

Supplemental material

Table 1. ^1H and ^{13}C chemical shifts of Ile (δI only), Leu and Val methyl groups in malate synthase G from *E.coli* at pH 7.1, 37 °C.^{a)}

Res.	^1H	^{13}C	^1H	^{13}C
I5	0.80	12.8		
L10	0.85	22.3	0.90	24.4
I12	-0.01	15.5		
V20	0.45	21.5	0.72	23.9
V24	0.52	20.5	0.12	22.5
L25	-0.30	20.0	0.28	24.5
L30	0.80	22.0	0.74	25.8
I42	0.66	14.6		
V43	0.65	20.8	1.03	24.7
L46	0.81	22.8	0.79	26.2
L53	0.71	22.2	0.29	25.9
L54	0.65	19.9	1.08	24.8
I60	0.75	12.0		
L64	0.73	24.5	0.88	25.3
V75	0.79	20.5	0.79	21.9
L85	-0.23	20.0	-0.10	24.7
L88	0.81	23.5	0.65	25.3
L91	0.89	24.5	0.88	25.3
V92	0.66	18.5	0.74	20.6
V98	0.83	20.2	0.97	22.2
V100	0.94	21.2	0.84	22.1
I105	0.79	10.2		
I109	0.70	14.4		
L117	0.56	25.3	0.57	26.4
V118	-0.86	17.6	0.21	19.3
V119	0.67	18.8	0.72	21.5
L128	0.59	24.2	0.55	24.9
L138	0.75	23.1	0.73*	26.2*
L142	-0.47	21.8	0.44	27.9
I147	0.24	13.5		
I148	0.37	11.3		
V155	0.91	19.7	0.93	20.9
V166	0.82	21.1	0.90	22.7
I167	0.81	14.1		
V170	1.16	22.2	1.36	25.5
L174	0.82*	23.7*	-	-
L178	0.71	26.7	0.59*	26.7*
L180	0.34	22.6	-0.10	24.3
V188	0.39	21.6	0.72	23.6
V189	0.52	18.7	0.71	21.3
V193	0.19	19.3	0.68	19.3
V194	0.75	20.2	0.84	20.3
L198	0.65	22.5	0.80	26.0

I200	0.73	16.0		
L202	0.48	22.6	0.75	24.7
L210	0.89	22.4	1.07	28.0
V217	0.86	21.8	0.78	21.9
I229	0.54	10.5		
L230	0.66	21.7	-0.52	24.0
L231	1.05	24.7	0.86	25.3
L236	0.68	22.4	0.78	25.1
I238	0.48	13.7		
L240	0.70	24.3	0.61	24.8
I242	0.65	12.3		
I248	0.73	12.2		
I256	0.88	11.6		
V259	0.64	19.9	0.63	21.1
I260	0.63	11.0		
V261	0.90	20.9	0.88	22.2
I265	0.36	9.4		
I268	0.63	13.5		
L269	0.63	22.3	0.86	26.8
V275	0.76	21.3	0.81	23.1
V278	0.62	18.0	0.40	20.9
I284	0.73	13.1		
L285	0.88	23.5	0.93	24.5
L286	0.86	25.6	0.75	26.1
L290	-	-	-	-
L291	0.58	25.2	0.75	26.2
L293	0.76	23.9	0.91	25.4
L298	1.03	23.5	0.81	25.1
I309	0.77	13.2		
V310	0.84	20.8	0.73	21.1
L313	0.79	23.9	0.92*	25.0*
I327	0.56	13.0		
L329	0.61	22.2	0.19	25.2
L334	0.81	21.3	0.76	27.6
L335	0.62	22.0	0.80	25.1
I337	0.84	14.5		
V340	0.85*	18.8*	1.00	20.5
L343	0.97	22.9	0.72	25.7
I346	0.57	13.7		
V348	0.14	20.9	0.38	21.4
I349	0.76	14.8		
I357	0.78*	15.7*		
I361	0.98	12.7		
L362	1.09	24.0	0.75	27.3
V365	-0.11	20.3	0.55	21.8
I370	0.85	13.7		
L372	0.84	23.0	1.02	25.7
L375	0.70	22.0	0.86	25.5
V377	1.20	20.5	1.06	21.3
V386	0.65	19.3	0.70	21.0
I388	0.27	12.7		
V389	0.41	20.5	0.70	22.3
V399	0.97	20.6	0.89	21.9
L405	-	-	-	-
I409	0.53	13.0		
L413	0.79	22.0	0.70	26.0

L420	0.35	22.4	0.45	24.7
I424	0.72	14.8		
L433	0.87	25.4	0.95	27.1
L435	0.79	21.4	1.18	27.4
I439	0.77	13.7		
V446	0.96	21.2	1.11	22.7
I449	0.62	14.1		
L454	0.43*	21.5*	0.37*	24.8*
V464	0.65	17.9	0.45	20.4
L471	1.06	22.1	0.90	25.9
I482	0.63	14.2		
V490	0.89	19.5	0.83	20.9
L491	0.27	20.6	0.54	25.0
L494	0.65	22.2	0.61	25.9
L498	0.60	23.2	0.74	25.0
I504	0.70	13.2		
L514	0.92	22.3	1.05	25.9
L526	0.08	22.3	0.09	23.4
V535	0.89	17.9	1.11	24.8
L543	0.23	21.4	0.55	25.1
L546	0.24	20.4	0.76	25.2
V553	1.10	20.0	1.07	22.9
V556	0.85	20.8	0.88	21.8
I560	0.58	13.7		
L572	1.04	23.3	0.71	26.4
L573	0.97	24.3	0.93	25.6
L576	1.20	24.6	0.81	24.8
L577	0.72	22.4	0.77	26.7
I579	0.74	14.6		
V581	0.51	20.2	0.51	20.5
I592	0.81	13.6		
L596	1.04*	24.8*	1.03	26.8
V600	0.73	22.4	0.95	25.0
I603	0.48	14.3		
L604	0.73	23.0	0.89	27.7
V607	1.02	23.0	1.10	26.6
V608	1.31	20.6	1.14	21.9
V611	0.85	21.7	1.33	25.1
I615	0.75	12.5		
V620	0.93	22.8	-	-
I623	0.77	14.5		
V626	0.79	20.7	0.86	21.5
L628	0.66	23.4	0.87	25.4
L635	1.00	25.2	0.85*	27.4*
I637	0.62*	14.6*		
I642	0.63	15.9		
L646	0.84	23.6	0.81	25.1
I650	0.56	8.0		
L651	1.04	25.2	1.18	28.4
V656	0.75	22.3	1.10	24.2
L660	0.46	23.3	0.70	25.8
V666	0.88	19.6	1.11	21.9
V667	1.04	22.5	1.11	23.3
L696	0.89	24.0	0.72	26.6
I697	0.55	14.7		
L699	0.86	22.1	0.89	24.9

V701	1.02	19.7	1.02	21.4
L711	1.00	22.7	0.79	25.7
L712	0.04	22.9	0.16	24.6
L717	0.94	23.6	0.96	25.1
L724 ^{b)}	0.85	22.9	0.92	24.7

^{a)} ¹H and ¹³C chemical shifts are referenced indirectly against TSP. Methyls that could not be assigned are marked “-”; methyls with tentative assignments are labeled with asterisks.

Stereospecific assignments for the methyl groups of Val and Leu are not available yet.

^{b)} L724 belongs to the linker between the C-terminus of MSG and the hexa-histidine tag.