Supplementary Appendix

This appendix has been provided by the authors to give readers additional information about their work.

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Supplementary Appendix

Acquired resistance to KRAS G12C inhibition in cancer

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SUPPLEMENTARY METHODS

Cell lines and KRAS^{G12C} inhibitors: 293T cells were from ATCC and cultured in DMEM with 10% FBS. The Ba/F3 cell line is a murine pro-B-cell line that was acquired from DSMZ (# ACC-300) and cultured in RPMI 1640 with 10% FBS and 10 ng/ml of murine IL3 (PeproTech; #213-13), except as otherwise indicated in the context of the screen. Ba/F3 cells require exogenous IL3 for survival at baseline; however, ectopic expression of oncogenes can confer IL3-independent proliferation and survival. MRTX1257 was provided by Mirati. The adagrasib (MRTX849) and sotarasib (AMG510) were purchased from MEDCHEM EXPRESS (# HY-130149 and HY-114277).

Individual plasmid mutagenesis and generation of Ba/F3 stable cell lines. QuikChange Lightning Site-Directed Mutagenesis Kit (Agilent; # 210519) was used to generate individual mutations from pMT025_KRAS^{G12C} plasmid template and sequences were confirmed by sanger sequencing. The mutant plasmids were transfected with packaging plasmids psPAX2 and pMD2.G in 293T cells and virus supernatant was harvested two days later. Ba/F3 cells were transduced by lentivirus with 8ug/ml DEAE-Dextran hydrochloride (Sigma Aldrich; # 30461) and puromycin selection was done at 1ug/ml 24 hour post viral infection to generate stable cell lines.

Consensus sequence of KRAS^{G12C} used as the template to generate the deep mutational scanning library: The open reading frame (ORF) of the KRAS4B reference sequence (NM_004985.5) was used as a template. Codon 12 (GGT) was mutated from Gly into Cys (TGT) and silent mutations were introduced at 6 wobble positions within 330-348. The final template DNA sequence for generation of the KRAS^{G12C} mutational scanning library is indicated below and the G12C and silent mutations are underlined:

ATGACTGAATATAAACTTGTGGTAGTTGGAGCTTGTGGCGTAGGCAAGAGTGCCTT
GACGATACAGCTAATTCAGAATCATTTTGTGGACGAATATGATCCAACAATAGAGG
ATTCCTACAGGAAGCAAGTAGTAATTGATGGAGAAACCTGTCTCTTGGATATTCTC
GACACAGCAGGTCAAGAGGAGTACAGTGCAATGAGGGACCAGTACATGAGGACTG
GGGAGGGCTTTCTTTGTGTATTTGCCATAAATAATACTAAATCATTTGAAGATATTC
ACCATTATAGAGAACAAATTAAAAGAGTTAAGGACTCTGAAGATGTACCCATGGTG
CTGGTCGGCAACAAATGTGATTTGCCTTCTAGAACAGTAGACACAAAACAGGCTCA
GGACTTAGCAAGAAGTTATGGAATTCCTTTTATTGAAACATCAGCAAAGACAAGACA
GGGTGTTGATGATGCCTTCTATACATTAGTTCGAGAAATTCGAAAACATAAAGAAAA
GATGAGCAAAGATGGTAAAAAGAAGAAAAAGAAGTCAAAGACAAAGTGTGTAATTA
TGTAG

Design and generation of KRAS^{G12C} deep mutational scanning library: To design a lentiviral library encoding all possible alleles with a single amino acid substitution in the KRAS^{G12C} backbone allele, we selected one codon for each of 19 missense mutations and one nonsense (stop) codon at each amino acid position of the open reading frame (ORF) of KRAS^{G12C}, using the reference sequence indicated above. In addition, we also designed synonymous mutations at every amino position for which silent changes could

be achieved with 2 or 3 nucleotide changes (n = 30 total silent mutations in the library). The starting variant library was synthesized at Twist BioScience as a pool of linear ORF fragments and was cloned into the pMT_025 vector (Addgene #158579). The resulting pooled plasmid DNA ORF variant library was sequenced via Illumina Nextera XT platform to determine the distribution of variants within the library. The final library contained 3704 total unique variants, with all amino acid positions represented except for codons at positions S65, E98, T158 of the protein. 293T viral packaging cells were transfected using TransIT-LT1 transfection reagent (Mirus Bio) with three plasmids: the pooled ORF pDNA library, a packaging plasmid containing gag, pol and rev genes (psPAX2, Addgene), and an envelope plasmid containing VSV-G (pMD2.G, Addgene). Media was changed 6-8 hours after transfection and virus was harvested 24 hours thereafter.

Deep mutational scanning screen for $KRAS^{G12C}$ resistance mutations in Ba/F3 cells. Deep mutational scanning is an approach that utilizes massively parallel sequencing to simultaneously measure the functional impact of many variants in a protein in a single experiment.[1-3] To perform deep mutational scanning of the $KRAS^{G12C}$ protein, we utilized the above described lentiviral library encoding nearly all possible alleles with a single amino acid substitution in the $KRAS^{G12C}$ backbone allele. A positive-selection screen for mutations in $KRAS^{G12C}$ that confer resistance to $KRAS^{G12C}$ inhibition was performed in Ba/F3 cells cultured for 7 days in the absence of IL3 and in the presence of one of two $KRAS^{G12C}$ inhibitors, MRTX1257 (a compound highly related to adagrasib)[4] or sotorasib. Briefly, Ba/F3 cells were cultured in RPMI medium with 10% FBS and 10 ng/ml of murine IL3 were mixed with 8ug/ml DEAE-Dextran hydrochloride and the lentiviral mutagenesis library at a multiplicity of infection (MOI) of around 0.14 in 12 well plates and spin-infection was performed at 2000 rpm for 2 hours at 30°C. Ba/F3 cells were transduced with this library at a representation of over 1000 cells per allele in triplicate. New media was added and the plates were incubated overnight at 37°C, 5% CO_2. On the following day, cells were washed with PBS and changed into IL3 medium with 1ug/ml puromycin. After two days with puromycin selection, cells were harvested at full representation as the IL3 arm. The remaining cells were washed with PBS and changed into culture medium without IL3. Two days after IL3 removal, cells were divided into three arms and treated with DMSO, MRTX1257 at 20 nM or sotorasib at 800 nM. Medium with each drug or DMSO was changed every three days. Cells were harvested after 6 days of drug treatment for genomic DNA isolation, library preparation and deep sequencing.

Nextera sequencing and data processing. Genomic DNA was harvested for each time point in the screen and alleles were PCR amplified. PCR reactions were set up in 96-well plates using two primers: Forward: 5'-ATTCTCCTTGGAATTTGCCCTT-3'; Reverse: 5'-CATAGCGTAAAAGGAGCAACA-3'. and Q5 DNA polymerase (New England Biolabs). All PCR reactions for each gDNA sample were pooled, concentrated with a PCR cleanup kit (QIAGEN), and separated by gel electrophoresis. Bands of the expected size were excised and DNA was purified using a QIAquick kit (QIAGEN) followed by an AMPure XP kit (Beckman Coulter). Nextera reactions were performed according to the Illumina Nextera XT protocol and sequenced using an Illumina Nextseq flowcell at a depth

corresponding to a sample average of 1300 perfectly mapping reads for each individual library variant. The reads were processed with a second-generation variant calling software called AnalyzeSaturationMutagenesis (as part of GATK, downloadable at (https://github.com/broadinstitute/gatk/releases). Raw read pairs were aligned to the ORF reference sequence and those that exactly matched to library variant sequences (perfect throughout both paired reads) were used to count the reads attributable to each variant.

Variant analysis from deep mutational scanning screen: Reads were aligned to KRAS reference sequence and collapsed to reads per amino acid at each position and for each variant amino acid. Abundance of each variant was calculated by the fraction of its read compared to the total reads of all variants in each sample. Log2 Fold Change was the fold change between reads from Day 6 compared to Day 0 before IL3 removal. Log2 Fold Change data for each allele were imported in R (version 4.0.2) and were then Z-score normalized independently for each arm representing the abundance of each allele at the endpoint of the drug-treated arms compared with the early pretreatment time point. Relative enrichment was plotted in relation to the primary amino acid sequence of the $KRAS^{G12C}$ protein. The heatmaps were generated using the pheatmap R package (https://cran.r-project.org/web/packages/pheatmap/index.html).

Z-score threshold for resistance: To identify the alleles inducing resistance to each of the $KRAS^{G12C}$ inhibitors in the screen, we used as cutoff values the average Z-score + 2 standard deviations of all the silent mutations in each treated arm. The cutoff values for resistance to both inhibitors were a Z-score of 1.25 for MRTX1257 and 1.5 for sotorasib.

Drug response curves for $KRAS^{G12C}$ inhibitors and validation of resistance mutations: Ba/F3 cells were seeded at 1000 cells/well in 96-well plates (Corning; # 3903) and directly treated with $KRAS^{G12C}$ inhibitors by adding adagrasib (0.1nM to 10μM) or sotorasib (1nM to 10μM) with a Tecan D300e drug dispenser. Viability was assessed 5 days post-treatment using the CellTiter-Glo 2.0 (Promega; # G9242) on a FLUOstar Omega microplate reader according to the manufacturer's protocol. Percentage viability was calculated by normalizing treated wells to DMSO treated control samples. Curves were fit with nonlinear sigmoid functions, forcing the low-concentration asymptote to 100% viability to represent the DMSO control treatment using a four-parameter curve in GraphPad Prism.

Calculation of IC50, AUC and relative resistance score: The IC_{50} values for each drug were determined with GraphPad Prism using a four-parameters drug response curve. Viability data for each allele with each inhibitor were imported in R (version 4.0.2) and treated with the nplr R package (https://cran.r-project.org/web/packages/nplr/index.html) to calculate the AUC of the fitted curves. The relative resistance score (RRS) for each allele were generated through the scaling of all the AUC values between the AUC values of $KRAS^{G12C}$ and $KRAS^{G12R}$, using the following formula:

$$\text{Relative Resistance Score} = \frac{(AUC\ of\ allele - AUC\ of\ KRAS\ G12C)}{(AUC\ of\ KRAS\ G12R - AUC\ of\ KRAS\ G12C)}$$

G12C serves as a sensitive control with an RRS of 0, and G12R is the strongest resistance mutation in the validation list with an RRS of 1.

Mapping of phenotypic data onto structures:

Mapping and graphical display of phenotypic data from the deep mutational scanning experiments onto KRAS crystal structures were performed with the UCSF Chimera package. Phenotypes were mapped using the 'define by attribute' and 'render by attribute' functions of the program. For each amino acid position in the structure, we indicated degree of maximal resistance phenotype per position and indicated the z-score of that Log-(2)-fold-change as an intensity of the color red. The number of substitutions producing resistance phenotypes above the Z score threshold defined above (2 standard deviations above from the average z-score of silent mutations: 1.25 for MRTX1257 and 1.5 for sotorasib) were represented as a gradient using 0.25 to 2 width of the worm size representing 2 to 19 substitutions scoring at that position. Phenotypes were mapped onto PDB 6UT0[5] (illustrating KRAS bound to analogue compound adagrasib) for MRTX1257 resistant mutations and PDB 6OIM [6] for sotorasib resistant mutations.

Immunoblotting. Cells were lysed in RIPA Lysis and Extraction Buffer (Life Technologies; # 89900) with Halt Phosphatase Inhibitor Cocktail (Life Technologies; #78420) and Halt Protease Inhibitor Cocktail (Life Technologies; # 87785) and lysates were run on NuPAGE™ 10%, Bis-Tris, 1.5 mm, Mini Protein Gel (Life Technologies; # NP0316BOX). Experiments were done at least three repeats for each line. The antibodies used from Cell Signaling Technology were phospho-p44/42 MAPK (#4370S), p44/42 MAPK (#4695), phospho-Akt (Ser473) (#4060), Akt (#9272), phospho-S6 (Ser240/244) (#2215), S6 (5G10) (#2217) and Vinculin (#4650S). Anti-KRAS rabbit polyclonal antibody was from Proteintech (# 12063-1-AP).

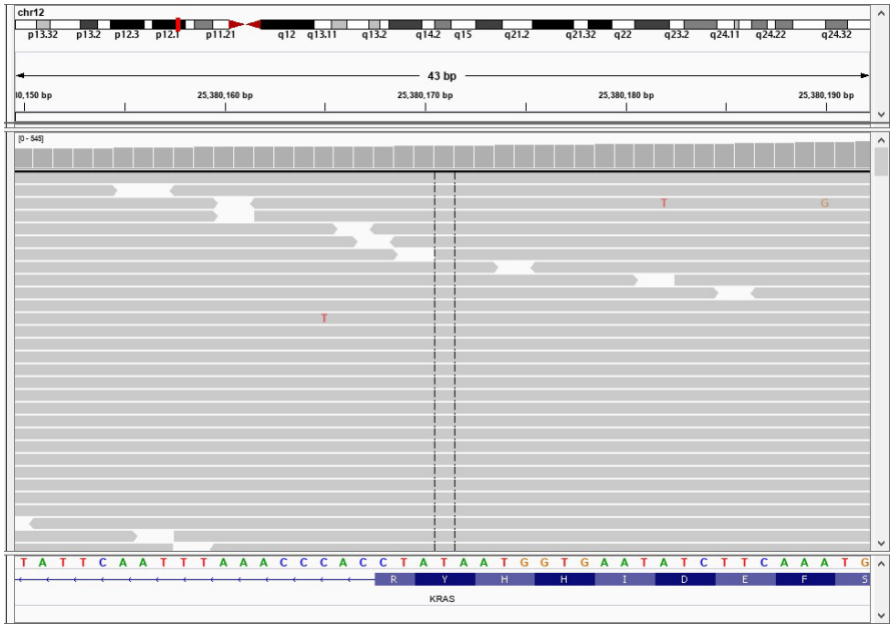
Fluorescence In-Situ Hybridization (FISH). FISH analysis was performed on formalin-fixed paraffin-embedded (FFPE) tissue. The slide was baked overnight at 50°C, deparaffinized, and rehydrated through a graded ethanol series. The sample underwent pretreatment and protease digestion using the Cytocell Tissue Pretreatment Kit, followed by dehydration through a graded ethanol series. Following the addition of Empire Genomics' KRAS/CEN12 probe, the sample was denatured and hybridized overnight. After post-hybridization washing, the slide was counterstained with 4′,6-diamidino-2-phenylindole (DAPI). FISH images were captured using a 60x oil objective (BZ-X800 fluorescent microscope, Keyence).

FoundationOne Liquid CDx. NGS of ctDNA was performed on ≥ 20ng of ctDNA extracted from blood plasma to create adapted sequencing libraries before hybrid capture and sample-multiplexed sequencing to a median unique exon coverage depth of >6,000X for up to 70 genes.[7] Results were analyzed for base substitutions, short insertions and deletions (indels), copy number alterations, and rearrangements. Testing was performed in a CLIA-certified/CAP-accredited laboratory (Foundation Medicine Inc., Cambridge, MA).

Figure S1

A

Pretreatment



B

Resistance to adagrasib

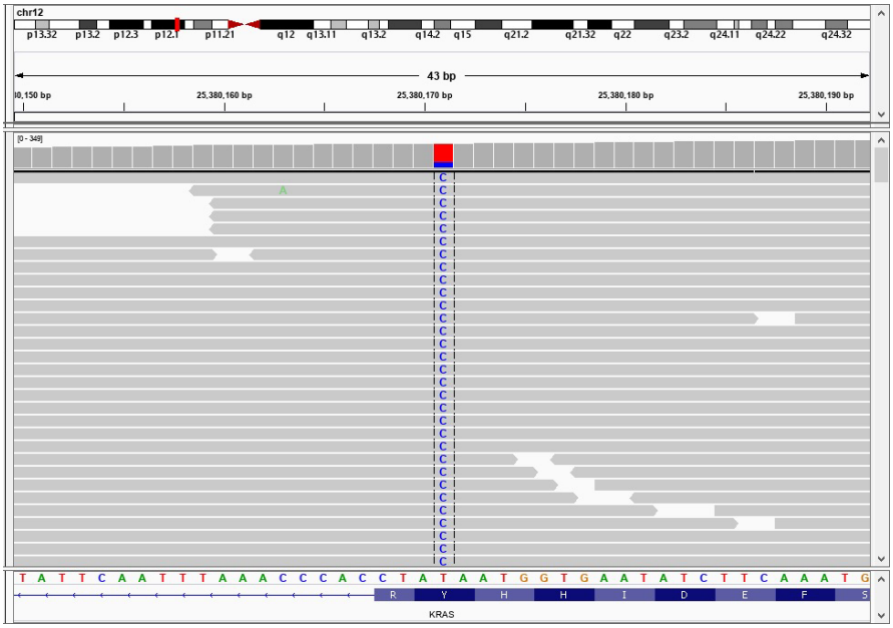


Figure S1. Y96C alignments in IGV for Case 1. Integrative Genomics Viewer (IGV) plots of *KRAS* DNA sequence encoding amino acid position 96 from the (**A**) pretreatment and (**B**) adagrasib-resistant samples for case 1. Antisense readings are shown demonstrating the TAT to TGT (Y96C) mutation identified after resistance.

Figure S2

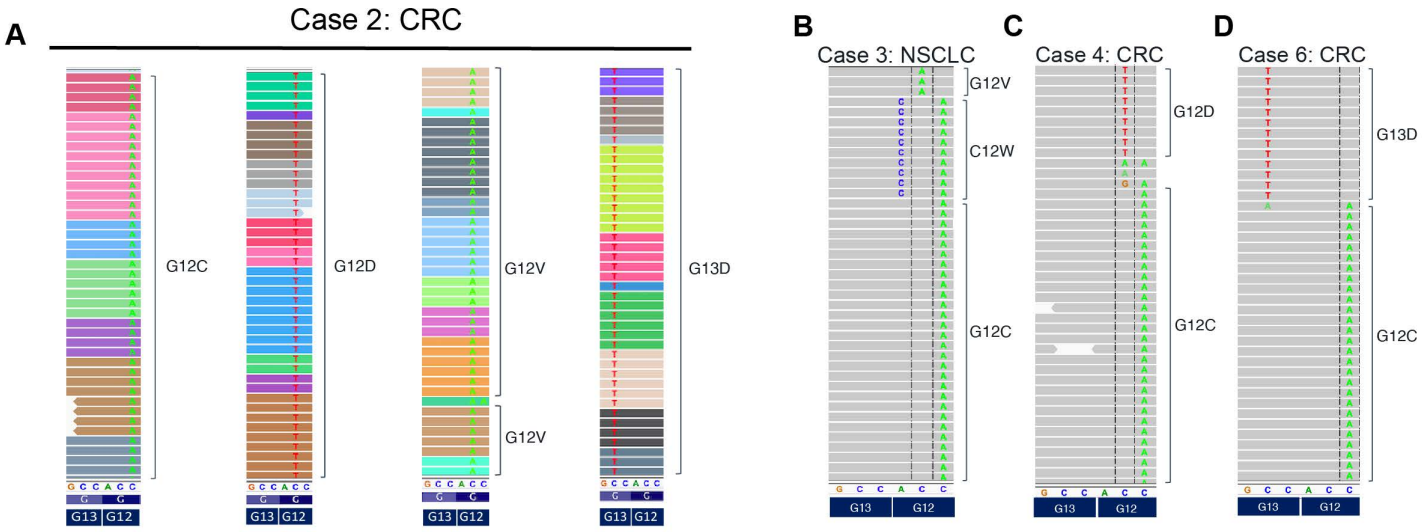


Figure S2. Cis/trans status for selected *KRAS* mutations at codons 12 and 13. Integrative Genomics Viewer (IGV) plots (antisense reading) of *KRAS* codons 12 and 13 showing the cis/trans (same sequence read vs. different sequence read) status of acquired mutations for (**A**) case 2, (**B**) case 3, (**C**) case 4, and (**D**) case 6. Case 2 demonstrates the GGT to TGT mutation (encoding for G12C), the GGT to GAT mutation in trans (encoding for G12D), the GGT to GTT mutation in trans (encoding for G12V) and the GGC to GAC mutation in trans (encoding for G13D). In addition, sequence reads from case 2 also demonstrated a G12R (c.34G>C) mutation, although it could not be determined whether this arose through a c.34_36 GGT (Gly) to CGT (Arg) mutation or a TGT (Cys) to CGT (Arg) mutation (data not shown, Table S1). Case 3 demonstrates the TGT to TGG mutation in cis, resulting in a C12W mutation (noted as G12W in reference to the wild type KRAS sequence) and the GGT to GTT mutation in trans (encoding for G12V). Cases 4 and 6 show a G12D and G13D mutation in trans, respectively.

Figure S3

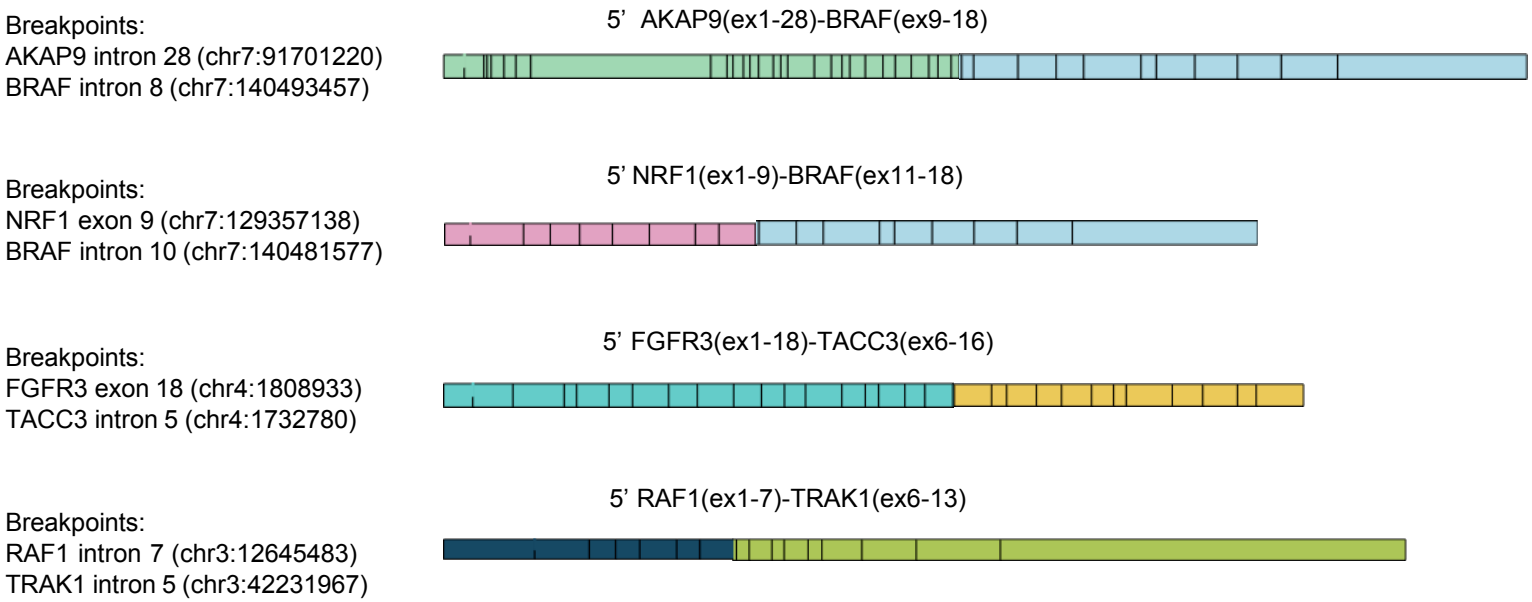


Figure S3. Schematic of selected gene fusions identified in case 6. Schematic depictions are shown for several chromosomal rearrangements identified in case 6 (CRC) through FoundationOne Liquid testing. Analysis based on the hg19 reference human genome assembly.

Figure S4

A

SPECIMEN:

1. FFPE Block A1
2. Approximate Tumor %: 30

DIAGNOSIS:

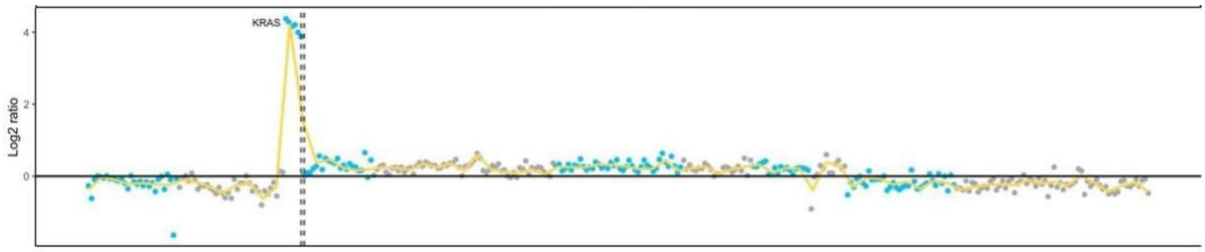
1. Poorly-differentiated non-small cell carcinoma, consistent with adenocarcinoma

INTERPRETATION:

1. Tier I Variants (Strong Clinical Significance) identified:

GRCh37 Position	Gene	RefSeq	Variant (Coding)	Variant (Protein)	VAF (%)	COSMIC ID
12:25398285	KRAS	NM_004985.4	c.34G>T	p.G12C	39.4	COSM516

B



C

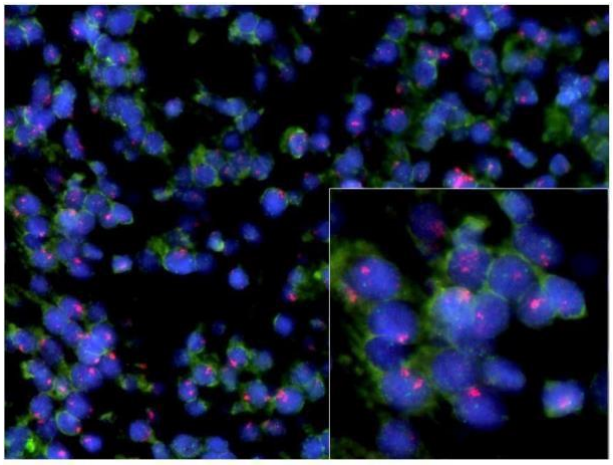


Figure S4. *KRAS*^{G12C} amplification at adagrasib resistance for case 7. (**A**) This de-identified pretreatment genomics report for case 7 demonstrates a tumor content of ~30% and a *KRAS*^{G12C} variant allele fraction (VAF) of 39.4%. The tissue had been exhausted and was not available for further analysis. (**B**) At adagrasib resistance, this DFCI OncoPanel copy plot indicated high-level focal *KRAS*^{G12C} amplification, with an estimated ~45 copies of the *KRAS*^{G12C} mutant allele (*KRAS*^{G12C} VAF was 95%). (**C**) Fluorescence in situ hybridization (FISH) evaluation of *KRAS* (performed at Boundless Bio) at adagrasib resistance shows intense, heterogeneous amplifications of *KRAS* in tumor cells (red), with both punctate and highly aggregated patterns present across the tissue; two normal copies of centromere 12 (green) were present in most nuclei, counterstained with DAPI (blue). The inset shows higher magnification.

Figure S5

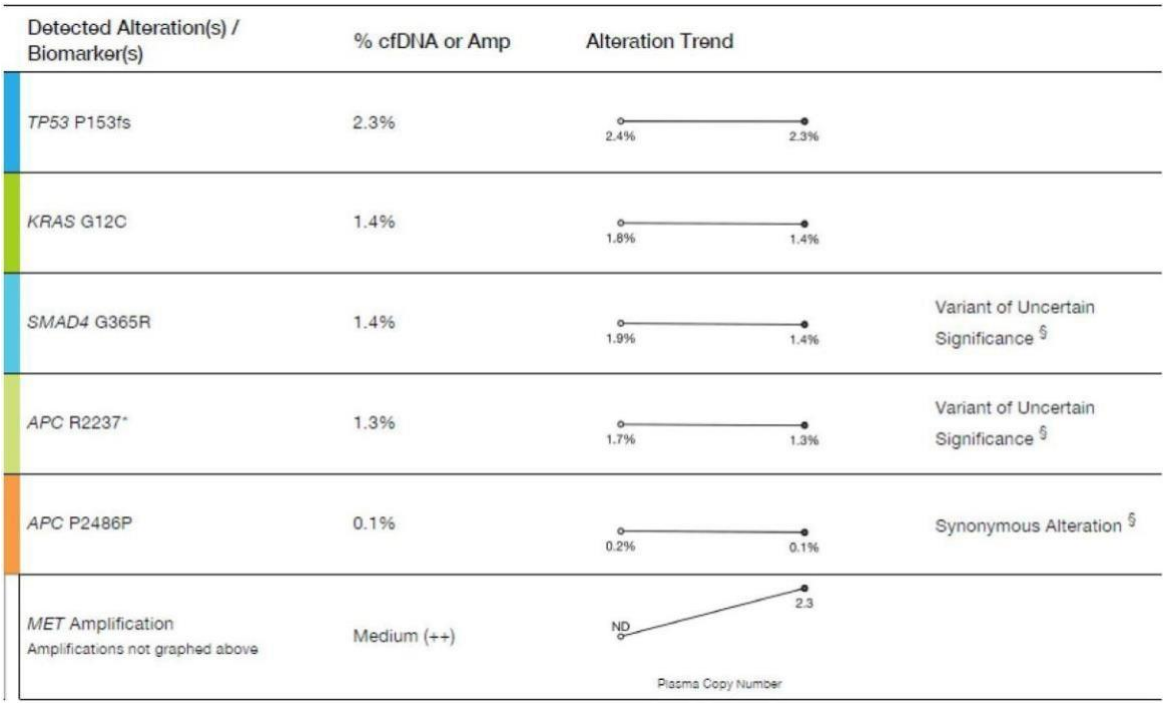


Figure S5. Acquired *MET* amplification in case 10. This de-identified Guardant360 circulating tumor DNA report shows acquired *MET* amplification as the only apparent genomic change between baseline prior to adagrasib initiation (left points on Alteration Trend lines) to the time of adagrasib resistance (right points on Alteration Trend lines).

Figure S6

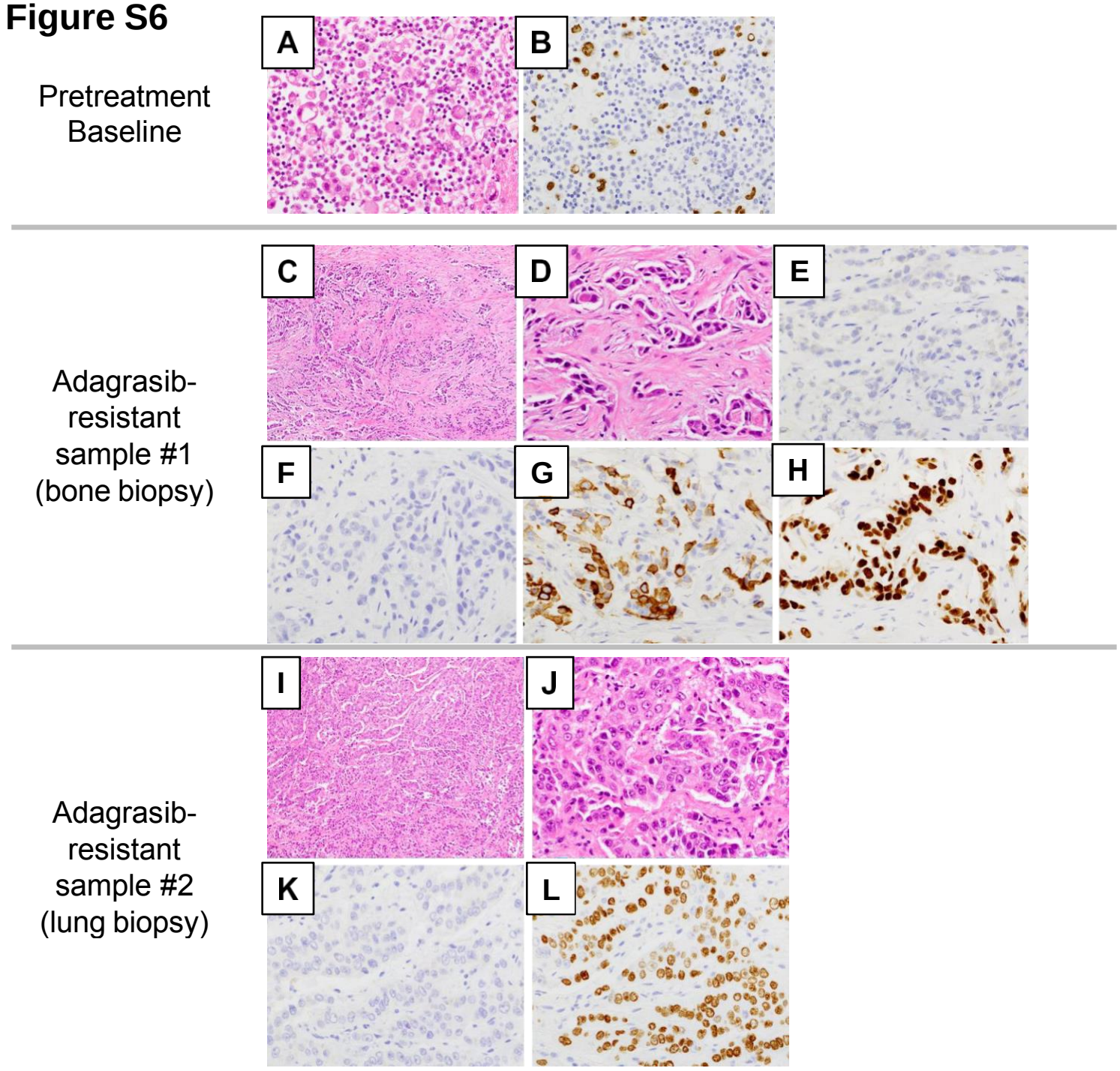


Figure S6. Lung squamous cell transformation observed in case 12. (**A**) Prior to adagrasib initiation, right pleural fluid contained scattered malignant cells consistent with adenocarcinoma in a background of reactive mesothelial cells and chronic inflammation (hematoxylin-eosin, 400× magnification). (**B**) Immunohistochemistry for TTF1 highlights the nuclei of the metastatic lung adenocarcinoma (400× magnification). (**C**) At time of adagrasib resistance, a right iliac wing core biopsy demonstrates groups of malignant cells amongst fibrous stroma (hematoxylin-eosin, 100× magnification). (**D**) At high magnification, tumor cells show a squamoid appearance with defined cell borders (hematoxylin-eosin, 400× magnification). By immunohistochemistry, tumor cells are negative for TTF1 (**E**) and Napsin A (**F**) but show multifocal staining for cytokeratin 5/6 (**G**) and strong diffuse staining for p40 (**H**), confirming the presence of squamous differentiation. (**I**) A right upper lobe lung biopsy at the time of adagrasib resistance demonstrates cohesive nests of malignant cells (hematoxylin-eosin, 100× magnification). (**J**) At high magnification, tumor cells show a poorly-differentiated non-small cell histology with conspicuous nucleoli (hematoxylin-eosin, 400× magnification). By immunohistochemistry, tumor cells are negative for TTF1 (**K**) and show diffuse strong staining for p40 (**L**), confirming squamous differentiation. All immunohistochemical stains (for TTF1, Napsin A, cytokeratin 5/6, and p40) were performed on routine automated diagnostic staining platforms.

Figure S7

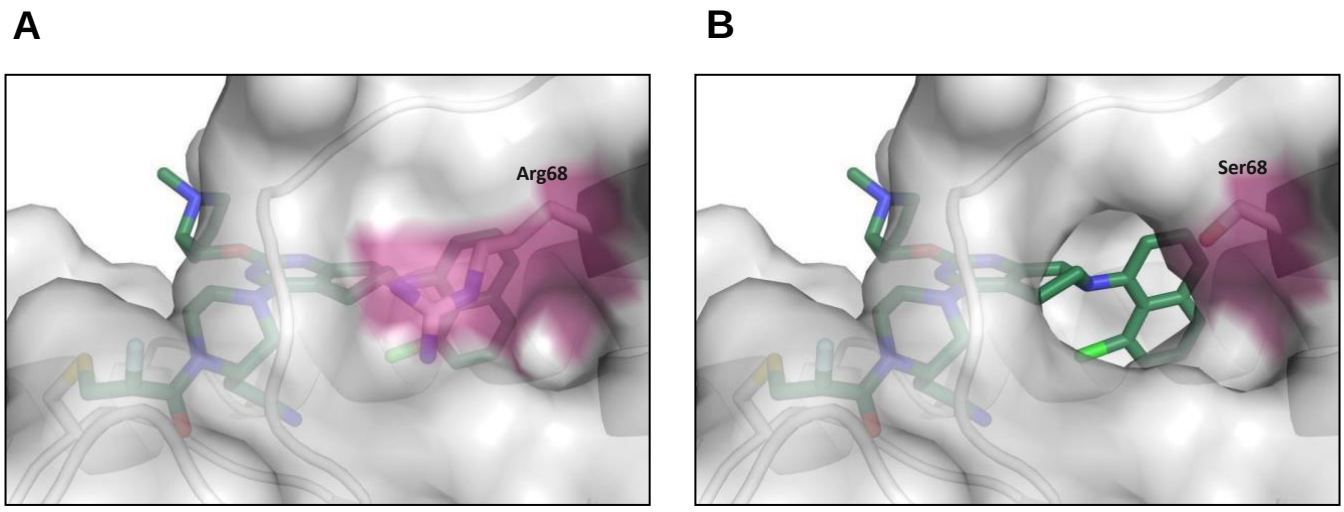


Figure S7. Structural basis of adagrasib resistance of KRAS R68S mutation. **(A)** A comparison of adagrasib (green sticks) bound to KRAS G12C (PDB code 6ut0) and (**B**) to a model of the G12C/R68S double mutant. The surface corresponding to residue 68 is highlighted in purple. The R68 sidechain packs against both the piperidine and naphthyl moieties of adagrasib. Mutation of the arginine residue to the smaller serine removes these favorable Van der Walls interactions and reduces shape complementarity to the Switch II pocket. Furthermore, R68 may play a role in maintaining the binding nascent conformation of the Switch II pocket through scaffolding effects anchored by hydrogen bonds to the backbone of residues A59 and Q61 (not shown).

Figure S8

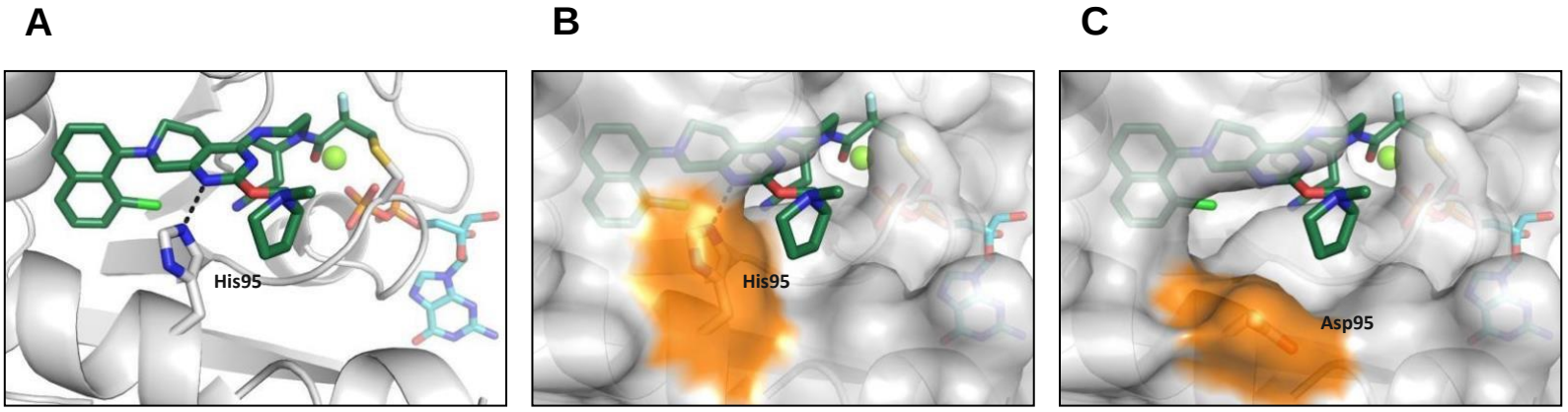


Figure S8. Structural basis of adagrasib resistance for the KRAS H95D mutation. (**A, B**) A comparison of adagrasib (green sticks) bound to KRAS G12C (PDB code 6ut0) and (**C**) to a model of the G12C/H95D double mutant. The surface corresponding to residue 95 is highlighted in orange. Mutation of the histidine residue to an aspartate disrupts a favorable hydrogen bond interaction to adagrasib's pyrimidine moiety (black dashed line in **A** and **B**). Asp95 (**C**) likely swings out of the binding site without being held in place with the hydrogen bond. This leads to an additional loss of binding energy via diminished shape complementarity of the Switch II pocket and loss of the scaffolding interaction with the pyrrolidine ring.

Figure S9

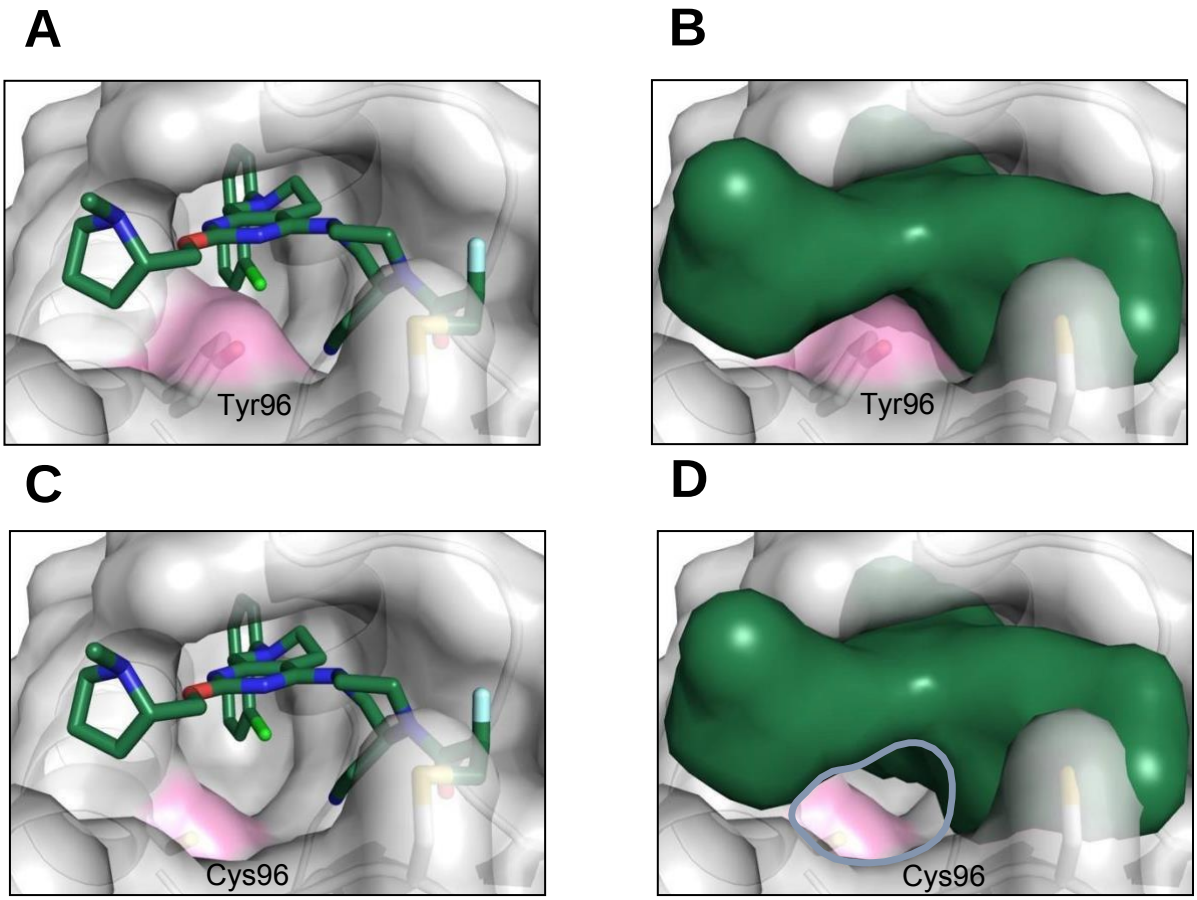


Figure S9. Structural basis of adagrasib resistance of KRAS Y96C mutation. A comparison of adagrasib (green sticks and surface) bound to KRAS G12C (PDB code 6ut0) (panels **A** and **B**) and to a model of the G12C/Y96C double mutant (panels **C** and **D**). The surface corresponding to residue 96 is highlighted in pink. Mutation of the much larger tyrosine to a cysteine in the bottom of the Switch II pocket creates a cavity (highlighted by the grey line in panel **D**) that removes a substantial amount of Van der Walls interaction energy including an edge/face interaction between the tyrosine and the pyrimidine moiety of adagrasib.

Figure S10

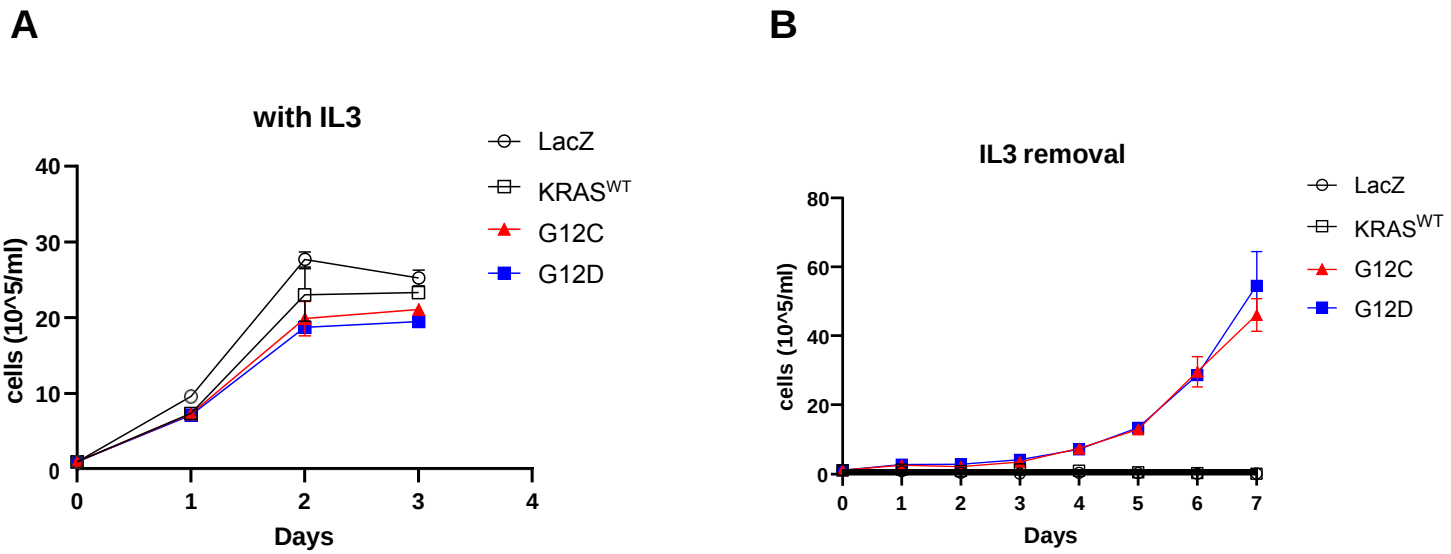


Figure S10. KRAS^{G12C} mediates IL3-independent survival of Ba/F3 cells. Ba/F3 cells were lentivirally transduced with LacZ, KRAS^{wt}, KRAS^{G12C} or KRAS^{G12D} and were cultured in 6-well plates in the presence (**A**) or absence (**B**) of IL3. Cell number was counted daily. The curves were shown as mean ± SEM from three independent experiments. The cells reached maximum density on day 3 with IL3 (A).

Figure S11

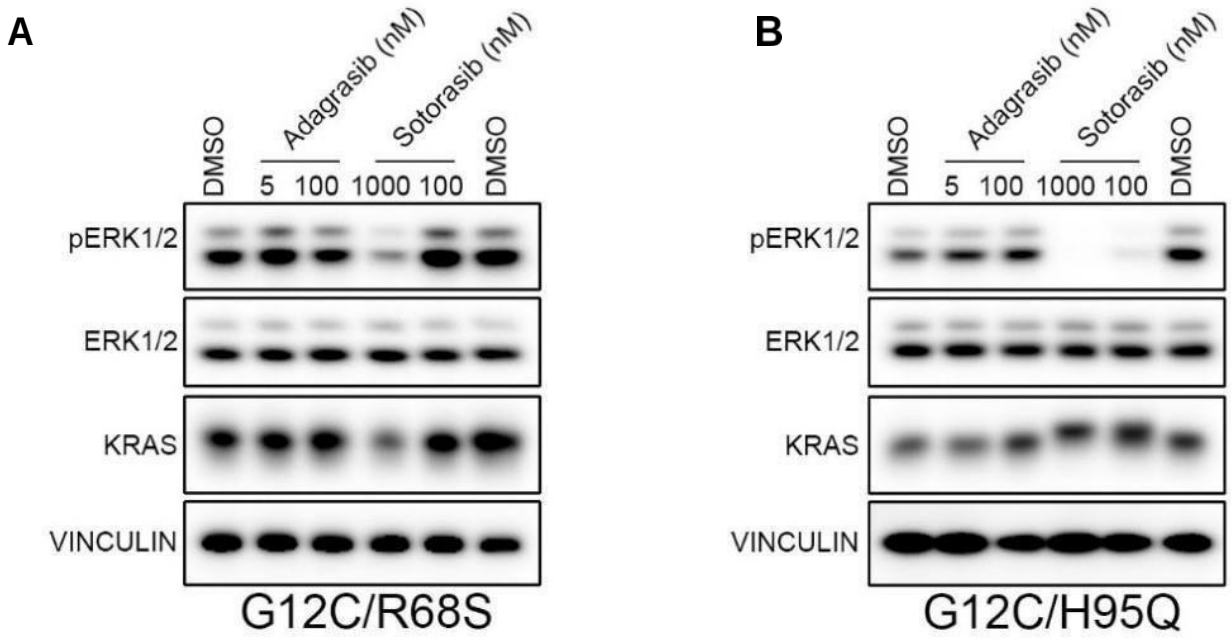


Figure S11. Immunoblot results for G12C/R68S and G12C/H95Q treated with KRAS^{G12C} inhibitors. Ba/F3 cells expressing KRAS$^{G12C/R68S}$ (**A**) or KRAS$^{G12C/H95Q}$ **(B)** were treated with adagrasib or sotorasib for 6 hours and immunoblots were performed to assess the ERK phosphorylation and total KRAS protein levels.

Figure S12

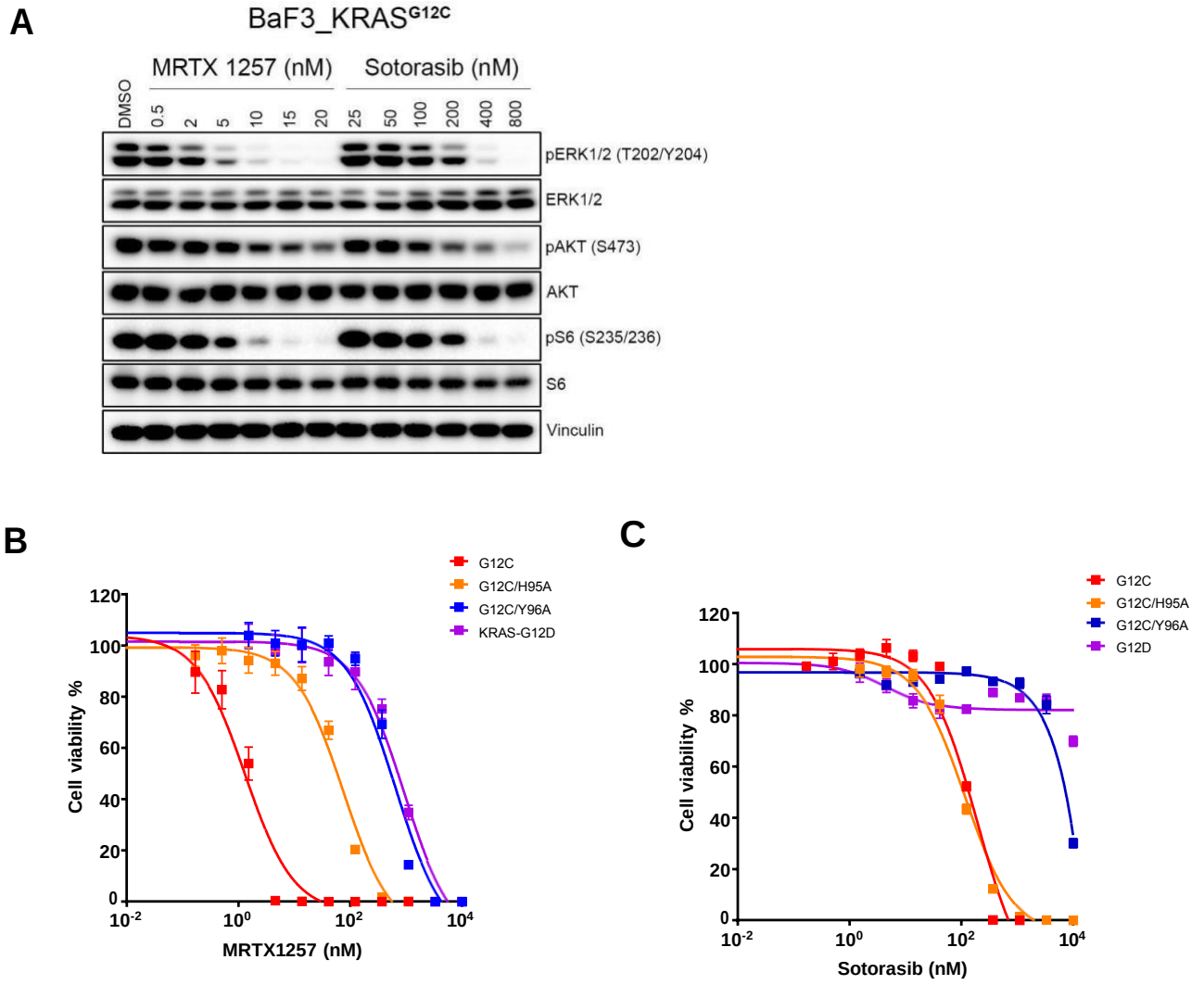


Figure S12. Optimization of KRAS^{G12C} inhibitor doses for the mutagenesis screen in Ba/F3 cells. (**A**) Ba/F3_KRAS^{G12C} cells were treated with indicated concentrations of MRTX1257 or sotorasib for 6 hours and KRAS effector signaling pathways were assessed by immunoblot. The drug response curves for MRTX1257 (**B**) and Sotorasib (**C**). Ba/F3 cells expressing the indicated alleles of KRAS^{G12C}, KRAS$^{G12C/H95A}$, KRAS$^{G12C/Y96A}$ or KRAS^{G12D} were seeded into 96-well plates and treated with increasing doses of (B) MRTX1257 or (C) sotorasib for 5 days and analyzed by CellTiter-Glo assays. Based on these data, MRTX1257 at 20 nM and sotorasib at 800nM was used in the screen.

Figure S13

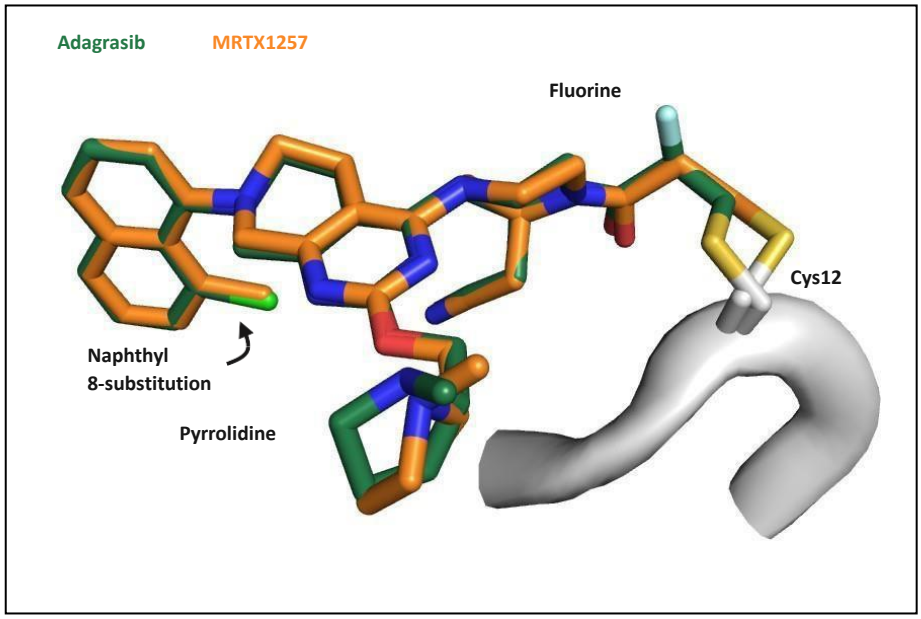


Figure S13. Structural comparison of adagrasib and MRTX1257. An overlay of adagrasib (PDB code 6ut0) and MRTX1257 bound to KRAS G12C. During the optimization of MRTX1257 to adagrasib, the 8-methyl group of the naphthyl was replaced with a chlorine and a fluorine was added to the acrylamide. Neither feature substantially changes the molecular interactions with the protein, and we believe that resistance mutations that affect MRTX1257 would have similar effects against adagrasib. This hypothesis is supported by the overlay of the two crystal structures as the only variations are a slight change in the position of the pyrrolidine moiety and the orientation of the covalent bond to Cys12. Both are commonly observed heterogeneities in this crystallographic system, observed across (and within) several related co-crystal structures over the course of the program.

Figure S14

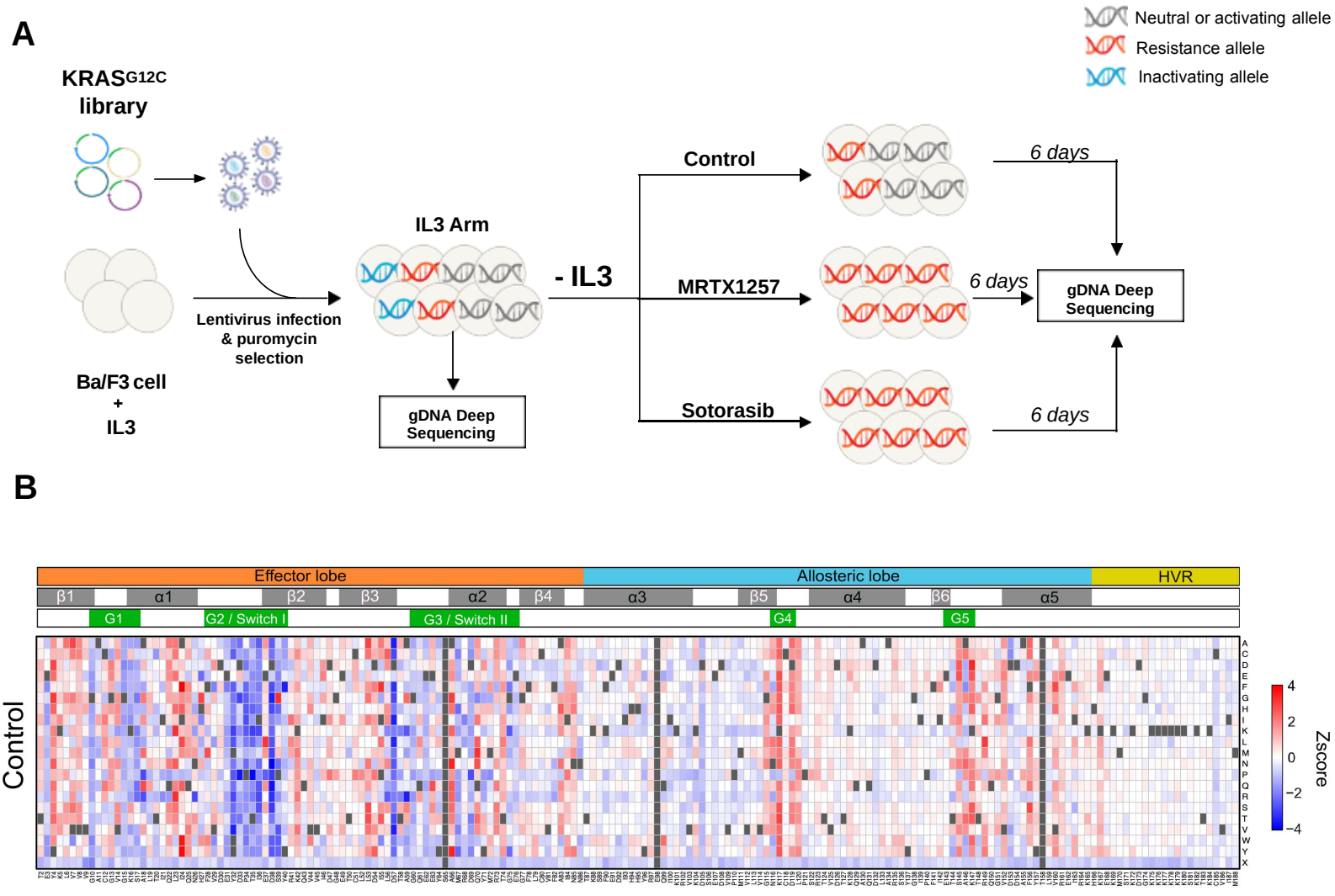


Figure S14. The workflow of KRAS^{G12C} deep mutational scanning screen in Ba/F3 cells. (**A**) Screen workflow. Parental Ba/F3 cells were first cultured with mIL3 and then transduced with the KRAS^{G12C} mutagenesis lentiviral library followed by puromycin selection. Some cells were harvested immediately after puromycin selection to establish the full representation of the alleles in the library at an early IL3-treated time point ("IL3 arm") and to use this time point as a baseline for allele abundance in comparison to drug-treated endpoints. Next, the remaining cells were changed into mIL3-free medium. Cells that survived in the absence of mIL3 (only cells with oncogenic G12C alleles) were further divided into three arms of the screen: 1) DMSO control arm; 2) MRTX1257 arm treated with 20 nM of MRTX1257; 3) Sotorasib arm treated with 800 nM of Sotorasib. There were three replicate samples for each arm. (**B**) Z-scores of DMSO control arm were shown as a heatmap. The red indicated enrichment while the blue indicated depletion of alleles after IL3 removal, which suggest increase or decrease of KRAS^{G12C} activity by these mutations, respectively.

Figure S15

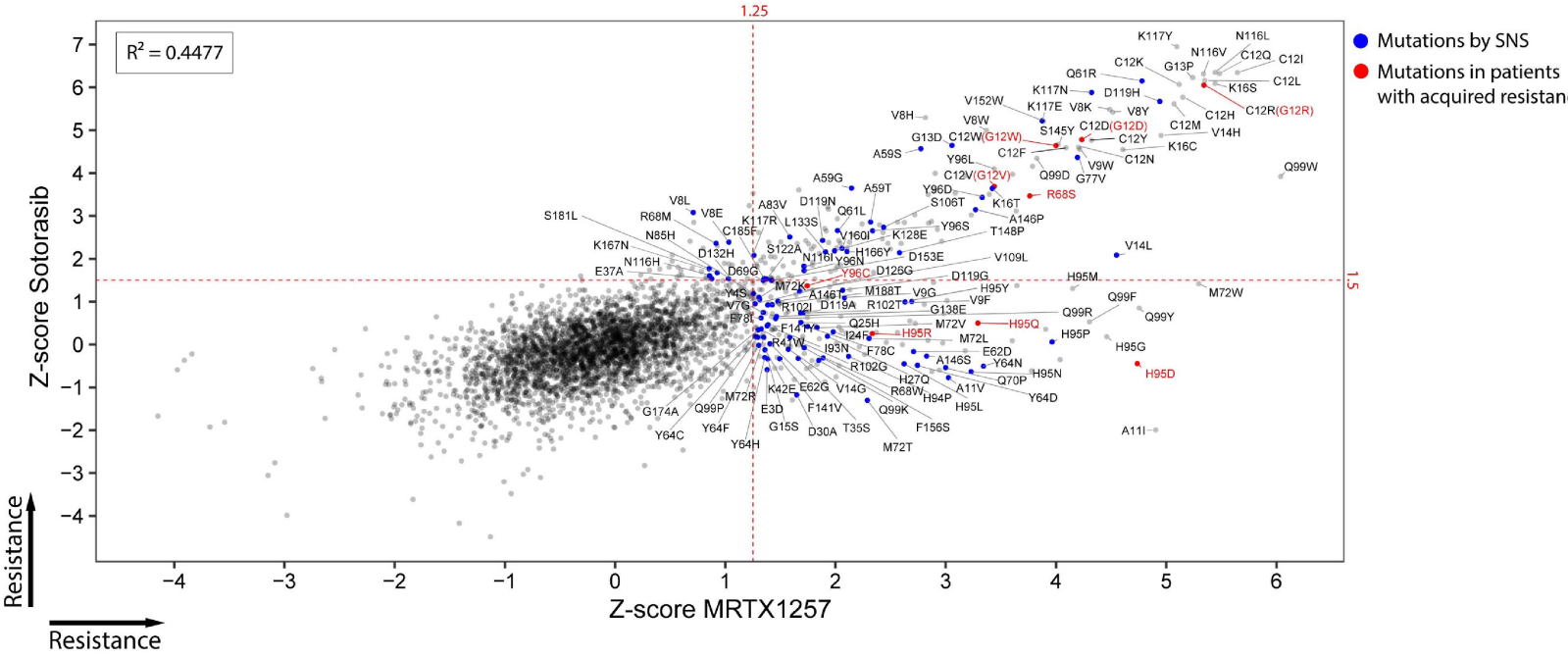


Figure S15. The correlation of Z-scores from the MRTX1257- and sotorasib-treated arms. Scatter plot showing the Z-scores for mutations from the sotorasib resistance screen (y-axis) versus the Z-scores from screen with the adagrasib-related compound MRTX1257 (x-axis). The blue dots indicate putative resistance mutations arising from a single nucleotide substitution (SNS), the most common mechanism of missense mutation in human cancers. Red dots mark the clinically identified mutations in patients with acquired resistance to adagrasib.
Dotted red lines indicate a threshold for statistical significance of resistance alleles, defined as the mean + 2 standard deviations (SD) of the Z-scores for all negative control silent mutations in each treated arm of the screen. At this Z-score threshold, 95/298 MRTX1257-resistance mutations and 41/164 sotorasib-resistance mutations could occur by single nucleotide substitution.

Figure S16

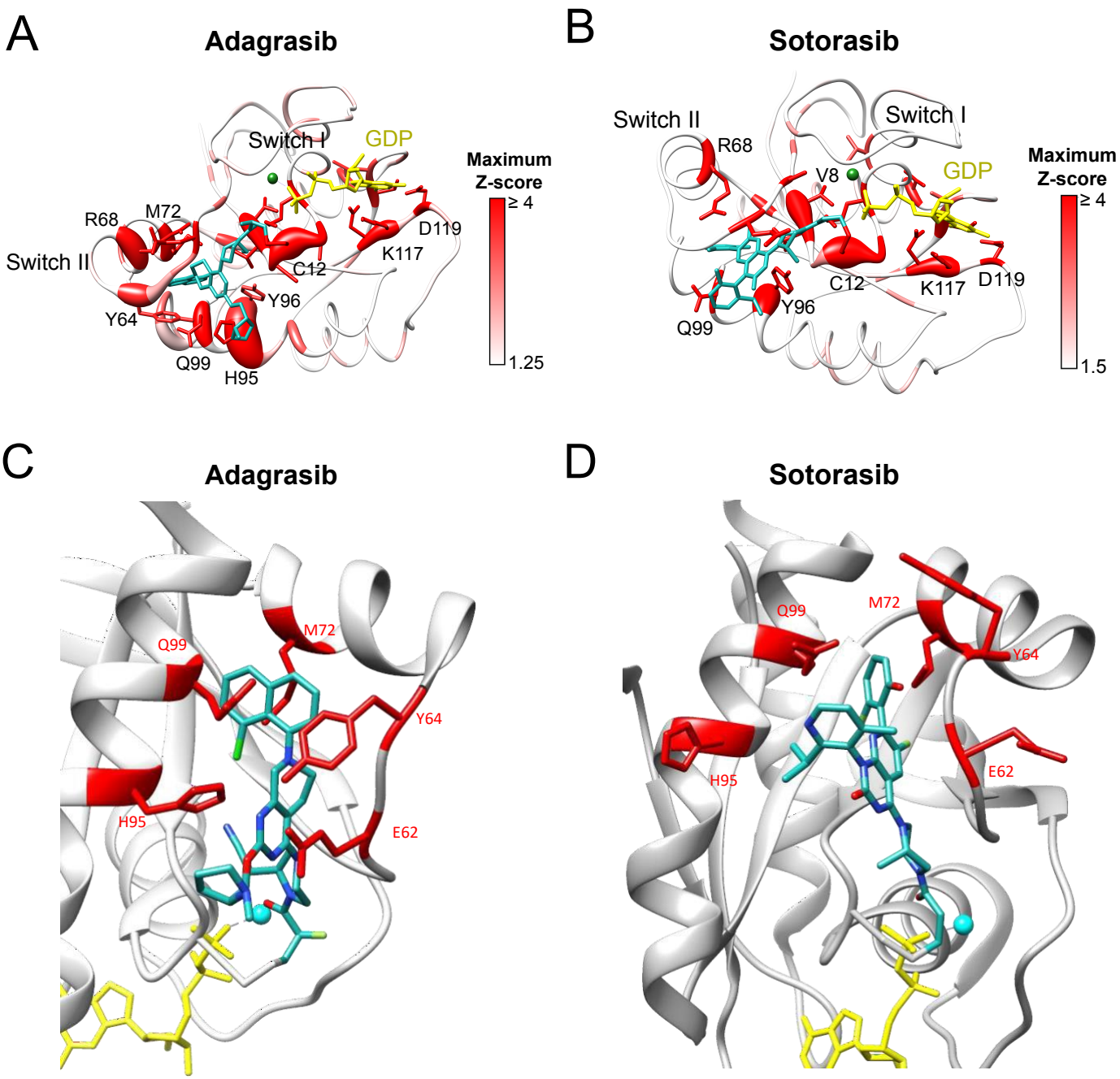


Figure S16. Structural mapping of deep mutational scanning results identifying on-target resistance mutations to KRAS^{G12C} inhibitors. (A-B) Putative second-site resistance mutations identified in the deep mutational scanning screen indicated in Figure 5 were mapped onto crystal structures of KRAS^{G12C} bound to adagrasib **(A)** or sotorasib **(B)**. Maximum Z-score at each position (most resistant allele) is indicated by the degree of red coloration and the size of each position corresponds to the number of mutations scoring as resistant in the screen **(Supplementary Methods, Table S3)**. **(C-D)** Conformation difference in the binding sites of adagrasib **(C)** and sotorasib **(D)**. Side chains of E62, Y64, M72, H95 and Q99 residues in KRAS^{G12C} are represented in red sticks in each binding sites for adagrasib and sotorasib.

Figure S17

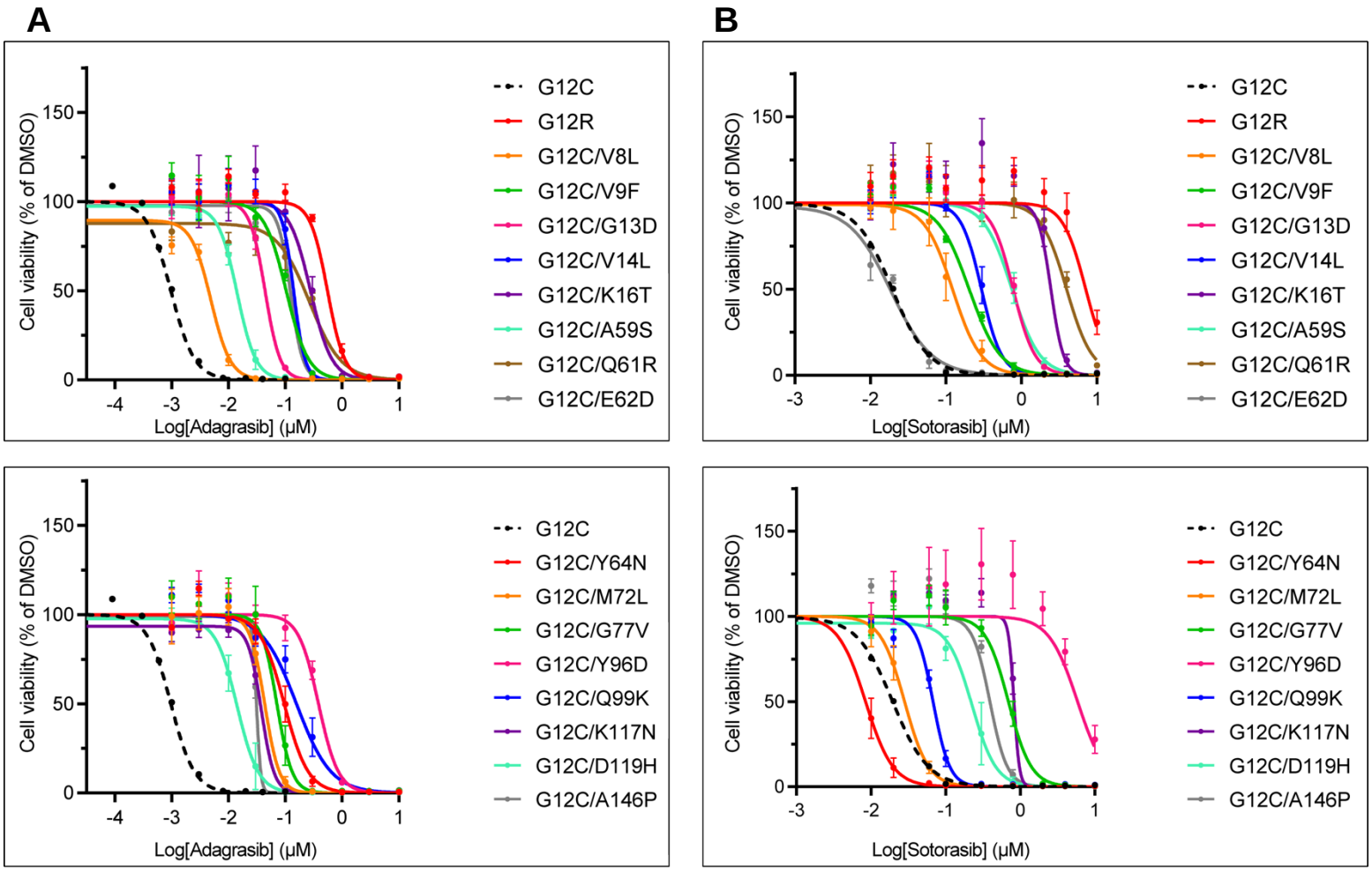


Figure S17. Drug response curves in Ba/F3 stable cell lines. Ba/F3 cells expressing the indicated variant were treated with (**A**) adagrasib or (**B**) sotorasib for 5 days and CellTiterGlo assays were performed. Drug-response curves for G12C allele in Figure 4C and 4D are shown as dotted line for reference. The curves are shown as mean ± SEM from at least three independent experiments.

Figure S18

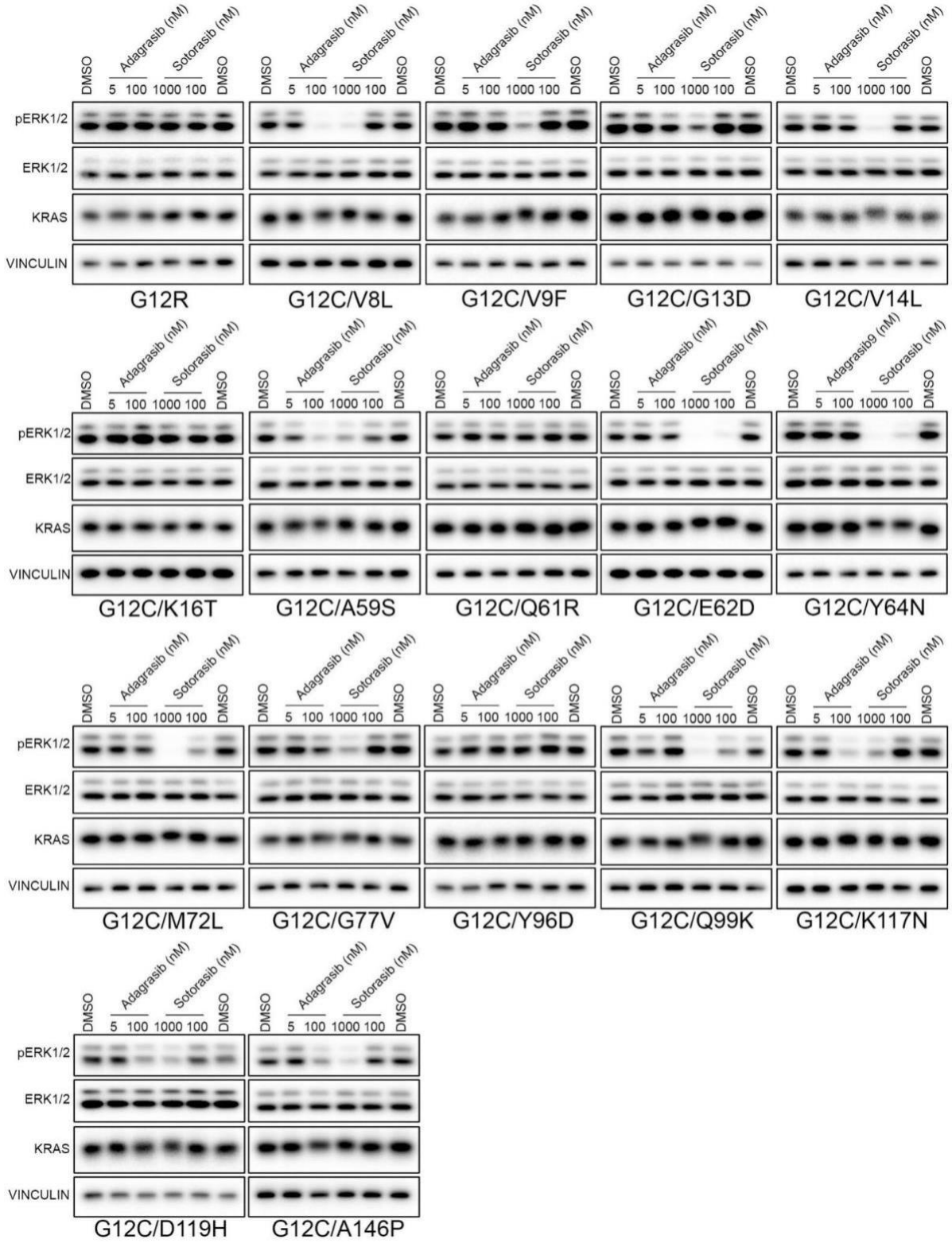


Figure S18. Immunoblot results for G12C variants after 6-hour treatment with KRAS^{G12C} inhibitors. Ba/F3 cells expressing indicated variants were treated with adagrasib or sotorasib for 6 hours and immunoblots were performed to assess the ERK phosphorylation and total KRAS protein levels.

Figure S19

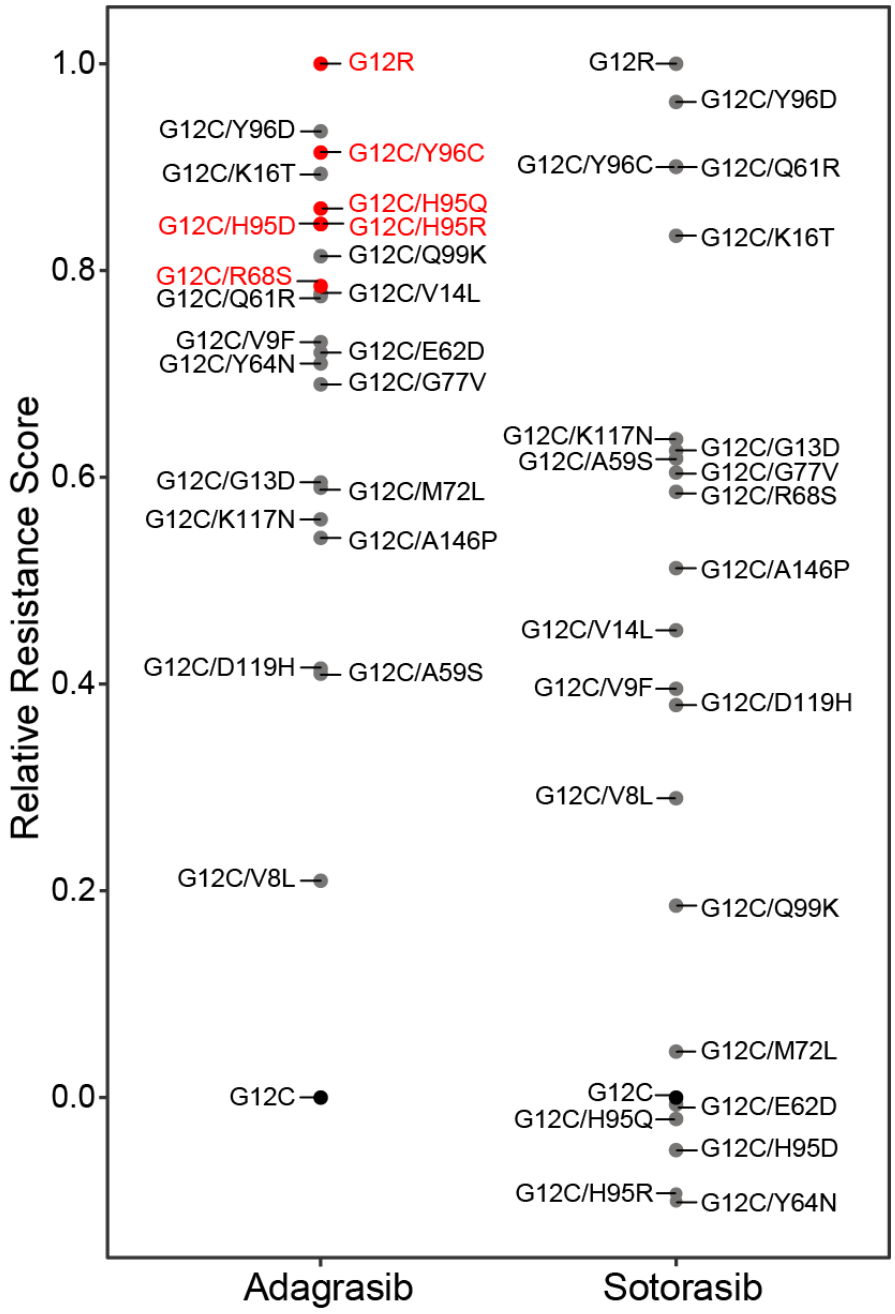


Figure S19: Summary of validation of results from the deep mutational scanning screen. A summary of the relative resistance scores is shown for each allele expressed in cells treated with adagrasib or sotorasib. Relative resistance score is defined as the fraction of resistance conferred by each allele, with maximal resistance defined by the differential sensitivity of the insensitive G12R allele (which does not covalently bind adagrasib or sotorasib) and the sensitive G12C allele **(Supplementary Methods, Table S6)**. A higher relative resistance score suggests stronger resistance potential. The mutations colored in red were observed clinically in the patients described in the study.

Table S1. Summary of testing platforms and genomic/histologic findings among the 38 patients.

Case	Tumor Type	Sequencing Platform at Baseline	Sequencing Platform at Resistance	Sample Available at Time of Resistance		Acquired KRAS alterations	Acquired RTK/MAPK/PI3K alterations	Acquired fusions	Histologic transformation
				Tissue	ctDNA				
Cases where KRAS G12C was detected at resistance:									
1	NSCLC	DFCI OncoPanel	DFCI OncoPanel	Yes	No	Y96C	---	---	No
2	CRC	Henry Ford Illumina Assay	Guardant360	No	Yes	H95Q H95R Q61H G13D G12D G12R G12V	BRAF V600E MAP2K1 K57N MAP2K1 K57T RIT1 P128L PTEN G209V	CCDC6-RET	Not assessed
3	NSCLC	FoundationOne Liquid CDx	FoundationOne Liquid CDx	No	Yes	H95D R68S G12W G12V	BRAF V600E	---	Not assessed
4	CRC	N/A	FoundationOne Liquid CDx	No	Yes	H95R G12D	MAP2K1 I99_K104del	---	Not assessed
5	CRC	Resolution Bioscience ctDx	Resolution Bioscience ctDx; Guardant Omni	No	Yes	G12D G13D	MAP2K1 K57N EGFR A289V	EML4-ALK	Not assessed
6	CRC	FoundationOne CDx	FoundationOne Liquid CDx	No	Yes	G13D	NRAS Q61K MAP2K1 E102_I103del	FGFR3-TACC AKAP-BRAF NRF1-BRAF RAF1-CCDC176 RAF1-TRAK1	Not assessed
7	NSCLC	DFCI OncoPanel	DFCI OncoPanel; Resolution Bioscience ctDx	Yes	Yes	KRAS G12C amplification	---	---	No
8	CRC	Resolution Bioscience ctDx	Resolution Bioscience ctDx	No	Yes	KRAS G12C amplification	---	---	Not assessed
9	NSCLC	MSK-IMPACT	MSK-IMPACT	Yes	No	---	MET amplification	---	No
10	NSCLC	Guardant360	Guardant360	No	Yes	---	MET amplification	---	Not assessed
11	NSCLC	DFCI OncoPanel	DFCI OncoPanel, Guardant360	Yes	Yes	---	---	---	Yes, adenocarcinoma to squamous cell carcinoma
12	NSCLC	MGH SNaPshot & Solid Fusion Assay	MGH SNaPshot & Solid Fusion Assay	Yes	No	---	---	---	Yes, adenocarcinoma to squamous cell carcinoma
13	NSCLC	Guardant360	Guardant360	Yes	Yes	---	MAP2K1 E102_103del	---	No
14	CRC	FoundationOne CDx	Tempus xT	Yes	No	---	PTEN N48K PIK3R1 S361fs	---	No

15	NSCLC	Resolution Bioscience ctDx	Resolution Bioscience ctDx	No	Yes	---	RET M918T	---	Not assessed
18	NSCLC	Guardant360	Guardant360	No	Yes	---	---	---	Not assessed
19	NSCLC	Henry Ford Illumina Assay	Henry Ford Illumina Assay	Yes	No	---	---	---	No
20	NSCLC	Henry Ford Illumina Assay	Guardant360	Yes	Yes	---	---	---	No
21	NSCLC	FoundationOne CDx	Guardant360	No	Yes	---	---	---	Not assessed
22	CRC	FoundationOne CDx	Guardant360	No	Yes	---	---	---	Not assessed
23	NSCLC	MSK-IMPACT	Resolution Bioscience ctDx; MSK-ACCESS	No	Yes	---	---	---	Not assessed
24	NSCLC	MSK-IMPACT	MSK-ACCESS	No	Yes	---	---	---	Not assessed
25	NSCLC	MSK-IMPACT	MSK-IMPACT	Yes	No	---	---	---	No
26	CRC	MSK-IMPACT	Resolution Bioscience ctDx; MSK-ACCESS	No	Yes	---	---	---	Not assessed
27	NSCLC	FoundationOne Liquid CDx; Caris	FoundationOne Liquid CDx	No	Yes	---	---	---	Not assessed
28	CRC	Resolution Bioscience ctDx	Resolution Bioscience ctDx	No	Yes	---	---	---	Not assessed
29	NSCLC	Resolution Bioscience ctDx	Resolution Bioscience ctDx	No	Yes	---	---	---	Not assessed
30	NSCLC	Resolution Bioscience ctDx	Resolution Bioscience ctDx	No	Yes	---	---	---	Not assessed
31	NSCLC	Resolution Bioscience ctDx	Resolution Bioscience ctDx	No	Yes	---	---	---	Not assessed
32	NSCLC	Resolution Bioscience ctDx	Resolution Bioscience ctDx	No	Yes	---	---	---	Not assessed
33	CRC	Resolution Bioscience ctDx	Resolution Bioscience ctDx	No	Yes	---	---	---	Not assessed
34	NSCLC	Resolution Bioscience ctDx	Resolution Bioscience ctDx	No	Yes	---	---	---	Not assessed
Cases where KRAS G12C was not detected at resistance:									
35	NSCLC	FoundationOne CDx	Guardant360	No	Yes	---	---	---	Not assessed
36	NSCLC	N/A	Guardant360	No	Yes	---	---	---	Not assessed
37	NSCLC	Tempus xF	Tempus xF	No	Yes	---	---	---	Not assessed
38	NSCLC	Guardant360	Guardant360	No	Yes	---	---	---	Not assessed
16	NSCLC	Resolution Bioscience ctDx	Resolution Bioscience ctDx; Guardant Omni	No	Yes	G12D	PIK3CA H1047R	---	Not assessed
17	Appendiceal	Guardant Omni	Guardant Omni	No	Yes	---	NF1 R2637*	---	Not assessed

Table S2. Detailed deep mutational scanning screen results.

Mutation	Zscore MRTX1257	Zscore Sotorasib	Zscore Control
T2A	-0.30794	-0.4119	0.3111
T2C	-0.50447	0.55517	0.3144
T2D	0.29036	0.19821	1.13175
T2E	-0.0649	-0.36654	0.81215
T2F	-0.10609	0.24591	0.6235
T2G	-0.22073	-1.36377	0.35112
T2H	-0.00154	0.24266	0.56694
T2I	0.33979	0.90523	1.16526
T2K	0.16673	0.20068	0.42076
T2L	0.80642	-0.00737	1.09175
T2M	-0.63476	-1.22401	1.08386
T2N	0.05708	0.55071	0.87575
T2P	-0.81568	-0.79592	0.68124
T2Q	1.29472	0.33992	0.81743
T2R	-0.5614	-0.43685	-0.5659
T2S	-0.56012	-0.63989	0.32776
T2T	NA	NA	NA
T2V	-0.55416	-0.9905	0.32798
T2W	-0.79453	-0.514	0.29287
T2Y	0.99829	0.41731	0.79369
T2X	-1.97088	-1.5186	-1.2024
E3A	-0.53627	0.30844	-0.89562
E3C	0.01519	0.36292	-0.12038
E3D	1.37878	-0.58135	0.08741
E3E	NA	NA	NA
E3F	-1.05065	-0.29308	-1.82259
E3G	-0.5574	-0.14979	-0.58067
E3H	-2.66134	-0.86174	-1.56069
E3I	-0.82172	-1.17847	-1.5229
E3K	-0.70223	-0.42448	-0.82711
E3L	-0.96699	-0.82697	-1.03792
E3M	-1.20053	-0.67931	-1.27731
E3N	-1.02206	-0.97793	-0.85835
E3P	-0.96792	-0.42628	-1.00876
E3Q	-0.6698	0.56509	-1.05551
E3R	-0.98094	-0.57334	-1.1512
E3S	-0.85121	-0.27776	-0.5519
E3T	-0.59683	0.22229	-0.6219
E3V	-0.93685	-0.79198	-0.78527
E3W	-0.54043	-0.24773	-1.64574
E3Y	-1.52118	-0.55417	-1.61016
E3X	0.10468	0.39877	-0.92907

Y4A	-0.10764	0.12065	1.65401
Y4C	0.10354	-0.27867	1.16724
Y4D	0.64938	0.57653	2.89117
Y4E	0.37647	0.07323	2.27502
Y4F	0.72348	0.36106	0.3944
Y4G	0.36085	0.56725	3.08293
Y4H	0.25106	0.64549	2.44675
Y4I	-0.41987	0.31332	1.18671
Y4K	0.12645	-0.21185	1.95468
Y4L	1.19976	1.5479	1.8475
Y4M	-0.23007	-0.44103	1.43413
Y4N	0.22125	0.44569	2.50929
Y4P	1.4645	1.31481	1.13723
Y4Q	0.4439	-0.05387	2.18706
Y4R	2.60653	0.00342	1.86838
Y4S	1.31147	1.06168	2.08482
Y4T	0.27738	0.11668	2.35009
Y4V	-0.23578	-1.12782	1.32617
Y4W	0.59624	1.7315	1.77286
Y4Y	NA	NA	NA
Y4X	-0.05542	0.03733	-0.39517
K5A	-0.03941	0.05695	0.46289
K5C	1.00289	-0.47226	1.10154
K5D	-0.03508	-0.08343	0.75159
K5E	-0.61503	-0.25879	0.58223
K5F	0.22751	-0.30959	0.32951
K5G	0.65021	-0.54674	0.86192
K5H	-0.61488	0.13633	0.23525
K5I	0.03269	-0.50534	1.76856
K5K	NA	NA	NA
K5L	-0.1211	-0.68989	0.87364
K5M	-0.14788	-0.6312	0.45426
K5N	0.1716	0.27915	0.6099
K5P	0.95839	0.45376	0.9412
K5Q	-0.02475	0.53189	0.37015
K5R	-0.03903	-0.22183	-0.22538
K5S	-0.47774	-0.41374	0.31983
K5T	-0.29414	0.90725	1.36754
K5V	0.25208	-0.14105	1.54365
K5W	-0.63891	-0.11305	-0.22516
K5Y	-0.06319	0.7434	-0.0228
K5X	0.34639	-0.10448	-0.70663
L6A	0.42586	0.58769	2.18447

L6C	-0.87834	-0.03271	0.92768
L6D	0.74818	0.3309	-0.4481
L6E	0.54693	0.13978	0.44139
L6F	0.3684	-0.36332	0.59972
L6G	0.67346	0.49078	1.74719
L6H	0.5132	0.66026	0.95439
L6I	0.10116	0.29815	0.58931
L6K	-0.09347	-0.16921	-0.78716
L6L	-0.27678	0.36792	-0.02776
L6M	-0.53261	-0.5824	-0.21808
L6N	0.97091	1.01822	0.3286
L6P	0.80782	1.17129	1.40849
L6Q	-0.74413	-0.12877	-0.11654
L6R	-0.06609	-0.47829	-0.61672
L6S	-0.3513	0.03078	1.61118
L6T	-0.19985	-0.33321	1.41342
L6V	-0.26096	-0.96248	0.5257
L6W	-0.28187	0.39396	-0.18161
L6Y	-0.22742	0.0292	1.03024
L6X	-0.39423	0.50785	-0.82441
V7A	0.03757	-0.56949	2.89408
V7C	0.06503	-0.34573	2.00831
V7D	0.19687	0.0874	0.65427
V7E	0.62067	0.4608	0.16064
V7F	-0.29376	-0.27052	0.10618
V7G	1.34397	0.75387	2.07814
V7H	-0.91102	-0.89839	1.2531
V7I	-0.82334	0.12893	-0.32589
V7K	-0.88193	-0.84458	1.07259
V7L	-0.55506	-0.39464	-0.69973
V7M	0.16199	-0.28478	1.23603
V7N	-0.67224	-0.83272	0.4219
V7P	-0.78708	-0.2728	-0.40734
V7Q	0.42669	0.96983	1.29487
V7R	-0.69341	-0.93014	1.62558
V7S	0.43419	0.18109	2.19256
V7T	-0.30317	0.71289	1.33069
V7V	NA	NA	NA
V7W	-0.62615	-0.0124	-1.8346
V7Y	-0.86534	-0.82161	0.148
V7X	-0.43788	-0.06423	-0.73029
V8A	0.33521	0.86474	1.9007
V8C	0.03191	0.43557	1.97461

V8D	0.14123	1.07025	1.06619
V8E	1.03204	2.39584	0.93987
V8F	2.24057	2.81955	0.80602
V8G	-0.03049	0.70156	1.31838
V8H	2.81539	5.3025	1.19486
V8I	0.07267	0.56498	1.08848
V8K	4.48745	5.49216	0.93241
V8L	0.70927	3.08771	1.03712
V8M	0.23241	1.63023	1.44448
V8N	1.39241	2.39664	1.1502
V8P	1.94502	1.35739	0.25656
V8Q	1.25313	3.53615	1.12323
V8R	0.27596	0.23572	-0.89515
V8S	1.93542	3.16217	1.7209
V8T	1.6671	3.61392	1.61513
V8V	NA	NA	NA
V8W	3.36883	5.00353	0.10316
V8Y	4.51515	5.42902	0.72118
V8X	0.44619	0.47711	-0.66114
V9A	-0.38046	-0.3492	0.70737
V9C	0.32312	0.41242	0.95114
V9D	1.0748	0.69651	-0.04354
V9E	1.10402	0.78753	-0.84991
V9F	2.62984	1.00013	0.27391
V9G	2.08102	1.09735	0.88512
V9H	3.63819	3.11909	1.33473
V9I	0.19177	-0.09012	-0.53877
V9K	3.39473	3.51342	0.17801
V9L	-0.69812	-0.55885	-0.96373
V9M	0.66347	0.87143	-0.54506
V9N	-0.33	0.0379	0.03301
V9P	-0.64593	-0.35404	0.15575
V9Q	2.96289	2.41618	0.6178
V9R	3.23025	3.02915	0.24721
V9S	-0.34723	-0.32036	-0.15105
V9T	-0.08787	0.5043	-0.12356
V9V	NA	NA	NA
V9W	4.21605	4.5624	0.70094
V9Y	2.49768	2.23599	-0.17751
V9X	0.54253	-0.23932	-1.71475
G10A	0.79238	0.14687	-0.73914
G10C	0.45484	-0.24228	-1.13507
G10D	-0.63757	-0.60795	-1.21413

G10E	-0.32051	-0.54636	-1.67136
G10F	0.30747	-0.48918	-1.65378
G10G	NA	NA	NA
G10H	0.4574	-0.41983	-1.4873
G10I	-0.96474	-1.61003	-1.43116
G10K	0.72788	1.18066	-1.16687
G10L	1.02065	-0.26857	-1.65964
G10M	-1.1552	-1.26995	-1.31191
G10N	-0.11811	0.48587	-1.97316
G10P	-1.3494	-1.21313	-1.21873
G10Q	0.02335	-0.28371	-1.39887
G10R	0.29424	0.90097	-1.42504
G10S	-0.20769	0.54986	-0.78016
G10T	-0.48158	-0.17903	-1.19004
G10V	-0.57484	-0.49741	-1.15311
G10W	-0.70722	-0.39613	-1.84299
G10Y	0.64788	0.43018	-1.51269
G10X	-1.05819	-1.07423	-1.99427
A11A	NA	NA	NA
A11C	0.13523	-0.8076	-0.94301
A11D	0.00622	1.12229	-0.41281
A11E	-0.65096	0.13702	-0.32579
A11F	-0.83289	0.21644	-0.64382
A11G	-0.07364	-1.02479	0.47775
A11H	0.00405	-0.72091	-0.3465
A11I	4.90494	-1.98839	1.42969
A11K	1.3026	2.62053	0.53069
A11L	1.16239	0.93652	-1.06206
A11M	-1.06778	-1.16765	-1.33828
A11N	-0.15421	0.99765	0.20066
A11P	-0.83932	-0.65352	-0.04886
A11Q	-0.10512	0.26303	-1.07668
A11R	1.41474	1.54931	0.19894
A11S	-1.2214	-1.89416	-0.15306
A11T	0.53693	0.79816	-0.91109
A11V	3.02403	-0.76681	0.23989
A11W	1.09852	0.56101	0.36667
A11Y	0.11599	-0.3864	-0.92149
A11X	-0.16806	-0.88765	-0.60299
C12A	1.28343	1.87729	-0.60485
C12C	NA	NA	NA
C12D	4.23448	4.7892	0.85756
C12E	3.78622	4.16407	0.35157

C12F	4.10719	4.60501	0.64362
C12G	0.51712	-0.29855	-0.96469
C12H	5.15009	5.77734	1.28756
C12I	5.64539	6.35227	2.05373
C12K	5.11718	6.07943	1.32479
C12L	5.34901	6.16885	1.69334
C12M	5.07075	5.62338	1.39419
C12N	4.20393	4.60777	0.54759
C12P	-0.06489	-0.45688	-1.1015
C12Q	5.48242	6.33159	2.1528
C12R	5.34249	6.06084	1.32865
C12S	0.66344	1.02028	-0.90762
C12T	2.39851	2.79957	-0.60727
C12V	3.44017	3.69739	0.04068
C12W	3.99963	4.64992	0.72788
C12Y	4.30468	4.77757	0.63139
C12X	0.2495	-0.18296	-0.89116
G13A	-0.47194	-0.85173	0.37341
G13C	-1.07778	-0.67183	-1.40087
G13D	3.0562	4.65388	2.05791
G13E	1.50383	2.40261	1.85306
G13F	-0.06586	0.94726	1.29803
G13G	NA	NA	NA
G13H	1.35489	1.44456	1.52964
G13I	-0.22604	-0.35836	0.59923
G13K	1.85221	2.13082	-0.7246
G13L	0.77175	1.28661	0.99951
G13M	-0.48447	-0.88374	0.61894
G13N	0.75275	0.10574	1.67297
G13P	5.2401	6.23707	1.66509
G13Q	1.55091	0.71847	1.54001
G13R	0.16842	-0.39635	-0.37212
G13S	-0.81868	-0.12513	-0.70509
G13T	-0.71994	-0.17424	-0.70476
G13V	0.07843	0.54313	0.76301
G13W	0.3883	-0.00277	1.23153
G13Y	0.5826	0.75028	1.15323
G13X	0.22855	-0.25534	-1.39249
V14A	-0.52629	-0.1519	1.08187
V14C	-0.97814	-0.36561	1.65298
V14D	-0.72471	0.53205	0.76299
V14E	-0.26415	-0.14951	0.6712
V14F	-0.47856	-0.14662	-0.96657

V14G	1.57138	-0.10385	1.6602
V14H	4.95217	4.88681	1.77258
V14I	0.9262	1.43637	1.64258
V14K	0.27392	-0.60766	-1.5516
V14L	4.54913	2.09299	1.17405
V14M	-1.74936	-1.7552	-1.25043
V14N	-0.66363	-0.06099	1.75691
V14P	2.87084	2.87714	0.77571
V14Q	-0.71725	-0.98351	0.93654
V14R	1.19666	1.20741	-0.78531
V14S	-1.51082	-1.5341	1.81914
V14T	0.49325	0.22542	1.85188
V14V	NA	NA	NA
V14W	0.31506	0.36835	-1.10985
V14Y	-0.09483	-0.89871	-0.59409
V14X	-0.01019	0.27859	-0.33722
G15A	-0.71627	-1.96742	-1.43078
G15C	-0.13673	-0.0531	-1.34069
G15D	-1.33071	-1.36578	-1.90497
G15E	-0.88791	-0.88991	-1.52671
G15F	-0.67912	-0.8235	-1.65711
G15G	NA	NA	NA
G15H	-0.427	-0.15218	-1.28573
G15I	-0.56447	-1.05889	-1.5216
G15K	-0.29264	-0.55302	-1.33708
G15L	-0.36946	0.35267	-1.02294
G15M	-0.54194	0.11945	-0.97815
G15N	-0.58701	-0.59026	-1.34546
G15P	-0.36924	-0.61944	-1.32024
G15Q	-0.31027	-0.39773	-1.02539
G15R	-0.13649	-0.50312	-0.78117
G15S	1.38451	-0.32895	-1.19064
G15T	-0.28757	-0.59992	-0.8195
G15V	-0.41477	-0.48824	-1.03326
G15W	0.20677	-0.81365	-0.93811
G15Y	-0.80882	-0.81153	-1.37821
G15X	-0.34785	-0.51665	-0.80975
K16A	0.36835	0.81426	-1.39014
K16C	4.60613	4.55506	0.90859
K16D	-0.26791	-0.92754	-1.62152
K16E	-0.54737	-0.77926	-1.19759
K16F	-0.37399	-1.0302	-1.16568
K16G	-0.63177	0.4011	-1.17365

K16H	-0.00245	-1.93314	-1.49367
K16I	-0.34619	-1.25834	-1.70192
K16K	NA	NA	NA
K16L	0.76696	0.25158	-1.1002
K16M	0.41255	0.33421	-0.59524
K16N	-1.19921	-0.29568	-0.84423
K16P	0.11387	0.57447	-0.7329
K16Q	-0.41535	-0.66013	-1.06697
K16R	-0.53565	0.03557	-1.49667
K16S	5.44312	6.10078	1.56222
K16T	3.42174	3.64911	0.70844
K16V	-0.20547	-1.58092	-1.57533
K16W	-0.11184	-0.48906	-0.70787
K16Y	-0.98801	-0.28388	-1.2048
K16X	0.14261	-0.66025	-0.49066
S17A	-0.66657	0.01059	-1.5191
S17C	0.46854	-0.03543	-0.57007
S17D	-0.24981	-1.18635	-1.40367
S17E	-0.61277	0.0114	-1.14862
S17F	-0.38544	-0.31921	-1.27825
S17G	-0.59167	-1.0806	-2.12697
S17H	0.23212	-0.06637	-1.14113
S17I	0.67241	-0.09256	-0.85027
S17K	-0.1787	-2.1589	-1.96229
S17L	-0.91109	-0.5716	-1.70749
S17M	0.11713	0.05025	-1.37816
S17N	-0.18682	-0.69371	-1.5603
S17P	-0.90949	-1.01885	-1.03501
S17Q	-0.45715	-0.67766	-2.2196
S17R	-1.26276	-1.76068	-2.24862
S17S	-0.17911	-0.53261	0.27992
S17T	-0.34641	0.04205	0.02884
S17V	-1.20933	-0.684	-1.21117
S17W	0.49332	0.52605	-1.51307
S17Y	0.17825	-0.02072	-1.04763
S17X	-0.41559	-0.47657	-0.62231
A18A	NA	NA	NA
A18C	-0.67418	-0.7504	-0.53266
A18D	0.48708	0.42625	1.05469
A18E	0.2675	-2.81794	-0.33979
A18F	-0.49466	-0.43505	-1.43236
A18G	-0.40266	0.72059	2.13232
A18H	-0.4046	-0.33669	-1.19324

A18I	-0.78224	0.41999	1.71495
A18K	-0.25972	-1.17643	-0.95107
A18L	-0.90806	-0.79205	-1.3782
A18M	-0.82525	-1.12248	2.25047
A18N	-0.04451	-0.42406	-0.3955
A18P	-1.09332	-2.37557	-2.82965
A18Q	0.73153	1.04305	2.84662
A18R	-0.98643	-1.46204	-2.78523
A18S	-1.88199	-0.59216	-1.33127
A18T	-1.63224	-0.17728	0.35657
A18V	0.14656	-0.46644	1.46921
A18W	-0.65773	-0.4577	-0.08799
A18Y	-1.63046	-1.78574	-1.32022
A18X	-1.33375	-1.68939	-1.34404
L19A	1.05261	0.94149	0.53467
L19C	-0.89543	-1.32857	-0.37417
L19D	0.36804	-0.72611	-0.38298
L19E	0.00835	-0.2494	0.24076
L19F	0.88814	0.89455	0.35729
L19G	-0.5379	-1.29787	1.13032
L19H	-0.16584	-1.14484	1.0699
L19I	-0.64509	0.84254	-0.64071
L19K	-0.96712	-0.6356	0.40609
L19L	-0.30513	-0.45966	-0.33663
L19M	-0.14717	0.36728	0.29176
L19N	-1.4025	-1.21839	1.09315
L19P	-0.25993	-0.69253	-1.16043
L19Q	2.21549	-0.0492	1.44248
L19R	-0.0166	-0.7132	-1.00449
L19S	-1.00798	0.34394	-0.68761
L19T	-1.12539	-0.7149	-1.06709
L19V	-0.67519	-0.88414	0.06887
L19W	0.41164	1.00537	0.53723
L19Y	0.65353	-0.0321	0.87298
L19X	-0.21876	-0.03679	-0.52589
T20A	0.97599	-0.43342	0.69619
T20C	-0.91982	-0.6033	-1.66266
T20D	1.21658	3.24719	0.12713
T20E	0.67803	0.81959	-0.37436
T20F	0.3725	0.03481	0.10705
T20G	-1.30281	0.39569	-0.20387
T20H	0.70043	0.2045	-1.08596
T20I	-0.35391	-0.30683	-0.72859

T20K	0.76447	-0.79078	-1.16916
T20L	-0.30781	-0.46924	-0.38182
T20M	0.64857	-0.0853	0.23182
T20N	0.4608	1.04277	0.67675
T20P	0.52615	0.49716	-0.52923
T20Q	0.39431	0.79285	-0.54688
T20R	-0.29788	-1.97732	-1.18744
T20S	-0.15965	0.19364	0.72761
T20T	NA	NA	NA
T20V	-0.57483	0.07849	-0.69016
T20W	0.47277	-0.82105	-1.05743
T20Y	-0.68758	-2.40995	-1.01191
T20X	-0.88158	-0.7847	-0.77713
I21A	-0.74703	-0.09618	0.42482
I21C	1.21547	0.04388	0.92398
I21D	-0.14362	-0.23061	-0.03827
I21E	-0.57327	-0.34327	0.31736
I21F	-0.5757	1.03807	-1.11907
I21G	-0.67987	-0.42782	-0.06577
I21H	2.45981	0.05603	-0.34569
I21I	NA	NA	NA
I21K	0.47255	0.15625	0.17927
I21L	-1.86201	-1.40951	0.01958
I21M	1.00229	0.95171	0.17065
I21N	0.99424	1.24591	0.61757
I21P	-0.58417	-0.9993	-1.33846
I21Q	-0.56261	-1.51426	-0.23198
I21R	-0.37787	-0.05979	-1.83017
I21S	0.13243	-0.93467	0.0487
I21T	0.16217	-0.80509	0.20802
I21V	-0.45577	-0.72866	0.36756
I21W	-0.0679	0.61195	0.14925
I21Y	-1.13135	-1.82136	-0.4313
I21X	0.96093	-0.15362	-0.85058
Q22A	0.45781	0.08674	2.14929
Q22C	-1.17573	-0.58833	0.88371
Q22D	-0.629	0.38991	1.86719
Q22E	0.68188	-0.71798	1.77466
Q22F	-0.45311	-0.35726	1.22616
Q22G	0.68303	-1.38953	1.36418
Q22H	0.00826	0.35087	0.33274
Q22I	-1.66474	0.18652	0.5199
Q22K	-0.31478	-0.80635	-1.25104

Q22L	-1.83971	-1.38182	0.2796
Q22M	-0.36632	-0.68107	-1.07476
Q22N	-0.28883	-1.59635	2.00814
Q22P	-0.00584	-0.12576	-1.49398
Q22Q	NA	NA	NA
Q22R	-1.28001	-1.26513	-1.59105
Q22S	0.81562	-0.82949	1.84393
Q22T	0.51194	0.68237	1.56974
Q22V	-0.18576	-0.30162	0.20672
Q22W	-0.7177	-1.57203	1.44741
Q22Y	-0.99406	-1.12792	0.74256
Q22X	-0.58825	0.34857	-0.88442
L23A	1.90313	-0.86633	2.15653
L23C	-0.54143	-0.98833	2.15394
L23D	-0.12192	-0.91489	0.66903
L23E	-1.15522	-0.60021	2.23936
L23F	-1.76991	-0.20563	-0.031
L23G	-0.16064	-1.03135	1.31922
L23H	-0.34783	0.25338	2.29522
L23I	-0.40771	-0.54116	0.86295
L23K	0.09887	-0.27599	3.22615
L23L	-1.28197	-1.35516	-0.31041
L23M	0.28279	-0.08139	0.50524
L23N	2.72377	0.49965	2.55581
L23P	-1.60378	-0.5862	-0.94344
L23Q	-0.2399	0.146	1.95575
L23R	1.061	0.75343	3.2171
L23S	0.34777	-0.68275	2.18834
L23T	0.16298	-0.07404	1.89425
L23V	-0.39199	-0.44878	1.19175
L23W	-0.46003	-0.12383	-0.8403
L23Y	-0.16476	0.20173	-0.3394
L23X	0.31234	-0.32064	-1.19634
I24A	NA	NA	NA
I24C	-0.28185	0.15382	0.19342
I24D	0.64623	-0.11697	0.82081
I24E	-0.24785	-0.25829	0.4398
I24F	1.97877	0.30148	4.80254
I24G	-0.6052	-0.06397	1.78145
I24H	0.70341	0.98328	2.50513
I24I	NA	NA	NA
I24K	-0.45498	-0.54777	0.96813
I24L	-0.52438	0.57804	2.81246

I24M	0.41993	0.42698	1.77708
I24N	0.44914	-0.43015	0.17634
I24P	0.18145	0.26436	-1.1936
I24Q	0.6237	-0.6945	2.48512
I24R	-1.31237	-0.65797	0.559
I24S	-0.16842	-0.63108	0.56472
I24T	-0.74084	-0.55692	0.15161
I24V	-1.2492	-1.56947	-0.07576
I24W	1.64151	1.17057	3.64556
I24Y	1.51709	0.97405	3.82765
I24X	-0.22201	-0.39555	-0.56401
Q25A	0.34509	0.04403	0.75184
Q25C	0.62874	-0.08621	1.28152
Q25D	-0.014	-0.20313	-0.2939
Q25E	-0.16802	0.02027	-0.91042
Q25F	1.1844	0.83853	1.7961
Q25G	-0.29459	0.07244	1.5704
Q25H	1.68558	0.52184	1.13347
Q25I	0.13622	0.9242	0.96268
Q25K	0.02241	0.13423	1.15235
Q25L	1.0182	-0.21986	1.46745
Q25M	0.52603	-0.38509	1.56259
Q25N	-0.65616	-0.13895	-0.52604
Q25P	-0.59978	-1.1391	-1.00913
Q25Q	NA	NA	NA
Q25R	-0.05353	-0.68858	0.16675
Q25S	0.69958	1.78735	0.15589
Q25T	0.90736	-0.5953	1.31578
Q25V	0.37635	-0.52187	2.00022
Q25W	0.76854	0.15898	1.55665
Q25Y	1.01298	0.66387	1.68337
Q25X	-0.48404	-0.66863	-0.8735
N26A	-0.80078	-0.49657	-0.8223
N26C	-0.77379	-0.59963	-0.4025
N26D	-0.11922	0.07382	-0.34786
N26E	0.11935	-0.35578	0.43794
N26F	-0.55114	0.21165	0.21902
N26G	-2.33201	-1.17125	-0.87968
N26H	0.22786	0.21354	-1.4061
N26I	-0.14417	-0.76557	1.05183
N26K	-0.63185	0.38571	-1.5492
N26L	0.39092	-0.66774	1.04844
N26M	0.51988	0.77691	1.57161

N26N	NA	NA	NA
N26P	-0.42149	-1.06422	0.59021
N26Q	-1.37337	-0.14059	0.1722
N26R	-1.44328	0.14381	-2.84436
N26S	-0.21992	-0.16706	0.27035
N26T	-0.61678	-0.89375	1.63762
N26V	-0.73562	-0.30136	0.92413
N26W	0.53558	0.3729	-0.8712
N26Y	0.34876	1.32975	-0.29575
N26X	-0.27276	-1.36672	-1.00267
H27A	-0.98674	-1.52792	-0.45853
H27C	-1.12207	-0.89851	-0.78255
H27D	-0.17375	-0.90012	-0.26617
H27E	-1.35848	-1.11204	-2.29439
H27F	-0.95977	-0.27871	0.3418
H27G	0.0305	-0.5637	2.88532
H27H	NA	NA	NA
H27I	-0.47343	-0.64048	-1.86697
H27K	0.38997	-0.25658	0.8297
H27L	-1.10374	-0.6123	-1.34218
H27M	-0.88541	-0.41414	-0.86044
H27N	-0.27144	-0.14104	1.27434
H27P	-0.22962	-1.24657	-0.88095
H27Q	1.92585	0.1977	0.19551
H27R	-0.46777	-0.52538	-0.41068
H27S	-0.11698	-0.62347	-0.47911
H27T	-1.79482	-0.38355	-0.6719
H27V	-0.92078	-1.09481	-1.07367
H27W	0.39032	0.4617	1.71857
H27Y	-0.60869	-0.49548	0.43845
H27X	-0.5898	-1.57693	-0.49706
F28A	-0.24306	-0.92524	-0.02256
F28C	0.12621	-1.08956	1.30586
F28D	-0.30104	-0.45591	-0.61024
F28E	-0.65644	-1.1585	-0.8985
F28F	NA	NA	NA
F28G	-0.00393	-0.25768	-0.63833
F28H	-0.01491	-0.83724	1.14358
F28I	-0.2903	-0.72613	0.50321
F28K	-0.68777	-1.76001	-1.05904
F28L	-1.58459	-1.16243	0.52616
F28M	-1.07042	-0.36898	2.76403
F28N	-0.26055	-0.71829	-0.93631

F28P	-0.19701	0.06827	-0.6696
F28Q	-1.06531	-1.1461	-0.42998
F28R	-0.39467	0.44285	0.35538
F28S	0.08792	-0.7099	-0.65135
F28T	-0.49925	-1.5736	0.0985
F28V	0.50396	-0.39244	0.68334
F28W	-0.01355	-0.90477	1.85981
F28Y	-1.06206	-1.31602	1.10568
F28X	0.3821	-0.12094	-0.63791
V29A	-0.89112	-1.15542	-0.11194
V29C	-3.14861	-3.04871	0.20681
V29D	-0.38966	-0.76659	1.67719
V29E	-0.79775	-0.48841	0.02559
V29F	-1.99905	-0.90623	-1.98489
V29G	0.23924	0.05727	1.09239
V29H	-0.84064	-0.15371	-0.17148
V29I	-1.01324	-1.51901	0.20824
V29K	0.01691	-1.07542	-0.20004
V29L	-0.74644	-0.035	-1.54145
V29M	-0.16667	-0.60467	-0.10557
V29N	-0.79818	-0.01212	0.08188
V29P	-1.35442	-0.75864	0.69774
V29Q	-0.24415	-0.18602	0.32986
V29R	-0.35317	-1.02314	-0.51454
V29S	-1.30241	-0.80991	1.05511
V29T	0.01848	-0.61496	1.36234
V29V	NA	NA	NA
V29W	-1.19647	-1.33456	-1.83359
V29Y	-1.06203	-1.24328	-1.18894
V29X	0.07833	-0.44526	-0.44822
D30A	1.64828	-1.17076	-0.72822
D30C	-0.52818	-0.77799	0.1583
D30D	NA	NA	NA
D30E	-0.27755	-0.10461	-0.11699
D30F	-0.5853	-2.18289	0.78149
D30G	-0.06221	-0.82957	-0.4095
D30H	-0.64065	-0.37569	-0.00853
D30I	-0.10165	0.03075	0.35013
D30K	-0.66859	-0.97492	0.71235
D30L	-1.14785	-0.54635	0.74081
D30M	0.65043	1.21816	0.52652
D30N	-1.21324	-1.91131	0.2767
D30P	-0.33403	0.12921	-1.0702

D30Q	-0.70579	-0.57569	-0.37029
D30R	0.19094	-0.04376	0.46321
D30S	-0.97554	-0.93946	-0.76705
D30T	-0.87375	-1.83422	0.68353
D30V	-0.19807	-0.42499	0.29169
D30W	-1.26418	-1.59232	0.15153
D30Y	-0.05842	-0.5675	0.5099
D30X	-0.21115	-0.7105	-1.20569
E31A	-1.34654	-1.23353	-1.16586
E31C	-0.62278	-0.15959	-1.00793
E31D	-0.17135	-0.19332	-0.45794
E31E	NA	NA	NA
E31F	-1.53407	-1.20421	-2.00189
E31G	1.05018	-0.67964	-0.8374
E31H	-0.42249	-0.89135	-0.88582
E31I	-0.94712	-0.31652	-1.05109
E31K	-0.56209	-0.46728	-1.53432
E31L	-0.57327	-2.00439	-1.49753
E31M	0.0278	0.32476	-1.1793
E31N	-0.39713	-0.29035	-0.82391
E31P	-1.31471	-1.67138	-0.13984
E31Q	0.08001	-0.15036	-0.742
E31R	-1.2966	-1.52611	-1.37098
E31S	-1.08743	-1.91914	-1.24763
E31T	-0.72635	-1.13333	-0.46441
E31V	-1.67605	-0.88376	-0.87587
E31W	-1.06336	-0.5489	-1.61185
E31Y	-0.41897	-0.17648	-1.66202
E31X	0.18454	-0.37164	-0.61288
Y32A	-0.26641	-0.15357	-1.90992
Y32C	0.09441	0.18201	-2.54758
Y32D	0.31152	-0.76896	-0.23858
Y32E	0.10734	0.44677	0.06235
Y32F	-0.82985	-0.64336	-2.54931
Y32G	-0.88438	-1.15097	-2.11088
Y32H	-0.5299	-0.96684	-1.89868
Y32I	-0.25102	-0.15361	-1.94595
Y32K	-0.49195	-0.98261	-3.02054
Y32L	-0.89096	-0.71605	-2.66472
Y32M	NA	NA	NA
Y32N	-0.90306	-0.56721	-2.10345
Y32P	-0.44292	-0.90562	-2.57592
Y32Q	-0.89684	-0.91713	-2.20403

Y32R	-0.96205	-1.44147	-2.87991
Y32S	-1.46094	-1.07057	-2.28002
Y32T	-1.20385	-0.4863	-2.20699
Y32V	-0.36655	-0.25458	-3.47481
Y32W	NA	NA	NA
Y32Y	NA	NA	NA
Y32X	0.02289	0.17748	-0.72624
D33A	-0.89236	-1.34781	-2.2007
D33C	-2.02939	-1.72458	-1.37972
D33D	NA	NA	NA
D33E	0.0464	0.15465	0.99938
D33F	-1.2636	-0.90708	-0.73466
D33G	-0.60491	-1.06434	-2.90314
D33H	-0.60492	-0.50553	-0.56383
D33I	-0.43749	-0.86398	-0.79456
D33K	-0.40938	-0.56507	-1.71309
D33L	-1.1838	-1.41797	-1.088
D33M	-0.67238	-0.3928	-0.54227
D33N	-0.40786	0.39873	-1.02159
D33P	-0.60814	-1.7564	-3.67057
D33Q	-1.38897	-0.25681	-0.764
D33R	-0.94119	-1.25894	-1.38741
D33S	-1.59538	-0.84566	-1.54446
D33T	-0.26578	-0.55672	-2.09068
D33V	-0.06964	0.6493	-0.85324
D33W	-0.62556	-0.2135	-0.69639
D33Y	-0.40021	0.10782	-0.87659
D33X	-0.35435	-0.82796	-0.84421
P34A	-1.43596	-1.18928	0.16118
P34C	-1.85325	-1.84343	-1.55976
P34D	-0.90429	-0.57803	-2.10466
P34E	-0.69231	-0.8266	-0.88882
P34F	-0.66141	-0.72666	-2.34934
P34G	-0.56708	-1.35374	-2.55252
P34H	-1.13087	-4.48162	-2.61396
P34I	-2.00689	-1.45194	-2.73703
P34K	-1.39371	-2.71184	-2.56994
P34L	-1.22176	-0.66452	-2.06238
P34M	-1.27825	-2.06152	-1.23512
P34N	-0.72041	0.49397	-2.29869
P34P	NA	NA	NA
P34Q	-0.1908	-0.43107	-1.46952
P34R	-1.2634	-0.92606	-1.75008

P34S	-1.20818	-0.67851	-1.67374
P34T	-1.61982	-1.48325	-1.10003
P34V	-0.0689	-0.00404	-1.92461
P34W	-1.19678	-0.76181	-2.09263
P34Y	0.00195	-0.55931	-1.65021
P34X	0.44545	0.06238	-0.86879
T35A	-0.79627	-0.73761	-1.66548
T35C	-0.47055	-0.87036	-0.80344
T35D	-1.93351	-1.40018	-1.36103
T35E	-0.82966	-0.91858	-1.77314
T35F	-0.54987	-1.65934	-1.67356
T35G	-1.06507	-0.17981	-1.84768
T35H	0.82596	1.1307	-2.42218
T35I	-0.65549	-1.27074	-1.54684
T35K	-0.92606	-1.28111	-2.97202
T35L	0.12742	0.10461	-2.33372
T35M	-0.94107	-0.56027	-1.03518
T35N	-0.34733	-0.29153	-1.36337
T35P	-1.72901	-1.2571	-3.9112
T35Q	-0.21315	-0.92896	-1.73241
T35R	-0.91255	-1.05367	-2.03987
T35S	1.66167	-0.31682	-1.34142
T35T	NA	NA	NA
T35V	-1.0426	-0.87884	-1.59497
T35W	-0.49468	-0.3786	-1.12732
T35Y	-0.7054	-1.04861	-1.82412
T35X	-0.93811	-1.13295	-0.789
I36A	-0.43815	-1.13451	-2.51883
I36C	-0.54587	-0.17636	-1.88575
I36D	-0.42071	0.07593	-1.76947
I36E	-0.26271	0.22202	-1.77611
I36F	-0.87637	-0.96017	-2.00857
I36G	-1.25274	-0.81614	-1.81946
I36H	0.57968	0.17582	-2.08105
I36I	NA	NA	NA
I36K	-1.90478	-0.84547	-2.83418
I36L	-2.04401	-1.64065	-1.589
I36M	-0.45563	-0.54872	-0.49481
I36N	-0.1131	-0.15328	-2.26176
I36P	0.46287	-0.68672	-1.7885
I36Q	-1.62737	-0.62083	-2.59139
I36R	-0.93465	0.43676	-2.83361
I36S	-1.99768	-1.39239	-2.71171

I36T	-0.94813	-0.21827	-1.85245
I36V	-0.89808	-0.37002	-1.35806
I36W	-2.0508	-0.52367	-1.66114
I36Y	0.27546	-0.48551	-1.69036
I36X	-0.98165	-0.66974	-0.87639
E37A	0.87678	1.54085	1.65838
E37C	1.54933	1.23953	0.79409
E37D	0.11494	0.50582	0.03503
E37E	NA	NA	NA
E37F	1.11016	0.64694	0.78607
E37G	0.04024	-0.46562	0.55883
E37H	-1.30877	0.50453	0.35596
E37I	-0.09185	0.63226	0.51262
E37K	0.81584	1.14159	0.32187
E37L	2.02888	2.43148	3.1524
E37M	1.17762	1.20701	1.62775
E37N	-0.66151	0.0868	0.16465
E37P	-1.08537	0.05904	-2.5442
E37Q	-0.69822	-0.71074	1.70155
E37R	1.23224	1.14199	0.13431
E37S	-1.11443	-0.26007	1.29708
E37T	-0.24981	-0.28804	-0.12388
E37V	0.16538	0.34752	0.33471
E37W	-0.5504	-0.17611	-0.95741
E37Y	-0.3165	-0.12588	0.44785
E37X	-0.25207	-0.30034	-1.16477
D38A	-0.49683	-0.21832	-2.5598
D38C	-0.75097	-0.44657	-2.21455
D38D	NA	NA	NA
D38E	-0.47349	-0.06584	-0.74653
D38F	-0.91537	-1.75449	-2.73696
D38G	-0.89358	-1.70529	-3.49472
D38H	-1.17217	-0.7722	-2.87215
D38I	-0.92902	-0.85819	-1.84485
D38K	-0.94009	-0.33406	-2.33676
D38L	-0.21961	-0.53832	-2.67019
D38M	-0.37545	-1.48907	-2.89473
D38N	-1.98358	-1.60962	-3.92367
D38P	-0.90045	-1.29954	-3.0655
D38Q	-1.0323	-0.91221	-3.72233
D38R	-0.28192	-0.48552	-3.24577
D38S	-1.01933	-0.37268	-3.10629
D38T	-0.44714	0.10922	-2.15708

D38V	-0.64543	-0.03942	-1.22174
D38W	-0.95114	-0.97287	-2.54452
D38Y	-1.43216	-1.43138	-2.62348
D38X	-0.69829	-1.38135	-0.46599
S39A	0.26454	0.11696	-0.59801
S39C	-1.27758	-1.5496	-1.17162
S39D	-1.41484	-1.49316	-1.46066
S39E	-1.0649	-1.08562	-1.89118
S39F	-1.7633	-2.06847	-1.68861
S39G	-0.18304	-0.01196	3.21417
S39H	-1.32798	-0.90186	-2.33368
S39I	-0.94063	-1.30031	-1.45391
S39K	-1.1601	-1.23402	-0.1884
S39L	-0.65111	-0.67999	0.43568
S39M	-0.82744	-1.39568	1.02084
S39N	-0.39185	-1.70876	-2.25052
S39P	NA	NA	NA
S39Q	-0.24373	0.232	-0.84438
S39R	-2.97626	-3.98152	-1.71365
S39S	-0.73362	-0.96358	-0.66517
S39T	0.02838	0.13388	-0.9109
S39V	-1.02573	-2.15985	-2.70524
S39W	-2.29554	-1.47321	-2.52033
S39Y	-0.57484	-2.25306	-2.42957
S39X	0.20063	-0.42572	-1.27267
Y40A	-1.32472	0.3292	-1.55433
Y40C	0.28824	0.1494	-1.51234
Y40D	0.1718	-0.8412	-1.2194
Y40E	0.64566	0.34336	-0.25445
Y40F	-1.17093	-0.46189	-3.4546
Y40G	0.09871	0.63356	-0.40508
Y40H	-0.6356	-2.09388	-0.46378
Y40I	-1.36148	-0.71806	-0.99273
Y40K	-0.43192	-0.38003	-0.52088
Y40L	-0.73316	-0.12023	-0.79447
Y40M	-0.62804	-1.02546	-0.91791
Y40N	-0.44521	-0.92787	-1.27205
Y40P	-0.84432	-0.68482	-0.92585
Y40Q	-0.6856	-1.60883	-0.22836
Y40R	-0.3656	-0.35705	-0.80284
Y40S	-0.25635	-0.04778	-0.24278
Y40T	-0.13175	0.21352	-0.58557
Y40V	-0.24583	-0.09773	-0.99215

Y40W	-0.24141	-0.79535	-0.31781
Y40Y	NA	NA	NA
Y40X	-0.21241	-0.28839	-0.64337
R41A	-0.32501	-0.62196	0.21701
R41C	1.1811	0.92669	0.81962
R41D	0.09415	-0.75879	-0.98757
R41E	0.83622	0.02308	-0.52515
R41F	0.7694	-0.41352	0.78548
R41G	0.46047	0.5315	0.25385
R41H	0.14782	-0.07843	-0.11388
R41I	0.9415	0.47335	2.19182
R41K	-0.08032	-0.24818	0.36543
R41L	1.57062	1.63877	1.90271
R41M	1.1216	0.68088	1.43854
R41N	-0.35644	-0.28091	-0.87656
R41P	-0.03295	-0.33308	0.47102
R41Q	0.04734	-0.19331	0.49352
R41R	-0.37612	-0.14438	0.39151
R41S	0.61447	0.13248	-0.24866
R41T	-0.02662	-0.66803	-0.09244
R41V	0.03808	-0.76902	0.88038
R41W	1.32633	0.36846	0.95584
R41Y	1.34278	-0.0012	0.03076
R41X	-0.20589	0.12721	-0.57512
K42A	0.77548	0.81117	0.94466
K42C	0.57779	-0.5295	1.8146
K42D	1.01182	0.58044	0.91823
K42E	1.35924	-0.11853	0.85086
K42F	0.26072	0.43587	1.50367
K42G	1.74973	0.77221	0.68829
K42H	0.85449	0.54042	0.87101
K42I	0.27177	0.43066	1.46204
K42K	NA	NA	NA
K42L	-0.28756	-0.78845	1.56494
K42M	0.99858	0.38379	2.15212
K42N	0.5455	-0.17002	1.68967
K42P	0.18079	-0.94103	1.62637
K42Q	-0.28923	0.03953	1.45677
K42R	0.28153	0.73384	2.13376
K42S	1.17972	0.47357	1.50533
K42T	0.04795	-0.33175	0.9134
K42V	0.73957	-0.07646	2.16066
K42W	1.05901	0.53206	1.34217

K42Y	0.65486	0.00879	1.02068
K42X	-0.20556	-0.46201	-0.24262
Q43A	-0.72331	-0.86786	-0.39516
Q43C	-0.36693	-0.62556	0.73729
Q43D	-1.75442	-1.23137	-0.42254
Q43E	0.17613	0.47052	-0.75076
Q43F	1.3646	0.73604	-0.11859
Q43G	-0.04173	-0.1726	0.31258
Q43H	-0.01702	0.24286	-0.10818
Q43I	-0.24322	0.21791	-0.5277
Q43K	0.5685	-0.23994	0.02447
Q43L	0.28993	0.19297	-0.27665
Q43M	-0.75775	-1.57821	-0.13901
Q43N	-0.16926	-0.77645	-0.65071
Q43P	0.8556	0.02578	0.46396
Q43Q	NA	NA	NA
Q43R	-0.34543	-1.01208	0.12906
Q43S	-0.92079	-0.73079	-0.4034
Q43T	-0.8952	-0.19034	-0.32869
Q43V	-0.56393	-0.40435	-0.58282
Q43W	-0.85307	-0.47724	-0.64719
Q43Y	-0.12427	0.06838	-0.28484
Q43X	0.17028	0.01404	-0.29636
V44A	-0.47269	-0.64531	1.23797
V44C	0.00949	-0.23946	0.65873
V44D	0.96788	-0.63312	0.99901
V44E	-0.04225	-0.35577	0.76929
V44F	-0.7202	-1.39677	-0.39394
V44G	0.4658	1.10117	1.14849
V44H	-0.44051	-0.52933	1.79644
V44I	-0.55128	0.26945	-0.17003
V44K	-0.81823	-0.17303	0.21665
V44L	0.02488	0.46198	0.41508
V44M	0.59416	0.12781	0.26062
V44N	0.58106	1.61899	1.14254
V44P	-0.34543	-0.36551	0.94182
V44Q	-0.5208	-0.28867	0.72809
V44R	-0.40666	-0.38441	0.87617
V44S	-0.35493	0.94023	0.83997
V44T	-0.74819	-0.40255	0.45987
V44V	NA	NA	NA
V44W	-0.76575	-0.3088	1.92215
V44Y	-1.15137	-0.36654	0.35233

V44X	0.3029	0.37503	-0.57606
V45A	-0.84406	-0.39324	-0.45215
V45C	-0.29632	-0.36241	0.29352
V45D	-0.93996	-0.20596	-0.46543
V45E	-0.38199	0.16793	-0.46884
V45F	0.40758	0.35874	-0.3751
V45G	-1.7516	-1.94485	-0.63743
V45H	-0.20618	-0.31185	-0.29566
V45I	0.11222	-0.36816	-0.76436
V45K	0.07018	0.45596	0.29234
V45L	0.14145	0.09754	-0.63356
V45M	-0.32067	-0.51227	-0.4385
V45N	-0.88201	-0.78288	-0.52577
V45P	-1.72983	-0.45558	-0.91424
V45Q	-0.55602	0.06716	-0.60492
V45R	-0.19483	-0.21526	0.2261
V45S	-0.81192	0.12169	-0.41878
V45T	0.1916	0.47199	0.24401
V45V	NA	NA	NA
V45W	-1.07873	-0.60172	-0.39503
V45Y	-0.46161	-1.00787	-1.08147
V45X	0.18357	-0.17704	-0.39934
I46A	0.31212	-0.48563	0.19281
I46C	0.17577	-0.25336	-0.1167
I46D	-0.69251	0.0536	1.67859
I46E	0.4676	0.02237	1.9666
I46F	0.52881	-0.14341	-0.55447
I46G	-0.04575	-0.64979	1.41745
I46H	-1.63487	-0.43413	-0.19911
I46I	NA	NA	NA
I46K	-1.23689	-0.44866	0.00493
I46L	-0.26498	0.81289	-0.38832
I46M	-0.18984	0.14614	-0.01324
I46N	0.96005	0.83692	0.71119
I46P	0.38655	0.60461	1.07852
I46Q	-1.44748	-1.06764	-0.09184
I46R	-0.26091	-0.90723	-0.61285
I46S	-0.70493	-0.45463	0.51935
I46T	-0.50743	-0.33579	0.2708
I46V	0.06851	-0.13128	-0.05357
I46W	0.9694	0.19828	-1.18302
I46Y	-0.1187	0.01357	-0.70763
I46X	0.0841	-0.22291	-0.64768

D47A	-0.79425	-0.86892	0.84755
D47C	-1.20225	-1.61505	0.65081
D47D	NA	NA	NA
D47E	-0.83607	-0.10853	-0.00705
D47F	-1.21568	-1.21952	0.56573
D47G	-0.51829	-0.26506	0.50594
D47H	-1.29198	-0.60602	0.35419
D47I	0.4631	0.4363	1.68411
D47K	-0.01655	-0.29226	-0.1727
D47L	-0.71614	-0.50948	1.16975
D47M	-1.01599	-0.44026	1.22294
D47N	-0.08262	0.20626	-0.09037
D47P	0.0662	-0.32346	2.16548
D47Q	-1.99644	-0.15028	0.30107
D47R	-0.29921	-1.12363	0.22393
D47S	-1.89509	-0.54358	-0.69167
D47T	-0.7306	-0.04358	0.20159
D47V	-2.06696	-0.20381	1.36305
D47W	-1.00219	-0.293	0.54018
D47Y	-0.73918	-0.47923	0.60527
D47X	-1.55101	-2.48261	-0.88642
G48A	-0.87623	-0.0936	-0.16004
G48C	-1.26539	-0.59331	-0.15984
G48D	-0.40507	-1.90496	0.6486
G48E	-1.04292	-0.79302	-0.07972
G48F	-2.1105	-1.60997	-0.11686
G48G	NA	NA	NA
G48H	-0.40035	0.00556	0.23421
G48I	-0.36065	0.05187	0.47887
G48K	-0.55657	0.09399	0.58153
G48L	0.12575	-0.34516	-0.111
G48M	-1.11565	0.91829	0.28935
G48N	-0.65008	-0.07358	0.30924
G48P	0.35092	0.72695	1.49326
G48Q	-0.22168	1.06379	-0.10907
G48R	-0.05885	-0.47732	0.40355
G48S	-0.68087	0.44709	0.088
G48T	-0.9036	0.83426	0.18716
G48V	0.12115	-0.63809	0.31262
G48W	-0.71557	-0.77782	-0.16293
G48Y	-0.10188	-0.44707	0.2802
G48X	0.37561	0.01264	-0.8724
E49A	-0.77203	-0.5672	0.82959

E49C	0.0158	0.12578	0.58941
E49D	-0.01429	0.20085	0.20405
E49E	NA	NA	NA
E49F	-0.28774	-0.46389	0.37765
E49G	-1.35522	-0.81075	0.08023
E49H	-0.54766	-0.36794	0.26752
E49I	0.19626	-0.02478	1.57159
E49K	-0.80729	-0.66301	0.18887
E49L	0.37309	0.21774	0.33602
E49M	-0.47164	-1.41584	0.29671
E49N	0.29905	-0.97884	0.07962
E49P	-0.99097	-0.61967	0.40052
E49Q	-0.65888	-1.70617	0.35862
E49R	-0.78696	-0.41375	-9.00E-05
E49S	-0.52183	-1.19961	0.64484
E49T	-0.35775	0.37196	0.79415
E49V	-0.62828	0.63586	1.3209
E49W	-1.11426	0.28103	0.6083
E49Y	-0.17059	-0.29399	0.30127
E49X	-0.17714	-0.05706	-0.70376
T50A	-0.41927	-0.00415	0.54371
T50C	-0.20858	-0.94237	-0.2387
T50D	0.26216	0.27826	0.30007
T50E	-1.46708	-1.1575	-0.5623
T50F	-0.95531	-0.87896	-0.72416
T50G	-0.30837	-1.52914	-0.20821
T50H	0.19307	-0.47792	-0.56294
T50I	-1.18715	-0.44596	-0.35265
T50K	-0.54584	-0.22966	-0.05854
T50L	-1.0998	-0.65966	-0.50108
T50M	0.31469	-1.92777	-1.19966
T50N	-0.07579	0.33621	-0.14203
T50P	0.27255	0.90028	0.3141
T50Q	-0.45359	-0.11291	-0.21521
T50R	0.25363	0.89533	0.09058
T50S	-0.89463	-0.43537	-0.01391
T50T	NA	NA	NA
T50V	-0.62544	0.22446	-0.17269
T50W	0.11023	0.55284	-0.64221
T50Y	-0.46065	-1.22155	0.14924
T50X	-0.13299	-0.08708	-0.44737
C51A	0.19241	0.06334	-0.40088
C51C	NA	NA	NA

C51D	-0.34942	0.22303	1.25055
C51E	0.83077	1.54173	1.22752
C51F	-1.27838	-1.39581	0.94166
C51G	-0.77922	-0.53362	0.23437
C51H	-0.65759	-1.04707	0.06035
C51I	-0.25729	-0.1929	0.09055
C51K	-0.96054	-0.09033	0.47162
C51L	-0.01669	-0.69828	0.88337
C51M	0.70496	0.0844	0.43461
C51N	-0.38669	-0.2356	0.55469
C51P	-0.00736	-0.14698	2.00397
C51Q	-1.2384	-0.29979	0.69052
C51R	-1.03706	-0.15806	0.47646
C51S	0.09322	0.38972	-0.07594
C51T	0.60143	0.81489	0.26572
C51V	-0.23137	-0.93802	-0.03728
C51W	-0.02004	-0.2619	0.44277
C51Y	0.38017	-0.89511	0.36735
C51X	0.02394	0.75769	-0.77863
L52A	0.00101	-0.79112	0.00775
L52C	-0.04551	-0.81486	0.00903
L52D	-0.43104	-1.61587	-0.20776
L52E	1.04914	-0.57616	-0.69067
L52F	-0.41716	0.31324	0.59203
L52G	-0.93909	-0.36535	-0.24008
L52H	-0.13669	-0.09895	-0.09184
L52I	0.01032	-0.1916	0.92679
L52K	-0.91017	0.07875	0.65377
L52L	0.10502	0.41592	-0.04523
L52M	-1.019	0.39945	0.03868
L52N	-0.75838	-0.44183	-0.67802
L52P	0.46535	0.33936	1.85274
L52Q	-0.06163	-0.44847	0.66357
L52R	1.04305	0.23453	0.81752
L52S	-0.17377	0.61573	-0.12214
L52T	0.48916	-0.68888	-0.05843
L52V	-0.20993	0.50057	0.03226
L52W	-0.25019	-0.64091	-0.79057
L52Y	0.56353	-1.04078	0.73163
L52X	0.05518	-0.42707	-0.69377
L53A	0.47432	0.20726	2.89422
L53C	-0.2103	0.03634	2.16783
L53D	-0.35918	-0.56739	-0.5715

L53E	1.44937	2.04855	0.84084
L53F	-0.05938	-0.28861	1.61171
L53G	0.92955	0.83741	2.17083
L53H	0.95459	1.20875	-0.10619
L53I	1.41958	0.6528	2.06251
L53K	0.59474	0.57087	0.25973
L53L	-1.09664	-0.84724	-0.03914
L53M	0.30768	0.38595	0.31957
L53N	0.67995	2.41765	2.12341
L53P	0.32524	0.80201	1.2334
L53Q	1.33407	0.19067	1.53968
L53R	-0.66818	-1.13697	-0.81533
L53S	0.38654	0.79273	2.7809
L53T	-0.08743	0.98773	2.72323
L53V	0.06692	-0.06826	2.20287
L53W	0.48151	1.19721	1.12941
L53Y	0.15849	0.30695	1.71927
L53X	-0.14596	-1.50944	-1.06277
D54A	-0.62239	-0.67943	0.94519
D54C	-0.17538	-1.09959	1.23071
D54D	NA	NA	NA
D54E	0.00773	-0.25924	-0.5226
D54F	0.01369	-0.15297	2.05226
D54G	-1.67728	-1.0721	1.05079
D54H	-1.69013	-0.6968	0.18645
D54I	-0.50635	0.034	1.55932
D54K	-0.00277	-0.06838	1.33166
D54L	-0.6477	-0.29228	-0.15751
D54M	-0.97001	-1.58879	0.93512
D54N	-1.81065	-1.78249	-0.91427
D54P	0.55027	1.00694	2.08685
D54Q	-0.81797	0.36625	0.67155
D54R	-1.11468	-1.36714	0.55324
D54S	-1.5132	-0.65505	0.03587
D54T	-0.69581	-0.37029	0.93642
D54V	0.00655	-0.6632	1.73061
D54W	-1.22613	-0.24407	0.75562
D54Y	-0.20758	0.34004	2.48938
D54X	0.01995	-0.25426	-0.82732
I55A	2.05429	0.33705	2.08303
I55C	1.14629	1.31803	1.55463
I55D	-0.22758	-1.80241	-0.90945
I55E	0.07884	-0.60609	-0.28076

I55F	0.69333	-0.67101	3.23896
I55G	-0.2142	0.16836	-1.37712
I55H	1.2104	0.84699	0.41222
I55I	NA	NA	NA
I55K	0.17084	0.2338	-0.39878
I55L	-1.07541	-0.16665	2.22914
I55M	-0.54291	-0.16976	0.80118
I55N	0.59522	0.59293	1.06944
I55P	NA	NA	NA
I55Q	-0.49512	-0.46772	-0.5284
I55R	-0.01196	-1.04719	-0.68268
I55S	0.18156	-1.32926	1.69841
I55T	-0.53629	-1.16439	2.6038
I55V	-1.17309	-0.03502	0.64015
I55W	-1.76076	-2.3368	-1.8562
I55Y	0.17363	0.23919	0.24798
I55X	-0.45071	-0.73674	-0.52155
L56A	-0.07348	0.14026	1.02255
L56C	0.28431	0.75149	2.51714
L56D	0.42263	0.20015	1.69417
L56E	0.71407	2.85721	-0.05383
L56F	0.46234	0.40676	-0.78792
L56G	0.51899	2.09627	0.49472
L56H	-0.82611	-0.76668	1.71111
L56I	-0.56375	0.10944	1.91986
L56K	-0.62811	-1.32907	-1.91224
L56L	-1.74248	-1.11553	-0.50217
L56M	-0.55709	0.79543	-0.80144
L56N	1.80305	2.29681	1.90036
L56P	-0.7499	-0.94768	-0.79965
L56Q	-0.73902	-0.20862	-1.43108
L56R	-2.11964	-0.4893	-2.5076
L56S	0.31722	0.8988	1.53762
L56T	9.00E-05	0.15413	0.23178
L56V	-0.27242	0.27407	0.78478
L56W	-1.33762	-1.04168	-0.2034
L56Y	-1.29111	-0.78771	0.21121
L56X	0.53469	-0.01473	-0.79577
D57A	-0.89827	-0.94315	-3.52372
D57C	0.11766	1.10759	-2.81662
D57D	NA	NA	NA
D57E	0.04657	0.17936	-0.56849
D57F	-1.08692	-0.67393	-3.20581

D57G	-0.78449	-1.84622	-2.82224
D57H	-1.09643	-0.82827	-2.00801
D57I	-0.04638	0.05881	-3.51641
D57K	-0.40253	-0.48776	-2.0773
D57L	-1.18187	-2.29547	-3.40495
D57M	-1.19876	-1.63765	-2.17718
D57N	-0.35974	0.44934	-2.62698
D57P	-0.01158	-1.91916	-2.27007
D57Q	0.075	-0.91094	-1.7052
D57R	0.09503	-1.56892	-2.07862
D57S	-0.85308	-0.58741	-2.11359
D57T	-1.23583	-0.47853	-2.83346
D57V	-0.71799	-0.07425	-3.48034
D57W	-0.78309	-1.40006	-2.05978
D57Y	-0.90962	-1.2081	-2.30125
D57X	-0.53946	-1.09014	-1.01386
T58A	-0.37309	-0.09657	1.25636
T58C	-0.17709	0.05987	0.4426
T58D	-1.0587	-1.05891	-1.17695
T58E	0.48364	0.38355	0.49455
T58F	-0.25515	-0.67748	-0.12026
T58G	-0.24809	-0.13474	-0.05121
T58H	-0.28544	-0.18503	-1.05649
T58I	-0.66053	0.07296	-0.03345
T58K	0.01785	0.07973	-1.96635
T58L	-0.66318	-0.53039	-0.26698
T58M	-0.27898	0.34975	-0.15885
T58N	0.96545	-0.67066	-0.48894
T58P	-1.71609	-1.10206	-1.50371
T58Q	0.40259	0.3561	-0.39359
T58R	0.1289	-0.54206	-1.95676
T58S	0.36542	-0.29271	1.26945
T58T	NA	NA	NA
T58V	-0.47662	-0.46826	1.25636
T58W	0.3966	-0.98905	-1.13888
T58Y	-0.45409	-0.22424	-0.28622
T58X	-0.43057	-0.30004	-0.59573
A59A	NA	NA	NA
A59C	-0.98173	-0.74723	0.37249
A59D	-0.0426	-0.31679	-0.54824
A59E	-0.04259	-0.09417	-0.31092
A59F	-0.64047	-0.91839	-1.00169
A59G	2.14543	3.65627	2.24563

A59H	0.06137	-1.42201	-0.40356
A59I	0.58692	0.00628	-0.44984
A59K	-0.24859	0.40886	-2.6205
A59L	0.17883	-0.25009	-0.52078
A59M	-0.59488	-0.70971	-1.45061
A59N	-0.0339	0.3936	0.61436
A59P	0.27135	0.14311	-0.21334
A59Q	-0.28322	-0.67449	-0.2508
A59R	-1.29452	-0.7176	-3.50347
A59S	2.77387	4.57712	1.95999
A59T	2.31743	2.86442	1.31528
A59V	-0.27254	-1.10522	-1.18864
A59W	-0.72765	-0.85938	-1.59394
A59Y	-0.59002	-1.30157	-1.32601
A59X	-0.9518	-1.14283	-0.82731
G60A	-0.20618	-0.04475	-1.41651
G60C	-0.05617	-0.37815	-0.95289
G60D	0.35972	-0.06221	-0.31726
G60E	-0.65695	-0.60043	-0.93133
G60F	-0.48881	-1.02606	-0.84178
G60G	NA	NA	NA
G60H	0.07158	-0.20179	-0.63158
G60I	-0.73962	-0.44711	-0.92764
G60K	0.21286	-0.23935	-1.47769
G60L	-0.44232	-0.17639	-1.3212
G60M	0.08385	-0.00026	-0.91334
G60N	0.30176	0.2351	-0.70016
G60P	0.63548	0.80001	-1.54929
G60Q	-0.70054	-0.16669	-0.52736
G60R	-0.21947	-0.43773	-1.67753
G60S	0.60654	-0.32531	-1.1822
G60T	0.14725	-0.10619	-1.45142
G60V	0.72007	0.3405	-1.01292
G60W	0.87808	0.40434	-0.88064
G60Y	-0.00752	0.13618	-0.66293
G60X	1.08958	0.41833	-0.89346
Q61A	-0.68291	-0.82044	-0.59414
Q61C	0.26789	0.43581	0.3509
Q61D	-0.74642	0.14003	0.28302
Q61E	0.41553	0.27495	-0.82267
Q61F	0.11241	-0.28742	-0.72517
Q61G	-0.0373	0.01854	-0.94775
Q61H	0.3872	0.51177	0.27552

Q61I	1.08127	0.54526	1.12172
Q61K	-0.7489	0.0416	-0.52869
Q61L	2.01734	2.66656	1.78105
Q61M	1.91578	2.65514	1.08247
Q61N	1.24989	1.43046	-0.00268
Q61P	-0.17077	-0.55113	-1.18812
Q61Q	NA	NA	NA
Q61R	4.7804	6.15824	1.44152
Q61S	1.22413	1.17899	0.31338
Q61T	0.09591	0.5535	-0.28068
Q61V	0.09079	0.32868	0.1275
Q61W	1.22012	0.70255	-0.20436
Q61Y	-0.27623	0.31878	-0.35126
Q61X	1.73716	-0.55408	-0.90488
E62A	-0.41442	-0.43887	-1.19183
E62C	-0.11748	-0.02119	-0.94365
E62D	2.70769	-0.15759	0.30596
E62E	NA	NA	NA
E62F	-0.49569	-1.0617	-1.28379
E62G	1.40418	0.02371	-0.97454
E62H	0.7372	0.99265	-0.89491
E62I	-0.27018	-0.17875	-1.2618
E62K	0.15092	-0.36257	-1.31422
E62L	-0.08607	-0.38401	-0.8581
E62M	0.10073	-0.02569	-1.26765
E62N	0.53237	-0.19	-0.90955
E62P	0.63267	-0.80389	-0.83292
E62Q	-0.2677	0.32923	-1.42285
E62R	0.91588	0.48024	-0.8277
E62S	0.10802	0.16297	-0.81229
E62T	-0.28606	-0.61229	-0.91637
E62V	-0.60806	-2.11271	-1.22115
E62W	-0.18916	-0.933	-1.17232
E62Y	-0.55962	-0.48007	-1.30648
E62X	-0.35916	-1.10178	-0.68695
E63A	0.42949	-0.3854	1.21297
E63C	0.90728	1.04411	0.9625
E63D	0.77172	0.49221	0.66797
E63E	NA	NA	NA
E63F	1.41797	0.35729	-0.8345
E63G	1.19788	-0.11615	0.67703
E63H	1.84836	1.04134	-0.75533
E63I	0.17098	0.3605	0.17903

E63K	0.82904	1.34541	0.94766
E63L	1.19574	-0.84075	0.39176
E63M	1.02069	0.27274	0.15314
E63N	0.45547	-0.27677	-0.35485
E63P	0.87037	0.17774	-1.49281
E63Q	1.07449	-0.01689	2.7477
E63R	2.16613	0.94016	1.16741
E63S	0.01582	0.39978	1.81596
E63T	0.43861	0.33076	1.04485
E63V	-0.36796	-0.50035	0.56274
E63W	-0.35492	0.34349	-0.88752
E63Y	1.49681	1.44329	-1.06637
E63X	0.16011	-0.23969	-0.90878
Y64A	0.16707	0.23746	-1.20647
Y64C	1.27059	0.19242	-0.62358
Y64D	2.74318	-0.47923	-0.26503
Y64E	2.14688	0.19504	0.3126
Y64F	1.3035	-0.01261	0.32656
Y64G	-0.58382	-1.1048	-1.09988
Y64H	1.35798	-0.29642	-0.61489
Y64I	1.44902	-0.54251	0.85767
Y64K	1.55488	0.20077	-0.64055
Y64L	3.60335	0.09481	1.16216
Y64M	0.81718	-0.54006	-0.3313
Y64N	3.34185	-0.50027	0.04456
Y64P	0.40438	-0.2504	-1.2871
Y64Q	1.30644	0.17256	0.48722
Y64R	1.26532	0.01123	-0.78548
Y64S	-0.02356	-0.08456	-1.04139
Y64T	1.83158	-0.45798	1.12181
Y64V	-0.61232	-0.64424	-0.0836
Y64W	0.58153	-0.55592	-1.07701
Y64Y	NA	NA	NA
Y64X	-0.60746	-1.3065	-0.85467
S65A	NA	NA	NA
S65C	NA	NA	NA
S65D	NA	NA	NA
S65E	NA	NA	NA
S65F	NA	NA	NA
S65G	NA	NA	NA
S65H	NA	NA	NA
S65I	NA	NA	NA
S65K	NA	NA	NA

S65L	NA	NA	NA
S65M	NA	NA	NA
S65N	NA	NA	NA
S65P	NA	NA	NA
S65Q	NA	NA	NA
S65R	NA	NA	NA
S65S	NA	NA	NA
S65T	NA	NA	NA
S65V	NA	NA	NA
S65W	NA	NA	NA
S65Y	NA	NA	NA
S65X	NA	NA	NA
A66A	NA	NA	NA
A66C	-0.31794	0.56496	0.53079
A66D	1.74329	0.63575	1.48634
A66E	-0.46864	-0.46561	1.77173
A66F	0.23737	-0.03835	0.67424
A66G	0.35881	-0.13116	3.00709
A66H	0.05703	0.69215	2.18462
A66I	-0.30154	-0.35125	0.16128
A66K	0.76707	0.06704	2.41734
A66L	-0.18584	0.43186	0.80777
A66M	0.57054	0.57586	1.17625
A66N	-0.0535	-0.24746	3.3879
A66P	-0.50817	-0.04777	1.74682
A66Q	-0.48758	-0.47944	2.5729
A66R	-0.77132	0.70295	2.46278
A66S	-0.62829	0.50684	2.25574
A66T	-0.02184	-0.36388	2.0442
A66V	-1.79602	-1.66442	1.10363
A66W	0.27332	0.68063	0.32964
A66Y	1.33231	1.28416	3.39497
A66X	-0.25536	-0.71658	-0.96521
M67A	-1.23567	-1.19861	-1.06359
M67C	-1.6222	-0.39586	-1.99393
M67D	-0.92422	-0.33588	-1.12488
M67E	-0.38087	-1.03315	-1.2945
M67F	-2.07196	-0.85544	-0.57552
M67G	-0.10383	-0.10406	-0.38001
M67H	-0.6713	-0.25291	-2.26929
M67I	-0.88388	-0.10657	-1.11665
M67K	-0.71256	-0.05261	-1.44374
M67L	-0.22802	-0.52909	-0.69657

M67M	NA	NA	NA
M67N	-0.59723	-0.37333	-0.12591
M67P	0.28033	0.79029	-1.48573
M67Q	-1.3456	-1.06941	-1.58545
M67R	-0.06832	-0.2931	-1.68522
M67S	-0.96765	-0.89211	-1.02107
M67T	-0.47694	0.23159	-1.3007
M67V	-0.04341	0.15291	-1.9843
M67W	-0.71195	-0.89658	-1.20524
M67Y	-0.18889	-0.4405	-2.39016
M67X	0.46231	0.14658	-0.70256
R68A	2.59457	2.36504	0.07717
R68C	1.96737	1.12311	0.11364
R68D	3.90642	0.36227	0.2104
R68E	3.77802	-0.61126	0.48133
R68F	2.93616	0.46119	-0.97488
R68G	0.77864	0.44941	-0.17212
R68H	2.97199	0.04146	0.35824
R68I	-0.92776	0.97925	-1.98775
R68K	-0.14143	0.58592	-0.86029
R68L	1.47845	1.55914	-1.45919
R68M	0.91599	2.36743	-0.03327
R68N	3.17357	3.94107	-0.43191
R68P	3.01091	1.0315	-0.47517
R68Q	1.29038	1.82861	0.36321
R68R	-0.62818	0.26584	0.01666
R68S	3.76125	3.47463	0.36503
R68T	-0.01373	0.62601	-0.30032
R68V	-0.4869	-0.2868	-0.26015
R68W	1.8878	-0.30779	-0.9525
R68Y	2.87387	-0.62553	-0.9227
R68X	-0.34739	-0.74961	-0.83972
D69A	0.45918	0.74222	-1.3917
D69C	-0.613	-0.05577	-1.75591
D69D	NA	NA	NA
D69E	0.05754	-0.12985	-0.20317
D69F	0.34245	0.59178	-1.41287
D69G	1.34379	1.50579	-1.39207
D69H	0.23984	0.0337	-1.24709
D69I	-0.36904	0.45928	-1.21902
D69K	-0.33101	0.05	-1.54989
D69L	-0.36882	0.50567	-1.23611
D69M	-0.29038	1.28185	-1.32155

D69N	0.22101	0.05169	0.2302
D69P	-1.0941	-0.99667	-2.72197
D69Q	0.1002	-0.31031	-1.0384
D69R	-1.51523	0.10978	-1.31301
D69S	-1.16092	-1.22821	-0.70467
D69T	-0.80569	0.12799	-2.04069
D69V	-0.61355	0.89637	-1.56235
D69W	-0.00105	0.0603	-1.26479
D69Y	0.05066	0.20517	-1.85725
D69X	0.05017	-0.20795	-0.72158
Q70A	-1.51553	-0.74135	1.64748
Q70C	-0.79496	-1.05573	1.35403
Q70D	-0.51899	-0.44575	-0.10025
Q70E	-0.37339	-0.82056	0.78519
Q70F	-1.85441	-1.8139	1.04836
Q70G	-1.02851	-0.70425	-1.85729
Q70H	-0.49658	-0.19033	0.80831
Q70I	0.77797	-0.14791	2.12451
Q70K	-0.63394	0.70106	0.0039
Q70L	-0.36645	-1.0142	2.48856
Q70M	-0.27588	-0.25341	3.26006
Q70N	0.89844	0.08553	2.64559
Q70P	2.99881	-0.53252	0.7414
Q70Q	NA	NA	NA
Q70R	-0.38236	-0.2255	0.46049
Q70S	-0.71738	-0.56902	1.6922
Q70T	0.04406	-0.1861	2.30141
Q70V	-0.32935	0.15664	1.78694
Q70W	-0.58649	-0.03544	-1.03902
Q70Y	0.10901	-0.20328	0.10648
Q70X	-0.43066	-0.62127	-0.7664
Y71A	-1.18739	0.28952	-0.15648
Y71C	0.17921	0.0525	-0.84478
Y71D	0.51408	0.07285	1.65103
Y71E	-1.82577	-0.55603	0.44994
Y71F	-0.81944	-0.79241	-1.11529
Y71G	0.03086	0.29235	-1.42357
Y71H	-0.54953	0.21404	1.04387
Y71I	-0.66741	0.62635	0.57439
Y71K	-0.95533	-0.03621	-1.07982
Y71L	-1.17121	-0.73363	-0.01811
Y71M	-2.03602	-1.63374	0.53204
Y71N	-0.57468	-1.0844	-0.18437

Y71P	-0.69556	0.5566	-1.65209
Y71Q	-0.02704	-1.43165	-1.47223
Y71R	-0.94091	-1.28991	-1.42346
Y71S	-0.27969	-0.1628	-0.51999
Y71T	-0.91097	0.26804	1.25802
Y71V	-0.39857	-0.95897	1.07559
Y71W	0.48758	0.05407	-0.46197
Y71Y	NA	NA	NA
Y71X	0.20614	-0.68999	-1.00783
M72A	0.14652	-1.7229	-0.06115
M72C	2.00415	-0.74913	0.67815
M72D	2.18393	0.42819	-0.57794
M72E	0.45396	-0.77381	-0.61864
M72F	-0.30306	0.40559	1.52978
M72G	0.10168	-0.98157	-1.35224
M72H	0.32526	0.05453	1.0645
M72I	0.95789	-0.3	0.39719
M72K	1.30598	1.10714	-0.52846
M72L	2.30373	0.15053	0.7062
M72M	NA	NA	NA
M72N	-0.19941	-0.36501	-0.46528
M72P	0.77876	-0.79604	-1.80601
M72Q	-0.27868	0.33296	-0.57942
M72R	1.34865	0.17289	-0.27289
M72S	1.85239	0.13922	-0.00346
M72T	2.28845	-1.29617	-0.42319
M72V	1.83183	0.40361	0.35435
M72W	5.29518	1.42561	1.26957
M72Y	-0.28625	0.97393	0.81019
M72X	0.34025	-0.42051	-0.87438
R73A	-0.75621	-0.19911	1.65618
R73C	-1.10607	-0.00017	1.74828
R73D	0.18982	1.17795	1.31476
R73E	-0.50364	-0.48043	1.2684
R73F	0.19433	0.4134	-1.24379
R73G	-2.66556	-0.78031	0.98534
R73H	-0.20151	0.09543	-0.6636
R73I	-0.2597	0.55972	0.12997
R73K	0.14257	-0.03795	0.07175
R73L	0.00683	-0.42689	0.08123
R73M	-0.03165	0.04391	0.51766
R73N	-1.15931	-0.68847	1.50549
R73P	1.608	-1.28781	-0.02819

R73Q	0.40915	0.60981	2.03884
R73R	0.35704	0.22894	0.25105
R73S	-0.20375	0.5368	2.0945
R73T	1.10943	0.59176	1.82642
R73V	-0.03345	0.31554	1.84262
R73W	0.42881	0.2111	0.15381
R73Y	0.38794	-0.58929	-0.54327
R73X	0.05416	-0.00397	-0.78381
T74A	-0.28491	-0.55838	1.19904
T74C	-0.69639	0.15829	1.14089
T74D	0.12406	0.15444	0.2412
T74E	-0.78553	-0.13802	0.94921
T74F	-0.24168	0.31566	1.67322
T74G	-0.07672	0.26409	0.80081
T74H	-0.74904	-0.69855	0.95789
T74I	-0.24334	0.13021	1.4623
T74K	-0.73014	-0.64996	1.39725
T74L	-0.11298	0.13641	2.05756
T74M	0.55122	0.31841	1.5819
T74N	-0.17736	-0.02953	0.77414
T74P	-0.00873	-0.07093	1.07209
T74Q	-1.45275	-0.02475	1.00237
T74R	-0.59438	0.41111	1.33136
T74S	-0.06454	-0.18197	0.5296
T74T	NA	NA	NA
T74V	-0.8173	0.06636	1.06908
T74W	0.73377	1.06779	1.1403
T74Y	-0.19803	-0.23276	1.6513
T74X	0.40189	0.59655	-1.33739
G75A	-0.11909	0.65798	-0.85299
G75C	-0.37827	-0.42864	-0.99109
G75D	1.25904	-0.99636	-1.53202
G75E	-0.23797	-1.18246	-0.54743
G75F	-0.06586	-0.31383	-2.15434
G75G	NA	NA	NA
G75H	-0.52389	-0.22309	-1.56408
G75I	-0.86896	-1.34617	-0.32491
G75K	-1.24463	-1.24456	-2.62588
G75L	-0.68139	-0.26634	-0.96485
G75M	-0.34694	-0.78808	-1.30184
G75N	-0.98694	-0.44121	-0.86132
G75P	-0.84376	-0.39464	0.02861
G75Q	-0.91449	-1.01628	0.36193

G75R	-0.62352	-0.05334	-0.87434
G75S	-0.47841	-0.06041	-1.1899
G75T	-0.63531	-1.01487	-0.69097
G75V	-0.09998	0.72483	0.18292
G75W	0.21794	0.54366	-0.67539
G75Y	-0.27471	-0.22996	-2.2946
G75X	-0.73759	-0.48888	-0.74062
E76A	-0.72795	-0.00706	-1.20513
E76C	-1.19676	-0.52699	-0.72215
E76D	-0.25463	-0.57716	-0.22504
E76E	NA	NA	NA
E76F	-0.91326	-0.68515	-0.48136
E76G	-0.16011	-0.32649	-1.07652
E76H	0.40317	1.01065	-0.85489
E76I	-0.31774	0.10892	-0.40371
E76K	-0.85726	-0.74762	-0.97785
E76L	-1.0985	-0.88336	-1.08219
E76M	0.17281	-0.55783	-0.69904
E76N	-0.57373	-0.28754	-0.66298
E76P	1.25944	1.06504	-0.54758
E76Q	-0.50525	-0.0902	-0.74719
E76R	-0.37797	-0.24147	-1.17906
E76S	-0.33741	-0.1975	-0.83399
E76T	1.50435	-0.54082	0.62323
E76V	-1.25207	-0.73452	-0.51677
E76W	-0.20865	-1.01356	-0.15315
E76Y	0.16356	-0.26021	-0.34595
E76X	-0.18547	-0.50124	-0.62978
G77A	-0.01421	0.30321	1.79217
G77C	-0.29403	1.06893	1.15883
G77D	-0.06196	-0.89359	-0.70812
G77E	0.17444	0.26661	-0.5832
G77F	2.5631	2.86255	1.11223
G77G	NA	NA	NA
G77H	1.04282	1.29213	0.82928
G77I	2.34438	1.68757	0.71685
G77K	0.75214	0.64129	-0.52148
G77L	1.40316	0.96826	0.79129
G77M	1.15948	1.92427	1.2552
G77N	1.28473	0.39578	1.06675
G77P	-0.46976	-1.08791	-0.83348
G77Q	-0.16444	0.0322	-0.14642
G77R	0.11015	0.31543	-0.5272

G77S	0.18054	1.36094	0.67459
G77T	2.01632	2.94104	0.59172
G77V	4.19469	4.37404	1.18985
G77W	0.67436	0.47329	-0.2398
G77Y	3.60652	3.98042	1.05662
G77X	-0.11957	-0.20908	-0.94111
F78A	1.2663	-0.10602	0.39754
F78C	1.74662	0.42757	0.68375
F78D	-0.47151	0.33479	-0.19308
F78E	1.34262	0.25258	-0.44761
F78F	NA	NA	NA
F78G	-0.44041	0.23992	-0.23285
F78H	2.00791	0.02504	1.11657
F78I	1.32464	0.62622	0.05297
F78K	0.53979	-0.2079	-0.43204
F78L	-0.05928	-1.04585	-0.1054
F78M	1.0065	0.94903	0.3179
F78N	-0.49176	-0.43382	0.44333
F78P	0.05933	0.32406	-0.58209
F78Q	0.69482	0.17303	-0.40548
F78R	0.52156	0.73315	-0.91698
F78S	0.49716	0.53064	0.33102
F78T	0.43743	-0.5333	0.75159
F78V	0.88125	-0.69456	0.53817
F78W	0.11681	-0.2961	0.46982
F78Y	-0.63196	-0.51607	0.36795
F78X	-0.72097	-0.66552	-0.82622
L79A	-0.54694	-0.02901	0.58519
L79C	0.19084	-0.15165	0.52837
L79D	0.64021	0.48798	-0.88693
L79E	-0.41736	0.0475	-0.24896
L79F	-0.78387	-0.87323	0.80875
L79G	0.43975	0.07379	0.39617
L79H	-0.92412	0.29604	-0.20276
L79I	-0.54908	-0.07921	0.1534
L79K	-0.07994	-0.06146	-0.54248
L79L	-0.05437	0.06292	-0.13068
L79M	-0.38034	0.17527	-0.12602
L79N	-0.77652	-0.25889	-0.2344
L79P	0.07555	0.50519	-0.57577
L79Q	-0.65506	-0.39822	0.26951
L79R	0.60832	-0.17122	-0.87559
L79S	-0.98019	-0.29753	0.14706

L79T	-0.18694	0.75471	0.25891
L79V	-0.03645	0.71564	0.34962
L79W	0.53343	0.90242	1.27647
L79Y	-0.39034	-0.08369	1.18522
L79X	0.26938	0.23195	-1.01773
C80A	-0.83722	-0.48012	-0.05715
C80C	NA	NA	NA
C80D	-0.97065	-0.66725	-0.58328
C80E	-0.09618	0.60434	-0.14245
C80F	0.00321	-0.14716	0.11279
C80G	0.13871	0.56353	-0.03314
C80H	-0.98495	-0.58428	-0.41878
C80I	0.4419	0.4629	0.32644
C80K	-0.899	-0.64725	0.08452
C80L	0.20911	0.59102	-0.03101
C80M	-0.27519	0.13716	0.31383
C80N	-0.69848	-0.99203	-0.58641
C80P	-1.35607	-0.22542	-0.24103
C80Q	-0.97427	-0.87579	-0.29389
C80R	0.75975	0.6648	-0.57276
C80S	-1.04368	-0.34106	-0.14546
C80T	-0.30492	-0.94823	-0.01084
C80V	0.02464	0.1886	0.33677
C80W	-0.34692	0.45595	-0.67248
C80Y	0.80707	0.20685	-0.08916
C80X	0.97588	0.49502	-0.98749
V81A	-0.79709	-0.29484	0.10284
V81C	-0.34238	-0.22346	0.00256
V81D	0.26695	-0.15263	-0.86701
V81E	-0.7794	-1.21353	-0.7191
V81F	0.51805	1.95362	0.46773
V81G	-1.27885	-0.31758	0.02249
V81H	-0.07405	-0.56734	-0.90945
V81I	0.45358	-0.25068	0.48943
V81K	-0.29022	0.40066	-0.84886
V81L	0.1991	-0.77706	-0.19207
V81M	-0.4562	-0.17039	0.10735
V81N	-1.27367	-1.08388	0.28346
V81P	-0.0015	-0.09884	-0.51722
V81Q	-0.49878	0.18961	-0.29533
V81R	-0.07068	0.32302	-0.84914
V81S	-0.57683	-0.36461	0.72016
V81T	-1.05755	-1.03207	0.40628

V81V	NA	NA	NA
V81W	0.29405	-0.14928	-0.70082
V81Y	-0.90039	-0.13343	-1.02889
V81X	0.71368	-0.06133	-0.87317
F82A	-0.66112	0.00638	-0.18015
F82C	-1.50273	-0.55802	-0.34957
F82D	-0.22629	-0.364	-0.84458
F82E	-1.02491	-0.33877	-0.78874
F82F	NA	NA	NA
F82G	-0.19943	0.52952	0.67932
F82H	-0.91238	-0.12768	0.00123
F82I	-0.20518	-0.3738	0.42372
F82K	-0.51526	-0.71167	-0.68962
F82L	1.24738	1.50229	-0.04314
F82M	-0.80303	-0.55714	-0.21728
F82N	-0.44655	-0.77906	-1.24317
F82P	0.11296	-0.40564	-0.63892
F82Q	0.1932	0.24497	-0.97093
F82R	-1.02778	-1.24595	-1.48461
F82S	-0.37806	-0.58044	-0.0329
F82T	-0.54555	-0.15521	-0.15061
F82V	-0.0253	-0.60489	0.04044
F82W	-0.67922	-0.44222	0.15226
F82Y	-0.19595	0.22601	0.28014
F82X	0.11279	0.11065	-0.94267
A83A	NA	NA	NA
A83C	-0.13609	-0.72504	0.37728
A83D	-0.08589	-0.25248	-0.44266
A83E	-0.7145	0.20936	-0.37942
A83F	0.04002	-0.46217	-0.76915
A83G	0.16595	-0.27788	1.45263
A83H	0.79856	2.25205	2.52012
A83I	-0.19314	0.36022	1.45046
A83K	0.36734	0.62785	1.7179
A83L	0.31057	0.68182	-0.03539
A83M	-0.91993	-0.06193	-0.80562
A83N	-0.42356	1.28262	2.19999
A83P	-0.97522	-0.25482	-0.92142
A83Q	-0.85526	-0.23846	1.77491
A83R	-0.30848	-0.38653	1.44772
A83S	-0.49585	0.18141	0.52811
A83T	-0.65673	-0.02651	1.57056
A83V	1.58477	2.51855	1.81057

A83W	0.20634	-1.48433	-1.23076
A83Y	-0.29455	0.07774	-0.5899
A83X	-0.42064	-1.18727	-0.41568
I84A	-0.32755	-0.07301	1.76407
I84C	-0.14143	-0.27565	1.47284
I84D	-0.91882	-0.08135	0.7024
I84E	-0.74335	-0.57681	1.01306
I84F	0.98336	1.18472	1.38021
I84G	-0.75131	-0.12564	1.49665
I84H	-0.01892	-0.31287	1.369
I84I	NA	NA	NA
I84K	-0.85388	-0.26965	0.63343
I84L	-1.14327	-0.67821	-0.40119
I84M	0.7282	1.09608	1.10059
I84N	-0.22898	0.00314	0.4366
I84P	-0.66377	-0.63733	2.10962
I84Q	0.56016	1.57533	0.78419
I84R	0.11016	-0.38101	0.38717
I84S	-0.08292	0.92501	1.07427
I84T	-0.87341	-0.14159	0.91671
I84V	-0.36678	-0.47357	-0.0385
I84W	-0.36922	-0.13634	1.51464
I84Y	0.7841	-0.71533	1.78487
I84X	-0.35792	-0.84641	-0.47007
N85A	-1.10444	-0.73395	0.92044
N85C	-0.04527	0.90983	0.69124
N85D	-1.3547	-0.24418	-0.38685
N85E	0.88901	0.40336	-0.52255
N85F	-1.24534	-0.28105	1.39234
N85G	-0.78636	0.1889	1.742
N85H	1.25434	1.1969	2.07832
N85I	0.07902	0.28407	0.76705
N85K	0.01272	0.62986	1.05914
N85L	-1.2546	-0.79369	0.98849
N85M	-0.33254	-0.24372	1.70835
N85N	NA	NA	NA
N85P	-0.7259	0.20204	0.72892
N85Q	-0.48587	0.28505	0.99855
N85R	-1.09573	-0.71077	0.58529
N85S	0.18833	-0.17754	0.43755
N85T	-0.87111	-0.02229	0.38225
N85V	-0.23889	0.57353	0.48423
N85W	-0.1444	0.51175	-0.0217

N85Y	-1.17618	-1.05958	2.06617
N85X	0.15166	0.09552	-0.79048
N86A	-0.29489	-0.05577	-0.10826
N86C	-1.82901	-1.48042	-0.56063
N86D	-0.48526	0.65663	-0.84385
N86E	-0.29335	-0.90526	-0.60807
N86F	-0.57455	-0.31821	-0.91971
N86G	-0.7214	0.57256	-0.17611
N86H	-1.26412	0.29601	-0.27217
N86I	0.02233	-0.0682	-0.78929
N86K	-0.12406	0.07177	0.20738
N86L	-1.11204	-0.13423	-1.1305
N86M	-0.68505	-0.71764	-1.38771
N86N	NA	NA	NA
N86P	-0.06994	-0.56127	-1.0245
N86Q	-0.53754	-0.0635	-0.12641
N86R	-0.79541	0.87041	-0.18828
N86S	0.15528	0.0349	0.01096
N86T	0.13456	0.43087	0.02542
N86V	-0.31385	0.29111	-0.26724
N86W	-0.54565	0.12327	-1.31273
N86Y	-1.33559	-0.16297	-0.88298
N86X	-0.24025	-0.81411	-0.84435
T87A	0.34776	-0.02814	-0.1353
T87C	0.45766	0.06198	-0.29063
T87D	-0.25015	-1.32821	0.54142
T87E	-0.89979	-0.42361	0.06527
T87F	-0.07116	-0.00381	-0.21833
T87G	-0.67888	0.87088	-0.33529
T87H	-1.5637	-1.90526	0.08503
T87I	-0.97404	-0.41413	-0.0502
T87K	-1.26972	-0.64909	0.06598
T87L	-0.60345	-1.49643	0.05023
T87M	0.24981	0.13352	-0.04591
T87N	-0.31024	0.39843	0.22786
T87P	0.24396	0.32329	0.06079
T87Q	-1.01418	0.44892	0.00793
T87R	-0.20382	-1.74395	-0.76496
T87S	-1.14159	-0.0676	-0.24303
T87T	NA	NA	NA
T87V	-0.61475	-0.36008	0.04733
T87W	-0.43915	-0.04809	-0.59889
T87Y	-0.9115	-0.68542	0.02413

T87X	-0.10818	-0.56167	-0.98804
K88A	-0.13304	-1.18568	0.08329
K88C	-0.38706	0.7594	-0.56292
K88D	0.09627	-0.28714	0.68835
K88E	-4.14742	-1.6651	0.66357
K88F	-1.01162	-0.14722	0.25519
K88G	-0.66279	0.95379	-0.16726
K88H	-0.15024	-0.75084	-0.10853
K88I	0.74076	1.4288	0.61555
K88K	NA	NA	NA
K88L	-0.75424	-0.30021	0.16069
K88M	0.5857	-0.86148	0.23264
K88N	-0.05409	0.03209	0.25544
K88P	-1.86396	-1.3597	0.60897
K88Q	-0.95541	-0.27022	-0.06165
K88R	-1.45261	-0.09604	0.26097
K88S	-1.162	-1.12496	0.15812
K88T	-1.0801	-0.60973	0.28149
K88V	-0.34573	-0.35166	-0.37452
K88W	0.36412	0.46973	0.73821
K88Y	-0.04263	0.68277	0.13292
K88X	-1.2081	-1.88022	-0.38811
S89A	-0.63739	-0.22083	0.64064
S89C	0.45165	-0.21419	-0.14461
S89D	-1.06088	-0.25184	-1.20556
S89E	0.01268	-0.20435	-0.1415
S89F	-0.27905	0.16349	-0.26473
S89G	-0.64829	-1.46566	0.3911
S89H	-0.32957	-0.05738	0.23497
S89I	-0.87316	-1.25925	-0.48519
S89K	-0.83864	-0.39611	0.4974
S89L	-0.41431	0.09213	-0.46078
S89M	-0.80977	-1.19238	-0.37522
S89N	-0.9226	0.21502	-0.04653
S89P	-0.7977	-0.83083	0.26263
S89Q	-0.49205	-2.17934	-0.24445
S89R	-0.36082	0.34025	-0.33163
S89S	-0.90894	0.30279	-0.20974
S89T	-0.83338	-3.02137	-0.24634
S89V	0.2172	0.71667	-0.58639
S89W	-0.17893	0.05827	0.78189
S89Y	-0.93964	-0.44278	0.34765
S89X	-0.34649	-0.31426	-0.58629

F90A	-2.74243	-0.55771	-0.36756
F90C	0.62884	0.51056	-0.3315
F90D	-0.23802	-0.2134	-0.90788
F90E	0.01727	0.15129	0.34451
F90F	NA	NA	NA
F90G	-0.7201	-0.89668	-0.19691
F90H	-3.8391	-0.21375	-0.05707
F90I	-0.5744	-0.35358	-0.03833
F90K	NA	NA	NA
F90L	-3.08616	-2.75493	-0.8679
F90M	-1.61304	-0.61332	0.05546
F90N	0.21847	-0.00442	-0.21415
F90P	-0.25791	0.57914	-1.04337
F90Q	-0.94284	-3.47385	-0.30102
F90R	0.26944	-0.85135	-0.89625
F90S	-3.6751	-1.91746	-0.91583
F90T	0.15505	-0.58084	-0.0658
F90V	0.01603	-1.24451	-0.05202
F90W	0.47502	0.39297	0.71859
F90Y	-0.93834	0.95354	0.38613
F90X	-0.60079	-1.41645	-1.29278
E91A	-1.09167	-0.82383	-0.05119
E91C	-1.15209	0.2491	-0.17978
E91D	-0.12028	0.5794	0.04412
E91E	NA	NA	NA
E91F	-0.25055	0.19172	-0.43727
E91G	-0.76086	0.29622	0.02619
E91H	-1.09781	-2.25415	-0.15394
E91I	-1.60371	-2.29077	-0.4062
E91K	-1.5761	-0.27538	-0.51323
E91L	-0.46452	0.0366	-0.17559
E91M	-0.56361	-1.68163	0.30945
E91N	-1.08311	-2.25398	-0.08909
E91P	-0.11158	1.10898	-0.40062
E91Q	0.49396	0.57286	-0.05137
E91R	-0.75254	-0.39763	-0.41429
E91S	-2.63116	-1.71785	-0.3901
E91T	-0.76865	0.67086	0.13814
E91V	0.47031	0.76035	-0.13786
E91W	-0.83412	-0.6191	-0.14955
E91Y	-0.97724	-1.28747	-0.27181
E91X	0.06684	-0.19696	-0.83259
D92A	0.48616	-0.4706	-0.04752

D92C	0.70819	0.66989	-0.29535
D92D	NA	NA	NA
D92E	-0.89391	-0.2535	0.09958
D92F	0.64533	-0.30119	-0.45845
D92G	0.10803	-0.66104	0.1154
D92H	0.40153	0.46524	0.23143
D92I	1.30974	-0.26994	-0.02944
D92K	2.98077	0.72616	-0.66991
D92L	2.56132	0.28747	0.08804
D92M	1.56879	-0.02739	0.22606
D92N	0.12326	-0.30549	-0.4272
D92P	1.70269	0.19659	0.22506
D92Q	-0.42331	-0.80106	0.16688
D92R	2.37107	0.28796	-0.66002
D92S	0.74111	-0.10249	0.11655
D92T	0.3612	-0.21759	-0.19746
D92V	0.60307	-0.49336	-0.04366
D92W	-0.34669	-0.56486	-1.18729
D92Y	0.46211	0.35052	-0.68187
D92X	-0.52023	-0.07813	-0.77747
I93A	-0.01577	-1.10438	-0.29903
I93C	-0.73248	0.26074	0.24941
I93D	0.17039	0.99853	-0.77376
I93E	0.33555	-0.97698	-0.69839
I93F	-0.29959	0.65706	-0.1849
I93G	-0.98423	-1.10092	-0.19615
I93H	-1.29266	-2.2091	-0.92366
I93I	NA	NA	NA
I93K	0.15123	0.21188	-0.73285
I93L	-0.40181	-0.29384	0.69018
I93M	0.2046	1.31358	0.72855
I93N	1.37852	0.44446	-0.40838
I93P	-0.09979	0.26512	-0.63327
I93Q	-0.36638	0.82309	0.20746
I93R	0.49838	0.69024	-0.93345
I93S	-0.19356	0.46192	-0.36219
I93T	-0.12708	0.50947	0.11205
I93V	-0.4452	0.02205	-0.46702
I93W	0.14914	-0.65575	-0.59997
I93Y	-0.31735	-0.18976	-0.5695
I93X	0.35569	0.41266	-0.43034
H94A	-0.53958	-0.17795	-0.02825
H94C	-0.26038	-0.88832	0.01124

H94D	-0.82654	0.05521	0.29761
H94E	-0.75968	0.015	0.56338
H94F	-0.71514	-0.39847	0.91782
H94G	-0.42063	0.07016	0.06715
H94H	NA	NA	NA
H94I	0.77654	-0.97707	0.83473
H94K	-0.08208	-0.38884	-0.53895
H94L	0.01284	0.95403	0.57221
H94M	-0.24673	1.11182	0.7541
H94N	-0.2174	0.62708	-0.25702
H94P	2.11847	-0.27069	0.00121
H94Q	-0.10801	0.69582	0.07556
H94R	0.15375	0.44634	-0.32406
H94S	-0.07017	0.68979	0.00994
H94T	0.07749	0.11436	0.01943
H94V	-0.85387	-0.62798	0.03326
H94W	-0.51186	-1.42921	0.74352
H94Y	0.16156	-0.48036	0.40008
H94X	-0.24958	-0.97835	-0.76669
H95A	2.941	-0.58895	0.07018
H95C	3.17605	-0.1412	0.24306
H95D	4.73715	-0.43884	1.0077
H95E	4.03688	-0.34673	0.72606
H95F	1.66871	-0.0059	-0.17361
H95G	4.4604	0.19004	0.56594
H95H	NA	NA	NA
H95I	1.78708	-0.36789	-0.51757
H95K	1.82345	0.43327	-0.70196
H95L	2.62187	-0.44472	-0.09789
H95M	4.15005	1.31265	0.71603
H95N	3.22913	-0.62773	0.04233
H95P	3.9644	0.06664	0.25881
H95Q	3.2913	0.50564	0.20543
H95R	2.3326	0.26213	-0.15519
H95S	3.64529	1.38086	-0.03738
H95T	2.83858	0.1012	-0.34265
H95V	2.80512	0.94577	-0.17734
H95W	1.99089	1.44642	0.62494
H95Y	2.69147	1.01219	0.30568
H95X	0.82343	1.03319	-0.79427
Y96A	2.42475	2.47172	-0.54909
Y96C	1.74261	1.3756	-0.978
Y96D	3.33037	3.44021	0.02889

Y96E	1.03562	1.4002	-1.35879
Y96F	0.89869	0.24662	0.1723
Y96G	1.41074	1.56914	-0.68978
Y96H	0.67785	0.29146	-1.06282
Y96I	1.34577	2.05093	-1.03103
Y96K	2.04367	2.36442	-0.86944
Y96L	3.43988	4.1063	0.01424
Y96M	2.90369	4.00067	-0.04645
Y96N	1.71421	1.73189	-0.91672
Y96P	0.14199	0.57646	-1.24826
Y96Q	2.1639	2.56549	-0.46115
Y96R	1.93745	2.38458	-0.66763
Y96S	2.33549	2.66077	-0.35033
Y96T	2.89703	3.62621	-0.30425
Y96V	2.01042	2.26089	-0.51389
Y96W	1.92867	3.22005	0.2716
Y96Y	NA	NA	NA
Y96X	0.37782	-0.66025	-0.7336
R97A	-1.25236	-0.52544	0.0367
R97C	-0.58483	-0.08208	0.21643
R97D	-0.50174	-0.61687	0.02185
R97E	-1.4813	-0.43356	0.58775
R97F	-0.0028	-1.00559	0.64547
R97G	0.06104	0.11505	0.23086
R97H	-0.79387	0.29988	0.44182
R97I	0.89608	0.37407	-0.30217
R97K	-0.96787	-0.28398	0.0274
R97L	0.52572	-0.00038	0.37762
R97M	-0.45733	0.14502	-0.34319
R97N	0.0602	0.59558	0.45915
R97P	2.67462	0.55534	0.48066
R97Q	-0.54892	0.13413	0.78388
R97R	0.7419	0.58338	0.16778
R97S	-0.02562	-0.14646	0.12834
R97T	-0.24585	0.21184	0.27282
R97V	-0.68188	-1.49447	0.44874
R97W	-0.975	-1.27007	0.57675
R97Y	0.55093	0.36146	1.02562
R97X	-0.03798	0.54006	-0.36049
E98A	NA	NA	NA
E98C	NA	NA	NA
E98D	NA	NA	NA
E98E	NA	NA	NA

E98F	NA	NA	NA
E98G	NA	NA	NA
E98H	NA	NA	NA
E98I	NA	NA	NA
E98K	NA	NA	NA
E98L	NA	NA	NA
E98M	NA	NA	NA
E98N	NA	NA	NA
E98P	NA	NA	NA
E98Q	NA	NA	NA
E98R	NA	NA	NA
E98S	NA	NA	NA
E98T	NA	NA	NA
E98V	NA	NA	NA
E98W	NA	NA	NA
E98Y	NA	NA	NA
E98X	NA	NA	NA
Q99A	2.19058	0.19602	0.6018
Q99C	-0.50266	0.64055	0.54561
Q99D	3.82622	4.35295	0.21573
Q99E	0.2292	0.06684	-1.41746
Q99F	4.30275	0.53566	1.0393
Q99G	2.76124	0.3274	-0.01561
Q99H	-0.12826	0.02637	0.12623
Q99I	2.04685	0.66535	0.18619
Q99K	1.84697	-0.3655	-0.66471
Q99L	1.01796	0.07062	0.83444
Q99M	1.19838	0.30863	0.71565
Q99N	0.85858	1.04649	0.83032
Q99P	1.29243	0.17539	-0.59855
Q99Q	NA	NA	NA
Q99R	1.45588	0.61153	-0.91396
Q99S	1.99807	1.76149	0.5079
Q99T	1.12874	1.41134	-0.50037
Q99V	1.17947	-0.0544	-0.23239
Q99W	6.03734	3.92598	2.25802
Q99Y	4.75478	0.8579	1.04991
Q99X	-1.17737	-1.03979	-0.96407
I100A	-0.68345	-0.16562	0.60055
I100C	0.59627	0.60284	-0.18521
I100D	-0.62166	-0.90289	-1.01175
I100E	-0.18563	-0.12202	-1.0621
I100F	-0.77721	0.83305	-0.1045

I100G	-0.78213	0.15668	0.0357
I100H	0.90203	0.7617	-0.73691
I100I	NA	NA	NA
I100K	0.05084	0.31709	-1.13666
I100L	-0.45677	-0.43602	0.40049
I100M	-0.26671	0.33645	1.16685
I100N	0.05919	0.8358	-0.51942
I100P	0.10287	0.67065	-0.79828
I100Q	-1.39642	0.38519	-1.03313
I100R	0.38835	0.58614	-0.61709
I100S	0.08392	-0.92549	0.13458
I100T	-0.9468	-0.59499	-0.2881
I100V	0.54841	0.61119	-0.28223
I100W	-0.07054	0.42538	-0.39453
I100Y	0.12765	-0.20579	-0.24432
I100X	0.05263	-0.32876	-0.61396
K101A	-0.91307	-1.40631	0.04165
K101C	-0.10808	0.42871	-0.05818
K101D	-0.88738	0.1167	-0.14629
K101E	-1.07045	-1.27626	0.25939
K101F	0.16242	1.06142	-0.05093
K101G	-0.60914	-0.35052	0.29484
K101H	1.42642	0.72595	-0.19967
K101I	-0.00965	-0.452	0.10125
K101K	NA	NA	NA
K101L	-0.56357	-0.09406	-0.08897
K101M	0.51381	0.27886	-0.13022
K101N	-0.23832	-0.68591	0.08622
K101P	0.29124	-1.35332	-0.8561
K101Q	-0.1035	0.56595	-0.36349
K101R	-1.80744	-0.28596	-0.16041
K101S	-0.82225	-0.64089	-0.18006
K101T	-0.79192	-2.91297	0.07908
K101V	-0.66343	-0.28121	-0.27603
K101W	-0.14853	-0.38097	0.36553
K101Y	0.09083	-0.85403	0.39489
K101X	0.28956	0.23474	-0.76554
R102A	1.57177	0.7806	-0.76128
R102C	1.27937	0.22386	-0.7139
R102D	0.94294	0.12217	-0.09555
R102E	1.46806	-0.29491	0.07084
R102F	1.02048	-0.15348	-0.70299
R102G	1.58621	0.1766	0.14213

R102H	1.487	0.2357	-0.7504
R102I	1.4255	0.9341	-0.35385
R102K	0.58933	-1.02183	-0.34634
R102L	1.1183	-0.23242	-0.65004
R102M	1.59186	-0.04225	-0.3217
R102N	0.86463	0.00192	-0.73633
R102P	0.56557	0.2915	-1.09234
R102Q	0.97145	-1.25613	-0.63247
R102R	1.68097	1.32137	0.19591
R102S	0.35892	0.021	-1.00612
R102T	1.70469	0.73674	-0.65187
R102V	1.01882	-0.5184	-0.73742
R102W	0.64433	-0.3481	-0.79771
R102Y	0.90839	-0.5568	-0.21363
R102X	-0.00918	0.0859	-0.98707
V103A	0.73151	-0.34577	-0.15613
V103C	0.64496	0.92606	-0.55876
V103D	0.81307	-0.72667	-0.87723
V103E	2.09564	0.27392	0.09172
V103F	0.91664	0.64482	-0.89868
V103G	0.03818	-0.55367	-0.75343
V103H	1.45217	0.36172	-0.37931
V103I	-0.33495	-0.06866	-0.5398
V103K	0.96669	0.0429	-0.89578
V103L	0.1567	-1.05738	-1.06069
V103M	1.04067	0.65815	-0.75285
V103N	1.14606	0.18081	-0.37969
V103P	0.61548	-2.4564	-1.14334
V103Q	2.88857	1.45346	-0.0699
V103R	0.92215	1.17183	-0.66428
V103S	0.46511	-0.90515	-0.77619
V103T	0.79455	-0.24588	-0.01959
V103V	NA	NA	NA
V103W	1.92554	1.08346	-0.03141
V103Y	0.69956	-0.97479	-1.11445
V103X	0.07846	-0.39982	-1.03069
K104A	-0.84243	-1.37845	0.83396
K104C	-0.54062	-0.36164	1.12177
K104D	0.594	0.17452	-0.88213
K104E	-0.83915	0.03327	-0.20853
K104F	-0.77739	-1.08594	0.37551
K104G	-0.02377	0.36913	-0.08622
K104H	0.31576	-0.66431	0.38597

K104I	-0.95476	-2.08227	0.46521
K104K	NA	NA	NA
K104L	-0.04093	0.54474	0.44506
K104M	0.19669	-0.15899	1.04185
K104N	-0.1028	-0.1577	0.17602
K104P	0.59219	-0.58962	-1.37895
K104Q	-0.6872	-2.23883	-0.99424
K104R	-0.20824	-0.86816	-1.11704
K104S	-0.00171	-0.12865	0.5106
K104T	-0.51563	0.5575	0.10265
K104V	1.24543	-0.38833	1.21174
K104W	-0.10271	0.46064	0.57561
K104Y	-0.21992	-0.11213	0.86382
K104X	0.38687	-0.73975	-0.84655
D105A	-0.97478	-0.99477	-1.20323
D105C	-0.65309	-1.00029	-0.9977
D105D	NA	NA	NA
D105E	-0.14357	-0.03823	0.90178
D105F	-1.10008	-0.12659	-1.07193
D105G	-0.36544	-0.3401	-0.76068
D105H	-1.26221	-0.47128	-1.2339
D105I	-0.3987	0.57154	-1.19709
D105K	0.14102	1.13208	-1.13324
D105L	-0.69966	0.22104	-1.10427
D105M	0.04097	-0.09858	-0.82074
D105N	-0.01619	-0.15719	-1.32642
D105P	-0.10477	0.36934	-0.94481
D105Q	-0.80689	-0.4358	-0.91477
D105R	-0.19835	-0.28586	-1.21947
D105S	0.7645	0.66172	-1.29266
D105T	0.19647	0.73863	-0.76795
D105V	-0.46236	-1.2844	-1.12359
D105W	-0.54797	-0.14627	-1.17286
D105Y	-0.45413	0.27369	-0.91449
D105X	0.43607	0.47277	-0.9372
S106A	-0.50239	-0.59757	0.22611
S106C	0.00636	0.35987	0.05076
S106D	0.24372	0.00023	0.32952
S106E	-0.02741	0.59061	0.15535
S106F	-0.96569	-2.1688	0.512
S106G	-0.13724	0.12002	0.19783
S106H	0.73956	0.1801	0.14854
S106I	-0.00965	0.03452	-0.10731

S106K	-0.34806	0.63036	-0.13447
S106L	0.11619	0.34136	-0.00657
S106M	0.50033	-0.07205	-0.16481
S106N	0.13493	0.14419	-0.04997
S106P	-0.58038	-0.72469	-0.31189
S106Q	-0.24547	-0.60595	-0.22482
S106R	-0.96545	0.52927	0.06093
S106S	0.00034	0.20024	-0.26506
S106T	2.4365	2.74256	0.00713
S106V	-0.27923	-0.16952	-0.01008
S106W	-0.19105	-0.43814	0.66512
S106Y	-0.5813	-0.20275	0.45819
S106X	0.56792	0.30254	-0.98778
E107A	-0.13481	-0.38037	-0.48442
E107C	0.00259	-0.12742	-0.16297
E107D	0.09039	-0.2832	0.15032
E107E	NA	NA	NA
E107F	-1.7328	-1.55564	-0.6232
E107G	-0.23822	-1.20797	-0.61991
E107H	-0.84903	-0.80336	-0.50868
E107I	-0.63199	0.0119	-0.51649
E107K	-0.53388	-0.59592	-0.51509
E107L	0.5868	0.65667	-0.67428
E107M	-0.34794	0.32451	-0.43996
E107N	-0.07436	0.18407	-0.33959
E107P	-0.41372	-0.81772	-0.47745
E107Q	-0.82002	0.13182	-0.53908
E107R	-1.1848	-1.00235	-0.75774
E107S	0.11885	-0.22529	-0.44493
E107T	-0.71378	-0.78019	-0.46706
E107V	0.06032	0.06704	-0.72684
E107W	-0.33053	0.46275	-0.61473
E107Y	-1.00137	-0.33965	-0.71796
E107X	0.89744	-0.02285	-0.50509
D108A	-0.30743	0.45586	-0.24265
D108C	-0.85451	-0.19287	-0.19229
D108D	NA	NA	NA
D108E	-0.55599	-0.19856	0.34888
D108F	-0.54065	0.16832	0.0823
D108G	-0.43078	-0.5937	-0.37818
D108H	-0.39825	-1.019	0.15421
D108I	-0.23177	0.20731	-0.27292
D108K	-0.45498	-0.32217	-0.38208

D108L	0.33524	0.96694	-0.07631
D108M	-0.39253	0.17773	-0.25338
D108N	-0.76844	-0.20747	-0.18289
D108P	-0.54698	-0.42872	-0.58927
D108Q	0.59533	-0.96627	-0.0511
D108R	-0.77608	-0.08442	-0.25865
D108S	-0.24728	0.00036	-0.16576
D108T	0.71836	0.63449	-0.26319
D108V	-0.81789	0.17439	-0.18603
D108W	0.00244	0.18358	-0.01851
D108Y	-0.29288	1.04314	-0.22019
D108X	0.3325	0.73386	-1.27707
V109A	0.42449	-0.02637	0.32441
V109C	0.09955	-0.79297	-0.16112
V109D	0.01396	0.15291	-0.8045
V109E	0.65328	0.6527	-0.2555
V109F	0.78612	0.63901	0.07848
V109G	0.38601	-0.86545	-0.11854
V109H	-1.12596	-0.26909	-0.30255
V109I	-0.01182	0.40935	-0.06225
V109K	-0.04609	-0.01609	-1.00125
V109L	1.67415	1.24678	-0.11863
V109M	0.18124	0.15733	0.46734
V109N	-0.30813	-0.47432	0.0446
V109P	0.06096	0.12027	0.71183
V109Q	-1.26346	-0.69965	0.04637
V109R	0.02599	-1.10249	-0.52566
V109S	0.5617	0.21813	-0.35728
V109T	-1.08292	-0.22901	-0.27075
V109V	NA	NA	NA
V109W	0.29382	-0.588	0.24804
V109Y	0.25118	-0.15974	-0.05105
V109X	0.10658	-0.28478	-0.8952
P110A	-0.72863	-0.47485	-0.55871
P110C	-0.49519	-0.72175	-0.57935
P110D	-0.43781	-0.98244	-0.39438
P110E	0.30862	0.82056	-0.34999
P110F	0.18966	0.39561	-0.29588
P110G	-0.76987	0.17461	-0.30939
P110H	-0.18647	-0.26675	0.02
P110I	-0.53447	0.27384	-0.44241
P110K	-0.05434	-0.68231	-1.1577
P110L	-1.19556	0.15101	-0.68114

P110M	-0.503	-0.53639	-0.52352
P110N	0.06082	0.0966	-0.64217
P110P	NA	NA	NA
P110Q	-0.5259	0.32694	-0.87709
P110R	-0.1525	0.72165	-0.98784
P110S	-0.39238	-1.29654	-0.36177
P110T	-0.93889	-0.1883	-0.82669
P110V	-0.67213	0.16669	-0.21219
P110W	-0.9213	-0.36991	-0.51336
P110Y	-0.37487	0.02572	-0.00386
P110X	-0.3096	-0.13933	-1.01998
M111A	-0.76006	0.92416	-0.80945
M111C	1.2397	0.72663	-0.01127
M111D	-0.33225	-0.25176	-0.69916
M111E	-0.26377	0.1361	-0.24596
M111F	-0.24258	0.97988	-0.40355
M111G	0.0886	-0.6137	-0.60686
M111H	-1.03343	-0.81492	-0.1913
M111I	-0.28266	-0.07851	0.45817
M111K	-0.45951	-0.74795	-0.85118
M111L	-0.31178	-0.15085	0.0647
M111M	NA	NA	NA
M111N	-1.18558	-0.79945	-0.15997
M111P	0.03883	0.22134	-0.63957
M111Q	0.03343	0.1755	-0.12927
M111R	0.11266	-0.98006	-0.61489
M111S	-0.73269	-0.94077	-0.63248
M111T	0.46207	0.02137	0.30789
M111V	-0.96674	-0.0145	-0.05065
M111W	-0.90487	0.43667	0.40944
M111Y	0.08021	0.13065	-0.2876
M111X	0.01817	0.25256	-0.79074
V112A	0.02432	0.22422	0.1617
V112C	-0.56036	-0.15176	-0.18897
V112D	0.08504	-0.25078	-0.57068
V112E	-0.75101	-1.63784	-0.96604
V112F	-0.28987	0.11955	0.53818
V112G	-0.81924	0.23811	-0.49343
V112H	0.49453	0.49783	-0.48495
V112I	-0.74037	-0.83824	0.06293
V112K	1.77491	-0.50824	-0.80483
V112L	-0.31476	0.04131	-0.17975
V112M	0.33634	0.62271	0.29486

V112N	-1.51297	-0.34882	-0.41297
V112P	0.4123	-0.20324	-0.14988
V112Q	-0.39552	-0.60783	-0.66109
V112R	0.41357	-0.25685	-0.51314
V112S	0.00135	0.07299	-0.21041
V112T	-1.12605	-0.54671	-0.20938
V112V	NA	NA	NA
V112W	0.72595	0.66918	-0.60362
V112Y	2.03287	-0.48973	0.56386
V112X	-0.82093	0.07612	-0.26573
L113A	-0.69969	-0.11613	0.09728
L113C	-0.08033	-0.67844	-0.03925
L113D	-0.11149	-0.43809	-0.92597
L113E	-0.396	-0.25294	-0.63682
L113F	-0.02764	0.2501	0.18308
L113G	0.52953	0.59714	-0.43522
L113H	0.11916	-0.05933	-0.54331
L113I	-0.38173	0.14914	0.34737
L113K	0.08966	-0.28184	-1.01106
L113L	-0.14598	0.63584	-0.15871
L113M	0.37149	0.37784	0.67956
L113N	0.3462	0.83438	-0.78668
L113P	-0.30623	-0.88968	-0.37677
L113Q	0.57977	-0.32935	-0.24117
L113R	-0.13715	-0.49402	-0.5297
L113S	-0.40334	-1.09734	-0.01002
L113T	-0.93393	-0.32639	0.15085
L113V	-1.20409	0.32022	0.49658
L113W	-0.82064	-0.09498	0.96932
L113Y	0.5386	-0.28224	0.27284
L113X	-0.32833	0.58543	-0.63311
V114A	-0.08016	-0.20082	0.25695
V114C	-0.87126	-0.26834	0.43179
V114D	-0.86399	-1.03543	-0.44792
V114E	-0.67792	-1.50423	-0.45275
V114F	0.10193	-0.46313	-0.72837
V114G	-0.21986	-0.21564	-0.29138
V114H	0.14424	-0.43493	-0.5714
V114I	-0.68686	-0.14082	-0.0157
V114K	-0.27508	-0.75385	-0.76067
V114L	-0.0564	-0.28967	-0.03038
V114M	1.52513	1.83752	0.39773
V114N	0.40043	-0.85093	0.69549

V114P	0.53237	1.17775	-0.76257
V114Q	-0.02329	0.17973	-0.60287
V114R	0.13472	0.5177	-0.82932
V114S	-0.52012	-1.20985	0.14524
V114T	1.17995	1.45488	0.43868
V114V	NA	NA	NA
V114W	0.57003	0.51334	-0.70506
V114Y	0.84919	1.28179	-0.67473
V114X	0.2541	-0.37129	-0.75881
G115A	0.33048	0.34885	0.54821
G115C	0.14303	0.4086	0.89078
G115D	0.44343	-0.85705	0.04962
G115E	0.86962	0.68922	1.75071
G115F	-0.64644	0.3382	1.23039
G115G	NA	NA	NA
G115H	-0.62605	0.64081	1.30408
G115I	0.80204	0.6305	1.6854
G115K	0.06004	0.24444	1.30998
G115L	0.12156	-0.69787	1.71364
G115M	-0.85018	-0.32625	1.15915
G115N	0.90809	0.15592	1.84741
G115P	-0.41454	0.23272	0.26006
G115Q	-0.41288	0.61569	0.90371
G115R	-0.36513	0.19637	1.10054
G115S	-0.84435	0.22078	0.89913
G115T	-0.80583	-1.10384	0.77818
G115V	-0.6066	-0.1455	1.4498
G115W	-1.02003	-0.41362	-0.03659
G115Y	-0.42728	-1.16997	1.0576
G115X	0.02842	-0.17486	-0.74421
N116A	1.54134	1.36117	1.21398
N116C	2.43123	2.62152	1.5231
N116D	-0.02109	0.59589	-0.23302
N116E	1.02553	0.95377	-0.51004
N116F	-0.39914	-1.22698	-1.35165
N116G	0.0389	-0.90874	1.36284
N116H	0.85673	1.61205	1.62662
N116I	1.71311	1.83362	-0.5249
N116K	-0.08767	0.25825	-0.62291
N116L	5.44244	6.3576	2.14022
N116M	2.12733	2.39397	1.75844
N116N	NA	NA	NA
N116P	0.14773	0.01144	-1.12676

N116Q	-0.1965	0.43485	0.79332
N116R	-0.15532	-0.56649	-1.40669
N116S	-0.1309	-0.17798	1.21888
N116T	0.74376	0.7582	1.57564
N116V	5.33835	6.32183	1.63304
N116W	-0.30154	-0.39764	-1.37692
N116Y	-0.58263	-1.00658	-0.93289
N116X	0.54178	0.45608	-0.73927
K117A	0.88133	1.15901	2.27167
K117C	1.79424	1.92807	2.4184
K117D	2.71925	3.03338	1.56589
K117E	3.87363	5.22722	2.77842
K117F	1.06257	1.86238	2.56766
K117G	2.28462	2.5079	2.44052
K117H	1.72967	2.43048	2.57713
K117I	0.46248	0.83961	2.43984
K117K	NA	NA	NA
K117L	2.84169	3.50615	2.46168
K117M	-0.50026	0.05408	2.14488
K117N	4.32249	5.88891	2.42486
K117P	-0.45453	-0.20932	-1.02807
K117Q	0.05237	0.51406	2.08975
K117R	1.26028	2.09016	1.6935
K117S	1.41054	2.05742	2.70152
K117T	0.70855	1.36142	2.89841
K117V	0.21539	0.17506	2.2732
K117W	0.23603	1.41715	2.50255
K117Y	5.09625	6.95855	2.63945
K117X	0.17736	0.1424	-0.96099
C118A	0.02016	0.07625	-0.24112
C118C	NA	NA	NA
C118D	-0.26268	0.85006	0.15705
C118E	0.0762	-0.42124	0.26616
C118F	-0.05303	-0.04748	0.79425
C118G	-0.74462	-0.27511	0.12012
C118H	-0.05975	0.32916	0.16734
C118I	-0.71689	-0.19443	-0.18678
C118K	0.46375	0.28388	0.27305
C118L	-0.57591	-0.12502	-0.28915
C118M	-0.13617	-0.03492	0.57169
C118N	-0.9161	0.11701	0.43626
C118P	1.95595	1.70971	0.61643
C118Q	0.10503	0.19693	0.39494

C118R	-0.74571	-0.56318	-0.19059
C118S	0.01405	0.16057	0.00709
C118T	1.2052	1.12348	-0.23253
C118V	0.09803	0.00454	-0.1
C118W	-0.02334	0.0638	0.38593
C118Y	-0.86913	-0.20541	0.35314
C118X	0.57252	-0.52141	-0.64717
D119A	1.68257	0.73942	2.26323
D119C	0.75419	0.71043	1.64175
D119D	NA	NA	NA
D119E	0.06987	0.3909	1.81689
D119F	0.4218	0.10052	1.99816
D119G	2.06408	1.27263	1.98711
D119H	4.94122	5.68044	2.36624
D119I	0.20365	0.46158	-0.03002
D119K	0.14431	0.42467	1.4758
D119L	-0.37194	-0.33385	2.10847
D119M	0.42767	1.48513	2.15984
D119N	1.88258	2.4354	1.86834
D119P	0.00011	0.18677	-0.9929
D119Q	0.85714	1.38494	1.86526
D119R	0.15807	-0.25354	1.05797
D119S	-0.11565	-0.18575	1.94757
D119T	1.60384	1.59716	2.03003
D119V	-0.41251	-0.15405	0.16437
D119W	0.82897	1.0234	0.45424
D119Y	1.06336	1.22898	1.66472
D119X	-0.6906	-0.66407	-0.7981
L120A	-0.60856	0.25716	1.63656
L120C	-0.54035	0.66777	1.70425
L120D	0.16139	0.92868	1.22773
L120E	0.85707	0.49415	1.4236
L120F	0.09552	0.02268	1.14499
L120G	0.39596	0.78486	1.35885
L120H	2.13092	1.28606	1.44309
L120I	0.25883	0.65585	0.36237
L120K	-0.1598	-0.19009	1.15408
L120L	0.11463	-0.18253	0.09811
L120M	0.59207	-0.15981	0.98433
L120N	-0.97529	0.07326	1.80677
L120P	0.41823	0.58101	1.9184
L120Q	0.11173	-0.08879	1.37009
L120R	-0.66763	-0.18138	0.59654

L120S	-0.27025	0.56688	1.75194
L120T	1.13171	1.28536	1.74657
L120V	0.23595	-0.83998	1.1091
L120W	0.47109	0.37266	1.27501
L120Y	0.54343	0.1424	1.9094
L120X	0.18129	0.06848	-0.74024
P121A	-0.80331	-0.19886	-0.20357
P121C	0.09697	-0.66428	-0.41489
P121D	-0.87449	0.08973	0.10341
P121E	-0.16264	-0.11062	-0.0923
P121F	-0.29071	-0.33668	-0.32952
P121G	-0.43064	0.40458	-0.20546
P121H	0.23943	-0.22258	-0.32711
P121I	1.44572	0.37447	-0.32774
P121K	-0.94892	0.62288	-0.00437
P121L	-1.05581	-0.87917	-0.42139
P121M	-1.03626	-0.8739	-0.60706
P121N	-0.95149	0.1636	-0.17424
P121P	NA	NA	NA
P121Q	0.00134	0.43486	0.13274
P121R	-0.37399	-0.30151	-0.48205
P121S	0.23313	-1.21776	-0.00967
P121T	-0.3831	-0.41942	0.02381
P121V	-0.9824	0.35403	-0.26912
P121W	-0.82767	0.22973	-0.65583
P121Y	-0.2174	-0.34908	-0.2855
P121X	-0.00912	-0.62362	-1.17032
S122A	1.3767	1.53732	-0.02885
S122C	0.15432	0.12181	-0.0846
S122D	-0.3231	0.462	-0.09069
S122E	-0.0801	-0.40616	0.06901
S122F	-0.2683	0.11734	-0.26968
S122G	0.14211	-0.19643	0.25674
S122H	-0.01376	0.39044	0.1343
S122I	-0.1641	0.01888	-0.03532
S122K	-0.46078	0.93393	0.01748
S122L	-0.37368	0.31102	0.22741
S122M	0.44816	-0.04494	-0.09348
S122N	0.45295	0.79998	0.52581
S122P	0.12073	0.39858	1.38186
S122Q	-0.07779	0.50143	-0.10151
S122R	0.23547	0.26259	0.04105
S122S	0.10532	1.1073	0.06008

S122T	-0.15071	0.07531	0.21088
S122V	-0.36236	-0.73751	-0.50214
S122W	-0.92137	-0.74276	-0.16221
S122Y	-0.0326	0.2194	-0.31499
S122X	0.08028	-0.00245	-0.75091
R123A	-0.66287	1.37796	0.99479
R123C	-0.39283	0.4062	0.75397
R123D	1.16955	1.35158	0.58121
R123E	0.39435	-0.22222	0.9086
R123F	-0.88184	-0.62594	0.44158
R123G	-0.648	-0.96045	0.50745
R123H	-0.1137	0.29161	0.20083
R123I	-0.36017	0.02505	0.79068
R123K	-0.10451	-0.42717	0.37056
R123L	1.44749	1.47421	0.81001
R123M	-0.71449	0.37365	0.60238
R123N	0.33799	0.90203	0.99521
R123P	-0.49891	-0.09927	1.21043
R123Q	-0.13613	0.71467	0.45516
R123R	-0.33416	-0.22814	0.09061
R123S	-0.13794	-1.7919	0.55398
R123T	-1.17889	-1.72105	0.72729
R123V	0.49705	0.33867	0.24821
R123W	-0.57548	-0.13349	-0.44771
R123Y	-0.00714	0.58179	0.04328
R123X	-0.41991	0.03784	-0.85326
T124A	-0.49476	0.4376	0.14701
T124C	-0.55691	-0.56957	0.13874
T124D	0.00158	-0.8549	0.45849
T124E	0.67073	-0.08815	0.12549
T124F	-0.93231	-1.11288	0.00474
T124G	0.11093	0.25077	0.41729
T124H	0.15068	-0.94036	0.28454
T124I	0.85748	0.47424	0.38491
T124K	-0.17759	1.07748	0.2547
T124L	-0.21646	-0.54621	0.17299
T124M	0.18464	0.37278	0.00181
T124N	1.00821	0.09889	0.06252
T124P	-0.63624	-0.17555	-0.19388
T124Q	0.64611	0.77654	0.66425
T124R	-0.02151	0.0498	0.01205
T124S	0.12395	1.18998	-0.0329
T124T	NA	NA	NA

T124V	-0.35655	0.42933	0.49005
T124W	-0.24559	0.80756	-0.03462
T124Y	-0.969	-0.47719	-0.03531
T124X	-0.32436	-0.19493	-0.88901
V125A	-1.50267	-0.92613	0.0928
V125C	0.00195	-0.42506	0.48535
V125D	-1.90573	-1.26969	0.60482
V125E	-0.91861	0.09025	0.75523
V125F	-0.45194	-0.16965	0.52813
V125G	-0.96443	0.557	0.61901
V125H	-0.89203	-0.29172	0.44749
V125I	-0.13404	-0.0987	0.08488
V125K	-0.37808	0.01518	0.29075
V125L	-0.33193	-0.3415	-0.01493
V125M	-0.57403	-0.01646	0.27964
V125N	-1.54859	0.13362	0.65755
V125P	0.22504	0.52142	0.66287
V125Q	-0.49658	-0.32991	-0.00235
V125R	-0.96641	-0.40738	0.04179
V125S	-0.32081	-0.17542	0.53902
V125T	0.33122	0.49584	0.19726
V125V	NA	NA	NA
V125W	-0.37479	-1.0613	0.8478
V125Y	0.85732	-0.08954	0.71793
V125X	0.67932	0.30896	-0.58016
D126A	-0.4798	-0.82445	-0.40384
D126C	-0.16051	0.72302	0.03416
D126D	NA	NA	NA
D126E	0.52317	0.04009	0.05536
D126F	-1.14129	-0.31593	-0.23929
D126G	1.27036	0.95864	-0.2146
D126H	-0.68061	-1.36577	-0.34866
D126I	-1.41357	-4.16516	-0.6519
D126K	-0.27744	-0.23059	-0.57984
D126L	-0.0932	0.00937	0.16742
D126M	-0.3957	0.41985	-0.16432
D126N	0.72852	0.70211	-0.22738
D126P	0.65057	0.94095	0.12519
D126Q	0.23784	0.52451	-0.37231
D126R	0.57538	-0.09437	-0.52667
D126S	-0.60799	-0.48773	-0.17164
D126T	0.04687	0.05331	-0.49522
D126V	0.33331	0.4724	-0.1945

D126W	-0.40567	-0.20543	-0.32571
D126Y	0.36544	-0.07702	-0.27873
D126X	0.54143	0.01574	-0.53273
T127A	-0.44444	-0.26364	-0.12444
T127C	-0.47911	-0.0154	-0.28739
T127D	-0.25737	-0.11505	0.68115
T127E	-1.33912	-0.48692	-0.3145
T127F	-0.15191	-1.12364	-0.22393
T127G	0.6146	0.73501	-0.38426
T127H	-1.1345	0.05708	-0.10783
T127I	0.16996	0.6146	-0.1017
T127K	-0.05743	0.44368	-0.46867
T127L	-0.7894	-0.23152	0.22814
T127M	-0.40028	-0.07066	0.16304
T127N	-0.02981	-1.41943	-0.27682
T127P	-1.11625	-0.06542	-0.11584
T127Q	-0.88236	-1.11397	-0.05313
T127R	-0.13233	0.73495	-0.04904
T127S	-0.67852	-0.95664	-0.18967
T127T	NA	NA	NA
T127V	-0.30087	1.50761	0.36796
T127W	-0.88632	-0.4874	-0.53347
T127Y	-0.0684	0.3029	-0.03406
T127X	-0.2268	-0.23221	-0.96971
K128A	-0.36656	-0.36653	0.55701
K128C	-2.05192	-0.92879	0.44399
K128D	-0.05618	-0.78808	0.93343
K128E	1.99077	2.19311	1.39598
K128F	0.39356	1.21246	0.37249
K128G	-0.34576	0.01205	0.49761
K128H	-0.32781	-0.12544	0.50259
K128I	-0.46305	-0.58192	0.40219
K128K	NA	NA	NA
K128L	-0.80873	0.18401	0.3559
K128M	-0.00496	-0.42346	0.55981
K128N	0.00249	0.5228	0.53494
K128P	1.06868	1.19688	0.10185
K128Q	0.16552	-0.10085	0.91674
K128R	0.60633	0.50419	0.12272
K128S	-0.44613	-0.35242	0.56381
K128T	0.66029	-0.43331	0.6651
K128V	0.35955	-0.29993	0.66208
K128W	2.26404	-0.22646	0.76766

K128Y	0.50625	0.45654	0.42565
K128X	0.50917	-0.9371	-0.64653
Q129A	1.00951	1.38001	0.28777
Q129C	0.06284	-0.65325	0.27274
Q129D	0.16805	-0.06939	0.69319
Q129E	-0.63353	-0.39458	0.4251
Q129F	0.32518	1.53757	0.8247
Q129G	-0.83735	-0.07344	0.1554
Q129H	-0.06277	0.56341	0.14364
Q129I	-0.29438	-0.27742	0.22959
Q129K	-0.48576	0.23958	-0.3005
Q129L	-0.22829	0.5547	-0.00965
Q129M	-0.12188	-1.02959	0.08944
Q129N	-0.40141	-0.18865	0.22201
Q129P	-0.78406	-0.62476	0.3793
Q129Q	NA	NA	NA
Q129R	-0.45795	0.48744	-0.40547
Q129S	-0.84944	-0.80362	0.08977
Q129T	-0.84199	0.43639	0.06422
Q129V	0.10219	-0.03026	0.53543
Q129W	-0.06274	-0.45775	-0.17411
Q129Y	0.21207	-0.80343	0.4448
Q129X	0.50272	-0.47955	-1.04429
A130A	NA	NA	NA
A130C	-0.44471	-0.27279	-0.2049
A130D	-0.22755	-0.27243	0.38853
A130E	0.09925	0.53216	0.01883
A130F	-0.53645	-0.60579	0.15304
A130G	-0.6635	0.49182	-0.0817
A130H	-0.71515	-0.07052	-0.11451
A130I	0.19943	-0.17875	0.01121
A130K	0.29031	-0.36609	-0.18922
A130L	-0.03777	-0.26551	-0.26483
A130M	-0.31249	-0.24161	-0.0714
A130N	-0.69867	-0.52824	0.35967
A130P	-1.24855	-0.38384	0.36928
A130Q	0.04541	0.03407	0.07362
A130R	-1.23185	-0.87011	-0.22511
A130S	0.07162	-0.13742	0.2105
A130T	0.36769	0.06333	-0.1013
A130V	-0.48229	-0.22327	0.1292
A130W	-0.71759	-0.13605	0.09709
A130Y	-0.36144	-0.38738	0.38565

A130X	0.48749	0.20829	-0.6338
Q131A	0.28377	0.16614	-0.29441
Q131C	0.15522	-0.35796	-0.16833
Q131D	2.01616	1.83813	0.48863
Q131E	0.48507	0.69345	0.20449
Q131F	-0.4156	-0.40848	-0.23486
Q131G	-1.13172	-0.77705	0.04181
Q131H	0.34412	0.25104	0.07972
Q131I	-0.00483	-0.09616	-0.05831
Q131K	-0.92388	-0.47568	-0.48827
Q131L	-0.25396	-0.0853	-0.02979
Q131M	-0.39047	-0.0796	0.14494
Q131N	0.51024	0.50861	-0.12811
Q131P	-0.52785	-1.16164	0.5937
Q131Q	NA	NA	NA
Q131R	0.15321	-0.55885	-0.36011
Q131S	0.17344	-0.41548	0.30033
Q131T	-0.9036	0.23877	0.1848
Q131V	-0.02253	0.31476	-0.09629
Q131W	-0.69775	-0.47712	0.05239
Q131Y	0.21084	0.20701	0.13305
Q131X	0.47083	-0.26981	-0.70294
D132A	0.1449	0.87586	-0.27742
D132C	-0.51391	0.43941	-0.67246
D132D	NA	NA	NA
D132E	-0.39739	0.45677	-0.11729
D132F	-1.31418	-0.89989	-0.39429
D132G	0.01372	0.45374	-0.55019
D132H	1.02843	1.54307	-0.83382
D132I	-0.15796	-0.74502	-0.22357
D132K	-0.24885	-0.2714	-0.7155
D132L	-0.37688	-0.23189	-0.37648
D132M	-0.0484	0.36113	-0.3419
D132N	-0.59737	-0.72954	-0.53361
D132P	-0.74373	0.09485	-0.60594
D132Q	0.53866	-0.86044	-0.64626
D132R	0.09908	0.07878	-0.72114
D132S	-0.90637	-0.59086	-0.62222
D132T	-0.16974	-0.0476	-0.32898
D132V	-0.18355	-0.32687	-0.27843
D132W	-0.84794	-0.44126	-0.32567
D132Y	-0.12631	-0.33603	-0.37774
D132X	-0.02176	-0.31096	-0.69954

L133A	-0.56313	0.40387	0.06308
L133C	-0.98519	-0.52545	0.06127
L133D	-0.20723	-0.28157	0.17987
L133E	-0.05955	-0.29405	-0.16642
L133F	0.18945	0.40471	0.24821
L133G	-0.53869	-0.71496	-0.62673
L133H	-0.07423	-1.04983	-0.23829
L133I	-0.5395	-1.13733	0.32459
L133K	-1.35246	-0.578	-0.69841
L133L	-0.24574	-0.29866	-0.24568
L133M	-0.58039	0.11588	-0.05564
L133N	0.2431	-0.25381	-0.28907
L133P	0.6346	0.46989	-0.17323
L133Q	-0.36087	0.59226	-0.46292
L133R	0.19744	-0.34768	-0.42303
L133S	1.90889	2.16874	0.42794
L133T	-1.363	-0.56556	0.28678
L133V	-0.66238	-0.24163	0.3772
L133W	-0.2903	-0.05809	0.96674
L133Y	0.99563	0.44874	0.49196
L133X	0.19722	1.03752	-0.56677
A134A	NA	NA	NA
A134C	-0.76994	-0.57104	0.23385
A134D	-0.29459	-0.56253	-0.13115
A134E	-0.36219	-0.27818	0.11114
A134F	-0.74507	-1.30828	0.31755
A134G	0.66068	0.47362	-0.22286
A134H	-0.08787	0.55747	0.00516
A134I	0.53469	0.57938	0.12978
A134K	0.11751	1.0927	-0.2696
A134L	0.21203	-0.57651	0.2878
A134M	0.83357	0.65774	0.00888
A134N	0.10588	-0.74644	0.11947
A134P	-0.02371	0.12839	-0.03548
A134Q	-0.49289	-0.35824	-0.18707
A134R	-0.00808	-0.24152	-0.54396
A134S	0.3503	-0.26412	-0.01734
A134T	-0.32288	1.27248	0.01608
A134V	0.54233	1.40121	0.10459
A134W	-0.08551	0.27304	0.13689
A134Y	0.04373	1.04528	0.50484
A134X	-0.46881	-0.16211	-0.99073
R135A	0.35892	0.98657	0.50471

R135C	-0.69551	-0.44952	0.73402
R135D	-0.13525	-0.27874	1.20307
R135E	-0.69381	-0.52921	0.68175
R135F	-0.16824	-0.75272	0.62191
R135G	-0.3098	0.39799	0.22045
R135H	-0.21741	0.6082	0.36649
R135I	0.51912	0.18471	0.84285
R135K	0.2291	0.87453	0.1958
R135L	0.24044	-1.36328	0.49169
R135M	0.11222	-1.8148	0.68994
R135N	1.75477	2.35421	0.55099
R135P	0.46326	0.11004	0.42553
R135Q	-0.24418	-0.02729	0.3289
R135R	0.12491	0.64663	-0.00042
R135S	0.00855	0.92194	0.62827
R135T	-0.52121	-0.35769	0.58061
R135V	0.13675	0.20358	0.28723
R135W	-0.17056	-0.42933	1.19317
R135Y	0.07613	-0.06857	0.75187
R135X	0.5408	-1.22065	-0.69468
S136A	0.52184	0.19607	0.23001
S136C	0.37902	-0.42332	0.23707
S136D	-0.04476	0.49113	0.37309
S136E	-0.22854	-0.38721	0.01518
S136F	0.0095	0.71304	0.50262
S136G	-0.45014	-0.25043	0.13092
S136H	0.56654	0.99707	0.11706
S136I	-1.25648	-1.21867	0.32835
S136K	-1.5829	-0.64139	-0.58314
S136L	-0.97864	-0.18428	-0.10256
S136M	-1.34485	0.15216	0.40384
S136N	0.61353	-0.13505	0.39916
S136P	0.02515	-0.01917	-0.44654
S136Q	-0.36209	-0.03041	-0.06121
S136R	-0.1116	-0.3918	-0.48
S136S	0.07871	0.06831	0.07803
S136T	-1.2357	-1.42782	-0.19235
S136V	-0.32772	0.18633	0.32298
S136W	0.65964	1.08527	1.15351
S136Y	0.75301	-0.21462	0.84439
S136X	-0.25202	-0.02386	-0.42233
Y137A	0.34602	1.11354	-0.11563
Y137C	-0.13072	0.17808	-0.34611

Y137D	-0.91274	-0.12973	-0.27683
Y137E	-1.02754	-0.01135	-0.07451
Y137F	-0.393	-1.09649	-0.21554
Y137G	0.31083	0.10607	-0.22115
Y137H	-0.56156	-0.02837	0.15481
Y137I	-0.30384	-0.13041	-0.31134
Y137K	-0.59812	0.14863	-0.55487
Y137L	-0.46216	-0.22534	-0.53973
Y137M	-0.96722	-0.50545	-0.12027
Y137N	0.15992	-0.51751	-0.18808
Y137P	-1.25568	-0.05583	-0.43702
Y137Q	-0.56628	-0.60008	-0.36651
Y137R	0.72626	0.54503	-0.46852
Y137S	0.03769	0.34712	-0.05879
Y137T	-0.46337	-0.00846	-0.10983
Y137V	0.14598	0.26566	-0.40454
Y137W	-0.29848	-0.04592	0.24569
Y137Y	NA	NA	NA
Y137X	-0.71099	0.39704	-0.9318
G138A	0.89489	-0.19507	0.17326
G138C	-0.19961	0.53617	0.29316
G138D	-0.53234	-0.34285	0.56912
G138E	1.46445	0.66177	0.70111
G138F	0.19136	0.79787	0.63462
G138G	NA	NA	NA
G138H	-0.82052	-0.03286	0.06237
G138I	-0.28154	-0.55732	0.1707
G138K	0.32218	0.16046	-0.43771
G138L	-0.34549	0.52524	0.43314
G138M	-0.13779	0.77014	0.34252
G138N	0.13646	-0.62804	0.43976
G138P	-0.04515	-1.29859	0.36333
G138Q	-0.07124	-0.09652	0.06388
G138R	0.03057	0.27831	-0.37658
G138S	1.26732	1.1659	0.30914
G138T	-0.18899	-0.50997	0.325
G138V	-1.17855	-1.15204	0.11121
G138W	-0.45888	-0.22101	0.36482
G138Y	-0.57039	-0.54768	0.2574
G138X	-0.11364	-0.89779	-0.44769
I139A	-0.00665	0.6969	-0.23522
I139C	0.9397	0.83182	0.02809
I139D	-0.63045	-0.24288	-0.0755

I139E	0.16476	0.05555	0.102
I139F	1.24174	1.07322	0.30126
I139G	-0.11985	0.45627	-0.44466
I139H	-0.92564	-1.05585	-0.20606
I139I	NA	NA	NA
I139K	-0.01379	-0.23874	-0.25145
I139L	-0.10666	-0.39966	0.27862
I139M	-0.14188	0.71892	0.03315
I139N	-0.8866	-1.54989	0.14268
I139P	0.10103	-0.69366	-0.05608
I139Q	-0.28694	-0.78374	-0.49512
I139R	-2.30461	-0.70374	-0.43652
I139S	-0.6206	0.50937	-0.1729
I139T	0.15159	0.31713	-0.36507
I139V	0.1956	0.56309	-0.066
I139W	1.11988	1.11745	-0.45989
I139Y	0.84651	-0.82976	-0.57115
I139X	0.28664	-0.07356	-0.77637
P140A	-0.46487	-0.709	0.12646
P140C	0.72958	1.27251	0.31804
P140D	0.982	-1.08642	0.40843
P140E	-0.74497	0.0545	0.8946
P140F	-0.47158	-0.04219	0.4569
P140G	0.81103	-0.60849	0.08874
P140H	-0.13544	-0.18998	0.20182
P140I	-0.91711	-0.55068	-0.22091
P140K	-0.44229	-0.67424	-0.14625
P140L	-0.49194	-0.40885	-0.28552
P140M	-0.12303	0.60596	0.10309
P140N	-0.18406	0.37951	0.11351
P140P	NA	NA	NA
P140Q	0.12453	-1.632	0.11164
P140R	-0.68038	0.11129	-0.34123
P140S	0.7389	1.21575	0.3729
P140T	-0.33724	-1.23123	0.14663
P140V	-0.81098	-1.10632	-0.04795
P140W	0.36088	0.48498	0.09158
P140Y	-0.60942	-1.72205	0.51625
P140X	-0.19767	-0.81626	-0.78087
F141A	-1.0444	-0.63038	0.01829
F141C	-0.85793	0.15791	-0.22194
F141D	-0.8842	-0.23119	-0.09669
F141E	0.01328	-0.18637	0.11843

F141F	NA	NA	NA
F141G	0.5378	-0.07104	-0.12463
F141H	0.69488	-0.21142	0.10465
F141I	0.53826	0.72004	0.22582
F141K	-0.87065	-0.90408	-0.89351
F141L	-0.08136	0.63785	-0.08331
F141M	-1.89917	-0.92977	-0.08285
F141N	-0.83737	-0.14451	-0.16799
F141P	-0.8786	0.17353	-0.72646
F141Q	-0.54677	0.15581	-0.22828
F141R	0.21258	-0.42144	-0.15274
F141S	-0.51081	-0.94102	-0.12289
F141T	-1.13076	-0.08353	0.30165
F141V	1.49313	-0.32521	0.00687
F141W	-0.29035	-0.22047	-0.02072
F141Y	1.38829	0.46877	0.15996
F141X	-0.09486	-0.17236	-0.67001
I142A	-0.46587	-0.76667	0.35725
I142C	2.62456	2.85379	-0.11079
I142D	0.01608	-0.63813	0.26742
I142E	-0.24674	0.22406	0.7877
I142F	0.70916	-0.09752	1.72809
I142G	-0.22539	0.19591	0.30847
I142H	0.91033	0.39059	0.41437
I142I	NA	NA	NA
I142K	-0.39752	-0.81882	-0.14781
I142L	-0.84962	1.19444	-0.16301
I142M	-0.5093	-0.26142	0.53001
I142N	0.5284	-0.06099	0.08808
I142P	-0.56784	-0.19465	-0.40562
I142Q	-0.62901	-1.00101	0.21491
I142R	-0.79675	-0.348	-0.33439
I142S	-0.0891	-0.31433	0.31464
I142T	-0.34298	0.03595	0.08008
I142V	-0.85417	0.39882	-0.16167
I142W	-0.73309	0.0229	0.45242
I142Y	0.57339	0.45092	0.89881
I142X	-0.39007	-1.18553	-0.44688
E143A	-0.50726	-0.21753	-0.08317
E143C	-1.79197	-0.62639	-0.29829
E143D	-0.04947	-0.29459	0.18671
E143E	NA	NA	NA
E143F	0.14551	-1.6968	0.11245

E143G	0.05886	0.55482	-0.02298
E143H	-0.07136	-0.11087	0.15911
E143I	-0.65109	-0.48257	-0.15178
E143K	0.3932	0.54093	-0.70103
E143L	-0.23904	0.27256	0.22175
E143M	-0.02806	-0.16974	-0.35112
E143N	-1.69659	-0.62708	-0.02293
E143P	0.1276	-0.02843	-0.02318
E143Q	1.06066	0.36609	-0.16123
E143R	-0.76042	0.39957	-0.14403
E143S	-0.4795	0.49408	-0.18682
E143T	-0.03205	-0.23333	-0.10465
E143V	-0.90797	-1.47654	0.38339
E143W	-0.88131	-0.28736	-0.03972
E143Y	-0.18334	-0.76309	0.03414
E143X	0.78351	0.63023	-0.36219
T144A	0.64804	0.51801	0.44292
T144C	0.40652	0.11925	0.37036
T144D	0.09619	-0.26605	-0.88393
T144E	0.17865	-0.39558	-0.68282
T144F	0.71345	0.16152	-1.21477
T144G	-0.46903	0.08866	0.26519
T144H	-0.09936	-0.15694	-1.15426
T144I	0.31809	0.30581	1.5006
T144K	0.53103	0.87953	-0.50564
T144L	-0.17715	-0.79146	1.01158
T144M	0.27224	0.86811	0.30024
T144N	0.18991	0.41691	1.50893
T144P	0.81294	-0.29767	0.1688
T144Q	0.01133	0.23494	0.18338
T144R	0.41201	0.34542	-1.20101
T144S	-0.29724	-0.48986	0.27744
T144T	NA	NA	NA
T144V	-0.16605	-0.19757	0.93095
T144W	-0.27348	0.52418	-1.10612
T144Y	0.00095	-1.07217	-1.39652
T144X	0.05036	0.0875	-0.66145
S145A	-0.27583	-0.53376	1.75795
S145C	0.12883	0.29265	1.77847
S145D	1.77937	2.23514	2.59516
S145E	0.92701	1.25357	2.64525
S145F	3.08663	3.54095	1.48375
S145G	1.32181	1.97095	1.46748

S145H	2.84398	2.8404	1.52425
S145I	0.20998	-0.37177	1.90069
S145K	0.5473	-0.2076	1.38551
S145L	0.36666	0.34007	-0.70637
S145M	0.31248	1.74147	1.50835
S145N	2.10705	2.26106	1.94491
S145P	-1.22178	-1.64969	-1.08816
S145Q	-0.13917	-0.13122	1.48197
S145R	1.24875	1.25563	1.0352
S145S	-0.07243	0.13573	0.08865
S145T	-0.11652	-0.19148	1.29252
S145V	0.5687	0.25581	1.90661
S145W	0.87045	0.83392	0.92664
S145Y	4.02102	4.6778	1.94249
S145X	-0.29883	-1.49514	-0.60791
A146A	NA	NA	NA
A146C	0.65904	0.62341	2.09454
A146D	0.46015	-0.18318	-1.28633
A146E	-0.11152	-1.30553	-1.26628
A146F	-0.15542	0.07676	-1.8289
A146G	0.59744	0.94293	1.91307
A146H	-0.47255	-1.48392	-0.91116
A146I	-0.58426	0.15694	-0.47691
A146K	-0.83838	-0.72297	-1.18913
A146L	-0.20467	0.19916	-0.59453
A146M	0.93138	1.03483	1.78968
A146N	0.99093	1.9031	2.33367
A146P	3.26983	3.15411	1.61416
A146Q	-0.03214	1.0538	-0.70154
A146R	-0.28534	-0.7387	-0.80654
A146S	2.82585	-0.26582	1.33093
A146T	1.47669	1.01322	2.31588
A146V	0.49211	1.2579	1.75975
A146W	0.56217	0.93569	-1.42074
A146Y	-0.50804	1.13049	-1.16477
A146X	-0.09641	0.09873	-0.85342
K147A	-1.41974	-1.94486	0.63914
K147C	-0.01809	0.54046	1.04957
K147D	0.75076	0.97257	3.4272
K147E	0.42	1.0437	2.71186
K147F	0.08897	0.1092	1.84665
K147G	0.30752	0.35768	2.12827
K147H	0.05546	0.19689	2.53412

K147I	-0.13317	0.47496	0.87172
K147K	NA	NA	NA
K147L	-0.3757	0.53861	0.34302
K147M	0.52671	0.2425	0.5806
K147N	0.4163	0.69798	1.82921
K147P	-1.83274	-3.60781	2.03207
K147Q	0.48127	0.2706	2.10129
K147R	-0.44506	0.05737	0.7706
K147S	0.50144	0.96975	2.57422
K147T	-1.01609	0.3058	2.48611
K147V	-1.05564	-0.47632	0.47813
K147W	0.36669	0.67005	2.3474
K147Y	-0.14077	0.25073	1.81285
K147X	0.04017	-0.01175	-0.87747
T148A	0.69752	-0.63868	0.43756
T148C	-0.02435	0.27616	0.75068
T148D	-0.00949	0.04503	0.55561
T148E	0.18216	0.6915	-0.38254
T148F	-0.65241	-0.78806	-0.3256
T148G	0.68644	0.55741	1.67698
T148H	-0.37058	0.08032	-0.30474
T148I	0.19965	-0.66961	-0.04057
T148K	-0.04796	-0.94615	0.84879
T148L	-0.5454	-0.05941	-0.01172
T148M	-0.5952	0.71888	0.22096
T148N	0.04168	1.24229	0.66536
T148P	2.58029	2.14991	1.33785
T148Q	1.42959	0.35231	0.18586
T148R	0.37758	0.10395	0.29566
T148S	-0.22537	-0.51513	0.95184
T148T	NA	NA	NA
T148V	-0.45766	0.4197	0.07455
T148W	0.02481	-0.13864	-1.02787
T148Y	-0.89402	-0.3809	-0.74204
T148X	-0.30695	0.22292	-0.56324
R149A	0.92342	1.04667	0.16729
R149C	-0.20583	-0.44226	0.94425
R149D	-0.16817	-0.47965	-0.10698
R149E	0.42166	0.05533	0.50543
R149F	-0.0944	0.81206	1.57498
R149G	0.49814	0.42495	0.44112
R149H	1.78905	1.85644	1.11724
R149I	-0.11837	0.37108	2.22716

R149K	-0.42543	-0.69814	-0.19417
R149L	0.48206	0.38525	3.0653
R149M	0.09059	0.53388	2.04361
R149N	0.0281	0.24948	0.66898
R149P	-3.54169	-1.80761	-0.8452
R149Q	-0.02991	0.42762	1.0272
R149R	0.04689	0.36708	0.01451
R149S	0.47133	-0.28858	-0.00202
R149T	1.0956	0.2008	0.77738
R149V	-0.07639	0.72783	1.56529
R149W	-0.85991	-0.13684	1.63699
R149Y	0.20735	-0.13866	2.05126
R149X	0.37903	0.23216	-0.79053
Q150A	0.63968	-0.1677	0.25735
Q150C	0.18187	-0.05249	0.30683
Q150D	-0.29395	0.41262	0.18093
Q150E	0.60098	0.51452	0.66242
Q150F	-0.15911	0.44955	-0.11991
Q150G	0.32715	0.47403	0.71323
Q150H	0.05801	0.43893	0.24487
Q150I	0.68306	-0.08604	0.40926
Q150K	0.28131	-0.79941	0.30841
Q150L	-0.24301	-0.37446	0.16842
Q150M	-0.70623	-0.28246	-0.19685
Q150N	-0.39108	-0.85448	0.46769
Q150P	0.38349	0.015	1.29345
Q150Q	NA	NA	NA
Q150R	-0.27237	-0.03159	0.19955
Q150S	-0.34983	0.24337	-0.10321
Q150T	0.22813	0.46233	0.18537
Q150V	1.03076	1.88583	0.47815
Q150W	-0.81253	-0.06723	0.01587
Q150Y	0.04377	-0.24423	0.21151
Q150X	-1.09415	-1.05064	-1.03322
G151A	0.53565	0.1459	-0.31734
G151C	-0.72808	-0.93821	-0.68663
G151D	-0.35621	1.16419	0.92141
G151E	-0.59083	0.36678	1.02735
G151F	0.26391	-0.29145	-0.40098
G151G	NA	NA	NA
G151H	-0.27015	0.00327	-0.09254
G151I	0.00374	-0.23922	1.55715
G151K	-0.06457	0.18043	-0.50703

G151L	-1.30999	-0.36521	0.30709
G151M	-0.0615	0.33493	-0.05617
G151N	-0.8088	-0.7098	0.05804
G151P	0.18136	-0.26084	1.5708
G151Q	-0.12763	0.77697	-0.22448
G151R	-0.69057	0.16789	-0.35671
G151S	0.89833	0.7312	-0.34455
G151T	-0.65235	-0.36662	0.91476
G151V	0.83475	0.47146	1.43504
G151W	-1.11053	-1.07477	-0.64721
G151Y	-1.30166	-1.0762	-0.57854
G151X	-0.00948	-0.52298	-0.63466
V152A	-0.04408	-0.77812	1.64946
V152C	0.42178	-0.63652	0.49757
V152D	0.42443	0.39058	1.7093
V152E	0.58306	0.57015	1.92967
V152F	0.77648	0.91012	1.63271
V152G	0.37639	0.2669	1.46851
V152H	2.92325	2.69698	1.77956
V152I	-0.75539	0.25384	1.34672
V152K	1.65189	2.36388	0.82211
V152L	0.32433	0.21197	0.46782
V152M	1.90148	2.71434	0.72404
V152N	0.82251	0.98144	1.29969
V152P	-0.18896	0.41147	1.31209
V152Q	1.06483	1.22585	1.08675
V152R	1.42888	1.76984	0.28561
V152S	0.52547	0.9391	1.13773
V152T	-0.30553	0.27333	0.93577
V152V	NA	NA	NA
V152W	3.88539	5.21221	1.33582
V152Y	-0.23932	0.2184	1.22582
V152X	0.34822	0.06581	-0.85414
D153A	-1.13146	-0.1098	-1.55594
D153C	-3.97125	-0.58469	-1.77389
D153D	NA	NA	NA
D153E	1.41923	1.50388	0.6205
D153F	0.35056	0.22943	-0.43909
D153G	-0.03558	0.18804	-0.12772
D153H	0.5716	1.09937	-1.3633
D153I	-0.53472	0.24928	-1.0427
D153K	-0.34177	0.44424	-0.29161
D153L	-0.11225	0.20139	-0.57676

D153M	-0.44562	-0.43743	-0.52396
D153N	-0.0187	0.91797	-0.09023
D153P	0.08527	1.07861	-1.30347
D153Q	0.43061	1.06092	0.04808
D153R	-0.36463	0.45685	-0.31093
D153S	-1.70955	-0.63591	-0.54509
D153T	-0.38844	0.2015	-0.77439
D153V	-0.61864	-0.57372	-1.44701
D153W	-0.42241	0.11234	-0.81435
D153Y	-0.73328	-0.02136	-1.21309
D153X	0.46297	-0.75404	-1.03053
D154A	-0.04689	0.44858	-0.46342
D154C	0.34389	0.47375	-0.2577
D154D	NA	NA	NA
D154E	0.0946	0.33283	0.1007
D154F	-1.15566	-1.08748	-0.07591
D154G	0.60204	0.3844	-0.19593
D154H	-1.36187	-0.1063	-0.5757
D154I	-0.38072	0.41519	-0.19995
D154K	0.60598	1.6197	-0.76566
D154L	0.36061	0.9917	-0.38686
D154M	0.38688	1.04053	-0.57922
D154N	-0.79833	-0.31496	-0.43602
D154P	-0.42136	-0.37424	0.15141
D154Q	-0.03364	0.74337	-0.76085
D154R	-0.45964	-0.80601	-0.35248
D154S	-0.65568	-0.86882	-0.24256
D154T	-0.62274	-1.64557	-0.54172
D154V	-0.51255	-0.06973	-0.47549
D154W	-0.616	0.52331	-0.10436
D154Y	-0.02318	0.20245	-0.19592
D154X	-0.6429	-0.95924	-1.1421
A155A	NA	NA	NA
A155C	-0.32296	-0.10596	0.41307
A155D	0.5273	0.7874	-0.77255
A155E	-0.66365	0.08369	-0.4033
A155F	-0.38731	-0.34444	-0.4124
A155G	-0.67054	-0.35486	-0.3212
A155H	0.72469	0.46733	-0.04968
A155I	0.01475	-0.02347	0.18287
A155K	-0.53496	-0.58903	-0.73106
A155L	0.57034	0.21145	0.53682
A155M	-0.14607	0.69296	0.07499

A155N	-0.37244	-0.1355	0.32828
A155P	0.39613	1.3853	1.40855
A155Q	0.61867	1.02653	0.57169
A155R	-0.12178	0.46017	-0.86877
A155S	0.04811	-0.07428	0.0763
A155T	0.199	-0.41422	0.16734
A155V	-0.50167	0.05345	0.40123
A155W	1.06161	1.47649	-0.87317
A155Y	0.63716	0.18868	-0.73869
A155X	0.47239	-0.0467	-1.09859
F156A	0.92573	0.76376	2.47137
F156C	1.20569	0.75221	2.16279
F156D	0.34801	-0.2573	-0.79546
F156E	0.71759	0.55838	1.8723
F156F	NA	NA	NA
F156G	0.3567	0.26328	1.84893
F156H	1.36063	1.91364	1.01494
F156I	-0.48683	-0.32536	0.77292
F156K	0.24843	0.13427	-0.35429
F156L	0.84956	-0.60954	2.23628
F156M	0.15821	0.29999	1.54191
F156N	0.48627	0.77213	1.43749
F156P	1.6966	0.12416	1.44126
F156Q	0.30944	-0.14541	2.08387
F156R	0.33475	0.41928	-0.72095
F156S	1.71637	-0.06792	2.83935
F156T	1.08689	0.99396	1.6515
F156V	0.22443	0.35648	1.01339
F156W	0.68937	1.07039	1.2443
F156Y	0.20596	0.17239	0.23897
F156X	0.05656	-0.07463	-0.69189
Y157A	-0.28861	-0.54833	0.16004
Y157C	-0.0724	0.85662	-0.08641
Y157D	-0.07002	-0.0601	1.25468
Y157E	0.26257	0.41437	1.76509
Y157F	0.46231	0.75737	-0.12942
Y157G	0.7437	-0.2185	0.72843
Y157H	0.0848	0.81908	0.26709
Y157I	-0.0417	0.33763	0.24162
Y157K	-0.63692	0.29936	-0.35386
Y157L	0.45675	0.33335	0.3626
Y157M	0.02455	0.79524	-0.15462
Y157N	0.26962	-0.18321	0.86675

Y157P	1.04613	-0.01236	0.93274
Y157Q	-0.48088	-0.31199	0.69174
Y157R	0.97779	1.49621	-0.3095
Y157S	0.53713	-0.66201	0.57717
Y157T	0.01669	-0.27152	0.93206
Y157V	0.99016	0.86884	0.66033
Y157W	0.15693	0.0334	0.28879
Y157Y	NA	NA	NA
Y157X	0.14226	0.51823	-0.97367
T158A	NA	NA	NA
T158C	NA	NA	NA
T158D	NA	NA	NA
T158E	NA	NA	NA
T158F	NA	NA	NA
T158G	NA	NA	NA
T158H	NA	NA	NA
T158I	NA	NA	NA
T158K	NA	NA	NA
T158L	NA	NA	NA
T158M	NA	NA	NA
T158N	NA	NA	NA
T158P	NA	NA	NA
T158Q	NA	NA	NA
T158R	NA	NA	NA
T158S	NA	NA	NA
T158T	NA	NA	NA
T158V	NA	NA	NA
T158W	NA	NA	NA
T158Y	NA	NA	NA
T158X	NA	NA	NA
L159A	-1.32549	-0.08583	-0.0063
L159C	0.5328	1.32644	0.11385
L159D	1.27248	0.41589	-0.48327
L159E	0.1662	0.37498	-0.24729
L159F	0.4971	0.93542	0.86809
L159G	0.54987	0.88538	0.73341
L159H	-0.10208	0.00167	-0.57392
L159I	-0.16234	-0.7977	-0.18739
L159K	0.1732	-0.64462	-0.83646
L159L	-0.6185	-0.22059	0.31799
L159M	0.31286	0.32611	-0.08234
L159N	-0.83164	0.17233	-0.47265
L159P	-0.37389	0.40375	-0.40958

L159Q	-0.30439	-0.48935	-0.44112
L159R	-0.29969	0.24179	-0.76931
L159S	0.52238	1.22653	0.34709
L159T	0.71949	0.04577	-0.08631
L159V	0.22101	0.8031	0.24887
L159W	0.96062	0.83876	0.9562
L159Y	1.31171	1.28932	0.17724
L159X	0.19592	-0.18347	-0.58756
V160A	-0.53779	-1.01131	1.45686
V160C	-0.3636	0.31166	-0.01863
V160D	0.12935	0.0868	-0.22455
V160E	-0.31668	-0.07939	1.60293
V160F	0.96814	0.94831	2.87044
V160G	0.35647	-0.09498	1.55616
V160H	0.81945	0.22476	2.18105
V160I	2.05895	2.24994	0.30742
V160K	0.28183	-0.19853	0.58354
V160L	0.17083	0.3798	0.77907
V160M	0.31735	0.09194	1.49831
V160N	-0.21505	-0.30713	1.35365
V160P	-0.65124	0.42515	-0.30723
V160Q	0.64688	-0.76333	1.55549
V160R	0.45046	0.81806	1.08199
V160S	-0.19271	-0.87769	0.96014
V160T	-0.62276	0.45167	0.47522
V160V	NA	NA	NA
V160W	-0.21462	-0.21518	1.56085
V160Y	1.12587	1.04615	1.77418
V160X	0.00284	-0.09838	-0.78661
R161A	-0.35991	-0.19747	0.49532
R161C	0.39909	0.49226	0.93948
R161D	0.35977	0.10644	1.24669
R161E	0.23166	0.31237	1.98246
R161F	0.2795	1.48781	0.88933
R161G	-1.07201	-0.90631	0.87627
R161H	1.52549	0.04853	0.7228
R161I	0.1037	-1.54941	0.91703
R161K	-0.28904	0.0986	0.30498
R161L	0.06126	1.1204	0.66336
R161M	-0.70143	-0.17419	0.37659
R161N	-1.81321	-0.17034	0.44721
R161P	-0.67535	0.75139	0.85097
R161Q	0.0027	0.27224	1.03548

R161R	1.62023	1.92316	0.26015
R161S	-1.01436	0.1637	0.99896
R161T	-0.1658	0.4597	0.74269
R161V	0.21471	-0.50022	0.79539
R161W	-0.61158	-0.92634	0.37142
R161Y	0.15986	0.1296	0.69262
R161X	1.48846	0.94848	-0.90866
E162A	-0.03233	0.92536	-0.05483
E162C	-0.4716	-0.21006	-0.40234
E162D	0.2992	0.50341	0.33835
E162E	NA	NA	NA
E162F	0.26023	-1.07633	-0.30238
E162G	0.26922	-0.42426	0.02104
E162H	-1.13841	-0.3229	0.00712
E162I	0.49407	-0.28455	0.00947
E162K	0.53233	0.07262	-0.32931
E162L	0.12537	-0.64808	0.03943
E162M	0.03346	0.5948	-0.37439
E162N	-1.31284	-0.76705	0.17552
E162P	-0.26216	0.19617	0.21548
E162Q	0.60926	0.2468	-0.34657
E162R	-0.30771	0.10326	-0.44025
E162S	-0.09536	-0.02085	-0.08994
E162T	-0.32204	0.21782	-0.42045
E162V	-0.14673	-0.51481	0.38159
E162W	-0.54872	-0.3946	-0.50934
E162Y	-1.05065	-1.19001	-0.32641
E162X	0.9875	0.25041	-0.59587
I163A	-0.47187	-0.04925	-0.67114
I163C	-1.19689	-0.68738	-0.06518
I163D	0.82241	1.56692	-0.31225
I163E	0.70944	0.58416	0.22112
I163F	0.44407	-0.80295	1.38544
I163G	0.89535	0.25284	-0.60858
I163H	-0.264	0.02794	0.85541
I163I	NA	NA	NA
I163K	-0.30173	0.45916	-0.16661
I163L	0.80558	0.87346	1.384
I163M	-0.198	0.19761	0.99488
I163N	-0.07998	-1.16004	0.44301
I163P	-1.16986	-0.52827	-0.66726
I163Q	0.36049	0.79194	0.4456
I163R	0.05791	-0.32151	-0.25924

I163S	-1.00749	-3.19586	-1.24543
I163T	-0.81765	-0.93075	-0.11932
I163V	0.02263	0.34087	-0.53866
I163W	0.04675	0.1063	1.30656
I163Y	0.44694	-0.01406	1.35364
I163X	0.72856	0.45618	-0.71281
R164A	-0.81178	-1.12054	0.21622
R164C	-0.30975	0.09987	0.25744
R164D	0.01362	0.62022	0.3575
R164E	0.29881	0.67117	0.17273
R164F	2.47557	2.36754	0.67449
R164G	-0.30597	0.13534	0.49097
R164H	0.67272	0.12925	0.14312
R164I	0.17299	-0.1663	0.24305
R164K	-0.26764	-0.51716	-0.2998
R164L	-0.29486	-1.26652	0.06297
R164M	-0.57649	0.0402	0.17452
R164N	-0.2569	-0.08851	0.22059
R164P	-0.41776	-0.47998	-0.24701
R164Q	0.67142	0.49133	0.28601
R164R	-0.16936	0.29045	0.08765
R164S	-0.6163	-0.43672	0.16095
R164T	-0.05851	1.2585	0.21584
R164V	0.53331	-0.32458	0.00017
R164W	-0.75586	0.33539	0.16398
R164Y	-0.67353	0.72187	0.06756
R164X	0.33227	0.30991	-0.66757
K165A	0.25643	0.4208	-0.21333
K165C	-0.67847	-0.64935	0.20783
K165D	-0.4044	-0.7284	0.27565
K165E	0.53431	0.47343	0.49585
K165F	-0.27818	-0.4358	0.30229
K165G	-0.03806	0.67594	0.45975
K165H	-0.93366	1.13985	-0.3389
K165I	0.04978	0.11637	0.1863
K165K	NA	NA	NA
K165L	0.91834	1.04568	0.80906
K165M	1.62572	-0.80943	0.32265
K165N	0.13986	-0.12797	0.24794
K165P	-0.07185	-0.38705	0.04172
K165Q	0.59932	0.10185	0.18198
K165R	0.64959	-1.07557	0.22395
K165S	-0.59436	-0.59021	0.25899

K165T	0.21596	-0.16323	1.23618
K165V	0.42289	0.52976	0.50722
K165W	-0.18429	-0.21465	-0.1142
K165Y	-0.02669	0.09925	0.52835
K165X	-0.21785	-0.38862	-1.01585
H166A	0.15322	-0.29556	0.18885
H166C	0.07169	0.31645	0.0193
H166D	-0.98058	-2.22893	-0.11539
H166E	-1.66881	-2.61935	0.32625
H166F	-0.81406	-0.96881	-0.15488
H166G	-1.62131	0.65318	-0.04691
H166H	NA	NA	NA
H166I	0.23931	-0.85309	0.36691
H166K	0.54342	0.26398	-0.30188
H166L	0.26659	-0.10995	0.21601
H166M	-0.14647	0.71873	0.25593
H166N	-0.01291	-1.18047	0.21736
H166P	-0.07323	0.84278	0.10431
H166Q	0.50842	0.24023	0.24309
H166R	-1.78185	-0.2854	0.10881
H166S	-0.64726	-1.81321	-0.30141
H166T	-1.68273	-1.60109	-0.12969
H166V	-1.22036	-0.15643	0.59878
H166W	-1.14214	-1.01891	-0.04271
H166Y	2.10337	2.17538	0.94683
H166X	0.74237	0.46419	-0.47168
K167A	0.63794	0.35477	0.53425
K167C	-0.38139	0.32808	0.79443
K167D	-0.31084	0.55448	1.3713
K167E	0.59819	0.47658	1.35205
K167F	0.56657	0.47641	1.44877
K167G	0.2115	-0.8548	0.35521
K167H	0.3775	1.06787	0.26506
K167I	-0.00425	-1.3608	1.05841
K167K	NA	NA	NA
K167L	0.54686	0.4194	1.44514
K167M	-0.27334	1.27178	1.36957
K167N	0.92572	1.68191	0.9808
K167P	0.07548	-0.14492	0.17926
K167Q	-0.76801	-1.19412	0.99207
K167R	1.12294	1.24893	0.63506
K167S	0.21407	0.38812	0.97137
K167T	-0.09386	0.30968	1.11277

K167V	0.57192	0.40023	1.36998
K167W	-0.06212	-1.68079	0.91358
K167Y	0.57512	-0.4052	1.28308
K167X	0.32711	1.3184	-0.83817
E168A	0.78909	0.30965	0.13525
E168C	-2.26463	0.37284	-0.52061
E168D	0.70524	-0.00384	-0.02642
E168E	NA	NA	NA
E168F	-1.69117	-0.59103	-0.56121
E168G	-0.73133	0.48785	-0.19392
E168H	0.21777	0.7321	-0.24328
E168I	0.89001	1.29255	-0.37221
E168K	-1.48635	-2.12785	-0.04212
E168L	2.04536	1.85861	-0.28554
E168M	-1.10531	-0.88867	-0.38581
E168N	-1.22769	-2.58301	0.31719
E168P	-0.24388	-0.35956	0.7521
E168Q	-0.46576	0.07421	-0.09449
E168R	-0.20924	-0.58851	0.06493
E168S	-0.37906	-0.32209	0.09867
E168T	-1.31595	0.11534	-0.3096
E168V	-3.90774	-0.36329	-0.47125
E168W	0.49179	1.81207	0.1194
E168Y	0.04242	-0.40594	0.88901
E168X	0.05455	0.53485	-0.9508
K169A	2.03072	0.41502	-0.06977
K169C	0.38685	-1.71925	-0.79447
K169D	-0.72741	-1.00185	0.14788
K169E	-1.01842	-1.0042	0.01699
K169F	-0.77127	-0.06979	-0.00562
K169G	-1.08313	-0.93067	-0.17295
K169H	0.0971	-0.36888	-0.19375
K169I	-0.24647	-0.639	-0.23943
K169K	NA	NA	NA
K169L	-2.08156	-0.92661	-0.21177
K169M	0.16346	-0.23313	0.25265
K169N	0.0718	0.01229	0.09139
K169P	-0.3141	-1.08001	-0.16606
K169Q	1.00042	0.44557	0.26916
K169R	0.0287	-0.17894	0.15281
K169S	0.31248	-0.32898	-0.19261
K169T	0.52617	-0.8725	0.04622
K169V	0.15095	-0.17603	0.09989

K169W	-0.09932	0.10667	-0.22485
K169Y	-0.51153	-0.0017	0.30185
K169X	-0.20048	-0.23639	-0.85544
M170A	-1.04534	0.58142	0.19668
M170C	-0.03101	0.07479	0.27526
M170D	-0.47247	-0.31755	-0.18225
M170E	-0.1499	1.01122	0.00355
M170F	0.29735	0.13953	0.30172
M170G	-0.50542	0.75986	0.25309
M170H	-0.86063	-0.27692	0.11382
M170I	0.31726	1.08827	0.26046
M170K	0.11935	0.52	0.0646
M170L	-0.19005	0.57168	0.08373
M170M	NA	NA	NA
M170N	-0.37353	-0.40291	-0.21963
M170P	-0.93465	-0.41721	0.02291
M170Q	0.42183	0.39176	-0.04643
M170R	-0.0648	0.16545	0.27248
M170S	0.41583	0.40294	-0.07283
M170T	-0.43376	-0.58894	0.22618
M170V	0.1351	-0.84737	-0.1831
M170W	-0.86985	-0.97543	-0.02204
M170Y	0.16399	0.49898	-0.01664
M170X	0.4023	-0.46819	-0.8722
S171A	0.01277	-0.8497	-0.53275
S171C	-0.06319	0.07783	0.55168
S171D	-0.43848	-0.01193	-0.24315
S171E	-0.56333	0.73087	-0.05827
S171F	0.6278	0.92621	-0.24827
S171G	-0.07949	-0.96914	-0.12761
S171H	0.05877	-0.46273	-0.2646
S171I	0.56111	-0.05579	-0.18558
S171K	-0.32513	-0.99601	-0.82846
S171L	-0.65949	-1.79262	0.28807
S171M	0.43424	-0.72086	0.02789
S171N	-0.4205	0.54611	0.04448
S171P	1.15856	1.01052	0.35764
S171Q	0.01556	0.91238	0.2282
S171R	-0.10168	-0.20211	-0.08844
S171S	0.03187	0.43285	0.02918
S171T	-0.33076	0.93371	-0.48446
S171V	-0.68865	-1.01021	-0.42523
S171W	0.46194	0.18868	0.31809

S171Y	-0.08666	-0.39148	0.01123
S171X	0.08984	0.67989	-0.62659
K172A	-0.9742	0.19861	-0.05538
K172C	-0.02336	-0.01164	0.29037
K172D	0.45385	-0.0122	0.26035
K172E	-1.01056	-0.58266	-0.08085
K172F	0.04583	-0.48771	0.0986
K172G	-0.25899	-0.04777	0.32042
K172H	0.96271	0.84767	0.0387
K172I	0.36015	0.25593	0.19521
K172K	NA	NA	NA
K172L	0.01742	0.88843	0.06125
K172M	0.46679	0.19651	-0.19482
K172N	0.79748	0.37765	0.17901
K172P	0.68909	-0.80241	0.19068
K172Q	-0.08637	0.23173	0.06183
K172R	0.5259	-0.00619	0.03107
K172S	-0.2414	-0.44815	0.06375
K172T	0.09432	0.81642	-0.07932
K172V	1.71602	-0.20304	0.02223
K172W	0.03879	-0.21943	-0.01693
K172Y	-0.0023	-0.6955	0.7426
K172X	0.26393	0.4842	-0.91214
D173A	-0.92014	-0.73223	-0.17009
D173C	-0.69698	-0.11234	-0.23928
D173D	NA	NA	NA
D173E	0.6541	1.04689	0.22254
D173F	0.1192	-0.4846	0.09485
D173G	-0.19509	0.32587	-0.1818
D173H	-0.24219	-0.66236	-0.45225
D173I	0.62459	0.57465	-0.06165
D173K	-0.71215	0.76645	0.17034
D173L	-0.67648	-3.09811	-0.15415
D173M	-0.9435	-0.44754	-0.13119
D173N	-0.0665	0.40159	0.01619
D173P	-0.0671	1.01201	-0.03586
D173Q	0.16885	-0.1718	-0.06788
D173R	-0.94177	-0.12997	-0.04378
D173S	-0.41282	0.58626	0.11845
D173T	-1.1157	0.25971	0.06632
D173V	-0.20175	-0.23975	0.01276
D173W	0.08563	-0.92544	0.12017
D173Y	0.01094	0.33802	-0.02479

D173X	1.41236	1.11768	-0.7633
G174A	1.29951	0.34973	0.48039
G174C	0.29396	0.71295	0.52353
G174D	-0.33403	0.56504	0.31806
G174E	-0.30677	-0.57993	0.20346
G174F	0.20532	0.86428	-0.41609
G174G	NA	NA	NA
G174H	-0.74221	0.41383	-0.43037
G174I	-0.53893	-0.47624	0.10767
G174K	0.20073	0.87066	0.1
G174L	-0.39962	0.20184	0.02065
G174M	0.17456	-0.49761	0.02445
G174N	-0.45131	-0.92745	-0.24612
G174P	0.41554	-0.84654	0.31578
G174Q	-0.19802	-0.35628	0.364
G174R	-0.37053	0.66513	0.08476
G174S	0.84263	0.34872	0.3205
G174T	0.18642	-0.16844	0.109
G174V	0.15953	0.18184	0.41756
G174W	0.12624	0.71339	-0.34989
G174Y	-1.17945	0.13185	0.04724
G174X	0.50195	-0.69695	-1.07674
K175A	-1.49911	-0.08862	-0.33763
K175C	0.0422	0.8035	-0.3106
K175D	0.44023	0.72916	-0.23577
K175E	0.00561	-0.43065	-0.00334
K175F	0.40538	1.7653	0.19197
K175G	-0.81694	-0.2114	-0.34517
K175H	0.28208	-0.19598	-0.00711
K175I	-0.09372	-0.15808	-0.32689
K175K	NA	NA	NA
K175L	0.14533	0.29345	-0.44856
K175M	0.28123	0.04943	-0.32487
K175N	-0.23471	-0.38244	0.15666
K175P	-0.13191	-0.05882	-0.0332
K175Q	-1.17902	-0.92738	-0.28069
K175R	0.23689	0.4274	-0.04721
K175S	1.79011	1.28077	0.25957
K175T	-0.00612	0.97418	-0.08785
K175V	-0.3436	-0.76933	-0.30443
K175W	-1.18992	-0.17662	0.0311
K175Y	0.32343	0.10249	-0.22993
K175X	-0.2003	-1.13245	-1.19867

K176A	0.39192	-0.421	0.10028
K176C	-0.48847	-0.10285	0.10385
K176D	0.19055	0.03632	-0.03567
K176E	-0.18868	0.07686	-0.32009
K176F	-0.88773	-0.00382	0.46663
K176G	-0.42823	0.34636	-0.03957
K176H	0.46848	0.20701	-0.81137
K176I	0.31938	-0.76118	-0.10151
K176K	NA	NA	NA
K176L	0.25812	-0.2789	-0.40138
K176M	0.1257	-0.46326	-0.08749
K176N	0.28128	0.30762	0.1205
K176P	-0.84654	-0.74743	-0.16358
K176Q	0.06629	-0.15452	0.01655
K176R	-0.55594	-0.0859	0.10017
K176S	0.17982	-0.01425	-0.10867
K176T	0.52488	-0.006	-0.11392
K176V	0.16386	-0.08822	0.22362
K176W	-0.43692	0.02717	0.07544
K176Y	0.1233	-0.08924	-0.00233
K176X	-0.21546	0.01406	-0.96166
K177A	-0.00818	0.13942	-0.28102
K177C	0.01928	0.25332	-0.26688
K177D	0.11921	0.69642	0.21854
K177E	-0.18557	0.41515	-0.20224
K177F	-0.21156	-0.88167	-0.29609
K177G	0.42721	0.75368	-0.41426
K177H	-0.30311	-0.10156	0.36744
K177I	0.37928	0.5072	0.30408
K177K	NA	NA	NA
K177L	0.19763	0.46233	-0.18458
K177M	0.1538	-0.13044	0.0265
K177N	0.65786	1.08495	0.23403
K177P	0.01533	-0.68319	-0.27553
K177Q	-0.78276	-0.14503	-0.27936
K177R	0.12169	0.13232	-0.45424
K177S	0.03173	0.21634	0.34761
K177T	-2.54284	-0.11249	0.02466
K177V	0.70493	0.48766	0.10968
K177W	-0.35429	-0.04536	0.39711
K177Y	0.16712	-0.20024	-0.15105
K177X	0.57315	-0.27609	-0.97338
K178A	-0.7998	-0.01192	0.10772

K178C	0.36009	1.23967	0.27598
K178D	-0.87681	-0.40859	0.01041
K178E	-0.58404	0.42777	-0.39547
K178F	-0.40617	1.15053	-0.16063
K178G	-0.35864	0.35631	-0.11194
K178H	-1.21307	-1.46723	-0.49263
K178I	0.24441	0.23586	0.11874
K178K	NA	NA	NA
K178L	-0.42785	0.21516	-0.95192
K178M	-0.21731	-0.79572	-0.38291
K178N	-0.16241	0.10466	0.05685
K178P	-0.48562	-0.22906	0.05618
K178Q	0.14017	1.05564	0.20376
K178R	-0.75993	0.08868	-0.46762
K178S	-0.33215	0.34688	-0.08687
K178T	-0.15856	-0.05496	-0.28668
K178V	0.87253	-0.21466	0.24069
K178W	0.14228	-0.14625	-0.12528
K178Y	0.85263	0.95906	-0.35781
K178X	0.44413	-0.10529	-1.23155
K179A	0.15739	1.46938	-0.38925
K179C	-0.43436	0.57246	0.03245
K179D	-0.10061	-0.73085	0.14933
K179E	-0.98087	-1.17631	-0.10863
K179F	-1.42466	-1.61746	0.10102
K179G	0.8404	-0.22524	-0.30392
K179H	-1.21416	0.03111	0.12606
K179I	0.25115	1.33794	0.22098
K179K	NA	NA	NA
K179L	-0.22441	0.34797	0.13425
K179M	0.5683	1.03005	0.3977
K179N	0.50864	0.72068	0.04564
K179P	0.41756	1.3903	0.11589
K179Q	-0.78706	-1.34543	0.35933
K179R	-0.14618	-0.12862	0.60988
K179S	0.30959	0.11355	0.18369
K179T	-0.28175	0.29309	-0.14492
K179V	0.37814	0.8049	0.34273
K179W	-0.46899	0.49036	0.03367
K179Y	0.45798	0.76589	0.75857
K179X	-0.61159	0.08696	-1.254
K180A	-0.03335	0.35454	-0.23315
K180C	-0.64643	-0.61391	-0.05942

K180D	-0.42934	-0.37024	-0.07389
K180E	-0.06297	1.09419	0.00497
K180F	0.02558	-0.36019	-0.22583
K180G	-0.31616	0.66961	0.01824
K180H	-0.42071	-0.31344	-0.10114
K180I	0.56281	0.48575	0.22116
K180K	NA	NA	NA
K180L	-0.12161	0.11122	0.15181
K180M	-0.23909	-0.78691	0.13461
K180N	-0.08433	0.17693	0.32353
K180P	0.77156	1.08315	0.03763
K180Q	-0.69593	-0.5553	0.06261
K180R	-0.89127	-0.6525	-0.50505
K180S	-0.24364	-0.50921	-0.17161
K180T	-0.20591	0.71813	-0.33446
K180V	0.26576	0.00759	0.18065
K180W	-0.36343	-0.77199	-0.14824
K180Y	-0.55877	-2.43395	-0.45495
K180X	0.31049	-0.54728	-0.70809
S181A	0.03878	0.16482	0.06414
S181C	0.82565	0.26918	-0.32189
S181D	-1.06465	-1.14429	-0.40002
S181E	-0.52519	-0.75155	-0.55652
S181F	0.19563	0.49449	-0.10292
S181G	-0.70983	-0.02258	-0.20084
S181H	0.0415	-0.44169	0.15059
S181I	-0.028	0.55319	0.1201
S181K	-0.0054	0.5306	-0.18135
S181L	0.85306	1.77577	-0.23153
S181M	-0.17242	0.94351	-0.35128
S181N	-0.72808	-0.03766	0.2359
S181P	-1.88652	0.16747	0.20361
S181Q	0.37215	1.15875	0.21623
S181R	-0.33366	0.23471	0.02188
S181S	-0.32395	0.42562	-0.1846
S181T	-0.37692	0.39911	-0.18814
S181V	-0.16003	-0.21034	0.12498
S181W	0.13655	-0.67099	-0.63608
S181Y	-0.18959	-1.12575	-0.18252
S181X	0.4923	0.38082	-1.1491
K182A	0.52794	0.29427	0.05674
K182C	-0.42647	-0.80973	-0.66226
K182D	1.48883	0.96889	0.1169

K182E	-0.51019	0.54546	0.16976
K182F	0.25449	-0.33028	-0.13763
K182G	0.4954	0.02941	-0.10563
K182H	0.07727	0.19974	-0.0324
K182I	0.31565	0.7083	-0.0246
K182K	NA	NA	NA
K182L	-0.29755	0.17619	0.08512
K182M	0.21579	0.00962	-0.15136
K182N	-0.34882	0.24943	0.09098
K182P	-0.64369	-0.66894	0.01045
K182Q	-0.69882	-0.11092	0.04742
K182R	0.06042	0.41242	-0.02643
K182S	-1.26971	-0.31323	-0.04757
K182T	-0.42081	-0.6589	-0.00818
K182V	0.35908	1.18408	0.02504
K182W	-0.64166	-0.56897	-0.19426
K182Y	-0.56981	-0.70067	-0.05001
K182X	0.41516	0.63781	-0.6782
T183A	0.05773	-0.02171	-0.09708
T183C	0.33951	-0.21233	-0.17787
T183D	-0.31184	1.60406	0.03803
T183E	-0.25781	0.10628	-0.29173
T183F	-0.42968	0.47948	-0.4815
T183G	-1.00581	-0.23283	0.00693
T183H	0.57024	1.81383	-0.17252
T183I	0.0945	-0.27308	-0.11413
T183K	0.13639	0.30981	0.00467
T183L	0.92745	2.30592	-0.10048
T183M	0.92159	0.87004	0.36349
T183N	-0.08138	-0.94512	0.03215
T183P	-1.37634	-0.07389	-0.13547
T183Q	0.06394	-0.17073	0.03742
T183R	0.06828	0.82557	-0.05978
T183S	-0.10078	-0.65462	-0.21093
T183T	NA	NA	NA
T183V	0.91406	0.3932	-0.02516
T183W	-0.30319	0.24594	-0.48498
T183Y	-0.65733	-0.21577	-0.09551
T183X	0.28384	0.31382	-0.74813
K184A	0.23149	0.162	0.18566
K184C	1.81249	1.53876	-0.34904
K184D	0.84804	-0.57621	0.07779
K184E	0.21955	-0.85576	0.03704

K184F	-0.32877	0.29243	0.00273
K184G	-0.95321	0.30707	0.10942
K184H	0.22251	0.64843	0.19549
K184I	-0.32269	0.50757	0.14043
K184K	NA	NA	NA
K184L	0.01335	0.27074	-0.05556
K184M	-0.10704	0.11235	0.24144
K184N	0.42172	0.32169	0.39936
K184P	-0.23391	-0.46929	0.03373
K184Q	0.06383	-0.16261	0.1077
K184R	0.04066	0.2176	-0.18616
K184S	-0.24438	-0.84366	-0.20795
K184T	0.04858	0.24179	0.08659
K184V	0.40836	0.78795	0.50545
K184W	-0.20376	-0.79837	-0.07941
K184Y	0.47034	-0.0335	-0.08688
K184X	0.93278	0.64594	-0.62498
C185A	0.70135	0.5709	-0.83972
C185C	NA	NA	NA
C185D	-0.59558	-1.07057	-0.08626
C185E	0.3397	0.4017	-0.75481
C185F	1.35256	1.5481	-0.58869
C185G	0.73627	0.44655	-0.67872
C185H	0.3544	-0.97647	-0.70691
C185I	0.31153	0.02571	-0.7825
C185K	-0.11568	-0.3788	-0.46357
C185L	0.78413	0.1655	-0.4808
C185M	0.04441	0.59796	-0.41509
C185N	-0.11547	-0.04377	-0.60895
C185P	-0.4752	0.32783	-0.83886
C185Q	1.10135	0.7051	-0.96324
C185R	-0.2991	0.41314	-0.63211
C185S	0.09282	0.10436	-0.71432
C185T	0.51361	-0.40722	-0.50323
C185V	-0.20653	-0.16447	-0.63548
C185W	-0.29025	-0.13363	-0.32923
C185Y	0.48597	-0.40728	-0.67105
C185X	-0.07158	0.47776	-0.51735
V186A	-0.30572	-0.72148	-0.07567
V186C	0.45091	0.09364	-0.21882
V186D	-0.02592	-0.37809	-0.28077
V186E	0.21536	-0.17185	0.31653
V186F	0.24753	-0.76261	0.38633

V186G	-0.15628	-1.39818	-0.11796
V186H	-0.15892	-0.10282	-0.11062
V186I	-0.29511	-1.10932	0.14628
V186K	0.07958	0.07222	-0.11183
V186L	-0.51184	0.99041	-0.33935
V186M	0.1471	0.90196	0.10179
V186N	-0.99289	0.46359	-0.19031
V186P	-0.10573	-0.09612	0.08088
V186Q	-0.4879	0.09084	-0.23872
V186R	-0.84537	-0.14489	-0.11874
V186S	1.49509	1.47353	-0.50333
V186T	-0.33638	0.45193	0.0975
V186V	NA	NA	NA
V186W	-0.49775	0.83763	-0.56544
V186Y	0.40655	-0.06795	-0.10657
V186X	0.94844	0.50162	-0.12008
I187A	0.14495	0.15321	0.02469
I187C	0.19176	-0.06317	-0.16044
I187D	-0.42392	-0.4506	-0.85428
I187E	0.1935	0.64009	-0.60984
I187F	-0.15881	0.27255	-0.36399
I187G	-0.18501	-0.14094	-0.70377
I187H	-0.04815	0.24367	-0.36458
I187I	NA	NA	NA
I187K	0.20614	0.30493	-0.77297
I187L	0.14915	0.59544	0.49611
I187M	0.03564	0.07982	0.07439
I187N	-0.40054	-1.60451	0.14066
I187P	0.36516	0.38662	0.00806
I187Q	-0.35584	0.25377	-0.35464
I187R	0.27212	1.11745	-0.29756
I187S	-0.65368	-0.22627	-0.16312
I187T	-0.09923	0.65039	0.02222
I187V	0.43093	-0.06533	-0.468
I187W	-1.0057	0.33967	-0.13898
I187Y	-0.38499	-0.4923	-0.1654
I187X	0.78365	1.70881	-0.92109
M188A	1.42629	1.55079	0.19273
M188C	0.42088	0.42986	0.19214
M188D	-0.26046	-0.3497	-0.45003
M188E	-0.25864	-0.24044	-0.00422
M188F	-0.74085	0.21996	-0.41825
M188G	-0.29332	-0.49992	-0.32902

M188H	0.67763	-1.19281	-0.24906
M188I	1.17631	-0.13489	0.37467
M188K	0.35787	0.0872	0.17305
M188L	-1.21674	0.12151	-0.18238
M188M	NA	NA	NA
M188N	-0.1548	-0.15775	-0.06213
M188P	0.19446	-0.54971	-0.68323
M188Q	0.05519	-1.13308	-0.03288
M188R	0.48481	-0.43889	-0.32835
M188S	0.30922	0.52213	0.25231
M188T	1.38432	0.92974	0.02883
M188V	-0.01454	0.57309	0.00079
M188W	-0.55664	0.32402	-0.2426
M188Y	-0.01481	0.55333	-0.31997
M188X	0.16707	0.21145	-0.36912

Table S3. Maximum Z-score and number of resistance mutations at each amino acid position

Residue	Maximum Zscore MRTX1257	Maximum Zscore Sotorasib	Number of resistant mutations MRTX1257	Number of resistant mutations Sotorasib
T2	1.294723677	0.905233059	1	0
E3	1.378775723	0.565090836	1	0
Y4	2.606531914	1.731500312	3	2
K5	1.00289144	0.9072493	0	0
L6	0.97090953	1.171290227	0	0
V7	1.343973249	0.96982655	1	0
V8	4.515145885	5.492160713	10	12
V9	4.216054787	4.562403382	8	6
G10	1.020652934	1.180662778	0	0
A11	4.904944436	2.620531567	4	2
C12	5.645392764	6.352267957	16	16
G13	5.240096516	6.237065461	6	4
V14	4.952165849	4.886813525	4	3
G15	1.384510886	0.352668955	1	0
K16	5.443122677	6.100775535	3	3
S17	0.672409833	0.526047819	0	0
A18	0.731530656	1.043045625	0	0
L19	2.215486835	1.005370096	1	0
T20	1.216581203	3.247190233	0	1
I21	2.459810797	1.245906505	1	0
Q22	0.815621979	0.682374068	0	0
L23	2.72377033	0.753428202	2	0
I24	1.97876553	1.170569503	3	0
Q25	1.68558115	1.787351735	1	1
N26	0.535583853	1.329752084	0	0
H27	1.92585348	0.461704215	1	0
F28	0.5039588	0.44285048	0	0
V29	0.23924404	0.057265763	0	0
D30	1.648282328	1.218159969	1	0
E31	1.050182409	0.324760213	0	0
Y32	0.311515168	0.44677409	0	0
D33	0.046403201	0.649303904	0	0
P34	0.445445416	0.493968537	0	0
T35	1.661672699	1.130699919	1	0
I36	0.579682921	0.436758568	0	0
E37	2.028880067	2.431481664	2	2

D38	-0.219606328	0.109219756	0	0
S39	0.264535832	0.232004114	0	0
Y40	0.645660569	0.633562678	0	0
R41	1.570619911	1.638768545	3	1
K42	1.749729976	0.811171658	2	0
Q43	1.364604672	0.736037459	1	0
V44	0.967877691	1.61899417	0	1
V45	0.407580738	0.471991252	0	0
I46	0.969397222	0.836920043	0	0
D47	0.463103306	0.436301795	0	0
G48	0.37561348	1.06379089	0	0
E49	0.373091803	0.63586306	0	0
T50	0.314686782	0.900276963	0	0
C51	0.830774084	1.541727872	0	1
L52	1.049143402	0.615732859	0	0
L53	1.449374898	2.417649239	3	2
D54	0.550265979	1.006944813	0	0
I55	2.054289983	1.318031886	1	0
L56	1.803054277	2.85720548	1	3
D57	0.117655301	1.107591441	0	0
T58	0.965452768	0.383554049	0	0
A59	2.773872135	4.577123945	3	3
G60	1.089577556	0.800013487	0	0
Q61	4.780400631	6.158236851	3	3
E62	2.707686203	0.992645974	2	0
E63	2.166134801	1.443293674	4	0
Y64	3.603354576	0.237455831	12	0
S65	NA	NA	0	0
A66	1.743293017	1.284158177	2	0
M67	0.46231462	0.79028957	0	0
R68	3.906419214	3.941071483	13	6
D69	1.343785293	1.505793823	1	0
Q70	2.99881265	0.701059313	1	0
Y71	0.514082127	0.626352909	0	0
M72	5.295180633	1.425614047	9	0
R73	1.607998317	1.177954923	1	0
T74	0.733772662	1.067788841	0	0
G75	1.259043408	0.724833892	1	0
E76	1.504350591	1.065044903	2	0
G77	4.194685582	4.374040729	7	6
F78	2.007908558	0.949033457	5	0
L79	0.640213138	0.902417719	0	0
C80	0.975881486	0.664804593	0	0
V81	0.713681572	1.953615766	0	1
F82	1.247376538	1.502288541	0	0

A83	1.584771783	2.518554615	1	2
I84	0.983363425	1.575325861	0	1
N85	1.254343714	1.196901385	1	0
N86	0.155281742	0.870406438	0	0
T87	0.457656706	0.870881389	0	0
K88	0.740760556	1.428800811	0	0
S89	0.451646257	0.71667481	0	0
F90	0.62884367	0.953539667	0	0
E91	0.493957554	1.108980026	0	0
D92	2.980766421	0.726159688	6	0
I93	1.378524018	1.313576647	1	0
H94	2.118471117	1.111820004	1	0
H95	4.737153117	1.446420973	19	0
Y96	3.439876703	4.106299126	15	14
R97	2.674616832	0.595575846	1	0
E98	NA	NA	0	0
Q99	6.037337873	4.352952341	11	3
I100	0.902031783	0.835804034	0	0
K101	1.426420579	1.061420058	1	0
R102	1.704690625	1.321369868	8	0
V103	2.88856742	1.453455038	4	0
K104	1.245427576	0.557501117	0	0
D105	0.764504708	1.132081802	0	0
S106	2.436500411	2.742559647	1	1
E107	0.897441209	0.656669625	0	0
D108	0.718357451	1.043144856	0	0
V109	1.674145014	1.246781552	1	0
P110	0.308622245	0.820556823	0	0
M111	1.239703153	0.979883004	0	0
V112	2.032867738	0.669184856	2	0
L113	0.579768001	0.834378098	0	0
V114	1.525133454	1.837519988	1	1
G115	0.908093717	0.689219377	0	0
N116	5.442438422	6.357595369	6	6
K117	5.096251082	6.958554517	10	11
C118	1.95595303	1.709711313	1	1
D119	4.94121766	5.680439172	5	3
L120	2.130918786	1.286062241	1	0
P121	1.445721304	0.622883088	1	0
S122	1.376695868	1.53731968	1	1
R123	1.447488703	1.474213693	1	0
T124	1.008205096	1.189982227	0	0
V125	0.857320078	0.557000106	0	0
D126	1.270358172	0.958639746	1	0
T127	0.61460264	1.507610311	0	0

K128	2.264038086	2.19311207	2	1
Q129	1.009514787	1.537569213	0	1
A130	0.487485441	0.532158205	0	0
Q131	2.016163492	1.838134659	1	1
D132	1.028427329	1.543065726	0	1
L133	1.908886943	2.168741502	1	1
A134	0.833572184	1.401214413	0	0
R135	1.754767628	2.354212032	1	1
S136	0.753006607	1.085265185	0	0
Y137	0.726262886	1.11353737	0	0
G138	1.464454465	1.165903166	2	0
I139	1.241736075	1.11745158	0	0
P140	0.981999635	1.272512033	0	0
F141	1.493127244	0.720043225	2	0
I142	2.624562528	2.853785198	1	1
E143	1.060659635	0.630230773	0	0
T144	0.812936907	0.879525784	0	0
S145	4.021020389	4.677795988	6	7
A146	3.269827459	3.154111607	3	2
K147	0.75076462	1.043701648	0	0
T148	2.580292791	2.149906273	2	1
R149	1.789049729	1.856442052	1	1
Q150	1.030763709	1.885831591	0	1
G151	0.898329383	1.164194861	0	0
V152	3.885392635	5.212214537	5	5
D153	1.419226001	1.503880836	1	0
D154	0.605975785	1.619697305	0	1
A155	1.061614878	1.476490529	0	0
F156	1.716365072	1.913638795	3	1
Y157	1.046131039	1.496208391	0	0
T158	NA	NA	0	0
L159	1.311710931	1.326440871	2	0
V160	2.058949895	2.249941904	1	1
R161	1.620234691	1.92315781	1	0
E162	0.987504486	0.925363412	0	0
I163	0.895345416	1.566918209	0	1
R164	2.475570491	2.367538352	1	1
K165	1.625724778	1.139854014	1	0
H166	2.103370244	2.175375132	1	1
K167	1.122944382	1.681905935	0	1
E168	2.045356525	1.85861207	1	2
K169	2.030717206	0.445572633	1	0
M170	0.421826836	1.088267379	0	0
S171	1.158564366	1.010523441	0	0
K172	1.71602381	0.888431637	1	0

D173	1.412362148	1.117681961	0	0
G174	1.299510448	0.870655883	1	0
K175	1.790114931	1.76529801	1	1
K176	0.524881204	0.346359188	0	0
K177	0.704932766	1.084947279	0	0
K178	0.872532347	1.239672096	0	0
K179	0.840400789	1.469381215	0	0
K180	0.771558625	1.094194234	0	0
S181	0.853058616	1.775771508	0	1
K182	1.488828547	1.184075398	1	0
T183	0.927447046	2.305922738	0	3
K184	1.812486727	1.538759804	1	1
C185	1.352558129	1.548101213	1	1
V186	1.495088244	1.473534671	1	0
I187	0.783646714	1.708807479	0	0
M188	1.426293692	1.550786649	2	1

Table S4. Alleles selected for validation experiments and their Z-scores in screen data.

Allele	Zscore MRTX1257	Zscore Sotorasib
C12R	5.34	6.06
G12C/V8L	0.71	3.09
G12C/V9F	2.63	1.00
G12C/G13D	3.06	4.65
G12C/V14L	4.55	2.09
G12C/K16T	3.42	3.65
G12C/A59S	2.77	4.58
G12C/Q61R	4.78	6.16
G12C/E62D	2.71	-0.16
G12C/Y64N	3.34	-0.50
G12C/R68S	3.76	3.47
G12C/M72L	2.30	0.15
G12C/G77V	4.19	4.37
G12C/H95D	4.74	-0.44
G12C/H95Q	3.29	0.51
G12C/H95R	2.33	0.26
G12C/Y96C	1.74	1.38
G12C/Y96D	3.33	3.44
G12C/Q99K	1.85	-0.37
G12C/K117N	4.32	5.89
G12C/D119H	4.94	5.68
G12C/A146P	3.27	3.15
Cutoff	1.25	1.50

The Z-score for each allele in the drug treated arm are listed. The Z-score below cutoff was indicated in grey.

Table S5. Summary of IC50 for individual alleles with each G12C inhibitor as measured in Ba/F3 single-allele drug resistance assays.

	IC50 ± SD (nM)	
Allele	Adagrasib	Sotorasib
G12C	1.01 ± 0.18	19.81 ± 3.46
G12R	598.03 ± 92.92	7116.33 ± 1177.58
G12C/V8L	4.46 ± 1.21	128.62 ± 60.06
G12C/V9F	108.7 ± 10.67	202 ± 32.35
G12C/G13D	44.59 ± 4.93	786.5 ± 93.08
G12C/V14L	162.93 ± 54.97	290.93 ± 65.62
G12C/K16T	289.47 ± 73.54	2524 ± 479.25
G12C/A59S	14.46 ± 3.55	766.1 ± 191.67
G12C/Q61R	258.67 ± 64.11	3998.33 ± 259.72
G12C/E62D	115.6 ± 11.43	18.57 ± 5.23
G12C/Y64N	97.45 ± 46.33	9.57 ± 3.46
G12C/R68S	147.07 ± 19.03	643.27 ± 236.65
G12C/M72L	42.02 ± 10.17	29.09 ± 8.41
G12C/G77V	70.75 ± 29.8	699.07 ± 163.14
G12C/H95D	234.3 ± 51.8	14.43 ± 4.61
G12C/H95Q	233.82 ± 67.37	17.05 ± 2.71
G12C/H95R	213.2 ± 52.26	8.6 ± 2.15
G12C/Y96C	332.9 ± 39.76	3814 ± 577.59
G12C/Y96D	376.64 ± 82.57	6920.67 ± 2029.04
G12C/Q99K	171.43 ± 56.85	65.82 ± 6.32
G12C/K117N	36.98 ± 4.62	846.7 ± 51.48
G12C/D119H	16.26 ± 8.83	242.63 ± 154.01
G12C/A146P	30.66 ± 1.6	406.17 ± 61.66

Table S6. Summary of AUC, AUC change relative to $KRAS^{G12C}$ and Relative Resistance Score for each allele. Data are derived from dose-response curves from Ba/F3 single-allele drug resistance assays.

	Adagrasib			Sotorasib		
Allele	AUC ± SD	AUC relative to G12C	Relative resistance score	AUC ± SD	AUC relative to G12C	Relative resistance score
G12C	1.1 ± 0.071	1.00	0.00	0.3 ± 0.052	1.00	0.00
G12R	3.8 ± 0.061	3.60	1.00	2.8 ± 0.111	8.11	1.00
G12C/V8L	1.6 ± 0.146	1.60	0.21	1.1 ± 0.246	3.06	0.29
G12C/V9F	3.1 ± 0.032	2.90	0.73	1.3 ± 0.035	3.81	0.40
G12C/G13D	2.7 ± 0.052	2.60	0.59	1.9 ± 0.03	5.45	0.63
G12C/V14L	3.2 ± 0.068	3.10	0.78	1.5 ± 0.075	4.21	0.45
G12C/K16T	3.5 ± 0.068	3.40	0.89	2.4 ± 0.103	6.93	0.83
G12C/A59S	2.2 ± 0.097	2.10	0.41	1.9 ± 0.107	5.40	0.62
G12C/Q61R	3.2 ± 0.282	3.00	0.78	2.6 ± 0.05	7.40	0.90
G12C/E62D	3.1 ± 0.163	2.90	0.72	0.3 ± 0.077	0.95	-0.01
G12C/Y64N	3 ± 0.206	2.90	0.71	0.1 ± 0.088	0.26	-0.10
G12C/R68S	3.2 ± 0.082	3.10	0.78	1.8 ± 0.132	5.17	0.59
G12C/M72L	2.7 ± 0.072	2.60	0.59	0.4 ± 0.114	1.31	0.04
G12C/G77V	2.9 ± 0.346	2.80	0.69	1.8 ± 0.08	5.30	0.60
G12C/H95D	3.4 ± 0.147	3.23	0.85	0.2 ± 0.081	0.64	-0.05
G12C/H95Q	3.4 ± 0.277	3.30	0.86	0.3 ± 0.036	0.85	-0.02
G12C/H95R	3.4 ± 0.11	3.22	0.85	0.1 ± 0.033	0.31	-0.09
G12C/Y96C	3.6 ± 0.042	3.40	0.91	2.6 ± 0.018	7.41	0.90
G12C/Y96D	3.6 ± 0.079	3.50	0.93	2.7 ± 0.113	7.85	0.96
G12C/Q99K	3.3 ± 0.16	3.10	0.81	0.8 ± 0.036	2.32	0.19
G12C/K117N	2.6 ± 0.041	2.50	0.56	1.95 ± 0.048	5.53	0.64
G12C/D119H	2.2 ± 0.208	2.10	0.41	1.3 ± 0.28	3.70	0.38
G12C/A146P	2.6 ± 0.046	2.40	0.54	1.64 ± 0.057	4.64	0.51

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