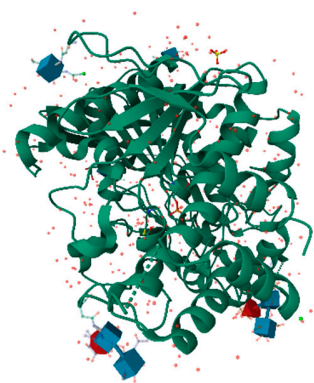



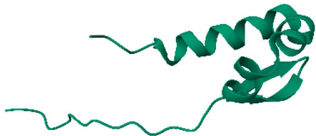
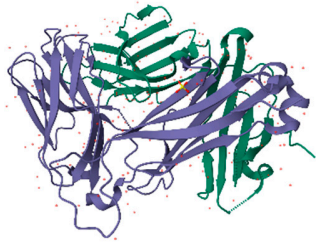


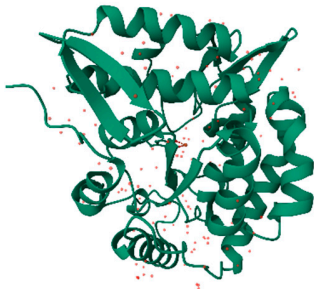
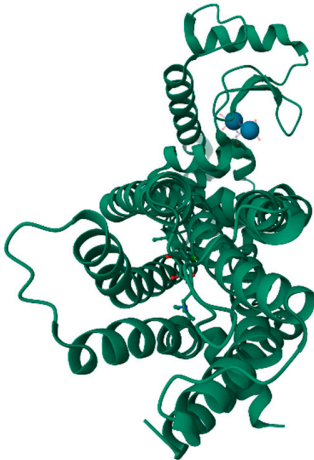
Table S1. Protein, Hormone, Gene, and their Receptors used in AutoDock analysis

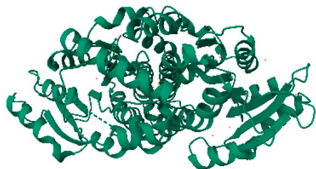

Target (Protein, Hormone, Gene, and their Receptors) from PDB (3D Structures)				PDB Information
Cholinesterase	Target Protein	1P0P		<p>1P0P</p> <p>Crystal structure of soman-aged human butyryl cholinesterase in complex with the substrate analog butyrylthiocholine</p> <ul style="list-style-type: none"> • PDB DOI: https://doi.org/10.2210/pdb1P0P/pdb • Classification: HYDROLASE • Organism(s): <u>Homo sapiens</u> • Expression System: <u>Cricetulus griseus</u> • Mutation(s): Yes • Deposited: 2003-04-10 Released: 2003-08-05 • Deposition Author(s): <u>Nicolet, Y., Lockridge, O., Masson, P., Fontecilla-Camps, J.C., Nachon, F.</u> <p>Experimental Data Snapshot</p> <ul style="list-style-type: none"> • Method: X-RAY DIFFRACTION • Resolution: 2.30 Å • R-Value Free: 0.242 • R-Value Work: 0.199 • R-Value Observed: 0.199

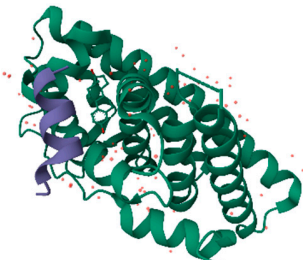

	Target Receptor	6EP4		<p>6EP4</p> <p>Human butyrylcholinesterase in complex with decamethonium</p> <ul style="list-style-type: none">• PDB DOI: https://doi.org/10.2210/pdb6EP4/pdb• Classification: HYDROLASE• Organism(s): <u>Homo sapiens</u>• Expression System: <u>Cricetulus griseus</u>• Mutation(s): Yes• Deposited: 2017-10-10 Released: 2017-12-13• Deposition Author(s): <u>Nachon, F.</u>, <u>Brazzolotto, X.</u>, <u>Wandhammer, M.</u>, <u>Trovaslet-Leroy, M.</u>, <u>Rosenberry, T.L.</u>, <u>Macdonald, I.R.</u>, <u>Darvesh, S.</u>• Funding Organization(s): French Ministry of Defense <p>Experimental Data Snapshot</p> <ul style="list-style-type: none">• Method: X-RAY DIFFRACTION• Resolution: 2.30 Å• R-Value Free: 0.217• R-Value Work: 0.179• R-Value Observed: 0.181
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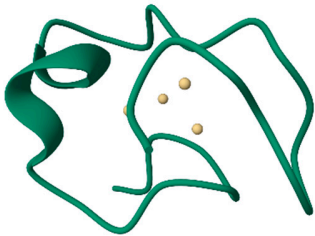
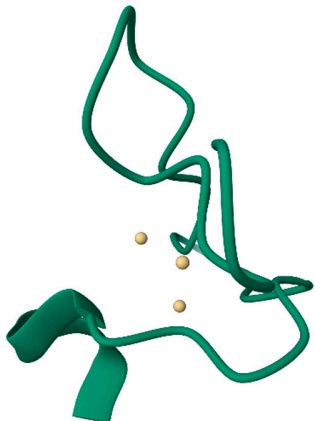
P53	Target Protein	7VOU		<p>7VOU</p> <p><i>The crystal structure of human forkhead box protein in complex with DNA I</i></p> <ul style="list-style-type: none"> • PDB DOI: https://doi.org/10.2210/pdb7VOU/pdb • NDB: 7VOU • Classification: <u>TRANSCRIPTION/DNA</u> • Organism(s): Homo sapiens • Expression System: Escherichia coli • Mutation(s): No • Deposited: 2021-10-14 Released: 2022-08-17 • Deposition Author(s): Choi, Y., Yoon, H.J., Lee, H.H. • Funding Organization(s): National Research Foundation (NRF, Korea) <p>Experimental Data Snapshot</p> <ul style="list-style-type: none"> • Method: X-RAY DIFFRACTION • Resolution: 3.10 Å • R-Value Free: 0.280 • R-Value Work: 0.221 • R-Value Observed: 0.227
		2LY4		<p>2LY4</p> <p><i>HMGB1-facilitated p53 DNA binding occurs via HMG-box/p53 transactivation domain interaction and is regulated by the acidic tail</i></p> <ul style="list-style-type: none"> • PDB DOI: https://doi.org/10.2210/pdb2LY4/pdb • BMRB: 18709 • Classification: <u>NUCLEAR PROTEIN/ANTITUMOUR PROTEIN</u> • Organism(s): Homo sapiens • Expression System: Escherichia coli • Mutation(s): No • Deposited: 2012-09-12 Released: 2012-10-31 • Deposition Author(s): Rowell, J.P., Simpson, K.L., Stott, K., Watson, M., Thomas, J.O. <p>Experimental Data Snapshot</p> <ul style="list-style-type: none"> • Method: SOLUTION NMR • Conformers Calculated: 100 • Conformers Submitted: 10 • Selection Criteria: structures with the lowest energy

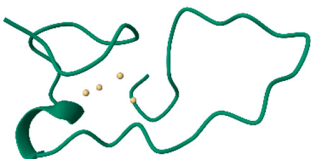
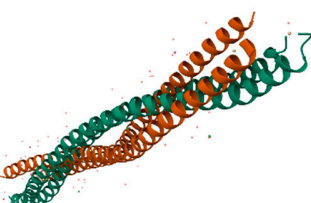
		2JTX		<p>2JTX</p> <p><i>NMR structure of the TFIIIE-alpha carboxyl terminus</i></p> <ul style="list-style-type: none"> • PDB DOI: https://doi.org/10.2210/pdb2JTX/pdb • Classification: TRANSCRIPTION • Organism(s): <i>Homo sapiens</i> • Expression System: <i>Escherichia coli</i> • Mutation(s): No • Deposited: 2007-08-08 Released: 2007-12-11 • Deposition Author(s): Di Lello, P., Omichinski, J.G. <p>Experimental Data Snapshot</p> <ul style="list-style-type: none"> • Method: SOLUTION NMR • Conformers Calculated: 50 • Conformers Submitted: 20 • Selection Criteria: structures with the lowest energy
Target Receptor		6VTH		<p>6VTH</p> <p><i>p53-specific T cell receptor</i></p> <ul style="list-style-type: none"> • PDB DOI: https://doi.org/10.2210/pdb6VTH/pdb • Classification: IMMUNE SYSTEM • Organism(s): <i>Homo sapiens</i> • Expression System: <i>Escherichia coli</i> • Mutation(s): No • Deposited: 2020-02-12 Released: 2020-06-17 • Deposition Author(s): Wu, D., Gallagher, D.T., Gowthaman, R., Pierce, B.G., Mariuzza, R.A. • Funding Organization(s): National Institutes of Health/National Institute of General Medical Sciences (NIH/NIGMS) <p>Experimental Data Snapshot</p> <ul style="list-style-type: none"> • Method: X-RAY DIFFRACTION • Resolution: 2.36 Å • R-Value Free: 0.264 • R-Value Work: 0.211 • R-Value Observed: 0.214

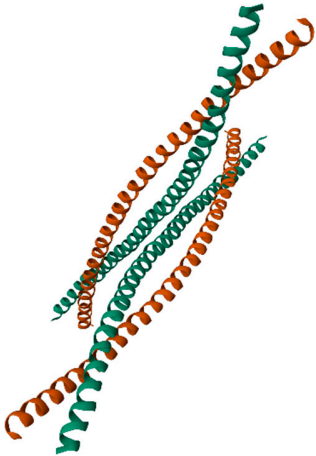
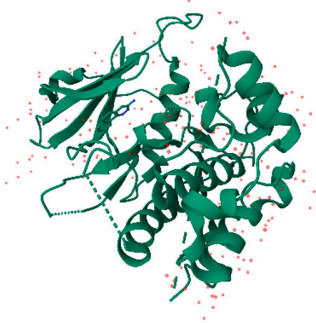
Dopamine	Target Protein	5PAH		<p>5PAH</p> <p><i>HUMAN PHENYLALANINE HYDROXYLASE CATALYTIC DOMAIN DIMER WITH BOUND DOPAMINE INHIBITOR</i></p> <ul style="list-style-type: none"> • PDB DOI: https://doi.org/10.2210/pdb5PAH/pdb • Classification: MONOOXYGENASE • Organism(s): <u>Homo sapiens</u> • Expression System: <u>Escherichia coli</u> • Mutation(s): No • Deposited: 1998-08-20 Released: 1999-04-27 • Deposition Author(s): <u>Erlandsen, H., Flatmark, T., Stevens, R.C.</u> <p>Experimental Data Snapshot</p> <ul style="list-style-type: none"> • Method: X-RAY DIFFRACTION • Resolution: 2.10 Å • R-Value Free: 0.200 • R-Value Work: 0.163 • R-Value Observed: 0.163
	Target Receptor	3PBL		<p>3PBL</p> <p><i>Structure of the human dopamine D3 receptor in complex with eticlopride</i></p> <ul style="list-style-type: none"> • PDB DOI: https://doi.org/10.2210/pdb3PBL/pdb • Classification: HYDROLASE/HYDROLASE INHIBITOR • Organism(s): <u>Homo sapiens, Tequatrovirus T4</u> • Expression System: <u>Spodoptera frugiperda</u> • Mutation(s): Yes • Membrane Protein: <u>Yes</u> • Deposited: 2010-10-20 Released: 2010-11-03 • Deposition Author(s): <u>Chien, E.Y.T., Liu, W., Han, G.W., Katritch, V., Zhao, Q., Cherezov, V., Stevens, R.C., Accelerated Technologies Center for Gene to 3D Structure (ATCG3D), GPCR Network (GPCR)</u> <p>Experimental Data Snapshot</p> <ul style="list-style-type: none"> • Method: X-RAY DIFFRACTION • Resolution: 2.89 Å • R-Value Free: 0.272 • R-Value Work: 0.243 • R-Value Observed: 0.245

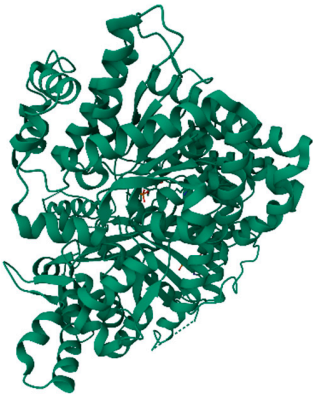
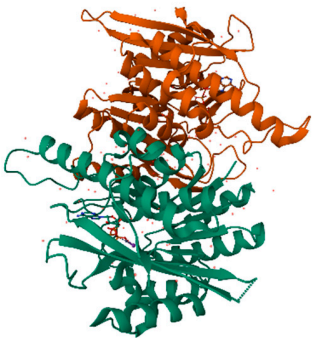
Estrogen	Target Protein	1FDW		<p>1FDW</p> <p><i>HUMAN 17-BETA-HYDROXYSTEROID-DEHYDROGENASE TYPE 1 MUTANT H221Q COMPLEXED WITH ESTRADIOL</i></p> <ul style="list-style-type: none"> • PDB DOI: https://doi.org/10.2210/pdb1FDW/pdb • Classification: DEHYDROGENASE • Organism(s): <u>Homo sapiens</u> • Expression System: <u>Spodoptera frugiperda</u> • Mutation(s): Yes • Deposited: 1998-01-16 Released: 1998-05-27 • Deposition Author(s): <u>Mazza, C., Breton, R., Housset, D., Fontecilla-Camps, J.-C.</u> <p>Experimental Data Snapshot</p> <ul style="list-style-type: none"> • Method: X-RAY DIFFRACTION • Resolution: 2.70 Å • R-Value Free: 0.263 • R-Value Work: 0.178
	Target Receptor	1L2J		<p>1L2J</p> <p><i>Human Estrogen Receptor beta Ligand-binding Domain in Complex with (R,R)-5,11-cis-diethyl-5,6,11,12-tetrahydrochrysene-2,8-diol</i></p> <ul style="list-style-type: none"> • PDB DOI: https://doi.org/10.2210/pdb1L2J/pdb • Classification: transcription receptor • Organism(s): <u>Homo sapiens</u> • Expression System: <u>Escherichia coli</u> • Mutation(s): No • Deposited: 2002-02-21 Released: 2002-05-01 • Deposition Author(s): <u>Shiau, A.K., Barstad, D., Radek, J.T., Meyers, M.J., Nettles, K.W., Katzenellenbogen, B.S., Katzenellenbogen, J.A., Agard, D.A., Greene, G.L.</u> <p>Experimental Data Snapshot</p> <ul style="list-style-type: none"> • Method: X-RAY DIFFRACTION • Resolution: 2.95 Å • R-Value Free: 0.299 • R-Value Work: 0.259


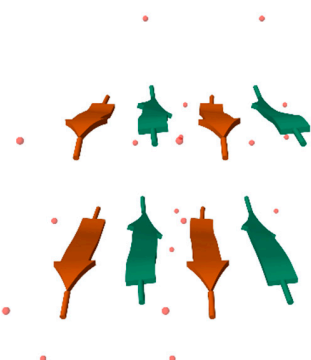
		4J26		<p>4J26</p> <p><i>Estrogen Receptor in complex with proline-flanked LXXLL peptides</i></p> <ul style="list-style-type: none"> • PDB DOI: https://doi.org/10.2210/pdb4J26/pdb • Classification: HORMONE RECEPTOR/PEPTIDE • Organism(s): <i>Homo sapiens</i> • Expression System: <i>Escherichia coli</i> • Mutation(s): No • Deposited: 2013-02-04 Released: 2013-03-13 • Deposition Author(s): Fuchs, S., Nguyen, H.D., Phan, T., Burton, M., Nieto, L., de Vries-van Leeuwen, I., Schmidt, A., Goodarzifard, M., Agten, S., Rose, R., Ottmann, C., Milroy, L.G., Brunsvel, L. <p>Experimental Data Snapshot</p> <ul style="list-style-type: none"> • Method: X-RAY DIFFRACTION • Resolution: 2.30 Å • R-Value Free: 0.242 • R-Value Work: 0.203 • R-Value Observed: 0.205
		4J24		<p>4J24</p> <p><i>Estrogen Receptor in complex with proline-flanked LXXLL peptides</i></p> <ul style="list-style-type: none"> • PDB DOI: https://doi.org/10.2210/pdb4J24/pdb • Classification: HORMONE RECEPTOR/PEPTIDE • Organism(s): <i>Homo sapiens</i> • Expression System: <i>Escherichia coli</i> • Mutation(s): No • Deposited: 2013-02-04 Released: 2013-03-13 • Deposition Author(s): Fuchs, S., Nguyen, H.D., Phan, T., Burton, M., Nieto, L., de Vries-van Leeuwen, I., Schmidt, A., Goodarzifard, M., Agten, S., Rose, R., Ottmann, C., Milroy, L.G., Brunsvel, L. <p>Experimental Data Snapshot</p> <ul style="list-style-type: none"> • Method: X-RAY DIFFRACTION • Resolution: 2.10 Å • R-Value Free: 0.224 • R-Value Work: 0.190 • R-Value Observed: 0.192

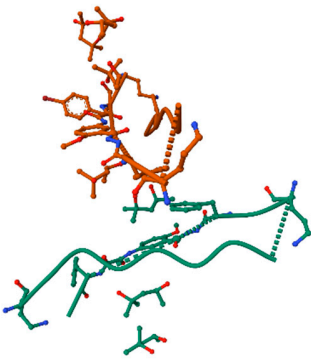

Metallothionein	Target Protein	1MHU		<p>1MHU</p> <p><i>THE THREE-DIMENSIONAL STRUCTURE OF HUMAN [113CD7] METALLOTHIONEIN-2 IN SOLUTION DETERMINED BY NUCLEAR MAGNETIC RESONANCE SPECTROSCOPY</i></p> <ul style="list-style-type: none"> • PDB DOI: https://doi.org/10.2210/pdb1MHU/pdb • BMRB: 1154 • Classification: METALLOTHIONEIN • Organism(s): <u>Homo sapiens</u> • Mutation(s): No • Deposited: 1990-05-14 Released: 1991-04-15 • Deposition Author(s): <u>Braun, W., Messerle, B.A., Schaeffer, A., Vasak, M., Kaegi, J.H.R., Wuthrich, K.</u> <p>Experimental Data Snapshot</p> <ul style="list-style-type: none"> • Method: SOLUTION NMR • Conformers Submitted: 1
	Target Receptor	2MHU		<p>2MHU</p> <p><i>THE THREE-DIMENSIONAL STRUCTURE OF HUMAN [113CD7] METALLOTHIONEIN-2 IN SOLUTION DETERMINED BY NUCLEAR MAGNETIC RESONANCE SPECTROSCOPY</i></p> <ul style="list-style-type: none"> • PDB DOI: https://doi.org/10.2210/pdb2MHU/pdb • Classification: METALLOTHIONEIN • Organism(s): <u>Homo sapiens</u> • Mutation(s): No • Deposited: 1990-05-14 Released: 1991-04-15 • Deposition Author(s): <u>Braun, W., Messerle, B.A., Schaeffer, A., Vasak, M., Kaegi, J.H.R., Wuthrich, K.</u> <p>Experimental Data Snapshot</p> <ul style="list-style-type: none"> • Method: SOLUTION NMR • Conformers Submitted: 1

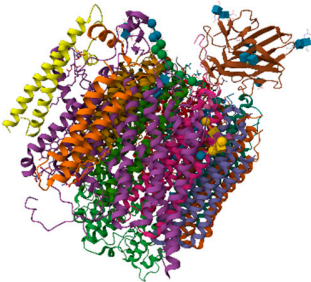
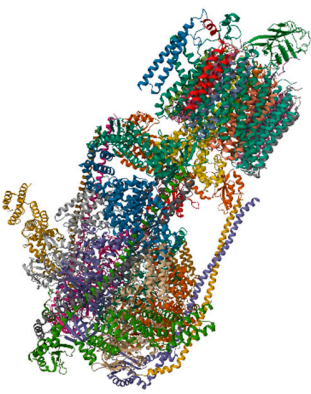
		2F5H		<p>2F5H</p> <p><i>Solution structure of the alpha-domain of human Metallothionein-3</i></p> <ul style="list-style-type: none"> • PDB DOI: https://doi.org/10.2210/pdb2F5H/pdb • Classification: METAL BINDING PROTEIN • Organism(s): <i>Homo sapiens</i> • Expression System: <i>Escherichia coli</i> BL21 • Mutation(s): No • Deposited: 2005-11-25 Released: 2006-05-30 • Deposition Author(s): Wang, H., Zhang, Q., Cai, B., Li, H.Y., Sze, K.H., Huang, Z.X., Wu, H.M., Sun, H.Z. <p>Experimental Data Snapshot</p> <ul style="list-style-type: none"> • Method: SOLUTION NMR • Conformers Calculated: 30 • Conformers Submitted: 10 • Selection Criteria: best converged structures
Keratin	Target Protein	6EC0		<p>6EC0</p> <p><i>Crystal structure of the wild-type heterocomplex between coil 1B domains of human intermediate filament proteins keratin 1 (KRT1) and keratin 10 (KRT10)</i></p> <ul style="list-style-type: none"> • PDB DOI: https://doi.org/10.2210/pdb6EC0/pdb • Classification: PROTEIN FIBRIL • Organism(s): <i>Homo sapiens</i> • Expression System: <i>Escherichia coli</i> BL21(DE3) • Mutation(s): No • Deposited: 2018-08-07 Released: 2019-05-15 • Deposition Author(s): Eldirany, S.A., Lomakin, I.B., Bunick, C.G. • Funding Organization(s): National Institutes of Health/National Institute of Arthritis and Musculoskeletal and Skin Diseases (NIH/NIAMS), Other private <p>Experimental Data Snapshot</p> <ul style="list-style-type: none"> • Method: X-RAY DIFFRACTION • Resolution: 2.98 Å • R-Value Free: 0.300 • R-Value Work: 0.281 • R-Value Observed: 0.282

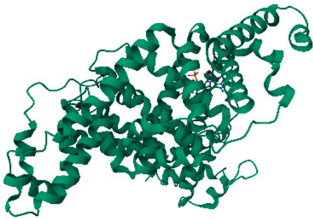
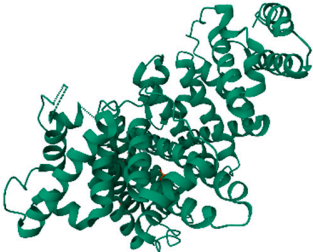
	Target Receptor	4ZRY		<p>4ZRY</p> <p><i>Crystal structure of the heterocomplex between coil 2B domains of human intermediate filament proteins keratin 1 (KRT1) and keratin 10 (KRT10)</i></p> <ul style="list-style-type: none"> • PDB DOI: https://doi.org/10.2210/pdb4ZRY/pdb • Classification: <u>PROTEIN FIBRIL</u> • Organism(s): <u>Homo sapiens</u> • Expression System: <u>Escherichia coli BL21(DE3)</u> • Mutation(s): No • Deposited: 2015-05-12 Released: 2016-05-18 • Deposition Author(s): <u>Bunick, C.G., Steitz, T.A.</u> • Funding Organization(s): Dermatology Foundation <p>Experimental Data Snapshot</p> <ul style="list-style-type: none"> • Method: X-RAY DIFFRACTION • Resolution: 3.30 Å • R-Value Free: 0.277 • R-Value Work: 0.273 • R-Value Observed: 0.273
Protein kinase enzyme	Target Protein	1P4F		<p>1P4F</p> <p><i>DEATH ASSOCIATED PROTEIN KINASE CATALYTIC DOMAIN WITH BOUND INHIBITOR FRAGMENT</i></p> <ul style="list-style-type: none"> • PDB DOI: https://doi.org/10.2210/pdb1P4F/pdb • Classification: <u>TRANSFERASE</u> • Organism(s): <u>Homo sapiens</u> • Expression System: <u>Escherichia coli</u> • Mutation(s): No • Deposited: 2003-04-23 Released: 2004-09-28 • Deposition Author(s): <u>Velentza, A.V., Wainwright, M.S., Zasadzki, M., Mirzoeva, S., Haiech, J., Focia, P.J., Egli, M., Watterson, D.M.</u> <p>Experimental Data Snapshot</p> <ul style="list-style-type: none"> • Method: X-RAY DIFFRACTION • Resolution: 1.90 Å • R-Value Free: 0.233 • R-Value Work: 0.185 • R-Value Observed: 0.186

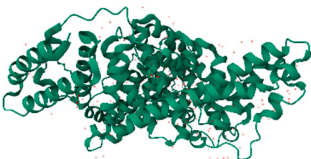
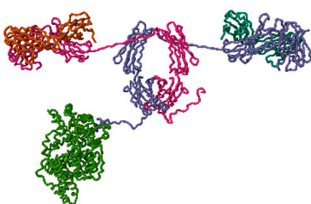
		5IKP		<p>5IKP</p> <p><i>Crystal structure of human brain glycogen phosphorylase bound to AMP</i></p> <ul style="list-style-type: none"> • PDB DOI: https://doi.org/10.2210/pdb5IKP/pdb • Classification: TRANSFERASE • Organism(s): <u>Homo sapiens</u> • Expression System: <u>Escherichia coli</u> • Mutation(s): No • Deposited: 2016-03-03 Released: 2016-07-20 • Deposition Author(s): <u>Mathieu, C., Li de la Sierra-Gallay, I., Xu, X., Haouz, A., Rodrigues-Lima, F.</u> <p>Experimental Data Snapshot</p> <ul style="list-style-type: none"> • Method: X-RAY DIFFRACTION • Resolution: 3.40 Å • R-Value Free: 0.295 • R-Value Work: 0.202 • R-Value Observed: 0.207
	Target Receptor	1LHR		<p>1LHR</p> <p><i>Crystal Structure of Pyridoxal Kinase complexed with ATP</i></p> <ul style="list-style-type: none"> • PDB DOI: https://doi.org/10.2210/pdb1LHR/pdb • Classification: TRANSFERASE • Organism(s): <u>Ovis aries</u> • Mutation(s): No • Deposited: 2002-04-17 Released: 2003-02-11 • Deposition Author(s): <u>Liang, D.C., Jiang, T., Li, M.H.</u> <p>Experimental Data Snapshot</p> <ul style="list-style-type: none"> • Method: X-RAY DIFFRACTION • Resolution: 2.60 Å • R-Value Free: 0.222 • R-Value Work: 0.193 • R-Value Observed: 0.198

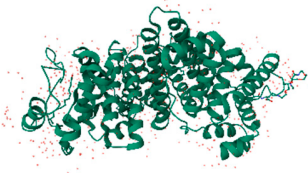
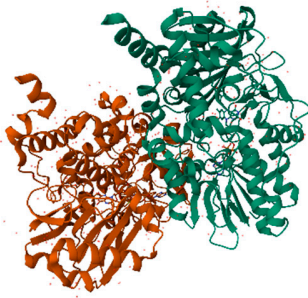
		6E0R		<p>6E0R</p> <p><i>hALK in complex with compound 7 N-((1S)-1-(5-fluoropyridin-2-yl)ethyl)-1-(5-methyl-1H-pyrazol-3-yl)-3-(oxetan-3-ylsulfonyl)-1H-pyrrolo[2,3-b]pyridin-6-amine</i></p> <ul style="list-style-type: none"> • PDB DOI: https://doi.org/10.2210/pdb6E0R/pdb • Classification: PROTEIN BINDING • Organism(s): <u>Homo sapiens</u> • Expression System: <u>unidentified baculovirus</u> • Mutation(s): No • Deposited: 2018-07-06 Released: 2019-05-01 • Deposition Author(s): <u>Lane, W., Saikatendu, K.</u> <p>Experimental Data Snapshot</p> <ul style="list-style-type: none"> • Method: X-RAY DIFFRACTION • Resolution: 2.30 Å • R-Value Free: 0.296 • R-Value Work: 0.237 • R-Value Observed: 0.241
Beta Amyloid	Target Protein	5TXJ		<p>5TXJ</p> <p><i>Polymorphic form 1 of amyloid-beta derived peptide - IFAE DV</i></p> <ul style="list-style-type: none"> • PDB DOI: https://doi.org/10.2210/pdb5TXJ/pdb • Classification: DE NOVO PROTEIN • Organism(s): <u>Homo sapiens</u> • Mutation(s): No • Deposited: 2016-11-16 Released: 2017-11-15 • Deposition Author(s): <u>Sangwan, S., Sawaya, M.R., Eisenberg, D.</u> <p>Experimental Data Snapshot</p> <ul style="list-style-type: none"> • Method: X-RAY DIFFRACTION • Resolution: 1.13 Å • R-Value Free: 0.157 • R-Value Work: 0.145 • R-Value Observed: 0.146



		3T4G		<p>3T4G</p> <p><i>AIIGLMV segment from Alzheimer's Amyloid-Beta displayed on 54-membered macrocycle scaffold</i></p> <ul style="list-style-type: none"> • PDB DOI: https://doi.org/10.2210/pdb3T4G/pdb • Classification: UNKNOWN FUNCTION • Mutation(s): No • Deposited: 2011-07-26 Released: 2012-10-31 • Deposition Author(s): Zhao, M., Liu, C., Cheng, P.N., Eisenberg, D., Nowick, J.S. <p>Experimental Data Snapshot</p> <ul style="list-style-type: none"> • Method: X-RAY DIFFRACTION • Resolution: 1.70 Å • R-Value Free: 0.274 • R-Value Work: 0.236 • R-Value Observed: 0.240
Target Receptor		3Q7G		<p>3Q7G</p> <p><i>Crystal Structure of E2 domain of Human Amyloid Precursor-Like Protein 1 in complex with SOS (sucrose octasulfate)</i></p> <ul style="list-style-type: none"> • PDB DOI: https://doi.org/10.2210/pdb3Q7G/pdb • Classification: SIGNALING PROTEIN • Organism(s): Homo sapiens • Expression System: Escherichia coli • Mutation(s): No • Deposited: 2011-01-04 Released: 2011-06-22 • Deposition Author(s): Xue, Y., Ha, Y. <p>Experimental Data Snapshot</p> <ul style="list-style-type: none"> • Method: X-RAY DIFFRACTION • Resolution: 2.30 Å • R-Value Free: 0.261 • R-Value Work: 0.217 • R-Value Observed: 0.222

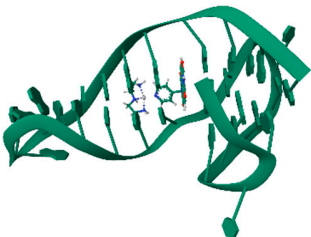
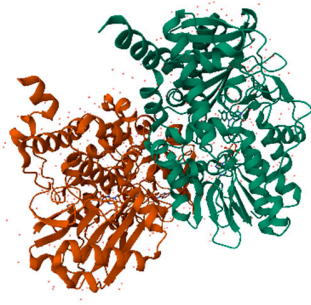
ATPase	Target Receptor	6WL W		<p>6WLW</p> <p><i>The Vo region of human V-ATPase in state 1 (focused refinement)</i></p> <ul style="list-style-type: none"> • PDB DOI: https://doi.org/10.2210/pdb6WLW/pdb • EM Map EMD-21844: EMDB EMDataResource • Classification: MEMBRANE PROTEIN • Organism(s): Homo sapiens • Mutation(s): No • Membrane Protein: Yes • Deposited: 2020-04-20 Released: 2020-11-11 • Deposition Author(s): Wang, L., Wu, H., Fu, T.-M. <p>Experimental Data Snapshot</p> <ul style="list-style-type: none"> • Method: ELECTRON MICROSCOPY • Resolution: 3.00 Å • Aggregation State: PARTICLE • Reconstruction Method: SINGLE PARTICLE
		6WM 3		<p>6WM3</p> <p><i>Human V-ATPase in state 2 with SidK and ADP</i></p> <ul style="list-style-type: none"> • PDB DOI: https://doi.org/10.2210/pdb6WM3/pdb • EM Map EMD-21848: EMDB EMDataResource • Classification: MEMBRANE PROTEIN • Organism(s): Homo sapiens, Legionella pneumophila subsp. pneumophila str. Philadelphia 1 • Mutation(s): No • Membrane Protein: Yes • Deposited: 2020-04-20 Released: 2020-11-11 • Deposition Author(s): Wang, L., Wu, H., Fu, T.M. <p>Experimental Data Snapshot</p> <ul style="list-style-type: none"> • Method: ELECTRON MICROSCOPY • Resolution: 3.40 Å • Aggregation State: PARTICLE • Reconstruction Method: SINGLE PARTICLE

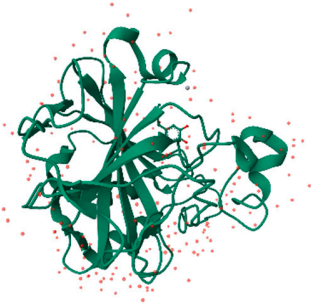
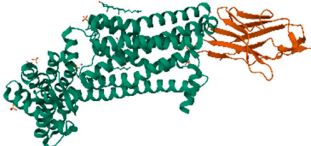
Albumin	Target Protein	5UJB		<p>5UJB</p> <p><i>Structure of a Mcl-1 Inhibitor Binding to Site 3 of Human Serum Albumin</i></p> <ul style="list-style-type: none"> • PDB DOI: https://doi.org/10.2210/pdb5UJB/pdb • Classification: TRANSPORT PROTEIN • Organism(s): <u>Homo sapiens</u> • Expression System: <u>Homo sapiens</u> • Mutation(s): No • Deposited: 2017-01-17 Released: 2017-05-03 • Deposition Author(s): <u>Zhao, B.</u> • Funding Organization(s): National Institutes of Health/National Cancer Institute (NIH/NCI) <p>Experimental Data Snapshot</p> <ul style="list-style-type: none"> • Method: X-RAY DIFFRACTION • Resolution: 2.70 Å • R-Value Free: 0.215 • R-Value Work: 0.174 • R-Value Observed: 0.177
		6M5D		<p>6M5D</p> <p><i>Human serum albumin (apo form)</i></p> <ul style="list-style-type: none"> • PDB DOI: https://doi.org/10.2210/pdb6M5D/pdb • Classification: PEPTIDE BINDING PROTEIN • Organism(s): <u>Homo sapiens</u> • Expression System: <u>Homo sapiens</u> • Mutation(s): No • Deposited: 2020-03-10 Released: 2020-11-18 • Deposition Author(s): <u>Ito, S., Senoo, A., Nagatoishi, S., Yamamoto, M., Tsumoto, K., Wakui, N.</u> • Funding Organization(s): Japan Agency for Medical Research and Development (AMED) <p>Experimental Data Snapshot</p> <ul style="list-style-type: none"> • Method: X-RAY DIFFRACTION • Resolution: 2.60 Å • R-Value Free: 0.264 • R-Value Work: 0.230 • R-Value Observed: 0.232


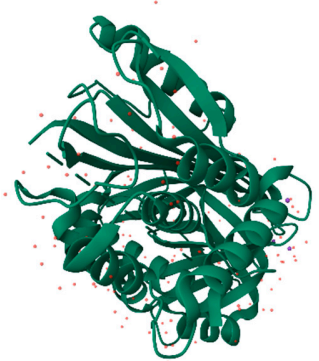
	Target Receptor	6HSC		<p>6HSC</p> <p><i>Structure of Human Serum Albumin in complex with Aristolochic Acid at 1.9 Å resolution</i></p> <ul style="list-style-type: none"> • PDB DOI: https://doi.org/10.2210/pdb6HSC/pdb • Classification: TRANSPORT PROTEIN • Organism(s): <u>Homo sapiens</u> • Expression System: <u>Homo sapiens</u> • Mutation(s): No • Deposited: 2018-09-29 Released: 2019-10-23 • Deposition Author(s): <u>Pomyalov, S., Sidorenko, V.S., Grollman, A.P., Shoham, G.</u> <p>Experimental Data Snapshot</p> <ul style="list-style-type: none"> • Method: X-RAY DIFFRACTION • Resolution: 1.90 Å • R-Value Free: 0.286 • R-Value Work: 0.238 • R-Value Observed: 0.240
		2ESG		<p>2ESG</p> <p><i>Solution structure of the complex between immunoglobulin IgA1 and human serum albumin</i></p> <ul style="list-style-type: none"> • PDB DOI: https://doi.org/10.2210/pdb2ESG/pdb • Classification: IMMUNE SYSTEM/TRANSPORT PROTEIN • Organism(s): <u>Homo sapiens</u> • Expression System: <u>Escherichia coli</u> • Mutation(s): No • Deposited: 2005-10-26 Released: 2006-01-31 • Deposition Author(s): <u>Almogren, A., Furtado, P.B., Sun, Z., Perkins, S.J., Kerr, M.A.</u> <p>Experimental Data Snapshot</p> <ul style="list-style-type: none"> • Method: SOLUTION SCATTERING

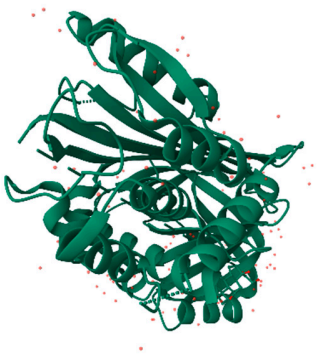

		6YG9		<p>6YG9</p> <p><i>CRYSTAL STRUCTURE OF HUMAN SERUM ALBUMIN (HSA) IN COMPLEX WITH GN-07.</i></p> <ul style="list-style-type: none"> • PDB DOI: https://doi.org/10.2210/pdb6YG9/pdb • Classification: <u>TRANSPORT PROTEIN</u> • Organism(s): <u>Homo sapiens</u> • Mutation(s): No • Deposited: 2020-03-27 Released: 2021-01-13 • Deposition Author(s): <u>Schreuder, H.A., Liesum, A.</u> <p>Experimental Data Snapshot</p> <ul style="list-style-type: none"> • Method: X-RAY DIFFRACTION • Resolution: 1.89 Å • R-Value Free: 0.313 • R-Value Work: 0.239 • R-Value Observed: 0.243
Mono amino oxidase (MAO)	Target Protein	2BK3		<p>2BK3</p> <p><i>Human Monoamine Oxidase B in complex with Farnesol</i></p> <ul style="list-style-type: none"> • PDB DOI: https://doi.org/10.2210/pdb2BK3/pdb • Classification: <u>OXIDOREDUCTASE</u> • Organism(s): <u>Homo sapiens</u> • Expression System: <u>Komagataella pastoris</u> • Mutation(s): No • Membrane Protein: <u>Yes</u> • Deposited: 2005-02-10 Released: 2005-02-14 • Deposition Author(s): <u>Binda, C., Edmondson, D.E., Mattevi, A.</u> <p>Experimental Data Snapshot</p> <ul style="list-style-type: none"> • Method: X-RAY DIFFRACTION • Resolution: 1.80 Å • R-Value Free: 0.249 • R-Value Work: 0.225 • R-Value Observed: 0.226

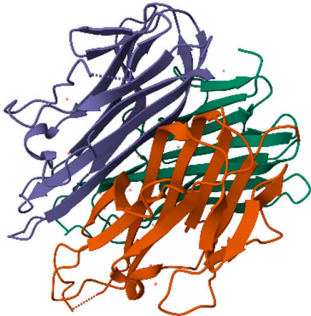
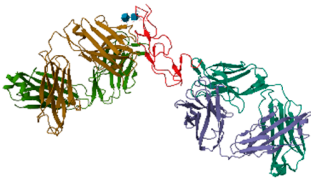
		2BXS		<p>2BXS</p> <p><i>Human Monoamine Oxidase A in complex with Clorgyline, Crystal Form B</i></p> <ul style="list-style-type: none"> • PDB DOI: https://doi.org/10.2210/pdb2BXS/pdb • Classification: OXIDOREDUCTASE • Organism(s): <u>Homo sapiens</u> • Expression System: <u>Komagataella pastoris</u> • Mutation(s): No • Membrane Protein: <u>Yes</u> • Deposited: 2005-07-27 Released: 2005-08-09 • Deposition Author(s): <u>De Colibus, L., Binda, C., Edmondson, D.E., Mattevi, A.</u> <p>Experimental Data Snapshot</p> <ul style="list-style-type: none"> • Method: X-RAY DIFFRACTION • Resolution: 3.15 Å • R-Value Free: 0.330 • R-Value Work: 0.268 • R-Value Observed: 0.271
		7DJU		<p>7DJU</p> <p><i>NMR solution structure of the 1:1 complex of a platinum(II) compound bound to 5'-end of Myc1234 G-quadruplex reveals the mechanism of conformational switch and dynamic binding of G-quadruplex</i></p> <ul style="list-style-type: none"> • PDB DOI: https://doi.org/10.2210/pdb7DJU/pdb • NDB: <u>7DJU</u> • Classification: DNA • Organism(s): <u>Homo sapiens</u> • Mutation(s): No • Deposited: 2020-11-22 Released: 2022-01-12 • Deposition Author(s): <u>Liu, W., Mao, Z.W.</u> • Funding Organization(s): National Natural Science Foundation of China (NSFC), Ministry of Education (MoE, China) <p>Experimental Data Snapshot</p> <ul style="list-style-type: none"> • Method: SOLUTION NMR • Conformers Calculated: 100 • Conformers Submitted: 20 • Selection Criteria: structures with the lowest energy

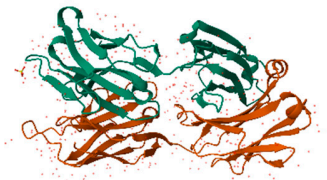

	Target Receptor	7EL7		<p>7EL7</p> <p><i>NMR solution structure of the 1:1 complex of a quadruplex-duplex hybrid MYT1L and a platinum(II) ligand L1Pt(dien)</i></p> <ul style="list-style-type: none"> • PDB DOI: https://doi.org/10.2210/pdb7EL7/pdb • NDB: 7EL7 • Classification: DNA • Organism(s): Homo sapiens • Mutation(s): No • Deposited: 2021-04-08 Released: 2021-12-15 • Deposition Author(s): Liu, L.-Y., Liu, W., Mao, Z.-W. • Funding Organization(s): National Science Foundation (NSF, China) <p>Experimental Data Snapshot</p> <ul style="list-style-type: none"> • Method: SOLUTION NMR • Conformers Calculated: 100 • Conformers Submitted: 15 • Selection Criteria: structures with the lowest energy
		2VRM		<p>2VRM</p> <p><i>Structure of human MAO B in complex with phenylethylhydrazine</i></p> <ul style="list-style-type: none"> • PDB DOI: https://doi.org/10.2210/pdb2VRM/pdb • Classification: OXIDOREDUCTASE • Organism(s): Homo sapiens • Expression System: Komagataella pastoris • Mutation(s): No • Membrane Protein: Yes • Deposited: 2008-04-09 Released: 2008-04-22 • Deposition Author(s): Binda, C., Wang, J., Li, M., Hubalek, F., Mattevi, A., Edmondson, D.E. <p>Experimental Data Snapshot</p> <ul style="list-style-type: none"> • Method: X-RAY DIFFRACTION • Resolution: 2.30 Å • R-Value Free: 0.246 • R-Value Work: 0.200 • R-Value Observed: 0.201

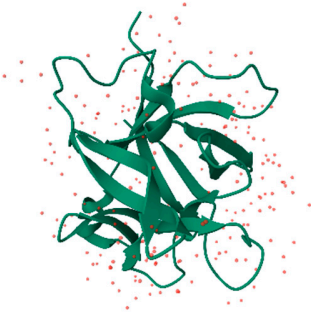
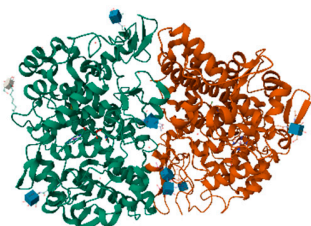
adrenaline	Target Protein	2HKK		<p>2HKK</p> <p><i>Carbonic anhydrase activators: Solution and X-ray crystallography for the interaction of adrenaline with various carbonic anhydrase isoforms</i></p> <ul style="list-style-type: none"> • PDB DOI: https://doi.org/10.2210/pdb2HKK/pdb • Classification: <u>LYASE</u> • Organism(s): <u>Homo sapiens</u> • Mutation(s): No • Deposited: 2006-07-05 Released: 2007-05-22 • Deposition Author(s): <u>Temperini, C., Innocenti, A., Vullo, D., Scozzafava, A., Supuran, C.T.</u> <p>Experimental Data Snapshot</p> <ul style="list-style-type: none"> • Method: X-RAY DIFFRACTION • Resolution: 1.90 Å • R-Value Free: 0.233 • R-Value Work: 0.186 • R-Value Observed: 0.188
		7BTS		<p>7BTS</p> <p><i>Structure of human beta1 adrenergic receptor bound to epinephrine and nanobody 6B9</i></p> <ul style="list-style-type: none"> • PDB DOI: https://doi.org/10.2210/pdb7BTS/pdb • Classification: <u>MEMBRANE PROTEIN</u> • Organism(s): <u>Tequatrovirus T4, Homo sapiens, Vicugna pacos</u> • Expression System: <u>Spodoptera frugiperda</u> • Mutation(s): Yes • Membrane Protein: <u>Yes</u> • Deposited: 2020-04-02 Released: 2020-12-02 • Deposition Author(s): <u>Xu, X., Kaindl, J., Clark, M., Hubner, H., Hirata, K., Sunahara, R., Gmeiner, P., Kobilka, B.K., Liu, X.</u> <p>Experimental Data Snapshot</p> <ul style="list-style-type: none"> • Method: X-RAY DIFFRACTION • Resolution: 3.13 Å • R-Value Free: 0.259 • R-Value Work: 0.235 • R-Value Observed: 0.237

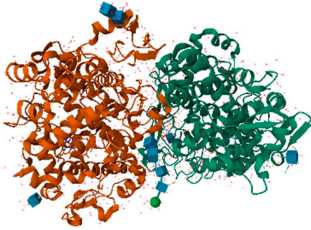
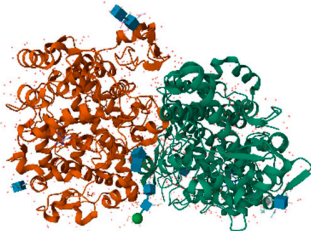
	Target Receptor	2RH1		<p>2RH1</p> <p><i>High resolution crystal structure of human B2-adrenergic G protein-coupled receptor.</i></p> <ul style="list-style-type: none"> • PDB DOI: https://doi.org/10.2210/pdb2RH1/pdb • Classification: <u>MEMBRANE PROTEIN / HYDROLASE</u> • Organism(s): <u>Homo sapiens, Tequatrovirus T4</u> • Expression System: <u>Spodoptera frugiperda</u> • Mutation(s): Yes • Membrane Protein: <u>Yes</u> • Deposited: 2007-10-05 Released: 2007-10-30 • Deposition Author(s): <u>Cherezov, V., Rosenbaum, D.M., Hanson, M.A., Rasmussen, S.G.F., Thian, F.S., Kobilka, T.S., Choi, H.J., Kuhn, P., Weis, W.I., Kobilka, B.K., Stevens, R.C., Accelerated Technologies Center for Gene to 3D Structure (ATCG3D), GPCR Network (GPCR)</u> <p>Experimental Data Snapshot</p> <ul style="list-style-type: none"> • Method: X-RAY DIFFRACTION • Resolution: 2.40 Å • R-Value Free: 0.232 • R-Value Work: 0.196 • R-Value Observed: 0.198
Cortisol	Target Protein	2VDX		<p>2VDX</p> <p><i>Crystal Structure of the reactive loop Cleaved Corticosteroid Binding Globulin</i></p> <ul style="list-style-type: none"> • PDB DOI: https://doi.org/10.2210/pdb2VDX/pdb • Classification: <u>TRANSPORT PROTEIN</u> • Organism(s): <u>Homo sapiens</u> • Expression System: <u>Escherichia coli BL21(DE3)</u> • Mutation(s): No • Deposited: 2007-10-13 Released: 2008-05-06 • Deposition Author(s): <u>Zhou, A., Wei, Z., Read, R.J.</u> <p>Experimental Data Snapshot</p> <ul style="list-style-type: none"> • Method: X-RAY DIFFRACTION • Resolution: 1.84 Å • R-Value Free: 0.241 • R-Value Work: 0.192 • R-Value Observed: 0.194



	Target Receptor	2VDY		<p>2VDY</p> <p><i>Crystal structure of the reactive loop cleaved Corticosteroid Binding Globulin complexed with Cortisol</i></p> <ul style="list-style-type: none"> • PDB DOI: https://doi.org/10.2210/pdb2VDY/pdb • Classification: TRANSPORT PROTEIN • Organism(s): <u>Homo sapiens</u> • Expression System: <u>Escherichia coli BL21(DE3)</u> • Mutation(s): No • Deposited: 2007-10-13 Released: 2008-05-13 • Deposition Author(s): <u>Zhou, A., Wei, Z., Read, R.J.</u> <p>Experimental Data Snapshot</p> <ul style="list-style-type: none"> • Method: X-RAY DIFFRACTION • Resolution: 2.30 Å • R-Value Free: 0.271 • R-Value Work: 0.210 • R-Value Observed: 0.213
		4P6X		<p>4P6X</p> <p><i>Crystal Structure of cortisol-bound glucocorticoid receptor ligand binding domain</i></p> <ul style="list-style-type: none"> • PDB DOI: https://doi.org/10.2210/pdb4P6X/pdb • Classification: HORMONE RECEPTOR/HORMONE ACTIVATOR • Organism(s): <u>Homo sapiens</u> • Expression System: <u>Escherichia coli K-12</u> • Mutation(s): Yes • Deposited: 2014-03-25 Released: 2014-04-16 • Deposition Author(s): <u>He, Y., Zhou, X.E., Tolbert, W.D., Powell, K., Melcher, K., Xu, H.E.</u> • Funding Organization(s): National Institutes of Health/National Institute of Diabetes and Digestive and Kidney Disease (NIH/NIDDK), AAF <p>Experimental Data Snapshot</p> <ul style="list-style-type: none"> • Method: X-RAY DIFFRACTION • Resolution: 2.50 Å • R-Value Free: 0.276 • R-Value Work: 0.246 • R-Value Observed: 0.248

TNF- α	Target Cytokine	6RMJ		<p>6RMJ</p> <p><i>Crystal structure of human NGR-TNF</i></p> <ul style="list-style-type: none"> • PDB DOI: https://doi.org/10.2210/pdb6RMJ/pdb • Classification: CYTOKINE • Organism(s): <u>Homo sapiens</u> • Expression System: <u>Escherichia coli</u> <u>BL21(DE3)</u> • Mutation(s): No • Deposited: 2019-05-07 Released: 2019-10-09 • Deposition Author(s): <u>Degano, M., Garau, G.</u> <p>Experimental Data Snapshot</p> <ul style="list-style-type: none"> • Method: X-RAY DIFFRACTION • Resolution: 2.65 Å • R-Value Free: 0.253 • R-Value Work: 0.209 • R-Value Observed: 0.211
	Target Receptor	5TLJ		<p>5TLJ</p> <p><i>COMPLEX BETWEEN HUMAN CD27 AND FAB FRAGMENTS OF ANTIBODIES M2177 AND M2191</i></p> <ul style="list-style-type: none"> • PDB DOI: https://doi.org/10.2210/pdb5TLJ/pdb • Classification: IMMUNE SYSTEM • Organism(s): <u>Mus musculus</u>, <u>Homo sapiens</u> • Expression System: <u>Homo sapiens</u>, <u>unidentified baculovirus</u> • Mutation(s): No • Deposited: 2016-10-11 Released: 2017-02-08 • Deposition Author(s): <u>Tepljakov, A., Obmolova, G., Malia, T., Gilliland, G.L.</u> <p>Experimental Data Snapshot</p> <ul style="list-style-type: none"> • Method: X-RAY DIFFRACTION • Resolution: 3.50 Å • R-Value Free: 0.356 • R-Value Work: 0.283 • R-Value Observed: 0.287

		6PE7		<p>6PE7</p> <p><i>Crystal Structure of ABBV-323 FAB</i></p> <ul style="list-style-type: none"> • PDB DOI: https://doi.org/10.2210/pdb6PE7/pdb • Classification: IMMUNE SYSTEM • Organism(s): <u>Homo sapiens</u> • Expression System: <u>Homo sapiens</u> • Mutation(s): No • Deposited: 2019-06-20 Released: 2019-08-14 • Deposition Author(s): <u>Argiriadi, M.A.</u> <p>Experimental Data Snapshot</p> <ul style="list-style-type: none"> • Method: X-RAY DIFFRACTION • Resolution: 1.74 Å • R-Value Free: 0.230 • R-Value Work: 0.196 • R-Value Observed: 0.198
IL-1 β	Target Receptor	4GAF		<p>4GAF</p> <p><i>Crystal structure of EBI-005, a chimera of human IL-1beta and IL-1Ra, bound to human Interleukin-1 receptor type 1</i></p> <ul style="list-style-type: none"> • PDB DOI: https://doi.org/10.2210/pdb4GAF/pdb • Classification: SIGNALING PROTEIN • Organism(s): <u>Homo sapiens</u> • Expression System: <u>Escherichia coli</u> • Mutation(s): No • Deposited: 2012-07-25 Released: 2013-02-20 • Deposition Author(s): <u>Hou, J., Townson, S.A., Kovalchin, J.T., Masci, A., Kiner, O., Shu, Y., King, B., Thomas, C., Garcia, K.C., Furfine, E.S., Barnes, T.M.</u> <p>Experimental Data Snapshot</p> <ul style="list-style-type: none"> • Method: X-RAY DIFFRACTION • Resolution: 2.15 Å • R-Value Free: 0.271 • R-Value Work: 0.215 • R-Value Observed: 0.218

		4GAI		<p>4GAI</p> <p><i>Crystal structure of EBI-005, a chimera of human IL-1beta and IL-1Ra</i></p> <ul style="list-style-type: none"> • PDB DOI: https://doi.org/10.2210/pdb4GAI/pdb • Classification: <u>SIGNALING PROTEIN</u> • Organism(s): <u>Homo sapiens</u> • Expression System: <u>Escherichia coli</u> • Mutation(s): No • Deposited: 2012-07-25 Released: 2013-02-20 • Deposition Author(s): <u>Hou, J., Townson, S.A., Kovalchin, J.T., Masci, A., Kiner, O., Shu, Y., King, B., Thomas, C., Garcia, K.C., Furfine, E.S., Barnes, T.M.</u> <p>Experimental Data Snapshot</p> <ul style="list-style-type: none"> • Method: X-RAY DIFFRACTION • Resolution: 1.49 Å • R-Value Free: 0.219 • R-Value Work: 0.187 • R-Value Observed: 0.189
COX-2	Target Protein	5JW1		<p>5JW1</p> <p><i>Crystal structure of Celecoxib bound to S121P murine COX-2 mutant</i></p> <ul style="list-style-type: none"> • PDB DOI: https://doi.org/10.2210/pdb5JW1/pdb • Classification: <u>OXIDOREDUCTASE</u> • Organism(s): <u>Mus musculus</u> • Expression System: <u>Spodoptera frugiperda</u> • Mutation(s): Yes • Deposited: 2016-05-11 Released: 2016-10-26 • Deposition Author(s): <u>Malkowski, M.G., Orlando, B.J.</u> <p>Experimental Data Snapshot</p> <ul style="list-style-type: none"> • Method: X-RAY DIFFRACTION • Resolution: 2.82 Å • R-Value Free: 0.226 • R-Value Work: 0.189 • R-Value Observed: 0.191

	Target Receptor	4E1G		<p>4E1G</p> <p><i>X-ray crystal structure of alpha-linolenic acid bound to the cyclooxygenase channel of cyclooxygenase-2</i></p> <ul style="list-style-type: none"> • PDB DOI: https://doi.org/10.2210/pdb4E1G/pdb • Classification: OXIDOREDUCTASE • Organism(s): <u>Mus musculus</u> • Expression System: <u>Spodoptera frugiperda</u> • Mutation(s): Yes • Deposited: 2012-03-06 Released: 2012-04-25 • Deposition Author(s): <u>Vecchio, A.J., Malkowski, M.G.</u> <p>Experimental Data Snapshot</p> <ul style="list-style-type: none"> • Method: X-RAY DIFFRACTION • Resolution: 2.10 Å • R-Value Free: 0.203 • R-Value Work: 0.159 • R-Value Observed: 0.161
		3TZI		<p>3TZI</p> <p><i>X-ray crystal structure of arachidonic acid bound in the cyclooxygenase channel of G533V murine COX-2</i></p> <ul style="list-style-type: none"> • PDB DOI: https://doi.org/10.2210/pdb3TZI/pdb • Classification: OXIDOREDUCTASE • Organism(s): <u>Mus musculus</u> • Expression System: <u>Spodoptera frugiperda</u> • Mutation(s): Yes • Deposited: 2011-09-27 Released: 2012-04-25 • Deposition Author(s): <u>Vecchio, A.J., Malkowski, M.G.</u> <p>Experimental Data Snapshot</p> <ul style="list-style-type: none"> • Method: X-RAY DIFFRACTION • Resolution: 2.15 Å • R-Value Free: 0.210 • R-Value Work: 0.170 • R-Value Observed: 0.172

LOX	Target Receptor	1YPO		<p>1YPO</p> <p><i>Human Oxidized Low Density Lipoprotein Receptor LOX-1 P3 1 21 Space Group</i></p> <ul style="list-style-type: none"> • PDB DOI: https://doi.org/10.2210/pdb1YPO/pdb • Classification: IMMUNE SYSTEM • Organism(s): <u>Homo sapiens</u> • Expression System: <u>Escherichia coli</u> • Mutation(s): No • Deposited: 2005-01-31 Released: 2005-02-08 • Deposition Author(s): <u>Park, H., Adsit, F.G., Boyington, J.C.</u> <p>Experimental Data Snapshot</p> <ul style="list-style-type: none"> • Method: X-RAY DIFFRACTION • Resolution: 3.00 Å • R-Value Free: 0.285 • R-Value Work: 0.228 • R-Value Observed: 0.228
		1YPU		<p>1YPU</p> <p><i>Human Oxidized Low Density Lipoprotein Receptor LOX-1 C2 Space Group</i></p> <ul style="list-style-type: none"> • PDB DOI: https://doi.org/10.2210/pdb1YPU/pdb • Classification: IMMUNE SYSTEM • Organism(s): <u>Homo sapiens</u> • Expression System: <u>Escherichia coli</u> • Mutation(s): No • Deposited: 2005-01-31 Released: 2005-02-08 • Deposition Author(s): <u>Park, H., Adsit, F.G., Boyington, J.C.</u> <p>Experimental Data Snapshot</p> <ul style="list-style-type: none"> • Method: X-RAY DIFFRACTION • Resolution: 2.05 Å • R-Value Free: 0.238 • R-Value Work: 0.183 • R-Value Observed: 0.183