Model Building Report

This document lists the results for the homology modelling project "Neuroglobin" submitted to SWISS-MODEL workspace on April 24, 2018, 6:24 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:

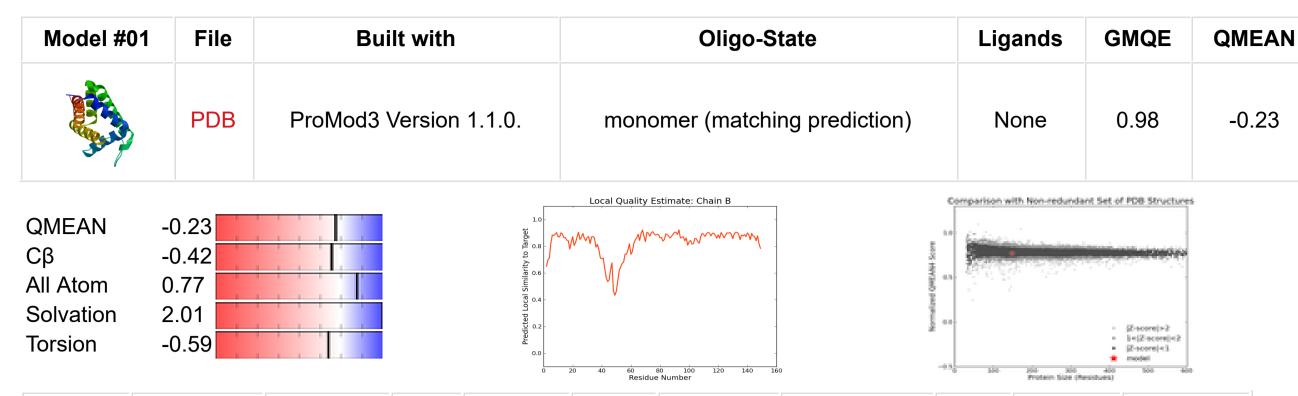
The following model was built (see Materials and Methods "Model Building"):

- 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). [M] [1055]
- 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). [m]
- 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). • Benkert, P., Biasini, M., Schwede, T. Toward the estimation of the absolute quality of individual protein structure models.
- Bioinformatics 27, 343-350 (2011). [M] [10] • 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). Im moss

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 1055 templates were found (Table T2).

Models



Template Seq Identity Oligo-state QSQE Found by Method Resolution Seq Similarity Range Coverage Description 4mpm.1.B 100.00 homo-dimer 0.57 HHblits X-ray 1.74Å 2 - 149 1.00 Neuroglobin

Ligand	Added to Model	Description
HEM	× - Binding site not conserved.	PROTOPORPHYRIN IX CONTAINING FE
HEM	imes - Binding site not conserved.	PROTOPORPHYRIN IX CONTAINING FE

MERPEPELIRQSWRAVSRSPLEHGTVLFARLFALEPDLLPLFQYNCRQFSSPEDCLSSPEFLDHIRKVMLVIDAAVTNVE 4mpm.1.B MERPEPELIRQSWRAVSRSPLEHGTVLFARLFALEPDLLPLFQYNCRQFSSPEDCLSSPEFLDHIRKVMLVIDAAVTNVE

DLSSLEEYLASLGRKHRAVGVKLSSFSTVGESLLYMLEKCLGPAFTPATRAAWSQLYGAVVQAMSRGWDGE 4mpm.1.B DLSSLEEYLASLGRKHRAVGVKLSSFSTVGESLLYMLEKCLGPAFTPATRAAWSQLYGAVVQAMSRGWDGE

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 84 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 be searched against all profiles of the SMTL. A total of 990 templates were found.

For each identified template, the template's quality has been predicted from features of the target-template alignment. The templates

Template Selection

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.

BLAST

References

- 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
- Remmert, M., Biegert, A., Hauser, A., Söding, J. HHblits: lightning-fast iterative protein sequence searching by HMM-HMM

Table T1:

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

VKLSSFSTVGESLLYMLEKCLGPAFTPATRAAWSQLYGAVVQAMSRGWDGE

Table T2:

1oj6.2.A 1oj6.4.A 1oj6.4.A 1mpm.1.A 1oj6.1.A 4o35.1.A 3gkt.1.A 4o1t.1.A 4nzi.1.A 5f2a.1.A 4mu5.1.A	100.00 98.01 98.01 100.00 98.01 92.05 92.72	homo- dimer monomer monomer homo- dimer monomer	0.57	HHblits HHblits	X-ray X-ray	1.74Å	0.60	1.00	Neuroglobin
1oj6.4.A 4mpm.1.A 1oj6.1.A 4o35.1.A 3gkt.1.A 4o1t.1.A 4nzi.1.A 5f2a.1.A 4mu5.1.A	98.01 100.00 98.01 92.05 92.72	monomer homo- dimer		HHblits	X-rav	4.05%			
Impm.1.A 1oj6.1.A 4o35.1.A 3gkt.1.A 4o1t.1.A 4nzi.1.A 5f2a.1.A 4mu5.1.A	100.00 98.01 92.05 92.72	homo- dimer				1.95Å	0.59	1.00	NEUROGLOBIN
1oj6.1.A 4o35.1.A 3gkt.1.A 4o1t.1.A 4nzi.1.A 5f2a.1.A 4mu5.1.A	98.01 92.05 92.72	dimer		HHblits	X-ray	1.95Å	0.59	1.00	NEUROGLOBIN
4o35.1.A 3gkt.1.A 4o1t.1.A 4nzi.1.A 5f2a.1.A 4mu5.1.A	92.05 92.72	monomer	0.57	HHblits	X-ray	1.74Å	0.60	1.00	Neuroglobin
3gkt.1.A 4o1t.1.A 4nzi.1.A 5f2a.1.A mu5.1.A	92.72	111011011161		HHblits	X-ray	1.95Å	0.59	1.00	NEUROGLOBIN
4o1t.1.A 4nzi.1.A 5f2a.1.A mu5.1.A		monomer		HHblits	X-ray	1.80Å	0.57	1.00	Neuroglobin
4nzi.1.A 5f2a.1.A mu5.1.A	00.05	monomer		HHblits	X-ray	1.86Å	0.57	1.00	Neuroglobin
5f2a.1.A lmu5.1.A	92.05	monomer		HHblits	X-ray	1.60Å	0.57	1.00	Neuroglobin
lmu5.1.A	92.05	monomer		HHblits	X-ray	2.10Å	0.57	1.00	Neuroglobin
	92.05	monomer		HHblits	X-ray	2.10Å	0.57	1.00	Neuroglobin
lw92.1.A	92.05	monomer		HHblits	X-ray	1.80Å	0.57	1.00	Neuroglobin
	92.72	homo- hexamer	0.60	HHblits	X-ray	1.70Å	0.57	1.00	NEUROGLOBIN
lo2g.1.A	92.05	monomer		HHblits	X-ray	2.70Å	0.57	1.00	Neuroglobin
	27.97	monomer		HHblits	X-ray	3.09Å	0.33	0.95	HEMOGLOBIN (BETA SUBUNI
	27.97	monomer		HHblits	X-ray	2.00Å	0.33	0.95	HEMOGLOBIN (BETA CHAIN)
	27.97	monomer		HHblits	X-ray	2.80Å	0.33	0.95	HEMOGLOBIN BETA CHAIN
	27.97	monomer		HHblits	X-ray	2.30Å	0.33	0.95	PROTEIN (HEMOGLOBIN (BET CHAIN))
Bmjp.1.B	27.97	monomer		HHblits	X-ray	2.76Å	0.33	0.95	Hemoglobin subunit beta
	27.27	homo- dimer	0.07	HHblits	X-ray	2.30Å	0.33	0.95	Hemoglobin
3fs4.1.B	27.97	monomer		HHblits	X-ray	2.22Å	0.33	0.95	Hemoglobin subunit beta
1hbr.1.B	27.97	homo- dimer		HHblits	X-ray	2.30Å	0.33	0.95	PROTEIN (HEMOGLOBIN D)
y4g.1.B	22.38	monomer		HHblits	X-ray	1.91Å	0.32	0.95	Hemoglobin beta chain
hba.1.B	22.38	monomer		HHblits	X-ray	2.10Å	0.32	0.95	HEMOGLOBIN ROTHSCHILD (DEOXY) (BETA CHAIN)
1yih.1.B	22.38	monomer		HHblits	X-ray	2.00Å	0.32	0.95	Hemoglobin beta chain
abw.1.A	23.57	monomer		HHblits	X-ray	2.00Å	0.32	0.93	HEMOGLOBIN-BASED BLOOI SUBSTITUTE
1aby.1.A	23.57	monomer		HHblits	X-ray	2.60Å	0.32	0.93	HEMOGLOBIN
lygd.1.B	22.38	monomer		HHblits	X-ray	2.73Å	0.32	0.95	Hemoglobin beta chain
lo1p.1.B	22.38	monomer		HHblits	X-ray	1.80Å	0.32	0.95	Hemoglobin beta chain
1y5j.1.B	22.38	monomer		HHblits	X-ray	2.03Å	0.32	0.95	Hemoglobin beta chain
1ye0.1.B	23.08	monomer		HHblits	X-ray	2.50Å	0.32	0.95	Hemoglobin beta chain
Ic7d.1.A	23.57	monomer		HHblits	X-ray	1.80Å	0.32	0.93	PROTEIN (DEOXYHEMOGLOB (ALPHA CHAIN))
lyg5.1.B	22.38	monomer		HHblits	X-ray	2.70Å	0.32	0.95	Hemoglobin beta chain
1o1j.1.A	23.57	monomer		HHblits	X-ray	1.90Å	0.32	0.93	Hemoglobin Alpha chain
sw7.1.A	23.57	homo- dimer	0.25	HHblits	X-ray	1.85Å	0.32	0.93	Hemoglobin subunit alpha
o1n.1.A	23.57	monomer		HHblits	X-ray	1.80Å	0.32	0.93	Hemoglobin Alpha chain
o1m.1.A	23.57	monomer		HHblits	X-ray	1.85Å	0.32	0.93	Hemoglobin Alpha chain
cp5.1.A	17.12	monomer		HHblits	X-ray	2.10Å	0.30	0.97	PROTEIN (MYOGLOBIN)
lch5.1.A	17.12	monomer		HHblits	X-ray	2.10Å	0.30	0.97	PROTEIN (MYOGLOBIN)
bmg.1.A	17.81	monomer		HHblits	X-ray	1.88Å	0.30	0.97	Myoglobin
	17.12	monomer		HHblits	X-ray	1.90Å	0.30	0.97	MYOGLOBIN
lh07.1.A	16.44	monomer		HHblits	X-ray	1.14Å	0.29	0.97	Myoglobin
3o89.1.A	16.44	monomer		HHblits	X-ray	1.10Å	0.29	0.97	Myoglobin
lh1x.1.A	16.44	monomer		HHblits	X-ray	1.40Å	0.29	0.97	MYOGLOBIN
Bsdn.1.A	17.12	monomer		HHblits	X-ray	1.50Å	0.30	0.97	Myoglobin
5d5r.1.A	14.38	monomer		HHblits	X-ray	1.60Å	0.29	0.97	Myoglobin
	14.38	monomer		HHblits	-	1.60Å	0.29	0.97	Myoglobin
5yl3.1.A	14.38	monomer		HHblits	X-ray	1.50Å	0.29	0.97	Myoglobin
	14.38	monomer		HHblits	X-ray	1.90Å	0.29	0.97	Myoglobin
	14.38	monomer		HHblits	X-ray	1.06Å	0.29	0.97	Myoglobin
	14.38	monomer		HHblits	X-ray	1.23Å	0.29	0.97	Myoglobin

1a4f.1.B, 5vmm.1.C, 2pgh.1.C, 3o7n.1.A, 3s48.2.B, 5ojb.1.A, 1aby.1.A, 1aby.1.B, 2zlx.2.A, 2zfb.1.A, 1umo.1.B, 1umo.1.A, 5ohe.4.A, 1hrm.1.A, 1mlj.1.A, 3mju.1.B, 1mni.1.A, 3pt8.1.B, 3mju.1.A, 4v93.124.A, 1it3.1.A, 1abs.1.A, 1s0h.1.A, 1s56.1.A, 3nl7.1.B, 2qu0.1.D, 1lue.1.A, 1shr.1.D, 1shr.1.C, 1o1n.1.A, 1v4w.1.D, 5hy8.2.B, 2qmb.1.A, 4xs0.1.A, 4xs0.1.B, 1or4.1.A, 4bja.1.A, 4nk2.1.B, 3ok5.1.B, 1yzi.1.B, 3qzx.1.B, 3qzz.1.A, 1y4v.1.B, 4ltr.1.A, 1qpw.1.C, 1d8u.1.B, 1d8u.1.A, 4lto.1.C, 4mqk.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, 1bij.1.A, 1bij.1.B, 3zjh.1.A, 1ibe.1.A, 5jgg.1.B, 2nx0.1.A, 5e6e.1.B, 3zom.1.A, 4b4y.1.A, 1y8w.1.A, 1o1j.1.B, 1y8w.1.C, 4o8w.2.B, 3wtg.1.A, 1hdb.1.B, 3wtg.1.C, 2gnv.1.A, 2gnv.1.B, 4g1b.1.A, 4tyx.1.A, 4fwz.1.A, 2wy4.1.A, 1iop.1.A, 4f6d.1.A, 1cmy.1.B, 1cmy.1.A, 2v8a.1.A, 2rao.1.A, 5gai.1.K, 3uh3.1.B, 3uhc.1.A, 1xye.1.A, 3ugz.1.A, 5hk7.1.C, 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, 5eet.1.A, 4mqj.2.D, 1y7g.1.B, 2nrl.1.A, 5hk7.1.D, 1ngk.1.B, 5eys.1.A, 2zlv.1.C, 2zlv.1.B, 1cg5.1.A, 5urc.1.D, 1cg5.1.B, 1hv4.1.D, 1v5h.1.A, 4f4o.1.A, 4f4o.1.B, 1yhu.1.B, 1myj.2.A, 1yhu.1.A, 1yhu.1.D, 3ogb.1.A, 1do3.1.A, 1mnj.1.A, 3vrg.1.A, 1it2.1.A, 1gbv.1.B, 1hbr.1.B, 1hbr.1.A, 1y7d.1.B, 5hk7.1.A, 5hk7.1.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, 2r4w.1.A, 1y09.1.A, 3vre.1.A, 3vre.1.B, 5v3t.1.A, 5v3t.1.B, 1y45.1.B, 1v4x.1.A, 1v4x.1.B, 5x2t.1.D, 5x2t.1.A, 4v93.65.A, 5ile.1.A, 1mwb.1.A, 4zvb.1.A, 2ri4.3.A, 2xyk.1.A, 3uh5.1.B, 3ng6.1.B, 1y5k.1.B, 2ri4.1.D, 2ri4.1.C, 3ia3.1.B, 1jzk.1.A, 1cbl.1.D, 3gkv.1.A, 3gkv.1.B, 1v4u.1.B, 3s1i.1.A, 3s1i.1.B, 1c40.1.A, 5yzf.1.A, 1c40.1.B, 3w4u.1.B, 5tjf.1.A, 3w4u.1.A, 1moh.1.A, 5y6p.7.A, 3uh6.1.A, 3onz.1.B, 1vxa.1.A, 4ni0.1.A, 3fs4.1.A, 2d6c.1.A, 4mqc.1.A, 3ciu.1.D, 1ewa.1.A, 1cpw.1.A, 1y4q.1.B, 3wyo.1.B, 3wyo.1.A, 1yma.1.A, 3aq8.1.A, 2dc3.1.A, 2grf.1.A, 1lh1.1.A, 2dc3.1.B, 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3rgk.1.A, 4esa.1.A, 5x2r.1.C, 5x2r.1.A, 3gdj.1.A, 2spo.1.A, 3gdj.1.B, 4rol.1.D, 1rse.1.A, 3g53.1.A, 1spg.1.A, 1k1k.1.B, 1m9p.1.A, 1ash.1.A, 1m9p.1.B, 3qjd.1.A, 1co9.1.A, 3ozu.1.A, 2eku.1.A, 1ycb.1.A, 1ux9.1.A, 1ch3.1.A, 5x2s.2.D, 3s65.1.B, 1fhj.1.A, 3s65.1.D, 1ch9.1.A, 5x2s.2.C, 3szk.1.B, 5hk6.1.A, 3szk.1.A, 5ab8.1.A, 1mcy.1.A, 3v2v.1.A, 2mgf.1.A, 3gqg.1.B, 3gqg.1.A, 3myn.1.A, 2vyz.1.A, 2pgh.1.B, 3fs4.1.B, 2hbs.1.D, 2pgh.1.A, 3uhd.1.A, 2pgh.1.D, 2r1h.1.C, 3heo.1.A, 5d1v.1.A, 5vgt.2.A, 5f0b.1.A, 4v93.42.A, 1abw.1.B, 1dm1.1.A, 1abw.1.A, 1ux8.1.A, 4g51.1.C, 1y7z.1.B, 1jl6.1.A, 5kdq.1.D, 2aup.1.A, 3mym.1.A, 5v3u.1.A, 3zhw.1.A, 1a4f.1.A, 1x46.1.A, 1myg.1.A, 3hyu.1.B, 3hyu.1.C, 1y0a.1.A, 4ns2.1.A, 3kuo.1.A, 1b33.2.E, 3h58.1.A, 1fsl.2.A, 1o16.1.A, 5wog.1.A, 5ojc.1.A, 3gys.1.C, 5utd.1.A, 1ngk.1.H, 4yu3.1.A, 4yu3.1.B, 1rvw.1.A, 1rvw.1.B, 5m3l.1.L, 3uhr.1.A, 5ksj.1.B, 4fh7.1.A, 3whm.1.D, 2ksc.1.A, 4hrr.2.D, 1bvd.1.A, 1mob.1.A, 1yeo.1.A, 3qjc.1.B, 4v93.118.A, 2oif.1.A, 1gli.1.A, 6bme.1.A, 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