#### **Model Building Report**

This document lists the results for the homology modelling project "Hemoglobin a" submitted to SWISS-MODEL workspace on April 24, 2018, 9:05 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). [[ ] [ ] [ ]
- 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). [Million 10]
- 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). [m] [m]
- Benkert, P., Biasini, M., Schwede, T. Toward the estimation of the absolute quality of individual protein structure models. Bioinformatics 27, 343-350 (2011). [M] [m]
- 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).
- 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 1337 templates were found (Table T2).

# Models

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

Model #01	File Built with		Olig Sta			GMQE	QMEAN				
	PDB	ProMod3 \ 1.1.0		mono	ner 1 x HEM: PROTOPORPHYRIN IX CONTAINING FE;				ONTAINING	0.98	-0.41
QMEAN	-0.41			Target	1.0	stimate: Chain A		Comp	arison with Non-redundant Set of I	POB Structures	
<b>C</b> β	-0.58			arity to Te				50 Hg		Manager of the	
All Atom	1.20			Local Simil	0.4 -			8 1	11.5		
Solvation	2.10			dicted Lo	0.2			1		Z-score(»2	
orsion	-0.80			Pr	0.0					+(Z-score)+2  Z-score)+1  model	
					0 20 40 60 8 Residue	eo 100 120 140 160 e Number		-0.5	100 300 400 400 Protein Size (Residues)	1500 4000	
Template	Seq Identity	Oligo- state	Found by	Method	Resolution	Seq Similarity	Range	Coverage	Des	cription	

1bz1.1.A	100.00 monome	er HHblits X-ray	1.59Å	0.60	142	1.00	ALPHA CHAIN)		
Ligand	A	dded to Model				Desci	ription		
HEM		✓		PROTOPORPHYRIN IX CONTAINING FE					
HEM	× - Bindi	ing site not conserve	d.	PROTOPORPHYRIN IX CONTAINING FE					
HEM	× - Bindi	d.	PROTOPORPHYRIN IX CONTAINING FE						
HEM	× - Bindi	ing site not conserve	d.	PROTOPORPHYRIN IX CONTAINING FE					

1 00

PROTEIN (HEMOGLOBIN

MVLSPADKTNVKAAWGKVGAHAGEYGAEALERMFLSFPTTKTYFPHFDLSHGSAQVKGHGKKVADALTNAVAHVDDMPNA 1bz1.1.A MVLSPADKTNVKAAWGKVGAHAGEYGAEALERMFLSFPTTKTYFPHFDLSHGSAQVKGHGKKVADALTNAVAHVDDMPNA

Target LSALSDLHAHKLRVDPVNFKLLSHCLLVTLAAHLPAEFTPAVHASLDKFLASVSTVLTSKYR 1bz1.1.A LSALSDLHAHKLRVDPVNFKLLSHCLLVTLAAHLPAEFTPAVHASLDKFLASVSTVLTSKYR

#### **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 600 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 922 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 alignment. Nat Methods 9, 173-175 (2012). [[ ] [ ] [ ]

## Table T1:

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

 ${\tt MVLSPADKTNVKAAWGKVGAHAGEYGAEALERMFLSFPTTKTYFPHFDLSHGSAQVKGHGKKVADALTNAVAHVDDMPNALSALSDLHAHKLRVDPVNFK}$ LLSHCLLVTLAAHLPAEFTPAVHASLDKFLASVSTVLTSKYR

Table T2:

Template	Seq Identity	Oligo- state	QSQE	Found by	Method	Resolution	Seq Similarity	Coverage	Description
1bz1.1.A	100.00	monomer		HHblits	X-ray	1.59Å	0.60	1.00	PROTEIN (HEMOGLOBIN ALPHA CHAIN)
1bab.1.A	99.30	homo- dimer	0.76	HHblits	X-ray	1.50Å	0.60	1.00	HEMOGLOBIN THIONVILLE (DEOXY) (ALPHA CHAIN)
1c7d.1.A	99.30	monomer		HHblits	X-ray	1.80Å	0.60	1.00	PROTEIN (DEOXYHEMOGLOBII (ALPHA CHAIN))
1dxu.1.A	100.00	homo- dimer	0.77	HHblits	X-ray	1.70Å	0.60	0.99	HEMOGLOBIN (DEOXY) (ALPHA CHAIN)
3ia3.1.B	100.00	monomer		HHblits	X-ray	3.20Å	0.60	1.00	Hemoglobin subunit alpha
1z8u.1.B	100.00	monomer		HHblits	X-ray	2.40Å	0.60	1.00	Hemoglobin alpha chain
1z8u.2.B 4yu3.1.A	100.00 87.94	monomer		HHblits HHblits	X-ray X-ray	2.40Å 2.45Å	0.60	0.99	Hemoglobin alpha chain hemoglobin
4yu4.1.C	87.94	homo- dimer	0.63	HHblits	X-ray	2.80Å	0.57	0.99	hemoglobin
1fsx.1.A	87.94	homo- dimer	0.74	HHblits	X-ray	2.10Å	0.56	0.99	HEMOGLOBIN ALPHA CHAIN
1fsx.1.C	87.94	homo- dimer	0.74	HHblits	X-ray	2.10Å	0.56	0.99	HEMOGLOBIN ALPHA CHAIN
1iwh.1.A	87.94	monomer		HHblits	X-ray	1.55Å	0.56	0.99	Hemoglobin alpha chain
1hda.1.A	87.94	homo- dimer	0.77	HHblits	X-ray	2.20Å	0.56	0.99	HEMOGLOBIN (DEOXY) (ALPHA CHAIN)
1g09.1.C	87.94	homo- dimer	0.56	HHblits	X-ray	2.04Å	0.56	0.99	HEMOGLOBIN ALPHA CHAIN
1g08.1.A	87.94	monomer		HHblits	X-ray	1.90Å	0.56	0.99	HEMOGLOBIN ALPHA CHAIN
1g0a.1.A	87.94	homo- dimer	0.62	HHblits	X-ray	2.04Å	0.56	0.99	HEMOGLOBIN ALPHA CHAIN
5c6e.1.C	87.94	homo- dimer	0.68	HHblits	neutron diff.	2.00Å	0.56	0.99	Hemoglobin subunit alpha
3cy5.1.A	86.52	monomer		HHblits	X-ray	2.00Å	0.56	0.99	Hemoglobin subunit alpha-2
3cy5.1.C	86.52	monomer		HHblits	X-ray	2.00Å	0.56	0.99	Hemoglobin subunit alpha-2
3d1a.1.A	86.62	homo- dimer	0.38	HHblits	X-ray	2.61Å	0.56	1.00	Hemoglobin subunit alpha-1/2
3d1a.1.C	86.62	homo- dimer	0.38	HHblits	X-ray	2.61Å	0.56	1.00	Hemoglobin subunit alpha-1/2
2dhb.1.A	87.23	homo- dimer	0.67	HHblits	X-ray	2.80Å	0.56	0.99	HEMOGLOBIN (DEOXY) (ALPHA CHAIN)
1g0b.1.A	87.23	monomer		HHblits	X-ray	1.90Å	0.56	0.99	HEMOGLOBIN ALPHA CHAIN
1y8i.1.A	87.23	homo- dimer	0.52	HHblits	X-ray	2.60Å	0.56	0.99	Hemoglobin alpha chains
1y8i.1.C	87.23	homo- dimer	0.52	HHblits	X-ray	2.60Å	0.56	0.99	Hemoglobin alpha chains
2zlw.1.A	87.23	homo- dimer	0.63	HHblits	X-ray	2.90Å	0.56	0.99	Hemoglobin subunit alpha
3fh9.1.A	86.52	homo- dimer	0.69	HHblits	X-ray	1.62Å	0.56	0.99	Hemoglobin alpha chain
3gqr.2.A	85.11	monomer		HHblits	X-ray	2.40Å	0.56	0.99	Hemoglobin subunit alpha
3gqp.1.A	85.11	homo- dimer	0.75	HHblits	X-ray	2.00Å	0.56	0.99	Hemoglobin subunit alpha
3eu1.1.C	86.52	homo- dimer	0.37	HHblits	X-ray	3.00Å	0.56	0.99	Hemoglobin subunit alpha-1/2
3eu1.1.A	86.52	homo- dimer	0.37	HHblits	X-ray	3.00Å	0.56	0.99	Hemoglobin subunit alpha-1/2
2qu0.1.C	86.52	homo- dimer	0.60	HHblits	X-ray	2.70Å	0.56	0.99	Hemoglobin subunit alpha-1/2
2qu0.1.A	86.52	homo- dimer	0.60	HHblits	X-ray	2.70Å	0.56	0.99	Hemoglobin subunit alpha-1/2
3hrw.1.A	85.82	monomer		HHblits	X-ray	2.80Å	0.56	0.99	Hemoglobin subunit alpha
3hrw.1.C	85.82	monomer		HHblits	X-ray	2.80Å	0.56	0.99	Hemoglobin subunit alpha
4h2l.1.A	85.11	monomer		HHblits	X-ray	1.78Å	0.56	0.99	Alpha-globin
3gdj.1.A	84.40	homo- dimer	0.62	HHblits	X-ray	2.00Å	0.56	0.99	Hemoglobin subunit alpha
3lqd.1.A	82.98	homo- dimer	0.65	HHblits	X-ray	2.80Å	0.56	0.99	Hemoglobin subunit alpha
2rao.1.A	82.27	homo- dimer	0.62	HHblits	X-ray	2.00Å	0.56	0.99	Hemoglobin subunit alpha-1/2
1y01.1.B 2zlx.2.A	100.00 87.23	monomer monomer		HHblits HHblits	X-ray X-ray	2.80Å 2.80Å	0.60 0.56	1.00 0.99	Hemoglobin alpha chain Hemoglobin subunit alpha
5ker.1.A	85.11	homo- dimer	0.41	HHblits	X-ray	2.20Å	0.55	0.99	Alpha-globin
5ker.1.C	85.11	homo- dimer	0.41	HHblits	X-ray	2.20Å	0.55	0.99	Alpha-globin
5ker.2.A	85.11	homo-	0.32	HHblits	X-ray	2.20Å	0.55	0.99	Alpha-globin
3gou.1.A	83.69	homo-	0.55	HHblits	X-ray	3.00Å	0.55	0.99	Hemoglobin subunit alpha
3pel.1.A	83.69	homo-	0.60	HHblits	X-ray	1.90Å	0.55	0.99	Hemoglobin subunit alpha
•		dimer							
2ri4.3.A 3gys.1.C	86.52 85.11	monomer monomer		HHblits	X-ray X-ray	2.70Å 2.90Å	0.56	0.99	Hemoglobin subunit alpha-1/2 Hemoglobin subunit alpha
5eui.1.A	90.07	monomer		HHblits	X-ray	1.45Å	0.57	0.99	HBA protein

4hsw.1.A, 1bje.1.A, 5m3l.1.E, 2qmb.1.D, 2eb9.1.A, 2qmb.1.A, 3zjj.1.A, 2bk9.1.A, 2zlw.1.B, 1qpw.1.B, 1qpw.1.C, 1a4f.1.A, 5t82.1.A, 1a4f.1.B, 5m3l.1.A, 1h1x.1.A, 3o7n.1.A, 3s48.2.B, 5ojb.1.A, 1aby.1.A, 1aby.1.B, 3uhc.1.A, 1y0c.1.A, 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, 1x3k.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, 1jra.1.A, 1v4w.1.D, 5hy8.2.B, 1dxv.1.B, 4xs0.1.A, 4xs0.1.B, 1or4.1.A, 4bja.1.A, 3ok5.1.B, 1yzi.1.B, 3qzx.1.B, 3qzz.1.A, 1y4v.1.B, 1nej.1.B, 1m9p.1.A, 1m9p.1.B, 4mqk.1.A, 4mqk.1.B, 4mqk.1.C, 5v5r.1.A, 1jr8.1.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, 1y5k.1.B, 5jgg.1.B, 2nx0.1.A, 1oj6.2.A, 5e6e.1.B, 3zom.1.A, 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, 1cmy.1.B, 1cmy.1.A, 5yl3.1.A, 3uh3.1.B, 1wmu.1.B, 3ugz.1.A, 3zhw.2.A, 3ubc.1.A, 1umo.1.B, 3eu1.1.D, 3eu1.1.B, 2vyy.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, 1ngk.1.B, 5eys.1.A, 2zlv.1.C, 2zlv.1.B, 1cq5.1.A, 5urc.1.D, 4mqc.1.A, 1hv4.1.D, 1v5h.1.A, 4f4o.1.A, 4f4o.1.B, 1yhu.1.B, 1myj.2.A, 1yhu.1.A, 1yhu.1.D, 3wct.1.C, 1do3.1.A, 1mnj.1.A, 3fs4.1.B, 1yih.1.B, 3vrg.1.A, 1it2.1.A, 1gbv.1.B, 1hbr.1.B, 1hbr.1.A, 1y7d.1.B, 1hbs.1.D, 1hbs.1.C, 1hbs.1.B, 1hbs.1.A, 1ch9.1.A, 3wfx.1.A, 1s56.2.A, 5ee4.1.C, 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, 5x2t.1.C, 4b3w.1.A, 5ile.1.A, 4zvb.1.A, 1y5j.1.B, 3ng6.1.B, 1ibe.1.A, 2ri4.1.D, 1cbl.1.D, 3gkv.1.A, 3gkv.1.B, 1v4u.1.B, 3s1i.1.A, 4o2g.1.A, 3s1i.1.B, 1c40.1.A, 5yzf.1.A, 1c40.1.B, 3w4u.1.B, 5tjf.1.A, 3w4u.1.A, 1y4g.1.B, 1moh.1.A, 5y6p.7.A, 3vhb.1.A, 3uh6.1.A, 2pgh.1.C, 1vxa.1.A, 2hbs.1.D, 2d6c.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, 3hep.1.A, 2ohb.1.A, 4of9.1.A, 1urv.2.A, 2d6c.2.A, 1irc.1.A, 1ch1.1.A, 4ni0.1.A, 1ufj.1.A, 3zjl.1.A, 5muu.1.D, 3gou.1.D, 3gou.1.B, 1vwt.1.A, 1y8i.1.D, 1y8i.1.B, 3d1k.1.A, 5f0b.1.A, 3uhh.1.A, 4gau.1.A, 3ugy.1.A, 4hrt.2.C, 1xz5.1.A, 1v07.1.A, 3ag5.1.A, 1cgx.1.A, 5k1l.1.B, 5eui.1.B, 1hds.1.A, 3tld.1.A, 1hds.1.C, 1hds.1.B, 1hds.1.D, 5hu6.1.B, 4iro.1.A, 1hbg.1.A, 4iro.1.C, 5hbi.1.B, 1myi.1.A, 1tu9.1.A, 2ig3.1.A, 3a0g.1.B, 1w92.1.A, 1dxd.1.A, 1buw.1.A, 1buw.1.B, 1buw.1.D, 2evp.1.A, 3qm7.1.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, 3ggr.2.B, 2zs0.1.A, 2zs0.1.B, 2zs0.1.C, 3sdn.1.A, 1fsx.1.D, 1f6h.1.A, 2cmm.1.A, 3o89.1.A, 1mlm.1.A, 4xdi.1.A, 3zh0.1.A, 3wcu.1.C, 4esa.1.D, 3mjp.1.D, 3mjp.1.C, 5vmm.1.C, 3mjp.1.A, 2gkm.1.A, 7hbi.1.B, 2h35.1.B, 2r4w.1.A, 3bj2.1.D, 5x2r.3.A, 5x2r.3.B, 5x2r.3.C, 5x2r.3.D, 3rgk.1.A, 3dht.1.A, 4o1t.1.A, 5x2r.1.C, 5x2r.1.A, 5x2r.1.D, 3gdj.1.B, 4rol.1.D, 1rse.1.A, 3g53.1.A, 5oj9.1.A, 1k1k.1.B, 1ufp.1.A, 1b33.1.A, 1d8u.1.B, 1ash.1.A, 3bj1.1.C, 3qjd.1.A, 1co9.1.A, 3ozu.1.A, 3pi4.1.B, 2eku.1.A, 1ycb.1.A, 1vxb.1.A, 1ch3.1.A, 5x2s.2.D, 3s65.1.B, 1fhj.1.A, 3s65.1.D, 5x2s.2.A, 1y09.1.A, 3szk.1.B, 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, 3onz.1.B, 3fs4.1.A, 2pgh.1.A, 3uhd.1.A, 2pgh.1.D, 5m3l.1.L, 3heo.1.A, 5d1v.1.A, 1pmb.2.A, 3gqp.1.D, 4v93.42.A, 1abw.1.B, 1dm1.1.A, 1abw.1.A, 4g51.1.C, 1y7z.1.B, 1jl6.1.A, 5kdq.1.D, 2aup.1.A, 3mym.1.A, 3zhw.1.A, 1qpw.1.D, 1x46.1.A, 2h35.1.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, 1o16.1.A, 5wog.1.A, 5ojc.1.A, 1jzk.1.A, 5utd.1.A, 4h07.1.A, 4yu3.1.B, 1rvw.1.A, 1rvw.1.B, 3uhr.1.A, 5ksj.1.B, 3whm.1.D, 4hrr.2.D, 1bvd.1.A, 1mob.1.A, 5v5q.1.A, 1hbs.2.B, 3qjc.1.B, 4v93.118.A, 2oif.1.A, 1gli.1.A, 1ye1.1.B, 4f69.1.A, 1bbb.1.C, 5ohf.1.B, 1xch.1.A, 2ig3.2.A, 4pqb.1.A, 3sdh.1.A, 5eu2.1.A, 3at6.1.A, 1ux9.2.A, 6hbw.1.D, 6hbw.1.B, 1fn3.1.D, 1dxu.1.B, 1fn3.1.C, 3kun.2.A, 3ozi.1.A, 4it8.1.A, 3k3u.2.B, 1xzv.1.A, 3oj1.1.A, 4uf6.1.C, 1y8w.1.A, 2aa1.1.A, 2aa1.1.B, 1ch7.1.A, 2w6w.1.A, 3at5.1.A, 3at5.1.B, 3bj2.1.A, 5d5r.1.A, 1y8w.1.C, 1a3o.1.A, 1pbx.1.A, 1pbx.1.B, 4nzi.1.A, 2gln.1.B, 1c7d.1.A, 2gln.1.A, 1gcv.1.B, 1gcv.1.A, 1or6.1.A, 1ch5.1.A, 2w6y.1.A, 1gcw.1.D, 1gcw.1.C, 1gcw.1.B, 1gcw.1.A, 2h8d.1.D, 6bmg.1.A, 1mgn.1.A, 1o1m.1.A, 3wtg.1.B, 1dlw.1.A, 3gkt.1.A, 5ni1.1.B, 1it3.1.A, 3uhb.1.A, 2bkm.1.A, 1y83.1.B, 2gnv.1.A, 1fdh.1.B, 2wth.1.A, 1r1y.1.B, 4zva.1.A, 1r1y.1.A, 5x2s.3.C, 4n7o.1.A, 3dhr.4.B, 3dut.1.D, 2zfo.1.A, 2zfo.1.B, 2zfo.1.C, 1o1k.1.B, 1jzl.1.B, 2qsp.1.D, 3dhr.2.C, 5x2t.2.A, 5x2t.2.D, 1it2.2.A, 3mn0.1.A, 2vee.1.A, 2mgc.1.A, 1yg5.1.B, 1cik.1.A, 1ebt.1.A, 4mxl.1.A, 1gvh.1.A, 5oja.1.A, 2hhe.1.B, 1f5o.1.A, 1ofk.1.A, 2vml.1.A, 1uvx.1.A, 4v93.65.A, 1spg.1.B, 1spg.1.A, 1o1o.1.A, 1o1o.1.B, 4uiq.2.A, 2oh8.1.A, 1y5f.1.B, 1y4r.1.B, 3a2g.1.A, 1r1x.1.B, 5vlx.1.A, 2g3h.1.A, 1r1x.1.A, 5hlq.1.A, 1hbs.2.A, 1yeo.1.A, 1hbs.2.C, 1hbs.2.D, 5o18.1.A, 4wjg.2.G, 2e2y.1.A, 2d5x.1.B, 1mba.1.A, 5x2u.3.B, 2oha.1.A, 1jzm.1.A, 4u8u.1.B, 3zji.1.A, 3s48.1.B, 1urv.1.A, 3rjn.1.A, 5ilr.1.A, 3uh7.1.A, 1qxd.2.D, 4wch.1.A, 5hy8.1.B, 2b7h.1.A, 2b7h.1.B, 4mpm.1.A, 1g0b.1.B, 4mpm.1.B, 1jeb.1.A, 5v3v.1.A, 1jeb.1.C, 1jeb.1.B, 2fam.1.A, 1mlh.1.A, 3vm9.1.B, 5muu.1.K, 1ch2.1.A, 2olp.1.A, 3uht.1.A, 3gwn.1.A, 3zol.1.A, 3kuo.2.A, 1nz2.1.A, 4mqk.2.C, 1kr7.1.A, 3ag0.1.A, 1hv4.2.C, 3wfx.1.B, 1obm.1.A, 4xdi.2.A, 3vm9.1.A, 1oj6.1.A, 3pi1.1.B, 1cp0.1.A, 5jnz.1.A, 5jnz.1.B, 2xkg.1.A, 3qqq.1.B, 3qqq.1.A, 3qqr.2.A, 4uiq.1.A, 1ecn.1.A, 1d8u.1.A, 1lhs.1.A, 4fwy.1.A, 1cg8.1.A, 1cg8.1.B, 2mgj.1.A, 2w31.1.A, 4mqg.1.B, 1cp5.1.A, 1mnk.1.A, 3hxn.1.B, 3hxn.1.C, 4yu4.1.D, 1xy0.1.A, 3hxn.1.D, 1hba.1.B, 4mqh.1.A, 1or4.1.B, 1ith.1.A, 5ohf.1.A, 1mni.2.A, 3nmm.1.A, 2gnw.1.A, 2gnw.1.B, 1gbu.1.B, 3gqp.1.B, 2r4z.1.B, 5sw7.1.B, 5sw7.1.A, 4mqj.1.B, 2qu0.1.B, 3zjm.1.A, 1mti.1.A, 5utb.1.A, 3mvc.1.A, 1xye.1.A, 1wmu.1.A, 1h97.1.A, 1cio.1.A, 1fcs.1.A, 1o1i.1.B, 1o1i.1.A, 1mbi.1.A, 1myj.1.A, 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1xq5.1.A, 3gys.2.B, 5m3l.1.F, 5m3l.1.G, 5c6y.1.A, 3pt7.1.B, 2vyw.1.A, 2qfn.1.A, 2in4.1.A, 4g1v.1.A, 3hrw.1.B, 3hrw.1.D, 1hlm.1.A, 2qrw.1.B, 1a6g.1.A, 2qrw.1.A, 2r80.5.B, 2jho.1.A, 1ye2.1.B, 3uhe.1.A, 3wyo.2.B, 2rao.1.B, 1ofj.1.A, 1ngk.1.G, 1ngk.1.D, 3w4u.2.A, 1ngk.1.A, 3wct.1.B, 3ogb.1.A, 3wct.1.A, 3wct.1.D, 5ker.2.C, 4v93.102.A, 1ird.1.B, 5ker.2.D, 1v4u.1.A, 1hho.1.B, 1jy7.1.B, 1y2z.1.B, 5ufj.1.D, 5ufj.1.B, 2ekt.1.A, 2qrw.4.A, 5vmm.1.B, 1aj9.1.A, 4ni0.1.B, 5vmm.1.A, 1uc3.1.A, 2vhb.1.B, 5vmm.1.D, 5kd1.1.A, 3ozv.3.A, 1yen.1.A, 2bwh.1.A, 4kn3.1.A, 4h2l.1.B, 5f2a.1.A, 1moc.1.A, 1m6c.1.A, 3vrf.1.B, 2w31.1.B, 3vrf.1.A, 4v93.3.A, 5x2r.2.D, 5x2r.2.A, 5x2r.2.C, 3mjp.1.B, 1ux9.1.A, 1mlr.1.A, 2r1h.1.B, 2r1h.1.C, 3zjr.1.B, 1dwr.1.A, 1fsl.2.A, 1la6.1.B, 1mbs.1.A, 3qjb.1.A, 4hrr.1.B, 1kfr.1.A, 2c0k.1.A, 1i3d.1.A, 1yvq.1.D, 1hjt.1.A, 4uii.1.B, 1vhb.1.A, 4v93.1.A, 4uii.1.A, 1ye0.1.B, 1mlu.1.A, 5x2s.3.A, 2oh9.1.A, 6bb5.1.D, 5x2s.3.B, 3qje.1.B, 5x2s.3.D, 6bb5.1.A,

2hbs.2.B, 1gdl.1.A, 3ovu.1.C, 4o35.1.A, 5d1v.1.B, 2auq.1.A, 2r4x.1.A, 4u8u.1.A, 4u8u.1.C, 3k9z.1.A, 3at6.1.B, 1y8k.1.B, 1cbm.1.A, 1myf.1.A, 2zs0.1.D, 1a9w.1.B, 5b84.1.A, 1s5x.1.B, 1y0d.1.A, 2w6x.1.A, 3zh0.2.A, 2gtl.1.C, 1dxt.1.B, 1ch4.1.A, 1ch4.1.C, 3tm9.1.A, 3lqd.1.B, 4fh7.1.B, 2lhb.1.A, 3aq9.1.A, 3cy5.1.B, 3dut.2.B, 1bz1.1.B, 4pqc.1.A, 1sdl.1.D, 1moa.1.A, 1g08.1.B, 1sdl.1.C, 2m6z.1.B,

1j40.2.B, 3b75.2.D, 3b75.2.A, 3b75.2.B, 3d17.1.A, 3d17.1.B, 3d17.1.D, 2spo.1.A, 2zfo.1.D, 2r4w.1.B, 1a6k.1.A, 1y8h.1.B, 4f6i.1.A,

3pel.1.B, 5x2t.3.D, 5x2t.3.C, 5x2t.3.A, 2yrs.1.B, 3lhb.1.A, 5llz.1.A, 1myt.1.A, 1xq5.1.B, 1o1l.1.A, 1ygd.1.B, 2bmm.1.A, 1j40.2.D,

3ozv.3.B, 1ns6.1.A, 3bj3.1.A, 1si4.1.B, 3dhr.1.A, 3eok.1.B, 3eok.1.A, 2dhb.1.B

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The table above shows the top 50 filtered templates. A further 866 templates were found which were considered to be less suitable

for modelling than the filtered list.