Supplementary Table 3: Complete template alignments for HsABCB1 are shown in two runs of HsABCB1 modelling based on Sav1866. For details, see Material and Methods.

First round modeling for HsABCB1 based on Sav1866 (2hyd)

```
>P1;HsABCB1
sequence:HsABCB1:1:.:1280:.:.: : :
MDLEGDRNGGAKKKNFFKLNNKSEKDKKEKKPTVSVFSMFRYSNWLDKL-
YMVVGTLAAIIHGAGLPLMMLVFGEMTDIFANAGNLEDLMSNITNRSDIN
DTGFFMNLEEDMTRYAYYYSGIGAGVLVAAYIQVSFWCLAAGRQIHKIRK
QFFHAIMRQEIGWFDVHDVGELNTRLTDDVSKINEGIGDKIGMFFQSMAT
FFTGFIVGFTRGWKLTLVILAISPVLGLSAAVWAKILSSFTDKELLAYAK
AGAVAEEVLAAIRTVIAFGGQKKELERYNKNLEEAKRIGIKKAITANISI
GAAFLLIYASYALAFWYGTTLVLSGEYSIGQVLTVFFSVLIGAFSVGQAS
PSIEAFANARGAAYEIFKIIDNKPSIDSYSKSGHKPDNIK-GNLEFRNVH
FSYPSRKEVKILKGLNLKVQSGQTVALVGNSGCGKSTTVQLMQRLYDPTE
GMVSVDGQDIRTINVRFLREIIGVVSQEPVLFATTIAENIRYGRENVTMD
EIEKAVKEANAYDFIMKLPHKFDTLVGERGAQLSGGQKQRIAIARALVRN
PKILLLDEATSALDTESEAVVQVALDKARKGRTTIVIAHRLSTVRNADVI
AGFDDGVIVEKGNHDELMKEKGIYFKLVTMQTAGNEVELENAADESKSEI
DALEMSSNDSRSSLIRKRSTRRSVRGSQAQDRKLSTKEALDESIPPVSFW
RIMKLNLTEWPYFVVGVFCAIINGGLQPAFAIIFSKIIGVFTRIDDPETK
RQNSNLFSLLFLALGIISFITFFLQGFTFGKAGEILTKRLRYMVFRSMLR
QDVSWFDDPKNTTGALTTRLANDAAQVKGAIGSRLAVITQNIANLGTGII
ISFIYGWQLTLLLLAIVPIIAIAGVVEMKMLSGQALKDKKELEGAGKIAT
EAIENFRTVVSLTQEQKFEHMYAQSLQVPYRNSLRKAHIFGITFSFTQAM
MYFSYAGCFRFGAYLVAHKLMSFEDVLLVFSAVVFGAMAVGQVSSFAPDY
AKAKISAAHIIMIIEKTPLIDSYSTEGLMPNTL-EGNVTFGEVVFNYPTR
PDIPVLQGLSLEVKKGQTLALVGSSGCGKSTVVQLLERFYDPLAGKVLLD
GKEIKRLNVQWLRAHLGIVSQEPILFDCSIAENIAYGDNSRVVSQEEIVR
AAKEANIHAFIESLPNKYSTKVGDKGTQLSGGQKQRIAIARALVRQPHIL
LLDEATSALDTESEKVVQEALDKAREGRTCIVIAHRLSTIQNADLIVVFQ
NGRVKEHGTHQQLLAQKGIYFSMVSVQAGTKRQ*
>P1;sele
structureX:sele:632:.:689:.:.: : :
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---------------------------------GNEVELENAADESKSEI
DALEMSSNDSRSSLIRKRSTRRSVRGSQAQDRKLSTKEALD---------
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>P1;2hyd
structureX:2hyd:1:A:578:B:.: : :
-------------------------------------MIKRYLQFVKPYK
YRIFATIIVGIIKFGIPMLIPLL------------IKYAIDGVINNHALT
TDEKVHHLTIAIGIALFIFVIVRPPI---EFIRQYLAQWTSNKILYDIRK
KLYNHLQALSARFYANNQVGQVISRVINDVEQTKDFILTGLMNIWLDCIT
IIIALSIMFFLDVKLTLAALFIFPFYILTVYVFFGRLRKLTRERSQALAE
VQGFLHERVQGISVVKSFAIEDNEAKNFDKKNTNFLTRALKHTRWNAYSF
AAINTVTDIGPIIVIGVGAYLAISGSITVGTLAAFVGYLELLFGPLRRLV
ASFTTLTQSFASMDRVFQLIDE--DYDIKNGVGAQPIEIKQGRIDIDHVS
FQY-NDNEAPILKDINLSIEKGETVAFVGMSGGGKSTLINLIPRFYDVTS
GQILIDGHNIKDFLTGSLRNQIGLVQQDNILFSDTVKENILLGRPTATDE
EVVEAAKMANAHDFIMNLPQGYDTEVGERGVKLSGGQKQRLSIARIFLNN
PPILILDEATSALDLESESIIQEALDVLSKDRTTLIVAHRLSTITHADKI
VVIENGHIVETGTHRELIAKQGAYEHLYSIQ-------------------
------------NL---------------------------MIKRYLQFV
KPYKYRI--FATIIVGIIKFGIPMLIPLLIKYAIDGVINNHALTTDEKVH
HLTIAIGIALFIFVIVRPPIEFIRQYLAQWTSNKILYD-IRKKLYNHLQA
LSARFYAN--NQVGQVISRVINDVEQTKDFILTGLMNIWLDCITIIIALS
IMFFLDVKLTLAALFIFPFYILTVYVFFGRLRKLTRERSQALAEVQGFLH
ERVQGISVVKSFAIEDNEAKNFDKKNTNFLTRALKHTRWNAYSFAAINTV
TDIGPIIVIGVGAYLAISGSITVGTLAAFVGYLELLFGPLRRLVASFTTL
TQSFASMDRVFQLIDED--YDIKNGVGAQPIEIKQGRIDIDHVSFQYNDN
-EAPILKDINLSIEKGETVAFVGMSGGGKSTLINLIPRFYDVTSGQILID
GHNIKDFLTGSLRNQIGLVQQDNILFSDTVKENILLGRPT--ATDEEVVE
AAKMANAHDFIMNLPQGYDTEVGERGVKLSGGQKQRLSIARIFLNNPPIL
ILDEATSALDLESESIIQEALDVLSKDRTTLIVAHRLSTITHADKIVVIE
NGHIVETGTHRELIAKQGAYEHLYSIQNL----*
```

Second round modeling for HsABCB1 based on the first round model (sele2)

```
>P1;HsABCB1
sequence:HsABCB1:1:.:1280:.:.: : :
MDLEGDRNGGAKKKNFFKLNNKSEKDKKEKKPTVSVFSMFRYSNWLDKLY
MVVGTLAAIIHGAGLPLMMLVFGEMTDIFANAGNLEDLMSNITNRSDIND
TGFFMNLEEDMTRYAYYYSGIGAGVLVAAYIQVSFWCLAAGRQIHKIRKQ
FFHAIMRQEIGWFDVHDVGELNTRLTDDVSKINEGIGDKIGMFFQSMATF
FTGFIVGFTRGWKLTLVILAISPVLGLSAAVWAKILSSFTDKELLAYAKA
GAVAEEVLAAIRTVIAFGGQKKELERYNKNLEEAKRIGIKKAITANISIG
AAFLLIYASYALAFWYGTTLVLSGEYSIGQVLTVFFSVLIGAFSVGQASP
SIEAFANARGAAYEIFKIIDNKPSIDSYSKSGHKPDNIKGNLEFRNVHFS
YPSRKEVKILKGLNLKVQSGQTVALVGNSGCGKSTTVQLMQRLYDPTEGM
VSVDGQDIRTINVRFLREIIGVVSQEPVLFATTIAENIRYGRENVTMDEI
EKAVKEANAYDFIMKLPHKFDTLVGERGAQLSGGQKQRIAIARALVRNPK
ILLLDEATSALDTESEAVVQVALDKARKGRTTIVIAHRLSTVRNADVIAG
FDDGVIVEKGNHDELMKEKGIYFKLVTMQTAGNEVELENAADESKSEIDA
LEMSSNDSRSSLIRKRSTRRSVRGSQAQDRKLSTKEALDESIPPVSFWRI
MKLNLTEWPYFVVGVFCAIINGGLQPAFAIIFSKIIGVFTRIDDPETKRQ
NSNLFSLLFLALGIISFITFFLQGFTFGKAGEILTKRLRYMVFRSMLRQD
VSWFDDPKNTTGALTTRLANDAAQVKGAIGSRLAVITQNIANLGTGIIIS
```

```
FIYGWQLTLLLLAIVPIIAIAGVVEMKMLSGQALKDKKELEGAGKIATEA
IENFRTVVSLTQEQKFEHMYAQSLQVPYRNSLRKAHIFGITFSFTQAMMY
FSYAGCFRFGAYLVAHKLMSFEDVLLVFSAVVFGAMAVGQVSSFAPDYAK
AKISAAHIIMIIEKTPLIDSYSTEGLMPNTLEGNVTFGEVVFNYPTRPDI
PVLQGLSLEVKKGQTLALVGSSGCGKSTVVQLLERFYDPLAGKVLLDGKE
IKRLNVQWLRAHLGIVSQEPILFDCSIAENIAYGDNSRVVSQEEIVRAAK
EANIHAFIESLPNKYSTKVGDKGTQLSGGQKQRIAIARALVRQPHILLLD
EATSALDTESEKVVQEALDKAREGRTCIVIAHRLSTIQNADLIVVFQNGR
VKEHGTHQQLLAQKGIYFSMVSVQAGTKRQ*

>P1;sele
structureX:sele:1:.:30:.:.: : :
----MDNDGGAPPPPPTLV---VEEPKKAEIRGVAFK-------------
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>P1;sele2
structureX:sele2:38:.:1280:.:.: : :
-------------------------------------SMFRYSNWLDKLY
MVVGTLAAIIHGAGLPLMMLVFGEMTDIFANAGNLEDLMSNITNRSDIND
TGFFMNLEEDMTRYAYYYSGIGAGVLVAAYIQVSFWCLAAGRQIHKIRKQ
FFHAIMRQEIGWFDVHDVGELNTRLTDDVSKINEGIGDKIGMFFQSMATF
FTGFIVGFTRGWKLTLVILAISPVLGLSAAVWAKILSSFTDKELLAYAKA
GAVAEEVLAAIRTVIAFGGQKKELERYNKNLEEAKRIGIKKAITANISIG
AAFLLIYASYALAFWYGTTLVLSGEYSIGQVLTVFFSVLIGAFSVGQASP
SIEAFANARGAAYEIFKIIDNKPSIDSYSKSGHKPDNIKGNLEFRNVHFS
YPSRKEVKILKGLNLKVQSGQTVALVGNSGCGKSTTVQLMQRLYDPTEGM
VSVDGQDIRTINVRFLREIIGVVSQEPVLFATTIAENIRYGRENVTMDEI
EKAVKEANAYDFIMKLPHKFDTLVGERGAQLSGGQKQRIAIARALVRNPK
ILLLDEATSALDTESEAVVQVALDKARKGRTTIVIAHRLSTVRNADVIAG
FDDGVIVEKGNHDELMKEKGIYFKLVTMQTAGNEVELENAADESKSEIDA
LEMSSNDSRSSLIRKRSTRRSVRGSQAQDRKLSTKEALDESIPPVSFWRI
MKLNLTEWPYFVVGVFCAIINGGLQPAFAIIFSKIIGVFTRIDDPETKRQ
NSNLFSLLFLALGIISFITFFLQGFTFGKAGEILTKRLRYMVFRSMLRQD
```

```
VSWFDDPKNTTGALTTRLANDAAQVKGAIGSRLAVITQNIANLGTGIIIS
FIYGWQLTLLLLAIVPIIAIAGVVEMKMLSGQALKDKKELEGAGKIATEA
IENFRTVVSLTQEQKFEHMYAQSLQVPYRNSLRKAHIFGITFSFTQAMMY
FSYAGCFRFGAYLVAHKLMSFEDVLLVFSAVVFGAMAVGQVSSFAPDYAK
AKISAAHIIMIIEKTPLIDSYSTEGLMPNTLEGNVTFGEVVFNYPTRPDI
PVLQGLSLEVKKGQTLALVGSSGCGKSTVVQLLERFYDPLAGKVLLDGKE
IKRLNVQWLRAHLGIVSQEPILFDCSIAENIAYGDNSRVVSQEEIVRAAK
EANIHAFIESLPNKYSTKVGDKGTQLSGGQKQRIAIARALVRQPHILLLD
EATSALDTESEKVVQEALDKAREGRTCIVIAHRLSTIQNADLIVVFQNGR
VKEHG
```