



SWISS-MODEL Homology Modelling Report

Model Building Report

This document lists the results for the homology modelling project "Untitled Project" submitted to SWISS-MODEL workspace on Oct. 18, 2023, 8:59 a.m..The submitted primary amino acid sequence is given in Table T1.

If you use any results in your research, please cite the relevant publications:

- Waterhouse, A., Bertoni, M., Bienert, S., Studer, G., Tauriello, G., Gumienny, R., Heer, F.T., de Beer, T.A.P., Rempfer, C., Bordoli, L., Lepore, R., Schwede, T. SWISS-MODEL: homology modelling of protein structures and complexes. Nucleic Acids Res. 46(W1), W296-W303 (2018).
- Bienert, S., Waterhouse, A., de Beer, T.A.P., Tauriello, G., Studer, G., Bordoli, L., Schwede, T. The SWISS-MODEL Repository - new features and functionality. Nucleic Acids Res. 45, D313-D319 (2017).
- Studer, G., Tauriello, G., Bienert, S., Biasini, M., Johnner, N., Schwede, T. ProMod3 - A versatile homology modelling toolbox. PLOS Comp. Biol. 17(1), e1008667 (2021).
- Studer, G., Rempfer, C., Waterhouse, A.M., Gumienny, G., Haas, J., Schwede, T. QMEANDisCo - distance constraints applied on model quality estimation. Bioinformatics 36, 1765-1771 (2020).
- Bertoni, M., Kiefer, F., Biasini, M., Bordoli, L., Schwede, T. Modeling protein quaternary structure of homo- and hetero-oligomers beyond binary interactions by homology. Scientific Reports 7 (2017).

Results

The SWISS-MODEL template library (SMTL version 2023-10-12, PDB release 2023-10-06) was searched with for evolutionary related structures matching the target sequence in Table T1. For details on the template search, see Materials and Methods. Overall 95 templates were found (Table T2).

Models

The following model was built (see Materials and Methods "Model Building"):

Model #01	File	Built with	Oligo-State	Ligands	GMQE	QMEANDisCo Global
	PDB	ProMod3 3.3.0	homo-tetramer (matching prediction)	None	0.60	0.60 ± 0.05

Template	Seq Identity	Oligo-state	QSQE	Found by	Method	Resolution	Seq Similarity	Range	Coverage	Description
7zny.1.A	35.37	homo-tetramer	0.54	HHblits	EM	-	0.38	130 - 606	0.99	Hemagglutinin glycoprotein

The template contained no ligands.

Target	MSAQRERINAFYKGNPHNKNHRVILDRERLVIERPYILLGVLLVMFLSLIGLLAIAGIRLHRATVGTLEIQSRLNTNIEL
7zny.1.A	MLSYQDKVSFAFYKDNARANSSKLSLVTEEQGGRRPPYLLFVLLILLVGMALLAITGVRFHQVSTSNMEFSRLLKEDMEK
Target	TESIDHQTQDVLTPLFKIIGDEVGIRIPQKFSDLVKFISDKIKFLNPDREYDFRDLRWCMNPPERVKINFQDQCEYKAAV
7zny.1.A	SEAVHHQVIDVLTPLFKIIGDEIGRLRPQKLNEIKQFILQKTNNFNPREFDFRDLHWCINPPSIKVNFTNYCDTIGIR
Target	KSIEHIFESPLNKSKKLQSLTLGPGTGCQGRVTTRAHFSELTLTLMDLDEMKNHVSSVFTVVEEGLFGRITYTVWRSDAR
7zny.1.A	KSIASAA NPILLSALSGGRGDIFFPYRCSGATTSVGRVFPLSVLSMSLSIRTSEIINMLTAISDGVYGYKTYLLVPDYIE
Target	DPSTDPGIGHFLRVFEIGLVRLDGLGPPVFHMTNYLTVNMSDDYRRCLLAVGELKLTALCTSSETVTLSERGVPKRKPLV
7zny.1.A	GG----FDTQKIRVFEIGFIKRWLNDMPLLQTNTYMLPENSAKAVCTIAGELTLASLCVDESTVLLYHSDSGSQDGIL
Target	VVILNLAGPTLGGELYSVLPTSDLMVEKLYLSSHGRIKDEANWVPSTDVRDLQNKGECLVEACKTRPPSFCNGTGSG
7zny.1.A	VVTLGIFGATPMDQVEEVIPVAHPSVEKIHITNHRGFIKDSIATWMPALVSEKQEEQKNCLESACQRKSYPMCNTSWE
Target	PWSEGRIPAYGVIRVSLNSASDPGVVITSVFGPLIPHLSGMDLYNNPFSRAVWLAVPPYEQSFLGMINTIGFPNRAEVMP
7zny.1.A	PFGGGQLPSYGRLLPLDPSIDLQLNISFTYGPVILNGDGMYYESPLLD SGWLTIPPKNGTVLGLINKASRGDQFTVIP

Target 7zny.1.A	HILTTEIRGPRGRCHVPIELSRRVDDDIKIGSNMVILPTMDLRYITATYDVSRRHAIVVYIYDTGLSSSSYYYPVRLNFK HVLTFAPRESSGNCYLPIQTSQIMDKDVLTESNLVVLPTQNFRYVIATYDISRGDHAIVVYVYDPIRAISYTYPFRLTTK
Target 7zny.1.A	GNPLSLRIECFPWRHKVWCYHDCLIYNTITDEEVHTRGLTGIEVTCNPV GRPDFLRIECFVWDDDLWCHQFYRFEADSTNSTTSVENLVRIRFSCNRS
Target 7zny.1.B	MSAQRERINAFYKGNPHNKNHRVILDRERLVIERPYILLGVLLVMFSLIGLLAIAGIRLHRATVGTLEIQSRLNTNIEL MLSYQDKVSFAFYKDNARANSSKLSLVTEEQGGRRPPYLLFVLLILLVGIMALLAITGVRFHQVSTSNMEFSRLLKEDMEK
Target 7zny.1.B	TESIDHQT KDVL TPLFKIIGDEVGIRIPQKFSDLVKFISDKIKFLNPDREYDFRDLRWCMNPPERVKINFDQFCEYKAAV SEAVHHQVIDVL TPLFKIIGDEIGRLRPQKLNEIKQFILQKTNFFNPNREFDFRDLHWCINPPSKIKVNFNYCDTIGIR
Target 7zny.1.B	KSIEHIFESPLNKS KKLQSLTLGPGTGCQGRVTTRAHFSELTLTLMDLDEMKNHVSSVFTVVEEGLFGRTYTVWRSDAR KSIASAANPILLSALS GGRGDIFPPYRCGATTSVGRVFPLSVLSMSLSIRTSEIINMLTAISDGVYGKTYLLVPDYIE
Target 7zny.1.B	DPSTDPGIGHFLRVFEIGLV RDLGLGPPVFHMTNYLTVNMSDDYRRCLLAVGELKLTALCTSSETVTLSERGVPKRKPLV GG----FDTQKIRVFEIGFIKRWLNDMPLLQTNTYMLVPENSAKAVCTIAGELTLASLCVDESTVLLYHSDGSDQGIL
Target 7zny.1.B	VVILNLAGPTLGGE LYSVLPTS DLMVEKLYLSSHGIIKDDEANWVPSTDVRDLQNKGECLVEACKTRPPSFCNGTGSG VVTLGIFGATPMDQVEE VIPVAHPSVEKIHITNHRGFIKDSIATWMVPALVSEKQEEQKNCLESAQQRKSYPMCNTSWE
Target 7zny.1.B	PWSEGRIPAYGVIRVSLNSASDPGVVITSVFGLPIPHLSGMDLYNNPFSRAVWLAVPPYEQSFLGMINTIGFPNRAEVMP PFGGGQLPSYGR LTLPLDPSIDLQLNISFTYGPVILNGDGMYYESPLLD SGWLTIPPKNGTVLGLINKASRGDQFTVIP
Target 7zny.1.B	HILTTEIRGPRGRCHVPIELSRRVDDDIKIGSNMVILPTMDLRYITATYDVSRRHAIVVYIYDTGLSSSSYYYPVRLNFK HVLTFAPRESSGNCYLPIQTSQIMDKDVLTESNLVVLPTQNFRYVIATYDISRGDHAIVVYVYDPIRAISYTYPFRLTTK
Target 7zny.1.B	GNPLSLRIECFPWRHKVWCYHDCLIYNTITDEEVHTRGLTGIEVTCNPV GRPDFLRIECFVWDDDLWCHQFYRFEADSTNSTTSVENLVRIRFSCNRS
Target 7zny.1.C	MSAQRERINAFYKGNPHNKNHRVILDRERLVIERPYILLGVLLVMFSLIGLLAIAGIRLHRATVGTLEIQSRLNTNIEL MLSYQDKVSFAFYKDNARANSSKLSLVTEEQGGRRPPYLLFVLLILLVGIMALLAITGVRFHQVSTSNMEFSRLLKEDMEK
Target 7zny.1.C	TESIDHQT KDVL TPLFKIIGDEVGIRIPQKFSDLVKFISDKIKFLNPDREYDFRDLRWCMNPPERVKINFDQFCEYKAAV SEAVHHQVIDVL TPLFKIIGDEIGRLRPQKLNEIKQFILQKTNFFNPNREFDFRDLHWCINPPSKIKVNFNYCDTIGIR
Target 7zny.1.C	KSIEHIFESPLNKS KKLQSLTLGPGTGCQGRVTTRAHFSELTLTLMDLDEMKNHVSSVFTVVEEGLFGRTYTVWRSDAR KSIASAANPILLSALS GGRGDIFPPYRCGATTSVGRVFPLSVLSMSLSIRTSEIINMLTAISDGVYGKTYLLVPDYIE
Target 7zny.1.C	DPSTDPGIGHFLRVFEIGLV RDLGLGPPVFHMTNYLTVNMSDDYRRCLLAVGELKLTALCTSSETVTLSERGVPKRKPLV GG----FDTQKIRVFEIGFIKRWLNDMPLLQTNTYMLVPENSAKAVCTIAGELTLASLCVDESTVLLYHSDGSDQGIL
Target 7zny.1.C	VVILNLAGPTLGGE LYSVLPTS DLMVEKLYLSSHGIIKDDEANWVPSTDVRDLQNKGECLVEACKTRPPSFCNGTGSG VVTLGIFGATPMDQVEE VIPVAHPSVEKIHITNHRGFIKDSIATWMVPALVSEKQEEQKNCLESAQQRKSYPMCNTSWE
Target 7zny.1.C	PWSEGRIPAYGVIRVSLNSASDPGVVITSVFGLPIPHLSGMDLYNNPFSRAVWLAVPPYEQSFLGMINTIGFPNRAEVMP PFGGGQLPSYGR LTLPLDPSIDLQLNISFTYGPVILNGDGMYYESPLLD SGWLTIPPKNGTVLGLINKASRGDQFTVIP
Target 7zny.1.C	HILTTEIRGPRGRCHVPIELSRRVDDDIKIGSNMVILPTMDLRYITATYDVSRRHAIVVYIYDTGLSSSSYYYPVRLNFK HVLTFAPRESSGNCYLPIQTSQIMDKDVLTESNLVVLPTQNFRYVIATYDISRGDHAIVVYVYDPIRAISYTYPFRLTTK
Target 7zny.1.C	GNPLSLRIECFPWRHKVWCYHDCLIYNTITDEEVHTRGLTGIEVTCNPV GRPDFLRIECFVWDDDLWCHQFYRFEADSTNSTTSVENLVRIRFSCNRS
Target 7zny.1.D	MSAQRERINAFYKGNPHNKNHRVILDRERLVIERPYILLGVLLVMFSLIGLLAIAGIRLHRATVGTLEIQSRLNTNIEL MLSYQDKVSFAFYKDNARANSSKLSLVTEEQGGRRPPYLLFVLLILLVGIMALLAITGVRFHQVSTSNMEFSRLLKEDMEK
Target 7zny.1.D	TESIDHQT KDVL TPLFKIIGDEVGIRIPQKFSDLVKFISDKIKFLNPDREYDFRDLRWCMNPPERVKINFDQFCEYKAAV SEAVHHQVIDVL TPLFKIIGDEIGRLRPQKLNEIKQFILQKTNFFNPNREFDFRDLHWCINPPSKIKVNFNYCDTIGIR
Target 7zny.1.D	KSIEHIFESPLNKS KKLQSLTLGPGTGCQGRVTTRAHFSELTLTLMDLDEMKNHVSSVFTVVEEGLFGRTYTVWRSDAR KSIASAANPILLSALS GGRGDIFPPYRCGATTSVGRVFPLSVLSMSLSIRTSEIINMLTAISDGVYGKTYLLVPDYIE
Target 7zny.1.D	DPSTDPGIGHFLRVFEIGLV RDLGLGPPVFHMTNYLTVNMSDDYRRCLLAVGELKLTALCTSSETVTLSERGVPKRKPLV GG----FDTQKIRVFEIGFIKRWLNDMPLLQTNTYMLVPENSAKAVCTIAGELTLASLCVDESTVLLYHSDGSDQGIL

Target	VVILNLAGPTLGGELYSVLPTSDLMVEKLYLSSHRIKDEANWVVPSTDVRDLQNKGECLVEACKTRPPSFCNGTGSG
7zny.1.D	VVTLGIFGATPMDQVEEVIPVAHPSVEKIHITNHRGFIKDSIATWMVPALVSEKQEEQKNCLESACQRKSYPMCQNQTSWE
Target	PWSEGRIPAYGVIRVSLNSASDPGVVITSVFGPLIPHLSGMDLYNNPFSRAVWLAVPPYEQSFLGMINTIGFPNRAEVM
7zny.1.D	PFGGGQLPSYGRLTLPLDPSIDLQLNISFTYGPVILNGDGMDDYESPLDSGWLTIPPKNGTVLGLINKASRGDQFTVIP
Target	HILTTEIRGPRGRCHVPIELSRVDDDIKIGSNMVILPTMDLRYITATYDVSRRHAIVVYIYDTGLSSSYYPVRLNFK
7zny.1.D	HVLTFAPRESSGNCYLPIQTSQIMDKDVLTESNLVVLPTQNFRYVIATYDISRGDHAIVVYVYDPIRAISYTYPFRLTTK
Target	GNPLSLRIECFPWRHKVWCYHDCLIYNTITDEEVHTRGLTGIEVTCNPV
7zny.1.D	GRPDFLRIECFVWDDDLWCHQFYRFEADSTNSTTSVENLVRIRFSCNRS

Materials and Methods

Template Search

Template search with has been performed against the SWISS-MODEL template library (SMTL, last update: 2023-10-12, last included PDB release: 2023-10-06).

Model Building

Models are built based on the target-template alignment using ProMod3 (Studer et al.). Coordinates which are conserved between the target and the template are copied from the template to the model. Insertions and deletions are remodelled using a fragment library. Side chains are then rebuilt. Finally, the geometry of the resulting model is regularized by using a force field.

Model Quality Estimation

The global and per-residue model quality has been assessed using the QMEAN scoring function (Studer et al.).

Ligand Modelling

Ligands present in the template structure are transferred by homology to the model when the following criteria are met: (a) The ligands are annotated as biologically relevant in the template library, (b) the ligand is in contact with the model, (c) the ligand is not clashing with the protein, (d) the residues in contact with the ligand are conserved between the target and the template. If any of these four criteria is not satisfied, a certain ligand will not be included in the model. The model summary includes information on why and which ligand has not been included.

Oligomeric State Conservation

The quaternary structure annotation of the template is used to model the target sequence in its oligomeric form. The method (Bertoni et al.) is based on a supervised machine learning algorithm, Support Vector Machines (SVM), which combines interface conservation, structural clustering, and other template features to provide a quaternary structure quality estimate (QSQE). The QSQE score is a number between 0 and 1, reflecting the expected accuracy of the interchain contacts for a model built based a given alignment and template. Higher numbers indicate higher reliability. This complements the GMQE score which estimates the accuracy of the tertiary structure of the resulting model.

References

- BLAST**
 Camacho, C., Coulouris, G., Avagyan, V., Ma, N., Papadopoulos, J., Bealer, K., Madden, T.L. BLAST+: architecture and applications. BMC Bioinformatics 10, 421-430 (2009).  
- HHblits**
 Steinegger, M., Meier, M., Mirdita, M., Vöhringer, H., Haunsberger, S. J., Söding, J. HH-suite3 for fast remote homology detection and deep protein annotation. BMC Bioinformatics 20, 473 (2019).  

Table T1:

Primary amino acid sequence for which templates were searched and models were built.

MSAQRERINAFYKGNPHNKNHRVILDRERLVIERPYILLGVLLVMFLSLIGLLAIAGIRLHRATVGTLEIQSRLNTNIELTESIDHQTKDVLTPLFKIIG
 DEVGIRIPQKFSDLVKFISDKIKFLNPDREYDFRDLRWCMNPPERVKINFQFCEYKAAVKSIEHIFESPLNKSKKLQSLTLGPGTGCGRTVTRAHFSE
 LTLTLMDDLDMKHNVSSVFTVVEEGLFGRTYTVWRSRDARDPSTDPGIGHFLRVFEIGLVRDLGLGPPVFHMTNYLTVNMSDDYRCLLAVGELKLTALC

TSSETVTLSERGVPKRKPLVVVILNLAGPTLGGELYSVLPTSDLMVEKLYLSSHRGIKDDKANWVVPSTDVVDLQNKGECLVEACKTRPPSFCNGTGS
PWSEGRIPAYGVIRVSLNSASDPGVVITSVFGPLIPHLSGMDLYNNPFSRAVWLAVPPEYQSFLGMINTIGFPNRAEVMPHILTTEIRGPRGRCHVPIEL
SRVDDDIKIGSNMVLPTMDLRYITATYDVSRRHAIVYYIDTGLSSSYYPVRLNFKGNPLSLRIECFPWRHKVWCYHDCLIYNTITDEEVHTRGLT
GIEVTCNPV

Table T2:

Template	Seq Identity	Oligo-state	QSQE	Found by	Method	Resolution	Seq Similarity	Coverage	Description
7zny.1.A	35.37	homo-tetramer	0.54	HHblits	EM	NA	0.38	0.99	Hemagglutinin glycoprotein
2zb5.1.A	38.91	homo-dimer	0.52	HHblits	X-ray	3.00Å	0.40	0.76	Hemagglutinin protein
7zny.1.D	35.37	homo-tetramer	0.54	HHblits	EM	NA	0.38	0.99	Hemagglutinin glycoprotein
7zny.1.C	35.37	homo-tetramer	0.54	HHblits	EM	NA	0.38	0.99	Hemagglutinin glycoprotein
7zny.1.B	35.37	homo-tetramer	0.54	HHblits	EM	NA	0.38	0.99	Hemagglutinin glycoprotein
7zny.1.A	35.82	homo-tetramer	0.51	BLAST	EM	NA	0.39	0.99	Hemagglutinin glycoprotein
2zb5.1.A	39.08	homo-dimer	0.50	BLAST	X-ray	3.00Å	0.40	0.75	Hemagglutinin protein
7zny.1.D	35.82	homo-tetramer	0.51	BLAST	EM	NA	0.39	0.99	Hemagglutinin glycoprotein
7zny.1.C	35.82	homo-tetramer	0.51	BLAST	EM	NA	0.39	0.99	Hemagglutinin glycoprotein
7zny.1.B	35.82	homo-tetramer	0.51	BLAST	EM	NA	0.39	0.99	Hemagglutinin glycoprotein
2zb6.1.A	38.91	homo-dimer	0.45	HHblits	X-ray	2.60Å	0.40	0.76	Hemagglutinin protein
2zb6.1.A	39.08	homo-dimer	0.43	BLAST	X-ray	2.60Å	0.40	0.75	Hemagglutinin protein
3alz.2.E	38.91	homo-hexamer	0.27	HHblits	X-ray	4.52Å	0.40	0.76	Hemagglutinin
3alz.2.E	39.08	homo-hexamer	0.25	BLAST	X-ray	4.52Å	0.40	0.75	Hemagglutinin
2rkc.1.A	38.63	monomer	-	HHblits	X-ray	2.70Å	0.40	0.74	Hemagglutinin
4gjt.1.A	38.19	homo-dimer	0.45	HHblits	X-ray	3.10Å	0.40	0.74	Hemagglutinin glycoprotein
5yzc.1.B	22.22	homo-trimer	-	HHblits	X-ray	2.33Å	0.35	0.10	glycoprotein F1,measles virus fusion protein
6xye.1.B	26.23	homo-trimer	-	HHblits	EM	NA	0.36	0.10	Fusion glycoprotein F1
5yxw.1.B	22.22	homo-trimer	-	HHblits	X-ray	2.78Å	0.35	0.10	glycoprotein F1,measles virus fusion protein

The table above shows the top 19 filtered templates. A further 69 templates were found which were considered to be less suitable for modelling than the filtered list.
1e8t.1.A, 1e8t.1.B, 1e8v.1.B, 1v2i.1.A, 1v2i.1.B, 1v3b.1.A, 1z4v.1.A, 2rkc.1.A, 2vsk.1.A, 2vsm.1.A, 2vwd.1.A, 2x9m.1.A, 3alw.1.A, 3alx.1.A, 3alx.1.B, 3alx.1.C, 3alx.1.D, 3d11.1.A, 3d12.1.A, 3inb.1.A, 3inb.1.B, 3t1e.1.A, 3t1e.1.C, 3t1e.1.D, 4fzh.1.A, 4gjt.1.A, 4jf7.1.A, 4jf7.1.B, 4jf7.1.C, 4jf7.1.D, 4mmq.1.B, 4mza.1.A, 4mza.1.B, 4mze.1.A, 4uf7.1.A, 4wef.1.A, 4xjr.1.A, 4xjr.1.B, 5b2d.1.B, 5kv8.1.A, 5kv9.1.A, 5nop.1.A, 5nop.2.A, 6c0m.1.A, 6c0m.1.B, 6cmg.1.A, 6p72.1.A, 6p7y.1.A, 6pd4.1.A, 6pdl.3.A, 6sg8.1.A, 6thb.1.A, 6vy4.1.A, 6vy4.1.B, 6vy5.1.C, 6vy6.1.A, 7bwu.1.A, 7lze.1.A, 7syz.1.A, 7txz.1.A, 7txz.1.B, 7ty0.1.G, 7ty0.1.H, 7uj3.1.B, 7uja.1.A, 7zm5.1.A, 7zm6.1.A, 8k80.1.A, A0A7C3KN29.1.A