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Supporting information for article:

Structural basis of the dominant inheritance of hypermethioninemia associated with the Arg264His mutation in the MAT1A gene

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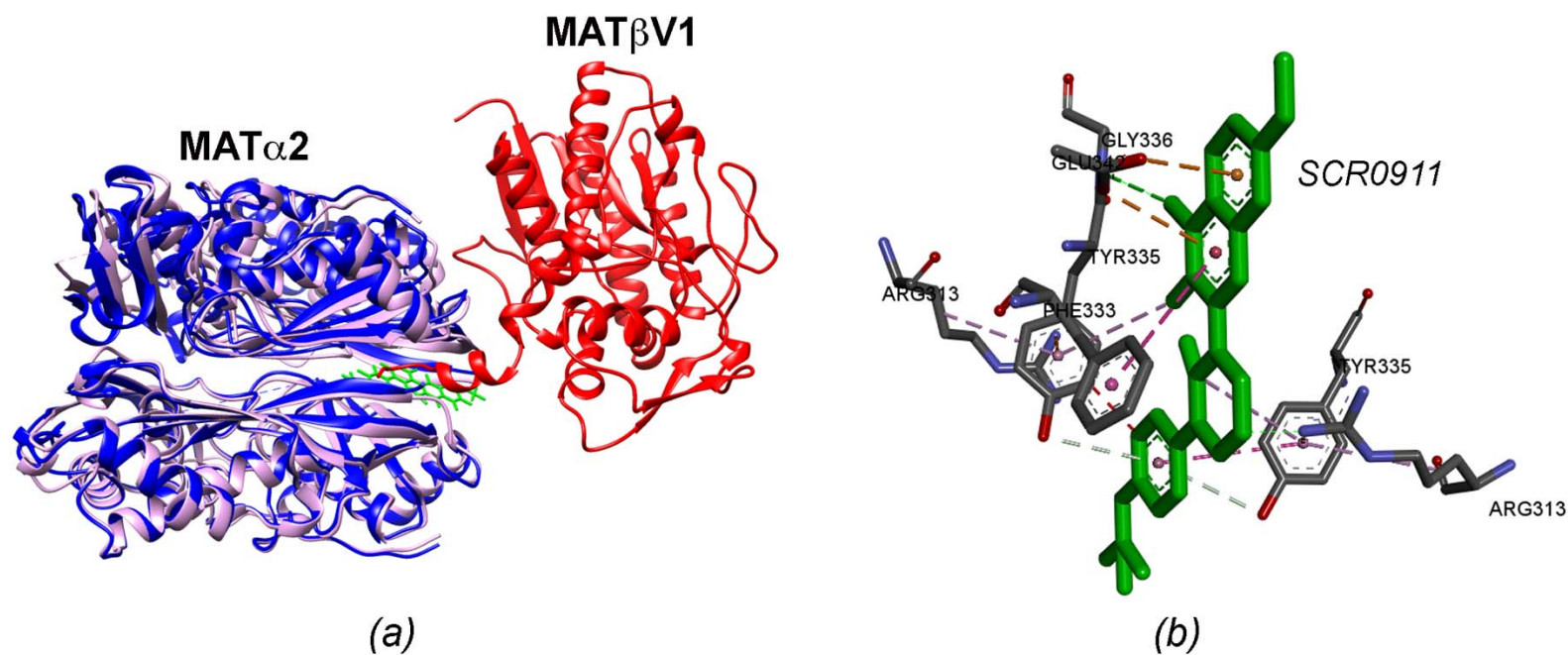


Figure S1 Molecular docking of SCR0911 binding site of the R264H mutant by PachtDock. **(a)** The R264H mutant (grey) is aligned with the complex structure of MAT α 2 (blue) and MAT β (red). SCR0911 is shown in a green stick. **(b)** SCR0911 and R264H interaction profiles obtained from PachtDock are shown. Protein ligand interactions are represented by green (H-bonds), pink (π - π stacking) and orange colour (electrostatic interactions).

Table S1 Dimer interface analysis showing residues involved in polar interactions.

wtMATα1				R264H			
Hydrogen bonds				Hydrogen bonds			
#	Chain A	Distance [Å]	Chain B	#	Chain A	Distance [Å]	Chain B
1	B:SER 329[OG]	3.39	A:MET 19[O]	1	B:THR 21[N]	3.24	A:GLN 317[OE1]
2	B:SER 319[OG]	3.03	A:MET 19[O]	2	B:THR 21[OG1]	3.19	A:SER 319[OG]
3	B:ARG 264[NH2]	3.34	A:GLU 57[OE1]	3	B:THR 21[OG1]	3.17	A:SER 329[OG]
4	B:GLN 183[NE2]	2.94	A:GLN 135[O]	4	B:LYS 61[NZ]	3.66	A:GLU 70[OE2]
5	B:ARG 264[NH2]	3.17	A:THR 262[O]	5	B:LEU 137[N]	3.84	A:GLU 23[OE2]
6	B:MET 19[N]	2.99	A:SER 329[OG]	6	B:LYS 181[NZ]	2.95	A:ASP 134[OD1]
7	B:GLN 190[NE2]	3.20	A:GLU 342[OE1]	7	B:LYS 181[NZ]	2.75	A:ASP 134[OD2]
8	B:MET 19[O]	3.36	A:GLN 317[NE2]	8	B:GLN 183[NE2]	2.76	A:TYR 320[O]
9	B:MET 19[O]	3.27	A:SER 319[OG]	9	B:ALA 259[N]	2.76	A:GLU 70[OE2]
10	B:MET 19[O]	3.49	A:SER 329[OG]	10	B:HIS 264[NE2]	2.97	A:GLU 57[OE1]
11	B:GLU 57[OE1]	3.19	A:ALA 259[N]	11	B:GLN 317[NE2]	2.96	A:THR 21[O]
12	B:GLU 57[OE2]	2.47	A:ARG 264[NH2]	12	B:SER 319[OG]	3.15	A:THR 21[OG1]
13	B:GLN 135[OE1]	2.41	A:THR 185[OG1]	13	B:SER 329[OG]	3.19	A:THR 21[OG1]
14	B:GLN 135[OE1]	3.26	A:THR 21[OG1]	14	B:SER 331[OG]	2.59	A:MET 19[O]
15	B:THR 185[OG1]	2.79	A:GLN 135[NE2]	15	B:GLN 317[OE1]	3.32	A:THR 21[N]
16	B:THR 262[O]	2.92	A:ARG 264[NH2]	16	B:GLU 70[OE2]	3.88	A:LYS 61[NZ]
17	B:SER 329[OG]	2.95	A:MET 19[N]	17	B:GLU 111[OE1]	3.55	A:LYS 61[NZ]
18	B:GLU 342[OE1]	3.06	A:GLN 190[NE2]	18	B:ASP 134[OD1]	3.21	A:LYS 181[NZ]
				19	B:ASP 134[OD2]	3.12	A:LYS 181[NZ]
				20	B:TYR 320[O]	2.81	A:GLN 183[NE2]
				21	B:GLU 342[OE1]	3.77	A:GLN 190[NE2]
				22	B:GLU 70[OE2]	2.85	A:ALA 259[N]
				23	B:GLU 57[OE1]	2.90	A:HIS 264[NE2]

				24	B:THR 21[O]	2.84	A:GLN 317[NE2]
				25	B:MET 19[O]	2.64	A:SER 331[OG]
	Salt-Bridges				Salt-Bridges		
#	Chain A		Chain B	#	Chain A	Distance [Å]	Chain B
1	B:ARG 264[NH1]	3.87	A:GLU 57[OE1]	1	B:LYS 61[NZ]	3.66	A:GLU 70[OE2]
2	B:ARG 264[NH2]	3.34	A:GLU 57[OE1]	2	B:LYS 181[NZ]	2.95	A:ASP 134[OD1]
3	B:GLU 57[OE2]	2.68	A:ARG 264[NH1]	3	B:LYS 181[NZ]	2.75	A:ASP 134[OD2]
4	B:GLU 57[OE2]	2.47	A:ARG 264[NH2]	4	B:HIS 264[NE2]	2.97	A:GLU 57[OE1]
				5	B:GLU 70[OE2]	3.88	A:LYS 61[NZ]