Letters in Applied NanoBioScience
Open-Access Journal (ISSN: 2284-6808)

Article
Volume 15, Issue 1, 2026, 48
https://doi.org/10.33263/LIANBS151.048

Glycolytic Inhibition may not be a Pathway for Covid-19 Inhibition of 2-Deoxyglucose: Evidence from Computational Studies

Pooventhiran Thangaiyan [1,2,3], Jesudoss Santhanasamy Kasparraj [3], Ali A Khairbek [4], Korada Rajashekaraiah Shadakshara Murthy [5], Renjith Thomas [6,7,*]

1 Centre of Molecular Medicine and Diagnostics (COMManD), Saveetha Dental College and Hospitals, Saveetha Institute of Medical and Technical Sciences, Saveetha University, Chennai 600077, India; pooventhiran134@gmail.com
2 Department of Mechanical Engineering, University Centre for Research & Development, Chandigarh University, Gharuan, Mohali, Punjab, India
3 Department of Chemistry, K. Ramakrishnan College of Engineering (Autonomous), Affiliated to Anna University Chennai, Samayapuram 621112, Tamilnadu, India
4 Department of Chemistry, Faculty of Science, Tishreen University, Lattakia, Syrian Arab Republic
5 Department of Chemical Engineering, Siddaganga Institute of Technology, Tumkur -572103, India krsmurthy@sit.ac.in
6 Department of Chemistry, St Berchmans College (Autonomous), Changanassery 686101, Kerala, India
7 Centre for Theoretical and Computational Chemistry, St Berchmans College (Autonomous), Changanassery 686101, Kerala, India
* Correspondence: renjith@sbcollege.ac.in;

Received: 1.08.2023; Accepted: 7.07.2024; Published: 30.03.2026

Abstract: Using 2-deoxyglucose (2DG) as a therapeutic agent, the SARS-CoV-2 disease was healed in the present study. *Coronaviridae* and *Nidovirales* are the families that contain SARS-CoV-2. Coronavirus disease 19 (COVID-19) is a respiratory disease caused by the virus. Humans and some animals can be infected by these viruses. People were first infected with SARS-CoV-2 in 2019. 2DG and glucose, both ring and chain conformers interact with human hexokinase (PDB ID: 1QAH), human phosphoglucose isomerase (PDB ID: 1JLH), human phosphofructokinase (PDB ID: 4WL0), human fructose 1,6-bisphosphate aldolase (PDB ID: 4ALD), human triose phosphate isomerase (PDB ID: 6NLH), human glyceraldehyde-3-phosphate dehydrogenase (PDB ID: 3GPD), human phosphoglycerate kinase (PDB ID: 3C3C), human phosphoglycerate mutase (PDB ID: 1YJX), and human enolase (PDB ID: 4ZCW) explained by binding affinities, active sites of protein residues, favorable noncovalent, unfavorable noncovalent, and unsatisfied noncovalent interactions shown in tables and figures. From the molecular docking result, 2DG does not affect the glycolysis cycle.

Keywords: 2-deoxy-d-glucose; SARS-CoV-2; *in silico*; docking.

1. Introduction

The spread of the n-CoV-2 virus, first reported in Wuhan, China, and the subsequent COVID-19 pandemic are affecting the entire human population, exceeding all proportions [1,2]. Initially, the healthcare community was unable to develop an effective solution to the pandemic. Later, many antiviral drugs were repurposed to treat this virus. Later, the specific proteins of n-CoV-2 were identified, and their crystal structures were made public, which accelerated further research into drug development. Computational chemistry has helped to a

large extent to ascertain the suitability of new drug candidates and the repurposing of existing drugs. Molecular docking, molecular dynamics, QSAR analysis, and chemoinformatic studies have helped a lot in that direction.

Recently, the Defence Research and Development Organisation of India (DRDO) has come up with a compound called 2-deoxyglucose (2DG) (Figure 1), which could heal COVID complications. It is an analog of glucose. This compound has only one oxygen less than that of glucose. Hence, it is supposed to mimic glucose in several biological functions. It is reported that the compound competitively binds with the phosphoglucoisomerase enzyme in the second stage of glycolysis, forming a primary metabolic block [3]. 2DG has been absorbed by the body with the help of glucose absorption promoters. Hence, tumors or other fast-growing cells have an increased tendency to absorb the molecule. It led to this molecule being investigated as a potential glycolytic inhibitor for the treatment of cancer [4]. Clinical trials have shown that the drug is well tolerated in humans compared with other anticancer drugs [5], but the mechanism of action of this compound is not fully understood. Many scientists do not agree that the glycolytic block is the mechanism of the drug action [6]. This drug is now widely used in COVID-19 patients following clinical trials, but no published data or preprints are available in the scientific or public domain, as far as the authors are aware. This manuscript is not meant to comment on the clinical efficacy of 2DG for the treatment of the pandemic, but instead to show that glycolysis inhibition is not the mechanism of action, based on computational chemistry studies. Recently, many research groups have conducted molecular docking studies of bioactive molecules, including ligands and metal complexes, that bind to human proteins [7–10].

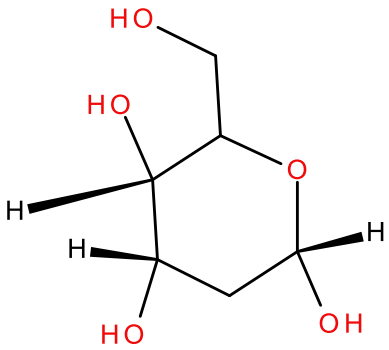

Figure 1. Structure (2D) of 2-deoxy glucose (2DG).

2. Materials and Methods

The open-chain and ring structures of 2DG and glucose were optimized at the B3LYP/6-311G(2d,p) level using Gaussian 09W [11], and these structures were used for further studies. It is believed that 2DG participates in glycolysis, like glucose, due to its structural similarity. Hence, we collected the structural files of the enzymes involved in the nine steps of human glycolysis from the protein data bank of the RCSB site [12]. The enzymes studied are human hexokinase (PDB ID: 1QAH) [13], human phosphoglucose isomerase (PDB ID: 1JLH) [14], human phosphofructokinase (PDB ID: 4WL0) [15], human fructose 1,6-bisphosphate aldolase (PDB ID: 4ALD) [16], human triose phosphate isomerase (PDB ID: 6NLH) [17], human glyceraldehyde-3-phosphate dehydrogenase (PDB ID: 3GPD) [18], human phosphoglycerate kinase (PDB ID: 3C3C) [19], human phosphoglycerate mutase (PDB ID: 1YJX) [20], and human enolase (PDB ID: 4ZCW) [21]. The molecular docking analysis

was performed using AutoDock Vina [22], BioDiscovery Studio, and other software packages [23].

3. Results and Discussion

3.1. Docking.

Molecular docking explains the biological applications of 2-deoxy-D-glucose (2DG) and D-glucose by structural (both chain and ring form) interactions with several proteins [24–33]. Table 1 shows the binding affinities of 2DG and glucose with human hexokinase (PDB ID: 1QAH) [13], human phosphoglucose isomerase (PDB ID: 1JLH)[14], human phosphofructokinase (PDB ID: 4WL0) [15], human fructose 1,6-bisphosphate aldolase (PDB ID: 4ALD) [16], human triose phosphate isomerase (PDB ID: 6NLH) [17], human glyceraldehyde-3-phosphate dehydrogenase (PDB ID: 3GPD) [18], human phosphoglycerate kinase (PDB ID: 3C3C) [19], human phosphoglycerate mutase (PDB ID: 1YJX) [20], and human enolase (PDB ID: 4ZCW) [21].

Table 1. Binding affinities of derivatives of 2DG and glucose.

Proteins with code	2DG_Chain	2DG_Ring	Glucose_Chain	Glucose_Ring
Human Hexokinase (PDB ID: 1QAH)	-4.4	-4.6	-5.0	-5.1
Human Phosphoglucose Isomerase (PDB ID: 1JLH)	-1.8	-1.9	-1.5	-2.0
Human Phosphofructokinase (PDB ID: 4WL0)	-5.5	-5.4	-5.6	-5.6
Human Fructose 1,6-bisphosphate Aldolase (PDB ID: 4ALD)	-5.4	-6.0	-5.2	-5.9
Human Triose Phosphate Isomerase (PDB ID: 6NLH)	-4.4	-5.0	-4.8	-5.4
Human Glyceraldehyde-3-Phosphate Dehydrogenase (PDB ID: 3GPD)	-4.8	-5.4	-5.1	-5.7
Human Phosphoglycerate Kinase (PDB ID: 3C3C)	-5.0	-5.2	-5.0	-5.8
Human Phosphoglycerate Mutase (PDB ID: 1YJX)	-5.1	-5.7	-5.1	-5.8
Human Enolase (PDB ID: 4ZCW)	-4.7	-6.3	-6.0	-6.4

Figures 2 and 3 display the skeletal structure and 2D structure of binding interactions of 2DG and D-glucose with human hexokinase protein. Figures S1a-S8a and Figures S1b-S8b show the skeletal structure and 2D structure of binding interactions of 2DG and glucose with human phosphoglucose isomerase, human phosphofructokinase, human fructose 1,6-bisphosphate aldolase, human triose phosphate isomerase, human glyceraldehyde-3-phosphate dehydrogenase, human phosphoglycerate kinase, human phosphoglycerate mutase, and human enolase, respectively.

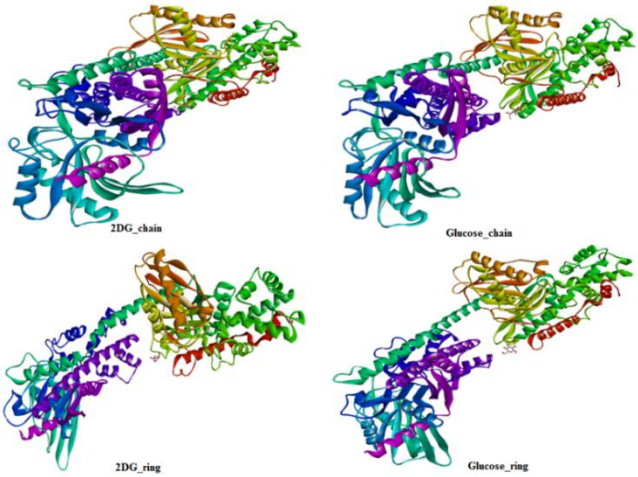

Figure 2. Skeletal structure of interactions of human hexokinase with 2DG and glucose.

Tables S1 and S2 show the label of protein residues (A and R are parent chains), and non-bond interactions are favorable, unfavorable, and unsatisfied bond interactions of 2DG and D-glucose with all referred proteins, respectively.

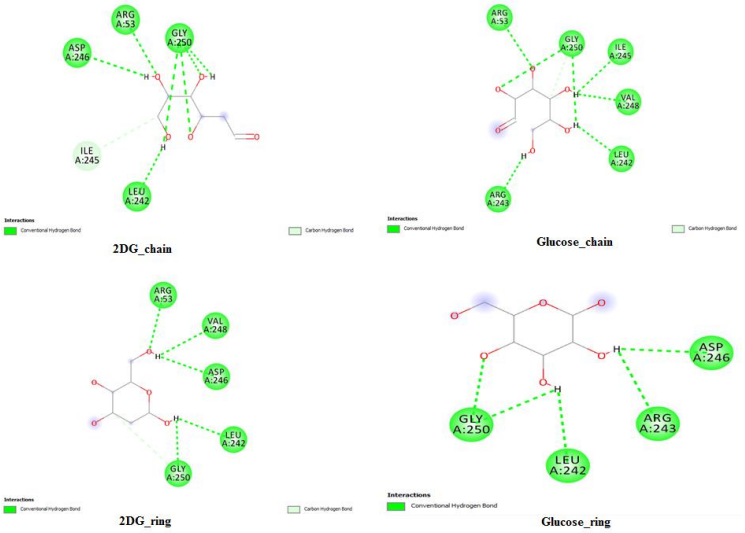

Figure 3. 2D structure of interactions of human hexokinase with 2DG and glucose.

3.1.1. Favourable non-bonds.

From Table S1 and Table S2 shows favourable non-bonds of 2DG_chain, glucose-chain, 2DG_rind and glucose_ring structure of interactions with human hexokinase protein having 9-conventional hydrogen bonds and 1-carbon hydrogen bond by five residues, 7-conventional hydrogen bonds and 1-carbon hydrogen bond by six residues, 5-conventional hydrogen bonds and 1-carbon hydrogen bond by five residues and 10-conventional hydrogen bonds by four residues respectively; similarly, with human phosphoglucose isomerase having 4-conventional hydrogen bonds by two residues, 4-conventional hydrogen bonds by two residues, 7-conventional hydrogen bonds by two residues and 3-conventional hydrogen bonds by one residue respectively; like, with human phosphofructokinase having 6-conventional hydrogen bonds and 2-carbon hydrogen bonds by four residues, 9-conventional hydrogen bonds and 1-carbon hydrogen bond by eight residues, 6-conventional hydrogen bonds and 1-carbon hydrogen bond by six residues and 5-conventional hydrogen bonds and 1-carbon hydrogen bond by six residues respectively; alike, with human fructose 1,6-bisphosphate aldolase having 10-conventional hydrogen bonds by seven residues, 10-conventional hydrogen bonds by six residues, 5-conventional hydrogen bonds and 1-carbon hydrogen bond by five residues and 7-conventional hydrogen bonds by six residues respectively; while, with human triose phosphate isomerase having 6-conventional hydrogen bonds and 1-carbon hydrogen bond by four residues, 9-conventional hydrogen bonds and 1-carbon hydrogen bond by six residues, 7-conventional hydrogen bonds by five residues and 4-conventional hydrogen bonds and 5-carbon hydrogen bonds by four residues respectively; likewise, with human glyceraldehyde-3-phosphate dehydrogenase having 7-conventional hydrogen bonds and -carbon hydrogen bonds by five residues, 5-conventional hydrogen bonds and 1-carbon hydrogen bond by four residues, 5-conventional hydrogen bonds by four residues and 8-conventional hydrogen bonds by six residues respectively; similarly, human phosphoglycerate kinase having 7-conventional hydrogen bonds by six residues, 11-conventional hydrogen bonds and 1-carbon hydrogen bond by eight residues, 7-conventional hydrogen bonds by six residues and 7-conventional hydrogen bonds by seven residues respectively; alike, with human

phosphoglycerate mutase having 7-conventional hydrogen bonds and 1-carbon hydrogen bond by six residues, 7-conventional hydrogen bonds by seven residues, 5-conventional hydrogen bonds and 1-carbon hydrogen bond by four residues and 7-conventional hydrogen bonds by five residues respectively; compatibly, with human enolase having 8-conventional hydrogen bonds by five residues, 12-conventional hydrogen bonds and 3-carbon hydrogen bonds by eleven residues, 10-conventional hydrogen bonds and 3-carbon hydrogen bonds by eight residues and 10-conventional hydrogen bonds and 3-carbon hydrogen bonds by ten residues respectively.

3.1.2. Unfavourable non-bonds.

From Table S1 and Table S2 shows unfavourable non-bonds of human hexokinase having one acceptor-acceptor with 2DG_chain and donor-donor with glucose_ring; alike, human fructose 1,6-bisphosphate aldolase having one and three donor-donor interactions with glucose_chain and glucose_ring respectively; like, human triose phosphate isomerase having one donor-donor interaction with 2DG_chain and glucose_chain each, and one acceptor-acceptor interaction with glucose_ring; similarly, human glyceraldehyde-3-phosphate dehydrogenase having two donor-donor interactions with 2DG_chain, two acceptor-acceptor with glucose_chain, and one donor-donor interactions with glucose_ring; likewise, human phosphoglycerate kinase having two, two, and three donor-donor interactions with 2DG_chain, glucose_chain, and glucose_ring respectively; alike, human phosphoglycerate mutase having one, three, and two donor-donor interactions with 2DG_chain, glucose_chain, and glucose_ring respectively; in the same way, human enolase having one donor-donor and acceptor-acceptor interactions with 2DG_chain and 2DG_ring, and one donor-donor interaction with glucose_chain. Tables S1 and S2 show unsatisfied non-bond sites of 2DG_chain, glucose-chain, 2DG_rind, and glucose_ring structure of interactions with all referred proteins [37–43].

From these results, 2-deoxy-D-glucose (2DG) does not affect the glycolysis cycle.

4. Conclusions

A variety of human proteins were studied using this *in silico* study, and 2-deoxy-D-glucose (2DG) was not found to interfere with the glycolysis cycle. Additionally, both ring and chain conformers contained 2DG and glucose docked with all nine human proteins. 2DG of the ring and chain with open and/or closed structures showed favorable non-bonds with different conventional and carbon-hydrogen bonds with the listed protein residues. Similarly, 2DG showed unfavorable non-bonds with a different number of steric hindrances between bulky sites and lone-pair hindrances if nucleophiles with the listed protein residues. This electrostatic information is required for the bioactivity of 2DG in the human body.

Supplementary Materials

The supplementary data associated with this article include Table S1, which lists the specific protein residues of human glycolytic enzymes that bind to 2DG and glucose molecules, and Table S2, which details the favorable and unfavorable non-bonding interaction parameters, including hydrogen bond distances and specific atom interactions for the ligand-protein complexes. Additionally, Figures S1 (a and b) through S8 (a and b) provide comprehensive visual representations of these molecular interactions, depicting both the 3D skeletal structures

and 2D interaction diagrams for human Phosphoglucose Isomerase, Phosphofructokinase, Fructose 1,6-bisphosphate Aldolase, Triose Phosphate Isomerase, Glyceraldehyde-3-Phosphate Dehydrogenase, Phosphoglycerate Kinase, Phosphoglycerate Mutase, and Enolase complexed with 2DG and glucose.

Author Contributions

Conceptualization, P.T.; methodology, P.T. and R.T.; software, R.T; validation, J.S.K., K.R.S.M. and R.T.; formal analysis, A.A.K. and K.R.S.M.; investigation, P.T. and J.S.K.; resources, R.T.; data curation, P.T, J.S.K. and K.R.S.M.; writing—original draft preparation, P.T., J.S.K., K.R.S.M. and R.T.; writing—review and editing, P.T., J.S.K., A.A.K., K.R.S.M. and R.T.; visualization, P.T. and J.S.K.; supervision, R.T.; project administration, R.T.. All authors have read and agreed to the published version of the manuscript.

Institutional Review Board Statement

Not applicable.

Informed Consent Statement

Not Applicable.

Data Availability Statement

Data supporting the findings of this study are available upon reasonable request from the corresponding author.

Funding

No funding received.

Acknowledgments

SEAGrid (www.seagrid.org) is acknowledged for computational resources and services for the selected results used in this publication.

Conflicts of Interest

The authors declare no conflict of interest.

References

1. Wu, Y.-C.; Chen, C.-S.; Chan, Y.-J. The outbreak of COVID-19: An overview. *J. Chin. Med. Assoc*. **2020**, *83*, 217–220, https://doi.org/10.1097/JCMA.0000000000000270.
2. Yuen, K.-S.; Ye, Z.W.; Fung, S.-Y.; Chan, C.-P.; Jin, D.-Y. SARS-CoV-2 and COVID-19: The most important research questions. *Cell Biosci*. **2020**, *10*, 40, https://doi.org/10.1186/s13578-020-00404-4.
3. Wick, A.N.; Drury, D.R.; Nakada, H.I.; Wolfe, J.B.; Britton, B.; Grabowski, R. Localization Of The Primary Metabolic Block Produced By 2-Deoxyglucose. *J. Biol. Chem*. **1957**, *224*, 963–969, https://doi.org/10.1016/S0021-9258(18)64988-9.
4. Pelicano, H.; Martin, D.S.; Xu, R.H.; Huang, P. Glycolysis inhibition for anticancer treatment. *Oncogene* **2006**, *25*, 4633–4646, https://doi.org/10.1038/sj.onc.1209597.
5. Raez, L.E.; Papadopoulos, K.; Ricart, A.D.; Chiorean, E.G.; DiPaola, R.S.; Stein, M.N.; Rocha Lima, C.M.; Schlesselman, J.J.; Tolba, K.; Langmuir, V.K.; Kroll, S.; Jung, D.T.; Kurtoglu, M.; Rosenblatt, J.;

Lampidis, T.J. A phase I dose-escalation trial of 2-deoxy-d-glucose alone or combined with docetaxel in patients with advanced solid tumors. *Cancer Chemother. Pharmacol.* **2013**, *71*, 523–530, https://doi.org/10.1007/s00280-012-2045-1.

6. Ralser, M.; Wamelink, M.M.; Struys, E.A.; Joppich, C.; Krobitsch, S.; Jakobs, C.; Lehrach, H. A catabolic block does not sufficiently explain how 2-deoxy-d-glucose inhibits cell growth. *Proc. Natl. Acad. Sci.* **2008**, *105*, 17807–17811, https://doi.org/10.1073/pnas.0803090105.
7. Medimagh, M.; Issaoui, N.; Gatfaoui, S.; Al-Dossary, O.; S. Kazachenko, A.; Marouani, H.; Wojcik, M.J. Molecular modeling and biological activity analysis of new organic-inorganic hybrid: 2-(3,4-dihydroxyphenyl) ethanaminium nitrate. *J. King Saud Univ. Sci.* **2021**, *33*, 101616, https://doi.org/10.1016/j.jksus.2021.101616.
8. Noureddine, O.; Issaoui, N.; Gatfaoui, S.; Al-Dossary, O.; Marouani, H. Quantum chemical calculations, spectroscopic properties and molecular docking studies of a novel piperazine derivative. *J. King Saud Univ. Sci.* **2021**, *33*, 101283, https://doi.org/10.1016/j.jksus.2020.101283.
9. Mhadhbi, N.; Issaoui, N.; Hamadou, W.S.; Alam, J.M.; Elhadi, A.S.; Adnan, M.; Naïli, H.; Badraoui, R. Physico-Chemical Properties, Pharmacokinetics, Molecular Docking and In-Vitro Pharmacological Study of a Cobalt (II) Complex Based on 2-Aminopyridine. *ChemistrySelect* **2022**, *7*, e202103592, https://doi.org/10.1002/slct.202103592.
10. Gatfaoui, S.; Issaoui, N.; Roisnel, T.; Marouani, H. Synthesis, experimental and computational study of a non-centrosymmetric material 3-methylbenzylammonium trioxonitrate. *J. Mol. Struct.* **2020**, *1225*, 129132, https://doi.org/10.1016/j.molstruc.2020.129132.
11. Frisch, M.J.; Trucks, G.W.; Schlegel, H.B.; Scuseria, G.E.; Robb, M.A.; Cheeseman, J.R.; Scalmani, G.; Barone, V.; Mennucci, B.; Petersson, G.A.; Nakatsuji, H.; Caricato, M.; Li, X.; Hratchian, H.P.; Izmaylov, A.F.; Bloino, J.; Zheng, G.; Sonnenberg, J.L.; Hada, M.; Ehara, M.; Toyota, K.; Fukuda, R.; Hasegawa, J.; Ishida, M.; Nakajima, T.; Honda, Y.; Kitao, O.; Nakai, H.; Vreven, T.; Montgomery Jr. J.A; Peralta, J.E.; Ogliaro, F.; Bearpark, M.; Heyd, J.J.; Brothers, E.; Kudin, K.N.; Staroverov, V.N.; Kobayashi, R.; Normand, J.; Raghavachari, K.; Rendell, A.; Burant, J.C.; Iyengar, S.S.; Tomasi, J.; Cossi, M.; Rega, N.; Millam, J.M.; Klene, M.; Knox, J.E.; Cross, J.B.; Bakken, V.; Adamo, C.; Jaramillo, J.; Gomperts, R.; Stratmann, R.E.; Yazyev, O.; Austin, A.J.; Cammi, R.; Pomelli, C.; Ochterski, J.W.; Martin, R.L.; Morokuma, K.; Zakrzewski, V.G.; Voth, G.A.; Salvador, P.; Dannenberg, J.J.; Dapprich, S.; Daniels, A.D.; Farkas, O.; Foresman, J.B.; Ortiz, J.V.; Cioslowski, J.; Fox, D.J. Gaussian09 Revision D.01. **2013**.
12. Burley, S.K.; Berman, H.M.; Bhikadiya, C.; Bi, C.; Chen, L.; Di Costanzo, L.; Christie, C.; Dalenberg, K.; Duarte, J.M.; Dutta, S.; Feng, Z.; Ghosh, S.; Goodsell, D.S.; Green, R.K.; Guranović, V.; Guzenko, D.; Hudson, B.P.; Kalro, T.; Liang, Y.; Lowe, R.; Namkoong, H.; Peisach, E.; Periskova, I.; Prlić, A.; Randle, C.; Rose, A.; Rose, P.; Sala, R.; Sekharan, M.; Shao, C.; Tan, L.; Tao, Y.-P.; Valasatava, Y.; Voigt, M.; Westbrook, J.; Woo, J.; Yang, H.; Young, J.; Zhuravleva, M.; Zardecki, C. RCSB Protein Data Bank: biological macromolecular structures enabling research and education in fundamental biology, biomedicine, biotechnology and energy. *Nucleic Acids Res.* **2019**, *47*, D464–D474, https://doi.org/10.1093/nar/gky1004.
13. Berman, H.; Henrick, K.; Nakamura, H. Announcing the worldwide Protein Data Bank. *Nat. Struct. Mol. Biol.* **2003**, *10*, 980, https://doi.org/10.1038/nsb1203-980.
14. Cordeiro, A.T.; Godoi, P.H.C.; Silva, C.H.T.P.; Garratt, R.C.; Oliva, G.; Thiemann, O.H. Crystal structure of human phosphoglucose isomerase and analysis of the initial catalytic steps. *Biochim. Biophys. Acta - Proteins Proteom.* **2003**, *1645*, 117–122, https://doi.org/10.1016/S1570-9639(02)00464-8.
15. Kloos, M.; Brüser, A.; Kirchberger, J.; Schöneberg, T.; Sträter, N. Crystal structure of human platelet phosphofructokinase-1 locked in an activated conformation. *Biochem. J.* **2015**, *469*, 421–432, https://doi.org/10.1042/BJ20150251.
16. Dalby, A.; Dauter, Z.; Littlechild, J.A. Crystal structure of human muscle aldolase complexed with fructose 1,6-bisphosphate: Mechanistic implications. *Protein Sci.* **1999**, *8*, 291–297, https://doi.org/10.1110/ps.8.2.291.
17. Roland, B.P.; Richards, K.R.; Hrizo, S.L.; Eicher, S.; Barile, Z.J.; Chang, T.-C.; Savon, G.; Bianchi, P.; Fermo, E.; Ricerca, B.M.; Tortorolo, L.; Vockley, J.; VanDemark, A.P.; Palladino, M.J. Missense variant in *TPI1* (Arg189Gln) causes neurologic deficits through structural changes in the triosephosphate isomerase catalytic site and reduced enzyme levels in vivo. *Biochim. Biophys. Acta - Mol. Basis Dis.* **2019**, *1865*, 2257–2266, https://doi.org/10.1016/j.bbadis.2019.05.002.
18. Mercer, W.D.; Winn, S.I.; Watson, H.C. Twinning in crystals of human skeletal muscle $_D$-glyceraldehyde-

3-phosphate dehydrogenase. *J. Mol. Biol*. **1976**, *104*, 277–283, https://doi.org/10.1016/0022-2836(76)90013-9.
19. Gondeau, C.; Chaloin, L.; Lallemand, P.; Roy, B.; Périgaud, C.; Barman, T.; Varga, A.; Vas, M.; Lionne, C.; Arold, S.T. Molecular basis for the lack of enantioselectivity of human 3-phosphoglycerate kinase. *Nucleic Acids Res*. **2008**, *36*, 3620–3629, https://doi.org/10.1093/nar/gkn212.
20. Wang, Y.; Wei, Z.; Liu, L.; Cheng, Z.; Lin, Y.; Ji, F.; Gong, W. Crystal structure of human B-type phosphoglycerate mutase bound with citrate. *Biochem. Biophys. Res. Commun*. **2005**, *331*, 1207–1215, https://doi.org/10.1016/j.bbrc.2005.03.243.
21. Leonard, P.G.; Satani, N.; Maxwell, D.; Lin, Y.-H.; Hammoudi, N.; Peng, Z.; Pisaneschi, F.; Link, T.M.; Lee, G.R.; Sun, D.; Prasad, B.A.B.; Di Francesco, M.E.; Czako, B.; Asara, J.M.; Wang, Y.A.; Bornmann, W.; DePinho, R.A.; Muller, F.L. SF2312 is a natural phosphonate inhibitor of enolase. *Nat. Chem. Biol*. **2016**, *12*, 1053–1058, https://doi.org/10.1038/nchembio.2195.
22. Trott, O.; Olson, A.J. AutoDock Vina: Improving the speed and accuracy of docking with a new scoring function, efficient optimization, and multithreading. *J. Comput. Chem*. **2009**, *31*, 455-461, https://doi.org/10.1002/jcc.21334.
23. Discovery Studio BIOVA, Discov. Stud. Client V17, San Diego, *Dassault Syst*. **2017**.
24. Pooventhiran, T.; Marondedze, E.F.; Govender, P.P.; Bhattacharyya, U.; Rao, D.J.; Aazam, E.S.; Kuthanapillil, J.M.; E, T.J.; Thomas, R. Energy and reactivity profile and proton affinity analysis of rimegepant with special reference to its potential activity against SARS-CoV-2 virus proteins using molecular dynamics. *J. Mol. Model*. **2021**, *27*, 276, https://doi.org/10.1007/s00894-021-04885-z.
25. Surendar, P.; Pooventhiran, T.; Al-Zaqri, N.; Rajam, S.; Jagadeeswara Rao, D.; Thomas, R. Synthesis of three quasi liquid Schiff bases between hexanal and adenine, cytosine, and *l*-leucine, structural interpretation, quantum mechanical studies and biological activity prediction. *J. Mol. Liq*. **2021**, *341*, 117305, https://doi.org/10.1016/j.molliq.2021.117305.
26. Suryanarayana, K.; Robert, A.R.; Kerru, N.; Pooventhiran, T.; Thomas, R.; Maddila, S.; Jonnalagadda, S.B. Design, synthesis, anticancer activity and molecular docking analysis of novel dinitrophenylpyrazole bearing 1,2,3-triazoles. *J. Mol. Struct*. **2021**, *1243*, 130865, https://doi.org/10.1016/j.molstruc.2021.130865.
27. Yeddu, S.P.; Thangaiyan, P.; Veeraiah, A.; Vijay, D.; Srikanth, K.E.; Irfan, A.; Thomas, R. Vibrational Spectral Studies , Quantum Mechanical Properties , and Biological Activity Prediction and Inclusion Molecular Self-Assembly Formation of N-N ' - Dimethylethylene Urea. *Biointerface Res. Appl. Chem*. **2022**, *12*, 3996–4017, https://doi.org/10.33263/BRIAC123.39964017.
28. Pooventhiran, T.; Bhattacharyya, U.; Rao, D.J.; Chandramohan, V.; Karunakar, P.; Irfan, A.; Mary, Y.S.; Thomas, R. Detailed spectra, electronic properties, qualitative non-covalent interaction analysis, solvatochromism, docking and molecular dynamics simulations in different solvent atmosphere of cenobamate. *Struct. Chem*. **2020**, *31*, 2475-2485, https://doi.org/10.1007/s11224-020-01607-8.
29. Loke, S.K.; Pagadala, E.; Srinivasadesikan, V.; Thanapaul, R.J.R.S.; Pooventhiran, T.; Thomas, R.; Naganjaneyulu, G.; Kottalanka, R.K. Unprecedented biological evaluation of Zn(II) complexes supported by "Self-adjustable" acyclic diiminodipyrromethane Schiff's bases: DFT, molecular docking; biological activity studies. *Inorg. Chem. Commun*. **2021**, *133*, 108936, https://doi.org/10.1016/j.inoche.2021.108936.
30. Bakht, M.A.; Pooventhiran, T.; Thomas, R.; Kamal, M.; Din, I.U.; Rehman, N.U.; Ali, I.; Ajmal, N.; Ahsan, M.J. Synthesis and Biological Evaluation of Octahydroquinazolinones as Phospholipase A2, and Protease Inhibitors: Experimental and Theoretical Exploration. *Molecules* **2023**, *28*, 1994, https://doi.org/10.3390/molecules28041944.
31. Begum, S.R.; Rao, D.J.; Rao, K.V.R.; Ramakrishna, Y.; Elangovan, N.; Pooventhiran, T.; Thomas, R. Spectral Characterization and Quantum Mechanical Studies of 5-Amino-2-(6-(2-Hydroxyethyl)-3-Oxononyl) Cyclohex-2-Enone Isolated from a Marine Algae. *Biointerface Res. Appl. Chem*. **2023**, *13*, 413, https://doi.org/10.33263/BRIAC135.413.
32. Daoudi, W.; Guo, L.; Azzouzi, M.; Pooventhiran, T.; Boutaybi, A.E.; Lamghafri, S.; Oussaid, A.; El Aatiaoui, A. Evaluation of the corrosion inhibition of mild steel by newly synthesized imidazo[1,2-a]pyridine derivatives: experimental and theoretical investigation. *J. Adhes. Sci. Technol*. **2023**, *37*, 2944-2967, https://doi.org/10.1080/01694243.2023.2175296.
33. Tabassum, S.; Thangaiyan, P.; Govindaraju, S.; Daniel, N.K.; Thomas, R. Pyrazole Derivative Containing Naphthalene Moiety: Cytotoxocity (Breast and Cervical Cancer), Antibacterial and Antifungal Studies Using Experimental and Theoretical Tools. *Polycycl. Aromat. Compd*. **2022**, *43*, 8544-8561,

https://doi.org/10.1080/10406638.2022.2149564.
34. Anaikutti, P.; Selvaraj, M.; Prabhakaran, J.; Pooventhiran, T.; Jeyakumar, T.C.; Thomas, R.; Makam, P. Indolyl-4H-chromenes: Multicomponent one-pot green synthesis, *in vitro* and *in silico*, anticancer and antioxidant studies. *J. Mol. Struct*. **2022**, *1266*, 133464, https://doi.org/10.1016/j.molstruc.2022.133464.
35. Surendar, P.; Pooventhiran, T.; Rajam, S.; Rao, D.J.; Manigandan, N.; Irfan, A.; Thomas, R. Organic quasi-liquid Schiff bases from biomolecules: Synthesis, structure and quantum mechanical studies. *Biointerface Res. Appl. Chem*. **2023**, *13*, 107, https://doi.org/10.33263/BRIAC132.107.
36. Surendar, P.; Pooventhiran, T.; Rajam, S.; Irfan, A.; Thomas, R. Schiff Bases from α-ionone with Adenine, Cytosine, and *l*-leucine Biomolecules: Synthesis, Structural Features, Electronic Structure, and Medicinal Activities. *J. Comput. Biophys. Chem*. **2022**, *21*, 1–22, https://doi.org/10.1142/S2737416522500016.
37. Alsalme, A.; Pooventhiran, T.; Al-Zaqri, N.; Rao, D.J.; Rao, S.S.; Thomas, R. Modelling the structural and reactivity landscapes of tucatinib with special reference to its wavefunction-dependent properties and screening for potential antiviral activity. *J. Mol. Model*. **2020**, *26*, 341, https://doi.org/10.1007/s00894-020-04603-1.
38. Al-Zaqri, N.; Pooventhiran, T.; Alsalme, A.; Warad, I.; John, A.M.; Thomas, R. Structural and physico-chemical evaluation of melatonin and its solution-state excited properties, with emphasis on its binding with novel coronavirus proteins. *J. Mol. Liq*. **2020**, *318*, 114082, https://doi.org/10.1016/j.molliq.2020.114082.
39. Alharthi, F.A.; Al-Zaqri, N.; Alsalme, A.; Al-Taleb, A.; Pooventhiran, T.; Thomas, R.; Rao, D.J. Excited-state electronic properties, structural studies, noncovalent interactions, and inhibition of the novel severe acute respiratory syndrome coronavirus 2 proteins in Ripretinib by first-principle simulations. *J. Mol. Liq*. **2021**, *324*, 115134, https://doi.org/10.1016/j.molliq.2020.115134.
40. Al-Zaqri, N.; Pooventhiran, T.; Alharthi, F.A.; Bhattacharyya, U.; Thomas, R. Structural investigations, quantum mechanical studies on proton and metal affinity and biological activity predictions of selpercatinib. *J. Mol. Liq*. **2021**, *325*, 114765, https://doi.org/10.1016/j.molliq.2020.114765.
41. Al-Zaqri, N.; Pooventhiran, T.; Rao, D.J.; Alsalme, A.; Warad, I.; Thomas, R. Structure, conformational dynamics, quantum mechanical studies and potential biological activity analysis of multiple sclerosis medicine ozanimod. *J. Mol. Struct*. **2021**, *1227*, 129685, https://doi.org/10.1016/j.molstruc.2020.129685.
42. Surendar, P.; Pooventhiran, T.; Rajam, S.; Bhattacharyya, U.; Bakht, M.A.; Thomas, R. Quasi liquid Schiff bases from *trans*-2-hexenal and cytosine and *l*-leucine with potential antieczematic and antiarthritic activities: Synthesis, structure and quantum mechanical studies. *J. Mol. Liq*. **2021**, *334*, 116448, https://doi.org/10.1016/j.molliq.2021.116448.
43. Srikanth, K.E.; Veeraiah, A.; Pooventhiran, T.; Thomas, R.; Solomon, K.A.; Soma Raju, C.J.; Latha, J.N.L. Detailed molecular structure (XRD), conformational search, spectroscopic characterization (IR, Raman, UV, fluorescence), quantum mechanical properties and bioactivity prediction of a pyrrole analogue. *Heliyon* **2020**, *6*, e04106, https://doi.org/10.1016/j.heliyon.2020.e04106.

Publisher's Note & Disclaimer

Supplementary materials

Table S1. Name and label of proteins residues binding with 2DG and glucose molecules.

Molecules	Label of protein residues
Human Hexokinase (PDB ID: 1QAH)	
2DG_chain	ARG A:53, LEU A:242, ILE A:245, ASP A:246 and GLY A:250
Glucose_chain	ARG A:50, LEU A:242, ARG A:243, ILE A:245, VAL A:248 and GLY A:250
2DG_ring	ARG A:53, LEU A:242, ASP A:246, VAL A:248 and GLY A:250
Glucose_ring	LEU A:242, ARG A:243, ASP A:246 and GLY A:250
Human Phosphoglucose Isomerase (PDB ID: 1JLH)	
2DG_chain	GLU A:226 and GLN A:230
Glucose_chain	GLN A:230 and LYS A:233
2DG_ring	GLN A:230 and LYS A:233
Glucose_ring	GLN A:230
Human Phosphofructokinase (PDB ID: 4WL0)	
2DG_chain	GLY A:545, SER A:546, ASP A:547 and GLU A:748
Glucose_chain	ASN A:541, VAL A:543, GLY A:545, SER A:546, ASP A:547, GLU A:748, GLN A:749 and TRP A:751
2DG_ring	VAL A:543, GLY A:545, SER A:546, ASP A:547, GLN A:738 and GLU A:748
Glucose_ring	GLY A:545, SER A:546, ASP A:547, ILE A:722, SER A:723 and GLU A:748
Human Fructose 1,6-bisphosphate Aldolase (PDB ID: 4ALD)	
2DG_chain	LYS A:229, SER A:271, GLY A:272, GLY A:273, SER A:300, GLY A:302 and ARG A:303
Glucose_chain	ARG A:42, LYS A:146, LYS A:229, SER A:300, GLY A:302 and ARG A:303
2DG_ring	LEU A:63, VAL A:69, ASN A:70, ILE A:73 and LYS A:100
Glucose_ring	ASP A:33, GLU A:34, ARG A:42, LYS A:229, SER A:300 and ARG A:303
Human Triose Phosphate Isomerase (PDB ID: 6NLH)	
2DG_chain	ASN A:11, GLN A:64, GLU A:97 and ARG A:98
Glucose_chain	GLY A:209, GLY A:210, VAL A:212, ILE A:230, GLY A:232 and ALA A:234
2DG_ring	GLU A:165, GLY A:209, GLY A:210, LEU A:230 and GLY A:232
Glucose_ring	ASN A:11, GLN A:64, GLU A:97 and ARG A:98
Human Glyceraldehyde-3-Phosphate Dehydrogenase (PDB ID: 3GPD)	
2DG_chain	GLY R:9, ASN R:33, ASP R:34, PRO R:35, THR R:98
Glucose_chain	ASP R:8, ASN R:33, ASP R:34 and PRO R:35
2DG_ring	ASN R:33, ASP R:34, GLU R:78 and THR R:98
Glucose_ring	ASP R:8, GLY R:9, ASN R:33, ASP R:34, THR R:98 and VAL R:100
Human Phosphoglycerate Kinase (PDB ID: 3C3C)	
2DG_chain	ASN A:25, ARG A:38, HIS A:62, ARG A:122, GLY A:166 and GLY A:396
Glucose_chain	ARG A:38, HIS A:62, ARG A:65, ARG A:122, GLY A:166, HIS A:169, GLY A:394 and GLY A:396
2DG_ring	ASP A:23, ASN A:25, ARG A:38, HIS A:169, ARG A:170 and GLY A:394
Glucose_ring	ARG A:38, HIS A:62, ARG A:65, GLY A:166, ARG A:170, GLY A:394, and GLY A:396
Human Phosphoglycerate Mutase (PDB ID: 1YJX)	
2DG_chain	ARG A:10, ASN A:17, ARG A:21, SER A:23, ARG A:90 and ASN A:188
Glucose_chain	ARG A:10, SER A:14, ARG A:21, SER A:23, ARG A:62, GLU A:89 and LYS A:100
2DG_ring	GLU A:89, ARG A:90, ARG A:116 and ASN A:188
Glucose_ring	ARG A:10, ASN A:17, ARG A:21, SER A:23 and GLU A:89
Human Enolase (PDB ID: 4ZCW)	
2DG_chain	ARG A:32, LYS A:120, GLU A:377, ASP A:378 and THR A:379
Glucose_chain	GLN A:166, GLU A:167, GLU A:210, ASP A:245, GLU A:293, ASP A:318, LYS A:343, HIS A:371, ARG A:372, SER A:373 and LYS A:394
2DG_ring	SER A:40, GLN A:166, GLU A:167, GLU A:210, LYS A:343, HIS A:371, ARG A:372 and SER A:373
Glucose_ring	GLY A:38, ALA A:39, SER A:40, GLU A:167, GLU A:210, ASP A:245, ASP A:318, LYS A:343, HIS A:371 and SER A:373

Table S2. Non-bond interactions of 2DG and glucose

FAVOURABLE NON-BOND						
Distance (Å)	**Category**	**Type**	**From**	**From Chemistry**	**To**	**To Chemistry**
Human Hexokinase (PDB ID: 1QAH)						
2DG_chain						
2.39	Hydrogen Bond	Conventional Hydrogen Bond	A:ARG53:HH12	H-Donor	:UNK0:O	H-Acceptor
2.34	Hydrogen Bond	Conventional Hydrogen Bond	A:ARG53:HH22	H-Donor	:UNK0:O	H-Acceptor
2.00	Hydrogen Bond	Conventional Hydrogen Bond	A:GLY250:HN	H-Donor	:UNK0:O	H-Acceptor

2.92	Hydrogen Bond	Conventional Hydrogen Bond	A:GLY250:HN	H-Donor	:UNK0:O	H-Acceptor
2.67	Hydrogen Bond	Conventional Hydrogen Bond	:UNK0:H	H-Donor	A:GLY250:O	H-Acceptor
2.32	Hydrogen Bond	Conventional Hydrogen Bond	:UNK0:H	H-Donor	:UNK0:O	H-Acceptor
2.93	Hydrogen Bond	Conventional Hydrogen Bond	:UNK0:H	H-Donor	A:ASP246:OD1	H-Acceptor
2.17	Hydrogen Bond	Conventional Hydrogen Bond	:UNK0:H	H-Donor	A:LEU242:O	H-Acceptor
2.65	Hydrogen Bond	Conventional Hydrogen Bond	:UNK0:H	H-Donor	A:GLY250:O	H-Acceptor
3.39	Hydrogen Bond	Carbon Hydrogen Bond	:UNK0:C	H-Donor	A:ILE245:O	H-Acceptor
Glucose_chain						
2.73	Hydrogen Bond	Conventional Hydrogen Bond	A:ARG53:HH22	H-Donor	:UNK0:O	H-Acceptor
2.52	Hydrogen Bond	Conventional Hydrogen Bond	A:GLY250:HN	H-Donor	:UNK0:O	H-Acceptor
2.02	Hydrogen Bond	Conventional Hydrogen Bond	:UNK0:H	H-Donor	A:ARG243:O	H-Acceptor
2.48	Hydrogen Bond	Conventional Hydrogen Bond	:UNK0:H	H-Donor	A:LEU242:O	H-Acceptor
2.54	Hydrogen Bond	Conventional Hydrogen Bond	:UNK0:H	H-Donor	A:GLY250:O	H-Acceptor
2.37	Hydrogen Bond	Conventional Hydrogen Bond	:UNK0:H	H-Donor	A:ILE245:O	H-Acceptor
2.08	Hydrogen Bond	Conventional Hydrogen Bond	:UNK0:H	H-Donor	A:VAL248:O	H-Acceptor
3.36	Hydrogen Bond	Carbon Hydrogen Bond	:UNK0:C	H-Donor	A:GLY250:O	H-Acceptor
2DG_ring						
2.40	Hydrogen Bond	Conventional Hydrogen Bond	A:ARG53:HH22	H-Donor	:UNK0:O	H-Acceptor
2.39	Hydrogen Bond	Conventional Hydrogen Bond	:UNK0:H	H-Donor	A:ASP246:O	H-Acceptor
2.69	Hydrogen Bond	Conventional Hydrogen Bond	:UNK0:H	H-Donor	A:VAL248:O	H-Acceptor
2.57	Hydrogen Bond	Conventional Hydrogen Bond	:UNK0:H	H-Donor	A:LEU242:O	H-Acceptor
2.36	Hydrogen Bond	Conventional Hydrogen Bond	:UNK0:H	H-Donor	A:GLY250:O	H-Acceptor
3.44	Hydrogen Bond	Carbon Hydrogen Bond	:UNK0:C	H-Donor	A:GLY250:O	H-Acceptor
Glucose_ring						
1.81	Hydrogen Bond	Conventional Hydrogen Bond	A:GLY250:HN	H-Donor	:UNK0:O	H-Acceptor
2.57	Hydrogen Bond	Conventional Hydrogen Bond	:UNK0:H	H-Donor	A:LEU242:O	H-Acceptor
2.42	Hydrogen Bond	Conventional Hydrogen Bond	:UNK0:H	H-Donor	A:GLY250:O	H-Acceptor
2.60	Hydrogen Bond	Conventional Hydrogen Bond	:UNK0:H	H-Donor	A:ARG243:O	H-Acceptor
2.38	Hydrogen Bond	Conventional Hydrogen Bond	:UNK0:H	H-Donor	A:ASP246:OD1	H-Acceptor
1.81	Hydrogen Bond	Conventional Hydrogen Bond	A:GLY250:HN	H-Donor	:UNK0:O	H-Acceptor
2.57	Hydrogen Bond	Conventional Hydrogen Bond	:UNK0:H	H-Donor	A:LEU242:O	H-Acceptor
2.42	Hydrogen Bond	Conventional Hydrogen Bond	:UNK0:H	H-Donor	A:GLY250:O	H-Acceptor
2.60	Hydrogen Bond	Conventional Hydrogen Bond	:UNK0:H	H-Donor	A:ARG243:O	H-Acceptor
2.38	Hydrogen Bond	Conventional Hydrogen Bond	:UNK0:H	H-Donor	A:ASP246:OD1	H-Acceptor
Human Phosphoglucose Isomerase (PDB ID: 1JLH)						
2DG_chain						
2.25	Hydrogen Bond	Conventional Hydrogen Bond	A:GLN230:HE22	H-Donor	:UNK0:O	H-Acceptor
3.08	Hydrogen Bond	Conventional Hydrogen Bond	:UNK0:H	H-Donor	A:GLN230:OE1	H-Acceptor

2.25	Hydrogen Bond	Conventional Hydrogen Bond	A:GLN230:HE22	H-Donor	:UNK0:O	H-Acceptor
3.08	Hydrogen Bond	Conventional Hydrogen Bond	:UNK0:H	H-Donor	A:GLN230:OE1	H-Acceptor
Glucose_chain						
2.11	Hydrogen Bond	Conventional Hydrogen Bond	A:GLN230:HE22	H-Donor	:UNK0:O	H-Acceptor
2.54	Hydrogen Bond	Conventional Hydrogen Bond	A:LYS233:HZ1	H-Donor	:UNK0:O	H-Acceptor
2.67	Hydrogen Bond	Conventional Hydrogen Bond	A:LYS233:HZ2	H-Donor	:UNK0:O	H-Acceptor
2.34	Hydrogen Bond	Conventional Hydrogen Bond	:UNK0:H	H-Donor	:UNK0:O	H-Acceptor
2DG_ring						
2.23	Hydrogen Bond	Conventional Hydrogen Bond	A:GLN230:HE22	H-Donor	:UNK0:O	H-Acceptor
2.41	Hydrogen Bond	Conventional Hydrogen Bond	A:LYS233:HZ2	H-Donor	:UNK0:O	H-Acceptor
2.52	Hydrogen Bond	Conventional Hydrogen Bond	:UNK0:H	H-Donor	A:GLN230:OE1	H-Acceptor
2.23	Hydrogen Bond	Conventional Hydrogen Bond	A:GLN230:HE22	H-Donor	:UNK0:O	H-Acceptor
2.41	Hydrogen Bond	Conventional Hydrogen Bond	A:LYS233:HZ2	H-Donor	:UNK0:O	H-Acceptor
2.52	Hydrogen Bond	Conventional Hydrogen Bond	:UNK0:H	H-Donor	A:GLN230:OE1	H-Acceptor
1.98	Hydrogen Bond	Conventional Hydrogen Bond	:UNK0:H	H-Donor	:UNK0:O	H-Acceptor
Clucose_ring						
2.70	Hydrogen Bond	Conventional Hydrogen Bond	A:GLN230:HE21	H-Donor	:UNK0:O	H-Acceptor
1.85	Hydrogen Bond	Conventional Hydrogen Bond	A:GLN230:HE22	H-Donor	:UNK0:O	H-Acceptor
2.68	Hydrogen Bond	Conventional Hydrogen Bond	A:GLN230:HE22	H-Donor	:UNK0:O	H-Acceptor
Human Phosphofructokinase (PDB ID: 4WL0)						
2DG_chain						
2.42	Hydrogen Bond	Conventional Hydrogen Bond	A:GLY545:HN	H-Donor	:UNK0:O	H-Acceptor
2.38	Hydrogen Bond	Conventional Hydrogen Bond	A:GLY545:HN	H-Donor	:UNK0:O	H-Acceptor
1.92	Hydrogen Bond	Conventional Hydrogen Bond	:UNK0:H	H-Donor	A:SER546:O	H-Acceptor
2.16	Hydrogen Bond	Conventional Hydrogen Bond	:UNK0:H	H-Donor	A:ASP547:OD1	H-Acceptor
2.80	Hydrogen Bond	Conventional Hydrogen Bond	:UNK0:H	H-Donor	A:GLU748:O	H-Acceptor
2.51	Hydrogen Bond	Conventional Hydrogen Bond	:UNK0:H	H-Donor	A:SER546:O	H-Acceptor
3.76	Hydrogen Bond	Carbon Hydrogen Bond	:UNK0:C	H-Donor	A:GLU748:O	H-Acceptor
3.25	Hydrogen Bond	Carbon Hydrogen Bond	:UNK0:C	H-Donor	A:SER546:O	H-Acceptor
Glucose_chain						
3.08	Hydrogen Bond	Conventional Hydrogen Bond	A:ASN541:HD22	H-Donor	:UNK0:O	H-Acceptor
2.37	Hydrogen Bond	Conventional Hydrogen Bond	A:GLY545:HN	H-Donor	:UNK0:O	H-Acceptor
2.13	Hydrogen Bond	Conventional Hydrogen Bond	A:SER546:HN	H-Donor	:UNK0:O	H-Acceptor
2.63	Hydrogen Bond	Conventional Hydrogen Bond	A:TRP751:HE1	H-Donor	:UNK0:O	H-Acceptor
3.05	Hydrogen Bond	Conventional Hydrogen Bond	:UNK0:H	H-Donor	A:VAL543:O	H-Acceptor
2.80	Hydrogen Bond	Conventional Hydrogen Bond	:UNK0:H	H-Donor	A:ASP547:OD1	H-Acceptor
2.07	Hydrogen Bond	Conventional Hydrogen Bond	:UNK0:H	H-Donor	A:GLU748:O	H-Acceptor
2.48	Hydrogen Bond	Conventional Hydrogen Bond	:UNK0:H	H-Donor	A:VAL543:O	H-Acceptor

2.25	Hydrogen Bond	Conventional Hydrogen Bond	:UNK0:H	H-Donor	A:SER546:O	H-Acceptor
3.33	Hydrogen Bond	Carbon Hydrogen Bond	A:GLN749:CA	H-Donor	:UNK0:O	H-Acceptor
2DG_ring						
2.49	Hydrogen Bond	Conventional Hydrogen Bond	A:GLY545:HN	H-Donor	:UNK0:O	H-Acceptor
2.27	Hydrogen Bond	Conventional Hydrogen Bond	A:GLY545:HN	H-Donor	:UNK0:O	H-Acceptor
2.20	Hydrogen Bond	Conventional Hydrogen Bond	A:SER546:HN	H-Donor	:UNK0:O	H-Acceptor
2.62	Hydrogen Bond	Conventional Hydrogen Bond	A:GLN738:HE22	H-Donor	:UNK0:O	H-Acceptor
2.48	Hydrogen Bond	Conventional Hydrogen Bond	:UNK0:H	H-Donor	A:VAL543:O	H-Acceptor
2.23	Hydrogen Bond	Conventional Hydrogen Bond	:UNK0:H	H-Donor	A:GLU748:O	H-Acceptor
2.94	Hydrogen Bond	Carbon Hydrogen Bond	:UNK0:C	H-Donor	A:ASP547:OD1	H-Acceptor
Glucose_ring						
2.35	Hydrogen Bond	Conventional Hydrogen Bond	A:GLY545:HN	H-Donor	:UNK0:O	H-Acceptor
2.40	Hydrogen Bond	Conventional Hydrogen Bond	A:SER723:HG	H-Donor	:UNK0:O	H-Acceptor
2.00	Hydrogen Bond	Conventional Hydrogen Bond	:UNK0:H	H-Donor	A:SER546:O	H-Acceptor
2.15	Hydrogen Bond	Conventional Hydrogen Bond	:UNK0:H	H-Donor	A:ASP547:OD1	H-Acceptor
2.56	Hydrogen Bond	Conventional Hydrogen Bond	:UNK0:H	H-Donor	A:ILE722:O	H-Acceptor
3.61	Hydrogen Bond	Carbon Hydrogen Bond	:UNK0:C	H-Donor	A:GLU748:O	H-Acceptor
Human Fructose 1,6-bisphosphate Aldolase (PDB ID: 4ALD)						
2DG_chain						
2.52	Hydrogen Bond	Conventional Hydrogen Bond	A:LYS229:HZ1	H-Donor	:UNK0:O	H-Acceptor
2.50	Hydrogen Bond	Conventional Hydrogen Bond	A:LYS229:HZ2	H-Donor	:UNK0:O	H-Acceptor
1.82	Hydrogen Bond	Conventional Hydrogen Bond	A:SER271:HG	H-Donor	:UNK0:O	H-Acceptor
3.09	Hydrogen Bond	Conventional Hydrogen Bond	A:GLY272:HN	H-Donor	:UNK0:O	H-Acceptor
1.87	Hydrogen Bond	Conventional Hydrogen Bond	A:GLY273:HN	H-Donor	:UNK0:O	H-Acceptor
2.39	Hydrogen Bond	Conventional Hydrogen Bond	A:GLY302:HN	H-Donor	:UNK0:O	H-Acceptor
2.37	Hydrogen Bond	Conventional Hydrogen Bond	A:ARG303:HN	H-Donor	:UNK0:O	H-Acceptor
2.50	Hydrogen Bond	Conventional Hydrogen Bond	:UNK0:H	H-Donor	:UNK0:O	H-Acceptor
2.16	Hydrogen Bond	Conventional Hydrogen Bond	:UNK0:H	H-Donor	:UNK0:O	H-Acceptor
2.43	Hydrogen Bond	Conventional Hydrogen Bond	:UNK0:H	H-Donor	A:SER300:O	H-Acceptor
Glucose_chain						
2.07	Hydrogen Bond	Conventional Hydrogen Bond	A:ARG42:HH12	H-Donor	:UNK0:O	H-Acceptor
2.29	Hydrogen Bond	Conventional Hydrogen Bond	A:ARG42:HH22	H-Donor	:UNK0:O	H-Acceptor
2.53	Hydrogen Bond	Conventional Hydrogen Bond	A:LYS146:HZ1	H-Donor	:UNK0:O	H-Acceptor
2.72	Hydrogen Bond	Conventional Hydrogen Bond	A:LYS146:HZ3	H-Donor	:UNK0:O	H-Acceptor
2.77	Hydrogen Bond	Conventional Hydrogen Bond	A:GLY302:HN	H-Donor	:UNK0:O	H-Acceptor
2.35	Hydrogen Bond	Conventional Hydrogen Bond	A:GLY302:HN	H-Donor	:UNK0:O	H-Acceptor
2.28	Hydrogen Bond	Conventional Hydrogen Bond	A:ARG303:HN	H-Donor	:UNK0:O	H-Acceptor
2.29	Hydrogen Bond	Conventional Hydrogen Bond	:UNK0:H	H-Donor	A:SER300:O	H-Acceptor

2.75	Hydrogen Bond	Conventional Hydrogen Bond	:UNK0:H	H-Donor	:UNK0:O	H-Acceptor
1.74	Hydrogen Bond	Conventional Hydrogen Bond	:UNK0:H	H-Donor	:UNK0:O	H-Acceptor
2DG_ring						
2.91	Hydrogen Bond	Conventional Hydrogen Bond	:UNK0:H	H-Donor	A:ASN70:O	H-Acceptor
2.84	Hydrogen Bond	Conventional Hydrogen Bond	:UNK0:H	H-Donor	A:ILE73:O	H-Acceptor
2.74	Hydrogen Bond	Conventional Hydrogen Bond	:UNK0:H	H-Donor	A:LYS100:O	H-Acceptor
2.15	Hydrogen Bond	Conventional Hydrogen Bond	:UNK0:H	H-Donor	:UNK0:O	H-Acceptor
1.88	Hydrogen Bond	Conventional Hydrogen Bond	:UNK0:H	H-Donor	A:LEU63:O	H-Acceptor
3.78	Hydrogen Bond	Carbon Hydrogen Bond	:UNK0:C	H-Donor	A:VAL69:O	H-Acceptor
Glucose_ring						
2.65	Hydrogen Bond	Conventional Hydrogen Bond	A:LYS229:HZ1	H-Donor	:UNK0:O	H-Acceptor
2.96	Hydrogen Bond	Conventional Hydrogen Bond	A:LYS229:HZ2	H-Donor	:UNK0:O	H-Acceptor
2.34	Hydrogen Bond	Conventional Hydrogen Bond	A:ARG303:HN	H-Donor	:UNK0:O	H-Acceptor
2.65	Hydrogen Bond	Conventional Hydrogen Bond	A:ARG303:HN	H-Donor	:UNK0:O	H-Acceptor
2.77	Hydrogen Bond	Conventional Hydrogen Bond	:UNK0:H	H-Donor	A:SER300:O	H-Acceptor
2.34	Hydrogen Bond	Conventional Hydrogen Bond	:UNK0:H	H-Donor	A:GLU34:OE2	H-Acceptor
2.19	Hydrogen Bond	Conventional Hydrogen Bond	:UNK0:H	H-Donor	A:ASP33:OD1	H-Acceptor
Human Triose Phosphate Isomerase (PDB ID: 6NLH)						
2DG_chain						
2.50	Hydrogen Bond	Conventional Hydrogen Bond	A:ASN11:HD21	H-Donor	:UNK0:O	H-Acceptor
2.63	Hydrogen Bond	Conventional Hydrogen Bond	A:ARG98:HH11	H-Donor	:UNK0:O	H-Acceptor
2.99	Hydrogen Bond	Conventional Hydrogen Bond	A:ARG98:HH12	H-Donor	:UNK0:O	H-Acceptor
2.11	Hydrogen Bond	Conventional Hydrogen Bond	:UNK0:H	H-Donor	A:GLN64:OE1	H-Acceptor
2.39	Hydrogen Bond	Conventional Hydrogen Bond	:UNK0:H	H-Donor	A:GLU97:OE1	H-Acceptor
3.08	Hydrogen Bond	Conventional Hydrogen Bond	:UNK0:H	H-Donor	A:GLN64:O	H-Acceptor
3.38	Hydrogen Bond	Carbon Hydrogen Bond	:UNK0:C	H-Donor	A:GLN64:O	H-Acceptor
Glucose_chain						
2.58	Hydrogen Bond	Conventional Hydrogen Bond	A:GLY232:HN	H-Donor	:UNK0:O	H-Acceptor
2.87	Hydrogen Bond	Conventional Hydrogen Bond	A:GLY232:HN	H-Donor	:UNK0:O	H-Acceptor
2.21	Hydrogen Bond	Conventional Hydrogen Bond	A:ALA234:HN	H-Donor	:UNK0:O	H-Acceptor
2.23	Hydrogen Bond	Conventional Hydrogen Bond	:UNK0:H	H-Donor	A:GLY209:O	H-Acceptor
2.50	Hydrogen Bond	Conventional Hydrogen Bond	:UNK0:H	H-Donor	A:GLY210:O	H-Acceptor
2.94	Hydrogen Bond	Conventional Hydrogen Bond	:UNK0:H	H-Donor	A:LEU230:O	H-Acceptor
2.41	Hydrogen Bond	Conventional Hydrogen Bond	:UNK0:H	H-Donor	A:VAL212:O	H-Acceptor
2.03	Hydrogen Bond	Conventional Hydrogen Bond	:UNK0:H	H-Donor	:UNK0:O	H-Acceptor
2.58	Hydrogen Bond	Conventional Hydrogen Bond	:UNK0:H	H-Donor	:UNK0:O	H-Acceptor
3.64	Hydrogen Bond	Carbon Hydrogen Bond	A:GLY232:CA	H-Donor	:UNK0:O	H-Acceptor
2DG_ring						
2.43	Hydrogen Bond	Conventional Hydrogen Bond	A:GLY232:HN	H-Donor	:UNK0:O	H-Acceptor

2.66	Hydrogen Bond	Conventional Hydrogen Bond	:UNK0:H	H-Donor	A:GLY209:O	H-Acceptor
2.63	Hydrogen Bond	Conventional Hydrogen Bond	:UNK0:H	H-Donor	A:GLY210:O	H-Acceptor
2.41	Hydrogen Bond	Conventional Hydrogen Bond	:UNK0:H	H-Donor	A:LEU230:O	H-Acceptor
2.58	Hydrogen Bond	Conventional Hydrogen Bond	:UNK0:H	H-Donor	A:GLU165:OE2	H-Acceptor
2.44	Hydrogen Bond	Conventional Hydrogen Bond	:UNK0:H	H-Donor	A:GLY209:O	H-Acceptor
2.11	Hydrogen Bond	Conventional Hydrogen Bond	:UNK0:H	H-Donor	A:LEU230:O	H-Acceptor
Glucose_ring						
2.56	Hydrogen Bond	Conventional Hydrogen Bond	A:ASN11:HD21	H-Donor	:UNK0:O	H-Acceptor
2.23	Hydrogen Bond	Conventional Hydrogen Bond	A:ASN11:HD21	H-Donor	:UNK0:O	H-Acceptor
2.37	Hydrogen Bond	Conventional Hydrogen Bond	A:ARG98:HH11	H-Donor	:UNK0:O	H-Acceptor
2.13	Hydrogen Bond	Conventional Hydrogen Bond	:UNK0:H	H-Donor	A:GLU97:OE1	H-Acceptor
3.69	Hydrogen Bond	Carbon Hydrogen Bond	A:ARG98:CD	H-Donor	:UNK0:O	H-Acceptor
3.55	Hydrogen Bond	Carbon Hydrogen Bond	:UNK0:C	H-Donor	A:GLN64:OE1	H-Acceptor
3.53	Hydrogen Bond	Carbon Hydrogen Bond	:UNK0:C	H-Donor	A:GLN64:OE1	H-Acceptor
3.38	Hydrogen Bond	Carbon Hydrogen Bond	:UNK0:C	H-Donor	A:GLN64:OE1	H-Acceptor
3.09	Hydrogen Bond	Carbon Hydrogen Bond	:UNK0:C	H-Donor	A:GLN64:O	H-Acceptor
Human Glyceraldehyde-3-Phosphate Dehydrogenase (PDB ID: 3GPD)						
2DG_chain						
1.81	Hydrogen Bond	Conventional Hydrogen Bond	R:ASN33:HD22	H-Donor	:UNK0:O	H-Acceptor
2.16	Hydrogen Bond	Conventional Hydrogen Bond	:UNK0:H	H-Donor	R:ASP34:OD1	H-Acceptor
2.77	Hydrogen Bond	Conventional Hydrogen Bond	:UNK0:H	H-Donor	R:PRO35:O	H-Acceptor
2.43	Hydrogen Bond	Conventional Hydrogen Bond	:UNK0:H	H-Donor	R:ASN33:O	H-Acceptor
2.939	Hydrogen Bond	Conventional Hydrogen Bond	:UNK0:H	H-Donor	R:THR98:O	H-Acceptor
2.52	Hydrogen Bond	Conventional Hydrogen Bond	:UNK0:H	H-Donor	R:ASP34:OD1	H-Acceptor
2.66	Hydrogen Bond	Conventional Hydrogen Bond	:UNK0:H	H-Donor	R:PRO35:O	H-Acceptor
3.72	Hydrogen Bond	Carbon Hydrogen Bond	R:ASP34:CA	H-Donor	:UNK0:O	H-Acceptor
3.36	Hydrogen Bond	Carbon Hydrogen Bond	R:PRO35:CD	H-Donor	:UNK0:O	H-Acceptor
3.45	Hydrogen Bond	Carbon Hydrogen Bond	R:PRO35:CD	H-Donor	:UNK0:O	H-Acceptor
Glucose_chain						
2.68	Hydrogen Bond	Conventional Hydrogen Bond	R:ASN33:HD21	H-Donor	:UNK0:O	H-Acceptor
2.19	Hydrogen Bond	Conventional Hydrogen Bond	R:ASN33:HD22	H-Donor	:UNK0:O	H-Acceptor
2.99	Hydrogen Bond	Conventional Hydrogen Bond	:UNK0:H	H-Donor	R:ASP8:OD1	H-Acceptor
2.53	Hydrogen Bond	Conventional Hydrogen Bond	:UNK0:H	H-Donor	R:ASP34:OD1	H-Acceptor
2.26	Hydrogen Bond	Conventional Hydrogen Bond	:UNK0:H	H-Donor	R:PRO35:O	H-Acceptor
3.71	Hydrogen Bond	Carbon Hydrogen Bond	R:ASP34:CA	H-Donor	:UNK0:O	H-Acceptor
2DG_ring						
2.69	Hydrogen Bond	Conventional Hydrogen Bond	R:ASN33:HD21	H-Donor	:UNK0:O	H-Acceptor
1.91	Hydrogen Bond	Conventional Hydrogen Bond	R:ASN33:HD22	H-Donor	:UNK0:O	H-Acceptor
2.16	Hydrogen Bond	Conventional Hydrogen Bond	R:THR98:HG1	H-Donor	:UNK0:O	H-Acceptor
2.89	Hydrogen Bond	Conventional Hydrogen Bond	:UNK0:H	H-Donor	R:ASP34:OD1	H-Acceptor
2.92	Hydrogen Bond	Conventional Hydrogen Bond	:UNK0:H	H-Donor	R:GLU78:O	H-Acceptor
Glucose_ring						

2.39	Hydrogen Bond	Conventional Hydrogen Bond	R:GLY9:HN	H-Donor	:UNK0:O	H-Acceptor
2.09	Hydrogen Bond	Conventional Hydrogen Bond	R:ASN33:HD22	H-Donor	:UNK0:O	H-Acceptor
2.53	Hydrogen Bond	Conventional Hydrogen Bond	:UNK0:H	H-Donor	R:THR98:O	H-Acceptor
2.58	Hydrogen Bond	Conventional Hydrogen Bond	:UNK0:H	H-Donor	R:THR98:O	H-Acceptor
2.03	Hydrogen Bond	Conventional Hydrogen Bond	:UNK0:H	H-Donor	:UNK0:O	H-Acceptor
2.66	Hydrogen Bond	Conventional Hydrogen Bond	:UNK0:H	H-Donor	R:ASP8:OD1	H-Acceptor
2.05	Hydrogen Bond	Conventional Hydrogen Bond	:UNK0:H	H-Donor	R:ASP34:OD1	H-Acceptor
2.24	Hydrogen Bond	Conventional Hydrogen Bond	:UNK0:H	H-Donor	R:ASN33:O	H-Acceptor
Human Phosphoglycerate Kinase (PDB ID: 3C3C)						
2DG_chain						
2.01	Hydrogen Bond	Conventional Hydrogen Bond	A:ARG38:HH12	H-Donor	:UNK0:O	H-Acceptor
3.00	Hydrogen Bond	Conventional Hydrogen Bond	A:ARG38:HH12	H-Donor	:UNK0:O	H-Acceptor
2.29	Hydrogen Bond	Conventional Hydrogen Bond	A:HIS62:HE2	H-Donor	:UNK0:O	H-Acceptor
2.34	Hydrogen Bond	Conventional Hydrogen Bond	A:ARG122:HH12	H-Donor	:UNK0:O	H-Acceptor
2.46	Hydrogen Bond	Conventional Hydrogen Bond	A:ARG122:HH22	H-Donor	:UNK0:O	H-Acceptor
2.50	Hydrogen Bond	Conventional Hydrogen Bond	A:GLY396:HN	H-Donor	:UNK0:O	H-Acceptor
2.48	Hydrogen Bond	Conventional Hydrogen Bond	:UNK0:H	H-Donor	A:GLY166:O	H-Acceptor
Glucose_chain						
2.19	Hydrogen Bond	Conventional Hydrogen Bond	A:ARG38:HH22	H-Donor	:UNK0:O	H-Acceptor
2.18	Hydrogen Bond	Conventional Hydrogen Bond	A:ARG38:HH22	H-Donor	:UNK0:O	H-Acceptor
2.53	Hydrogen Bond	Conventional Hydrogen Bond	A:HIS62:HE2	H-Donor	:UNK0:O	H-Acceptor
2.39	Hydrogen Bond	Conventional Hydrogen Bond	A:HIS62:HE2	H-Donor	:UNK0:O	H-Acceptor
2.14	Hydrogen Bond	Conventional Hydrogen Bond	A:ARG122:HH12	H-Donor	:UNK0:O	H-Acceptor
2.49	Hydrogen Bond	Conventional Hydrogen Bond	A:ARG122:HH22	H-Donor	:UNK0:O	H-Acceptor
2.31	Hydrogen Bond	Conventional Hydrogen Bond	A:HIS169:HE2	H-Donor	:UNK0:O	H-Acceptor
2.18	Hydrogen Bond	Conventional Hydrogen Bond	A:GLY396:HN	H-Donor	:UNK0:O	H-Acceptor
2.72	Hydrogen Bond	Conventional Hydrogen Bond	:UNK0:H	H-Donor	A:GLY394:O	H-Acceptor
1.81	Hydrogen Bond	Conventional Hydrogen Bond	:UNK0:H	H-Donor	:UNK0:O	H-Acceptor
1.85	Hydrogen Bond	Conventional Hydrogen Bond	:UNK0:H	H-Donor	A:GLY166:O	H-Acceptor
3.68	Hydrogen Bond	Carbon Hydrogen Bond	:UNK0:C	H-Donor	A:GLY166:O	H-Acceptor
2DG_ring						
1.97	Hydrogen Bond	Conventional Hydrogen Bond	A:ASN25:HD21	H-Donor	:UNK0:O	H-Acceptor
2.67	Hydrogen Bond	Conventional Hydrogen Bond	A:ARG38:HH12	H-Donor	:UNK0:O	H-Acceptor
2.55	Hydrogen Bond	Conventional Hydrogen Bond	A:HIS169:HE2	H-Donor	:UNK0:O	H-Acceptor
2.16	Hydrogen Bond	Conventional Hydrogen Bond	A:ARG170:HH21	H-Donor	:UNK0:O	H-Acceptor
2.48	Hydrogen Bond	Conventional Hydrogen Bond	A:ARG170:HH21	H-Donor	:UNK0:O	H-Acceptor
2.36	Hydrogen Bond	Conventional Hydrogen Bond	:UNK0:H	H-Donor	A:ASP23:OD2	H-Acceptor

2.77	Hydrogen Bond	Conventional Hydrogen Bond	:UNK0:H	H-Donor	A:GLY394:O	H-Acceptor
Glucose_ring						
2.50	Hydrogen Bond	Conventional Hydrogen Bond	A:ARG38:HH22	H-Donor	:UNK0:O	H-Acceptor
2.44	Hydrogen Bond	Conventional Hydrogen Bond	A:HIS62:HE2	H-Donor	:UNK0:O	H-Acceptor
3.05	Hydrogen Bond	Conventional Hydrogen Bond	A:ARG65:HH21	H-Donor	:UNK0:O	H-Acceptor
3.00	Hydrogen Bond	Conventional Hydrogen Bond	A:ARG170:HE	H-Donor	:UNK0:O	H-Acceptor
1.85	Hydrogen Bond	Conventional Hydrogen Bond	A:ARG170:HH21	H-Donor	:UNK0:O	H-Acceptor
2.69	Hydrogen Bond	Conventional Hydrogen Bond	:UNK0:H	H-Donor	A:GLY394:O	H-Acceptor
1.90	Hydrogen Bond	Conventional Hydrogen Bond	:UNK0:H	H-Donor	A:GLY166:O	H-Acceptor
Human Phosphoglycerate Mutase (PDB ID: 1YJX)						
2DG_chain						
2.20	Hydrogen Bond	Conventional Hydrogen Bond	A:ASN17:HD22	H-Donor	:UNK0:O	H-Acceptor
2.13	Hydrogen Bond	Conventional Hydrogen Bond	A:SER23:HN	H-Donor	:UNK0:O	H-Acceptor
2.92	Hydrogen Bond	Conventional Hydrogen Bond	A:ARG90:HH11	H-Donor	:UNK0:O	H-Acceptor
2.15	Hydrogen Bond	Conventional Hydrogen Bond	A:ASN188:HD22	H-Donor	:UNK0:O	H-Acceptor
2.71	Hydrogen Bond	Conventional Hydrogen Bond	:UNK0:H	H-Donor	A:ARG21:O	H-Acceptor
2.36	Hydrogen Bond	Conventional Hydrogen Bond	:UNK0:H	H-Donor	A:SER23:OG	H-Acceptor
2.29	Hydrogen Bond	Conventional Hydrogen Bond	:UNK0:H	H-Donor	:UNK0:O	H-Acceptor
3.39	Hydrogen Bond	Carbon Hydrogen Bond	:UNK0:C	H-Donor	A:SER23:OG	H-Acceptor
Glucose_chain						
2.41	Hydrogen Bond	Conventional Hydrogen Bond	A:ARG10:HH21	H-Donor	:UNK0:O	H-Acceptor
2.86	Hydrogen Bond	Conventional Hydrogen Bond	A:SER14:HG	H-Donor	:UNK0:O	H-Acceptor
2.38	Hydrogen Bond	Conventional Hydrogen Bond	A:ARG62:HH12	H-Donor	:UNK0:O	H-Acceptor
2.36	Hydrogen Bond	Conventional Hydrogen Bond	A:LYS100:HZ1	H-Donor	:UNK0:O	H-Acceptor
2.71	Hydrogen Bond	Conventional Hydrogen Bond	:UNK0:H	H-Donor	A:ARG21:O	H-Acceptor
2.34	Hydrogen Bond	Conventional Hydrogen Bond	:UNK0:H	H-Donor	A:GLU89:OE2	H-Acceptor
2.09	Hydrogen Bond	Conventional Hydrogen Bond	:UNK0:H	H-Donor	A:GLU89:OE2	H-Acceptor
2DG_ring						
2.37	Hydrogen Bond	Conventional Hydrogen Bond	A:ARG90:HH11	H-Donor	:UNK0:O	H-Acceptor
2.63	Hydrogen Bond	Conventional Hydrogen Bond	A:ARG116:HH11	H-Donor	:UNK0:O	H-Acceptor
2.57	Hydrogen Bond	Conventional Hydrogen Bond	:UNK0:H	H-Donor	A:ASN188:OD1	H-Acceptor
2.64	Hydrogen Bond	Conventional Hydrogen Bond	:UNK0:H	H-Donor	:UNK0:O	H-Acceptor
3.01	Hydrogen Bond	Conventional Hydrogen Bond	:UNK0:H	H-Donor	A:GLU89:OE2	H-Acceptor
3.46	Hydrogen Bond	Carbon Hydrogen Bond	:UNK0:C	H-Donor	A:ARG116:O	H-Acceptor
Glucose_ring						
2.49	Hydrogen Bond	Conventional Hydrogen Bond	A:ARG10:HH21	H-Donor	:UNK0:O	H-Acceptor
2.45	Hydrogen Bond	Conventional Hydrogen Bond	A:ASN17:HD22	H-Donor	:UNK0:O	H-Acceptor
1.87	Hydrogen Bond	Conventional Hydrogen Bond	A:SER23:HN	H-Donor	:UNK0:O	H-Acceptor

2.51	Hydrogen Bond	Conventional Hydrogen Bond	:UNK0:H	H-Donor	A:ARG21:O	H-Acceptor
2.59	Hydrogen Bond	Conventional Hydrogen Bond	:UNK0:H	H-Donor	A:SER23:OG	H-Acceptor
2.11	Hydrogen Bond	Conventional Hydrogen Bond	:UNK0:H	H-Donor	A:GLU89:OE2	H-Acceptor
2.65	Hydrogen Bond	Conventional Hydrogen Bond	:UNK0:H	H-Donor	A:SER23:OG	H-Acceptor
Human Enolase (PDB ID: 4ZCW)						
2DG_chain						
2.82	Hydrogen Bond	Conventional Hydrogen Bond	A:LYS120:HZ2	H-Donor	:UNK0:O	H-Acceptor
2.73	Hydrogen Bond	Conventional Hydrogen Bond	A:LYS120:HZ2	H-Donor	:UNK0:O	H-Acceptor
2.57	Hydrogen Bond	Conventional Hydrogen Bond	A:LYS120:HZ3	H-Donor	:UNK0:O	H-Acceptor
3.04	Hydrogen Bond	Conventional Hydrogen Bond	A:THR379:HN	H-Donor	:UNK0:O	H-Acceptor
2.57	Hydrogen Bond	Conventional Hydrogen Bond	A:THR379:HG1	H-Donor	:UNK0:O	H-Acceptor
2.46	Hydrogen Bond	Conventional Hydrogen Bond	:UNK0:H	H-Donor	A:ARG32:O	H-Acceptor
2.26	Hydrogen Bond	Conventional Hydrogen Bond	:UNK0:H	H-Donor	:UNK0:O	H-Acceptor
2.93	Hydrogen Bond	Conventional Hydrogen Bond	:UNK0:H	H-Donor	A:GLU377:O	H-Acceptor
Glucose_chain						
1.90	Hydrogen Bond	Conventional Hydrogen Bond	A:LYS343:HZ1	H-Donor	:UNK0:O	H-Acceptor
2.65	Hydrogen Bond	Conventional Hydrogen Bond	A:LYS343:HZ1	H-Donor	:UNK0:O	H-Acceptor
2.04	Hydrogen Bond	Conventional Hydrogen Bond	A:LYS343:HZ2	H-Donor	:UNK0:O	H-Acceptor
2.75	Hydrogen Bond	Conventional Hydrogen Bond	A:ARG372:HE	H-Donor	:UNK0:O	H-Acceptor
2.34	Hydrogen Bond	Conventional Hydrogen Bond	A:ARG372:HE	H-Donor	:UNK0:O	H-Acceptor
1.90	Hydrogen Bond	Conventional Hydrogen Bond	:UNK0:H	H-Donor	A:SER373:OG:B	H-Acceptor
3.00	Hydrogen Bond	Conventional Hydrogen Bond	:UNK0:H	H-Donor	A:GLU167:OE2	H-Acceptor
2.92	Hydrogen Bond	Conventional Hydrogen Bond	:UNK0:H	H-Donor	A:GLU210:OE1	H-Acceptor
2.49	Hydrogen Bond	Conventional Hydrogen Bond	:UNK0:H	H-Donor	A:ASP245:OD2	H-Acceptor
2.04	Hydrogen Bond	Conventional Hydrogen Bond	:UNK0:H	H-Donor	A:GLU293:OE2	H-Acceptor
2.64	Hydrogen Bond	Conventional Hydrogen Bond	:UNK0:H	H-Donor	A:ASP318:OD2	H-Acceptor
2.36	Hydrogen Bond	Conventional Hydrogen Bond	:UNK0:H	H-Donor	A:HIS371:O	H-Acceptor
3.60	Hydrogen Bond	Carbon Hydrogen Bond	A:HIS371:CD2	H-Donor	:UNK0:O	H-Acceptor
3.35	Hydrogen Bond	Carbon Hydrogen Bond	A:LYS394:CE	H-Donor	:UNK0:O	H-Acceptor
3.59	Hydrogen Bond	Carbon Hydrogen Bond	:UNK0:C	H-Donor	A:GLN166:OE1	H-Acceptor
2DG_ring						
2.21	Hydrogen Bond	Conventional Hydrogen Bond	A:LYS343:HZ2	H-Donor	:UNK0:O	H-Acceptor
2.52	Hydrogen Bond	Conventional Hydrogen Bond	A:HIS371:HE2	H-Donor	:UNK0:O	H-Acceptor
2.06	Hydrogen Bond	Conventional Hydrogen Bond	A:SER373:HG	H-Donor	:UNK0:O	H-Acceptor
3.07	Hydrogen Bond	Conventional Hydrogen Bond	A:SER373:HG:B	H-Donor	:UNK0:O	H-Acceptor
2.23	Hydrogen Bond	Conventional Hydrogen Bond	:UNK0:H	H-Donor	A:GLU210:OE1	H-Acceptor
2.83	Hydrogen Bond	Conventional Hydrogen Bond	:UNK0:H	H-Donor	A:GLN166:OE1	H-Acceptor
1.94	Hydrogen Bond	Conventional Hydrogen Bond	:UNK0:H	H-Donor	A:GLU167:OE2	H-Acceptor

2.95	Hydrogen Bond	Conventional Hydrogen Bond	:UNK0:H	H-Donor	A:SER40:O	H-Acceptor
2.70	Hydrogen Bond	Conventional Hydrogen Bond	:UNK0:H	H-Donor	A:SER40:OG	H-Acceptor
2.15	Hydrogen Bond	Conventional Hydrogen Bond	:UNK0:H	H-Donor	A:SER40:OG	H-Acceptor
3.77	Hydrogen Bond	Carbon Hydrogen Bond	A:ARG372:CA	H-Donor	:UNK0:O	H-Acceptor
2.67	Hydrogen Bond	Carbon Hydrogen Bond	:UNK0:C	H-Donor	A:SER373:OG	H-Acceptor
3.56	Hydrogen Bond	Carbon Hydrogen Bond	:UNK0:C	H-Donor	A:HIS371:O	H-Acceptor
Glucose_ring						
2.42	Hydrogen Bond	Conventional Hydrogen Bond	A:ALA39:HN	H-Donor	:UNK0:O	H-Acceptor
2.74	Hydrogen Bond	Conventional Hydrogen Bond	A:ALA39:HN	H-Donor	:UNK0:O	H-Acceptor
1.92	Hydrogen Bond	Conventional Hydrogen Bond	A:LYS343:HZ1	H-Donor	:UNK0:O	H-Acceptor
2.33	Hydrogen Bond	Conventional Hydrogen Bond	A:HIS371:HE2	H-Donor	:UNK0:O	H-Acceptor
2.80	Hydrogen Bond	Conventional Hydrogen Bond	A:SER373:N	H-Donor	:UNK0:O	H-Acceptor
1.86	Hydrogen Bond	Conventional Hydrogen Bond	:UNK0:H	H-Donor	A:GLU167:OE2	H-Acceptor
3.08	Hydrogen Bond	Conventional Hydrogen Bond	:UNK0:H	H-Donor	A:GLU210:OE2	H-Acceptor
2.31	Hydrogen Bond	Conventional Hydrogen Bond	:UNK0:H	H-Donor	A:GLU210:OE1	H-Acceptor
1.97	Hydrogen Bond	Conventional Hydrogen Bond	:UNK0:H	H-Donor	A:ASP318:OD2	H-Acceptor
2.23	Hydrogen Bond	Conventional Hydrogen Bond	:UNK0:H	H-Donor	A:SER40:OG	H-Acceptor
3.08	Hydrogen Bond	Carbon Hydrogen Bond	A:GLY38:CA	H-Donor	:UNK0:O	H-Acceptor
2.87	Hydrogen Bond	Carbon Hydrogen Bond	:UNK0:C	H-Donor	A:SER40:OG	H-Acceptor
3.70	Hydrogen Bond	Carbon Hydrogen Bond	:UNK0:C	H-Donor	A:ASP245:OD2	H-Acceptor
UNAVOURABLE NON-BOND						
Human Phosphoglucose Isomerase (PDB ID: 1JLH)						
2DG_chain						
2.85	Unfavorable	Unfavorable Acceptor-Acceptor	A:GLU226:OE1	H-Acceptor	:UNK0:O	H-Acceptor
Glucose_ring						
1.46	Unfavorable	Unfavorable Donor-Donor	A:GLN230:HE22	H-Donor	:UNK0:H	H-Donor
Human Fructose 1,6-bisphosphate Aldolase (PDB ID: 4ALD)						
Glucose_chain						
1.34	Unfavorable	Unfavorable Donor-Donor	A:LYS229:HZ1	H-Donor	:UNK0:H	H-Donor
Glucose_ring						
2.43	Unfavorable	Unfavorable Donor-Donor	A:GLU34:HN	H-Donor	:UNK0:H	H-Donor
1.73	Unfavorable	Unfavorable Donor-Donor	A:ARG42:HH12	H-Donor	:UNK0:H	H-Donor
2.41	Unfavorable	Unfavorable Donor-Donor	A:LYS229:HZ1	H-Donor	:UNK0:H	H-Donor
Human Triose Phosphate Isomerase (PDB ID: 6NLH)						
2DG_chain						
1.41	Unfavorable	Unfavorable Donor-Donor	A:ASN11:HD21	H-Donor	:UNK0:H	H-Donor
Glucose_chain						
1.39	Unfavorable	Unfavorable Donor-Donor	A:GLY232:HN	H-Donor	:UNK0:H	H-Donor
Glucose_ring						
2.95	Unfavorable	Unfavorable Acceptor-Acceptor	A:GLU97:OE1	H-Acceptor	:UNK0:O	H-Acceptor
Human Glyceraldehyde-3-Phosphate Dehydrogenase (PDB ID: 3GPD)						
2DG_chain						
1.90	Unfavorable	Unfavorable Donor-Donor	R:GLY9:HN	H-Donor	:UNK0:H	H-Donor
1.92	Unfavorable	Unfavorable Donor-Donor	R:ASN33:HD21	H-Donor	:UNK0:H	H-Donor

Glucose_chain						
2.79	Unfavorable	Unfavorable Acceptor-Acceptor	R:ASP34:OD1	H-Acceptor	:UNK0:O	H-Acceptor
2.81	Unfavorable	Unfavorable Acceptor-Acceptor	R:ASP34:OD1	H-Acceptor	:UNK0:O	H-Acceptor
Glucose_ring						
2.49	Unfavorable	Unfavorable Donor-Donor	R:VAL100:HN	H-Donor	:UNK0:H	H-Donor
Human Phosphoglycerate Kinase (PDB ID: 3C3C)						
2DG_chain						
1.12	Unfavorable	Unfavorable Donor-Donor	A:ASN25:HD21	H-Donor	:UNK0:H	H-Donor
2.33	Unfavorable	Unfavorable Donor-Donor	A:HIS62:HE2	H-Donor	:UNK0:H	H-Donor
Glucose_chain						
1.43	Unfavorable	Unfavorable Donor-Donor	A:ARG38:HH22	H-Donor	:UNK0:H	H-Donor
2.45	Unfavorable	Unfavorable Donor-Donor	A:ARG65:HH21	H-Donor	:UNK0:H	H-Donor
Glucose_ring						
0.87	Unfavorable	Unfavorable Donor-Donor	A:ARG65:HH21	H-Donor	:UNK0:H	H-Donor
2.41	Unfavorable	Unfavorable Donor-Donor	A:ARG170:HE	H-Donor	:UNK0:H	H-Donor
1.22	Unfavorable	Unfavorable Donor-Donor	A:GLY396:HN	H-Donor	:UNK0:H	H-Donor
Human Phosphoglycerate Mutase (PDB ID: 1YJX)						
2DG_chain						
2.35	Unfavorable	Unfavorable Donor-Donor	A:ARG10:HH21	H-Donor	:UNK0:H	H-Donor
Glucose_chain						
1.96	Unfavorable	Unfavorable Donor-Donor	A:SER23:HN	H-Donor	:UNK0:H	H-Donor
1.56	Unfavorable	Unfavorable Donor-Donor	:UNK0:H	H-Donor	:UNK0:H	H-Donor
1.82	Unfavorable	Unfavorable Donor-Donor	:UNK0:H	H-Donor	:UNK0:H	H-Donor
Glucose_ring						
2.06	Unfavorable	Unfavorable Donor-Donor	A:ASN17:HD22	H-Donor	:UNK0:H	H-Donor
1.58	Unfavorable	Unfavorable Donor-Donor	A:SER23:HN	H-Donor	:UNK0:H	H-Donor
Human Enolase (PDB ID: 4ZCW)						
2DG_chain						
1.59	Unfavorable	Unfavorable Donor-Donor	A:LYS120:HZ2	H-Donor	:UNK0:H	H-Donor
2.86	Unfavorable	Unfavorable Acceptor-Acceptor	A:ASP378:OD2	H-Acceptor	:UNK0:O	H-Acceptor
Glucose_chain						
2.38	Unfavorable	Unfavorable Donor-Donor	A:SER373:N	H-Donor		
2DG_ring						
2.26	Unfavorable	Unfavorable Donor-Donor	A:SER373:N	H-Donor	:UNK0:H	H-Donor
2.72	Unfavorable	Unfavorable Acceptor-Acceptor	A:SER40:O	H-Acceptor	:UNK0:O	H-Acceptor

UNSATISFIED SITE

Name	**Atoms**	**Unsatisfied type**
Human Hexokinase (PDB ID: 1QAH)		
2DG_chain		
:UNK0:O	O	Acceptor
Glucose_chain		
:UNK0:O	O	Acceptor
:UNK0:H	H	Donor
:UNK0:H	H	Donor
2DG_ring		
:UNK0:O	O	Acceptor
:UNK0:H	H	Donor

:UNK0:H	H	Donor
Glucose_Ring		
:UNK0:O	O	Acceptor
:UNK0:H	H	Donor
:UNK0:H	H	Donor
:UNK0:H	H	Donor
Human Phosphoglucose Isomerase (PDB ID: 1JLH)		
2DG_chain		
:UNK0:H	H	Donor
:UNK0:H	H	Donor
:UNK0:O	O	Acceptor
:UNK0:H	H	Donor
Glucose_chain		
:UNK0:H	H	Donor
:UNK0:H	H	Donor
:UNK0:H	H	Donor
:UNK0:H	H	Donor
2DG_ring		
:UNK0:H	H	Donor
:UNK0:H	H	Donor
:UNK0:H	H	Donor
Glucosr_ring		
:UNK0:H	H	Donor
:UNK0:H	H	Donor
:UNK0:H	H	Donor
:UNK0:H	H	Donor
:UNK0:H	H	Donor
Human Phosphofructokinase (PDB ID: 4WL0)		
Glucose_chain		
:UNK0:H	H	Donor
2DG_ring		
:UNK0:H	H	Donor
:UNK0:H	H	Donor
Glucose_ring		
:UNK0:O	O	Acceptor
:UNK0:H	H	Donor
:UNK0:H	H	Donor
:UNK0:H	H	Donor
Human Fructose 1,6-bisphosphate Aldolase (PDB ID: 4ALD)		
2DG_chain		
:UNK0:H	H	Donor
Glucose_chain		
:UNK0:H	H	Donor
:UNK0:H	H	Donor
2DG_ring		
:UNK0:O	O	Acceptor
:UNK0:H	H	Donor
Glucose_ring		
:UNK0:H	H	Donor
:UNK0:H	H	Donor
Human Triose Phosphate Isomerase (PDB ID: 6NLH)		
2DG_chain		
:UNK0:H	H	Donor
Glucose_chain		
:UNK0:H	H	Donor
2DG_ring		
:UNK0:O	O	Acceptor
:UNK0:H	H	Donor
Glucose_ring		
:UNK0:H	H	Donor
:UNK0:H	H	Donor
:UNK0:H	H	Donor
:UNK0:H	H	Donor
Human Glyceraldehyde-3-Phosphate Dehydrogenase (PDB ID: 3GPD)		
Glucose_chain		
:UNK0:O	O	Acceptor
:UNK0:H	H	Donor

:UNK0:H	H	Donor
2DG_ring		
:UNK0:O	O	Acceptor
:UNK0:H	H	Donor
:UNK0:H	H	Donor
Glucose_ring		
:UNK0:O	O	Acceptor
Human Phosphoglycerate Kinase (PDB ID: 3C3C)		
2DG_chain		
:UNK0:H	H	Donor
:UNK0:H	H	Donor
:UNK0:H	H	Donor
Glucose_chain		
:UNK0:H	H	Donor
:UNK0:H	H	Donor
:UNK0:H	H	Donor
2DG_ring		
:UNK0:H	H	Donor
:UNK0:H	H	Donor
Glucose_ring		
:UNK0:H	H	Donor
:UNK0:H	H	Donor
:UNK0:H	H	Donor
Human Phosphoglycerate Mutase (PDB ID: 1YJX)		
2DG_chain		
:UNK0:H	H	Donor
:UNK0:H	H	Donor
Glucose_chain		
:UNK0:H	H	Donor
:UNK0:H	H	Donor
2DG_ring		
:UNK0:O	O	Acceptor
:UNK0:H	H	Donor
:UNK0:H	H	Donor
Glucose_ring		
:UNK0:O	O	Acceptor
:UNK0:H	H	Donor
:UNK0:H	H	Donor
Human Enolase (PDB ID: 4ZCW)		
2DG_chain		
:UNK0:H	H	Donor
Glucose_chain		
:UNK0:H	H	Donor
2DG_ring		
:UNK0:H	H	Donor

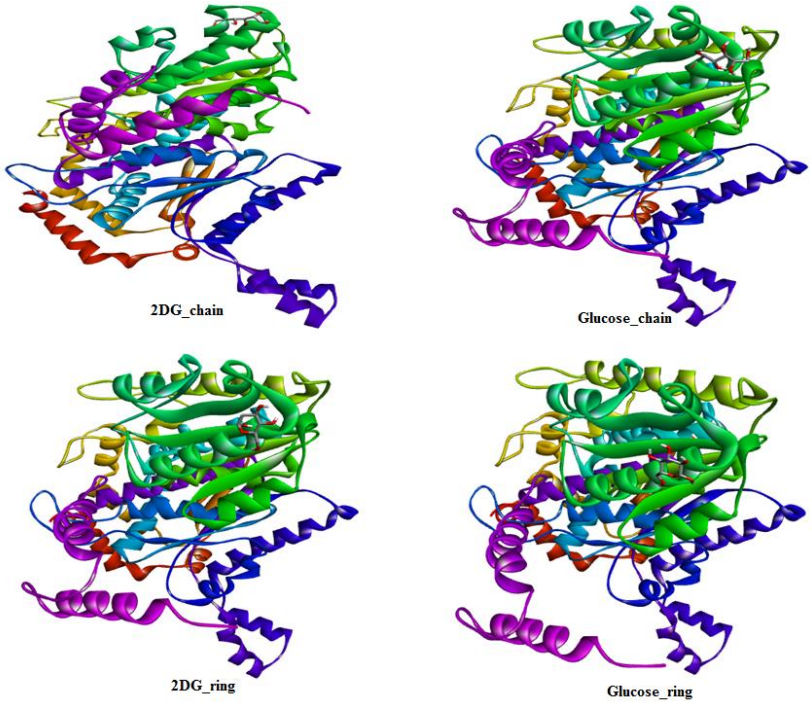

Figure S1a. Skeletal structure of interactions of human phosphoglucose isomerase with 2DG and Glucose.

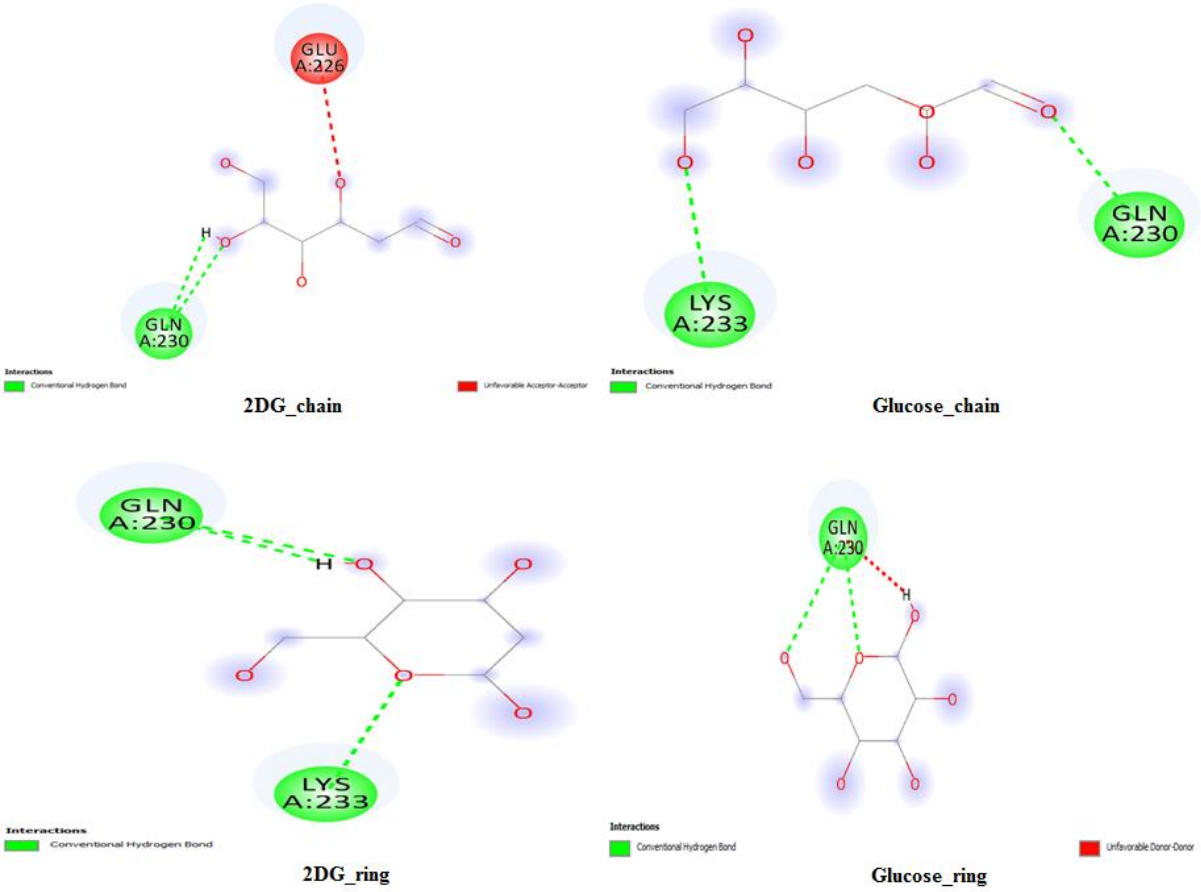

Figure S1b. 2Dl structure of interactions of human phosphoglucose isomerase with 2DG and Glucose.

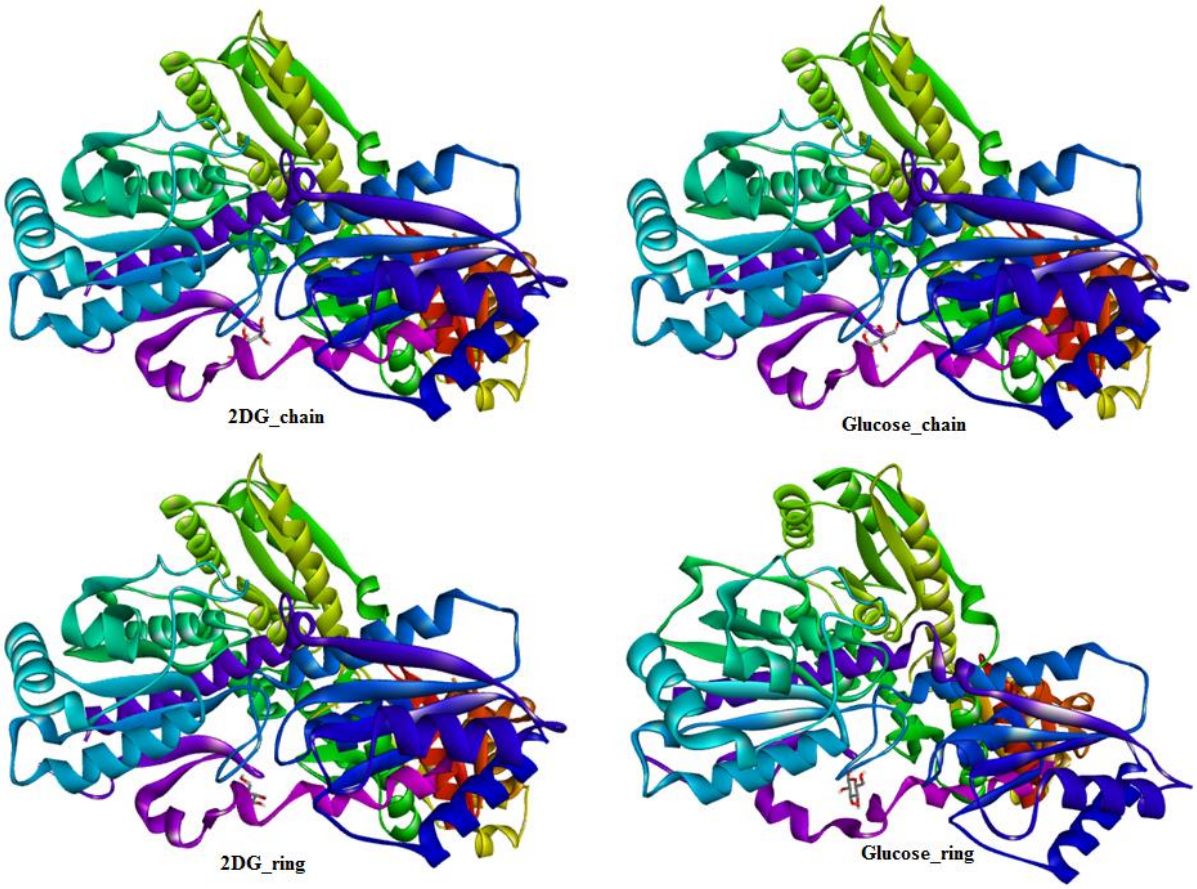

Figure S2a. Skeletal structure of interactions of human phosphofructokinase with 2DG and Glucose.

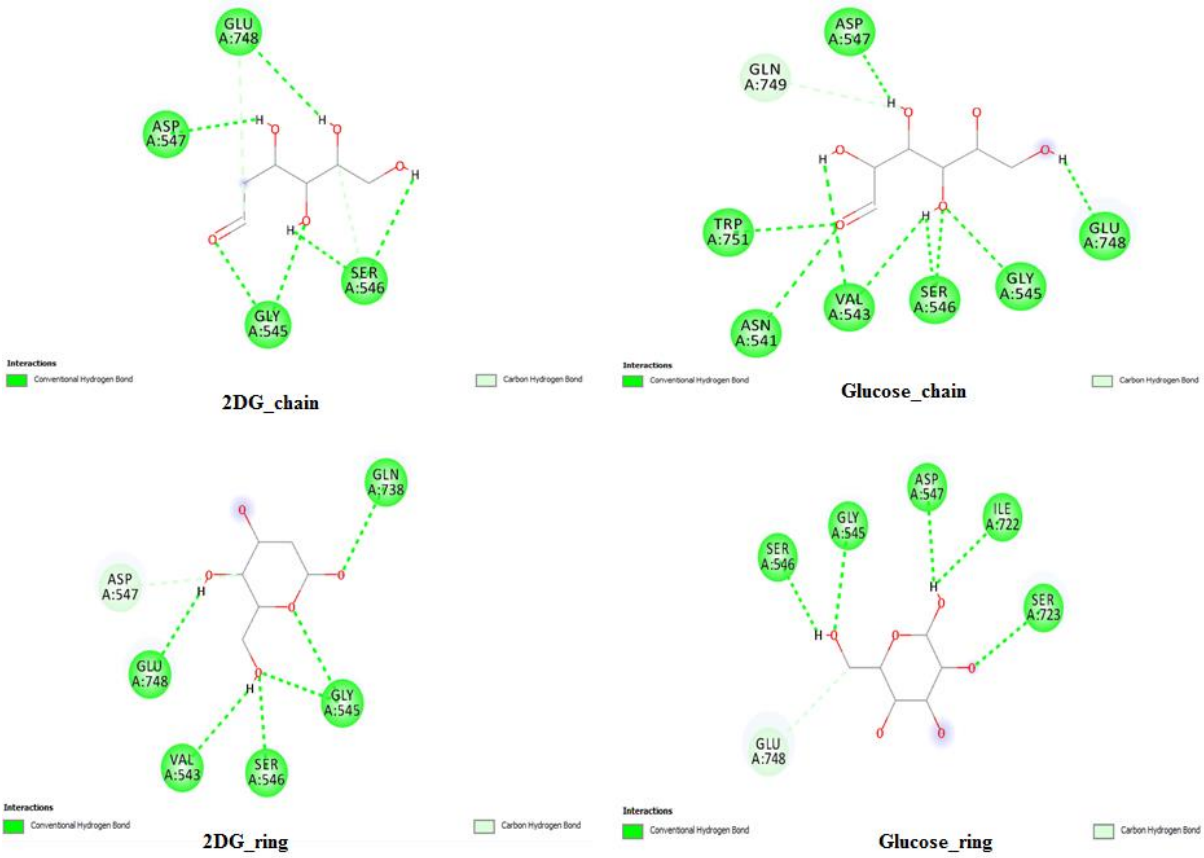

Figure S2b. 2D structure of interactions of human phosphofructokinase with 2DG and Glucose.

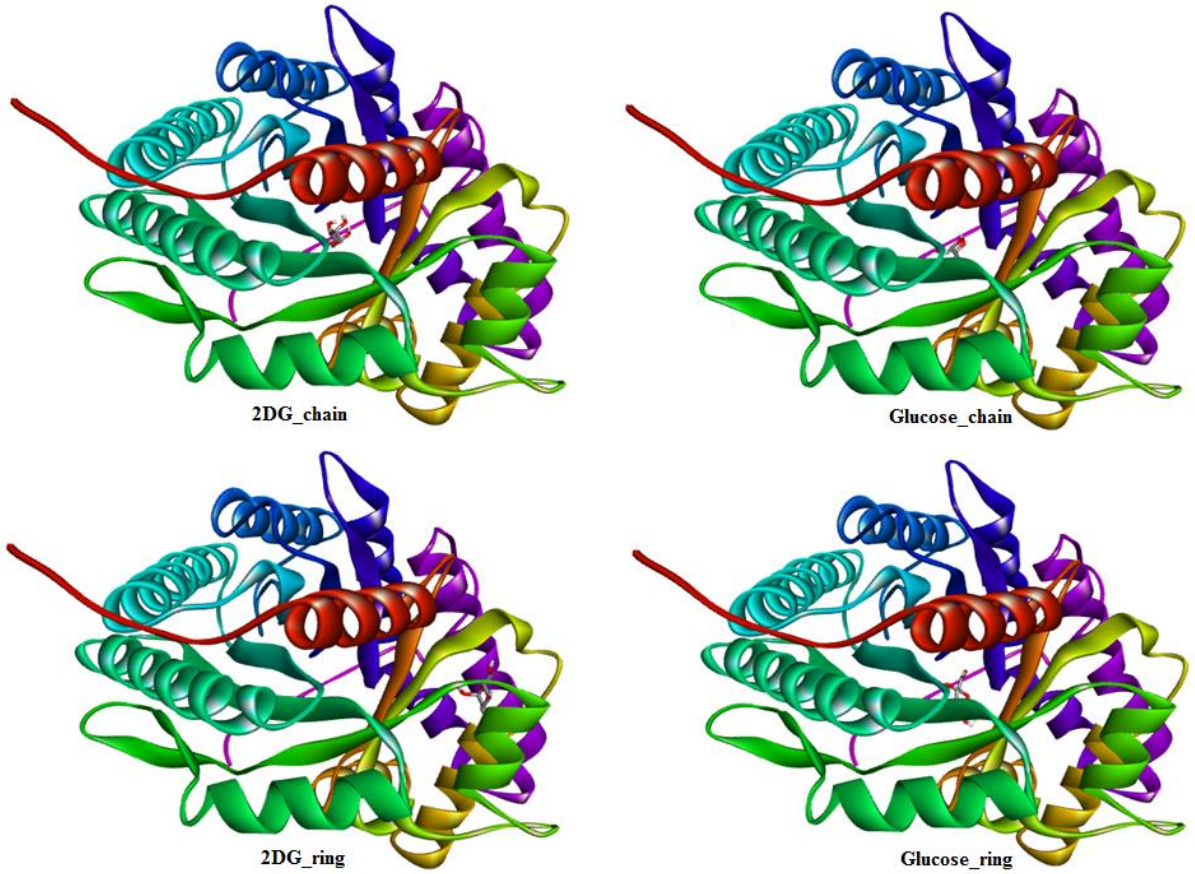

Figure S3a. Skeletal structure of interactions of human fructose 1,6-bisphosphate aldolase with 2DG and Glucose.

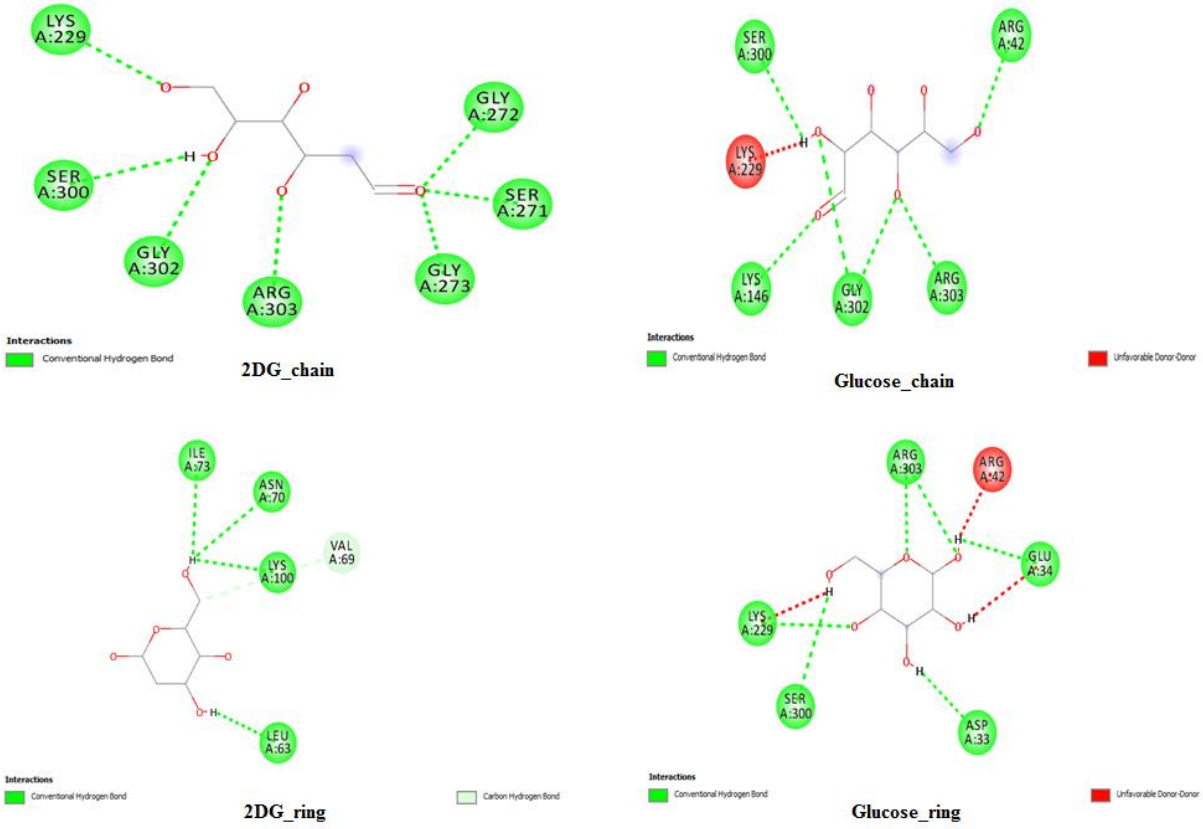

Figure S3b. 2D structure of interactions of human fructose 1,6-bisphosphate aldolase with 2DG and Glucose.

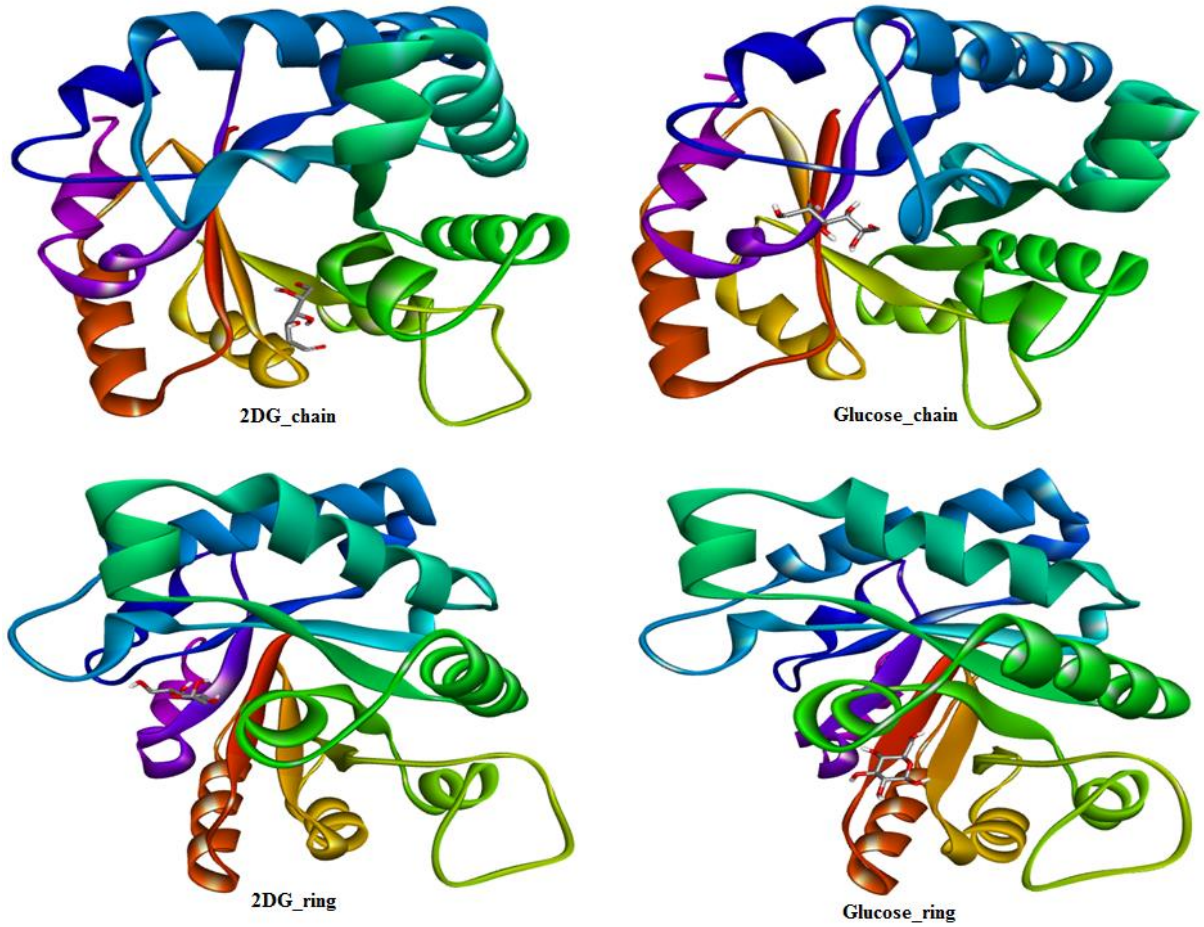

Figure S4a. Skeletal structure of interactions of human triose phosphate isomerase with 2DG and Glucose.

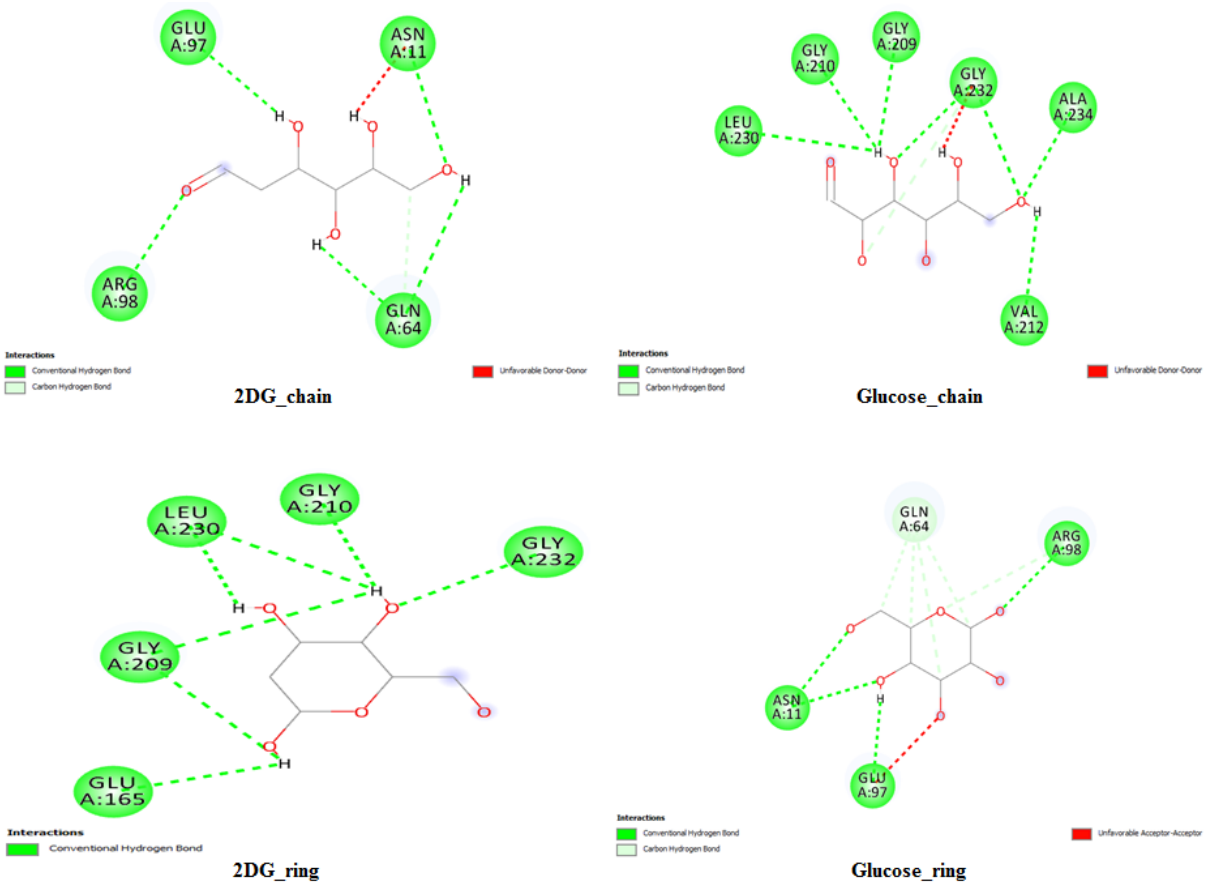

Figure S4b. 2D structure of interactions of human triose phosphate isomerase with 2DG and Glucose.

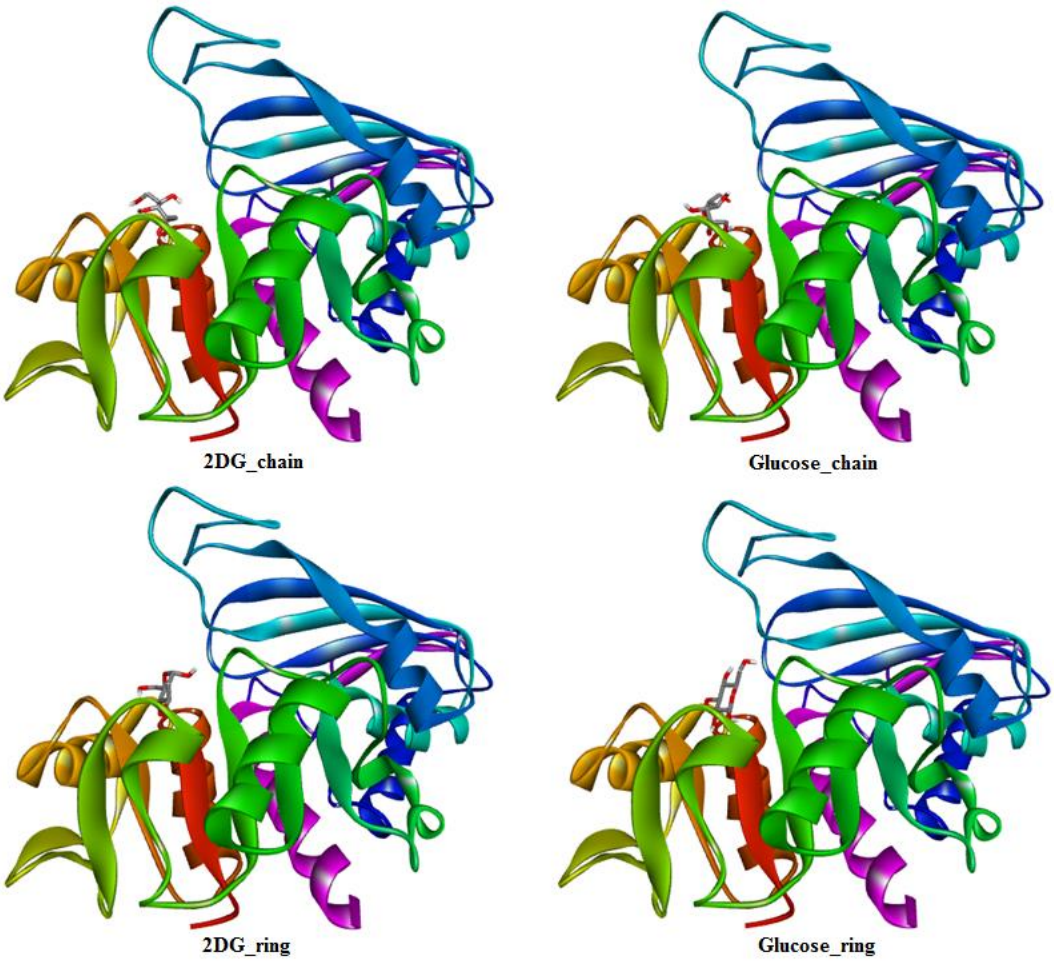

Figure S5a. Skeletal structure of interactions of human glyceraldehyde-3-phosphate dehydrogenase with 2DG and Glucose.

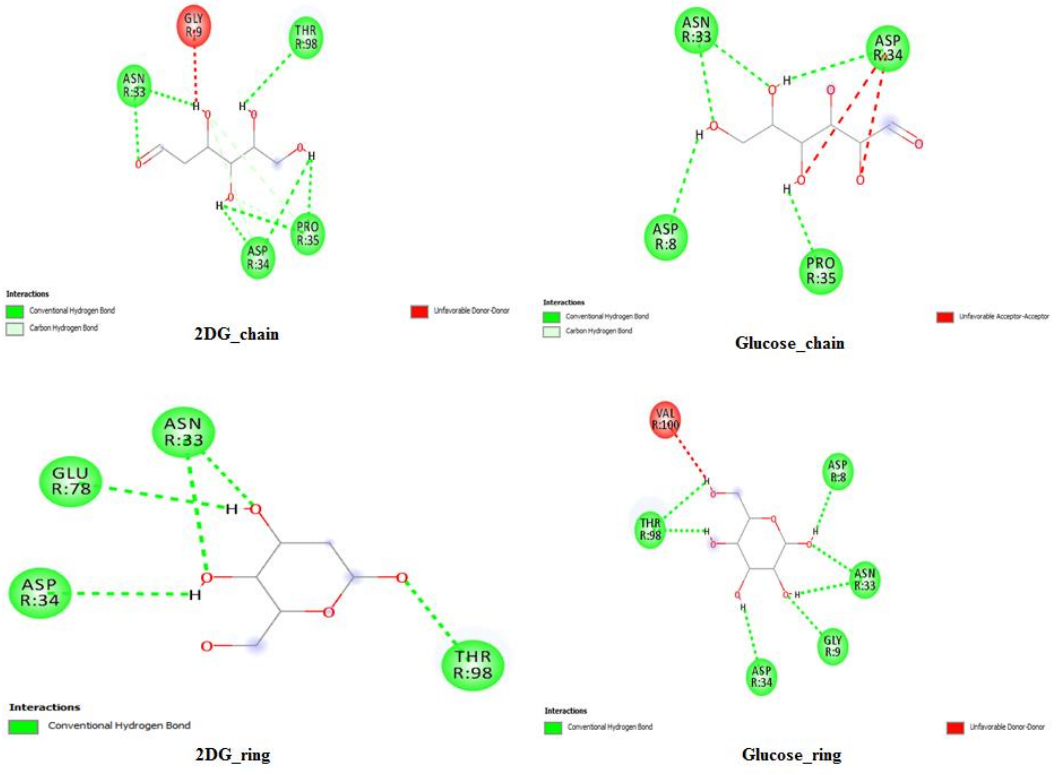

Figure S5b. 2D structure of interactions of human glyceraldehyde-3-phosphate dehydrogenase with 2DG and Glucose

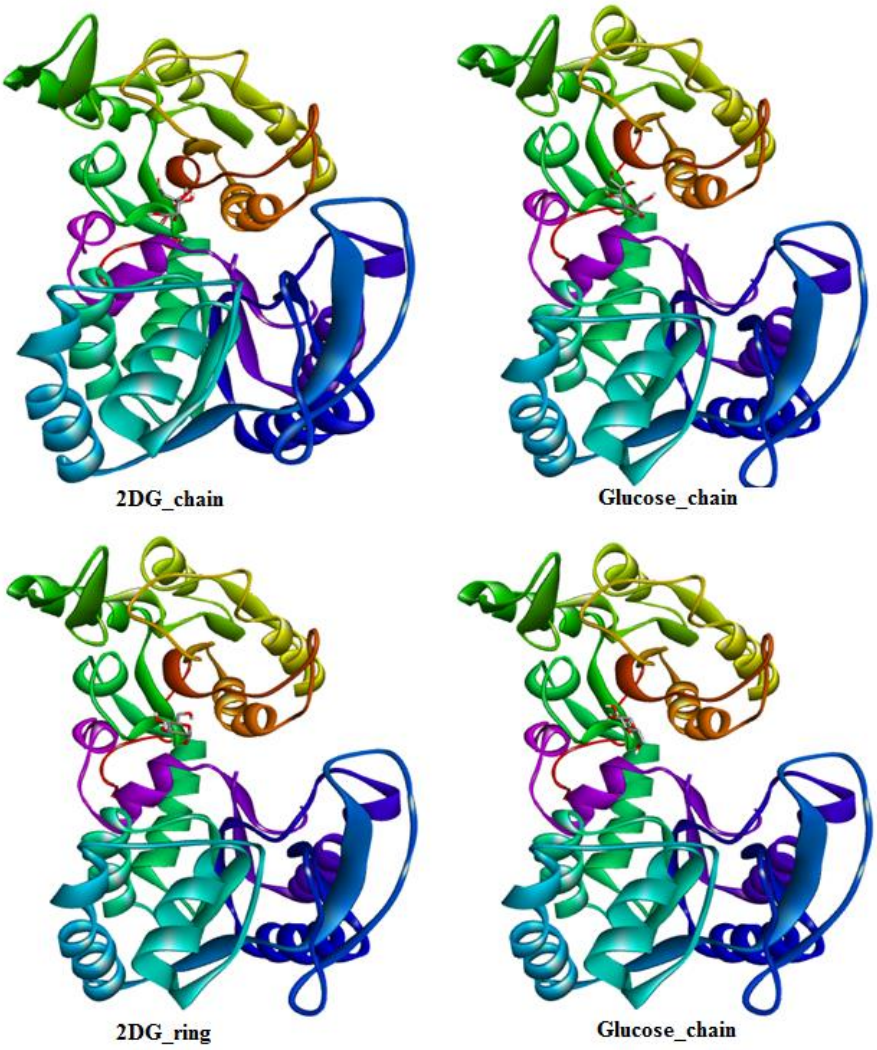

Figure S6a. Skeletal structure of interactions of human phosphoglycerate kinase with 2DG and Glucose.

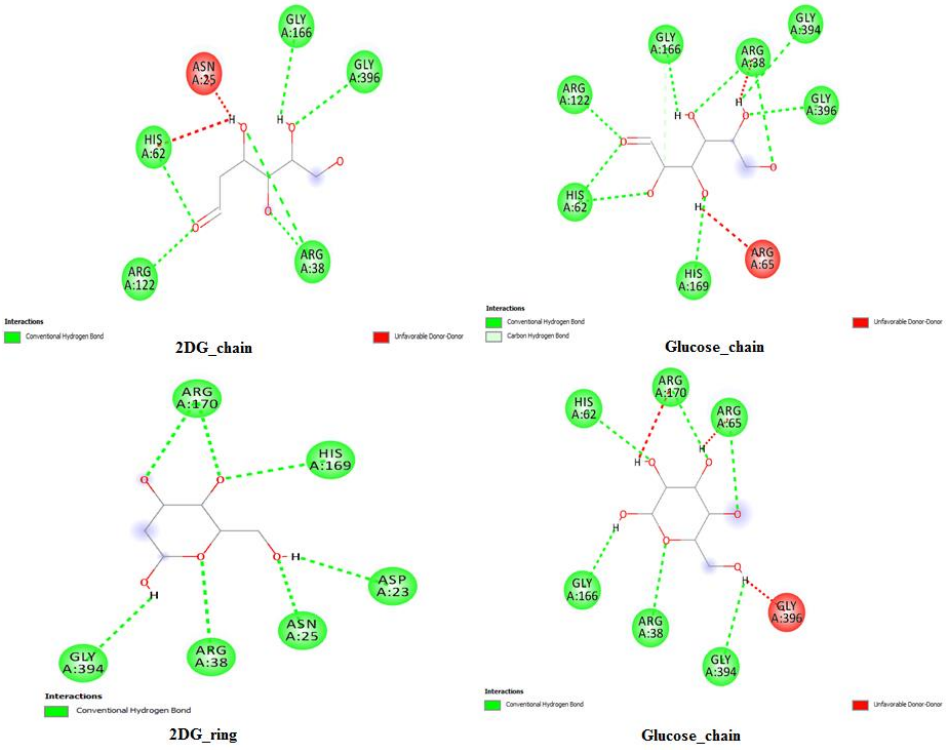

Figure S6b. 2D structure of interactions of human phosphoglycerate kinase with 2DG and Glucose

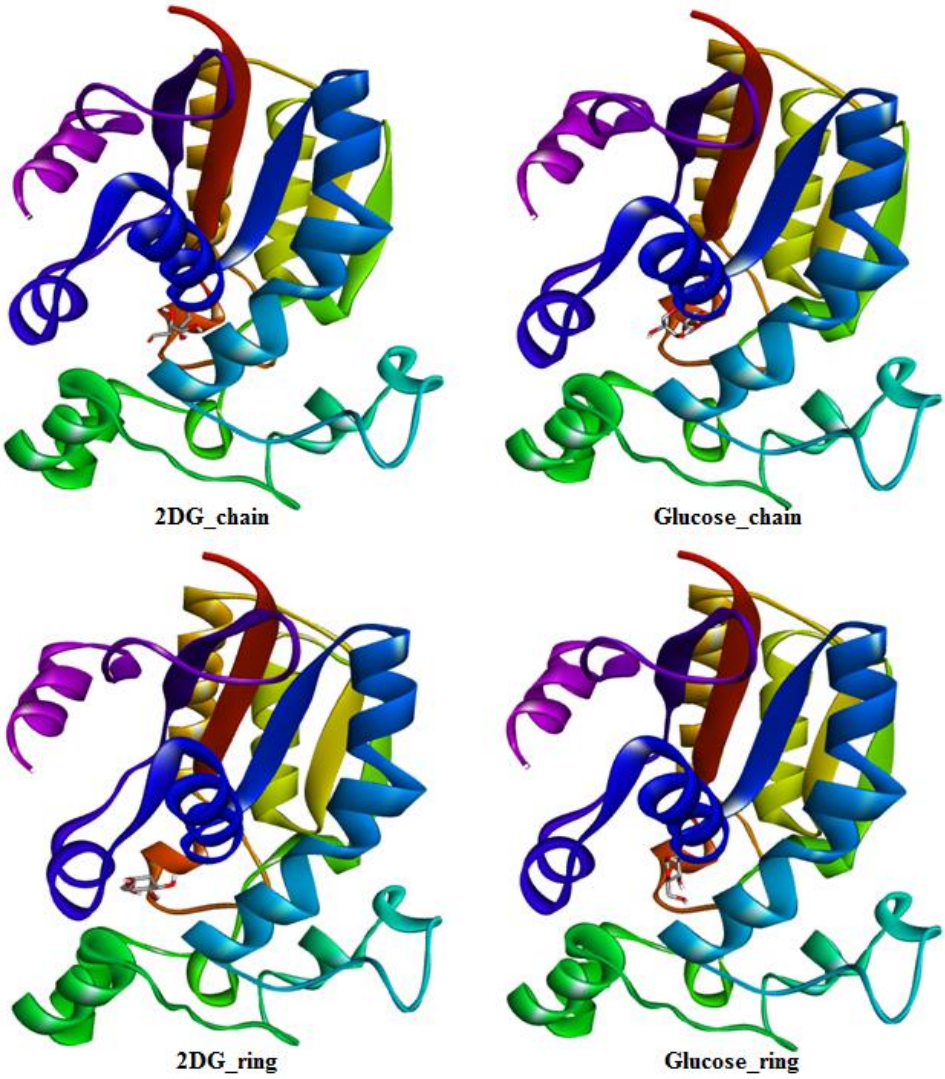

Figure S7a. Skeletal structure of interactions of human phosphoglycerate mutase with 2DG and Glucose.

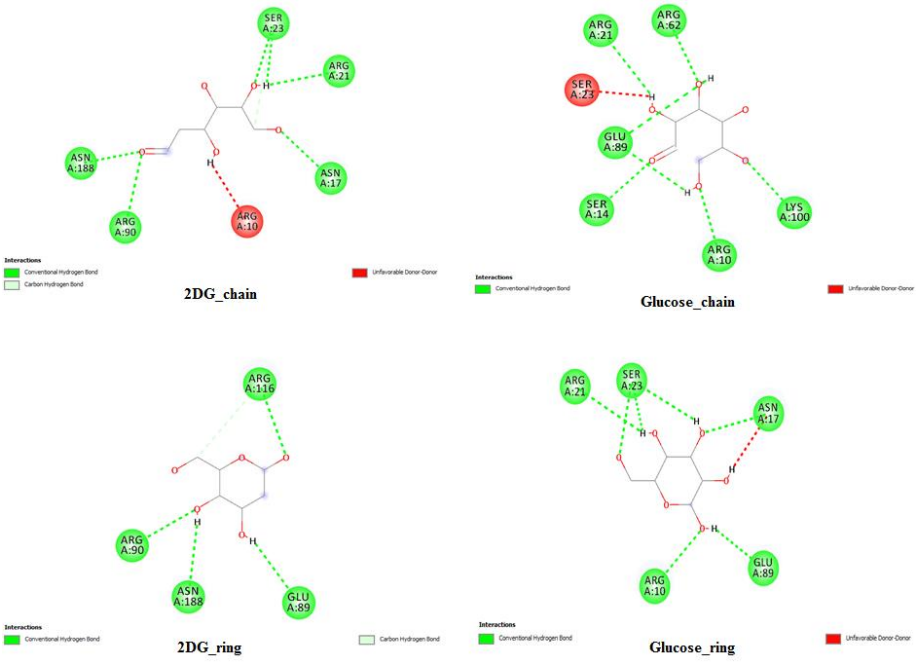

Figure S7b. 2D structure of interactions of human phosphoglycerate mutase with 2DG and Glucose.

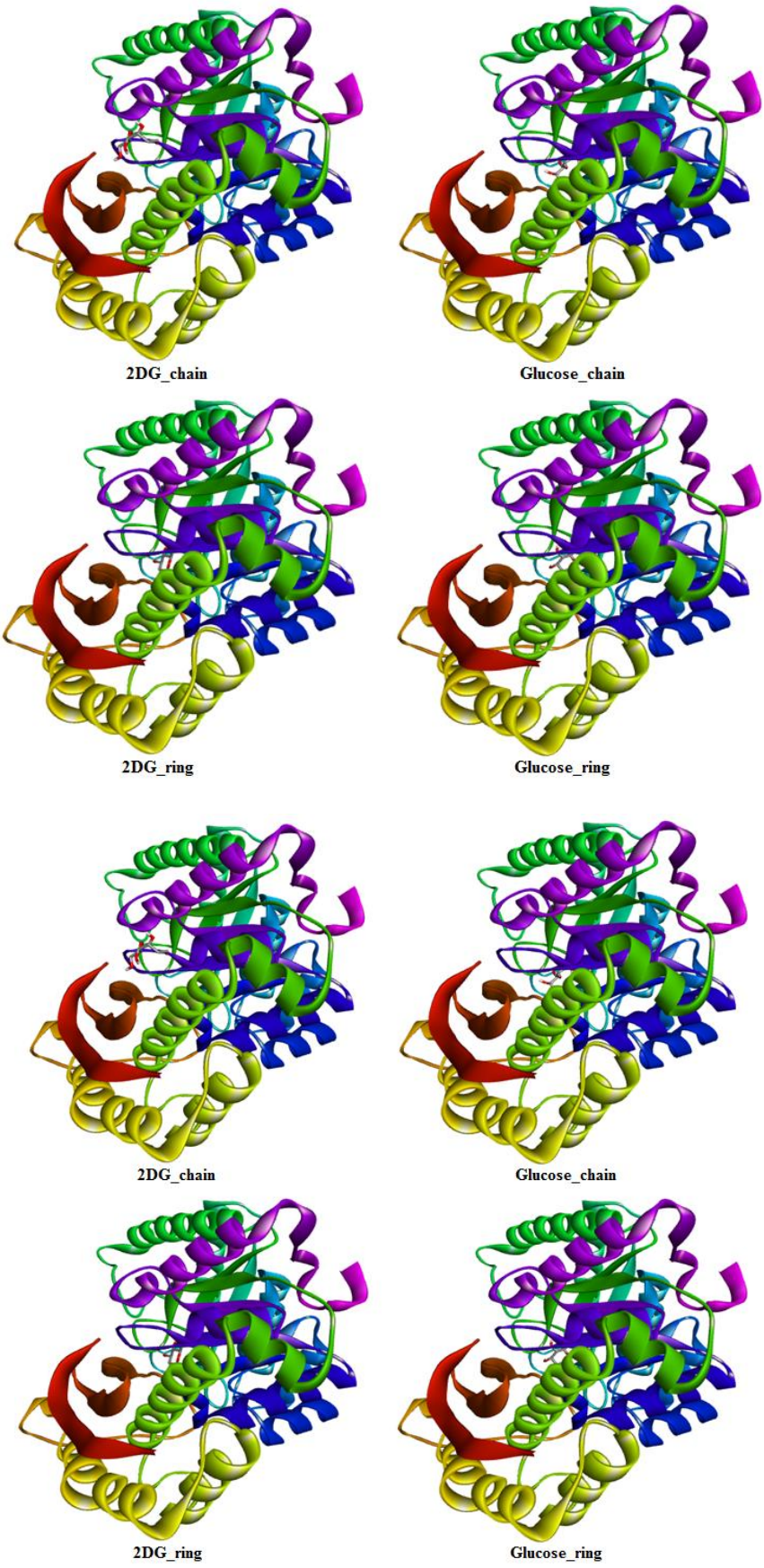

Figure S8a. Skeletal structure of interactions of human enolase with 2DG and Glucose.

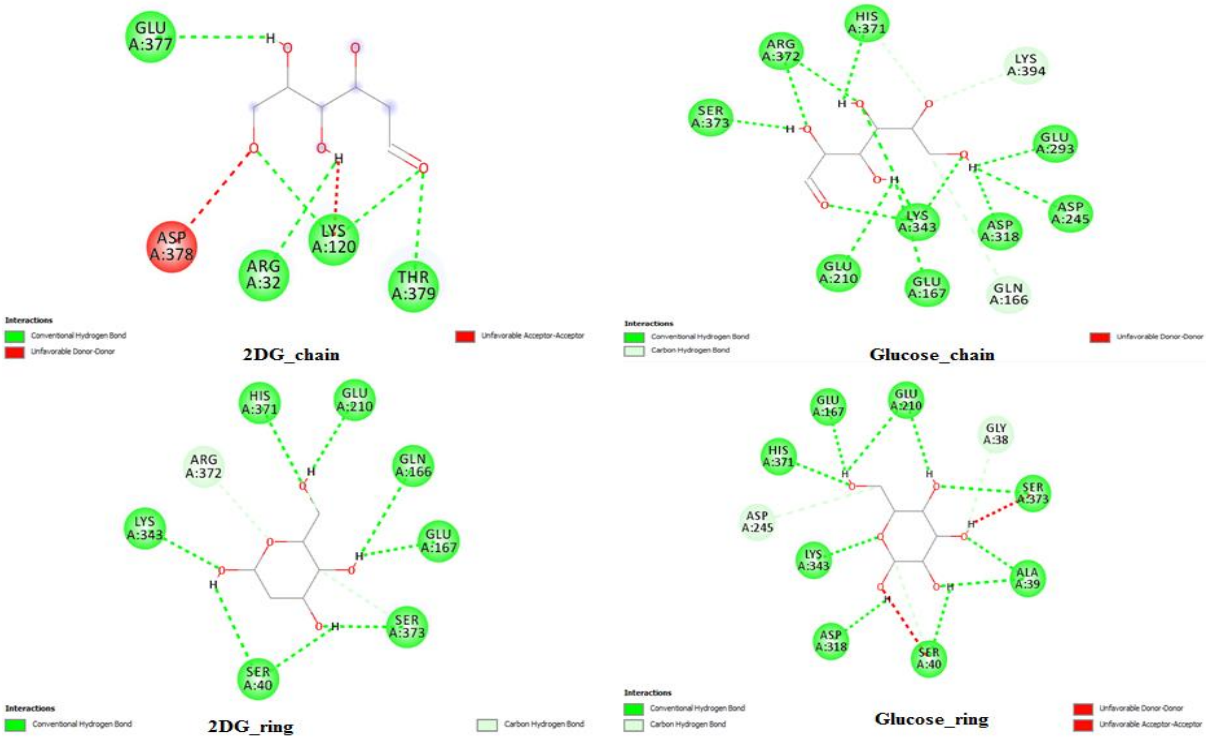

Figure S8b. 2D structure of interactions of human enolase with 2DG and Glucos.