SWISS-MODEL Homology Modelling Report

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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:

- 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). doi>
- 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). doi>
- 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). doi>
- Benkert, P., Biasini, M., Schwede, T. Toward the estimation of the absolute quality of individual protein structure models. Bioinformatics 27, 343-350 (2011). doi>
- 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). doi>

Results

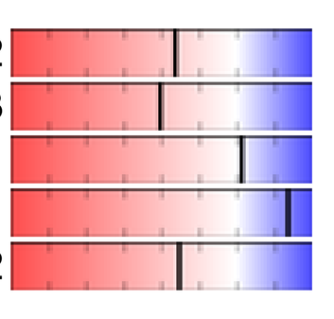
The SWISS-MODEL template library (SMTL version 2018-04-18, PDB release 2018-04-13) was searched with BLAST (Camacho et al.) and HHBlits (Remmert et al.) for evolutionary related structures matching the target sequence in Table T1. For details on the template search, see Materials and Methods. Overall 1055 templates were found (Table T2).

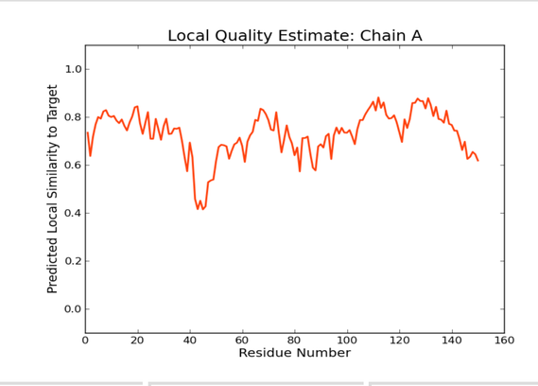
Models

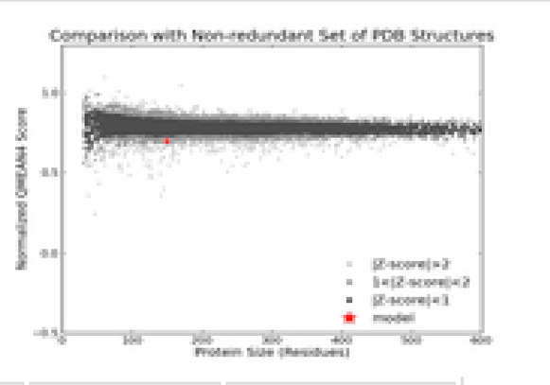
The following model was built (see Materials and Methods "Model Building"):

Model #02	File	Built with	Oligo-State	Ligands	GMQE	QMEAN
	PDB	ProMod3 Version 1.1.0.	monomer	None	0.63	-1.62

QMEAN	-1.62
Cβ	-2.03
All Atom	0.14
Solvation	1.37
Torsion	-1.52







Template	Seq Identity	Oligo-state	Found by	Method	Resolution	Seq Similarity	Range	Coverage	Description
6bmg.1.A	17.81	monomer	HHblits	X-ray	1.88Å	0.30	1 - 150	0.97	Myoglobin

Ligand	Added to Model	Description
ACT	× - Binding site not conserved.	ACETATE ION
ACT	× - Binding site not conserved.	ACETATE ION
ACT	× - Not biologically relevant.	ACETATE ION
ACT	× - Binding site not conserved.	ACETATE ION
ACT	× - Not biologically relevant.	ACETATE ION
ACT	× - Binding site not conserved.	ACETATE ION
CD	× - Not biologically relevant.	CADMIUM ION
CD	× - Not biologically relevant.	CADMIUM ION
CD	× - Binding site not conserved.	CADMIUM ION
CD	× - Binding site not conserved.	CADMIUM ION
CD	× - Binding site not conserved.	CADMIUM ION
CD	× - Binding site not conserved.	CADMIUM ION
HEM	× - Binding site not conserved.	PROTOPORPHYRIN IX CONTAINING FE
OXY	× - Binding site not conserved.	OXYGEN MOLECULE

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Target    MERPEPELIRQSWRAVSRSPLEHGTVLFARLFALEPDLLPLFQYNCRQFSSPEDCLSSPEFLDHIRKVMLVIDAAVTNVE
6bmg.1.A  LSEGEWQLVLHVWAKVEADIAGHGQDILIRLFKHHPETLEKFDR-FKHLKSEAEMKASEDLKKHGVTVLTALGAILKKKG

Target    DLSSLEEYLASLGRKHRA-VGVKLSSFSTVGESLLYMLEKCLGPAFTPATRAAWSQLYGAVVQAMSRGWDGE
6bmg.1.A  H---HEAELKPLAQSHATKHKIPIKYLEFISEAIIHVLHSRHPADFGADAQGAMSKALELFRKDIAAKYKE-
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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.

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). doi>
- **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). doi>

Table T1:

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

```
MERPEPELIRQSWRAVSRSPLEHGTVLFARLFALEPDLLPLFQYNCRQFSSPEDCLSSPEFLDHIRKVMLVIDAAVTNVEDLSSLEEYLASLGRKHRAVG
VKLSSFSTVGESLLYMLEKCLGPAFTPATRAAWSQLYGAVVQAMSRGWDGE
```

Table T2:

Template	Seq Identity	Oligo-state	QSQE	Found by	Method	Resolution	Seq Similarity	Coverage	Description
4mpm.1.B	100.00	homo-dimer	0.57	HHblits	X-ray	1.74Å	0.60	1.00	Neuroglobin
1oj6.2.A	98.01	monomer		HHblits	X-ray	1.95Å	0.59	1.00	NEUROGLOBIN
1oj6.4.A	98.01	monomer		HHblits	X-ray	1.95Å	0.59	1.00	NEUROGLOBIN
4mpm.1.A	100.00	homo-dimer	0.57	HHblits	X-ray	1.74Å	0.60	1.00	Neuroglobin
1oj6.1.A	98.01	monomer		HHblits	X-ray	1.95Å	0.59	1.00	NEUROGLOBIN
4o35.1.A	92.05	monomer		HHblits	X-ray	1.80Å	0.57	1.00	Neuroglobin
3gkt.1.A	92.72	monomer		HHblits	X-ray	1.86Å	0.57	1.00	Neuroglobin
4o1t.1.A	92.05	monomer		HHblits	X-ray	1.60Å	0.57	1.00	Neuroglobin
4nzi.1.A	92.05	monomer		HHblits	X-ray	2.10Å	0.57	1.00	Neuroglobin
5f2a.1.A	92.05	monomer		HHblits	X-ray	2.10Å	0.57	1.00	Neuroglobin
4mu5.1.A	92.05	monomer		HHblits	X-ray	1.80Å	0.57	1.00	Neuroglobin
1w92.1.A	92.72	homo-hexamer	0.60	HHblits	X-ray	1.70Å	0.57	1.00	NEUROGLOBIN
4o2g.1.A	92.05	monomer		HHblits	X-ray	2.70Å	0.57	1.00	Neuroglobin
1faw.1.B	27.97	monomer		HHblits	X-ray	3.09Å	0.33	0.95	HEMOGLOBIN (BETA SUBUNIT)
1a4f.1.B	27.97	monomer		HHblits	X-ray	2.00Å	0.33	0.95	HEMOGLOBIN (BETA CHAIN)
1hv4.1.D	27.97	monomer		HHblits	X-ray	2.80Å	0.33	0.95	HEMOGLOBIN BETA CHAIN
1c40.1.B	27.97	monomer		HHblits	X-ray	2.30Å	0.33	0.95	PROTEIN (HEMOGLOBIN (BETA CHAIN))
3mjp.1.B	27.97	monomer		HHblits	X-ray	2.76Å	0.33	0.95	Hemoglobin subunit beta
3wtg.1.B	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)
1y4g.1.B	22.38	monomer		HHblits	X-ray	1.91Å	0.32	0.95	Hemoglobin beta chain
1hba.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
1abw.1.A	23.57	monomer		HHblits	X-ray	2.00Å	0.32	0.93	HEMOGLOBIN-BASED BLOOD SUBSTITUTE
1aby.1.A	23.57	monomer		HHblits	X-ray	2.60Å	0.32	0.93	HEMOGLOBIN
1ygd.1.B	22.38	monomer		HHblits	X-ray	2.73Å	0.32	0.95	Hemoglobin beta chain
1o1p.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
1c7d.1.A	23.57	monomer		HHblits	X-ray	1.80Å	0.32	0.93	PROTEIN (DEOXYHEMOGLOBIN (ALPHA CHAIN))
1yg5.1.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
5sw7.1.A	23.57	homo-dimer	0.25	HHblits	X-ray	1.85Å	0.32	0.93	Hemoglobin subunit alpha
1o1n.1.A	23.57	monomer		HHblits	X-ray	1.80Å	0.32	0.93	Hemoglobin Alpha chain
1o1m.1.A	23.57	monomer		HHblits	X-ray	1.85Å	0.32	0.93	Hemoglobin Alpha chain
1cp5.1.A	17.12	monomer		HHblits	X-ray	2.10Å	0.30	0.97	PROTEIN (MYOGLOBIN)
1ch5.1.A	17.12	monomer		HHblits	X-ray	2.10Å	0.30	0.97	PROTEIN (MYOGLOBIN)
6bmg.1.A	17.81	monomer		HHblits	X-ray	1.88Å	0.30	0.97	Myoglobin
1moa.1.A	17.12	monomer		HHblits	X-ray	1.90Å	0.30	0.97	MYOGLOBIN
4h07.1.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
1h1x.1.A	16.44	monomer		HHblits	X-ray	1.40Å	0.29	0.97	MYOGLOBIN
3sdn.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
1nz3.1.A	14.38	monomer		HHblits	X-ray	1.60Å	0.29	0.97	Myoglobin
5yl3.1.A	14.38	monomer		HHblits	X-ray	1.50Å	0.29	0.97	Myoglobin
1nz2.1.A	14.38	monomer		HHblits	X-ray	1.90Å	0.29	0.97	Myoglobin
4twv.1.A	14.38	monomer		HHblits	X-ray	1.06Å	0.29	0.97	Myoglobin
3rj6.1.A	14.38	monomer		HHblits	X-ray	1.23Å	0.29	0.97	Myoglobin

The table above shows the top 50 filtered templates. A further 947 templates were found which were considered to be less suitable for modelling than the filtered list.
4hsw.1.A, 1bje.1.A, 3tm9.1.A, 2qmb.1.D, 2eb9.1.A, 5c6e.1.C, 1dxv.1.B, 3zjj.1.A, 2bk9.1.A, 2zlw.1.B, 1qpw.1.B, 1nej.1.B, 1qpw.1.D,
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,
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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,
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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,
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