

## Supplemental Information

### Outcome of the First wwPDB/CCDC/D3R Ligand

#### Validation Workshop

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## Supplemental References

- Heller, S., McNaught, A., Stein, S., Tchekhovskoi, D., and Pletnev, I. (2013). InChI—the worldwide chemical structure identifier standard. *J. Cheminform* 5, 7.
- Henderson, R., Sali, A., Baker, M.L., Carragher, B., Devkota, B., Downing, K.H., Egelman, E.H., Feng, Z., Frank, J., Grigorieff, N., et al. (2012). Outcome of the first electron microscopy validation task force meeting. *Structure* 20, 205–214.
- Henrick, K., Feng, Z., Bluhm, W.F., Dimitropoulos, D., Doreleijers, J.F., Dutta, S., Flippen-Anderson, J.L., Ionides, J., Kamada, C., Krissinel, E., et al. (2008). Remediation of the Protein Data Bank archive. *Nucleic Acids Res.* 36, D426–D433.
- Kleywegt, G.J., Harris, M.R., Zou, J.Y., Taylor, T.C., Wahlby, A., and Jones, T.A. (2004). The Uppsala electron-density server. *Acta Crystallogr. D Biol. Crystallogr.* 60, 2240–2249.
- Liebeschuetz, J., Hennemann, J., Olsson, T., and Groom, C.R. (2012). The good, the bad and the twisted: a survey of ligand geometry in protein crystal structures. *J. Comput. Aided. Mol. Des.* 26, 169–183.
- Malde, A.K., and Mark, A.E. (2011). Challenges in the determination of the binding modes of non-standard ligands in X-ray crystal complexes. *J. Comput. Aided. Mol. Des.* 25, 1–12.
- Montelione, G.T., Nilges, M., Bax, A., Guntert, P., Herrmann, T., Richardson, J.S., Schwieters, C.D., Vranken, W.F., Vuister, G.W., Wishart, D.S., et al. (2013). Recommendations of the wwPDB NMR validation task force. *Structure* 21, 1563–1570.
- Pozharski, E., Weichenberger, C.X., and Rupp, B. (2013). Techniques, tools and best practices for ligand electron-density analysis and results from their application to deposited crystal structures. *Acta Crystallogr. D Biol. Crystallogr.* 69, 150–167.
- Protein Data Bank. (1971). *Protein Data Bank. Nat. New Biol.* 233, 223.
- Read, R.J., Adams, P.D., Arendall, W.B., 3rd, Brunger, A.T., Emsley, P., Joosten, R.P., Kleywegt, G.J., Krissinel, E.B., Lutteke, T., Otwinowski, Z., et al. (2011). A new generation of crystallographic validation tools for the protein data bank. *Structure* 19, 1395–1412.
- Rupp, B. (2010). Scientific inquiry, inference and critical reasoning in the macromolecular crystallography curriculum. *J. Appl. Cryst.* 43, 1242–1249.
- Sehna, D., Svobodova Varekova, R., Pravda, L., Ionescu, C.M., Geidl, S., Horsky, V., Jaiswal, D., Wimmerova, M., and Koca, J. (2015). ValidatorDB: database of up-to-date validation results for ligands and non-standard residues from the Protein Data Bank. *Nucleic Acids Res.* 43, D369–D375.
- Sen, S., Young, J., Berrisford, J.M., Chen, M., Conroy, M.J., Dutta, S., Di Costanzo, L., Gao, G., Ghosh, S., Hudson, B.P., et al. (2014). Small molecule annotation for the Protein Data Bank. *Database (Oxford)* 2014, bau116.

- Sitzmann, M., Weidlich, I.E., Filippov, I.V., Liao, C., Peach, M.L., Ihlenfeldt, W.D., Karki, R.G., Borodina, Y.V., Cachau, R.E., and Nicklaus, M.C. (2012). PDB ligand conformational energies calculated quantum-mechanically. *J. Chem. Inf. Model.* 52, 739–756.
- Smart, O., and Bricogne, G. (2015). Achieving high quality ligand chemistry in protein-ligand crystal structures for drug design. In *Multifaceted Roles of Crystallography in Modern Drug Discovery*, P.D. Scapin G., Arnold E., ed. (Springer), pp. 165–181.
- Terwilliger, T.C., and Bricogne, G. (2014). Continuous mutual improvement of macromolecular structure models in the PDB and of X-ray crystallographic software: the dual role of deposited experimental data. *Acta Crystallogr. D Biol. Crystallogr.* 70, 2533–2543.
- UniProt Consortium. (2015). UniProt: a hub for protein information. *Nucleic Acids Res.* 43, D204–D212.
- Warren, G.L., Do, T.D., Kelley, B.P., Nicholls, A., and Warren, S.D. (2012). Essential considerations for using protein-ligand structures in drug discovery. *Drug Discov. Today* 17, 1270–1281.
- Weichenberger, C.X., Pozharski, E., and Rupp, B. (2013). Visualizing ligand molecules in Twilight electron density. *Acta Crystallogr. Sect. F Struct. Biol. Cryst. Commun.* 69, 195–200.
- Weininger, D. (1988). SMILES 1. Introduction and encoding rules. *J. Chem. Inf. Comput. Sci.* 28, 31–36.
- Westbrook, J.D., Shao, C., Feng, Z., Zhuravleva, M., Velankar, S., and Young, J. (2015). The Chemical Component Dictionary: complete descriptions of constituent molecules in experimentally determined 3D macromolecules in the Protein Data Bank. *Bioinformatics* 31, 1274–1278.
- Young, J.Y., Feng, Z., Dimitropoulos, D., Sala, R., Westbrook, J., Zhuravleva, M., Shao, C., Quesada, M., Peisach, E., and Berman, H.M. (2013). Chemical annotation of small and peptide-like molecules at the Protein Data Bank. *Database (Oxford)* 2013, bat079.
- Zheng, H., Chordia, M.D., Cooper, D.R., Chruszcz, M., Muller, P., Sheldrick, G.M., and Minor, W. (2014). Validation of metal-binding sites in macromolecular structures with the CheckMyMetal web server. *Nat. Protoc.* 9, 156–170.