

## Model Building Report

This document lists the results for the homology modelling project "Myoglobin" submitted to SWISS-MODEL workspace on April 24, 2018, 8:27 a.m..The submitted primary amino acid sequence is given in Table T1.

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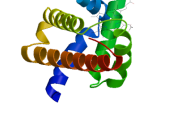
- Biasini, M., Bienert, S., Waterhouse, A., Arnold, K., Studer, G., Schmidt, T., Kiefer, F., Cassarino, T.G., Bertoni, M., Bordoli, L., Schwede, T. SWISS-MODEL: modelling protein tertiary and quaternary structure using evolutionary information. *Nucleic Acids Res.* 42, W252-W258 (2014). [\[Pub\]](#)
- 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). [\[Pub\]](#)
- Bienert, S., Waterhouse, A., de Beer, T.A., Tauriello, G., Studer, G., Bordoli, L., Schwede, T. The SWISS-MODEL Repository - new features and functionality. *Nucleic Acids Res.* 45, D313-D319 (2017). [\[Pub\]](#)
- Benkert, P., Biasini, M., Schwede, T. Toward the estimation of the absolute quality of individual protein structure models. *Bioinformatics* 27, 343-350 (2011). [\[Pub\]](#)
- 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). [\[Pub\]](#)

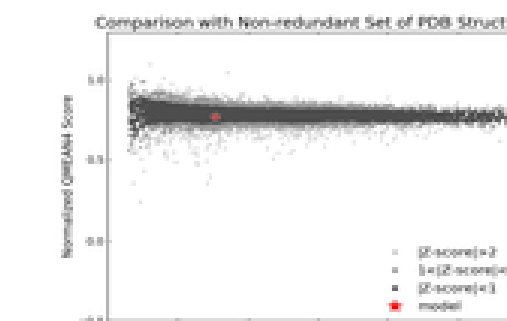
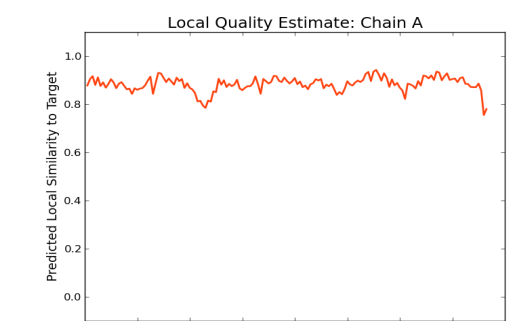
## Results

The SWISS-MODEL template library (SMTL version 2018-04-18, PDB release 2018-04-13) was searched with BLAST ([Camacho et al.](#)) and HHBlits ([Remmert et al.](#)) for evolutionary related structures matching the target sequence in Table T1. For details on the template search, see Materials and Methods. Overall 1281 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	QMEAN
	PDB	ProMod3 Version 1.1.0.	monomer	1 x HEM: PROTOPORPHYRIN IX CONTAINING FE;	0.99	-0.25
QMEAN	-0.25					
CP	1.04					
All Atom	1.68					
Solvation	1.77					
Torsion	-0.90					



Template	Seq Identity	Oligo-state	Found by Method	Resolution	Seq Similarity	Range	Coverage	Description
1mnh.1.A	100.00	monomer	HHblits	X-ray	2.30Å	0.60	1 - 153	1.00 MYOGLOBIN

Ligand	Added to Model	Description
HEM	✓	PROTOPORPHYRIN IX CONTAINING FE

Target GLSDGEWQLVLNVWGKVEADVAGHGQEVILRLFKGHPETLEKFDKFHLKSEDEMKASEDLKKVGNRVLTALGGILKKKG  
1mnh.1.A GLSDGEWQLVLNVWGKVEADVAGHGQEVILRLFKGHPETLEKFDKFHLKSEDEMKASEDLKKVGNRVLTALGGILKKKG

Target HHEAELTPLAQSHATKHKIPVKYLEFISEATIIQVLQSKHPGDFGADAGAMSKALELFRNDMAAKYKELGFG  
1mnh.1.A HHEAELTPLAQSHATKHKIPVKYLEFISEATIIQVLQSKHPGDFGADAGAMSKALELFRNDMAAKYKELGFG

## Materials and Methods

### Template Search

Template search with BLAST and HHBlits has been performed against the SWISS-MODEL template library (SMTL, last update: 2018-04-18, last included PDB release: 2018-04-13).

The target sequence was searched with BLAST against the primary amino acid sequence contained in the SMTL. A total of 426 templates were found.

An initial HHblits profile has been built using the procedure outlined in (Remmert et al.), followed by 1 iteration of HHblits against NR20. The obtained profile has then been searched against all profiles of the SMTL. A total of 898 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 ([Benkert et al.](#)). For improved performance, weights of the individual QMEAN terms have been trained specifically for SWISS-MODEL.

### 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). [\[Pub\]](#)
- HHblits**  
Remmert, M., Biegert, A., Hauser, A., Söding, J. HHblits: lightning-fast iterative protein sequence searching by HMM-HMM alignment. *Nat Methods* 9, 173-175 (2012). [\[Pub\]](#)

### Table T1:

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

GLSDGEWQLVLNVWGKVEADVAGHGQEVILRLFKGHPETLEKFDKFHLKSEDEMKASEDLKKVGNRVLTALGGILKKKGHHEAELTPLAQSHATKHKIPVKYLEFISEATIIQVLQSKHPGDFGADAGAMSKALELFRNDMAAKYKELGFG

### Table T2:

Template	Seq Identity	Oligo-state	QSQE	Found by Method	Resolution	Seq Similarity	Coverage	Description
1mnh.1.A	100.00	monomer		HHblits	X-ray	2.30Å	0.60	1.00 MYOGLOBIN
1mnj.1.A	98.69	monomer		HHblits	X-ray	2.20Å	0.60	1.00 MYOGLOBIN
1mni.1.A	98.69	monomer		HHblits	X-ray	2.07Å	0.60	1.00 MYOGLOBIN
1mni.2.A	98.69	monomer		HHblits	X-ray	2.07Å	0.60	1.00 MYOGLOBIN
1myg.1.A	98.69	monomer		HHblits	X-ray	1.75Å	0.60	1.00 MYOGLOBIN
1pmb.2.A	98.69	monomer		HHblits	X-ray	2.50Å	0.60	1.00 MYOGLOBIN
1myh.1.A	98.04	monomer		HHblits	X-ray	1.90Å	0.60	1.00 MYOGLOBIN
1fcs.1.A	86.18	monomer		BLAST	X-ray	1.60Å	0.56	0.99 MYOGLOBIN
3vm9.1.A	90.20	homo-dimer	0.66	HHblits	X-ray	1.05Å	0.57	1.00 Myoglobin
3vm9.1.B	90.20	homo-dimer	0.66	HHblits	X-ray	1.05Å	0.57	1.00 Myoglobin
1yma.1.A	90.20	monomer		HHblits	X-ray	2.00Å	0.57	1.00 MYOGLOBIN
1bje.1.A	90.20	monomer		HHblits	X-ray	1.80Å	0.57	1.00 MYOGLOBIN
1dwr.1.A	90.20	monomer		HHblits	X-ray	1.45Å	0.57	1.00 MYOGLOBIN
1mnk.1.A	98.69	monomer		HHblits	X-ray	2.20Å	0.60	1.00 MYOGLOBIN
5yl3.1.A	90.20	monomer		HHblits	X-ray	1.50Å	0.57	1.00 Myoglobin
3heo.1.A	91.50	monomer		HHblits	X-ray	2.00Å	0.58	1.00 Myoglobin
1fcs.1.A	85.62	monomer		HHblits	X-ray	1.60Å	0.56	1.00 MYOGLOBIN
3hep.1.A	90.85	monomer		HHblits	X-ray	1.95Å	0.58	1.00 Myoglobin
2w6w.1.A	84.97	monomer		HHblits	X-ray	1.99Å	0.56	1.00 MYOGLOBIN
1ufp.1.A	84.97	monomer		HHblits	X-ray	2.10Å	0.56	1.00 Myoglobin
2mgj.1.A	84.97	monomer		HHblits	X-ray	2.00Å	0.56	1.00 MYOGLOBIN
2jho.1.A	84.97	monomer		HHblits	X-ray	1.40Å	0.56	1.00 MYOGLOBIN
1emy.1.A	84.31	monomer		HHblits	X-ray	1.78Å	0.56	1.00 MYOGLOBIN
6brmg.1.A	85.53	monomer		BLAST	X-ray	1.88Å	0.56	0.99 Myoglobin
3rgk.1.A	92.16	monomer		HHblits	X-ray	1.65Å	0.58	1.00 Myoglobin
2eb9.1.A	84.97	monomer		HHblits	X-ray	1.80Å	0.56	1.00 Myoglobin
1mbs.1.A	86.93	monomer		HHblits	X-ray	2.50Å	0.56	1.00 MYOGLOBIN
2w6y.1.A	84.97	monomer		HHblits	X-ray	1.60Å	0.56	1.00 MYOGLOBIN
6brmg.1.A	84.97	monomer		HHblits	X-ray	1.88Å	0.55	1.00 Myoglobin
5ojc.1.A	80.92	monomer		BLAST	X-ray	1.25Å	0.54	0.99 Myoglobin
5ojc.1.A	80.39	monomer		HHblits	X-ray	1.25Å	0.54	1.00 Myoglobin

The table above shows the top 31 filtered templates. A further 869 templates were found which were considered to be less suitable for modelling than the filtered list.

4hsu.1.A, 5m3l.1.E, 2qmb.1.D, 2eb9.1.A, 5c6e.1.C, 1dxv.1.B, 3zji.1.A, 2bk9.1.A, 3gqp.1.D, 1qpw.1.B, 1qpw.1.C, 1qpw.1.D, 5f82.1.A, 1e4f.1.B, 5vmm.1.C, 5m9l.1.A, 1h1x.1.A, 3o7n.1.A, 3e48.2.B, 5ojb.1.A, 1aby.1.A, 1aby.1.B, 2z2.2.A, 2zfb.1.A, 1umo.1.B, 1umo.1.A, 5ohe.4.A, 1hmm.1.A, 1mji.1.A, 3mju.1.B, 3pt8.1.B, 3mju.1.A, 4v93.12A, 1h3.1.A, 1abs.1.A, 1s0h.1.A, 1s56.1.A, 3n17.1.B, 2qu0.1.D, 1lue.1.A, 1shr.1.D, 1shr.1.C, 1o1n.1.A, 1wh.1.A, 5hy8.2.B, 2qmb.1.A, 4xs0.1.A, 4xs0.1.B, 1o4.1.A, 4bja.1.A, 3ok5.1.B, 1yz1.1.B, 1y4v.1.B, 1nej.1.B, 1m9p.1.A, 1y4g.1.B, 1a4f.1.A, 4mqk.1.B, 4mqk.1.C, 5v5r.1.A, 3bcq.1.B, 3bcq.1.C, 2gl3.1.A, 3bcq.1.A, 3qqr.1.A, 3bcq.1.D, 1bj1.1.A, 1bj1.1.B, 1ibe.1.A, 5jgg.1.B, 2nx0.1.A, 1oj6.2.A, 5e6e.1.B, 4b4y.1.A, 1o1j.1.A, 1o1j.1.B, 5jgg.1.A, 3wtg.1.A, 1hdb.1.B, 3wtg.1.C, 1bzz.1.A, 2gnv.1.B, 4g1b.1.A, 4tyx.1.A, 1nz3.1.A, 4fwz.1.A, 2wy4.1.A, 1iop.1.A, 4f6d.1.A, 1cmv.1.B, 1cmv.1.A, 2rao.1.A, 3uh3.1.B, 3uhc.1.A, 1xye.1.A, 3ugz.1.A, 3zhw.2.A, 3ubc.1.A, 1y0c.1.A, 3eu1.1.D, 3eu1.1.C, 3eu1.1.B, 3eu1.1.A, 5o41.1.A, 4jac.1.A, 1mtk.1.A, 1or6.1.B, 5ee1.1.A, 4mqj.2.D, 1y7g.1.B, 2nrl.1.A, 1ngk.1.B, 5eys.1.A, 2zlv.1.C, 2zlv.1.B, 1cg5.1.A, 5urc.1.D, 4mqc.1.A, 1hvv.1.D, 1v5h.1.A, 4f4o.1.A, 4f4o.1.B, 1yhu.1.B, 5x2s.2.D, 1yhu.1.A, 1yhu.1.D, 3wct.1.C, 1do3.1.A, 3f64.1.A, 3s65.1.B, 3vrg.1.A, 1i12.1.A, 1gbv.1.B, 1hbr.1.A, 1hbr.1.A, 1y7d.1.B, 1hbs.1.D, 1hbs.1.C, 1hbs.1.B, 1hbs.1.A, 5x2s.2.A, 3wfx.1.A, 1s56.2.A, 2qsp.1.D, 1ngk.1.H, 4u8u.1.D, 5x2s.2.C, 3vre.1.A, 3vre.1.B, 4mu5.1.A, 1y45.1.B, 1v4x.1.A, 1v4x.1.B, 5x2t.1.D, 5x2t.1.A, 2h35.1.B, 5ile.1.A, 1faf.1.A, 1y5j.1.B, 2ri4.3.A, 3uh5.1.B, 3ng6.1.B, 1y5k.1.B, 2ri4.1.D, 2ri4.1.C, 3ia3.1.B, 1cbl.1.D, 4esa.1.A, 3gkv.1.A, 3gkv.1.B, 1v4u.1.B, 3s1l.1.A, 4o2g.1.A, 3s1l.1.B, 1c40.1.A, 5y2f.1.A, 1c40.1.B, 3w4u.1.B, 3w4u.1.A, 1moh.1.A, 3vnh.1.A, 3uh6.1.A, 3onz.1.B, 1vxa.1.A, 3s4.1.A, 2d6c.1.A, 3ciu.1.D, 1ewa.1.A, 1cpw.1.A, 1kmi.1.B, 1y4q.1.B, 3wyo.1.B, 3wyo.1.A, 5k36.1.A, 2dc3.1.A, 2gfr.1.A, 1h1t.1.A, 2dc3.1.B, 2ohb.1.A, 4o9f.1.A, 1urv.2.A, 2d6c.2.A, 1irc.1.A, 1y01.1.B, 1c0h.1.A, 4n10.1.A, 1ufj.1.A, 1v4w.1.D, 4mqk.1.A, 1ird.1.B, 3gou.1.B, 3gou.1.A, 1vvt.1.A, 1y8l.1.D, 1y8l.1.B, 4i8.1.A, 1y8l.1.A, 5f0b.1.A, 3uhh.1.A, 4qau.1.A, 3ugy.1.A, 4hrt.2.C, 1xz5.1.A, 1v07.1.A, 1ecn.1.A, 5k1l.1.B, 5eui.1.A, 5eui.1.B, 1hds.1.A, 3ld.1.A, 1hds.1.C, 1hds.1.B, 1hds.1.D, 1ofk.1.A, 4iro.1.A, 1hbg.1.A, 4iro.1.C, 2jxu.1.A, 5hbi.1.B, 1myi.1.A, 1tu9.1.A, 3a0g.1.B, 1w92.1.A, 1lf2.1.A, 1dxd.1.A, 1buw.1.A, 1buw.1.B, 1buw.1.D, 2evp.1.A, 3qmr.1.A, 5ker.1.D, 1a00.1.B, 5ker.1.B, 4twv.1.A, 2ef2.1.A, 1hac.1.B, 1hac.1.C, 2r50.2.A, 4hsw.2.A, 2r50.2.B, 1vre.1.A, 3gqr.2.A, 3gqr.2.B, 4o4b.1.A, 1fsx.1.A, 2zs0.1.A, 1fsx.1.C, 2zs0.1.C, 3sdn.1.A, 1fsx.1.D, 2qrw.1.A, 2cmm.1.A, 1m1m.1.A, 4xdi.1.A, 3zho.1.A, 3wcu.1.C, 4b3w.1.A, 3mjp.1.D, 3mjp.1.C, 3mjp.1.B, 3mjp.1.A, 7hbi.1.B, 2r4w.1.A, 5x2r.3.A, 5x2r.3.B, 3k9z.1.A, 5x2r.3.D, 5b84.1.A, 3dht.1.A, 4o1t.1.A, 5x2r.1.C, 5x2r.1.A, 3gdj.1.A, 5x2r.1.D, 3gdj.1.B, 4rol.1.D, 1rse.1.A, 3g53.1.A, 1spg.1.A, 1k1k.1.B, 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3mm.1.A, 2gnw.1.A, 2gnw.1.B, 1gbu.1.B, 2zlw.1.A, 3gqp.1.A, 3gqp.1.B, 2r4z.1.B, 5sw7.1.B, 5sw7.1.A, 4mqj.1.B, 2qu0.1.A, 2vvy.1.A, 2qu0.1.C, 2qu0.1.B, 1mti.1.A, 5utb.1.A, 3mvc.1.A, 1wmu.1.B, 1wmu.1.A, 1h97.1.A, 1o1i.1.B, 1o1i.1.A, 1mbi.1.A, 1myj.1.A, 1i13.3.A, 2zlx.1.B, 4gtb.3.A, 5ifg.1.D, 1dti.1.A, 4xdi.2.A, 2eb8.1.A, 1j3z.2.B, 1a01.1.B, 3ixf.1.A, 1j3f.1.A, 1ouu.1.B, 1ouu.1.A, 3d7o.1.A, 5b85.1.A, 3dht.1.D, 1co8.1.A, 4pg6.1.A, 4esa.1.A, 4g1v.1.A, 1gdl.1.A, 2zfb.1.B, 4fh7.1.B, 1wvp.1.A, 3wr1.1.A, 3wr1.1.B, 2gkn.1.A, 2lhb.1.A, 4hbi.1.A, 1out.1.B, 2ri4.2.B, 2ri4.2.D, 6hbi.1.A, 5nvi.1.A, 1hda.1.B, 1hda.1.A, 4esa.1.D, 2r50.1.A, 2qrw.2.A, 1myi.2.A, 1vrf.1.A, 5ker.1.A, 3m3a.1.A, 4v93.64.A, 5ifg.2.A, 1fsl.1.A, 5ker.1.C, 2mgc.1.A, 1bab.1.A, 4x0l.1.A, 1h1b.1.A, 1f6h.1.A, 5hu6.1.B, 1g08.1.A, 2r80.1.B, 2av0.1.A, 2d2m.1.D, 4ood.1.A, 1cg5.1.B, 3k8b.1.A, 2d2m.1.B, 3k8b.1.B, 1cio.1.A, 128u.1.B, 6b3y.1.A, 4kmw.1.A, 1bin.1.A, 4e0h.1.A, 2w72.1.C, 2w72.1.B, 2w72.1.A, 1lvf.1.A, 1fn3.1.A, 1xzu.1.A, 4hrr.1.A, 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