Supporting Information

Figure S1. a) PSI-BLAST result for rT-M386 and G210C lipase and b) multiple sequence alignment of target and template, 2HIH. (https://blast.ncbi.nlm.nih.gov)

a)

Description	Max score	Total score	Query cover	E value	Ident	Accession
Chain A, Crystal Structure Of Staphylococcus Hyicus Lipase	390	390	98%	5e-134	51%	2HIH_A
Chain A, Crystal Structure Of Lipase From Geobacillus Stearothermophilus T6 Methanol Stable Variant H86y/a269t	228	228	94%	3e-71	36%	4X7B_A
Chain A, Crystal Structure Of Lipase From Geobacillus Stearothermophilus T6 Methanol Stable Variant H86y/a269t/r374w	228	228	94%	5e-71	36%	4X85_A
Chain A, Structure Of Lipase 1 From Pelosinus Fermentans	219	219	94%	6e-68	39%	5AH0_A
Chain A, Structure Of Esta From Clostridium Botulinum	218	218	89%	2e-66	38%	5AH1_A
Chain A, Crystal Structure Of A Lipase From Geobacillus Sp. Sbs-4s	206	206	95%	2e-62	35%	3AUK_A
Chain A, Crystal Structure Of T1 Lipase	205	205	94%	3e-62	35%	2DSN_A
Chain A, An Organic Solvent Tolerant Lipase 42	205	205	94%	3e-62	35%	4FKB_A
Chain A, Crystallization And 3d Structure Elucidation Of Thermostable L2 Lipase From Thermophilic Locally Isolated Bacillus Sp. L2	205	205	94%	3e-62	35%	4FDM_A
Chain A, Crystal Structure Of D311e Lipase	204	204	94%	4e-62	35%	3UMJ_A

b)

Score	Expect	Method	Identities	Positives	Gaps
396 bits(927)	7e-113	Compositional matrix adjust.	196/383(51%)	223/383(58%)	7/383(1%)

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Query  6    KNQYPVVFVHGFVGLVGEDSFSMYPNYWGGTKYNVKQELTKLGYRVHEANVGAFSSNYDR  65
            KN  P VFVHGF G VGE       NYWGGTK N    L K GY   EA V A  SN +R
Sbjct  50   KNKDPFVFVHGFTGFVGEVA-AKGENYWGGTKANLRNHLRKAGYETYEASVSALASNHER  108

Query  66   AVELYYYIKGGRVDYGAAHAAKYGHKRYGRTYEGIMPDWEPGKKIHLVGHSMGGQTIRLM  125
            AVELYYY KGGRVDYGAAH  KYGH RYG TYEG++ DW PG  +H +GHSMGGQTIRL+
Sbjct  109  AVELYYYLKGGRVDYGAAHSEKYGHERYGKTYEGVLKDWKPGHPVHFIGHSMGGQTIRLL  168

Query  126  EHFLRNGNQEEIDYQRQYGGTVSDLFKGGQDNMVSTITTLGTPHNGTPAADKLGSTKFIK  185
            EH+LR G+  EI YQ Q GG +S+LFKGGQDNMV  ITT  TPHNGT A D  G T  I
Sbjct  169  EHYLRFGDKAEIAYQQQHGGIISELFKGGQDNMVTSITTIATPHNGTHASDDIGNTPTIR  228

Query  186  DTINRIGKIGGTKALDLELGFSQWGFKQKPNESYAEYAKRIANSKVWETEDQAVNDLTTA  245
            +                + G  +WGFK K  ES  +Y KRIA SK+W+ ED    DLT
Sbjct  229  NILYSFAQMSSHLG-TIDFGMDHWGFKRKDGESLTDYNKRIAESKIWDSEDTGLYDLTRE  287

Query  246  GAEKLNQMTTLNPNIVYTSYTGAATHTGPLGNEVPNI-RQFPLFDLTSRAIGGDDNKNVR  304
            GAEK NQ T LNPNI Y  YTG ATH   LG  + +   +F    LT   IG  D+   R
Sbjct  288  GAEKINQKTELNPNIYYKTYTGVATHETQLGKHIADLGMEFTKI-LTGNYIGSVDDILWR  346

Query  305  VNDGIVPVSSSLHPSDEAFKKVGM-MNLATDKGIWQVRPVQYDWDHLDLVGLDTTDYKRT  363
             NDG V   SS HPSDE  K +    N    KG WQV P    WDH D +G D  D K
Sbjct  347  PNDGLVSEISSQHPSDE--KNISVDENSELHKGTWQVMPTMKGWDHSDFIGNDALDTKHS  404

Query  364  GEELGQFYKSMINNMLKVEELDG  386
              EL  FY S  + ++ +E  +
Sbjct  405  AIELTNFYHSISDYLMRIEKAES  427
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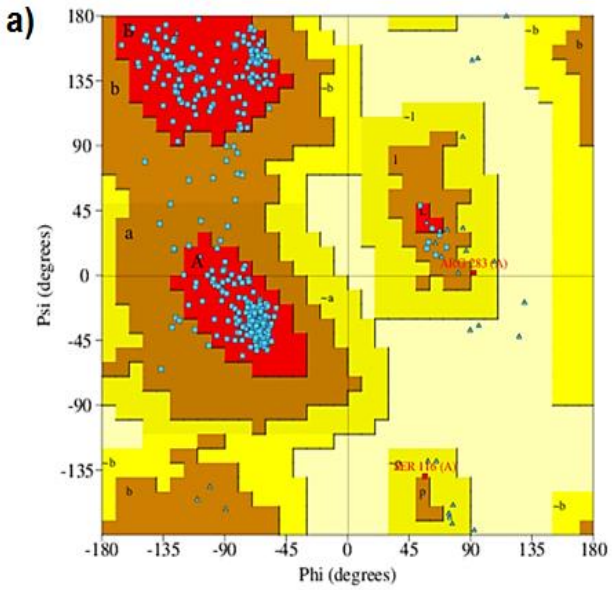
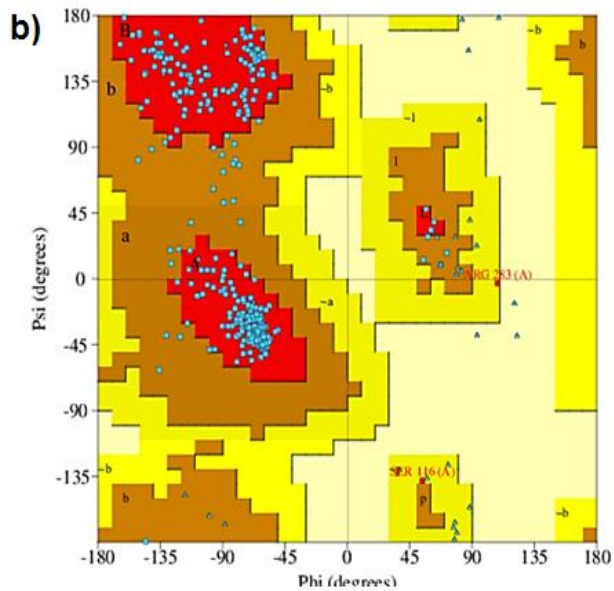
Figure S2. Ramachandran plot of a) rT-M386 b) G210C predicted models. Color are represented as follows; most favored region (red), additional allowed region (brown), generously allowed region (yellow) and disallowed region (white).



1. Ramachandran Plot statistics

		No. of residues	%-tage
Most favoured regions	[A,B,L]	293	89.3%*
Additional allowed regions	[a,b,l,p]	33	10.1%
Generously allowed regions	[~a,~b,~l,~p]	2	0.6%
Disallowed regions	[XX]	0	0.0%
Non-glycine and non-proline residues		328	100.0%
End-residues (excl. Gly and Pro)		1	
Glycine residues		43	
Proline residues		14	
Total number of residues		386	



1. Ramachandran Plot statistics

		No. of residues	%-tage
Most favoured regions	[A,B,L]	298	90.6%
Additional allowed regions	[a,b,l,p]	29	8.8%
Generously allowed regions	[~a,~b,~l,~p]	2	0.6%
Disallowed regions	[XX]	0	0.0%
Non-glycine and non-proline residues		329	100.0%
End-residues (excl. Gly and Pro)		1	
Glycine residues		42	
Proline residues		14	
Total number of residues		386	

Figure S3. Calcium binding site of a) rT-M386 b) G210C and **Zinc binding site of** c) rT-M386 d) G210C. The distances (Å) between each interaction are as indicated in the diagram. Figures are generated using the PDBsum (http://www.ebi.ac.uk/pdbsum).

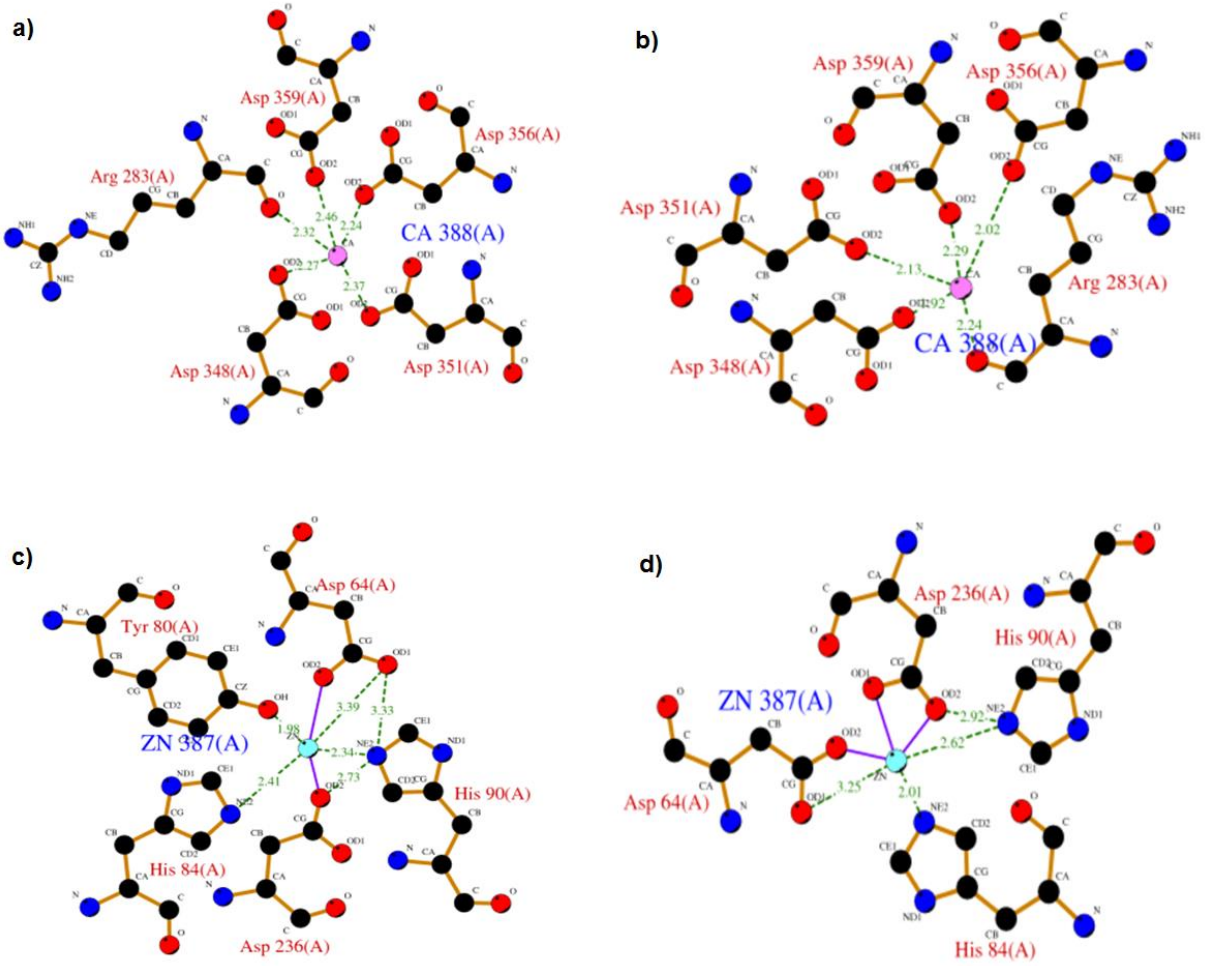


Figure S4. NetSurP results for a) rT-M386 and b) G210C. Residue 210 is highlighted in grey and the RSA value is shown in the box. Results are generated using NetSurP-2.0 (http://www.cbs.dtu.dk/services/NetSurfP/)