

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 Dec. 22, 2020, 9:58 p.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).
- Guex, N., Peitsch, M.C., Schwede, T. Automated comparative protein structure modeling with SWISS-MODEL and Swiss-PdbViewer: A historical perspective. Electrophoresis 30, S162-S173 (2009). Im ☐ ☐ ☐
- 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., 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 heterooligomers beyond binary interactions by homology. Scientific Reports 7 (2017). (2017)

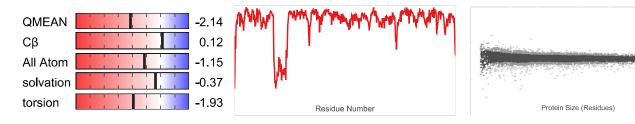
Results

The SWISS-MODEL template library (SMTL version 2020-12-16, PDB release 2020-12-11) was searched with BLAST (Camacho et al.) and HHBlits (Steinegger et al.) for evolutionary related structures matching the target sequence in Table T1. For details on the template search, see Materials and Methods. Overall 1630 templates were found (Table T2).

Models

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

Мо	del #01	File	Built with	Oligo-State	Ligands	GMQE	QMEAN
2		PDB	ProMod3 3.2.0	monomer	1 x SO4: SULFATE ION;	0.60	-2.14



Template	Seq Identity	Oligo- state	QSQE	Found by	Method	Resolution	Seq Similarity	Range	Coverage	Description
1qon.1.A	89.70	monomer	0.00	BLAST	X-ray	2.72Å	0.60	140 - 709	0.77	ACETYLCHOLINESTERASE

Included Ligands

Ligand	Description				
1 x SO4	SULFATE ION				

Excluded ligands

Ligand Name.Number	Reason for Exclusion	Description							
140.3	Not biologically relevant.	9-(3-IODOBENZYLAMINO)-1,2,3,4-TETRAHYDROACRIDINE							
NAG-NAG-BMA-BMA- BMA.1	Not biologically relevant.	beta-D-mannopyranose-(1-3)-[beta-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose							

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Target 1qon.1.A	MARFITSSSLSPSTTPSFASATASPAIASSLPRSKSTKATKARKTILSANSFKTSSLSSSSSSSSSSSSSSSSSSSSSSSSSSSSSSSSS
Target 1qon.1.A	SSKSRYSSSHLFNAFASLIPSSLAFSSLSFSSLTSTNDLYRGFFATLVILLRMSSVAYGITDRLIVQTTSGPVRGRAVTV
Target 1qon.1.A	QGREVHVFTGIPYAKPPVDDLRFRKPVPAEPWHGVLDATRLPATCVQERYEYFPGFSGEEIWNPNTNVSEDCLYMNIWAP QGREVHVYTGIPYAKPPVEDLRFRKPVPAEPWHGVLDATGLSATCVQERYEYFPGFSGEEIWNPNTNVSEDCLYINVWAP
Target 1qon.1.A	SKARLRHGRGANGVEHAAKTDPDHLIHSATPQNTTNGLPILIWIYGGGFMTGSATLDIYNADIMSAVGNVIVASFQYR AKARLRHGRGANGGEHPNGKQADTDHLIHNGNPQNTTNGLPILIWIYGGGFMTGSATLDIYNADIMAAVGNVIVASFQYR
Target 1qon.1.A	VGAFGFLHLSPVMPG-FEEEAPGNVGLWDQALALRWLKENARAFGGNPEWMTLFGESAGSSSVNAQLVSPVTRGLVKRGM VGAFGFLHLAPEMPSEFAEEAPGNVGLWDQALAIRWLKDNAHAFGGNPEWMTLFGESAGSSSVNAQLMSPVTRGLVKRGM
Target 1qon.1.A	MQSGTMNAPWSHMTSEKAVEIGKALINDCNCNASLLSENPQSVMACMRSVDAKTISVQQWNSYSGILSFPSAPTIDGAFF MQSGTMNAPWSHMTSEKAVEIGKALINDCNCNASMLKTNPAHVMSCMRSVDAKTISVQQWNSYSGILSFPSAPTIDGAFL
Target 1qon.1.A	TADPMTLMKTADMTGYDIMIGNVKDEGTYFLLYDFIDYFDKDEATSLPRDKYLEIMNNIFNKATQAEREAIIFQYTSWEG PADPMTLMKTADLKDYDILMGNVRDEGTYFLLYDFIDYFDKDDATALPRDKYLEIMNNIFGKATQAEREAIIFQYTSWEG
Target 1qon.1.A	NPGYQNQQQIGRAVGDHFFTCPTNEYAQALAERGAQVHYYYFTHRTSTSLWGEWMGVLHGDEIEYFFGQPLNTSLQYRPV NPGYQNQQQIGRAVGDHFFTCPTNEYAQALAERGASVHYYYFTHRTSTSLWGEWMGVLHGDEIEYFFGQPLNNSLQYRPV
Target 1qon.1.A	ERELGKRMLNSVIEFAKTGNPAVDGEEWPNFSKEDPVYYVFSTDEKTEKLQRGPLAKRCSFWNDYLPKVRSWVGSECENN ERELGKRMLSAVIEFAKTGNPAQDGEEWPNFSKEDPVYYIFSTDDKIEKLARGPLAARCSFWNDYLPKVRSWAGT
Target 1qon.1.A	NAASAAVNNINGQQYLLKWVIMLTIMVTCIFQ

Materials and Methods

Template Search

Template search with BLAST and HHBlits has been performed against the SWISS-MODEL template library (SMTL, last update: 2020-12-16, last included PDB release: 2020-12-11).

The target sequence was searched with BLAST against the primary amino acid sequence contained in the SMTL. A total of 163 templates were found.

An initial HHblits profile has been built using the procedure outlined in (Steinegger et al.), followed by 1 iteration of HHblits against Uniclust30 (Mirdita, von den Driesch et al.). The obtained profile has then be searched against all profiles of the SMTL. A total of 1475 templates were found.

Template Selection

For each identified template, the template's quality has been predicted from features of the target-template alignment. The templates with the highest quality have then been selected for model building.

Model Building

Models are built based on the target-template alignment using ProMod3. 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. In case loop modelling with ProMod3 fails, an alternative model is built with PROMOD-II (Guex et al.).

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). [A] [doi>]

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).

Uniclust30

Mirdita, M., von den Driesch, L., Galiez, C., Martin, M.J., Söding, J., Steinegger, M. Uniclust databases of clustered and deeply annotated protein sequences and alignments. Nucleic Acids Research 45, D170–D176 (2016).

Table T1:

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

MARFITSSSLSPSTTPSFASATASPAIASSLPRSKSTKATKARKTILSANSFKTSSLSSLSSSSSSPSLSSSPSFKSSSSSKSRYSSSHLFNAFASLIP SSLAFSSLSFSSLTSTNDLYRGFFATLVILLRMSSVAYGITDRLIVQTTSGPVRGRAVTVQGREVHVFTGIPYAKPPVDDLRFRKPVPAEPWHGVLDATR LPATCVQERYEYFPGFSGEEIWNPNTNVSEDCLYMNIWAPSKARLRHGRGANGVEHAAKTDPDHLIHSATPQNTTNGLPILIWIYGGGFMTGSATLDIYN ADIMSAVGNVIVASFQYRVGAFGFLHLSPVMPGFEEAPGNVGLWDQALALRWLKENARAFGGNPEWMTLFGESAGSSSVNAQLVSPVTRGLVKRGMMQS GTMNAPWSHMTSEKAVEIGKALINDCNCNASLLSENPQSVMACMRSVDAKTISVQQWNSYSGILSFPSAPTIDGAFFTADPMTLMKTADMTGYDIMIGNV KDEGTYFLLYDFIDYFDKDEATSLPRDKYLEIMNNIFNKATQAEREAIIFQYTSWEGNPGYQNQQQIGRAVGDHFFTCPTNEYAQALAERGAQVHYYYFT HRTSTSLWGEWMGVLHGDEIEYFFGQPLNTSLQYRPVERELGKRMLNSVIEFAKTGNPAVDGEEWPNFSKEDPVYYVFSTDEKTEKLQRGPLAKRCSFWN DYLPKVRSWVGSECENNNAASAAVNNINGQQYLLKWVIMLTIMVTCIFQ

Table T2:

Template	Seq Identity	Oligo- state	QSQE	Found by	Method	Resolution	Seq Similarity	Coverage	Description	
1qon.1.A	89.70	monomer	-	BLAST	X-ray	2.72Å	0.60	0.77	ACETYLCHOLINESTERASE	
1qon.1.A	89.72	monomer	-	HHblits	X-ray	2.72Å	0.59	0.77	ACETYLCHOLINESTERASE	
6xyy.1.A	89.55	monomer	-	HHblits	X-ray	2.70Å	0.59	0.77	Acetylcholinesterase	
6xyy.1.A	89.70	monomer	-	BLAST	X-ray	2.70Å	0.60	0.77	Acetylcholinesterase	
6xys.1.A	89.55	monomer	-	HHblits	X-ray	2.46Å	0.59	0.77	Acetylcholinesterase	
6xys.1.A	89.70	monomer	-	BLAST	X-ray	2.46Å	0.60	0.77	Acetylcholinesterase	
1qo9.1.A	89.72	monomer	-	HHblits	X-ray	2.70Å	0.59	0.77	ACETYLCHOLINESTERASE	
1qo9.1.A	89.70	monomer	-	BLAST	X-ray	2.70Å	0.60	0.77	ACETYLCHOLINESTERASE	
2whp.2.A	39.89	monomer	-	HHblits	X-ray	2.20Å	0.40	0.71	ACETYLCHOLINESTERASE	
1q83.1.A	39.63	homo- dimer	0.50	HHblits	X-ray	2.65Å	0.40	0.71	Acetylcholinesterase	
2c0p.2.A	39.89	monomer	-	HHblits	X-ray	2.50Å	0.40	0.71	ACETYLCHOLINESTERASE	
5ydh.1.A	40.08	homo- dimer	0.30	HHblits	X-ray	3.21Å	0.41	0.71	Acetylcholinesterase	
5ydj.1.A	39.92	homo- dimer	0.36	HHblits	X-ray	3.04Å	0.41	0.71	Acetylcholinesterase	
6h14.1.A	39.16	homo- dimer	0.43	HHblits	X-ray	1.86Å	0.41	0.70	Acetylcholinesterase	
5x61.1.A	39.85	homo- dimer	0.34	HHblits	X-ray	3.40Å	0.41	0.71	Acetylcholinesterase	
2w6c.1.A	39.09	monomer	-	HHblits	X-ray	2.69Å	0.41	0.70	ACETYLCHOLINESTERASE	
6o5s.1.A	38.91	homo- dimer	0.22	HHblits	X-ray	2.80Å	0.40	0.71	Acetylcholinesterase	
6qaa.1.A	41.30	monomer	-	BLAST	X-ray	1.90Å	0.41	0.72	Cholinesterase	
1f8u.1.A	38.65	monomer	-	HHblits	X-ray	2.90Å	0.40	0.71	ACETYLCHOLINESTERASE	
5ydi.1.A	39.85	homo- dimer	0.48	HHblits	X-ray	3.45Å	0.41	0.71	Acetylcholinesterase	
6tt0.1.A	39.09	monomer	-	HHblits	X-ray	2.80Å	0.41	0.70	Acetylcholinesterase	
2c0p.2.A	41.28	monomer	-	BLAST	X-ray	2.50Å	0.41	0.71	ACETYLCHOLINESTERASE	
2whp.2.A	41.28	monomer	-	BLAST	X-ray	2.20Å	0.41	0.71	ACETYLCHOLINESTERASE	

Template	Seq Identity	Oligo- state	QSQE	Found by	Method	Resolution	Seq Similarity	Coverage	Description
5fpq.2.B	40.30	homo- dimer	0.52	BLAST	X-ray	2.40Å	0.41	0.70	ACETYLCHOLINESTERASE
5hf5.1.A	40.30	homo- dimer	0.44	BLAST	X-ray	2.15Å	0.41	0.70	Acetylcholinesterase
5hf8.1.B	40.30	homo- dimer	0.46	BLAST	X-ray	2.80Å	0.41	0.70	Acetylcholinesterase
6f25.1.A	40.30	homo- dimer	0.49	BLAST	X-ray	3.05Å	0.41	0.70	Acetylcholinesterase
4bdt.2.E	38.84	homo- dimer	0.39	HHblits	X-ray	3.10Å	0.40	0.71	ACETYLCHOLINESTERASE
2jge.2.A	41.09	monomer	-	BLAST	X-ray	2.60Å	0.41	0.71	ACETYLCHOLINESTERASE
4b84.1.A	41.40	homo- dimer	0.48	BLAST	X-ray	2.60Å	0.41	0.71	ACETYLCHOLINESTERASE
4a16.1.A	41.40	homo- dimer	0.49	BLAST	X-ray	2.65Å	0.41	0.71	ACETYLCHOLINESTERASE
4tpk.1.A	40.84	monomer	-	BLAST	X-ray	2.70Å	0.41	0.73	Cholinesterase
5lkr.2.A	41.48	monomer	-	BLAST	X-ray	2.52Å	0.41	0.70	Cholinesterase
4xii.1.A	41.48	homo- dimer	0.41	BLAST	X-ray	2.70Å	0.41	0.70	Cholinesterase
3o9m.1.A	41.48	homo- tetramer	0.21	BLAST	X-ray	2.98Å	0.41	0.70	Cholinesterase
6arx.1.A	42.07	homo- dimer	0.66	BLAST	X-ray	2.30Å	0.42	0.70	Acetylcholinesterase
5ydh.1.A	42.42	homo- dimer	0.27	BLAST	X-ray	3.21Å	0.42	0.70	Acetylcholinesterase
3lii.1.A	40.30	homo- dimer	0.52	BLAST	X-ray	3.20Å	0.41	0.70	Acetylcholinesterase
5x61.1.A	42.42	homo- dimer	0.31	BLAST	X-ray	3.40Å	0.42	0.70	Acetylcholinesterase
2cek.1.A	41.39	monomer	-	BLAST	X-ray	2.20Å	0.42	0.69	ACETYLCHOLINESTERASE
5ydi.1.A	42.42	homo- dimer	0.50	BLAST	X-ray	3.45Å	0.42	0.70	Acetylcholinesterase
2pm8.1.A	41.67	homo- octamer	0.13	BLAST	X-ray	2.80Å	0.41	0.70	Cholinesterase
5ehx.1.A	41.39	monomer	-	BLAST	X-ray	2.10Å	0.42	0.69	Acetylcholinesterase
6eue.1.A	41.39	homo- dimer	0.46	BLAST	X-ray	2.00Å	0.42	0.69	Acetylcholinesterase
6fqn.1.A	41.39	homo- dimer	0.42	BLAST	X-ray	2.30Å	0.42	0.69	Acetylcholinesterase
1amn.1.A	41.39	monomer	-	BLAST	X-ray	2.80Å	0.42	0.69	ACETYLCHOLINESTERASE
6i2t.1.A	41.48	homo- tetramer	0.27	BLAST	EM	NA	0.41	0.70	Cholinesterase
6i2t.1.B	41.48	homo- tetramer	0.27	BLAST	EM	NA	0.41	0.70	Cholinesterase
4qwm.1.A	34.28	monomer	-	BLAST	X-ray	2.17Å	0.38	0.66	E3
5tym.1.A	34.48	monomer	-	BLAST	X-ray	1.84Å	0.38	0.66	Carboxylic ester hydrolase

The table above shows the top 50 filtered templates. A further 1,456 templates were found which were considered to be less suitable for modelling than the filtered list.

1a7u.1.A, 1a88.1.A, 1a8q.1.A, 1a8s.1.A, 1ac5.1.A, 1acj.1.A, 1akn.1.A, 1amn.1.A, 1aql.1.A, 1auo.1.A, 1auo.1.B, 1azw.1.A, 1b6g.1.A, 1bcr.1.A, 1bee.1.A, 1bn6.1.A, 1bro.1.A, 1brt.1.A, 1bu8.1.A, 1c2b.1.A, 1c2o.1.A, 1c4x.1.A, 1c7i.1.A, 1c7j.1.A, 1cex.1.A, 1cle.1.A, 1cpy.1.A, 1cqw.1.A, 1cqz.1.A, 1crl.1.A, 1cub.1.A, 1cud.1.A, 1cud.2.A, 1cud.3.A, 1cue.1.A, 1cug.1.A, 1cug.1.A, 1cuj.1.A, 1cvl.1.A, 1cuj.1.A, 1cuj.1

1va5.1.A, 1ve7.1.A, 1vkh.1.A, 1vz2.1.A, 1vz3.1.A, 1w52.1.A, 1wb4.1.A, 1wcy.1.A, 1whs.1.A, 1wht.1.A, 1wom.1.A, 1wpr.1.A, 1wpr.2.A, 1wpx.1.A, 1x2e.1.A, 1xfd.1.A, 1xkl.1.A, 1xkl.1.C, 1xqv.1.A, 1xqx.1.A, 1xqy.1.A, 1xrl.1.A, 1xro.1.A, 1xrq.1.A, 1xzd.1.A, 1xzf.1.A, 1xzg.1.A, 1xzi.1.A, 1xzj.1.A, 1y37.1.A, 1y7h.2.A, 1y7i.1.A, 1yaj.4.B, 1yas.1.A, 1yb6.1.A, 1ycd.1.A, 1yr2.1.A, 1ys2.1.A, 1ysc.1.A, 1z68.1.A, 1z68.1.B, 1zd3.1.A, 1zi8.1.A, 1zi9.1.A, 1zic.1.A, 1zix.1.A, 1zj4.1.A, 1zj5.1.A, 1zoi.1.A, 2ajc.3.C, 2b20.1.A, 2b4k.1.A, 2b61.1.A, 2bce.1.A, 2bgr.1.A, 2bkl.1.A, 2bub.1.A, 2buc.2.B, 2c7b.1.A, 2cek.1.A, 2cjp.1.A, 2cmf.1.B, 2cut.1.A, 2d0d.1.A, 2d80.1.A, 2d81.1.A, 2dcm.1.A, 2dsn.1.A, 2dst.1.A, 2dst.1.B, 2e3j.1.A, 2ecf.1.A, 2eep.1.A, 2es4.1.A, 2fj0.1.A, 2fuk.1.A, 2fx5.1.A, 2g5p.1.A, 2gbg.1.A, 2gyv.1.A, 2gzr.1.A, 2gzs.1.A, 2h1i.1.A, 2h1i.2.A, 2h7c.1.E, 2h7x.1.A, 2ha2.1.B, 2ha6.1.A, 2hdw.1.A, 2hfk.1.A, 2hih.1.A, 2hm7.1.A, 2hrq.2.A, 2hu5.1.B, 2hu8.1.A, 2i3d.1.A, 2j3q.1.A, 2j4c.1.A, 2j4f.1.A, 2jbw.1.A, 2jbw.2.A, 2jge.2.A, 2jid.1.A, 2k2q.1.B, 2nw6.1.A, 2o2g.1.A, 2o2i.1.A, 2o7r.1.A, 2ocg.1.A, 2ock.1.A, 2ocl.1.A, 2og1.1.A, 2ogs.1.A, 2ogt.1.A, 2ogz.1.B, 2ole.1.A, 2onc.1.A, 2oxe.1.A, 2pbl.1.A, 2pl5.1.A, 2pm8.1.A, 2ppl.1.A, 2pse.1.A, 2psf.1.A, 2psf.2.A, 2psh.1.A, 2psj.1.A, 2pu7.1.A, 2puh.1.A, 2pvs.1.A, 2pvs.2.A, 2q0x.1.A, 2qjr.1.A, 2qjw.1.A, 2qjw.1.B, 2qky.1.B, 2qm0.1.A, 2qm0.1.B, 2qmq.1.A, 2qr5.1.A, 2qru.1.A, 2qs9.1.A, 2qt9.1.A, 2qub.1.A, 2qvb.1.A, 2qxt.1.A, 2qzp.1.A, 2qzp.2.A, 2r11.1.A, 2r8b.1.A, 2rau.1.A, 2rht.1.A, 2rip.1.A, 2ron.1.A, 2uz0.1.A, 2v9z.1.A, 2vax.1.A, 2veo.1.A, 2vf2.1.A, 2w22.1.A, 2w6c.1.A, 2wfl.1.A, 2wfm.1.A, 2wid.1.A, 2wil.1.A, 2wj3.1.A, 2wm2.1.A, 2wqz.1.A, 2wqz.2.A, 2wtm.1.A, 2wtm.1.B, 2wtm.2.B, 2wug.1.A, 2x5x.1.A, 2xb6.1.A, 2xe4.1.A, 2xlc.1.A, 2xmb.1.A, 2xmq.1.A, 2xmr.1.A, 2xms.1.A, 2xmz.1.A, 2xqf.1.A, 2xt0.1.A, 2xua.1.A, 2xug.1.A, 2xuk.1.A, 2y6v.1.B, 2yij.1.A, 2yxp.1.A, 2yys.1.A, 2yys.2.A, 2z3z.1.A, 2z5g.1.A, 2z8x.1.A, 2z8z.1.A, 2zj6.1.A, 2zjf.1.A, 2zsh.1.A, 2zyh.1.A, 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