		0.91 / 0.67	0.80
5g6j	A-904	1.88	0.677	0.16	0.19	1.00	0.64 / 0.32		3.14	0.80
5kce	B-601	1.85	0.673	0.19	0.25	0.93	0.27 / 0.20 / 0.21 / 0.20		1.49 / 0.84 / 1.20	0.80
5ltp	B-59	1.70	0.689	0.19	0.21	1.00	0.69 / 0.24		1.20	0.79
4zvz	C-503	2.00	0.671	0.20	0.24	1.00	0.20 / 0.20 / 0.23 / 0.20		0.91 / 1.48 / 1.11	0.79
5dw1	B-500	1.55	0.715	0.16	0.20	1.00	0.59 / 0.20 / 0.21		2.00 / 1.37	0.79
5g10	A-1375	1.71	0.738	0.16	0.19	1.00	0.21 / 0.20 / 0.39		1.36 / 1.35	0.79
5ea9	A-401	1.71	0.701	0.18	0.22	1.00	0.47 / 0.33		0.78	0.79
5g09	B-1474	1.90	0.648	0.17	0.20	1.00	0.62 / 0.36		0.99	0.79
5g28	A-1275	1.57	0.737	0.15	0.19	1.00	0.58 / 0.20 / 0.22		1.08 / 0.98	0.79
5f91	C-501	2.00	0.632	0.15	0.19	1.00	0.53 / 0.24 / 0.20		0.67 / 1.14	0.79
5iy5	G-102	2.00	0.639	0.17	0.21	1.00	0.62 / 0.38		0.66	0.79
5ign	A-201	1.70	0.693	0.21	0.24	1.00	0.21 / 0.26 / 0.29 / 0.20		1.75 / 0.64 / 1.81	0.79
4zu5	B-202	1.80	0.796	0.21	0.24	0.25	0.36 / 0.28		1.13	0.79
5ecx	B-202	1.95	0.685	0.22	0.27	1.00	0.49 / 0.37		1.03	0.79
4y1u	A-202	1.76	0.705	0.18	0.23	1.00	0.54 / 0.32		0.95	0.79
5l9l	B-401	1.80	0.688	0.21	0.24	1.00	0.51 / 0.28 / 0.22		0.62 / 0.72	0.79
5t64	B-505	1.70	0.722	0.18	0.22	1.00	0.72 / 0.24		0.94	0.79
4xjl	B-502	1.85	0.698	0.19	0.21	1.00	0.33 / 0.24 / 0.22		1.29 / 1.01	0.78
5dyz	C-502	1.97	0.697	0.18	0.22	1.00	0.24 / 0.20 / 0.29 / 0.20		1.58 / 0.98 / 0.95	0.78
5ecq	E-301	1.66	0.697	0.23	0.23	1.00	0.78 / 0.22		1.06	0.78
4zyy	A-1101	1.85	0.660	0.17	0.20	0.84	0.41 / 0.20 / 0.23		0.47 / 1.49	0.78
5c8z	A-301	1.60	0.733	0.15	0.17	0.89	0.61 / 0.23		0.97	0.78
5lsc	B-404	1.50	0.735	0.14	0.17	0.98	0.42 / 0.49		0.70	0.78
4xnd	A-902	1.93	0.641	0.13	0.17	1.00	0.28 / 0.70		0.78	0.78
5iuc	B-602	1.25	0.785	0.16	0.18	1.00	0.22 / 0.20 / 0.32 / 0.20		0.65 / 0.87 / 1.08	0.78
5aez	A-903	1.47	0.939	0.14	0.15	1.00	0.67 / 0.29		2.61	0.77
5k2d	A-1213	1.90	0.753	0.17	0.21	1.00	0.42 / 0.20 / 0.38		0.91 / 1.11	0.77
5fh5	A-703	1.55	0.716	0.21	0.24	0.70 / 0.30	0.46 / 0.23 / 0.20	1.42	0.87 / 0.85	0.77
5ft4	A-1401	2.00	0.632	0.14	0.19	1.00	0.53 / 0.45		1.14	0.77
5fp1	A-1722	1.94	0.695	0.16	0.18	1.00	0.35 / 0.59		0.78	0.77
5i8b	A-1404	1.52	0.739	0.19	0.20	1.00	0.80 / 0.20		1.46	0.77
5b1s	D-501	1.58	0.703	0.19	0.23	1.00	0.26 / 0.20 / 0.38		2.12 / 2.24	0.77
5ltp	A-59	1.70	0.691	0.19	0.21	1.00	0.55 / 0.20 / 0.21		0.52 / 1.18	0.77
5eec	A-301	1.87	0.666	0.17	0.21	0.40 / 0.60	0.33 / 0.25 / 0.23	1.80	1.68 / 0.70	0.77
5k2d	A-1220	1.90	0.683	0.17	0.21	1.00	0.25 / 0.55 / 0.20		0.99 / 0.86	0.77
5faj	D-401	1.64	0.700	0.21	0.24	1.00	0.75 / 0.21		1.88	0.77
5f6u	A-201	1.55	0.741	0.18	0.20	1.00	0.20 / 0.24 / 0.23 / 0.20		1.38 / 0.54 / 1.17	0.76
5hat	L-500	2.00	0.639	0.21	0.25	1.00	0.29 / 0.23 / 0.35		1.29 / 0.99	0.76
5jj0	B-1205	1.72	0.697	0.22	0.25	1.00	0.38 / 0.20 / 0.40		0.78 / 0.67	0.76
5f2f	A-201	1.66	0.708	0.14	0.18	0.45 / 0.55	0.34 / 0.20 / 0.20 / 0.21	0.86	0.85 / 0.41 / 3.31	0.76
5dnk	A-601	1.90	0.651	0.20	0.25	1.00	0.31 / 0.20 / 0.26 / 0.20		1.31 / 0.68 / 0.89	0.76

PDB	Ligand	Resolution (Å)	Twilight score	Rwork	Rfree	Occupancy (deposited)	Occupancy (qFit)	RMSD A->B (Å) (deposited)	RMSD A->B (qFit)	Best Fisher z improvement
5hya	A-410	1.90	0.728	0.18	0.21	1.00	0.20 / 0.22 / 0.33 / 0.20		1.01 / 0.78 / 1.19	0.76
5g0i	B-1809	1.99	0.687	0.17	0.20	1.00	0.38 / 0.48		1.38	0.76
5k2d	A-1211	1.90	0.716	0.17	0.21	1.00	0.32 / 0.48 / 0.20		1.70 / 1.82	0.76
5bw6	B-401	1.82	0.657	0.17	0.21	1.00	0.67 / 0.24		1.27	0.76
5k2c	A-1201	1.90	0.654	0.17	0.21	1.00	0.22 / 0.20 / 0.29 / 0.26		0.81 / 0.98 / 1.35	0.76
4yda	A-201	1.95	0.674	0.19	0.24	1.00	0.56 / 0.27		0.98	0.75
4x3l	A-301	1.70	0.711	0.19	0.21	1.00	0.37 / 0.53		0.76	0.75
5sexy	A-306	1.55	0.738	0.13	0.17	0.55	0.21 / 0.20 / 0.20		1.52 / 0.82	0.75
5exbx	M-64	1.81	0.682	0.18	0.25	1.00	0.58 / 0.36		0.75	0.75
5dzi	B-900	1.90	0.649	0.18	0.21	1.00	0.52 / 0.20 / 0.23		1.37 / 1.03	0.75
5lb5	A-504	2.00	0.641	0.24	0.28	1.00	0.56 / 0.39		0.90	0.75
5etz	B-301	1.80	0.675	0.22	0.24	1.00	0.76 / 0.23		1.12	0.75
5fvn	A-418	1.45	0.791	0.16	0.18	1.00	0.60 / 0.33		0.71	0.75
5iu8	A-2427	2.00	0.686	0.18	0.20	1.00	0.57 / 0.20 / 0.23		1.32 / 1.07	0.75
5azp	C-501	1.69	0.813	0.16	0.18	1.00	0.20 / 0.20 / 0.20 / 0.20 / 0.20		1.04 / 0.86 / 1.11 / 1.51	0.74
5hgg	T-201	1.97	0.770	0.17	0.20	1.00	0.23 / 0.27 / 0.20 / 0.30		3.95 / 0.61 / 1.98	0.74
5u20	B-184	1.50	0.717	0.14	0.18	1.00	0.53 / 0.20 / 0.23		1.15 / 0.58	0.74
5i7r	B-402	1.73	0.700	0.17	0.21	1.00	0.48 / 0.28 / 0.20		1.19 / 0.96	0.74
5jmy	B-807	2.00	0.637	0.19	0.23	1.00	0.36 / 0.22 / 0.20 / 0.21		1.11 / 1.27 / 1.17	0.74
5d0e	A-303	1.48	0.742	0.19	0.23	0.93	0.42 / 0.20 / 0.29		2.99 / 0.81	0.74
4zmg	A-401	1.90	0.644	0.18	0.20	1.00	0.55 / 0.45		0.81	0.74
5g4o	A-1293	1.48	0.752	0.14	0.17	1.00	0.73 / 0.20		1.11	0.74
5j7p	C-201	1.85	0.678	0.18	0.20	1.00	0.61 / 0.26		0.88	0.74
4y6g	A-301	1.65	0.707	0.16	0.18	0.90	0.55 / 0.20		1.81	0.74
5fvn	B-409	1.45	0.777	0.16	0.18	1.00	0.20 / 0.22 / 0.29		1.12 / 1.30	0.74
5fvn	F-414	1.45	0.805	0.16	0.18	1.00	0.57 / 0.39		0.74	0.74
5d2r	A-523	1.90	0.655	0.18	0.22	1.00	0.62 / 0.28		0.95	0.73
5kp7	B-100	1.60	0.724	0.15	0.17	1.00	0.37 / 0.21 / 0.34		0.53 / 0.69	0.73
5m0p	A-502	1.95	0.678	0.16	0.20	1.00	0.71 / 0.22		0.88	0.73
5etl	B-204	1.82	0.698	0.20	0.24	1.00	0.80 / 0.20		4.83	0.73
5j7p	A-201	1.85	0.717	0.18	0.20	0.90	0.53 / 0.25		0.58	0.73
5j9a	A-404	2.00	0.629	0.14	0.18	1.00	0.35 / 0.25 / 0.36		0.87 / 0.93	0.73
5anw	A-1157	1.37	0.752	0.20	0.23	1.00	0.80 / 0.20		0.81	0.73
5iu8	A-2424	2.00	0.687	0.18	0.20	1.00	0.66 / 0.34		1.05	0.73
4ygg	A-201	1.90	0.676	0.20	0.24	1.00	0.70 / 0.24		0.70	0.73
4zqc	A-301	1.54	0.709	0.14	0.19	1.00	0.68 / 0.20		0.91	0.73
5fvn	B-414	1.45	0.786	0.16	0.18	1.00	0.49 / 0.34		0.96	0.73
5e0r	A-204	1.35	0.835	0.17	0.20	1.00	0.43 / 0.20 / 0.22		1.05 / 1.01	0.73
5ep2	A-401	1.42	0.749	0.16	0.18	1.00	0.23 / 0.21 / 0.44		1.42 / 1.15	0.73
5ert	A-801	2.00	0.630	0.18	0.21	1.00	0.69 / 0.28		0.61	0.73
5eyc	A-1401	1.80	0.669	0.19	0.25	1.00	0.72 / 0.27		1.53	0.73
5g4o	B-1292	1.48	0.756	0.14	0.17	1.00	0.54 / 0.20 / 0.20		1.42 / 1.28	0.73
5e93	B-408	1.41	0.733	0.15	0.17	1.00	0.58 / 0.41		0.78	0.72
5cft	A-204	1.50	0.727	0.15	0.17	1.00	0.73 / 0.27		0.88	0.72
5cvf	A-402	1.63	0.782	0.20	0.21	0.65	0.27 / 0.20		0.98	0.72
5azp	B-501	1.69	0.772	0.16	0.18	1.00	0.73 / 0.27		4.28	0.72
5dtk	B-301	1.60	0.750	0.15	0.17	0.69	0.37 / 0.20 / 0.20		1.39 / 1.29	0.72
5t6b	B-502	2.00	0.639	0.18	0.23	1.00	0.39 / 0.20 / 0.41		0.63 / 1.06	0.72
5t77	A-550	2.00	0.772	0.19	0.21	1.00	0.49 / 0.51		1.53	0.72
5enq	C-901	1.80	0.665	0.18	0.22	1.00	0.56 / 0.22 / 0.21		1.55 / 0.58	0.72
5jin	A-1205	1.85	0.667	0.20	0.24	1.00	0.37 / 0.56		0.69	0.72
5d15	B-301	1.50	0.732	0.20	0.21	0.24 / 0.76	0.64 / 0.24	0.84	0.92	0.71
5b2f	A-302	1.90	0.646	0.22	0.27	1.00	0.44 / 0.47		1.24	0.71
5efo	E-303	1.63	0.737	0.16	0.21	0.75	0.46 / 0.45		0.60	0.71
5k2c	A-1216	1.90	0.746	0.17	0.21	1.00	0.65 / 0.35		1.45	0.71
5cpn	A-402	1.80	0.675	0.18	0.22	1.00	0.56 / 0.38		0.83	0.71
5ivg	A-704	1.95	0.641	0.16	0.20	1.00	0.58 / 0.20 / 0.22		1.56 / 1.41	0.71
4yh2	B-301	1.72	0.685	0.16	0.19	1.00	0.68 / 0.23		0.81	0.71
5hzq	A-201	1.75	0.717	0.20	0.23	0.50 / 0.50	0.20 / 0.30 / 0.20 / 0.20	2.05	1.74 / 1.17 / 0.94	0.71
5d4o	A-201	1.80	0.665	0.21	0.23	1.00	0.47 / 0.42		0.51	0.70
5fvn	F-410	1.45	0.746	0.16	0.18	1.00	0.32 / 0.20 / 0.40		0.78 / 0.61	0.70

PDB	Ligand	Resolution (Å)	Twilight score	Rwork	Rfree	Occupancy (deposited)	Occupancy (qFit)	RMSD A->B (Å) (deposited)	RMSD A->B (qFit)	Best Fisher z improvement
5eci	E-301	1.56	0.714	0.21	0.23	1.00	0.80 / 0.20		0.76	0.70
5ivg	C-704	1.95	0.637	0.16	0.20	1.00	0.20 / 0.20 / 0.20 / 0.20 / 0.20		1.27 / 1.24 / 0.94 / 1.37	0.70
5lwm	A-1201	1.55	0.724	0.16	0.20	1.00	0.39 / 0.20 / 0.36		0.74 / 1.16	0.70
5an1	B-1220	2.00	0.647	0.21	0.26	1.00	0.69 / 0.28		0.75	0.70
5thv	A-404	1.87	0.683	0.17	0.21	1.00	0.22 / 0.20 / 0.56		1.37 / 0.82	0.70
5dq1	A-402	1.49	0.782	0.13	0.18	0.85	0.51 / 0.20 / 0.20		1.47 / 1.33	0.69
5ej4	C-601	1.77	0.683	0.18	0.22	1.00	0.48 / 0.25 / 0.25		1.80 / 0.57	0.69
5flj	F-301	1.82	0.723	0.16	0.21	0.80	0.44 / 0.37		1.43	0.69
5fok	A-1725	1.90	0.657	0.19	0.21	1.00	0.50 / 0.49		0.69	0.69
5il1	A-601	1.71	0.694	0.18	0.21	1.00	0.53 / 0.42		0.64	0.69
5lkd	B-401	1.68	0.693	0.16	0.20	1.00	0.55 / 0.29		0.82	0.69
5iu8	A-2429	2.00	0.698	0.18	0.20	1.00	0.37 / 0.20 / 0.20 / 0.23		1.13 / 1.30 / 1.39	0.69
5d3h	A-201	1.70	0.702	0.16	0.20	1.00	0.51 / 0.20 / 0.20		1.29 / 1.03	0.69
5g0v	B-1271	1.79	0.700	0.16	0.19	1.00	0.38 / 0.20 / 0.29		1.52 / 0.96	0.69
4yd7	A-405	1.42	0.788	0.12	0.15	0.76	0.45 / 0.29		1.21	0.69
5fal	A-502	1.86	0.673	0.15	0.19	1.00	0.65 / 0.30		1.05	0.69
5ixx	A-1001	1.43	0.742	0.17	0.18	1.00	0.53 / 0.20 / 0.24		1.15 / 0.62	0.69
5lf7	G-47	2.00	0.654	0.18	0.21	1.00	0.43 / 0.26 / 0.20		2.36 / 2.09	0.68
5g3n	B-1126	1.80	0.674	0.20	0.23	1.00	0.68 / 0.27		0.57	0.68
4s35	A-202	1.55	0.713	0.15	0.17	0.50 / 0.50	0.60 / 0.27	1.21	1.14	0.68
5fvn	F-420	1.45	0.760	0.16	0.18	1.00	0.25 / 0.28 / 0.35		1.03 / 0.88	0.68
5erv	A-801	1.80	0.665	0.16	0.20	0.59	0.49 / 0.20 / 0.20		1.07 / 1.01	0.68
5exb	D-64	1.81	0.690	0.18	0.25	1.00	0.34 / 0.30 / 0.33		0.86 / 0.99	0.68
5hya	A-422	1.90	0.787	0.18	0.21	1.00	0.35 / 0.28 / 0.31		1.63 / 2.61	0.68
5syw	A-111	1.85	0.659	0.15	0.18	0.55 / 0.15	0.53 / 0.40	0.58	0.54	0.68
4y9u	B-701	1.95	0.678	0.20	0.24	1.00	0.34 / 0.21 / 0.20 / 0.20		0.98 / 0.93 / 1.36	0.68
5dy3	A-401	1.82	0.683	0.15	0.19	1.00	0.60 / 0.20		0.85	0.68
5d4v	C-308	1.60	0.725	0.17	0.21	1.00	0.38 / 0.33 / 0.20		3.06 / 1.41	0.67
4zqc	B-402	1.54	0.726	0.14	0.19	0.80	0.20 / 0.20 / 0.32		1.37 / 0.87	0.67
4zs9	A-501	1.37	0.746	0.13	0.17	1.00	0.79 / 0.21		0.53	0.67
5fqqr	A-1546	1.88	0.678	0.21	0.24	1.00	0.62 / 0.37		1.29	0.67
5g3l	G-300	1.72	0.711	0.17	0.20	1.00	0.31 / 0.20 / 0.29		1.05 / 0.75	0.67
4d7b	B-1126	1.15	0.823	0.17	0.20	0.51	0.20 / 0.27 / 0.27		1.17 / 0.81	0.67
4zof	B-402	1.80	0.664	0.19	0.22	1.00	0.49 / 0.20 / 0.24		0.91 / 0.89	0.67
5hdj	A-400	1.89	0.649	0.17	0.21	1.00	0.80 / 0.20		0.85	0.67
5aqy	A-1389	1.56	0.735	0.17	0.20	1.00	0.71 / 0.22		0.60	0.67
5lf7	X-91	2.00	0.657	0.18	0.21	1.00	0.54 / 0.33		1.15	0.67
5lmc	A-502	1.90	0.645	0.17	0.17	1.00	0.45 / 0.55		0.77	0.67
5fvn	A-409	1.45	0.808	0.16	0.18	1.00	0.39 / 0.23 / 0.38		1.43 / 0.81	0.66
5iwg	A-403	1.66	0.703	0.19	0.21	1.00	0.49 / 0.20 / 0.26		1.07 / 1.11	0.66
4yqs	A-301	1.90	0.666	0.16	0.19	1.00	0.42 / 0.25 / 0.20		1.37 / 1.23	0.66
5jc1	B-502	1.65	0.698	0.18	0.20	1.00	0.76 / 0.22		1.90	0.66
5fok	B-1722	1.90	0.708	0.19	0.21	1.00	0.60 / 0.40		0.76	0.66
5t67	A-503	1.60	0.697	0.20	0.25	1.00	0.80 / 0.20		0.70	0.66
4yaf	B-703	1.91	0.648	0.21	0.24	1.00	0.45 / 0.20 / 0.28		0.45 / 0.55	0.66
5faz	A-202	1.40	0.849	0.22	0.26	1.00	0.22 / 0.20 / 0.27 / 0.31		1.05 / 0.78 / 1.43	0.66
5jyc	B-401	2.00	0.664	0.15	0.19	1.00	0.50 / 0.50		1.26	0.66
5k2c	A-1212	1.90	0.731	0.17	0.21	1.00	0.20 / 0.54 / 0.26		1.65 / 3.30	0.65
5t6b	D-503	2.00	0.670	0.18	0.23	1.00	0.56 / 0.20 / 0.24		0.74 / 0.86	0.65
5ds7	A-201	2.00	0.650	0.23	0.26	1.00	0.55 / 0.35		1.00	0.65
5iwg	B-403	1.66	0.698	0.19	0.21	1.00	0.64 / 0.35		1.08	0.65
4zj0	B-201	1.50	0.827	0.20	0.25	1.00	0.33 / 0.25 / 0.20 / 0.22		2.27 / 0.56 / 0.84	0.65
5g68	A-902	1.63	0.703	0.16	0.19	1.00	0.65 / 0.30		1.03	0.65
5j3z	B-401	1.80	0.683	0.17	0.20	1.00	0.57 / 0.39		0.70	0.65
5t6b	C-503	2.00	0.676	0.18	0.23	1.00	0.66 / 0.34		0.75	0.64
4yko	A-201	1.57	0.740	0.20	0.22	1.00	0.58 / 0.20 / 0.22		0.58 / 0.73	0.64
4yq4	A-301	1.89	0.658	0.17	0.20	1.00	0.52 / 0.20 / 0.20		1.52 / 1.71	0.64
5bph	C-401	1.70	0.686	0.18	0.21	1.00	0.77 / 0.20		0.92	0.64
5fvn	F-411	1.45	0.762	0.16	0.18	1.00	0.47 / 0.21 / 0.32		3.09 / 0.65	0.64
5hrw	A-801	1.80	0.673	0.20	0.24	1.00	0.73 / 0.23		0.80	0.64
5lmb	B-525	1.95	0.768	0.18	0.23	1.00	0.54 / 0.35		0.82	0.64

PDB	Ligand	Resolution (Å)	Twilight score	Rwork	Rfree	Occupancy (deposited)	Occupancy (qFit)	RMSD A->B (Å) (deposited)	RMSD A->B (qFit)	Best Fisher z improvement
5tc4	A-402	1.89	0.655	0.16	0.21	1.00	0.76 / 0.20		0.59	0.64
5kqr	A-301	1.33	0.804	0.17	0.19	1.00	0.63 / 0.21		0.69	0.64
5ley	U-47	1.90	0.692	0.19	0.23	1.00	0.52 / 0.32		1.27	0.64
5hzq	B-201	1.75	0.714	0.20	0.23	0.50 / 0.50	0.57 / 0.23	1.79	1.49	0.64
5syg	A-111	1.85	0.667	0.15	0.19	0.80 / 0.10	0.31 / 0.26 / 0.39	0.59	0.65 / 0.59	0.64
5c1r	B-403	1.80	0.665	0.17	0.21	1.00	0.62 / 0.34		0.93	0.63
5ke0	A-401	1.68	0.702	0.17	0.19	1.00	0.68 / 0.20		0.70	0.63
4zns	A-601	1.86	0.667	0.20	0.24	0.78	0.58 / 0.20		1.02	0.63
5hni	Y-1401	1.71	0.813	0.23	0.25	1.00	0.34 / 0.27 / 0.20		1.01 / 1.06	0.63
5epo	C-302	2.00	0.670	0.18	0.22	1.00	0.51 / 0.28 / 0.20		2.01 / 1.32	0.63
5g28	A-1268	1.57	0.711	0.15	0.19	1.00	0.26 / 0.25 / 0.21 / 0.27		0.54 / 0.44 / 1.29	0.63
5l02	B-111	1.90	0.650	0.17	0.21	0.80 / 0.10	0.37 / 0.20 / 0.36	0.58	0.63 / 0.60	0.63
5f9s	A-401	1.70	0.680	0.16	0.21	1.00	0.52 / 0.20 / 0.24		1.18 / 1.13	0.63
5ivq	A-101	1.57	0.737	0.19	0.22	1.00	0.31 / 0.20 / 0.20 / 0.20		0.93 / 0.59 / 0.86	0.63
4zvz	B-503	2.00	0.663	0.20	0.24	1.00	0.43 / 0.37		1.08	0.63
5fqp	A-1549	1.88	0.674	0.21	0.23	1.00	0.78 / 0.22		1.46	0.63
5ikm	A-311	1.90	0.655	0.15	0.18	1.00	0.74 / 0.20		0.73	0.63
4yaf	A-703	1.91	0.648	0.21	0.24	1.00	0.59 / 0.37		0.55	0.63
5b1s	C-501	1.58	0.706	0.19	0.23	1.00	0.23 / 0.20 / 0.21 / 0.27		1.25 / 2.32 / 0.89	0.63
5dkr	A-103	1.74	0.705	0.21	0.25	1.00	0.63 / 0.24		1.05	0.62
5efj	F-1	1.73	0.698	0.15	0.17	1.00	0.63 / 0.21		1.24	0.62
5g0o	A-760	1.85	0.678	0.19	0.23	1.00	0.61 / 0.21		0.93	0.62
5ecl	E-301	1.85	0.661	0.21	0.22	1.00	0.80 / 0.20		0.89	0.62
4y6g	B-401	1.65	0.686	0.16	0.18	1.00	0.67 / 0.30		1.12	0.62
5fvn	F-422	1.45	0.743	0.16	0.18	1.00	0.41 / 0.53		0.43	0.62
5exo	A-302	1.50	0.739	0.16	0.19	1.00	0.56 / 0.28		0.50	0.62
5kcq	B-501	2.00	0.663	0.19	0.22	1.00	0.46 / 0.22 / 0.27		2.22 / 2.19	0.62
5kk4	F-101	1.70	0.823	0.18	0.21	1.00	0.20 / 0.23 / 0.27 / 0.28		0.99 / 0.81 / 1.56	0.62
5fa7	A-301	1.67	0.688	0.18	0.21	1.00	0.54 / 0.20 / 0.20		0.76 / 0.88	0.62
4zof	B-403	1.80	0.720	0.19	0.22	0.75	0.27 / 0.20 / 0.28		0.70 / 0.75	0.62
5dvz	B-82	1.69	0.681	0.20	0.23	1.00	0.60 / 0.20 / 0.20		1.14 / 0.49	0.62
5k4z	A-401	1.64	0.701	0.19	0.20	1.00	0.58 / 0.36		0.96	0.62
4yaw	A-701	2.00	0.637	0.20	0.25	1.00	0.60 / 0.20 / 0.20		0.92 / 0.83	0.61
4zvz	D-503	2.00	0.660	0.20	0.24	1.00	0.20 / 0.30 / 0.32		1.00 / 0.69	0.61
5dwj	A-901	2.00	0.698	0.20	0.23	0.78	0.56 / 0.28		1.48	0.61
5ix0	C-404	1.72	0.714	0.18	0.20	1.00	0.51 / 0.20 / 0.20		1.30 / 1.35	0.61
5jss	E-406	1.19	0.786	0.10	0.12	0.70 / 0.30	0.56 / 0.24 / 0.20	0.37	0.45 / 0.55	0.61
5h85	A-1201	1.70	0.699	0.16	0.20	1.00	0.72 / 0.20		0.87	0.61
5ivg	D-704	1.95	0.637	0.16	0.20	1.00	0.40 / 0.20 / 0.20 / 0.20		1.17 / 1.64 / 1.25	0.61
5t6m	B-82	1.80	0.672	0.20	0.24	1.00	0.70 / 0.25		1.02	0.61
5e2n	A-307	1.53	0.743	0.18	0.21	1.00	0.46 / 0.33		0.91	0.61
5fp7	A-1344	2.00	0.666	0.16	0.21	1.00	0.47 / 0.20 / 0.24		1.61 / 1.43	0.61
5tg5	A-302	1.75	0.699	0.18	0.21	1.00	0.43 / 0.38		1.52	0.61
5e23	A-201	1.41	0.734	0.17	0.20	0.37	0.20 / 0.21 / 0.20		2.28 / 0.72	0.61
5g54	A-1271	2.00	0.667	0.18	0.23	1.00	0.55 / 0.45		0.81	0.61
4xug	A-300	1.65	0.692	0.17	0.19	1.00	0.52 / 0.20 / 0.20		1.27 / 0.97	0.61
4wv8	A-303	1.83	0.724	0.16	0.20	1.00	0.60 / 0.20 / 0.20		0.68 / 0.42	0.61
5i8g	A-1404	1.41	0.748	0.19	0.21	1.00	0.63 / 0.37		0.89	0.61
5d3y	A-501	1.95	0.658	0.21	0.26	1.00	0.74 / 0.25		0.91	0.60
5h02	A-301	1.78	0.680	0.18	0.20	1.00	0.68 / 0.20		1.03	0.60
5kf8	A-405	1.90	0.662	0.16	0.21	1.00	0.70 / 0.24		0.71	0.60
5t6b	A-502	2.00	0.640	0.18	0.23	1.00	0.43 / 0.20 / 0.37		1.03 / 1.04	0.60
5fvn	A-408	1.45	0.818	0.16	0.18	1.00	0.43 / 0.36		1.41	0.60
5e9q	C-4000	1.79	0.689	0.17	0.20	1.00	0.71 / 0.22		0.75	0.60
5ea9	A-409	1.71	0.678	0.18	0.22	1.00	0.80 / 0.20		0.81	0.60
5iu8	A-2413	2.00	0.755	0.18	0.20	1.00	0.56 / 0.44		0.94	0.60
5ix0	B-404	1.72	0.700	0.18	0.20	1.00	0.60 / 0.20 / 0.20		1.39 / 1.62	0.60
4yd3	A-402	1.25	0.788	0.11	0.13	1.00	0.76 / 0.24		1.19	0.60
5hin	A-401	1.60	0.698	0.16	0.18	1.00	0.46 / 0.53		0.78	0.60
5a5i	A-1493	2.00	0.674	0.21	0.25	1.00	0.64 / 0.20		1.57	0.60
5d3x	B-501	1.69	0.735	0.18	0.21	0.52	0.38 / 0.20		1.68	0.60

PDB	Ligand	Resolution (Å)	Twilight score	Rwork	Rfree	Occupancy (deposited)	Occupancy (qFit)	RMSD A->B (Å) (deposited)	RMSD A->B (qFit)	Best Fisher z improvement
5g2p	B-2000	1.89	0.647	0.16	0.20	1.00	0.54 / 0.46		1.16	0.60
5f58	A-201	1.54	0.770	0.19	0.23	1.00	0.41 / 0.28 / 0.20		1.01 / 0.56	0.59
5fvn	F-403	1.45	0.771	0.16	0.18	1.00	0.68 / 0.32		1.03	0.59
5ec8	C-4000	1.71	0.702	0.17	0.20	1.00	0.32 / 0.20 / 0.20 / 0.20		0.56 / 0.65 / 1.28	0.59
5cbw	A-206	1.80	0.707	0.17	0.21	1.00	0.35 / 0.20 / 0.22		1.05 / 1.38	0.59
5t77	A-535	2.00	0.671	0.19	0.21	1.00	0.28 / 0.20 / 0.40		0.78 / 0.59	0.59
4ybu	A-201	1.92	0.696	0.20	0.24	1.00	0.20 / 0.20 / 0.20 / 0.20		0.61 / 0.66 / 2.33	0.59
5b2f	C-302	1.90	0.649	0.22	0.27	1.00	0.68 / 0.27		1.28	0.59
5bst	A-601	1.61	0.698	0.20	0.22	1.00	0.66 / 0.31		0.86	0.58
5le5	U-47	1.80	0.701	0.18	0.21	1.00	0.51 / 0.36		2.06	0.58
5hg8	A-9001	1.42	0.752	0.21	0.21	1.00	0.78 / 0.20		1.38	0.58
5eci	C-301	1.56	0.716	0.21	0.23	1.00	0.76 / 0.24		0.75	0.58
5k0i	A-204	1.30	0.868	0.15	0.16	1.00	0.74 / 0.26		0.52	0.58
5fc4	A-403	1.50	0.744	0.16	0.20	1.00	0.57 / 0.22		0.71	0.58
5szy	A-200	2.00	0.635	0.20	0.21	1.00	0.71 / 0.20		0.93	0.58
4ykw	A-301	1.85	0.665	0.20	0.23	1.00	0.70 / 0.20		1.93	0.58
5fen	B-201	1.55	0.764	0.20	0.24	1.00	0.35 / 0.29 / 0.34		0.84 / 0.39	0.57
5fvn	D-417	1.45	0.774	0.16	0.18	1.00	0.65 / 0.35		4.34	0.57
5t77	A-529	2.00	0.738	0.19	0.21	1.00	0.60 / 0.27		1.87	0.57
5tck	B-801	1.95	0.644	0.20	0.24	1.00	0.80 / 0.20		1.21	0.57
4ujb	A-1351	1.95	0.644	0.16	0.19	1.00	0.71 / 0.22		1.28	0.57
4yko	B-201	1.57	0.743	0.20	0.22	1.00	0.47 / 0.20 / 0.33		0.62 / 0.53	0.57
5kq8	A-401	2.00	0.631	0.18	0.22	1.00	0.47 / 0.20 / 0.29		0.85 / 0.91	0.57
5dy9	E-101	1.60	0.823	0.17	0.20	0.59	0.24 / 0.35		0.98	0.57
5b2n	A-301	1.58	0.714	0.18	0.20	1.00	0.69 / 0.31		0.41	0.57
5d47	A-201	1.70	0.735	0.18	0.21	1.00	0.35 / 0.20 / 0.20		0.94 / 0.54	0.57
5lt7	A-1806	1.51	0.725	0.17	0.19	1.00	0.41 / 0.23 / 0.36		0.61 / 0.57	0.57
5d45	A-201	1.65	0.697	0.19	0.22	1.00	0.79 / 0.20		1.14	0.56
5j41	A-301	1.19	0.807	0.16	0.19	1.00	0.40 / 0.44		0.61	0.56
5kdu	A-1102	2.00	0.650	0.17	0.20	1.00	0.20 / 0.20 / 0.28 / 0.26		0.95 / 0.91 / 1.61	0.56
5ant	A-1157	2.00	0.638	0.21	0.25	1.00	0.32 / 0.20 / 0.48		0.53 / 1.04	0.56
5g67	A-1365	1.97	0.658	0.17	0.20	1.00	0.22 / 0.29 / 0.28 / 0.20		0.88 / 1.19 / 1.40	0.56
5hk9	D-401	1.80	0.679	0.17	0.20	0.94	0.32 / 0.20 / 0.38		0.88 / 1.24	0.55
5apg	A-1185	1.60	0.698	0.19	0.20	1.00	0.42 / 0.31 / 0.20		0.64 / 0.68	0.55
5iyz	A-501	1.80	0.661	0.17	0.20	1.00	0.74 / 0.20		0.67	0.55
5k4i	A-401	1.76	0.683	0.18	0.23	1.00	0.48 / 0.22 / 0.29		1.17 / 0.55	0.55
5kd6	B-501	1.84	0.691	0.18	0.23	1.00	0.20 / 0.20 / 0.44		2.01 / 0.77	0.55
5kpg	B-401	1.60	0.715	0.19	0.22	1.00	0.55 / 0.41		0.65	0.55
5sx7	B-111	1.95	0.642	0.15	0.19	1.00	0.38 / 0.23 / 0.28		0.49 / 0.74	0.55
5flq	A-1264	1.70	0.701	0.16	0.22	0.90	0.47 / 0.20		1.20	0.55
5kpg	A-401	1.60	0.704	0.19	0.22	1.00	0.58 / 0.42		0.64	0.55
5liw	X-402	1.75	0.671	0.18	0.21	1.00	0.46 / 0.21 / 0.20		0.66 / 2.14	0.55
4zbe	A-302	1.80	0.668	0.15	0.22	1.00	0.41 / 0.20 / 0.34		0.97 / 0.79	0.54
5iu8	A-2428	2.00	0.703	0.18	0.20	1.00	0.20 / 0.20 / 0.28 / 0.32		0.83 / 0.93 / 0.94	0.54
4yal	B-701	1.88	0.665	0.20	0.23	1.00	0.74 / 0.20		0.96	0.54
5hat	A-500	2.00	0.635	0.21	0.25	1.00	0.20 / 0.33 / 0.27		0.94 / 0.72	0.54
5t77	A-523	2.00	0.704	0.19	0.21	1.00	0.72 / 0.28		1.56	0.54
4z3f	A-201	1.80	0.720	0.20	0.23	1.00	0.21 / 0.26 / 0.20 / 0.20		1.40 / 1.51 / 0.80	0.54
5iru	A-202	2.00	0.649	0.22	0.27	1.00	0.66 / 0.20		0.81	0.54
5t64	A-506	1.70	0.697	0.18	0.22	1.00	0.69 / 0.23		1.05	0.54
5fvs	B-800	1.95	0.659	0.19	0.23	1.00	0.34 / 0.20 / 0.43		0.92 / 0.55	0.54
5ivc	A-601	1.57	0.715	0.17	0.18	1.00	0.56 / 0.20 / 0.20		1.73 / 1.29	0.54
5bqs	B-402	1.90	0.682	0.21	0.25	1.00	0.45 / 0.20 / 0.29		1.35 / 1.35	0.54
5ezg	A-302	1.84	0.665	0.18	0.21	1.00	0.60 / 0.31		1.10	0.53
5lpg	A-1102	1.70	0.709	0.22	0.25	1.00	0.67 / 0.25		1.17	0.53
5d4u	B-301	2.00	0.643	0.20	0.23	1.00	0.75 / 0.20		0.74	0.53
5an1	A-1220	2.00	0.658	0.21	0.26	1.00	0.47 / 0.25 / 0.20		0.88 / 0.77	0.53
5yl	A-404	1.83	0.656	0.14	0.20	1.00	0.56 / 0.44		1.32	0.53
5fvn	C-431	1.45	0.756	0.16	0.18	1.00	0.45 / 0.47		0.63	0.53
5b0w	A-306	1.70	0.793	0.20	0.22	1.00	0.42 / 0.38 / 0.20		0.84 / 0.57	0.53
5fvn	C-417	1.45	0.743	0.16	0.18	1.00	0.58 / 0.36		0.54	0.52

PDB	Ligand	Resolution (Å)	Twilight score	Rwork	Rfree	Occupancy (deposited)	Occupancy (qFit)	RMSD A->B (Å) (deposited)	RMSD A->B (qFit)	Best Fisher z improvement
5fh3	A-704	1.60	0.702	0.21	0.24	0.70 / 0.30	0.62 / 0.23	1.44	0.70	0.52
5el2	B-201	1.75	0.710	0.18	0.22	1.00	0.71 / 0.20		1.56	0.52
5hjs	A-301	1.72	0.795	0.21	0.24	1.00	0.22 / 0.27 / 0.20 / 0.20		1.74 / 1.82 / 2.02	0.52
5k2d	A-1205	1.90	0.677	0.17	0.21	1.00	0.64 / 0.36		1.32	0.52
5i9z	A-1001	1.70	0.687	0.16	0.20	1.00	0.77 / 0.20		1.16	0.52
5ihp	A-1001	1.85	0.655	0.17	0.20	1.00	0.54 / 0.20 / 0.20		0.99 / 1.12	0.52
5eic	B-1201	1.50	0.766	0.17	0.21	0.81	0.35 / 0.21 / 0.20		0.84 / 0.98	0.51
5t77	A-519	2.00	0.730	0.19	0.21	1.00	0.24 / 0.20 / 0.26 / 0.20		0.92 / 1.19 / 1.09	0.51
5k2d	A-1221	1.90	0.688	0.17	0.21	1.00	0.69 / 0.31		1.23	0.51
5fvn	F-424	1.45	0.793	0.16	0.18	1.00	0.44 / 0.45		0.55	0.51
5sxr	B-808	1.69	0.738	0.14	0.17	0.80	0.45 / 0.20		1.39	0.51
5hat	I-500	2.00	0.641	0.21	0.25	1.00	0.36 / 0.20 / 0.27		1.09 / 1.18	0.51
5kdu	A-1103	2.00	0.646	0.17	0.20	1.00	0.60 / 0.27		0.95	0.51
5ank	A-1299	1.90	0.668	0.20	0.24	1.00	0.64 / 0.20		1.37	0.51
5dtf	B-301	1.90	0.685	0.21	0.25	1.00	0.55 / 0.20 / 0.25		0.54 / 1.31	0.51
5e0r	A-203	1.35	0.770	0.17	0.20	1.00	0.52 / 0.25		1.20	0.51
4y5b	A-405	1.24	0.868	0.12	0.15	0.86	0.41 / 0.23 / 0.31		0.93 / 2.59	0.51
5i7r	A-402	1.73	0.727	0.17	0.21	1.00	0.74 / 0.20		1.22	0.51
5h9l	A-202	1.37	0.792	0.16	0.19	1.00	0.64 / 0.22		0.91	0.51
5fvn	C-413	1.45	0.746	0.16	0.18	1.00	0.57 / 0.29		0.97	0.50
5g6i	A-904	1.98	0.724	0.17	0.22	1.00	0.42 / 0.25 / 0.20		2.01 / 0.91	0.50
5eva	A-801	1.45	0.803	0.18	0.20	1.00	0.66 / 0.23		1.69	0.50
5iy5	P-307	2.00	0.666	0.17	0.21	1.00	0.42 / 0.25 / 0.33		0.70 / 0.87	0.50
5syx	B-111	1.77	0.671	0.14	0.17	0.70 / 0.10	0.72 / 0.22	0.61	0.64	0.50
5ey4	A-501	1.86	0.665	0.17	0.21	1.00	0.54 / 0.20 / 0.20		1.22 / 0.64	0.50
5fvn	D-404	1.45	0.878	0.16	0.18	1.00	0.63 / 0.37		1.04	0.50
4znh	B-601	1.93	0.669	0.20	0.25	0.90	0.32 / 0.21 / 0.31		0.81 / 0.57	0.50
5k2c	A-1213	1.90	0.685	0.17	0.21	1.00	0.57 / 0.43		0.65	0.50
5dbm	C-1201	1.86	0.666	0.17	0.22	1.00	0.74 / 0.20		0.98	0.50
5faf	A-302	1.10	0.823	0.19	0.20	1.00	0.57 / 0.20 / 0.21		3.05 / 0.39	0.50
5g0i	A-1808	1.99	0.662	0.17	0.20	1.00	0.27 / 0.62		0.46	0.50
5hzc	B-501	2.00	0.651	0.22	0.27	1.00	0.67 / 0.29		0.83	0.50
5hqe	A-401	1.62	0.705	0.16	0.18	1.00	0.76 / 0.20		1.43	0.49
4yaw	A-703	2.00	0.634	0.20	0.25	1.00	0.80 / 0.20		0.67	0.49
5elg	A-302	1.81	0.673	0.16	0.20	1.00	0.73 / 0.20		0.78	0.49
5ja3	B-202	1.81	0.721	0.23	0.27	0.94	0.30 / 0.20 / 0.47		1.25 / 0.56	0.49
5k0n	B-303	1.99	0.646	0.18	0.23	1.00	0.58 / 0.42		1.04	0.49
5jaz	B-501	1.40	0.755	0.19	0.21	1.00	0.57 / 0.20 / 0.20		0.74 / 2.08	0.49
5t8z	A-200	1.85	0.682	0.17	0.20	1.00	0.44 / 0.20 / 0.26		1.00 / 2.04	0.49
4xcf	H-302	1.43	0.756	0.14	0.17	0.90	0.22 / 0.20 / 0.24 / 0.25		3.29 / 0.83 / 1.07	0.49
5k2c	A-1214	1.90	0.696	0.17	0.21	1.00	0.44 / 0.56		0.85	0.49
5k9c	A-400	1.66	0.684	0.13	0.15	1.00	0.78 / 0.20		0.83	0.49
5t77	A-518	2.00	0.715	0.19	0.21	1.00	0.28 / 0.20 / 0.20 / 0.31		1.59 / 1.03 / 0.92	0.49
5cpl	B-401	1.57	0.707	0.14	0.16	1.00	0.52 / 0.20 / 0.20		0.88 / 0.69	0.49
4yb8	B-300	1.90	0.689	0.18	0.22	1.00	0.70 / 0.28		0.93	0.48
5f03	B-301	1.94	0.651	0.16	0.20	1.00	0.49 / 0.20 / 0.20		0.61 / 0.47	0.48
5fl0	B-1719	1.95	0.646	0.20	0.23	1.00	0.49 / 0.20 / 0.20		0.72 / 0.60	0.48
5ew8	A-803	1.63	0.697	0.19	0.21	1.00	0.75 / 0.20		1.07	0.48
5fvn	C-407	1.45	0.767	0.16	0.18	1.00	0.63 / 0.35		1.01	0.48
5fbg	B-701	1.97	0.667	0.16	0.19	1.00	0.50 / 0.20 / 0.20		2.05 / 1.56	0.48
5fbi	A-302	1.47	0.871	0.17	0.20	1.00	0.31 / 0.21 / 0.20 / 0.20		2.78 / 0.93 / 1.02	0.48
4xoc	A-501	1.42	0.736	0.15	0.18	1.00	0.68 / 0.30		1.18	0.48
5ioq	B-302	1.93	0.649	0.17	0.20	1.00	0.74 / 0.20		0.61	0.48
5dwj	B-900	2.00	0.685	0.20	0.23	0.81	0.51 / 0.20 / 0.20		4.92 / 1.07	0.48
5t64	B-502	1.70	0.683	0.18	0.22	1.00	0.56 / 0.41		0.60	0.48
4wi1	A-801	1.65	0.721	0.16	0.19	1.00	0.49 / 0.24 / 0.20		1.27 / 0.99	0.48
5ey5	D-501	1.97	0.655	0.18	0.23	1.00	0.55 / 0.37		1.16	0.48
5hg7	A-9001	1.85	0.673	0.22	0.25	1.00	0.56 / 0.20 / 0.24		1.06 / 0.85	0.47
4xja	A-705	1.98	0.647	0.17	0.20	1.00	0.20 / 0.20 / 0.20 / 0.20		0.99 / 1.11 / 1.18	0.47
5eyr	A-301	1.57	0.727	0.19	0.20	1.00	0.49 / 0.20 / 0.31		0.75 / 0.40	0.47
5eyy	A-304	1.90	0.664	0.16	0.18	1.00	0.29 / 0.20 / 0.48		0.53 / 0.42	0.47

PDB	Ligand	Resolution (Å)	Twilight score	Rwork	Rfree	Occupancy (deposited)	Occupancy (qFit)	RMSD A->B (Å) (deposited)	RMSD A->B (qFit)	Best Fisher z improvement
5itp	B-301	1.85	0.660	0.18	0.20	1.00	0.29 / 0.26 / 0.20 / 0.20		0.83 / 1.13 / 1.12	0.47
5szy	D-200	2.00	0.630	0.20	0.21	1.00	0.80 / 0.20		0.89	0.47
5hg5	A-9001	1.52	0.733	0.21	0.22	1.00	0.58 / 0.20 / 0.20		1.02 / 0.97	0.47
5kok	B-401	1.79	0.673	0.16	0.20	1.00	0.59 / 0.20 / 0.20		1.08 / 0.69	0.47
5le5	G-47	1.80	0.712	0.18	0.21	1.00	0.25 / 0.60		0.66	0.47
5t77	A-524	2.00	0.708	0.19	0.21	1.00	0.37 / 0.37 / 0.20		0.90 / 1.28	0.47
5j54	A-503	1.89	0.695	0.15	0.18	0.90	0.32 / 0.49		2.06	0.46
4yal	A-703	1.88	0.656	0.20	0.23	1.00	0.55 / 0.23 / 0.20		1.10 / 0.98	0.46
5drq	A-303	1.63	0.702	0.17	0.20	0.96	0.42 / 0.24 / 0.28		1.59 / 0.95	0.46
5e8w	A-601	1.86	0.657	0.17	0.19	1.00	0.58 / 0.34		0.36	0.46
5ixj	D-82	1.54	0.711	0.18	0.20	1.00	0.45 / 0.23 / 0.22		0.93 / 0.92	0.46
4yb8	D-300	1.90	0.651	0.18	0.22	1.00	0.80 / 0.20		1.37	0.46
5ej4	G-601	1.77	0.683	0.18	0.22	1.00	0.50 / 0.20 / 0.26		0.70 / 0.61	0.46
5f4n	A-301	1.91	0.654	0.15	0.19	1.00	0.75 / 0.24		0.96	0.46
5hvt	C-202	1.75	0.694	0.18	0.20	1.00	0.57 / 0.36		0.46	0.46
5t77	A-515	2.00	0.704	0.19	0.21	1.00	0.27 / 0.29 / 0.43		0.99 / 1.65	0.46
5byf	A-401	2.00	0.644	0.18	0.22	1.00	0.57 / 0.31		1.05	0.46
5j3z	A-401	1.80	0.680	0.17	0.20	1.00	0.54 / 0.44		0.69	0.46
5ihp	B-1001	1.85	0.669	0.17	0.20	1.00	0.69 / 0.20		1.49	0.45
5kok	A-401	1.79	0.670	0.16	0.20	1.00	0.80 / 0.20		0.84	0.45
5lf4	X-91	1.99	0.661	0.18	0.22	1.00	0.29 / 0.20 / 0.24 / 0.20		1.27 / 0.98 / 2.41	0.45
5hge	A-66	1.86	0.664	0.17	0.21	1.00	0.47 / 0.25 / 0.20		1.20 / 0.86	0.45
5g4m	B-1294	1.38	0.870	0.15	0.17	1.00	0.66 / 0.20		0.91	0.45
5fp1	A-1720	1.94	0.704	0.16	0.18	1.00	0.41 / 0.33 / 0.26		0.91 / 1.23	0.45
5lsa	A-303	1.50	0.716	0.17	0.21	1.00	0.65 / 0.33		0.63	0.45
5k2c	A-1206	1.90	0.699	0.17	0.21	1.00	0.49 / 0.51		0.57	0.45
5teg	B-401	1.30	0.769	0.19	0.21	1.00	0.75 / 0.20		0.42	0.45
5k4z	A-402	1.64	0.730	0.19	0.20	1.00	0.48 / 0.38		0.92	0.44
5lom	B-301	1.50	0.721	0.19	0.22	1.00	0.60 / 0.20 / 0.20		0.71 / 0.70	0.44
5drr	A-303	1.59	0.719	0.18	0.21	0.98	0.51 / 0.23 / 0.20		1.41 / 0.97	0.44
5fp4	A-1344	2.00	0.666	0.16	0.21	1.00	0.42 / 0.26 / 0.20		1.19 / 0.83	0.44
5i8o	H-302	1.80	0.729	0.16	0.21	0.70	0.23 / 0.21 / 0.20		0.66 / 0.41	0.44
4wv8	B-303	1.83	0.715	0.16	0.20	1.00	0.65 / 0.24		0.40	0.44
5lf4	J-91	1.99	0.655	0.18	0.22	1.00	0.20 / 0.20 / 0.31 / 0.26		0.97 / 0.65 / 1.41	0.44
5fdq	A-704	1.90	0.667	0.15	0.19	1.00	0.40 / 0.20 / 0.20 / 0.20		0.48 / 0.66 / 0.99	0.44
5jiy	A-1205	1.48	0.724	0.21	0.23	1.00	0.61 / 0.32		0.63	0.44
4yaf	A-701	1.91	0.659	0.21	0.24	1.00	0.42 / 0.24 / 0.29		0.89 / 0.78	0.44
5t6m	A-82	1.80	0.671	0.20	0.24	1.00	0.50 / 0.20 / 0.28		1.06 / 0.39	0.43
5l11	A-601	1.85	0.674	0.20	0.24	1.00	0.54 / 0.21 / 0.20		0.53 / 0.95	0.43
5fvn	A-407	1.45	0.878	0.16	0.18	1.00	0.61 / 0.23		1.42	0.43
5ie3	A-601	1.90	0.656	0.16	0.21	1.00	0.79 / 0.21		1.02	0.43
5hkb	B-401	1.65	0.692	0.19	0.22	0.84	0.28 / 0.20 / 0.21 / 0.20		1.98 / 0.93 / 2.01	0.43
5k2c	A-1210	1.90	0.778	0.17	0.21	1.00	0.68 / 0.32		3.92	0.43
5dgi	A-401	1.85	0.654	0.15	0.20	1.00	0.45 / 0.35 / 0.20		0.82 / 0.86	0.43
5fvn	C-428	1.45	0.741	0.16	0.18	1.00	0.53 / 0.36		0.86	0.43
5dkh	A-1503	1.70	0.716	0.20	0.24	1.00	0.69 / 0.20		1.21	0.42
5kok	B-403	1.79	0.681	0.16	0.20	1.00	0.70 / 0.20		0.53	0.42
5g2d	A-1271	1.80	0.729	0.18	0.21	1.00	0.70 / 0.30		2.90	0.42
5syk	B-111	1.80	0.662	0.15	0.18	0.80 / 0.20	0.59 / 0.35	0.59	0.61	0.42
4y9u	A-701	1.95	0.653	0.20	0.24	1.00	0.73 / 0.20		0.81	0.42
5lck	A-405	1.89	0.675	0.16	0.21	1.00	0.29 / 0.28 / 0.23		0.78 / 0.37	0.42
5ivg	B-704	1.95	0.636	0.16	0.20	1.00	0.20 / 0.20 / 0.20 / 0.20		1.14 / 0.96 / 1.66 / 1.44	0.42
5g54	A-1276	2.00	0.707	0.18	0.23	1.00	0.74 / 0.26		0.81	0.42
5jcj	D-302	1.76	0.708	0.18	0.23	0.80	0.58 / 0.20		1.48	0.42
5ey5	B-501	1.97	0.657	0.18	0.23	1.00	0.72 / 0.21		2.39	0.42
5fjg	A-1266	2.00	0.642	0.17	0.22	1.00	0.80 / 0.20		1.08	0.42
5axd	A-502	1.60	0.706	0.16	0.18	1.00	0.60 / 0.38		0.80	0.41
5syv	B-111	1.75	0.695	0.16	0.19	1.00	0.62 / 0.29		0.59	0.41
4uho	A-1460	1.24	0.838	0.11	0.12	0.80	0.43 / 0.27		0.49	0.41
4zsh	A-501	1.80	0.680	0.21	0.22	1.00	0.77 / 0.23		0.81	0.41
5fre	A-201	1.90	0.651	0.17	0.21	1.00	0.72 / 0.20		1.16	0.41

PDB	Ligand	Resolution (Å)	Twilight score	Rwork	Rfree	Occupancy (deposited)	Occupancy (qFit)	RMSD A->B (Å) (deposited)	RMSD A->B (qFit)	Best Fisher z improvement
5syt	A-514	2.00	0.715	0.22	0.25	1.00	0.23 / 0.36 / 0.40		1.29 / 0.75	0.41
5etz	A-301	1.80	0.680	0.22	0.24	1.00	0.75 / 0.25		1.14	0.41
5g28	A-1270	1.57	0.804	0.15	0.19	1.00	0.72 / 0.28		1.14	0.41
5g6a	A-902	1.92	0.686	0.16	0.19	1.00	0.58 / 0.35		1.59	0.41
5dtz	D-68	1.50	0.718	0.17	0.20	1.00	0.53 / 0.20 / 0.20		1.09 / 0.76	0.41
5ley	S-148	1.90	0.676	0.19	0.23	1.00	0.42 / 0.47		0.64	0.41
5g0i	A-1809	1.99	0.653	0.17	0.20	1.00	0.35 / 0.27 / 0.36		1.07 / 0.78	0.41
5thu	A-404	1.95	0.692	0.18	0.20	0.95	0.34 / 0.20 / 0.20 / 0.21		1.59 / 1.13 / 1.21	0.40
5h8g	A-421	2.00	0.636	0.16	0.20	1.00	0.60 / 0.20 / 0.20		1.47 / 0.61	0.40
5ioq	C-302	1.93	0.647	0.17	0.20	1.00	0.78 / 0.20		0.63	0.40
5dw1	C-501	1.55	0.709	0.16	0.20	1.00	0.80 / 0.20		1.12	0.40
5el2	A-203	1.75	0.731	0.18	0.22	1.00	0.66 / 0.24		1.54	0.40
5fvn	C-410	1.45	0.825	0.16	0.18	1.00	0.68 / 0.28		0.97	0.40
5fh8	C-801	1.55	0.711	0.19	0.22	1.00	0.67 / 0.33		0.49	0.40
5etn	A-206	1.40	0.762	0.18	0.22	1.00	0.74 / 0.20		0.96	0.40
5tvc	B-302	1.93	0.678	0.19	0.23	1.00	0.71 / 0.20		1.23	0.40
5g3l	D-200	1.72	0.690	0.17	0.20	1.00	0.50 / 0.30		0.56	0.39
5lb3	B-502	1.80	0.670	0.20	0.23	1.00	0.73 / 0.20		0.70	0.39
5fh8	D-801	1.55	0.706	0.19	0.22	1.00	0.80 / 0.20		1.80	0.39
4yb6	B-301	1.98	0.639	0.20	0.22	1.00	0.52 / 0.47		0.93	0.39
4zse	A-1101	1.97	0.640	0.19	0.21	1.00	0.57 / 0.20 / 0.20		0.46 / 0.81	0.39
5azp	C-504	1.69	0.755	0.16	0.18	1.00	0.36 / 0.20 / 0.20 / 0.20		1.84 / 0.79 / 0.81	0.39
5iu8	A-2405	2.00	0.648	0.18	0.20	1.00	0.32 / 0.36 / 0.32		0.82 / 0.69	0.39
5iy5	Z-101	2.00	0.665	0.17	0.21	1.00	0.67 / 0.30		1.18	0.39
4y1u	B-202	1.76	0.734	0.18	0.23	1.00	0.20 / 0.28 / 0.31		1.08 / 0.99	0.39
5dj9	A-505	1.55	0.712	0.16	0.19	1.00	0.21 / 0.20 / 0.38 / 0.20		0.82 / 0.59 / 0.79	0.39
5i7w	B-42	1.95	0.642	0.18	0.22	1.00	0.59 / 0.37		0.91	0.38
5tck	A-401	1.95	0.647	0.20	0.24	1.00	0.35 / 0.20 / 0.41		0.61 / 0.97	0.38
4uj9	A-1351	1.87	0.656	0.17	0.21	1.00	0.73 / 0.22		1.20	0.38
5ffh	B-202	1.68	0.733	0.22	0.27	1.00	0.64 / 0.36		1.00	0.38
5m96	A-501	1.77	0.671	0.19	0.21	1.00	0.57 / 0.43		0.82	0.38
5cx9	B-403	1.73	0.807	0.19	0.20	1.00	0.60 / 0.33		0.86	0.38
5dtf	P-4	1.90	0.686	0.21	0.25	1.00	0.76 / 0.24		0.59	0.38
5kf9	A-407	1.49	0.779	0.18	0.21	1.00	0.49 / 0.26		0.83	0.38
5li8	A-502	1.83	0.666	0.16	0.20	1.00	0.45 / 0.23 / 0.28		0.96 / 0.89	0.38
4yqj	A-301	1.94	0.646	0.15	0.20	1.00	0.77 / 0.20		0.89	0.37
5dwe	B-901	1.92	0.660	0.20	0.24	1.00	0.63 / 0.37		1.01	0.37
5fre	B-201	1.90	0.652	0.17	0.21	1.00	0.58 / 0.20 / 0.20		0.85 / 0.57	0.37
5fr0	A-1585	1.75	0.698	0.18	0.22	1.00	0.61 / 0.21		0.47	0.37
5flj	H-301	1.82	0.726	0.16	0.21	0.72	0.53 / 0.22		1.45	0.37
5cgb	B-301	1.60	0.706	0.16	0.18	1.00	0.74 / 0.21		0.79	0.37
5lmb	B-701	1.95	0.650	0.18	0.23	1.00	0.79 / 0.20		0.93	0.37
5fvn	B-408	1.45	0.744	0.16	0.18	1.00	0.40 / 0.35		0.57	0.36
5k2c	A-1209	1.90	0.690	0.17	0.21	1.00	0.37 / 0.20 / 0.43		0.69 / 0.56	0.36
4xje	A-201	1.88	0.649	0.17	0.19	1.00	0.57 / 0.23 / 0.20		0.93 / 0.91	0.36
5eck	E-301	1.54	0.708	0.16	0.18	1.00	0.74 / 0.20		0.76	0.36
5hat	K-500	2.00	0.651	0.21	0.25	1.00	0.60 / 0.28		0.95	0.36
5tvc	D-302	1.93	0.708	0.19	0.23	1.00	0.23 / 0.20 / 0.42		0.93 / 1.06	0.36
5sx7	A-111	1.95	0.644	0.15	0.19	0.70 / 0.10	0.60 / 0.35	0.61	0.54	0.36
5bph	A-401	1.70	0.680	0.18	0.21	1.00	0.70 / 0.25		0.91	0.36
5fen	A-201	1.55	0.757	0.20	0.24	1.00	0.70 / 0.30		0.69	0.36
4y1y	B-202	1.86	0.687	0.20	0.23	1.00	0.22 / 0.26 / 0.22 / 0.20		1.28 / 0.76 / 1.68	0.36
5fvn	B-401	1.45	0.884	0.16	0.18	1.00	0.72 / 0.28		0.85	0.36
4zvn	B-303	1.87	0.664	0.16	0.20	1.00	0.73 / 0.20		0.73	0.36
5dtz	A-68	1.50	0.718	0.17	0.20	1.00	0.47 / 0.20 / 0.21		0.90 / 1.10	0.36
5efo	F-303	1.63	0.753	0.16	0.21	0.75	0.55 / 0.33		0.53	0.36
5lb5	C-503	2.00	0.664	0.24	0.28	1.00	0.68 / 0.25		1.04	0.36
5ios	A-303	1.90	0.648	0.18	0.21	1.00	0.60 / 0.20 / 0.20		1.18 / 0.93	0.36
5t6m	D-82	1.80	0.679	0.20	0.24	1.00	0.68 / 0.20		0.46	0.36
5i6y	A-202	1.90	0.650	0.17	0.22	1.00	0.74 / 0.20		0.47	0.36
4ybp	A-201	1.83	0.683	0.19	0.24	1.00	0.68 / 0.20		0.97	0.35

PDB	Ligand	Resolution (Å)	Twilight score	Rwork	Rfree	Occupancy (deposited)	Occupancy (qFit)	RMSD A->B (Å) (deposited)	RMSD A->B (qFit)	Best Fisher z improvement
5hja	A-403	1.65	0.761	0.19	0.21	1.00	0.24 / 0.33 / 0.20 / 0.20		1.66 / 0.87 / 1.07	0.35
5teg	A-401	1.30	0.771	0.19	0.21	1.00	0.70 / 0.20		0.41	0.35
5t77	A-520	2.00	0.688	0.19	0.21	1.00	0.43 / 0.29 / 0.21		0.96 / 1.32	0.35
5tk7	A-203	1.90	0.695	0.19	0.22	1.00	0.44 / 0.20 / 0.21		1.27 / 1.24	0.35
5ftw	A-1257	1.80	0.659	0.18	0.24	1.00	0.80 / 0.20		0.62	0.35
5jjr	A-1003	1.99	0.639	0.18	0.23	1.00	0.80 / 0.20		0.68	0.35
5h9r	A-301	1.58	0.733	0.17	0.20	1.00	0.64 / 0.28		0.42	0.35
5g2d	A-1273	1.80	0.711	0.18	0.21	1.00	0.55 / 0.25 / 0.20		0.99 / 0.40	0.35
5fvn	F-423	1.45	0.774	0.16	0.18	1.00	0.60 / 0.30		0.52	0.34
5ghn	A-201	1.39	0.756	0.15	0.19	1.00	0.72 / 0.20		0.88	0.34
4y45	A-406	1.06	0.963	0.12	0.14	0.72	0.53 / 0.20		0.63	0.34
5syt	A-509	2.00	0.676	0.22	0.25	1.00	0.68 / 0.20		1.50	0.34
5ew8	B-802	1.63	0.698	0.19	0.21	1.00	0.55 / 0.20 / 0.20		1.07 / 0.80	0.34
5lf1	G-47	2.00	0.666	0.18	0.21	1.00	0.20 / 0.20 / 0.22 / 0.32		1.23 / 1.04 / 3.46	0.34
5jh2	A-401	1.72	0.680	0.17	0.21	1.00	0.65 / 0.25		0.85	0.34
5azb	A-302	1.60	0.736	0.18	0.22	1.00	0.50 / 0.28 / 0.20		0.63 / 0.78	0.34
4zrs	B-151	2.00	0.629	0.15	0.20	1.00	0.59 / 0.41		1.23	0.33
5l2f	B-301	1.77	0.693	0.18	0.19	1.00	0.41 / 0.20 / 0.35		0.82 / 0.68	0.33
5lf1	E-148	2.00	0.666	0.18	0.21	1.00	0.61 / 0.20		0.53	0.33
4y0i	A-501	1.66	0.690	0.17	0.20	0.92	0.68 / 0.20		0.66	0.33
5e0w	A-900	2.00	0.657	0.19	0.23	1.00	0.58 / 0.32		0.97	0.33
5i5v	B-401	1.94	0.639	0.17	0.23	1.00	0.59 / 0.35		1.17	0.33
4yai	B-501	1.60	0.829	0.14	0.16	1.00	0.60 / 0.30		0.64	0.33
4zam	A-301	1.42	0.790	0.17	0.19	1.00	0.24 / 0.36 / 0.20 / 0.20		0.97 / 0.96 / 0.64	0.33
5br5	A-301	2.00	0.667	0.21	0.25	1.00	0.80 / 0.20		1.04	0.33
5ios	A-302	1.90	0.650	0.18	0.21	1.00	0.65 / 0.29		1.01	0.33
5a8k	D-554	1.41	0.732	0.11	0.14	1.00	0.40 / 0.20 / 0.40		0.72 / 0.96	0.32
5hrx	B-801	1.73	0.695	0.21	0.25	1.00	0.64 / 0.26		0.71	0.32
5ja3	C-202	1.81	0.687	0.23	0.27	0.97	0.62 / 0.34		1.15	0.32
3x36	A-501	1.93	0.645	0.18	0.22	1.00	0.70 / 0.30		0.80	0.32
5bnm	A-402	1.70	0.784	0.24	0.27	1.00	0.45 / 0.20 / 0.24		1.13 / 0.97	0.32
5i2b	A-202	1.70	0.720	0.17	0.21	1.00	0.39 / 0.20 / 0.20		0.61 / 0.76	0.32
5bqq	A-203	1.44	0.812	0.15	0.17	1.00	0.42 / 0.24 / 0.20		1.84 / 1.20	0.32
5g0h	A-1801	1.60	0.718	0.15	0.17	0.91	0.54 / 0.20 / 0.20		1.21 / 1.08	0.32
4zsk	B-301	1.85	0.653	0.19	0.25	1.00	0.67 / 0.32		0.78	0.32
5byf	B-401	2.00	0.648	0.18	0.22	1.00	0.70 / 0.20		0.71	0.32
5drp	A-402	1.89	0.669	0.16	0.19	1.00	0.56 / 0.20 / 0.20		0.92 / 0.66	0.32
5fhn	A-305	1.60	0.706	0.16	0.19	1.00	0.77 / 0.20		0.67	0.32
5igm	A-301	1.60	0.716	0.22	0.27	1.00	0.74 / 0.20		0.96	0.32
5dw1	D-501	1.55	0.711	0.16	0.20	1.00	0.80 / 0.20		1.62	0.32
5hrw	B-801	1.80	0.675	0.20	0.24	1.00	0.70 / 0.20		0.51	0.32
5ixj	C-82	1.54	0.714	0.18	0.20	1.00	0.43 / 0.20 / 0.31		1.01 / 0.89	0.32
5afg	B-1030	1.90	0.651	0.18	0.23	1.00	0.76 / 0.20		0.47	0.32
4ui6	A-2113	1.80	0.679	0.15	0.19	1.00	0.69 / 0.21		0.90	0.31
5g54	A-1273	2.00	0.745	0.18	0.23	1.00	0.53 / 0.47		0.71	0.31
5ths	B-404	1.90	0.664	0.18	0.21	1.00	0.78 / 0.20		1.22	0.31
5cpn	B-402	1.80	0.672	0.18	0.22	1.00	0.58 / 0.34		0.81	0.31
5k2c	A-1203	1.90	0.673	0.17	0.21	1.00	0.52 / 0.25 / 0.20		1.18 / 0.67	0.31
5kit	A-501	1.60	0.725	0.14	0.18	1.00	0.59 / 0.20 / 0.20		0.95 / 1.36	0.31
5fkk	B-222	1.75	0.712	0.21	0.25	1.00	0.46 / 0.36		0.69	0.31
4z8d	B-401	2.00	0.648	0.16	0.22	1.00	0.55 / 0.45		0.69	0.31
5fh4	A-704	1.49	0.727	0.20	0.23	1.00	0.76 / 0.20		0.84	0.31
4zyx	A-1101	1.65	0.694	0.16	0.18	0.76	0.52 / 0.23		0.53	0.31
5d3t	A-201	1.93	0.663	0.17	0.20	1.00	0.67 / 0.22		0.80	0.31
5t77	A-532	2.00	0.711	0.19	0.21	1.00	0.69 / 0.29		0.85	0.31
4xjl	B-501	1.85	0.700	0.19	0.21	1.00	0.74 / 0.20		1.50	0.30
5exz	A-306	1.90	0.663	0.15	0.20	0.60	0.39 / 0.20		0.86	0.30
5k0c	A-304	1.95	0.644	0.18	0.23	1.00	0.62 / 0.34		1.06	0.30
5f2m	A-3001	1.92	0.672	0.16	0.21	0.37 / 0.63	0.29 / 0.28 / 0.20	0.18	1.11 / 0.74	0.30
5dl7	A-508	1.75	0.713	0.17	0.19	1.00	0.69 / 0.20		0.76	0.30
5ley	G-47	1.90	0.666	0.19	0.23	1.00	0.20 / 0.42 / 0.24		0.56 / 0.72	0.30

PDB	Ligand	Resolution (Å)	Twilight score	Rwork	Rfree	Occupancy (deposited)	Occupancy (qFit)	RMSD A->B (Å) (deposited)	RMSD A->B (qFit)	Best Fisher z improvement
5law	A-201	1.64	0.699	0.19	0.22	1.00	0.80 / 0.20		0.48	0.30
5e2m	A-302	1.41	0.748	0.18	0.21	0.50 / 0.50	0.40 / 0.25	1.97	0.97	0.30
5d3s	A-201	1.75	0.707	0.18	0.20	1.00	0.48 / 0.20 / 0.20		1.09 / 0.96	0.30
5cfs	A-204	1.70	0.687	0.17	0.19	1.00	0.75 / 0.20		0.88	0.30
5u5h	A-501	1.80	0.669	0.16	0.20	1.00	0.68 / 0.20		0.65	0.30
5k0n	D-305	1.99	0.639	0.18	0.23	1.00	0.73 / 0.27		0.55	0.30
5bmp	A-501	1.85	0.668	0.15	0.18	1.00	0.72 / 0.20		0.59	0.30
5c2k	A-503	1.42	0.736	0.18	0.21	1.00	0.33 / 0.63		0.85	0.30
5hat	H-500	2.00	0.640	0.21	0.25	1.00	0.34 / 0.20 / 0.35		0.64 / 0.63	0.29
4y3a	A-410	1.17	0.863	0.11	0.13	0.72	0.55 / 0.20		0.85	0.29
5ea9	B-401	1.71	0.709	0.18	0.22	1.00	0.56 / 0.20		1.05	0.29
5fvn	C-414	1.45	0.748	0.16	0.18	1.00	0.26 / 0.22 / 0.38		0.56 / 1.08	0.29
5fnl	A-1264	1.59	0.728	0.15	0.20	0.50 / 0.50	0.44 / 0.28	3.56	1.00	0.29
5co4	B-401	1.70	0.687	0.17	0.20	1.00	0.78 / 0.20		0.60	0.29
4y0i	C-503	1.66	0.686	0.17	0.20	0.93	0.69 / 0.21		1.09	0.29
5kok	A-402	1.79	0.689	0.16	0.20	1.00	0.55 / 0.30		0.30	0.29
5k0j	B-303	1.94	0.646	0.19	0.23	1.00	0.51 / 0.46		1.03	0.29
5jyc	A-401	2.00	0.662	0.15	0.19	1.00	0.43 / 0.20 / 0.34		1.17 / 0.70	0.29
5t0m	B-1205	1.90	0.659	0.18	0.22	1.00	0.75 / 0.20		0.59	0.29
5aee	A-1681	1.85	0.658	0.16	0.20	1.00	0.66 / 0.27		1.17	0.28
5seen	A-804	1.86	0.675	0.18	0.22	1.00	0.35 / 0.21 / 0.45		0.88 / 1.04	0.28
5azb	A-303	1.60	0.774	0.18	0.22	1.00	0.79 / 0.20		0.42	0.28
5e2k	A-303	1.40	0.765	0.17	0.19	1.00	0.33 / 0.20 / 0.24		1.05 / 1.65	0.28
5g2p	A-2000	1.89	0.645	0.16	0.20	1.00	0.67 / 0.33		1.11	0.28
5jf5	A-301	1.80	0.759	0.18	0.23	1.00	0.49 / 0.36		0.95	0.28
5b41	A-501	1.89	0.660	0.19	0.23	1.00	0.39 / 0.20 / 0.41		0.60 / 0.73	0.28
5d3j	A-201	1.70	0.705	0.18	0.21	1.00	0.71 / 0.20		0.86	0.28
5sey1	B-302	2.00	0.634	0.19	0.23	1.00	0.80 / 0.20		0.60	0.28
5foe	B-1426	1.98	0.637	0.20	0.25	1.00	0.49 / 0.20 / 0.22		0.84 / 0.84	0.28
5iu8	A-2423	2.00	0.729	0.18	0.20	1.00	0.70 / 0.30		1.01	0.28
5k2c	A-1223	1.90	0.708	0.17	0.21	1.00	0.70 / 0.30		1.09	0.28
5duw	D-201	1.70	0.685	0.15	0.18	1.00	0.76 / 0.20		0.69	0.28
5etz	A-307	1.80	0.750	0.22	0.24	1.00	0.33 / 0.67		0.54	0.28
5t6b	A-504	2.00	0.670	0.18	0.23	1.00	0.67 / 0.31		1.01	0.28
4yx6	A-601	1.86	0.664	0.17	0.20	1.00	0.80 / 0.20		0.78	0.27
5dh5	A-803	2.00	0.634	0.20	0.23	1.00	0.60 / 0.36		0.86	0.27
5tme	A-501	1.78	0.704	0.19	0.23	1.00	0.61 / 0.20		1.00	0.27
5b5s	A-301	1.50	0.728	0.15	0.20	1.00	0.68 / 0.32		0.42	0.27
5bw6	A-301	1.82	0.713	0.17	0.21	0.70	0.52 / 0.20		1.24	0.27
5d5s	A-403	1.70	0.706	0.17	0.21	0.88	0.41 / 0.23		2.13	0.27
5ekd	B-402	1.82	0.673	0.17	0.21	1.00	0.77 / 0.20		0.85	0.27
5k2c	A-1211	1.90	0.682	0.17	0.21	1.00	0.47 / 0.33 / 0.20		1.20 / 0.87	0.27
5etrm	A-202	1.46	0.732	0.20	0.24	1.00	0.74 / 0.26		0.78	0.26
4d7b	A-1126	1.15	0.818	0.17	0.20	0.49	0.47 / 0.20		0.74	0.26
4s35	B-202	1.55	0.718	0.15	0.17	1.00	0.79 / 0.20		0.66	0.26
5fra	D-201	2.00	0.638	0.18	0.21	1.00	0.49 / 0.20 / 0.31		0.60 / 0.74	0.26
5k0n	C-304	1.99	0.640	0.18	0.23	1.00	0.70 / 0.30		0.46	0.26
5hyl	B-201	1.80	0.667	0.16	0.21	1.00	0.75 / 0.23		0.76	0.26
5syw	B-111	1.85	0.666	0.15	0.18	0.90 / 0.10	0.72 / 0.28	0.59	0.61	0.26
5aqv	A-1382	1.75	0.682	0.18	0.20	1.00	0.54 / 0.20 / 0.20		0.54 / 0.35	0.26
5k2c	A-1208	1.90	0.700	0.17	0.21	1.00	0.60 / 0.20 / 0.20		1.02 / 0.78	0.26
5i90	A-501	1.22	0.778	0.14	0.16	1.00	0.75 / 0.20		1.15	0.26
5dzi	A-901	1.90	0.651	0.18	0.21	1.00	0.78 / 0.20		0.40	0.25
5jjr	A-1004	1.99	0.636	0.18	0.23	1.00	0.80 / 0.20		2.87	0.25
5i0j	A-201	1.80	0.662	0.17	0.21	1.00	0.70 / 0.30		0.97	0.25
5lbf	A-502	1.90	0.648	0.16	0.19	1.00	0.49 / 0.48		0.74	0.25
5syt	A-513	2.00	0.668	0.22	0.25	1.00	0.53 / 0.28		0.91	0.25
5d26	A-201	1.82	0.668	0.16	0.19	1.00	0.44 / 0.25 / 0.31		1.17 / 1.09	0.25
5cvt	A-97	1.78	0.672	0.14	0.16	1.00	0.78 / 0.20		0.51	0.25
5he4	A-501	1.53	0.731	0.20	0.22	1.00	0.74 / 0.20		2.00	0.25
5sym	A-301	1.55	0.791	0.18	0.20	1.00	0.51 / 0.34		0.71	0.25

PDB	Ligand	Resolution (Å)	Twilight score	Rwork	Rfree	Occupancy (deposited)	Occupancy (qFit)	RMSD A->B (Å) (deposited)	RMSD A->B (qFit)	Best Fisher z improvement
5k2d	A-1204	1.90	0.671	0.17	0.21	1.00	0.48 / 0.26 / 0.27		0.88 / 0.59	0.25
5c1r	A-403	1.80	0.668	0.17	0.21	0.75	0.57 / 0.21		0.94	0.24
5d4u	D-301	2.00	0.641	0.20	0.23	1.00	0.73 / 0.20		0.65	0.24
5jhn	A-1205	1.67	0.690	0.21	0.24	1.00	0.69 / 0.24		0.63	0.24
5f25	A-201	1.68	0.727	0.19	0.21	1.00	0.50 / 0.20 / 0.20		0.89 / 0.64	0.24
5fvn	C-408	1.45	0.799	0.16	0.18	1.00	0.69 / 0.22		0.96	0.24
5aqz	A-1389	1.65	0.708	0.19	0.22	1.00	0.74 / 0.22		0.49	0.24
5duv	A-201	1.90	0.656	0.16	0.20	1.00	0.74 / 0.24		0.49	0.24
5syn	B-301	1.64	0.700	0.22	0.25	1.00	0.68 / 0.20		0.44	0.24
5iey	A-1001	1.66	0.692	0.18	0.23	1.00	0.55 / 0.20 / 0.20		1.00 / 0.94	0.23
5fqc	A-600	1.45	0.743	0.16	0.18	1.00	0.52 / 0.20 / 0.28		1.14 / 0.63	0.23
5jhu	A-505	1.80	0.704	0.14	0.18	1.00	0.63 / 0.20		0.69	0.23
5kau	A-201	1.95	0.663	0.16	0.19	1.00	0.64 / 0.33		0.38	0.23
5sw4	B-111	1.90	0.648	0.14	0.17	1.00	0.65 / 0.32		0.64	0.23
4zn7	A-601	1.93	0.670	0.20	0.23	1.00	0.74 / 0.20		0.58	0.23
5t77	A-526	2.00	0.673	0.19	0.21	1.00	0.79 / 0.21		0.95	0.23
5fvn	E-407	1.45	0.787	0.16	0.18	1.00	0.54 / 0.30		0.57	0.23
5g6n	A-902	1.91	0.696	0.18	0.22	1.00	0.62 / 0.26		1.43	0.23
5fvn	D-425	1.45	0.777	0.16	0.18	1.00	0.57 / 0.23		0.80	0.23
5f1h	A-201	1.82	0.681	0.19	0.20	1.00	0.26 / 0.20 / 0.29 / 0.20		0.77 / 0.65 / 1.20	0.22
4xjl	B-504	1.85	0.659	0.19	0.21	1.00	0.80 / 0.20		1.11	0.22
4uhm	A-1458	1.33	0.837	0.11	0.13	0.80	0.48 / 0.24		0.48	0.22
4yqu	A-301	1.94	0.658	0.20	0.24	1.00	0.20 / 0.29 / 0.29 / 0.20		1.35 / 0.54 / 3.01	0.22
5eww	A-801	1.73	0.753	0.19	0.21	0.73	0.37 / 0.29		0.60	0.22
5fvt	A-800	1.83	0.675	0.17	0.21	1.00	0.76 / 0.20		1.79	0.22
5g2d	A-1272	1.80	0.715	0.18	0.21	1.00	0.80 / 0.20		0.83	0.22
5he5	B-502	1.55	0.715	0.19	0.20	1.00	0.55 / 0.20 / 0.20		2.03 / 0.32	0.22
5iu8	A-2418	2.00	0.735	0.18	0.20	1.00	0.80 / 0.20		1.07	0.22
5eu1	B-201	1.60	0.712	0.18	0.19	1.00	0.56 / 0.20 / 0.20		2.67 / 0.76	0.22
5fbg	A-701	1.97	0.647	0.16	0.19	1.00	0.78 / 0.20		0.81	0.22
5fra	F-201	2.00	0.640	0.18	0.21	1.00	0.44 / 0.54		0.70	0.22
5hdu	A-502	1.58	0.714	0.19	0.21	1.00	0.78 / 0.20		1.67	0.22
5ctx	B-303	1.60	0.725	0.19	0.22	1.00	0.52 / 0.31		0.97	0.22
4zs9	B-501	1.37	0.744	0.13	0.17	1.00	0.80 / 0.20		0.34	0.22
5g28	A-1274	1.57	0.775	0.15	0.19	1.00	0.69 / 0.31		1.03	0.22
5fvn	C-419	1.45	0.754	0.16	0.18	1.00	0.54 / 0.39		0.81	0.22
5l8l	A-501	1.67	0.701	0.19	0.22	1.00	0.69 / 0.26		0.87	0.22
5tkd	B-901	1.92	0.652	0.19	0.22	1.00	0.76 / 0.20		0.77	0.22
5ley	U-161	1.90	0.673	0.19	0.23	1.00	0.48 / 0.43		0.67	0.21
4yal	A-701	1.88	0.663	0.20	0.23	1.00	0.48 / 0.20 / 0.30		0.85 / 0.78	0.21
5etn	A-205	1.40	0.749	0.18	0.22	1.00	0.75 / 0.23		0.78	0.21
5g3l	G-200	1.72	0.711	0.17	0.20	1.00	0.61 / 0.20		1.12	0.21
5jr3	B-401	1.84	0.657	0.16	0.18	1.00	0.66 / 0.34		0.60	0.21
5etl	D-204	1.82	0.676	0.20	0.24	1.00	0.80 / 0.20		2.09	0.21
5epb	A-1202	1.50	0.785	0.17	0.19	1.00	0.72 / 0.20		1.04	0.21
4xq6	B-402	2.00	0.630	0.18	0.23	1.00	0.68 / 0.31		0.79	0.21
5jj0	A-1205	1.72	0.691	0.22	0.25	1.00	0.71 / 0.21		0.63	0.21
5t77	A-527	2.00	0.695	0.19	0.21	1.00	0.69 / 0.23		1.39	0.21
5d3y	B-501	1.95	0.668	0.21	0.26	1.00	0.80 / 0.20		0.48	0.20
5fjg	A-1273	2.00	0.742	0.17	0.22	1.00	0.80 / 0.20		0.84	0.20
5kl0	A-501	1.85	0.675	0.15	0.19	1.00	0.54 / 0.20		0.66	0.20
5i88	A-205	1.40	0.753	0.15	0.20	1.00	0.47 / 0.53		0.72	0.20
5le5	J-91	1.80	0.703	0.18	0.21	1.00	0.67 / 0.20		0.51	0.20
4ufg	I-563	1.65	0.726	0.16	0.19	1.00	0.35 / 0.20 / 0.43		0.54 / 1.06	0.20
5eif	A-301	1.50	0.717	0.16	0.19	1.00	0.66 / 0.33		0.61	0.20
5jzj	B-902	1.71	0.677	0.18	0.21	1.00	0.80 / 0.20		0.75	0.20
5ktw	C-1201	1.09	0.810	0.16	0.18	1.00	0.80 / 0.20		0.99	0.20
5iu8	A-2403	2.00	0.651	0.18	0.20	1.00	0.80 / 0.20		1.22	0.20
5l41	E-409	1.25	0.773	0.11	0.13	1.00	0.75 / 0.25		0.82	0.20
5ios	C-302	1.90	0.656	0.18	0.21	1.00	0.68 / 0.30		0.97	0.20
5kql	A-200	1.45	0.725	0.16	0.18	1.00	0.48 / 0.20 / 0.23		1.52 / 1.41	0.20

PDB	Ligand	Resolution (Å)	Twilight score	Rwork	Rfree	Occupancy (deposited)	Occupancy (qFit)	RMSD A->B (Å) (deposited)	RMSD A->B (qFit)	Best Fisher z improvement
5thv	B-404	1.87	0.677	0.17	0.21	1.00	0.80 / 0.20		0.88	0.20
5j47	A-703	1.99	0.649	0.18	0.22	1.00	0.73 / 0.20		0.91	0.19
5kut	A-601	1.69	0.681	0.22	0.24	1.00	0.69 / 0.26		0.84	0.19
5ltp	E-59	1.70	0.692	0.19	0.21	1.00	0.75 / 0.20		0.70	0.19
5eu1	A-201	1.60	0.709	0.18	0.19	1.00	0.65 / 0.29		0.55	0.19
5exz	A-307	1.90	0.709	0.15	0.20	0.67	0.35 / 0.20		0.87	0.19
5b7n	A-301	1.40	0.736	0.18	0.20	1.00	0.80 / 0.20		0.52	0.19
4zo6	B-801	2.00	0.670	0.18	0.26	1.00	0.63 / 0.20		0.70	0.19
5kru	A-201	1.60	0.706	0.18	0.22	1.00	0.80 / 0.20		0.64	0.19
5lf7	J-91	2.00	0.652	0.18	0.21	1.00	0.20 / 0.21 / 0.31 / 0.20		0.86 / 2.65 / 2.82	0.19
5t64	A-502	1.70	0.697	0.18	0.22	1.00	0.71 / 0.20		0.57	0.19
5an1	H-1220	2.00	0.643	0.21	0.26	1.00	0.73 / 0.20		0.79	0.19
4uff	I-563	1.55	0.748	0.16	0.19	1.00	0.31 / 0.64		1.03	0.19
5eif	C-4000	1.50	0.721	0.16	0.19	1.00	0.73 / 0.20		0.62	0.18
5li6	B-502	1.95	0.652	0.19	0.24	1.00	0.80 / 0.20		0.90	0.18
5lf1	J-91	2.00	0.661	0.18	0.21	1.00	0.20 / 0.20 / 0.20 / 0.20 / 0.20		2.35 / 2.03 / 4.94 / 5.72	0.18
5e9q	A-302	1.79	0.723	0.17	0.20	0.68	0.41 / 0.26		0.64	0.18
5kut	B-601	1.69	0.686	0.22	0.24	1.00	0.74 / 0.20		0.90	0.18
5toz	A-1201	1.98	0.637	0.18	0.22	1.00	0.75 / 0.20		0.91	0.18
5hfk	A-302	1.55	0.715	0.19	0.21	1.00	0.79 / 0.20		0.70	0.18
5kgu	A-202	1.90	0.648	0.18	0.23	1.00	0.60 / 0.36		0.89	0.18
4zl1	A-403	1.86	0.687	0.16	0.18	1.00	0.61 / 0.20		1.04	0.18
5f1h	B-201	1.82	0.668	0.19	0.20	1.00	0.45 / 0.29 / 0.20		0.71 / 0.39	0.18
5fok	B-1723	1.90	0.703	0.19	0.21	0.50	0.40 / 0.24		0.52	0.18
5hur	A-202	1.50	0.717	0.18	0.23	1.00	0.56 / 0.37		0.90	0.18
5f08	A-301	1.92	0.657	0.20	0.23	1.00	0.80 / 0.20		0.93	0.17
5syn	C-301	1.64	0.701	0.22	0.25	1.00	0.64 / 0.24		0.39	0.17
4y5g	A-401	1.47	0.761	0.12	0.16	0.88	0.64 / 0.20		2.04	0.17
5lf1	G-161	2.00	0.649	0.18	0.21	1.00	0.20 / 0.63		0.49	0.17
4ufe	I-563	1.59	0.741	0.16	0.18	1.00	0.76 / 0.20		0.44	0.17
4y4x	A-407	1.67	0.716	0.15	0.18	0.75	0.39 / 0.32		1.13	0.17
5a2c	A-1476	1.90	0.676	0.16	0.21	1.00	0.64 / 0.20		0.33	0.17
5k4x	A-401	1.37	0.760	0.20	0.21	1.00	0.60 / 0.20		1.85	0.17
5de3	A-201	1.42	0.742	0.21	0.23	1.00	0.65 / 0.28		0.77	0.17
5duw	B-201	1.70	0.687	0.15	0.18	1.00	0.74 / 0.23		0.71	0.17
4zno	B-401	1.86	0.685	0.19	0.23	1.00	0.80 / 0.20		0.56	0.17
5d25	A-201	1.70	0.684	0.18	0.20	1.00	0.75 / 0.20		1.18	0.17
5l7e	A-1106	1.86	0.658	0.18	0.20	1.00	0.80 / 0.20		1.00	0.17
5iw0	A-601	1.63	0.698	0.16	0.19	1.00	0.76 / 0.20		0.71	0.17
5lf7	E-148	2.00	0.649	0.18	0.21	1.00	0.20 / 0.45 / 0.25		0.89 / 0.51	0.17
5t77	A-552	2.00	0.686	0.19	0.21	1.00	0.40 / 0.60		1.19	0.17
5fwa	A-1446	1.80	0.665	0.17	0.19	1.00	0.79 / 0.20		0.70	0.16
5fpb	A-1341	1.91	0.667	0.16	0.20	1.00	0.67 / 0.20		1.05	0.16
5t77	A-541	2.00	0.731	0.19	0.21	1.00	0.73 / 0.27		1.25	0.16
5iu8	A-2426	2.00	0.748	0.18	0.20	1.00	0.80 / 0.20		1.31	0.16
5irc	F-201	1.72	0.678	0.17	0.21	1.00	0.56 / 0.42		0.80	0.16
5d3l	A-201	1.50	0.730	0.18	0.20	1.00	0.69 / 0.20		0.47	0.16
5k2d	A-1208	1.90	0.742	0.17	0.21	1.00	0.80 / 0.20		0.92	0.16
5ant	B-1157	2.00	0.646	0.21	0.25	1.00	0.80 / 0.20		0.69	0.16
5jf8	A-301	1.80	0.719	0.19	0.22	1.00	0.55 / 0.20 / 0.20		1.28 / 3.23	0.16
4znt	B-601	1.90	0.656	0.20	0.21	1.00	0.73 / 0.20		1.43	0.16
5g0n	B-800	1.94	0.664	0.18	0.22	1.00	0.76 / 0.20		1.28	0.16
5cpn	A-401	1.80	0.697	0.18	0.22	1.00	0.47 / 0.20 / 0.20		0.94 / 1.30	0.16
5flj	C-301	1.82	0.681	0.16	0.21	0.80	0.62 / 0.20		1.37	0.16
5hht	B-711	1.50	0.719	0.13	0.16	1.00	0.80 / 0.20		0.94	0.16
5fvn	E-411	1.45	0.811	0.16	0.18	1.00	0.72 / 0.22		0.61	0.15
5hat	D-500	2.00	0.646	0.21	0.25	1.00	0.47 / 0.20 / 0.20		1.41 / 1.14	0.15
5a8k	A-558	1.41	0.731	0.11	0.14	1.00	0.76 / 0.24		0.70	0.15
5eyp	A-501	1.90	0.646	0.17	0.21	1.00	0.76 / 0.20		0.80	0.15
5ezh	A-301	1.70	0.690	0.19	0.23	1.00	0.67 / 0.20		1.09	0.15
5igm	B-301	1.60	0.711	0.22	0.27	1.00	0.78 / 0.20		0.52	0.15

PDB	Ligand	Resolution (Å)	Twilight score	Rwork	Rfree	Occupancy (deposited)	Occupancy (qFit)	RMSD A->B (Å) (deposited)	RMSD A->B (qFit)	Best Fisher z improvement
5ers	A-801	1.70	0.679	0.15	0.18	1.00	0.79 / 0.20		0.68	0.15
5ktw	A-1201	1.09	0.809	0.16	0.18	1.00	0.80 / 0.20		1.21	0.15
4xym	B-300	1.90	0.649	0.20	0.24	1.00	0.78 / 0.20		0.97	0.15
5g2d	A-1266	1.80	0.725	0.18	0.21	1.00	0.80 / 0.20		1.06	0.15
5icc	A-401	1.90	0.646	0.16	0.21	1.00	0.80 / 0.20		1.19	0.15
5eyp	B-502	1.90	0.651	0.17	0.21	1.00	0.74 / 0.20		0.66	0.15
4zyu	A-1101	1.95	0.658	0.18	0.21	0.71	0.50 / 0.20		1.39	0.15
5igf	A-202	1.70	0.679	0.20	0.22	1.00	0.79 / 0.20		1.16	0.15
5ih9	A-401	1.79	0.672	0.17	0.20	1.00	0.79 / 0.20		0.92	0.15
5fh2	A-703	1.49	0.716	0.15	0.17	1.00	0.67 / 0.27		0.76	0.14
5etz	B-304	1.80	0.689	0.22	0.24	1.00	0.73 / 0.27		0.61	0.14
5lf4	G-47	1.99	0.659	0.18	0.22	1.00	0.65 / 0.24		0.77	0.14
5aee	B-1680	1.85	0.653	0.16	0.20	1.00	0.64 / 0.32		0.87	0.14
4xjp	A-502	1.60	0.708	0.16	0.19	1.00	0.76 / 0.20		0.66	0.14
5k2d	A-1215	1.90	0.772	0.17	0.21	1.00	0.59 / 0.41		1.13	0.14
4z15	B-2	1.60	0.704	0.18	0.21	1.00	0.55 / 0.39		0.93	0.14
5in3	B-418	1.73	0.709	0.20	0.23	0.70	0.42 / 0.20		1.16	0.14
5iu8	A-2422	2.00	0.752	0.18	0.20	1.00	0.78 / 0.22		0.66	0.14
5lf4	G-161	1.99	0.642	0.18	0.22	1.00	0.47 / 0.40		0.68	0.14
5i5x	B-401	1.65	0.691	0.18	0.22	1.00	0.76 / 0.20		1.35	0.14
5le5	S-148	1.80	0.707	0.18	0.21	1.00	0.51 / 0.34		0.54	0.14
5isl	A-601	1.69	0.701	0.17	0.20	1.00	0.56 / 0.20 / 0.21		0.61 / 0.60	0.14
5ku3	A-211	1.14	0.810	0.16	0.18	1.00	0.78 / 0.20		0.87	0.13
5lf4	S-148	1.99	0.667	0.18	0.22	1.00	0.98			0.13
4zen	A-501	1.93	0.648	0.16	0.20	1.00	0.61 / 0.35		1.09	0.13
5szy	B-201	2.00	0.633	0.20	0.21	1.00	0.76 / 0.20		0.84	0.13
5djt	A-602	1.40	0.743	0.15	0.17	1.00	0.78 / 0.20		0.78	0.13
5g54	A-1270	2.00	0.669	0.18	0.23	1.00	0.80 / 0.20		0.92	0.13
4ufv	B-1001	1.75	0.683	0.19	0.24	1.00	0.78 / 0.20		0.49	0.13
4xym	D-302	1.90	0.656	0.20	0.24	1.00	0.78 / 0.20		0.58	0.13
5ei3	A-301	1.71	0.703	0.17	0.19	1.00	0.59 / 0.20		0.83	0.13
5j22	A-202	1.90	0.649	0.18	0.24	1.00	0.77 / 0.20		0.75	0.13
5t6b	B-504	2.00	0.681	0.18	0.23	1.00	0.67 / 0.33		1.09	0.13
5ead	A-602	2.00	0.634	0.19	0.23	1.00	0.63 / 0.37		0.82	0.13
5t6b	C-502	2.00	0.636	0.18	0.23	1.00	0.79 / 0.20		0.42	0.12
4yaw	B-703	2.00	0.634	0.20	0.25	1.00	0.79 / 0.20		0.99	0.12
5d7x	A-802	1.35	0.827	0.17	0.18	1.00	0.60 / 0.20		1.76	0.12
5cx9	A-406	1.73	0.856	0.19	0.20	1.00	0.36 / 0.36		1.29	0.12
5aez	A-902	1.47	0.869	0.14	0.15	1.00	0.72 / 0.28		2.99	0.12
5tg2	A-201	1.75	0.687	0.18	0.23	1.00	0.73 / 0.20		0.60	0.12
5b1s	A-501	1.58	0.706	0.19	0.23	1.00	0.62 / 0.20		2.41	0.12
4s35	B-201	1.55	0.712	0.15	0.17	1.00	0.77 / 0.20		0.80	0.12
5ley	E-148	1.90	0.673	0.19	0.23	1.00	0.60 / 0.20		0.41	0.12
5j99	A-401	1.70	0.680	0.15	0.18	1.00	0.50 / 0.23 / 0.20		0.86 / 0.80	0.11
5k0j	A-302	1.94	0.646	0.19	0.23	1.00	0.76 / 0.20		0.55	0.11
4xjm	B-502	1.60	0.700	0.20	0.22	1.00	0.44 / 0.53		1.10	0.11
5g0a	A-1298	1.70	0.681	0.17	0.20	1.00	0.66 / 0.27		1.11	0.11
4yqc	A-301	1.89	0.652	0.16	0.18	1.00	0.63 / 0.31		0.82	0.11
5edl	A-201	1.95	0.640	0.20	0.22	1.00	0.68 / 0.20		0.42	0.11
5ej4	A-601	1.77	0.678	0.18	0.22	1.00	0.78 / 0.20		0.73	0.11
5e3k	A-501	1.70	0.708	0.15	0.20	1.00	0.73 / 0.20		0.93	0.11
5syn	D-301	1.64	0.698	0.22	0.25	1.00	0.64 / 0.21		0.87	0.11
5kut	C-601	1.69	0.691	0.22	0.24	1.00	0.72 / 0.21		0.83	0.11
5le5	G-161	1.80	0.676	0.18	0.21	1.00	0.65 / 0.20		0.55	0.10
5fc4	A-402	1.50	0.727	0.16	0.20	1.00	0.70 / 0.23		0.78	0.10
5fra	E-201	2.00	0.638	0.18	0.21	1.00	0.80 / 0.20		0.50	0.10
5g6m	A-902	1.77	0.757	0.16	0.20	1.00	0.47 / 0.38		0.91	0.10
5t77	A-544	2.00	0.690	0.19	0.21	1.00	0.78 / 0.22		1.37	0.10
5etz	D-301	1.80	0.680	0.22	0.24	1.00	0.77 / 0.22		0.48	0.10
5f12	A-201	1.50	0.726	0.18	0.21	1.00	0.73 / 0.23		0.76	0.10
5jtt	A-901	1.85	0.652	0.16	0.19	1.00	0.61 / 0.39		1.14	0.10

PDB	Ligand	Resolution (Å)	Twilight score	Rwork	Rfree	Occupancy (deposited)	Occupancy (qFit)	RMSD A->B (Å) (deposited)	RMSD A->B (qFit)	Best Fisher z improvement
5eyp	B-501	1.90	0.643	0.17	0.21	1.00	0.58 / 0.36		0.81	0.10
5jda	A-401	1.40	0.759	0.17	0.18	1.00	0.61 / 0.20		0.96	0.10
5lf7	U-161	2.00	0.662	0.18	0.21	1.00	0.32 / 0.28 / 0.40		3.33 / 2.53	0.10
4ylw	A-401	1.79	0.701	0.16	0.18	1.00	0.57 / 0.20		0.48	0.10
5g3m	B-1133	1.85	0.672	0.20	0.23	1.00	0.71 / 0.26		1.21	0.10
4zoj	A-402	1.96	0.637	0.22	0.26	1.00	0.75 / 0.23		0.89	0.10
5fvs	A-800	1.95	0.672	0.19	0.23	1.00	0.52 / 0.20 / 0.26		1.04 / 0.55	0.10
5iu8	A-2411	2.00	0.759	0.18	0.20	1.00	0.80 / 0.20		1.16	0.09
5syx	A-111	1.77	0.670	0.14	0.17	0.60 / 0.10	0.70 / 0.20	0.60	0.55	0.09
5job	A-201	1.45	0.727	0.16	0.18	1.00	0.76 / 0.21		0.87	0.09
5kcd	B-601	1.82	0.672	0.18	0.21	0.94	0.80 / 0.20		1.23	0.09
5syh	A-111	1.65	0.689	0.14	0.17	1.00	0.64 / 0.20		0.52	0.09
5jr3	A-401	1.84	0.656	0.16	0.18	1.00	0.47 / 0.52		0.59	0.08
4znv	A-601	1.77	0.674	0.18	0.20	0.95	0.77 / 0.20		0.88	0.08
5f91	A-501	2.00	0.633	0.15	0.19	1.00	0.77 / 0.20		1.12	0.08
4zsi	B-301	1.65	0.689	0.19	0.23	1.00	0.75 / 0.20		1.12	0.08
5enz	B-401	1.91	0.642	0.20	0.23	1.00	0.38 / 0.21 / 0.38		0.84 / 0.84	0.08
5t4f	B-811	1.90	0.646	0.16	0.19	1.00	0.75 / 0.20		0.87	0.08
5buc	B-301	1.87	0.743	0.15	0.20	1.00	0.54 / 0.20		0.59	0.08
5iif	A-202	1.85	0.658	0.20	0.24	1.00	0.75 / 0.20		0.53	0.08
5eqq	A-603	1.66	0.712	0.23	0.23	1.00	0.77 / 0.20		0.87	0.08
5fvn	D-412	1.45	0.823	0.16	0.18	1.00	0.48 / 0.20		0.86	0.08
5g2d	A-1270	1.80	0.785	0.18	0.21	1.00	0.74 / 0.26		0.92	0.08
5eco	E-301	1.80	0.674	0.22	0.24	1.00	0.72 / 0.24		0.57	0.07
5a8y	A-1001	1.90	0.655	0.16	0.22	1.00	0.78 / 0.20		0.48	0.07
5tr6	A-701	1.93	0.652	0.19	0.22	1.00	0.78 / 0.20		0.91	0.07
5fh0	A-703	1.60	0.699	0.20	0.23	1.00	0.68 / 0.24		0.79	0.07
5hx1	A-201	1.80	0.663	0.17	0.21	1.00	0.79 / 0.21		0.97	0.07
5t6m	C-402	1.80	0.739	0.20	0.24	1.00	0.37 / 0.52		0.77	0.07
5tf5	B-263	1.81	0.724	0.22	0.25	1.00	0.51 / 0.20		1.52	0.07
5cp1	B-403	1.57	0.702	0.14	0.16	1.00	0.49 / 0.49		0.78	0.06
5ft4	B-1401	2.00	0.631	0.14	0.19	1.00	0.54 / 0.45		1.07	0.06
5ifi	B-701	1.95	0.641	0.19	0.21	1.00	0.77 / 0.20		0.42	0.06
3sp5	A-232	1.80	0.672	0.16	0.21	1.00	0.52 / 0.47		0.76	0.06
4zmg	A-403	1.90	0.649	0.18	0.20	1.00	0.77 / 0.20		0.43	0.06
5u26	A-201	1.85	0.658	0.15	0.19	1.00	0.80 / 0.20		0.34	0.06
5b2e	B-302	1.80	0.666	0.18	0.22	1.00	0.67 / 0.20		0.67	0.06
5fg3	A-701	1.90	0.646	0.19	0.24	1.00	0.62 / 0.36		0.82	0.06
5le5	U-161	1.80	0.687	0.18	0.21	1.00	0.53 / 0.20 / 0.20		1.23 / 0.69	0.06
5fvn	D-410	1.45	0.827	0.16	0.18	1.00	0.80 / 0.20		0.98	0.06
5iu8	A-2419	2.00	0.725	0.18	0.20	1.00	0.80 / 0.20		0.58	0.06
4y3n	A-402	1.34	0.957	0.12	0.15	0.78	0.51 / 0.24		0.90	0.06
5ezh	A-302	1.70	0.692	0.19	0.23	1.00	0.72 / 0.27		1.06	0.06
5i5y	A-401	1.81	0.660	0.15	0.19	1.00	0.72 / 0.20		1.15	0.06
5lf1	U-161	2.00	0.659	0.18	0.21	1.00	0.46 / 0.43		2.44	0.06
5ktw	B-1201	1.09	0.812	0.16	0.18	1.00	0.79 / 0.20		0.46	0.06
5duw	C-201	1.70	0.685	0.15	0.18	1.00	0.80 / 0.20		0.81	0.05
5hjs	B-301	1.72	0.776	0.21	0.24	1.00	0.67 / 0.20		0.80	0.05
5jdc	B-302	1.78	0.808	0.21	0.24	1.00	0.68 / 0.21		0.36	0.05
5dtk	D-301	1.60	0.772	0.15	0.17	0.78	0.39 / 0.20 / 0.22		1.27 / 1.06	0.05
5kti	A-301	1.80	0.672	0.18	0.20	1.00	0.80 / 0.20		0.52	0.05
4znv	B-601	1.77	0.676	0.18	0.20	0.99	0.80 / 0.20		0.44	0.05
5fqc	B-600	1.45	0.741	0.16	0.18	1.00	0.73 / 0.20		0.80	0.05
5fvn	C-415	1.45	0.757	0.16	0.18	1.00	0.65 / 0.20		0.57	0.05
5g1x	A-1390	1.72	0.673	0.18	0.20	1.00	0.80 / 0.20		0.83	0.05
4y47	A-401	1.19	0.804	0.13	0.15	1.00	0.71 / 0.20		1.06	0.05
5k2d	A-1207	1.90	0.703	0.17	0.21	1.00	0.80 / 0.20		1.48	0.05
5ddc	A-601	1.62	0.698	0.16	0.19	1.00	0.20 / 0.39 / 0.36		0.72 / 0.72	0.04
5d7i	A-302	2.00	0.634	0.18	0.22	1.00	0.72 / 0.20		0.85	0.04
5he5	A-502	1.55	0.715	0.19	0.20	1.00	0.74 / 0.20		0.43	0.04
5d4o	A-203	1.80	0.661	0.21	0.23	1.00	0.49 / 0.47		0.90	0.04

PDB	Ligand	Resolution (Å)	Twilight score	Rwork	Rfree	Occupancy (deposited)	Occupancy (qFit)	RMSD A->B (Å) (deposited)	RMSD A->B (qFit)	Best Fisher z improvement
5fvn	F-418	1.45	0.762	0.16	0.18	1.00	0.64 / 0.20		0.49	0.04
5ecn	D-603	1.72	0.692	0.17	0.19	1.00	0.64 / 0.20		0.79	0.04
5j1z	A-202	1.73	0.674	0.17	0.21	1.00	0.78 / 0.20		0.89	0.04
5l9g	A-401	1.75	0.687	0.18	0.21	1.00	0.76 / 0.22		0.70	0.04
5dh5	B-803	2.00	0.640	0.20	0.23	1.00	0.78 / 0.21		0.89	0.03
5i5y	B-402	1.81	0.661	0.15	0.19	1.00	0.76 / 0.20		0.62	0.03
5etq	B-203	1.96	0.636	0.18	0.22	1.00	0.62 / 0.38		0.78	0.03
5k2c	A-1215	1.90	0.779	0.17	0.21	1.00	0.72 / 0.28		1.12	0.03
5t6m	B-402	1.80	0.684	0.20	0.24	1.00	0.71 / 0.20		0.81	0.03
5i1q	A-1701	1.50	0.720	0.19	0.21	1.00	0.68 / 0.32		0.71	0.03
5duf	A-301	1.50	0.723	0.17	0.18	1.00	0.67 / 0.27		0.98	0.03
5ej4	B-602	1.77	0.680	0.18	0.22	1.00	0.75 / 0.20		0.54	0.03
5dbm	A-1201	1.86	0.658	0.17	0.22	1.00	0.75 / 0.20		0.74	0.02
5ctv	E-101	1.05	0.848	0.13	0.15	1.00	0.64 / 0.20		0.79	0.02
4xcf	L-302	1.43	0.781	0.14	0.17	0.80	0.55 / 0.20		1.55	0.02
5fri	A-1501	2.00	0.635	0.16	0.19	1.00	0.80 / 0.20		0.63	0.02
5tbn	A-401	1.85	0.682	0.24	0.30	1.00	0.77 / 0.23		0.86	0.02
5l3u	E-409	1.23	0.776	0.10	0.12	1.00	0.80 / 0.20		0.86	0.02
5t1u	A-401	1.78	0.672	0.19	0.21	1.00	0.44 / 0.52		0.71	0.02
5aap	A-201	1.30	0.759	0.12	0.15	1.00	0.80 / 0.20		0.94	0.02
5hin	A-408	1.60	0.710	0.16	0.18	1.00	0.59 / 0.35		0.78	0.02
5jzj	A-703	1.71	0.677	0.18	0.21	1.00	0.80 / 0.20		0.85	0.02
4s35	A-201	1.55	0.707	0.15	0.17	1.00	0.51 / 0.29 / 0.20		0.78 / 0.78	0.01
5fvn	A-412	1.45	0.855	0.16	0.18	1.00	0.80 / 0.20		1.09	0.01
5l6e	A-601	1.90	0.653	0.16	0.18	1.00	0.76 / 0.24		0.59	0.01
5fjg	A-1271	2.00	0.664	0.17	0.22	1.00	0.80 / 0.20		0.79	0.01
5fvn	B-411	1.45	0.748	0.16	0.18	1.00	0.68 / 0.20		0.85	0.01
5jcx	A-302	1.43	0.785	0.14	0.18	0.80	0.48 / 0.20		1.47	0.00
5kmi	A-901	1.87	0.663	0.21	0.25	1.00	0.67 / 0.22		0.91	0.00
5g27	A-501	1.61	0.754	0.15	0.17	0.70 / 0.30	0.63	8.62		
5dog	A-304	1.70	0.796	0.16	0.21	0.50 / 0.50	0.59	4.08		
5hj1	A-301	1.50	0.761	0.19	0.22	0.50 / 0.50	1.00	1.90		
5mae	A-301	1.00	0.877	0.15	0.18	0.50 / 0.50	0.89	0.39		
5etp	A-201	1.05	0.817	0.11	0.13	0.50 / 0.50	0.96	0.34		
5bmh	A-101	1.60	0.706	0.16	0.18	0.50 / 0.50	0.92	0.22		
4mlo	A-304	1.65	0.729	0.17	0.19	1.00	0.97			
4rvj	B-101	1.60	0.702	0.17	0.20	1.00	0.98			
4rvj	D-101	1.60	0.701	0.17	0.20	1.00	0.97			
4s32	A-401	1.34	0.813	0.20	0.23	1.00	0.96			
4s33	A-401	1.48	0.776	0.20	0.24	0.50	0.68			
4ufv	A-1001	1.75	0.678	0.19	0.24	1.00	0.92			
4ufv	C-1001	1.75	0.686	0.19	0.24	1.00	0.91			
4ufw	A-1411	1.50	0.749	0.21	0.26	1.00	0.95			
4ufw	B-1411	1.50	0.747	0.21	0.26	1.00	0.95			
4ufw	C-1411	1.50	0.758	0.21	0.26	1.00	0.86			
4ufx	A-1000	1.49	0.720	0.16	0.20	1.00	0.99			
4ufx	B-1000	1.49	0.726	0.16	0.20	1.00	0.98			
4ufx	C-1000	1.49	0.724	0.16	0.20	1.00	0.93			
4ufy	A-2165	1.70	0.767	0.17	0.19	1.00	0.78			
4ufy	B-2165	1.70	0.790	0.17	0.19	1.00	0.76			
4uhg	A-2165	1.70	0.685	0.18	0.20	1.00	0.99			
4uhg	B-2165	1.70	0.688	0.18	0.20	1.00	0.93			
4ui3	A-2115	2.00	0.668	0.17	0.21	1.00	0.83			
4ui3	B-2116	2.00	0.659	0.17	0.21	1.00	0.80			
4ui5	A-2116	1.65	0.693	0.16	0.20	1.00	0.97			
4ui5	B-2116	1.65	0.693	0.16	0.20	1.00	0.93			
4ui6	B-2114	1.80	0.689	0.15	0.19	1.00	0.86			
4ui7	A-2116	1.80	0.683	0.17	0.20	1.00	0.97			
4ui7	B-2117	1.80	0.682	0.17	0.20	1.00	0.92			
4uj1	A-1351	1.77	0.687	0.17	0.20	1.00	0.90			
4uja	A-1351	1.93	0.645	0.16	0.21	1.00	0.77			

PDB	Ligand	Resolution (Å)	Twilight score	Rwork	Rfree	Occupancy (deposited)	Occupancy (qFit)	RMSD A->B (Å) (deposited)	RMSD A->B (qFit)	Best Fisher z improvement
4wv8	D-303	1.83	0.724	0.16	0.20	1.00	0.84			
4x3l	B-301	1.70	0.690	0.19	0.21	1.00	0.87			
4xeb	A-504	1.70	0.692	0.14	0.20	1.00	0.98			
4xem	A-501	1.28	0.768	0.16	0.18	1.00	1.00			
4xja	A-701	1.98	0.643	0.17	0.20	1.00	0.96			
4xje	A-202	1.88	0.658	0.17	0.19	1.00	1.00			
4xjl	A-502	1.85	0.657	0.19	0.21	1.00	1.00			
4xjm	A-502	1.60	0.700	0.20	0.22	1.00	1.00			
4xjo	A-501	1.50	0.721	0.19	0.21	1.00	0.98			
4xjo	A-502	1.50	0.729	0.19	0.21	1.00	0.96			
4xjo	B-501	1.50	0.725	0.19	0.21	1.00	1.00			
4xjo	B-502	1.50	0.726	0.19	0.21	1.00	0.98			
4xjp	A-501	1.60	0.700	0.16	0.19	1.00	0.97			
4xjp	B-502	1.60	0.704	0.16	0.19	1.00	0.98			
4xo7	A-402	1.75	0.756	0.16	0.21	0.70	0.59			
4xo7	B-402	1.75	0.784	0.16	0.21	0.70	0.64			
4xo8	A-501	1.70	0.685	0.17	0.20	1.00	0.95			
4xo8	B-501	1.70	0.685	0.17	0.20	1.00	0.96			
4xq6	A-401	2.00	0.632	0.18	0.23	1.00	0.98			
4xzw	A-401	1.50	0.728	0.17	0.20	1.00	1.00			
4xzw	A-402	1.50	0.792	0.17	0.20	1.00	0.86			
4y0i	D-501	1.66	0.686	0.17	0.20	0.94	0.92			
4y39	A-405	1.20	0.804	0.12	0.14	0.64	0.67			
4y3d	A-401	1.48	0.737	0.12	0.16	1.00	0.94			
4y45	A-405	1.06	0.843	0.12	0.14	1.00	0.89			
4y4b	A-406	1.11	0.963	0.12	0.14	1.00	1.00			
4y53	A-402	1.62	0.776	0.19	0.21	0.76	0.70			
4y53	A-403	1.62	0.815	0.19	0.21	0.79	0.76			
4y5b	A-403	1.24	0.978	0.12	0.15	1.00	0.91			
4y5b	A-404	1.24	0.835	0.12	0.15	0.83	0.81			
4y5m	A-401	1.28	0.816	0.12	0.15	1.00	0.88			
4y5m	A-402	1.28	0.904	0.12	0.15	1.00	0.97			
4y5n	A-401	1.29	0.788	0.12	0.15	1.00	0.95			
4y5p	A-404	1.23	0.835	0.12	0.15	1.00	0.92			
4y9h	A-301	1.43	0.740	0.20	0.22	1.00	1.00			
4y9h	A-309	1.43	0.766	0.20	0.22	1.00	1.00			
4yaf	B-701	1.91	0.660	0.21	0.24	1.00	0.91			
4yal	B-703	1.88	0.657	0.20	0.23	1.00	0.94			
4yb6	A-301	1.98	0.641	0.20	0.22	1.00	1.00			
4yb6	C-301	1.98	0.637	0.20	0.22	1.00	1.00			
4ycy	A-401	1.70	0.748	0.17	0.20	1.00	0.82			
4yd3	A-401	1.25	0.785	0.11	0.13	1.00	0.92			
4yfq	A-201	1.62	0.720	0.19	0.23	1.00	1.00			
4ykq	A-301	1.91	0.645	0.18	0.20	1.00	0.90			
4ykr	A-301	1.61	0.700	0.18	0.20	1.00	0.93			
4ykw	B-301	1.85	0.673	0.20	0.23	1.00	0.83			
4yqx	A-301	1.80	0.677	0.17	0.19	1.00	0.82			
4yky	A-301	1.78	0.687	0.17	0.19	1.00	0.87			
4ykz	A-301	1.85	0.658	0.17	0.21	1.00	0.99			
4yla	A-401	1.40	0.757	0.18	0.20	1.00	0.97			
4ylw	A-402	1.79	0.660	0.16	0.18	1.00	1.00			
4ync	A-401	1.50	0.718	0.16	0.17	1.00	0.99			
4yq0	A-301	1.76	0.686	0.17	0.19	1.00	0.82			
4yq1	A-301	2.00	0.636	0.19	0.22	1.00	0.99			
4yq6	A-301	1.90	0.661	0.18	0.21	1.00	0.96			
4yq7	A-301	1.80	0.669	0.18	0.21	1.00	0.91			
4yqi	A-301	1.92	0.648	0.17	0.20	1.00	0.96			
4yqt	A-301	1.60	0.704	0.18	0.21	1.00	0.99			
4ys9	B-501	2.00	0.635	0.21	0.22	1.00	0.97			
4ysn	A-1001	1.94	0.641	0.15	0.19	1.00	0.97			
4yx6	B-601	1.86	0.659	0.17	0.20	1.00	1.00			

PDB	Ligand	Resolution (Å)	Twilight score	Rwork	Rfree	Occupancy (deposited)	Occupancy (qFit)	RMSD A->B (Å) (deposited)	RMSD A->B (qFit)	Best Fisher z improvement
4z12	A-606	1.85	0.651	0.17	0.21	0.68	0.65			
4z12	A-607	1.85	0.698	0.17	0.21	0.69	1.00			
4z13	A-607	1.78	0.661	0.16	0.20	0.93	0.84			
4z1t	A-1	1.50	0.737	0.19	0.23	1.00	0.93			
4z1t	B-1	1.50	0.787	0.19	0.23	1.00	1.00			
4z54	A-301	1.83	0.657	0.17	0.20	1.00	0.97			
4z54	B-301	1.83	0.656	0.17	0.20	1.00	0.98			
4zam	A-302	1.42	0.792	0.17	0.19	0.80	1.00			
4zam	A-303	1.42	0.743	0.17	0.19	1.00	0.90			
4zea	A-419	1.20	0.848	0.14	0.16	0.77	0.81			
4zfi	A-201	2.00	0.636	0.20	0.24	1.00	0.98			
4zfi	B-201	2.00	0.635	0.20	0.24	1.00	0.96			
4zfi	C-201	2.00	0.633	0.20	0.24	1.00	1.00			
4zfi	D-201	2.00	0.637	0.20	0.24	1.00	0.97			
4zfm	A-501	1.40	0.804	0.13	0.16	0.70	0.61			
4zfm	B-501	1.40	0.798	0.13	0.16	0.70	0.58			
4zi3	B-301	2.00	0.640	0.19	0.24	1.00	0.93			
4zl1	A-402	1.86	0.648	0.16	0.18	1.00	1.00			
4zoj	B-403	1.96	0.720	0.22	0.26	0.50	0.65			
4zr2	A-201	1.80	0.707	0.18	0.22	1.00	1.00			
4zse	B-2001	1.97	0.639	0.19	0.21	1.00	0.87			
4zse	C-3001	1.97	0.640	0.19	0.21	1.00	0.93			
4zsi	A-301	1.65	0.689	0.19	0.23	1.00	0.95			
4zsk	A-301	1.85	0.662	0.19	0.25	1.00	0.89			
4zv5	B-101	1.57	0.756	0.23	0.26	1.00	0.97			
4zvl	A-303	1.90	0.657	0.15	0.19	1.00	0.92			
4zvl	B-301	1.90	0.670	0.15	0.19	1.00	0.90			
4zvn	A-303	1.87	0.668	0.16	0.20	1.00	0.92			
4zvz	A-503	2.00	0.660	0.20	0.24	1.00	0.80			
4zyz	A-1101	1.60	0.700	0.17	0.19	0.82	0.77			
4zz0	A-1101	1.65	0.691	0.16	0.19	1.00	0.91			
5a28	A-1002	1.48	0.726	0.20	0.25	1.00	0.95			
5a2b	A-1478	1.85	0.692	0.16	0.19	1.00	0.85			
5a5d	A-500	1.74	0.681	0.18	0.22	1.00	1.00			
5a5f	A-451	1.90	0.643	0.20	0.23	1.00	0.91			
5a6h	A-1264	1.57	0.709	0.15	0.19	0.90	0.85			
5a6h	A-1265	1.57	0.740	0.15	0.19	0.70	0.61			
5a8z	A-1001	2.00	0.638	0.19	0.24	1.00	1.00			
5aa8	A-2402	1.86	0.666	0.21	0.23	1.00	0.98			
5aa9	A-2402	1.93	0.647	0.20	0.24	1.00	0.97			
5ad1	A-500	1.32	0.754	0.14	0.18	1.00	0.99			
5aez	A-901	1.47	0.836	0.14	0.15	1.00	1.00			
5aez	A-905	1.47	0.921	0.14	0.15	1.00	0.89			
5ajc	C-103	1.70	0.698	0.15	0.19	1.00	0.88			
5ang	A-1299	1.90	0.666	0.20	0.24	1.00	0.93			
5anj	A-1299	1.60	0.702	0.20	0.23	1.00	0.96			
5anq	A-1353	2.00	0.654	0.19	0.23	1.00	0.77			
5anq	B-1354	2.00	0.654	0.19	0.23	1.00	0.80			
5ans	A-1157	1.60	0.707	0.21	0.24	1.00	1.00			
5anu	A-1158	1.80	0.685	0.21	0.26	1.00	0.93			
5apg	B-1185	1.60	0.700	0.19	0.20	1.00	0.90			
5aqf	A-1382	1.88	0.654	0.17	0.21	1.00	0.96			
5aqf	C-1382	1.88	0.654	0.17	0.21	1.00	0.98			
5aqw	A-1385	1.53	0.721	0.16	0.19	1.00	0.91			
5axa	A-502	1.55	0.721	0.19	0.23	1.00	0.94			
5axa	C-502	1.55	0.724	0.19	0.23	1.00	0.89			
5axb	A-502	1.65	0.689	0.15	0.18	1.00	1.00			
5axb	C-502	1.65	0.694	0.15	0.18	1.00	0.94			
5axc	A-503	1.55	0.730	0.18	0.21	1.00	0.95			
5axc	C-503	1.55	0.728	0.18	0.21	1.00	0.95			
5axd	C-502	1.60	0.707	0.16	0.18	1.00	0.91			

PDB	Ligand	Resolution (Å)	Twilight score	Rwork	Rfree	Occupancy (deposited)	Occupancy (qFit)	RMSD A->B (Å) (deposited)	RMSD A->B (qFit)	Best Fisher z improvement
5ayt	B-201	1.40	0.783	0.19	0.21	0.50	0.79			
5azb	A-301	1.60	0.763	0.18	0.22	1.00	0.98			
5b09	A-201	1.70	0.723	0.20	0.22	1.00	0.99			
5b0w	A-305	1.70	0.726	0.20	0.22	1.00	1.00			
5b0w	A-307	1.70	0.759	0.20	0.22	1.00	1.00			
5b0w	B-303	1.70	0.832	0.20	0.22	1.00	1.00			
5b0w	F-304	1.70	0.702	0.20	0.22	1.00	1.00			
5b0w	G-304	1.70	0.727	0.20	0.22	1.00	1.00			
5b2e	A-302	1.80	0.664	0.18	0.22	1.00	0.92			
5b2e	C-302	1.80	0.664	0.18	0.22	1.00	0.93			
5b2z	A-201	1.56	0.703	0.15	0.18	1.00	0.99			
5b30	A-201	1.60	0.697	0.17	0.20	1.00	0.97			
5b3y	A-401	1.90	0.650	0.17	0.19	1.00	1.00			
5b4o	A-201	1.37	0.803	0.18	0.20	1.00	0.90			
5b4o	B-201	1.37	0.820	0.18	0.20	1.00	0.87			
5b4o	B-202	1.37	0.831	0.18	0.20	1.00	0.83			
5b4o	C-201	1.37	0.785	0.18	0.20	1.00	0.86			
5b59	A-201	2.00	0.649	0.18	0.25	1.00	0.87			
5b6i	A-302	1.95	0.641	0.16	0.19	1.00	1.00			
5b6i	B-302	1.95	0.644	0.16	0.19	1.00	1.00			
5b7n	B-301	1.40	0.736	0.18	0.20	1.00	0.99			
5b7p	A-301	1.49	0.723	0.13	0.16	1.00	0.96			
5b7p	B-301	1.49	0.722	0.13	0.16	1.00	0.97			
5b7q	A-301	1.49	0.727	0.15	0.18	1.00	0.94			
5b7q	B-301	1.49	0.720	0.15	0.18	1.00	0.96			
5bmy	A-500	2.00	0.634	0.15	0.19	1.00	1.00			
5bn9	A-401	1.69	0.681	0.18	0.20	1.00	0.88			
5bph	B-401	1.70	0.688	0.18	0.21	1.00	0.84			
5bph	D-401	1.70	0.684	0.18	0.21	1.00	0.94			
5bpl	A-401	1.93	0.646	0.18	0.24	1.00	0.94			
5bpm	A-401	1.83	0.654	0.17	0.23	1.00	1.00			
5bqq	A-201	1.44	0.760	0.15	0.17	1.00	0.82			
5bqq	A-202	1.44	0.727	0.15	0.17	1.00	1.00			
5bqi	A-202	1.88	0.649	0.17	0.18	1.00	0.93			
5bqi	A-204	1.88	0.685	0.17	0.18	1.00	1.00			
5bsr	A-602	1.50	0.716	0.19	0.21	1.00	0.98			
5bsu	A-601	1.75	0.673	0.18	0.21	1.00	0.97			
5buc	A-303	1.87	0.687	0.15	0.20	1.00	0.88			
5bv6	A-501	1.94	0.638	0.18	0.21	1.00	0.96			
5bwz	A-404	1.59	0.717	0.14	0.16	1.00	0.92			
5bx1	A-201	1.90	0.695	0.20	0.24	1.00	0.88			
5bxu	B-101	1.35	0.802	0.16	0.19	1.00	0.84			
5c41	B-401	1.95	0.643	0.17	0.21	1.00	0.94			
5c41	C-401	1.95	0.642	0.17	0.21	1.00	0.96			
5c8w	A-302	1.80	0.662	0.16	0.20	1.00	1.00			
5c8w	B-303	1.80	0.663	0.16	0.20	1.00	1.00			
5c8w	C-302	1.80	0.666	0.16	0.20	1.00	1.00			
5c8w	D-302	1.80	0.670	0.16	0.20	1.00	0.99			
5c8w	E-302	1.80	0.666	0.16	0.20	1.00	1.00			
5c8w	F-302	1.80	0.670	0.16	0.20	1.00	1.00			
5ca3	B-1004	1.80	0.667	0.15	0.19	1.00	0.99			
5cbt	A-201	1.45	0.757	0.18	0.20	1.00	0.82			
5cbu	A-206	1.40	0.861	0.17	0.20	1.00	0.69			
5cbv	A-205	1.80	0.687	0.16	0.19	1.00	0.80			
5ccq	A-206	1.80	0.669	0.16	0.20	1.00	0.89			
5cfv	A-1201	1.80	0.682	0.18	0.23	1.00	1.00			
5cgb	A-301	1.60	0.706	0.16	0.18	1.00	0.94			
5cgp	A-4000	1.96	0.665	0.21	0.25	1.00	0.91			
5cli	A-200	1.95	0.648	0.14	0.17	1.00	0.83			
5clj	A-200	1.85	0.687	0.15	0.18	1.00	0.82			
5cm0	A-301	1.90	0.644	0.15	0.19	1.00	0.96			

PDB	Ligand	Resolution (Å)	Twilight score	Rwork	Rfree	Occupancy (deposited)	Occupancy (qFit)	RMSD A->B (Å) (deposited)	RMSD A->B (qFit)	Best Fisher z improvement
5cm0	B-301	1.90	0.642	0.15	0.19	1.00	0.96			
5cm0	C-301	1.90	0.646	0.15	0.19	1.00	0.93			
5co4	A-202	1.70	0.688	0.17	0.20	1.00	0.96			
5cph	A-301	1.20	0.810	0.17	0.19	1.00	0.85			
5cp1	A-401	1.57	0.716	0.14	0.16	1.00	0.92			
5cp1	A-402	1.57	0.703	0.14	0.16	1.00	1.00			
5cpm	A-402	1.50	0.718	0.15	0.19	1.00	0.99			
5cpm	B-402	1.50	0.720	0.15	0.19	1.00	0.97			
5cpn	B-401	1.80	0.693	0.18	0.22	1.00	0.91			
5cpo	A-402	1.65	0.690	0.16	0.19	1.00	0.99			
5cpo	B-402	1.65	0.692	0.16	0.19	1.00	0.97			
5ctj	B-97	1.93	0.646	0.14	0.17	1.00	0.96			
5cty	B-305	1.60	0.708	0.17	0.20	1.00	0.90			
5cu6	A-401	1.36	0.810	0.19	0.21	1.00	0.81			
5cuh	A-306	1.83	0.664	0.17	0.21	1.00	0.94			
5cuh	B-306	1.83	0.661	0.17	0.21	1.00	0.99			
5cvt	B-97	1.78	0.671	0.14	0.16	1.00	0.92			
5cvy	A-802	2.00	0.650	0.15	0.19	1.00	0.93			
5cx9	A-407	1.73	0.701	0.19	0.20	1.00	0.95			
5d0g	A-301	1.60	0.700	0.19	0.21	1.00	0.95			
5d0g	B-301	1.60	0.700	0.19	0.21	1.00	0.94			
5d29	A-818	1.80	0.671	0.17	0.21	1.00	0.93			
5d3p	A-201	1.95	0.642	0.18	0.20	1.00	1.00			
5d48	A-201	1.81	0.670	0.18	0.24	1.00	0.99			
5d4n	B-201	1.60	0.699	0.21	0.24	1.00	0.97			
5d4v	A-301	1.60	0.700	0.17	0.21	1.00	0.97			
5d4v	B-301	1.60	0.702	0.17	0.21	1.00	0.95			
5d4v	C-301	1.60	0.698	0.17	0.21	1.00	1.00			
5d4v	D-301	1.60	0.699	0.17	0.21	1.00	0.97			
5d7i	C-302	2.00	0.644	0.18	0.22	1.00	0.88			
5d86	A-1001	1.50	0.720	0.15	0.18	1.00	0.91			
5d87	A-401	1.50	0.716	0.15	0.18	1.00	0.93			
5d9j	A-203	1.85	0.674	0.18	0.23	1.00	0.90			
5d9x	A-301	1.68	0.718	0.19	0.23	1.00	0.79			
5db1	A-601	1.86	0.656	0.16	0.20	1.00	0.97			
5dbm	B-1201	1.86	0.657	0.17	0.22	1.00	1.00			
5dc5	B-403	1.94	0.659	0.18	0.21	1.00	0.99			
5dkh	B-1505	1.70	0.705	0.20	0.24	1.00	0.93			
5dkq	A-103	1.59	0.858	0.20	0.23	0.66	0.73			
5dl7	A-506	1.75	0.695	0.17	0.19	1.00	0.89			
5dl7	A-507	1.75	0.719	0.17	0.19	1.00	0.87			
5dl7	A-509	1.75	0.723	0.17	0.19	1.00	0.96			
5dl7	A-510	1.75	0.726	0.17	0.19	1.00	0.96			
5dl7	A-511	1.75	0.683	0.17	0.19	1.00	0.86			
5dq2	A-403	1.51	0.846	0.12	0.16	0.81	0.81			
5dr1	A-409	1.45	0.899	0.16	0.17	0.83	0.76			
5dr3	A-408	1.24	0.825	0.11	0.13	0.50	0.49			
5dr7	A-406	1.23	0.827	0.12	0.15	0.74	0.66			
5drf	A-65	1.14	0.820	0.14	0.17	1.00	0.80			
5drg	A-65	1.14	0.820	0.14	0.17	1.00	0.80			
5ds7	B-201	2.00	0.634	0.23	0.26	1.00	0.98			
5ds7	C-201	2.00	0.635	0.23	0.26	1.00	0.98			
5ds8	P-4	1.95	0.652	0.18	0.22	1.00	0.90			
5dtk	A-306	1.60	0.829	0.15	0.17	0.72	0.67			
5duv	C-201	1.90	0.651	0.16	0.20	1.00	0.99			
5duv	D-201	1.90	0.658	0.16	0.20	1.00	0.98			
5duw	A-201	1.70	0.683	0.15	0.18	1.00	0.98			
5dux	B-201	1.85	0.687	0.17	0.21	1.00	0.92			
5dvz	A-82	1.69	0.684	0.20	0.23	1.00	0.90			
5dxe	A-1000	1.50	0.727	0.18	0.20	1.00	0.97			
5dxe	B-1000	1.50	0.732	0.18	0.20	1.00	1.00			

PDB	Ligand	Resolution (Å)	Twilight score	Rwork	Rfree	Occupancy (deposited)	Occupancy (qFit)	RMSD A->B (Å) (deposited)	RMSD A->B (qFit)	Best Fisher z improvement
5dxg	A-1000	1.86	0.656	0.17	0.20	1.00	1.00			
5dxg	B-601	1.86	0.660	0.17	0.20	1.00	0.98			
5dxi	A-403	2.00	0.639	0.20	0.24	1.00	0.99			
5dxi	B-403	2.00	0.638	0.20	0.24	1.00	0.97			
5dxy	A-401	1.77	0.670	0.15	0.18	1.00	0.99			
5dy2	A-401	1.57	0.706	0.16	0.19	1.00	1.00			
5dy9	A-101	1.60	0.832	0.17	0.20	0.56	0.53			
5dy9	G-101	1.60	0.772	0.17	0.20	0.63	0.59			
5e0w	B-901	2.00	0.645	0.19	0.23	1.00	0.99			
5e1q	A-702	1.94	0.650	0.19	0.22	1.00	0.98			
5e1q	B-702	1.94	0.650	0.19	0.22	1.00	1.00			
5e3k	B-501	1.70	0.683	0.15	0.20	1.00	0.93			
5e78	B-503	2.00	0.671	0.18	0.21	1.00	0.80			
5e7x	A-301	1.80	0.734	0.18	0.22	1.00	1.00			
5e8x	A-601	1.45	0.750	0.19	0.21	1.00	0.92			
5e8z	A-601	1.51	0.751	0.18	0.21	1.00	0.82			
5e93	A-408	1.41	0.732	0.15	0.17	1.00	0.99			
5e95	A-201	1.40	0.733	0.16	0.19	1.00	1.00			
5ec8	A-301	1.71	0.684	0.17	0.20	1.00	0.92			
5eci	A-602	1.56	0.713	0.21	0.23	1.00	1.00			
5eci	D-602	1.56	0.712	0.21	0.23	1.00	1.00			
5eck	A-602	1.54	0.709	0.16	0.18	1.00	0.93			
5eck	C-301	1.54	0.708	0.16	0.18	1.00	0.92			
5eck	D-603	1.54	0.711	0.16	0.18	1.00	0.93			
5eck	F-301	1.54	0.707	0.16	0.18	1.00	0.92			
5ecm	E-301	1.60	0.713	0.23	0.25	1.00	1.00			
5ecn	A-603	1.72	0.689	0.17	0.19	1.00	0.94			
5ecn	F-301	1.72	0.687	0.17	0.19	1.00	0.81			
5eco	F-301	1.80	0.685	0.22	0.24	1.00	0.94			
5ecq	C-301	1.66	0.705	0.23	0.23	1.00	0.98			
5ecq	D-603	1.66	0.710	0.23	0.23	1.00	0.94			
5ecq	F-301	1.66	0.703	0.23	0.23	1.00	0.99			
5ecr	C-301	1.72	0.703	0.26	0.28	1.00	0.87			
5ecr	E-301	1.72	0.716	0.26	0.28	1.00	0.98			
5edd	A-202	1.97	0.635	0.16	0.21	1.00	0.99			
5ehp	A-601	1.85	0.662	0.18	0.21	1.00	0.95			
5ehp	B-601	1.85	0.667	0.18	0.21	1.00	0.92			
5ehr	A-601	1.70	0.689	0.20	0.22	1.00	0.95			
5ehr	B-601	1.70	0.689	0.20	0.22	1.00	0.95			
5ei4	A-202	1.05	0.910	0.17	0.19	0.50	0.43			
5eis	A-201	1.60	0.703	0.18	0.22	1.00	0.94			
5eiw	A-301	1.61	0.701	0.18	0.21	1.00	0.92			
5eiw	C-4000	1.61	0.741	0.18	0.21	1.00	0.90			
5ekd	A-401	1.82	0.670	0.17	0.21	1.00	1.00			
5ekd	B-401	1.82	0.676	0.17	0.21	1.00	1.00			
5elo	A-602	1.90	0.653	0.20	0.25	1.00	0.93			
5elo	B-602	1.90	0.668	0.20	0.25	1.00	0.93			
5elo	C-602	1.90	0.652	0.20	0.25	1.00	0.97			
5elo	D-602	1.90	0.663	0.20	0.25	1.00	0.98			
5elv	A-312	1.92	0.640	0.16	0.21	1.00	1.00			
5elv	B-312	1.92	0.640	0.16	0.21	1.00	1.00			
5en4	A-302	1.52	0.757	0.11	0.13	1.00	0.89			
5enz	A-401	1.91	0.645	0.20	0.23	1.00	0.95			
5eob	A-1401	1.75	0.682	0.17	0.20	1.00	0.98			
5epb	A-1201	1.50	0.741	0.17	0.19	1.00	0.88			
5eqd	B-501	1.83	0.658	0.17	0.20	1.00	0.95			
5eqt	A-401	1.94	0.646	0.22	0.24	1.00	0.94			
5er4	X-103	1.81	0.739	0.18	0.22	1.00	0.98			
5er9	B-501	1.69	0.685	0.19	0.22	1.00	0.97			
5err	A-801	1.65	0.689	0.16	0.18	1.00	0.93			
5et8	A-401	1.92	0.649	0.18	0.22	0.80	0.77			

PDB	Ligand	Resolution (Å)	Twilight score	Rwork	Rfree	Occupancy (deposited)	Occupancy (qFit)	RMSD A->B (Å) (deposited)	RMSD A->B (qFit)	Best Fisher z improvement
5etl	A-205	1.82	0.662	0.20	0.24	1.00	1.00			
5etl	B-203	1.82	0.665	0.20	0.24	1.00	1.00			
5etl	C-204	1.82	0.666	0.20	0.24	1.00	1.00			
5etl	D-203	1.82	0.670	0.20	0.24	1.00	1.00			
5etp	A-209	1.05	0.833	0.11	0.13	1.00	0.87			
5etq	A-203	1.96	0.636	0.18	0.22	1.00	1.00			
5etq	A-204	1.96	0.659	0.18	0.22	1.00	1.00			
5etq	B-204	1.96	0.660	0.18	0.22	1.00	1.00			
5etr	A-201	1.32	0.749	0.12	0.15	1.00	1.00			
5etr	A-202	1.32	0.755	0.12	0.15	1.00	0.99			
5etr	B-201	1.32	0.748	0.12	0.15	1.00	1.00			
5etr	B-202	1.32	0.756	0.12	0.15	1.00	1.00			
5ets	A-201	1.95	0.639	0.19	0.22	1.00	1.00			
5ets	A-202	1.95	0.648	0.19	0.22	1.00	1.00			
5ets	B-201	1.95	0.636	0.19	0.22	1.00	1.00			
5ets	B-202	1.95	0.645	0.19	0.22	1.00	1.00			
5ett	A-201	1.55	0.703	0.16	0.19	1.00	1.00			
5ett	A-202	1.55	0.717	0.16	0.19	1.00	0.99			
5ett	B-201	1.55	0.705	0.16	0.19	1.00	1.00			
5ett	B-202	1.55	0.710	0.16	0.19	1.00	1.00			
5etv	A-201	1.72	0.678	0.18	0.21	1.00	1.00			
5etv	A-202	1.72	0.687	0.18	0.21	1.00	1.00			
5etz	A-305	1.80	0.762	0.22	0.24	1.00	1.00			
5etz	D-304	1.80	0.836	0.22	0.24	1.00	1.00			
5eub	A-303	1.81	0.667	0.17	0.19	1.00	0.94			
5exb	A-64	1.81	0.685	0.18	0.25	1.00	0.90			
5exb	E-64	1.81	0.671	0.18	0.25	1.00	0.87			
5exb	F-64	1.81	0.678	0.18	0.25	1.00	0.85			
5sexy	A-307	1.55	0.762	0.13	0.17	0.70	0.73			
5ey3	B-506	1.90	0.700	0.20	0.24	0.67	0.65			
5ez6	B-204	1.80	0.662	0.18	0.21	1.00	1.00			
5ezg	A-301	1.84	0.665	0.18	0.21	1.00	1.00			
5f00	A-504	1.95	0.642	0.22	0.26	1.00	0.97			
5f01	A-504	1.52	0.714	0.19	0.21	1.00	0.96			
5f03	A-301	1.94	0.656	0.16	0.20	1.00	0.89			
5f0c	A-301	1.87	0.663	0.20	0.23	1.00	0.97			
5f0x	B-503	1.60	0.731	0.17	0.20	0.90	0.75			
5f0x	B-504	1.60	0.708	0.17	0.20	1.00	0.89			
5f12	B-201	1.50	0.721	0.18	0.21	1.00	0.95			
5f1g	A-401	1.76	0.677	0.17	0.19	1.00	0.90			
5f38	D-401	1.90	0.670	0.20	0.24	1.00	0.70			
5f41	A-1003	2.00	0.634	0.19	0.22	1.00	0.93			
5f6d	A-201	1.55	0.763	0.17	0.20	0.82	0.79			
5f6l	A-4001	1.90	0.666	0.17	0.21	1.00	0.91			
5f76	A-301	1.95	0.655	0.17	0.19	1.00	0.93			
5f76	B-301	1.95	0.648	0.17	0.19	1.00	0.97			
5f76	C-301	1.95	0.662	0.17	0.19	1.00	0.89			
5f7x	A-301	1.77	0.688	0.16	0.19	1.00	0.88			
5f7x	B-301	1.77	0.715	0.16	0.19	1.00	0.88			
5f7x	C-301	1.77	0.703	0.16	0.19	1.00	0.98			
5f8f	C-400	1.90	0.693	0.19	0.22	1.00	0.85			
5f9e	B-1001	2.00	0.643	0.20	0.23	1.00	0.95			
5fbc	A-601	1.75	0.685	0.13	0.18	0.80	0.71			
5fc4	A-401	1.50	0.715	0.16	0.20	1.00	1.00			
5fep	A-407	1.45	0.744	0.16	0.19	1.00	0.84			
5fez	A-408	1.35	0.750	0.12	0.14	1.00	0.99			
5ff0	A-409	1.49	0.724	0.15	0.17	1.00	0.94			
5ff2	A-408	1.47	0.728	0.17	0.19	1.00	0.98			
5fg6	A-705	1.10	0.819	0.18	0.20	1.00	0.78			
5fgu	A-66	1.90	0.654	0.18	0.20	1.00	0.96			
5fh1	A-703	1.55	0.710	0.18	0.22	1.00	0.95			

PDB	Ligand	Resolution (Å)	Twilight score	Rwork	Rfree	Occupancy (deposited)	Occupancy (qFit)	RMSD A->B (Å) (deposited)	RMSD A->B (qFit)	Best Fisher z improvement
5fh7	A-803	1.47	0.721	0.19	0.21	1.00	0.99			
5fh7	B-801	1.47	0.720	0.19	0.21	1.00	0.96			
5fh8	A-801	1.55	0.707	0.19	0.22	1.00	0.98			
5fh8	B-801	1.55	0.706	0.19	0.22	1.00	1.00			
5fhq	A-301	1.63	0.694	0.16	0.19	1.00	0.97			
5fhr	A-303	1.63	0.694	0.16	0.18	1.00	0.97			
5fhr	B-303	1.63	0.693	0.16	0.18	1.00	0.97			
5fhv	A-66	1.55	0.737	0.16	0.19		0.73			
5fjg	A-1270	2.00	0.685	0.17	0.22	1.00	1.00			
5fjg	A-1272	2.00	0.675	0.17	0.22	1.00	1.00			
5fjg	A-1274	2.00	0.711	0.17	0.22	1.00	0.92			
5fjg	A-1276	2.00	0.694	0.17	0.22	1.00	0.94			
5fkl	A-222	1.90	0.661	0.22	0.27	1.00	0.94			
5fkm	A-222	1.63	0.699	0.17	0.21	1.00	0.98			
5fkn	A-1209	1.80	0.676	0.22	0.26	1.00	0.92			
5fkn	B-1209	1.80	0.693	0.22	0.26	1.00	0.91			
5fko	A-1209	1.85	0.687	0.21	0.26	1.00	0.86			
5fl0	A-1718	1.95	0.649	0.20	0.23	1.00	0.86			
5fl1	A-1716	1.95	0.653	0.19	0.22	1.00	0.89			
5flj	A-301	1.82	0.720	0.16	0.21	0.82	0.81			
5flj	B-301	1.82	0.700	0.16	0.21	0.80	0.80			
5flj	D-301	1.82	0.685	0.16	0.21	0.85	0.84			
5flj	E-301	1.82	0.758	0.16	0.21	0.50	0.61			
5flj	I-301	1.82	0.687	0.16	0.21	0.81	0.83			
5flj	J-301	1.82	0.701	0.16	0.21	0.80	0.81			
5flj	K-301	1.82	0.704	0.16	0.21	0.76	0.76			
5flj	L-301	1.82	0.726	0.16	0.21	0.74	0.73			
5flt	A-1264	1.67	0.696	0.15	0.20	1.00	0.91			
5fns	A-1614	1.79	0.668	0.18	0.21	0.96	0.94			
5fnt	A-1615	1.79	0.664	0.17	0.20	1.00	0.92			
5foe	A-1428	1.98	0.637	0.20	0.25	1.00	0.93			
5fok	A-1723	1.90	0.662	0.19	0.21	1.00	1.00			
5fok	A-1724	1.90	0.679	0.19	0.21	1.00	0.98			
5fol	A-1544	1.77	0.679	0.20	0.23	1.00	0.94			
5fp1	A-1718	1.94	0.671	0.16	0.18	1.00	1.00			
5fp1	A-1719	1.94	0.710	0.16	0.18	1.00	0.86			
5fp1	A-1721	1.94	0.708	0.16	0.18	1.00	0.87			
5fp1	A-1723	1.94	0.672	0.16	0.18	1.00	1.00			
5fp1	A-1724	1.94	0.686	0.16	0.18	1.00	0.88			
5fp8	A-1341	1.98	0.642	0.16	0.21	1.00	0.82			
5fq5	A-1546	1.94	0.644	0.18	0.22	1.00	1.00			
5fq7	A-1546	1.99	0.648	0.19	0.23	1.00	0.94			
5fqv	A-1546	1.74	0.685	0.19	0.23	1.00	0.99			
5fra	A-201	2.00	0.633	0.18	0.21	1.00	0.96			
5fsx	B-1262	2.00	0.641	0.21	0.25	1.00	0.90			
5ftb	A-1434	1.38	0.738	0.17	0.18	1.00	0.90			
5ful	A-1446	1.89	0.650	0.17	0.19	1.00	0.95			
5fvn	A-403	1.45	0.933	0.16	0.18	1.00	1.00			
5fvn	A-404	1.45	0.819	0.16	0.18	1.00	1.00			
5fvn	A-405	1.45	0.781	0.16	0.18	1.00	1.00			
5fvn	A-406	1.45	0.920	0.16	0.18	1.00	1.00			
5fvn	A-410	1.45	0.805	0.16	0.18	1.00	1.00			
5fvn	A-414	1.45	0.759	0.16	0.18	1.00	0.67			
5fvn	A-417	1.45	0.781	0.16	0.18	1.00	0.82			
5fvn	A-419	1.45	0.841	0.16	0.18	1.00	0.89			
5fvn	A-420	1.45	0.922	0.16	0.18	1.00	0.90			
5fvn	B-403	1.45	0.812	0.16	0.18	1.00	0.77			
5fvn	B-405	1.45	0.826	0.16	0.18	1.00	1.00			
5fvn	B-407	1.45	0.758	0.16	0.18	1.00	0.78			
5fvn	B-412	1.45	0.754	0.16	0.18	1.00	0.93			
5fvn	B-413	1.45	0.813	0.16	0.18	1.00	0.80			

PDB	Ligand	Resolution (Å)	Twilight score	Rwork	Rfree	Occupancy (deposited)	Occupancy (qFit)	RMSD A->B (Å) (deposited)	RMSD A->B (qFit)	Best Fisher z improvement
5fvn	B-415	1.45	0.868	0.16	0.18	1.00	1.00			
5fvn	C-401	1.45	0.836	0.16	0.18	1.00	1.00			
5fvn	C-402	1.45	0.828	0.16	0.18	1.00	0.89			
5fvn	C-403	1.45	0.781	0.16	0.18	1.00	1.00			
5fvn	C-404	1.45	0.821	0.16	0.18	1.00	1.00			
5fvn	C-405	1.45	0.769	0.16	0.18	1.00	0.98			
5fvn	C-406	1.45	0.817	0.16	0.18	1.00	0.92			
5fvn	C-409	1.45	0.796	0.16	0.18	1.00	1.00			
5fvn	C-420	1.45	0.736	0.16	0.18	1.00	0.95			
5fvn	C-422	1.45	0.800	0.16	0.18	1.00	0.93			
5fvn	C-430	1.45	0.772	0.16	0.18	1.00	0.97			
5fvn	D-403	1.45	0.850	0.16	0.18	1.00	1.00			
5fvn	D-406	1.45	0.876	0.16	0.18	1.00	1.00			
5fvn	D-407	1.45	0.845	0.16	0.18	1.00	0.90			
5fvn	D-409	1.45	0.784	0.16	0.18	1.00	0.73			
5fvn	D-414	1.45	0.937	0.16	0.18	1.00	0.80			
5fvn	D-415	1.45	0.884	0.16	0.18	1.00	1.00			
5fvn	D-416	1.45	0.842	0.16	0.18	1.00	0.91			
5fvn	D-426	1.45	0.767	0.16	0.18	1.00	0.82			
5fvn	D-427	1.45	0.791	0.16	0.18	1.00	0.88			
5fvn	D-428	1.45	0.810	0.16	0.18	1.00	0.86			
5fvn	D-430	1.45	0.850	0.16	0.18	1.00	0.99			
5fvn	E-401	1.45	0.842	0.16	0.18	1.00	1.00			
5fvn	E-405	1.45	0.760	0.16	0.18	1.00	0.80			
5fvn	E-408	1.45	0.754	0.16	0.18	1.00	0.85			
5fvn	E-409	1.45	0.770	0.16	0.18	1.00	0.92			
5fvn	E-410	1.45	0.773	0.16	0.18	1.00	0.91			
5fvn	E-412	1.45	0.839	0.16	0.18	1.00	0.89			
5fvn	F-401	1.45	0.755	0.16	0.18	1.00	1.00			
5fvn	F-402	1.45	0.800	0.16	0.18	1.00	1.00			
5fvn	F-413	1.45	0.752	0.16	0.18	1.00	0.89			
5fvn	F-421	1.45	0.748	0.16	0.18	1.00	0.87			
5fvn	F-425	1.45	0.826	0.16	0.18	1.00	0.89			
5fvs	A-760	1.95	0.643	0.19	0.23	1.00	0.88			
5fvs	B-760	1.95	0.647	0.19	0.23	1.00	0.91			
5fvt	A-760	1.83	0.665	0.17	0.21	1.00	0.91			
5fvt	B-760	1.83	0.663	0.17	0.21	1.00	0.93			
5fvt	B-800	1.83	0.677	0.17	0.21	1.00	0.92			
5fw0	A-760	1.80	0.675	0.19	0.23	1.00	0.85			
5fw0	B-760	1.80	0.691	0.19	0.23	1.00	0.90			
5g09	A-1475	1.90	0.646	0.17	0.20	1.00	1.00			
5g09	D-1476	1.90	0.647	0.17	0.20	1.00	1.00			
5g0a	B-1298	1.70	0.680	0.17	0.20	1.00	0.93			
5g0a	C-1298	1.70	0.684	0.17	0.20	1.00	0.93			
5g0a	D-1298	1.70	0.682	0.17	0.20	1.00	0.89			
5g0n	A-760	1.94	0.644	0.18	0.22	1.00	0.93			
5g0n	B-760	1.94	0.645	0.18	0.22	1.00	0.93			
5g28	A-1272	1.57	0.775	0.15	0.19	1.00	1.00			
5g2d	A-1267	1.80	0.737	0.18	0.21	1.00	1.00			
5g2d	A-1269	1.80	0.739	0.18	0.21	1.00	1.00			
5g2g	A-1129	1.60	0.766	0.20	0.23	1.00	0.86			
5g2g	B-1129	1.60	0.754	0.20	0.23	1.00	0.83			
5g2p	C-2000	1.89	0.649	0.16	0.20	1.00	1.00			
5g2p	D-2000	1.89	0.647	0.16	0.20	1.00	1.00			
5g3w	B-377	1.60	0.840	0.13	0.17	0.60	0.52			
5g3w	D-373	1.60	0.851	0.13	0.17	0.50	0.50			
5g4i	A-1441	1.50	0.730	0.15	0.18	1.00	0.88			
5g4i	B-1440	1.50	0.723	0.15	0.18	1.00	0.86			
5g4r	A-1739	1.96	0.643	0.20	0.24	1.00	0.99			
5g4r	B-1739	1.96	0.643	0.20	0.24	1.00	0.97			
5g4r	C-1739	1.96	0.654	0.20	0.24	1.00	0.91			

PDB	Ligand	Resolution (Å)	Twilight score	Rwork	Rfree	Occupancy (deposited)	Occupancy (qFit)	RMSD A->B (Å) (deposited)	RMSD A->B (qFit)	Best Fisher z improvement
5g4r	D-1739	1.96	0.645	0.20	0.24	1.00	0.93			
5g54	A-1269	2.00	0.706	0.18	0.23	1.00	1.00			
5g54	A-1272	2.00	0.726	0.18	0.23	1.00	1.00			
5g54	A-1274	2.00	0.704	0.18	0.23	1.00	1.00			
5g54	A-1277	2.00	0.643	0.18	0.23	1.00	1.00			
5g68	A-905	1.63	0.763	0.16	0.19	1.00	0.88			
5g6a	A-904	1.92	0.663	0.16	0.19	1.00	0.97			
5g6b	A-904	1.80	0.676	0.16	0.20	1.00	0.96			
5g6h	A-902	1.91	0.754	0.16	0.19	1.00	0.90			
5g6k	A-902	1.95	0.749	0.17	0.22	1.00	0.96			
5g6m	A-904	1.77	0.678	0.16	0.20	1.00	0.96			
5ggk	A-301	1.30	0.787	0.15	0.18	1.00	0.97			
5ggk	B-301	1.30	0.778	0.15	0.18	1.00	0.96			
5ggl	B-301	1.27	0.816	0.15	0.16	1.00	1.00			
5gmd	A-1001	1.50	0.714	0.17	0.19	1.00	0.91			
5gmd	A-1003	1.50	0.742	0.17	0.19	1.00	0.73			
5gme	A-1001	1.70	0.678	0.17	0.20	1.00	0.91			
5gme	A-1002	1.70	0.767	0.17	0.20	1.00	0.81			
5gme	A-1003	1.70	0.692	0.17	0.20	1.00	0.89			
5gy7	A-401	1.43	0.730	0.13	0.16	1.00	1.00			
5gy7	B-401	1.43	0.729	0.13	0.16	1.00	1.00			
5gzg	A-201	2.00	0.667	0.20	0.26	1.00	0.97			
5h8q	B-302	1.90	0.649	0.18	0.21	1.00	0.96			
5ha7	B-402	1.65	0.724	0.17	0.20	0.60	0.64			
5hae	A-202	2.00	0.653	0.15	0.20	1.00	0.88			
5hd0	A-502	1.65	0.696	0.20	0.23	1.00	0.96			
5hd0	B-502	1.65	0.694	0.20	0.23	1.00	0.96			
5hdj	B-401	1.89	0.647	0.17	0.21	1.00	1.00			
5hdu	B-502	1.58	0.707	0.19	0.21	1.00	0.95			
5hdv	A-501	1.71	0.686	0.18	0.20	1.00	0.96			
5hdv	B-502	1.71	0.683	0.18	0.20	1.00	0.98			
5he4	B-502	1.53	0.726	0.20	0.22	1.00	0.96			
5he7	A-501	1.71	0.692	0.19	0.22	1.00	0.94			
5he7	B-501	1.71	0.686	0.19	0.22	1.00	0.98			
5hgp	A-301	1.95	0.672	0.19	0.22	0.17	0.85			
5hgt	A-202	1.75	0.671	0.17	0.21	1.00	0.99			
5hjm	A-401	1.76	0.677	0.18	0.20	1.00	0.98			
5hk9	A-401	1.80	0.803	0.17	0.20	0.56	0.36			
5hm0	A-201	1.39	0.760	0.19	0.23	1.00	0.92			
5hmz	A-1003	1.99	0.632	0.18	0.21	1.00	0.95			
5hq8	A-507	1.72	0.680	0.17	0.20	1.00	0.97			
5hqe	A-402	1.62	0.700	0.16	0.18	1.00	1.00			
5hr5	A-602	1.82	0.655	0.14	0.16	1.00	0.98			
5hr5	A-604	1.82	0.657	0.14	0.16	1.00	0.98			
5hrv	A-801	1.70	0.691	0.18	0.21	1.00	0.91			
5hrx	A-803	1.73	0.683	0.21	0.25	1.00	0.96			
5hs2	A-301	1.90	0.647	0.20	0.25	1.00	0.96			
5hsj	B-702	1.90	0.653	0.17	0.21	1.00	1.00			
5htz	A-501	1.95	0.641	0.20	0.23	1.00	0.98			
5htz	B-501	1.95	0.640	0.20	0.23	1.00	0.98			
5hu0	A-502	1.83	0.659	0.17	0.20	1.00	0.99			
5hu0	B-502	1.83	0.659	0.17	0.20	1.00	0.97			
5hu1	A-501	1.50	0.723	0.19	0.20	1.00	0.97			
5hu1	B-501	1.50	0.721	0.19	0.20	1.00	0.95			
5hvt	A-202	1.75	0.680	0.18	0.20	1.00	0.93			
5hvt	B-202	1.75	0.678	0.18	0.20	1.00	0.94			
5hx1	B-201	1.80	0.662	0.17	0.21	1.00	1.00			
5hyl	A-201	1.80	0.668	0.16	0.21	1.00	0.97			
5hz8	A-200	1.12	0.803	0.14	0.17	1.00	0.96			
5hzc	A-501	2.00	0.762	0.22	0.27	1.00	0.82			
5hzx	A-201	1.90	0.650	0.18	0.24	1.00	1.00			

PDB	Ligand	Resolution (Å)	Twilight score	Rwork	Rfree	Occupancy (deposited)	Occupancy (qFit)	RMSD A->B (Å) (deposited)	RMSD A->B (qFit)	Best Fisher z improvement
5hzx	B-201	1.90	0.650	0.18	0.24	1.00	1.00			
5hzz	C-201	1.80	0.664	0.16	0.21	1.00	0.99			
5hzz	D-201	1.80	0.662	0.16	0.21	1.00	1.00			
5i0h	A-801	1.80	0.659	0.17	0.19	1.00	1.00			
5i0h	B-801	1.80	0.662	0.17	0.19	1.00	0.95			
5i0j	B-201	1.80	0.663	0.17	0.21	1.00	1.00			
5i29	A-1701	1.21	0.787	0.20	0.22	1.00	1.00			
5i2h	A-501	1.55	0.886	0.16	0.20	1.00	0.75			
5i2h	B-501	1.55	0.869	0.16	0.20	1.00	0.74			
5i3v	A-404	1.62	0.722	0.21	0.23	1.00	0.99			
5i49	A-702	1.80	0.669	0.17	0.21	1.00	0.83			
5i4f	A-301	1.55	0.751	0.17	0.19	0.50	0.86			
5i4n	A-1000	1.54	0.708	0.17	0.19	1.00	0.96			
5i5v	A-401	1.94	0.640	0.17	0.23	1.00	0.93			
5i5x	A-401	1.65	0.687	0.18	0.22	1.00	0.95			
5i5x	A-402	1.65	0.700	0.18	0.22	1.00	0.81			
5i5x	B-402	1.65	0.709	0.18	0.22	1.00	0.76			
5i5y	A-402	1.81	0.664	0.15	0.19	1.00	0.97			
5i5y	B-401	1.81	0.660	0.15	0.19	1.00	0.94			
5i6d	A-401	1.64	0.693	0.16	0.19	1.00	1.00			
5i6d	A-402	1.64	0.694	0.16	0.19	1.00	1.00			
5i6d	B-401	1.64	0.691	0.16	0.19	1.00	0.97			
5i6d	B-402	1.64	0.695	0.16	0.19	1.00	1.00			
5i6d	C-401	1.64	0.694	0.16	0.19	1.00	0.94			
5i6d	C-402	1.64	0.703	0.16	0.19	1.00	0.98			
5i6d	D-401	1.64	0.688	0.16	0.19	1.00	0.99			
5i6d	D-402	1.64	0.702	0.16	0.19	1.00	1.00			
5i6w	A-202	1.90	0.648	0.18	0.24	1.00	0.99			
5i7r	A-401	1.73	0.687	0.17	0.21	1.00	0.96			
5i7r	B-401	1.73	0.677	0.17	0.21	1.00	0.96			
5i7u	A-812	1.95	0.638	0.15	0.19	1.00	1.00			
5i7u	B-812	1.95	0.638	0.15	0.19	1.00	0.95			
5i80	A-201	1.45	0.738	0.15	0.20	1.00	0.97			
5i83	A-1202	1.35	0.763	0.14	0.19	1.00	1.00			
5i90	B-501	1.22	0.777	0.14	0.16	1.00	0.97			
5i9o	A-202	1.95	0.637	0.20	0.24	1.00	1.00			
5i9o	B-202	1.95	0.641	0.20	0.24	1.00	1.00			
5i9p	A-202	1.85	0.655	0.19	0.23	1.00	1.00			
5i9w	A-1001	1.36	0.795	0.17	0.18	1.00	0.81			
5ia2	A-1001	1.62	0.703	0.16	0.20	1.00	0.99			
5ibd	A-407	1.77	0.673	0.15	0.19	1.00	0.99			
5ice	A-401	1.60	0.695	0.16	0.20	1.00	1.00			
5ice	A-402	1.60	0.702	0.16	0.20	1.00	1.00			
5icf	A-401	1.80	0.662	0.16	0.19	1.00	1.00			
5icf	A-402	1.80	0.731	0.16	0.19	0.80	0.62			
5icm	A-303	1.68	0.701	0.16	0.19	1.00	0.96			
5ie2	A-601	1.85	0.654	0.15	0.19	0.84	0.94			
5ie2	B-601	1.85	0.653	0.15	0.19	0.60	0.91			
5ie3	B-601	1.90	0.661	0.16	0.21	1.00	0.98			
5if9	A-1001	1.80	0.660	0.16	0.19	1.00	0.93			
5if9	B-1001	1.80	0.664	0.16	0.19	1.00	0.89			
5ifi	A-701	1.95	0.644	0.19	0.21	1.00	0.97			
5ifi	C-701	1.95	0.673	0.19	0.21	1.00	0.88			
5igb	A-202	1.80	0.663	0.19	0.23	1.00	0.98			
5igd	A-202	1.80	0.663	0.19	0.23	1.00	0.99			
5ige	A-202	1.80	0.663	0.19	0.21	1.00	0.96			
5igg	A-202	1.70	0.679	0.20	0.24	1.00	0.98			
5igk	A-202	1.70	0.684	0.16	0.20	1.00	0.95			
5ign	B-201	1.70	0.683	0.21	0.24	1.00	1.00			
5ilw	A-802	1.98	0.641	0.16	0.21	1.00	0.95			
5in3	A-402	1.73	0.692	0.20	0.23	1.00	0.93			

PDB	Ligand	Resolution (Å)	Twilight score	Rwork	Rfree	Occupancy (deposited)	Occupancy (qFit)	RMSD A->B (Å) (deposited)	RMSD A->B (qFit)	Best Fisher z improvement
5in3	B-402	1.73	0.680	0.20	0.23	1.00	0.88			
5ioc	A-201	1.90	0.649	0.18	0.24	1.00	0.98			
5iod	A-201	1.60	0.700	0.19	0.23	1.00	0.97			
5ioq	D-302	1.93	0.649	0.17	0.20	1.00	0.97			
5ior	A-302	1.95	0.637	0.16	0.19	1.00	0.99			
5ior	A-303	1.95	0.797	0.16	0.19	1.00	0.86			
5iru	C-202	2.00	0.646	0.22	0.27	1.00	0.86			
5ism	A-811	2.00	0.641	0.17	0.20	1.00	1.00			
5isr	A-202	1.90	0.648	0.18	0.24	1.00	0.97			
5iu8	A-2409	2.00	0.740	0.18	0.20	1.00	1.00			
5iu8	A-2412	2.00	0.761	0.18	0.20	1.00	0.98			
5iu8	A-2414	2.00	0.717	0.18	0.20	1.00	1.00			
5iu8	A-2415	2.00	0.753	0.18	0.20	1.00	1.00			
5iu8	A-2420	2.00	0.778	0.18	0.20	1.00	1.00			
5iu8	A-2421	2.00	0.716	0.18	0.20	1.00	1.00			
5iv3	A-506	1.86	0.651	0.18	0.22	1.00	0.97			
5iv4	A-501	1.79	0.666	0.16	0.21	1.00	0.95			
5ive	A-601	1.78	0.671	0.18	0.21	1.00	0.98			
5ivf	A-601	1.68	0.704	0.17	0.20	1.00	0.96			
5ivv	A-601	1.85	0.662	0.17	0.20	1.00	0.95			
5ivy	A-601	1.45	0.739	0.19	0.21	1.00	0.93			
5iwg	C-403	1.66	0.711	0.19	0.21	1.00	0.92			
5iy5	C-301	2.00	0.645	0.17	0.21	1.00	1.00			
5iy5	C-307	2.00	0.700	0.17	0.21	1.00	1.00			
5iy5	P-301	2.00	0.646	0.17	0.21	1.00	0.98			
5iy5	T-103	2.00	0.641	0.17	0.21	1.00	1.00			
5iyz	C-501	1.80	0.659	0.17	0.20	1.00	0.98			
5iyz	D-501	1.80	0.668	0.17	0.20	1.00	0.95			
5iyz	F-402	1.80	0.691	0.17	0.20	1.00	0.96			
5j3u	A-501	1.80	0.661	0.17	0.20	1.00	1.00			
5j3u	A-502	1.80	0.665	0.17	0.20	1.00	1.00			
5j41	A-302	1.19	0.785	0.16	0.19	1.00	0.93			
5j41	B-302	1.19	0.786	0.16	0.19	1.00	0.92			
5j42	A-401	1.70	0.685	0.16	0.20	1.00	0.96			
5j42	B-401	1.70	0.691	0.16	0.20	1.00	0.98			
5j5r	A-401	1.60	0.715	0.17	0.19	1.00	0.83			
5j5r	A-402	1.60	0.704	0.17	0.19	1.00	0.87			
5ja7	A-301	1.61	0.767	0.18	0.22	1.00	0.83			
5jav	A-202	1.89	0.652	0.19	0.25	1.00	0.97			
5jaz	A-501	1.40	0.752	0.19	0.21	1.00	0.91			
5jbi	A-501	1.70	0.693	0.18	0.21	1.00	0.88			
5cj	A-303	1.76	0.688	0.18	0.23	0.80	0.79			
5cj	B-302	1.76	0.693	0.18	0.23	0.80	0.75			
5jcu	A-112	1.93	0.684	0.18	0.24	0.80	1.00			
5jcu	B-112	1.93	0.652	0.18	0.24	0.74	1.00			
5jcu	D-112	1.93	0.680	0.18	0.24	0.77	1.00			
5jcx	B-302	1.43	0.757	0.14	0.18	0.80	0.75			
5jcx	D-302	1.43	0.797	0.14	0.18	0.80	0.64			
5jdc	A-302	1.78	0.786	0.21	0.24	1.00	0.85			
5jdc	D-302	1.78	0.815	0.21	0.24	1.00	0.80			
5je2	A-301	1.52	0.712	0.13	0.15	1.00	1.00			
5je2	B-301	1.52	0.711	0.13	0.15	1.00	1.00			
5jf2	A-301	2.00	0.722	0.16	0.20	1.00	0.67			
5jjs	A-1004	1.65	0.691	0.17	0.20	1.00	0.95			
5jmy	A-807	2.00	0.637	0.19	0.23	1.00	0.96			
5joh	A-302	1.99	0.646	0.23	0.25	1.00	0.93			
5jq2	B-502	2.00	0.662	0.17	0.22	1.00	0.97			
5jrh	A-702	1.64	0.697	0.17	0.21	1.00	0.98			
5jrh	B-702	1.64	0.699	0.17	0.21	1.00	0.98			
5jtu	A-901	1.85	0.654	0.17	0.20	1.00	0.85			
5jtu	A-902	1.85	0.656	0.17	0.20	1.00	0.84			

PDB	Ligand	Resolution (Å)	Twilight score	Rwork	Rfree	Occupancy (deposited)	Occupancy (qFit)	RMSD A->B (Å) (deposited)	RMSD A->B (qFit)	Best Fisher z improvement
5k03	A-301	1.81	0.679	0.20	0.25	1.00	0.98			
5k0c	B-302	1.95	0.644	0.18	0.23	1.00	0.97			
5k0i	A-201	1.30	0.766	0.15	0.16	1.00	1.00			
5k0i	A-202	1.30	0.757	0.15	0.16	1.00	1.00			
5k0i	A-203	1.30	0.904	0.15	0.16	1.00	0.87			
5k1p	A-501	1.50	0.728	0.17	0.20	0.91	0.85			
5k1x	A-501	1.95	0.642	0.20	0.23	1.00	0.94			
5k2c	A-1207	1.90	0.701	0.17	0.21	1.00	1.00			
5k2c	A-1217	1.90	0.733	0.17	0.21	1.00	1.00			
5k2c	A-1218	1.90	0.770	0.17	0.21	1.00	1.00			
5k2c	A-1220	1.90	0.671	0.17	0.21	1.00	1.00			
5k2c	A-1224	1.90	0.794	0.17	0.21	1.00	1.00			
5k2d	A-1201	1.90	0.652	0.17	0.21	1.00	0.97			
5k2d	A-1216	1.90	0.673	0.17	0.21	1.00	1.00			
5k2d	A-1217	1.90	0.787	0.17	0.21	1.00	1.00			
5k2d	A-1218	1.90	0.731	0.17	0.21	1.00	1.00			
5k2d	A-1219	1.90	0.769	0.17	0.21	1.00	1.00			
5k2d	A-1222	1.90	0.743	0.17	0.21	1.00	1.00			
5k2d	A-1224	1.90	0.743	0.17	0.21	1.00	1.00			
5k4x	A-402	1.37	0.747	0.20	0.21	1.00	0.97			
5k7u	A-601	1.70	0.696	0.16	0.19	1.00	0.94			
5kb3	A-301	1.40	0.759	0.14	0.17	1.00	1.00			
5kda	A-501	2.00	0.691	0.19	0.24	1.00	0.95			
5kds	G-102	1.60	0.716	0.16	0.19	1.00	0.88			
5kit	B-501	1.60	0.718	0.14	0.18	1.00	0.98			
5kix	A-201	1.75	0.671	0.18	0.22	1.00	0.99			
5kok	A-403	1.79	0.671	0.16	0.20	1.00	0.96			
5kok	B-402	1.79	0.692	0.16	0.20	1.00	0.86			
5kp3	A-201	1.70	0.731	0.23	0.25	1.00	0.85			
5kp3	B-201	1.70	0.785	0.23	0.25	1.00	0.79			
5kp4	B-201	1.71	0.728	0.20	0.24	1.00	0.83			
5kpr	A-402	1.83	0.655	0.17	0.19	1.00	1.00			
5kqf	A-501	1.98	0.646	0.22	0.25	1.00	0.96			
5kqg	A-200	1.50	0.717	0.17	0.19	1.00	0.97			
5kr7	A-403	1.90	0.651	0.19	0.23	1.00	0.89			
5kr7	B-403	1.90	0.650	0.19	0.23	1.00	0.93			
5ktx	A-1201	1.27	0.777	0.17	0.17	1.00	0.87			
5kuk	A-510	2.00	0.690	0.20	0.23	1.00	0.88			
5kva	B-301	1.83	0.663	0.16	0.19	1.00	0.99			
5kwk	A-601	1.90	0.693	0.22	0.29	1.00	0.94			
5kwk	B-601	1.90	0.671	0.22	0.29	1.00	1.00			
5kyi	A-201	1.70	0.678	0.18	0.20	1.00	1.00			
5kyl	A-202	1.85	0.654	0.18	0.22	1.00	1.00			
5l6d	A-601	1.85	0.657	0.16	0.19	1.00	1.00			
5l6f	A-509	1.80	0.730	0.15	0.18	1.00	0.80			
5l6f	A-510	1.80	0.708	0.15	0.18	1.00	0.83			
5l6f	A-511	1.80	0.670	0.15	0.18	1.00	0.95			
5l6f	A-512	1.80	0.708	0.15	0.18	1.00	0.77			
5l7h	A-1101	1.84	0.666	0.19	0.22	1.00	0.98			
5l7t	A-303	1.98	0.661	0.16	0.19	1.00	0.81			
5l7w	A-303	1.76	0.694	0.15	0.19	0.87	0.86			
5l7y	A-303	1.91	0.701	0.14	0.16	0.80	0.85			
5l7y	A-304	1.91	0.674	0.14	0.16	1.00	0.96			
5l8u	A-2001	1.85	0.672	0.17	0.19	1.00	0.92			
5l9m	A-301	1.93	0.648	0.16	0.20	1.00	0.94			
5lat	A-502	1.90	0.651	0.15	0.17	1.00	0.97			
5lb3	E-502	1.80	0.667	0.20	0.23	1.00	0.94			
5lb5	B-504	2.00	0.637	0.24	0.28	1.00	0.92			
5lb6	A-502	1.70	0.677	0.15	0.17	1.00	1.00			
5fbe	A-502	1.75	0.673	0.16	0.18	1.00	1.00			
5le5	E-148	1.80	0.708	0.18	0.21	1.00	0.78			

PDB	Ligand	Resolution (Å)	Twilight score	Rwork	Rfree	Occupancy (deposited)	Occupancy (qFit)	RMSD A->B (Å) (deposited)	RMSD A->B (qFit)	Best Fisher z improvement
5lf1	S-148	2.00	0.685	0.18	0.21	1.00	0.71 / 0.21		0.72	
5lf4	E-148	1.99	0.657	0.18	0.22	1.00	0.58 / 0.26		0.61	
5lf4	U-161	1.99	0.657	0.18	0.22	1.00	0.89			
5lf4	U-47	1.99	0.688	0.18	0.22	1.00	0.21 / 0.22 / 0.45		0.52 / 0.95	
5lf7	S-148	2.00	0.663	0.18	0.21	1.00	0.52 / 0.43		0.51	
5iu	X-402	1.75	0.683	0.21	0.25	1.00	0.87			
5lmb	A-525	1.95	0.686	0.18	0.23	1.00	0.88			
5lmb	A-701	1.95	0.647	0.18	0.23	1.00	1.00			
5luu	A-203	1.61	0.720	0.17	0.21	1.00	0.84			
5lvl	A-401	1.40	0.749	0.15	0.18	1.00	0.99			
5lx6	A-1101	1.25	0.791	0.21	0.21	1.00	0.95			
5lx6	B-1101	1.25	0.778	0.21	0.21	1.00	0.95			
5m0o	C-502	1.80	0.695	0.18	0.22	1.00	1.00			
5m12	A-604	1.53	0.734	0.19	0.22	1.00	0.86			
5m96	B-501	1.77	0.678	0.19	0.21	1.00	1.00			
5maj	A-301	1.00	0.856	0.14	0.17	1.00	0.93			
5mf6	A-410	1.87	0.699	0.19	0.22	1.00	0.90			
5mf6	B-408	1.87	0.688	0.19	0.22	1.00	0.85			
5mn4	A-1001	1.50	0.717	0.18	0.21	1.00	0.98			
5syn	A-301	1.64	0.699	0.22	0.25	1.00	0.86			
5syt	A-507	2.00	0.663	0.22	0.25	1.00	0.94			
5syt	A-515	2.00	0.703	0.22	0.25	1.00	0.91			
5sz1	A-307	1.55	0.716	0.16	0.19	1.00	0.85			
5szy	C-200	2.00	0.631	0.20	0.21	1.00	1.00			
5tok	A-1304	1.70	0.683	0.17	0.19	1.00	0.98			
5t4f	A-812	1.90	0.647	0.16	0.19	1.00	1.00			
5t67	A-502	1.60	0.699	0.20	0.25	1.00	1.00			
5t6b	D-502	2.00	0.636	0.18	0.23	1.00	0.97			
5t6m	D-403	1.80	0.694	0.20	0.24	1.00	0.81			
5t77	A-516	2.00	0.774	0.19	0.21	1.00	0.82			
5t77	A-521	2.00	0.738	0.19	0.21	1.00	1.00			
5t77	A-531	2.00	0.687	0.19	0.21	1.00	1.00			
5t77	A-534	2.00	0.641	0.19	0.21	1.00	1.00			
5t77	A-536	2.00	0.713	0.19	0.21	1.00	0.91			
5t77	A-537	2.00	0.655	0.19	0.21	1.00	1.00			
5t77	A-538	2.00	0.727	0.19	0.21	1.00	1.00			
5t77	A-539	2.00	0.737	0.19	0.21	1.00	0.98			
5t77	A-540	2.00	0.667	0.19	0.21	1.00	1.00			
5t77	A-542	2.00	0.693	0.19	0.21	1.00	1.00			
5t77	A-546	2.00	0.701	0.19	0.21	1.00	1.00			
5t77	A-547	2.00	0.674	0.19	0.21	1.00	1.00			
5t77	A-551	2.00	0.709	0.19	0.21	1.00	1.00			
5t7i	A-401	2.00	0.658	0.19	0.22	1.00	0.92			
5t7s	A-201	1.90	0.662	0.15	0.18	1.00	0.85			
5t8s	A-402	1.70	0.714	0.15	0.17	0.73	0.68			
5t8s	B-402	1.70	0.683	0.15	0.17	1.00	0.93			
5tg5	A-301	1.75	0.685	0.18	0.21	1.00	0.84			
5tg6	A-301	1.78	0.668	0.17	0.19	1.00	0.94			
5ths	A-404	1.90	0.667	0.18	0.21	1.00	0.97			
5tiu	A-701	1.49	0.729	0.19	0.20	1.00	0.93			
5tk8	A-201	1.64	0.739	0.18	0.20	1.00	0.87			
5tk9	A-202	1.84	0.704	0.18	0.22	1.00	0.78			
5tkd	A-901	1.92	0.649	0.19	0.22	1.00	0.95			
5tt7	A-901	1.77	0.676	0.21	0.24	1.00	0.96			
5u5t	A-501	1.60	0.712	0.17	0.20	1.00	0.97			
5u5t	B-503	1.60	0.704	0.17	0.20	1.00	1.00			
5u62	A-504	1.90	0.660	0.17	0.21	1.00	1.00			
5u62	B-501	1.90	0.651	0.17	0.21	1.00	1.00			
5ucv	A-302	1.80	0.670	0.17	0.21	1.00	0.94			

PDBID	Ligand	Receptor	Ligand Code	Resolution (Å)	Occupancies (deposited re-refined)	Occupancies (qFit refined)	Occupancies (Manually edited refined)	R-work (deposited re-refined)	R-work (qFit refined)	R-work (manually edited refined)	R-free (deposited re-refined)	R-free (qFit refined)	R-free (manually edited refined)	Ligand Energy (kcal/mol) qFit confs relative to single conf
4ykq	A-301	AbbVie-CSAR_HSP90	4EO	1.91	1	0.45/0.55	---	0.1686	0.1667	---	0.2003	0.2013	---	0.03
4fv3	A-401	ERK2	EK6	2.2	0.51/0.49	0.22/0.26/0.36/0.15	0.46/0.54	0.183	0.1894	0.1864	0.2318	0.2364	0.2361	4.83 / 10.5
4ev4	A-401	ERK2	MER	1.30	1	0.43/0.57	0.35/0.65	0.1203	0.117	0.117	0.1352	0.1459	0.1462	4.21
5fsi	A-1157	MTH1	8DG	1.63	1	0.57/0.26/0.16	0.69/0.31	0.1969	0.198	0.196	0.2101	0.2133	0.2098	0.78 / 0.59
5ezx	A-501	BACE-1	5T5	1.90	1	0.32/0.36/0.32	---	0.1875	0.1844	---	0.2216	0.2244	---	3.75
5dlv	A-930	Autotaxin (ENPP2)	5D5	2.00	0.41/0.28/0.31	0.53/0.47	---	0.1979	0.198	---	0.2421	0.2456	---	5.07
5cfw	A-201	BRD4	53W	1.15	1	0.23/0.39/0.38	0.62/0.38	0.1577	0.1625	0.1616	0.1952	0.1992	0.1992	5.46 / 2.52
4nr5	A-1201	BRD4	2LL	1.66	1	0.00/0.41/0.59	0.66/0.34	0.1952	0.1962	0.1997	0.237	0.2346	0.2339	2.85 / 1.76
4bw3	A-1172	BRD4	9BM	1.5	1	0.39 / 0.49	---	0.1475	0.1453	---	0.1926	0.1923	---	1.57

PDB ID	Ligand	Ligand Code	Resolution (Å)	Occupancies (deposited)	Occupancies (qFit)	RMSD vs A conformer (Å) (deposited)	RMSD vs A conformer (Å) (qFit)	Z-scores
4zc9	A-4000	4MW	0.99	0.86	0.20 / 0.20 / 0.20 / 0.20 / 0.20		3.99 / 4.95 / 3.70 / 5.73	5.24
5ad2	A-1169	ETU	2.01	0.50 / 0.50	0.44 / 0.39	12.33	1.55	2.56
5dlz	A-201	5D1	1.7	1	0.20 / 0.20 / 0.20 / 0.20 / 0.20		1.77 / 4.80 / 8.46 / 12.28	2.54
5kj0	A-201	6TB	1.51	1	0.38 / 0.21 / 0.23		1.38 / 1.10	2.49
4whw	A-201	3OT	1.35	1	0.32 / 0.20 / 0.20 / 0.20		1.74 / 1.45 / 1.82	2.46
4hxl	A-201	1A9	1.52	1	0.32 / 0.23 / 0.20 / 0.20		1.47 / 1.78 / 1.23	2.42
5lj2	A-204	6XW	1.19	1	0.41 / 0.20 / 0.30		2.65 / 0.64	2.33
4uiz	A-1171	N1D	1.19	1	0.31 / 0.21 / 0.20		2.03 / 3.35	2.11
4hxs	A-201	1A3	1.43	0.5	0.33 / 0.20 / 0.29		2.46 / 3.03	1.95
4bw3	A-1172	9BM	1.5	1	0.39 / 0.49		2.17	1.84
5hls	A-201	62G	2.18	1	0.46 / 0.46		1.11	1.71
4hxr	A-201	1A4	1.53	1	0.46 / 0.42		0.89	1.53
4bw1	A-1172	S5B	1.4	1	0.44 / 0.24 / 0.28		2.30 / 2.25	1.52
5f63	A-201	5W2	1.45	1	0.36 / 0.20 / 0.24 / 0.20		2.52 / 1.89 / 3.37	1.43
4cl9	A-1170	IES	1.4	1	0.36 / 0.24 / 0.20 / 0.20		1.18 / 0.56 / 0.81	1.28
4qr5	A-201	BNM	1.41	0.50 / 0.50	0.20 / 0.20 / 0.20 / 0.20 / 0.20	2.9	3.00 / 3.54 / 1.44 / 2.95	1.23
5u2e	A-201	837	1.99	1	0.28 / 0.20 / 0.23 / 0.22		1.42 / 1.40 / 1.87	1.23
4hby	A-201	13F	1.59	0.35 / 0.30 / 0.35	0.28 / 0.24 / 0.35	1.03 / 3.46	3.61 / 1.13	1.21
5coi	A-201	55K	1.62	1	0.41 / 0.20 / 0.35		1.19 / 0.60	1.21
5ad3	B-1169	K6K	1.49	1	0.40 / 0.21 / 0.30		0.75 / 0.68	1.17
4hxo	A-201	1A6	1.76	1	0.62 / 0.26		3.33	1.15
4hxm	A-201	1A8	1.5	1	0.60 / 0.20 / 0.20		3.41 / 3.44	1.14
5d24	A-201	L26	1.65	1	0.38 / 0.20 / 0.33		0.70 / 0.69	1.14
5cqf	A-201	EB3	1.6	1	0.51 / 0.44		1.14	1.13
4o75	A-201	2RC	1.55	1	0.30 / 0.24 / 0.20		0.83 / 0.94	1.06
4uiy	A-1172	5V2	1.3	0.50 / 0.50	0.47 / 0.42	0.45	0.67	1
4qr3	A-201	BNJ	1.37	1	0.64 / 0.22		3.87	0.99
5m39	A-201	7EA	1.38	1	0.49 / 0.23 / 0.25		0.83 / 2.29	0.95
2yel	A-1170	WSH	1.65	1	0.48 / 0.20 / 0.25		2.21 / 1.01	0.93
5khw	A-201	XNH	1.48	0.50 / 0.50	0.53 / 0.25	12.61	0.68	0.92
5a85	A-1169	78J	1.72	1	0.41 / 0.33 / 0.23		1.07 / 0.73	0.86
4bw2	A-1170	UTH	1.92	1	0.31 / 0.20 / 0.46		2.08 / 0.85	0.76
5ti4	A-201	7CM	1.62	1	0.44 / 0.29		1.41	0.72
4clb	A-1170	83T	1.6	1	0.54 / 0.21 / 0.24		1.19 / 1.05	0.7
5hq5	A-201	64Q	1.6	1	0.40 / 0.46		1.65	0.7
5dw2	A-201	5GD	1.12	0.70 / 0.30	0.58 / 0.20 / 0.20	2.56	0.75 / 0.70	0.68
5dlx	A-201	5D2	1.9	1	0.46 / 0.46		1.05	0.59
4o7b	A-201	2RJ	1.5	1	0.53 / 0.25		1.35	0.58
5bt4	A-201	2LO	1.5	1	0.65 / 0.21		0.79	0.57
5lj1	A-202	6XX	1.9	1	0.20 / 0.33 / 0.40		0.77 / 0.81	0.57
5fbx	A-201	5W4	1.85	1	0.68 / 0.29		0.98	0.56
5d3h	A-201	57G	1.7	1	0.51 / 0.20 / 0.22		1.29 / 1.03	0.55
5cy9	A-202	E0A	1.55	1	0.78 / 0.20		2.9	0.46
4o70	A-201	1QK	1.55	1	0.44 / 0.20 / 0.29		1.20 / 0.51	0.42
4lyw	A-1001	21Q	1.95	1	0.36 / 0.20 / 0.21 / 0.20		1.50 / 0.86 / 2.08	0.41
4qr4	A-201	BNK	1.28	1	0.67 / 0.20		1.27	0.41
5d3r	A-201	57C	2.2	1	0.32 / 0.30 / 0.34		0.70 / 1.23	0.35
5crm	A-203	EB5	1.99	1	0.68 / 0.22		0.48	0.31
4nuc	A-201	435	1.4	1	0.80 / 0.20		1.78	0.26
5d3j	A-201	L33	1.7	1	0.71 / 0.20		0.86	0.26
5d3t	A-201	56Y	1.93	1	0.69 / 0.20		0.8	0.26
3svf	A-1	WDR	1.98	1	0.69 / 0.21		1.72	0.24

PDB ID	Ligand	Ligand Code	Resolution (Å)	Occupancies (deposited)	Occupancies (qFit)	RMSD vs A conformer (Å) (deposited)	RMSD vs A conformer (Å) (qFit)	Z-scores
5cs8	A-201	EB8	1.62	1	0.63 / 0.27		0.79	0.24
5d26	A-201	L28	1.82	1	0.62 / 0.38		1.09	0.24
4yh3	A-201	Y80	1.6	0.8	0.57 / 0.20		0.63	0.23
5d3n	A-201	L40	2.15	1	0.34 / 0.30 / 0.30		0.85 / 0.56	0.21
5ti2	A-201	7CJ	1.65	1	0.57 / 0.20		1.37	0.2
5f62	A-201	5W1	1.35	1	0.20 / 0.23 / 0.28 / 0.20		0.64 / 0.88 / 1.13	0.19
5f60	A-201	5VZ	1.35	1	0.50 / 0.20 / 0.24		1.22 / 0.88	0.16
3p5o	A-1	EAM	1.6	1	0.72 / 0.23		0.46	0.14
5d3l	A-201	57F	1.5	1	0.70 / 0.20		0.47	0.14
4j0s	A-205	1H3	1.84	1	0.80 / 0.20		1.01	0.13
5acy	A-1172	9S3	2.01	1	0.34 / 0.36 / 0.30		0.98 / 0.84	0.13
3svg	A-169	ODR	1.68	1	0.97			
3u5j	A-1	08H	1.6	1	0.94			
3u5k	A-1	08J	1.8	1	0.87			
3u5l	A-1	08K	1.39	1	1			
3zyu	A-1173	1GH	1.5	1	1			
4bw4	A-1169	9B6	1.67	1	0.79			
4c66	A-1168	H4C	1.87	1	0.9			
4c67	A-1170	L5S	1.55	1	0.96			
4cfk	A-1170	LY2	1.55	1	0.94			
4cfl	A-1169	8DQ	1.32	1	1			
4e96.	A-201	0NS	1.92	1	0.97			
4f3i	A-203	0S6	1.4	1	1			
4hbx	A-201	14X	1.62	1	0.91			
4hxk	A-201	1AJ	1.61	1	0.87			
4lrg	A-201	1XB	2.21	1	0.94			
4men	A-202	25K	1.81	1	0.91			
4meo	A-203	DMS	1.72	1	0.79			
4mep	A-201	24Y	1.85	1	0.9			
4meq	A-202	25O	1.77	1	0.92			
4mr3	A-202	1K0	1.68	1	0.94			
4nud	A-201	NUD	1.2	1	0.93			
4nue	A-201	NUE	1.3	1	0.96			
4o71	A-201	CPB	1.36	1	0.96			
4o74	A-201	R78	1.45	1	0.9			
4o76	A-201	1M3	1.7	1	0.93			
4o77	A-201	2RE	2	1	0.97			
4o78	A-201	SAV	1.34	1	0.95			
4o7a	A-201	2RF	1.34	1	0.76			
4o7c	A-201	2RK	1.55	1	0.9			
4o7e	A-201	2RN	1.85	1	1			
4o7f	A-201	2RQ	1.8	1	0.92			
4ogi	A-202	R78	1.73	1	0.98			
4ogj	A-203	2TA	1.65	1	0.98			
4pce	A-302	2N0	1.29	1	0.93			
4pci	A-201	2NJ	1.25	1	1			
4qb3	A-201	30M	0.94	1	0.97			
4wiv	A-201	3P2	1.56	1	1			
4xy9	A-202	43U	1.83	1	0.93			
4xya	A-201	43S	2.05	1	1			
4z1q	A-201	558	1.4	1	0.89			
4z1s	A-201	559	1.06	1	0.96			

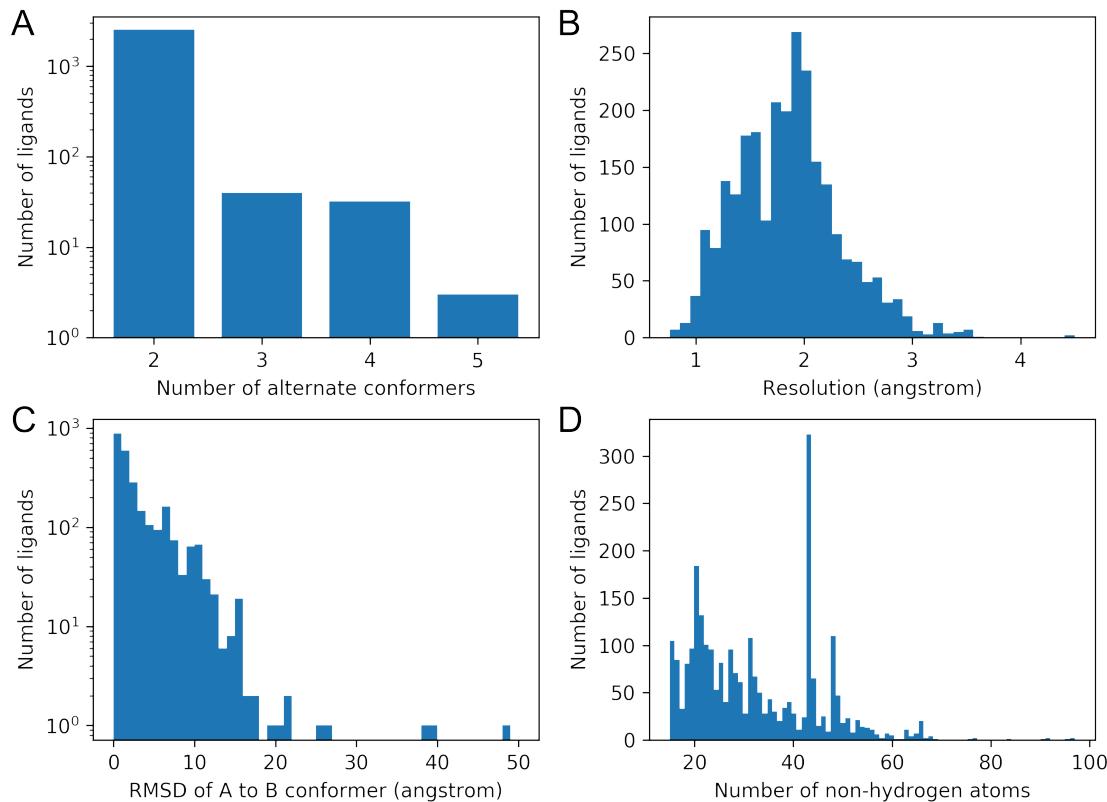
PDB ID	Ligand	Ligand Code	Resolution (Å)	Occupancies (deposited)	Occupancies (qFit)	RMSD vs A conformer (Å) (deposited)	RMSD vs A conformer (Å) (qFit)	Z-scores
4zw1	A-201	4V1	1.75	1	0.75			
5cpe	A-203	EB2	1.62	1	1			
5crz	A-204	EB7	2.12	1	0.91			
5d25	A-203	BU3	1.7	1	0.73			
5d3p	A-201	57E	1.95	1	1			
5dx4	A-201	E0C	2.3	1	0.95			
5egu	A-201	5NQ	2.21	1	1			
5ei4	A-202	5NV	1.05	0.5	0.43			
5eis	A-201	5OU	1.6	1	0.94			
5f5z	A-201	5VY	1.76	1	0.87			
5f61	A-203	5W0	1.45	1	0.97			
5hm0	A-201	62V	1.39	1	0.92			
5hq7	A-201	64S	1.9	1	0.89			
5igk	A-202	BMF	1.7	1	0.95			
5luu	A-203	77X	1.61	1	0.84			
5m3a	A-303	7E7.	1.65	1	0.93			
5ti3	A-205	7CG	1.7	1	0.68			
5ti5	A-201	7CN	1.83	1	0.91			
5ti6	A-201	7CO	1.7	1	0.82			
5ti7	A-201	7CQ	1.65	1	0.9			
5u28	A-201	82V	1.8	1	0.97			
5ula	A-201	5MJ	1.5	1	0.95			

## Supporting Information

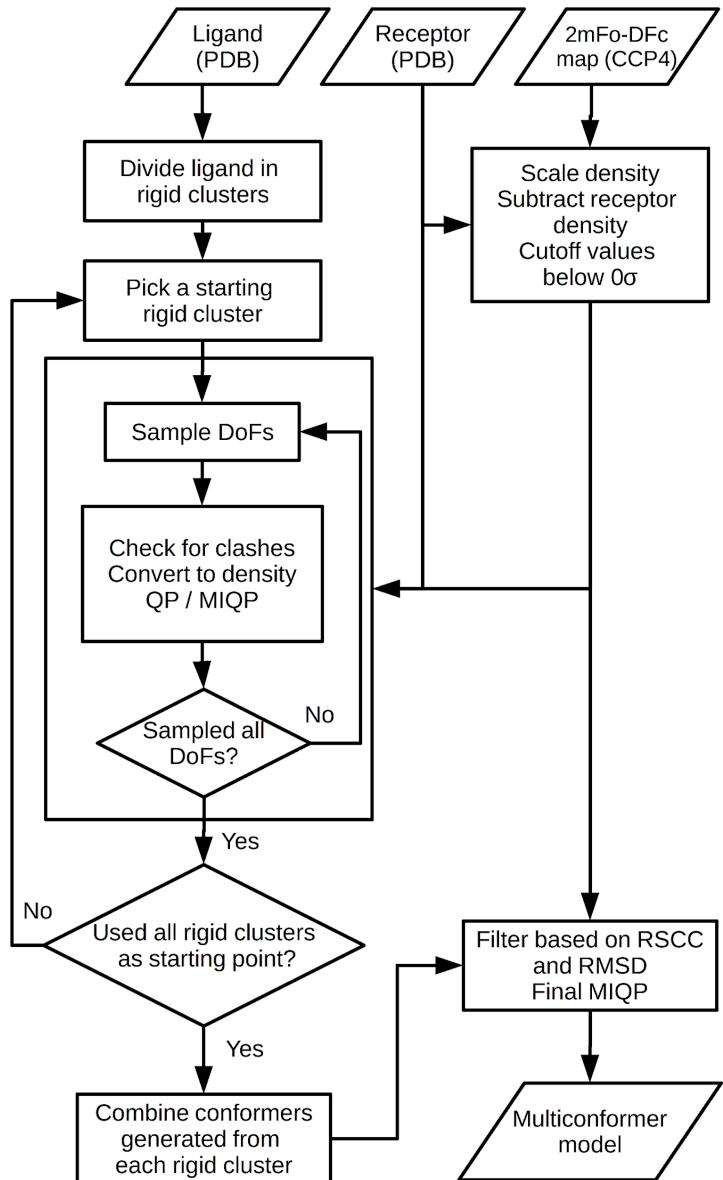
### *qFit-ligand* reveals widespread conformational heterogeneity of drug-like molecules in X-ray electron density maps

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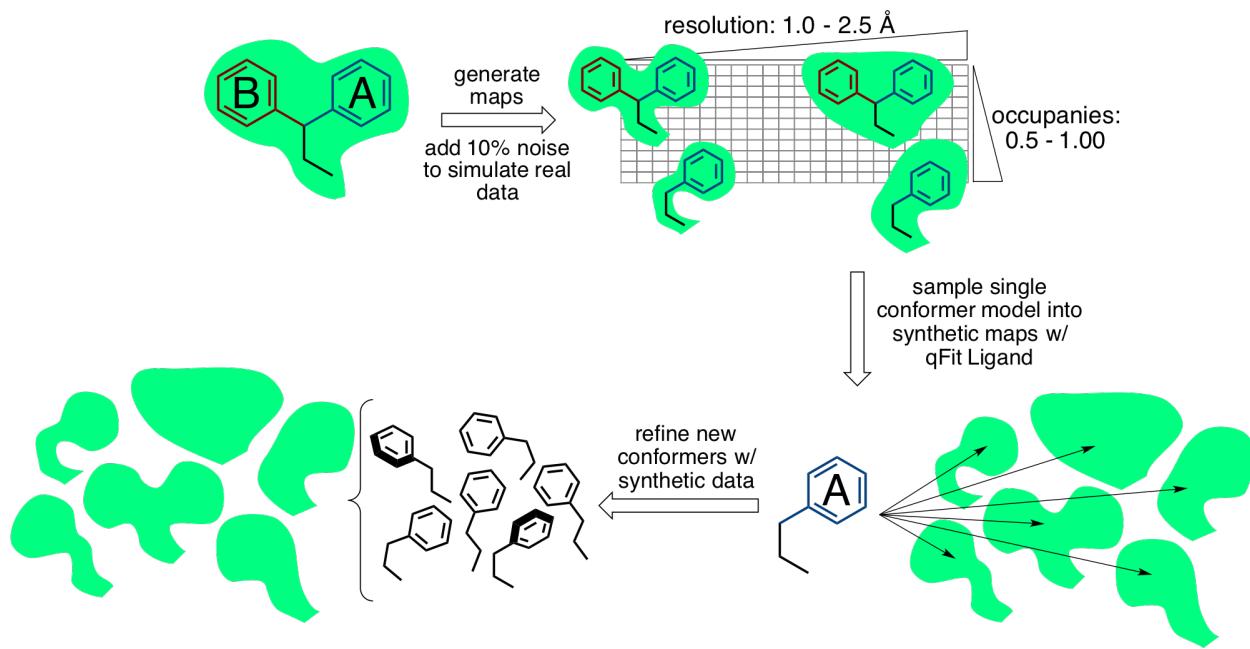
1. Schrödinger, New York, NY 10036, USA
2. Department of Bioengineering and Therapeutic Sciences, UCSF, San Francisco, CA 94158, USA
3. Department of Molecular and Cellular Physiology, Stanford University, Stanford, CA 94305, USA.
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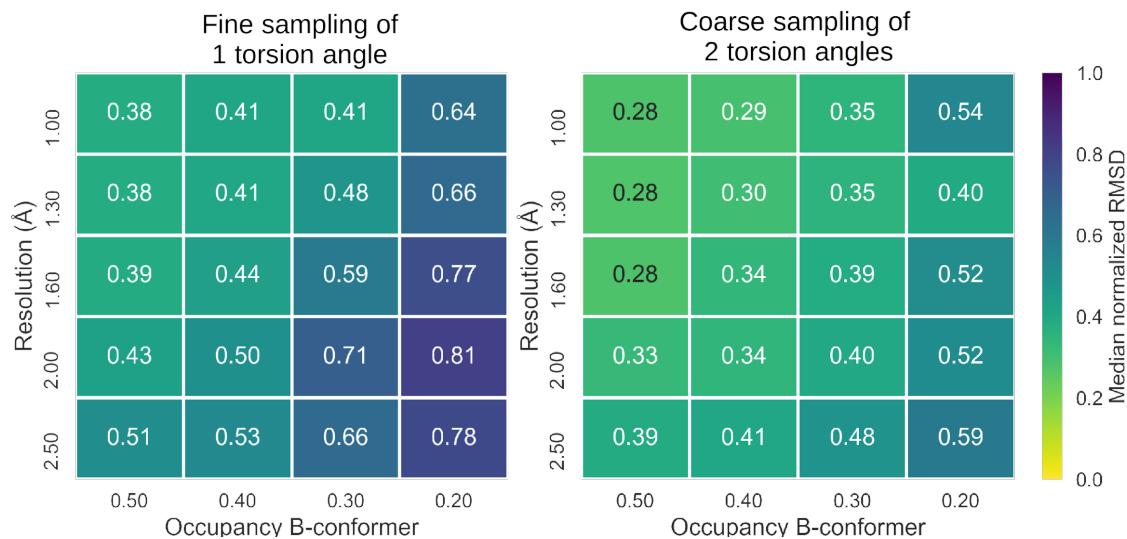
**Figure S1.** Overview of 2,611 multiconformer ligands deposited in the PDB as of June 2017. The most common ligands found were heme (240), NADP (48), and NAD<sup>+</sup> (46), while most other ligands only appear once (714) or twice (207 unique codes). A) Histogram of number of alternate conformers per ligand. The majority have two conformers (2,534), while less than 100 have three to five conformers. B) The resolution of the multi-conformer ligands ranges from 0.5 Å to 4.5 Å, with the mode at 2.0 Å. C) Histogram of RMSD between A and B conformer. Large RMSD values indicate alternate binding pockets instead of alternate conformations. D) Distribution of ligand size by the number of non-hydrogen atoms.



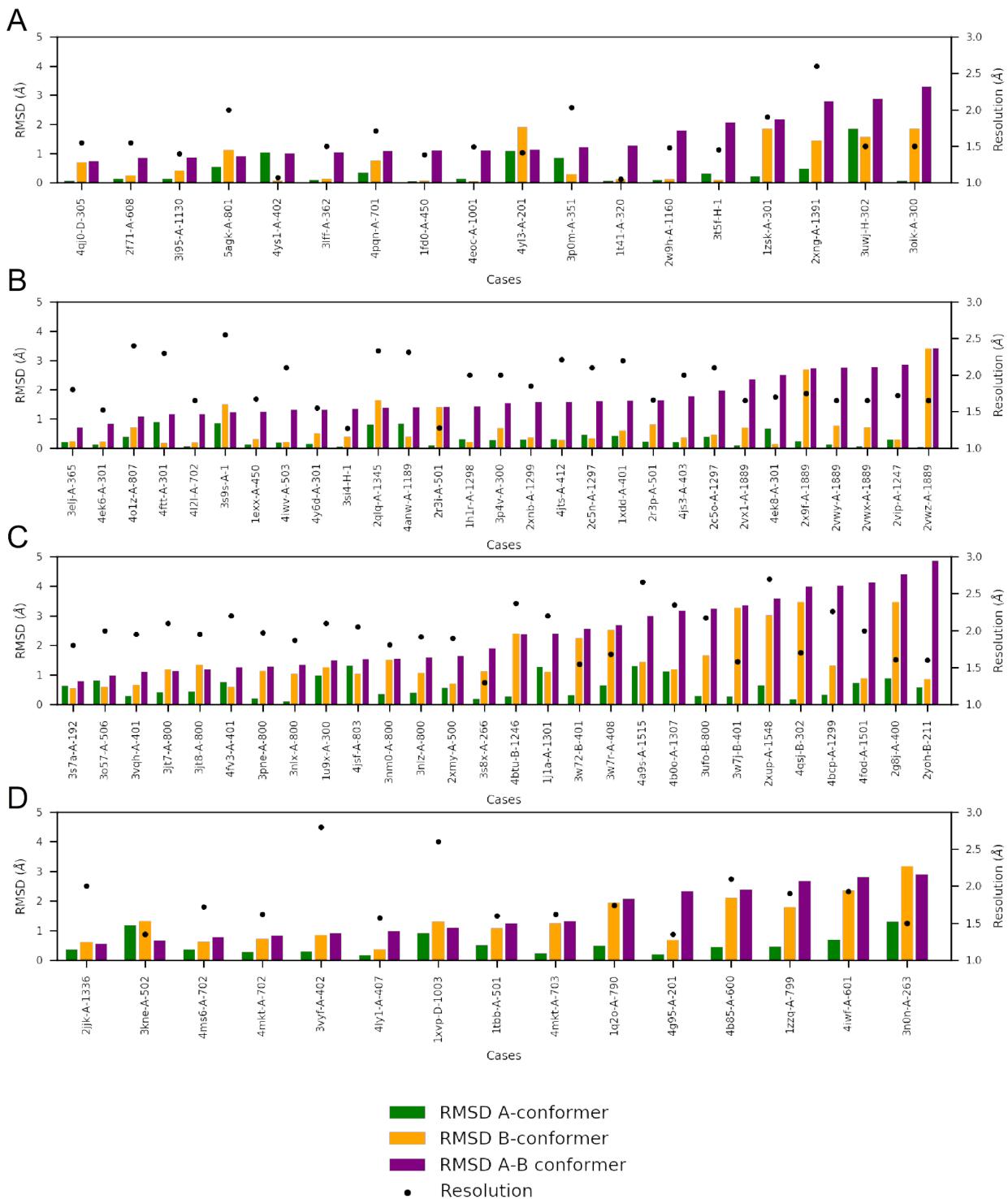
**Figure S2.** A detailed flowchart of the *qFit-ligand* algorithm. The algorithm first partitions the ligand into K rigid groups of atoms that are connected by rotatable bonds. It builds up the complete ligand starting from each rigid group in turn. In the first iteration, it performs a rigid body search for the rigid group. It checks for clashes and selects conformations and occupancies for the rigid group using QP/MIQP. It then samples dihedral angles of rigid groups connected to the selected initial rigid groups of atoms, and selects a subset of conformations including all rigid groups considered so far. It continues this process until all dihedral angles are sampled. It repeats the procedure starting from each of the K rigid groups. The up to 5K conformations starting from each rigid group are pooled, and a final filter is run to generate the final multi-conformer model.



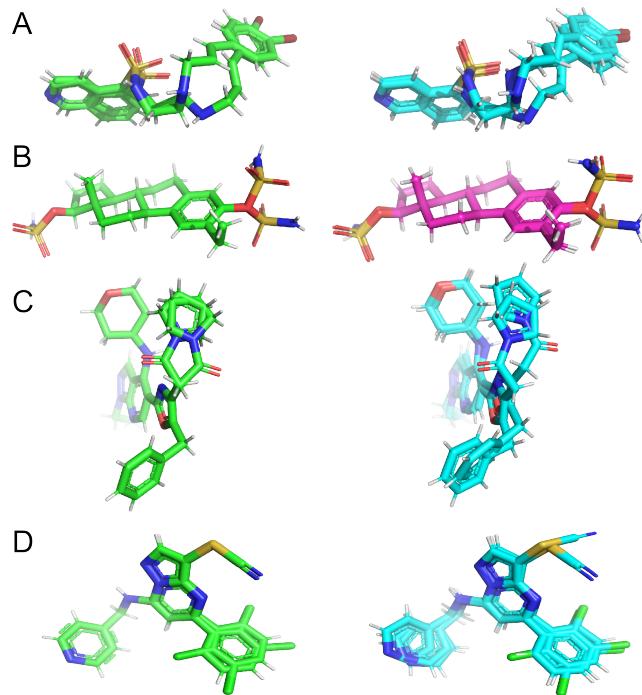
**Figure S3.** Generating simulated data for testing resolution and occupancy limits of *qFit-ligand*.



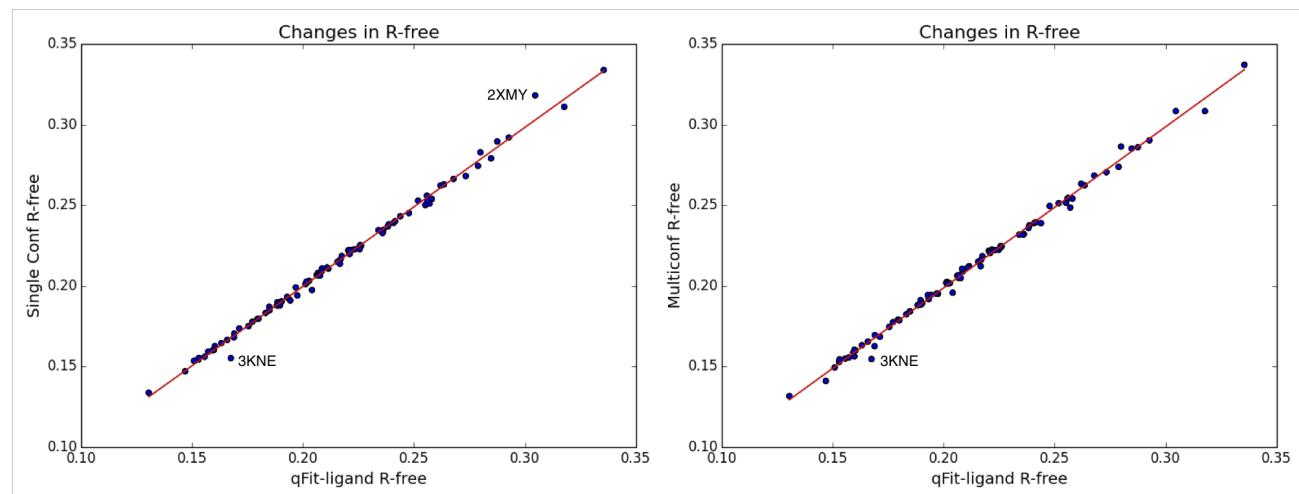
**Figure S4.** Performance of *qFit-ligand* before final rescoring round measured in median normalized RMSD when exhaustively sampling 1 torsion angle at a fine interval of 1 degree (left) and 2 torsion angles at a coarser interval of 6 degree (right).



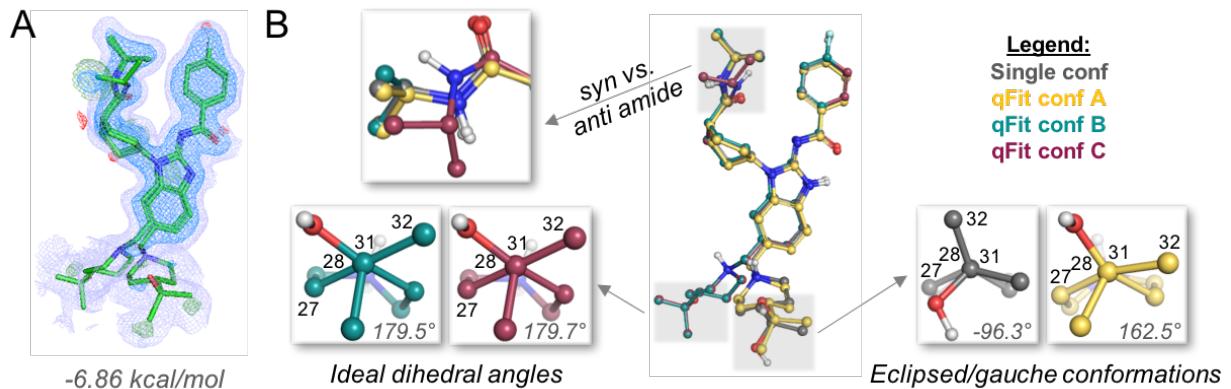
**Figure S5.** Barplots showing RMSD values for each case in the benchmark divided across the 4 categories (A: terminal end flips, B: ring flips, C: branching, D: disordered). Each case shows three bars, where the first two provide the RMSD between the final qFit-ligand and re-refined deposited A and B conformer, respectively, and the third bar shows the RMSD between the A and B conformer of the deposited structure. The black dot shown for each case indicates the resolution of the data. Cases are ordered by the height of the third bar.



**Figure S6.** Visual inspection of cases with  $nRMSD \sim 0.6$  suggest that their conformations are good starting points for further manual refinement. Left panels show the re-refined deposited multiconformer model, right panels show the refined *qFit-ligand* model with closest matched conformers. A) 3VQH branching case,  $nRMSD = 0.60$ ,  $RMSD = 0.66\text{\AA}$ . B) 3OIK terminal end flip case,  $nRMSD = 0.56$ ,  $RMSD = 0.83\text{\AA}$ . C) 3O57 branching case  $nRMSD = 0.59$ ,  $RMSD = 0.59\text{\AA}$ . D) 2R3P ring flip,  $nRMSD = 0.48$ ,  $RMSD = 0.79\text{\AA}$ .

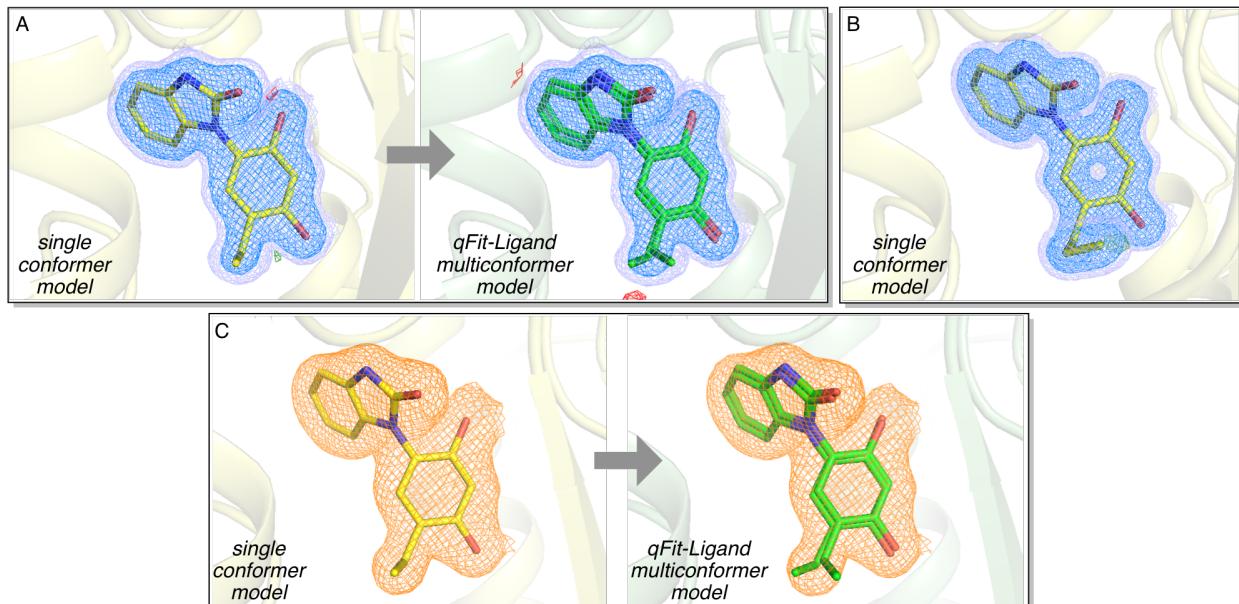


**Figure S7.** R-free values post-refinement of *qFit-ligand* multiconformer model vs. single conformer and deposited multiconformer models, respectively, from our benchmark dataset. Outliers are labeled.



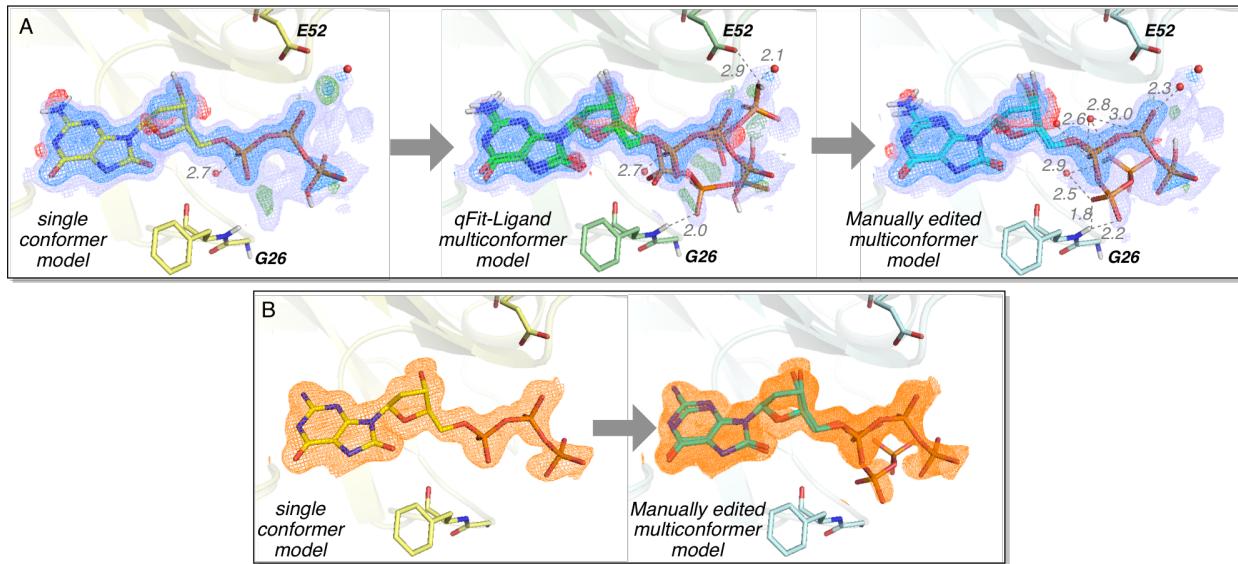
**Figure S8.** Branching ligand heterogeneity from the benchmark dataset (PDB ID 4FOD). A) Ligand conformations generated by *qFit-ligand* are significantly lower in energy (by ~7 kcal/mol) than the corresponding single conformer model. Electron densities are shown at  $1.5\sigma$  (blue) and  $0.3\sigma$  (purple). Positive (green) and negative (red) difference densities are shown at  $\pm 3.0\sigma$ . B) Evaluation of ligand conformations reveal that an *anti* amide conformation and ideal dihedral angles as opposed to *syn* amide conformation and eclipsed/gauche conformations help to significantly lower ligand conformational energies.

We examined HSP90 inhibitor CS301 (PDB ID 4YKQ) from the D3R dataset (**Figure S9A**). *qFit-ligand* detected two discrete conformations of the ethyl group in inhibitor CS301 (with occupancies split 45/55), which was hidden in the averaged electron density map (**Figure S9A** left panel). This terminal flip could be used as a design element for future ligands; for example, we imagine a derivative of the ligand with a cyclopropyl group in place of the ethyl group. Although this derivative was not synthesized, a derivative with a propyl group was found to occupy the space captured by our *qFit-ligand* multiconformer model (**Figure S9B**).

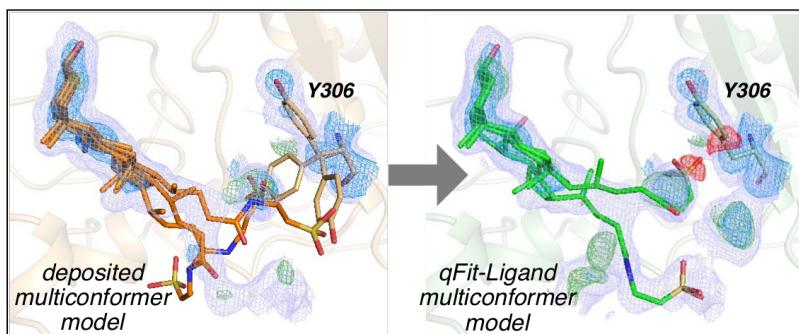


**Figure S9.** Prospective application of *qFit-ligand* to inhibitor CS301 bound to HSP90 (PDB ID 4YKQ). A) Two discrete conformations of the ethyl group found by *qFit-ligand*, supported by a  $2mF_o - DF_c$  map at  $0.3\sigma$  (purple). Difference density (green) in the single conformer model provides evidence for an unmodeled conformation. B) A derivative of inhibitor CS301, with a propyl group pointing to the right, provides further evidence that the alternate conformation found by *qFit-ligand* and shown in panel A is pre-sampled. C) OMIT maps for the single conformer and *qFit-ligand* multiconformer ligand models of 4YKQ are shown for comparison. The OMIT maps are near identical to our refined models. Electron densities are shown at  $1.5\sigma$  (blue),  $1.0\sigma$  (orange), and  $0.3\sigma$  (purple). Positive (green) and negative (red) difference densities are shown at  $\pm 3.0\sigma$ . Phenix was used to generate the OMIT maps using phenix.composite OMIT\_map.

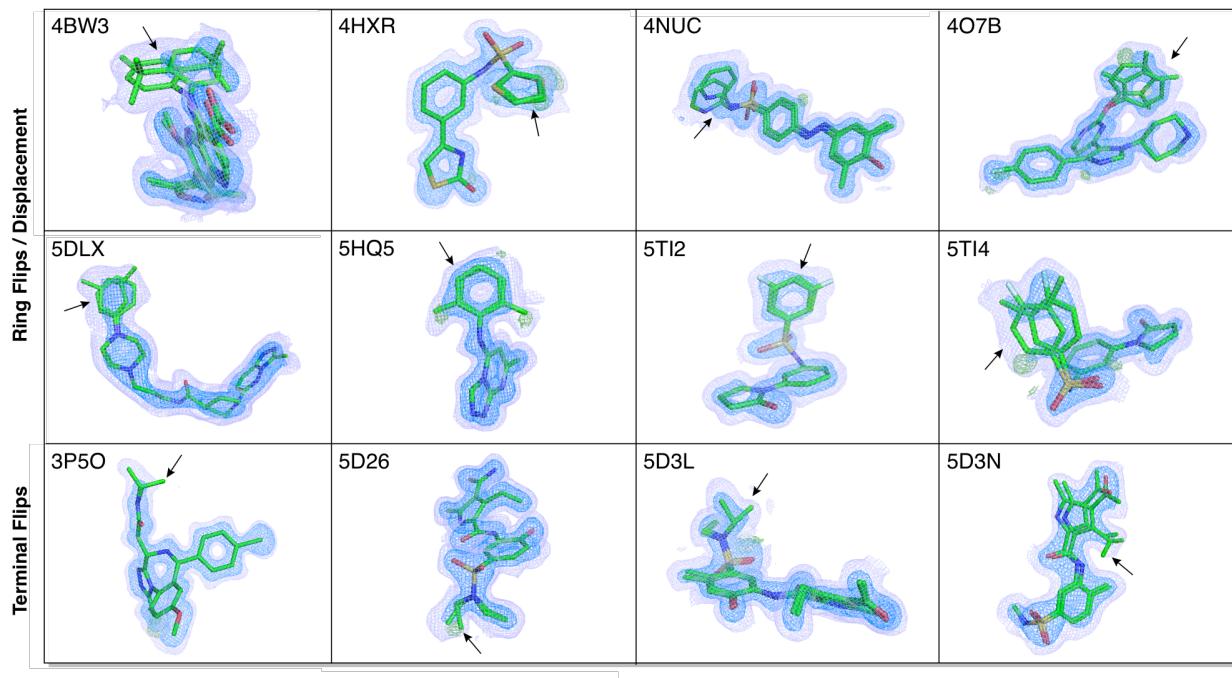
In the crystal structure of substrate 8-oxo-dGTP bound to MTH1 (PDB 5FSI), the electron density provides evidence of ligand disorder. Two of the alternate conformations of the phosphate tail selected by *qFit-ligand* better explain the ligand density and, furthermore, reveals protein-ligand interactions that were not captured in the single conformer model (**Figure S10**).



**Figure S10.** Prospective application of *qFit-ligand* to substrate 8-oxo-dGTP bound to MTH1 (PDB ID 5FSI). Single conformer, *qFit-ligand* multiconformer, and manually edited multiconformer models shown. B) OMIT maps for the single conformer and *qFit-ligand* multiconformer ligand models of 4YKQ are shown for comparison. The OMIT maps are near identical to those from our refined models. Electron densities are shown at  $1.5\sigma$  (blue),  $1.0\sigma$  (orange), and  $0.3\sigma$  (purple). Positive (green) and negative (red) difference densities are shown at  $\pm 3.0\sigma$ . Distances in Ångstroms. Phenix was used to generate the OMIT maps using phenix.composite\_omit\_map.

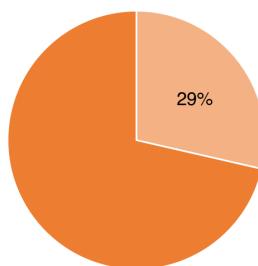


**Figure S11.** Left panel shows the deposited multiconformer model of ENPP2 (PDB ID 5DLV), which includes multiple conformations of the ligand and Y306. Upon inspection of the density, we removed two of the three Y306 and ligand conformations, then carried out *qFit-ligand* starting from the new single conformer model. Our algorithm creates ligand conformations that fit the density better than the manually curated, deposited multiconformer model. The presence of remaining positive difference densities are likely a result of unmodeled waters. Prospective application of *qFit-ligand* to an ENPP2-bound ligand (PDB ID 5DLV). Deposited multiconformer model and *qFit-ligand* multiconformer model shown. The deposited model has a very poor fit to the density, which is greatly improved by our automated method. Electron densities are shown at  $1.5\sigma$  (blue) and  $0.3\sigma$  (purple). Positive (green) and negative (red) difference densities are shown at  $\pm 3.0\sigma$ . Distances in Ångstroms.

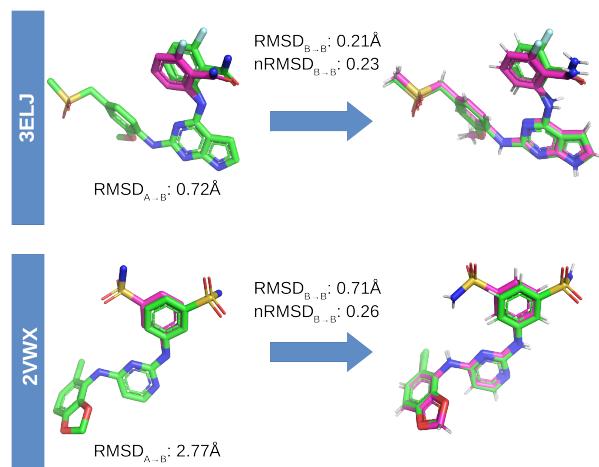


**Figure S12.** Twelve new binding conformations detected with high confidence for ligands bound to BRD4. Electron densities are shown at  $1.5\sigma$  (blue) and  $0.3\sigma$  (purple). Positive (green) difference densities are shown at  $\pm 3.0\sigma$ . Alternate conformations supported by density at  $0.3 \sigma$  contour levels are considered 'high confidence', while conformations supported by density at lower contour levels are considered possible.

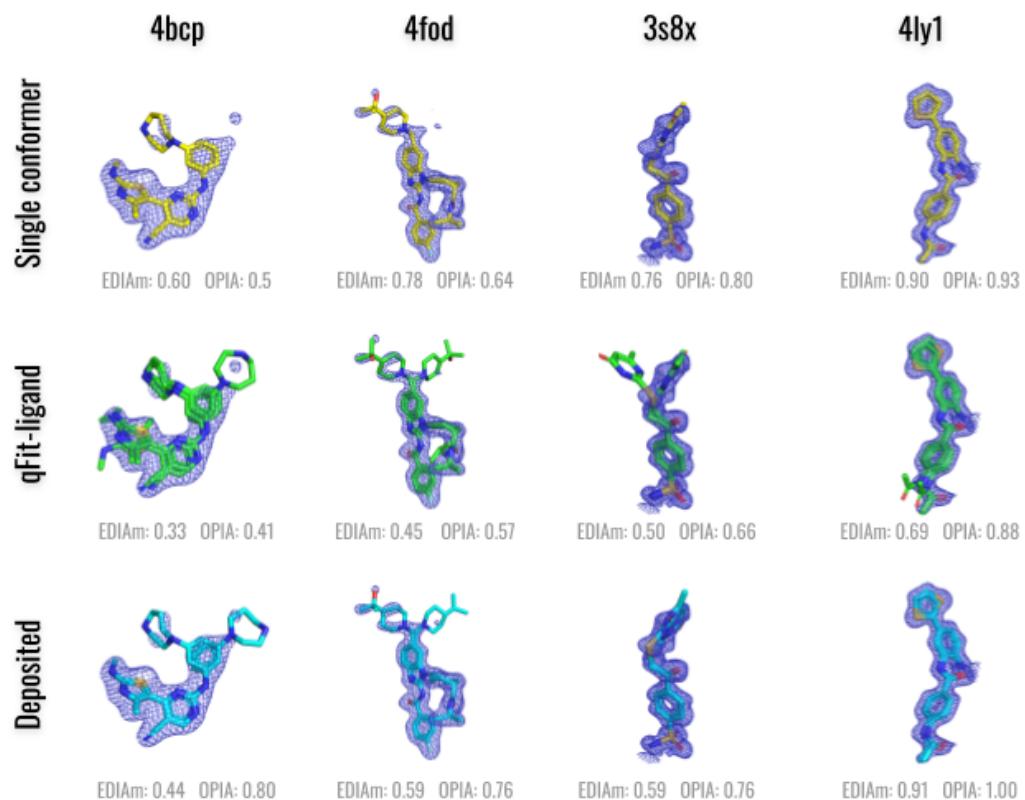
Percentage of BRD4 Structures with Possible Alternate Ligand Conformations



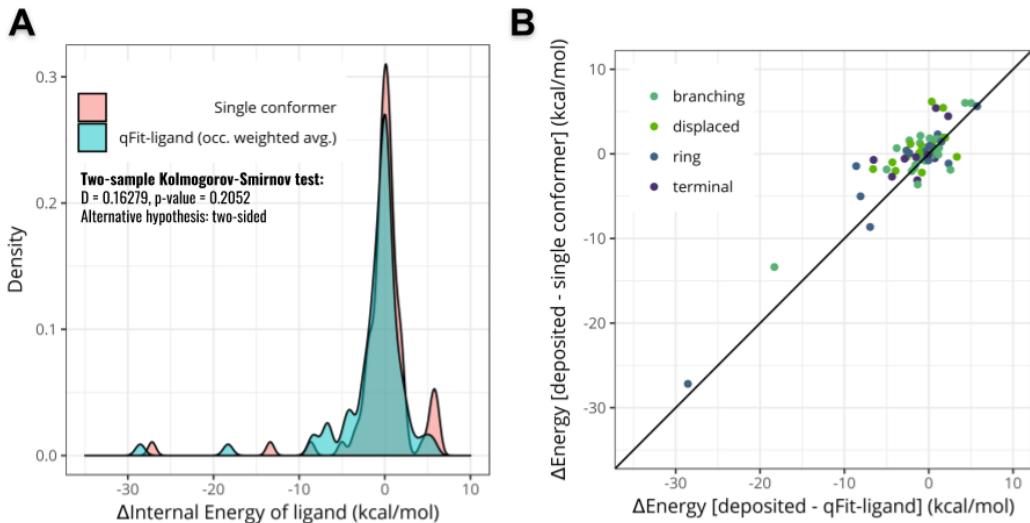
**Figure S13.** Possible alternate ligand conformations found in BRD4 structures. *qFit-ligand* was applied to a dataset of 126 crystal structures (100% sequence similarity to 5CFW) deposited in the PDB. Of those, *qFit-ligand* detected alternate conformations in 12 crystal structures with high confidence, and another 24 with possible alternate ligand conformations. Alternate conformations supported by density at  $0.3 \sigma$  contour levels are considered 'high confidence', while conformations supported by density at lower contour levels are considered possible.



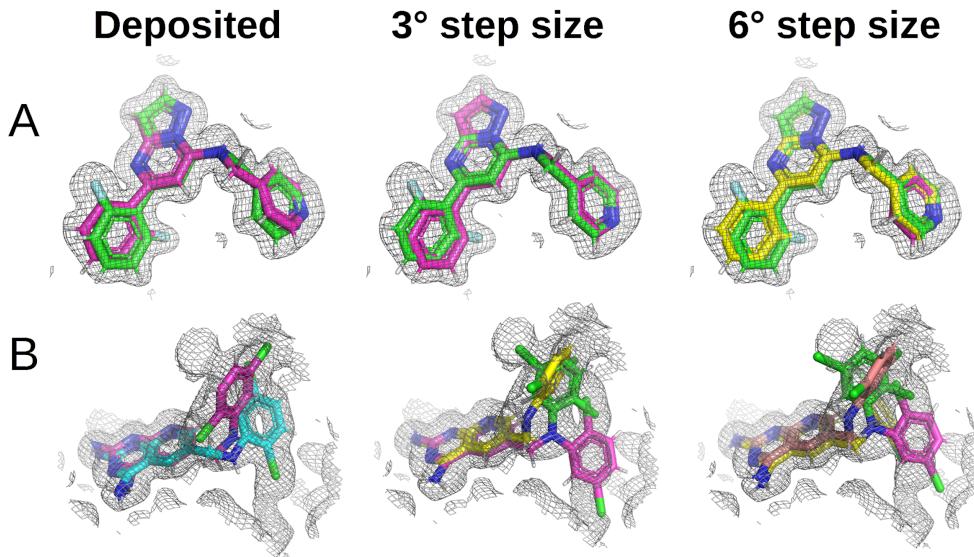
**Figure S14** Illustration of a case where A and B are very different, the normalization is different than if A and B are binding in nearly the same way.



**Figure S15.** Examples where the ligand EDIAm or OPIA decreased by modeling alternate conformations with *qFit-ligand*. The 2mFo-DFc maps are shown in blue at a contour level of  $1\sigma$ . For two of the cases (PDB IDs: 4bcp and 4fod) the output poses are similar to the deposited conformers, despite the lower EDIAm and OPIA scores.



**Figure S16. Automated *qFit-ligand* multi-conformer ligand internal energies are statistically indistinguishable from single conformer internal energies taken from our benchmark deposited models.** A) Distribution of  $\Delta$ Internal Energies of single conformers (red) and multiconformers output by *qFit-ligand* (blue). We subtracted the internal energy of each conformer from the occupancy-weighted average internal energy of the conformers in the deposited structure ( $\Delta$ ). Our two-sample Kolmogorov-Smirnov test comparing the two distributions had a p-value of 0.20, which is not sufficient to reject the null hypothesis. B) Comparison of the  $\Delta$ Internal Energies of single conformers against the  $\Delta$ Internal Energies of multiconformers output by *qFit-ligand*. Points are colored based on the type of their conformational heterogeneity.



**Figure S17. Finer sampling steps can improve multi-conformer models.** The deposited and *qFit-ligand* results after sampling with 2 DoFs at angular step sizes of 3° (denser) and 6° (default) for A) 2R3I; 1.28Å and B) 4G95; 1.35Å. The denser sampling protocol reduces model complexity (two conformers instead of three for 2R3I; three conformers instead of four for 4G95) while maintaining or improving average EDIA score (0.93; unchanged for 2R3I, 0.35; nearly doubled for 4G95). However, computational time increased from minutes to several hours, and memory requirements also significantly increased.

**Table S1.** Overview of benchmark cases and categorization of conformational change between alternate conformers.

**Table S2.** Performance of *qFit-ligand* on the benchmark using re-refined deposited data, showing quality metrics of re-refined single conformer structures, re-refined multiconformer deposited structures and refined *qfit-ligand* generated structures. The single conformer structures were generated by removing the ligand's B-conformer from the deposited data with subsequent refinement. Ligand energies of each conformation chosen by qFit-ligand relative to the single conformer ligand geometry is included, as well as the energy of the overall occupancy-weighted ligand multiconformer model.

**Table S3.** Results of applying *qFit-ligand* on a subset of the Twilight database. Entries are sorted by the highest found Fisher z-score. The *Twilight score*,  $R_{\text{work}}$  and  $R_{\text{free}}$  were retrieved from the Twilight database. Entries in the *RMSD A -> B (Å) (deposited)* column are non-empty if the ligand in the deposited PDB file has an alternate conformer modeled.

**Table S4.** Overview of prospective cases with an unmodeled alternate conformer found by *qFit-ligand*.

**Table S5.** BRD4 structures subjected to *qFit-ligand* approach, ordered by the Fisher z-score.