Supplemental Data

SD Table S1. Peptides from E2 selected for HDX-MS analysis

Peptides			Monoisotopic Mass [M+H] (Da)		Error (ppm)
No.	Position	Sequence	Experimental	Theoretical	
1	4-13	IKVPDIGADE	1056.5583	1056.5572	1.0
2	16-20	ITEIL	588.3607	588.3603	0.6
3	21-33, 124-136	VKVGDKVEAEQSL	1401.7587	1401.7584	0.2
4	34-43, 137-146, 238-247	ITVEGDK(Lip)ASM	1238.5456	1238.5465	-0.8
5	44-51	EVPSPQAG	784.3838	784.3836	0.2
6	56-69, 159-172	IKVNVGDKVSTGSL	1416.8063	1416.8057	0.5
7	70-80	IMIFDSADGAA	1110.5140	1110.5136	0.4
8	278-319	EVEGAAPAAAPAKQEAAVPAPAAKAEAPAAAPAAKAEGKSEF	3912.0152	3912.0138	0.4
9	325-338	YVHATPLIRRLARE	1694.9818	1694.9813	0.3
10	339-343	FGVNL	549.3035	549.3031	0.7
11	363-393	YVKEAIKRAEAAPAATGGGIPGMLPWPKVDF	3240.7231	3240.7238	-0.2
12	394-401	SKFGEIEE	938.4465	938.4466	-0.1
13	402-415	VELGRIQKISGANL	1497.8755	1497.8748	0.5
14	419-428	WVMIPHVTHF	1266.6456	1266.6452	0.3
15	439-461	FRKQQNEEAAKRKLDVKITPVVF	2744.5609	2744.5570	1.4
16	462-467	IMKAVA	632.3800	632.3800	0.0
17	471-476	EQMPRF	807.3831	807.3818	1.6
18	477-496	NSSLSEDGQRLTLKKYINIG	2236.1931	2236.1932	0.0
19	498-506	AVDTPNGLV	885.4677	885.4676	0.1
20	508-521	PVFKDVNKKGIIEL	1599.9482	1599.9469	0.8
21	548-566	TISSIGGLGTTHFAPIVNA	1855.9897	1855.9912	-0.8
22	567-572	PEVAIL	641.3873	641.3869	0.8
23	573-594	GVSKSAMEPVWNGKEFVPRLML	2475.2884	2475.2887	-0.1
24	599-613	SFDHRVIDGADGARF	1662.7989	1662.7983	0.4
25	614-623	ITIINNTLSD	1103.5931	1103.5943	-1.1

SD Table S2. Peptides from E3 selected for DXMS analysis

		Peptides	Monoisotopic Mass [M+H] (Da)		Error (ppm)
No.	Position	Sequence	Experimental	Theoretical	
1	2-9	STEIKTQV	905.4935	905.4938	-0.3
2	10-22	VVLGAGPAGYSAA	1132.6000	1132.5997	0.2
3	23-30	FRCADLGL	894.4504	894.4502	0.3
4	33-57	VIVERYNTLGGVCLNVGCIP SKALL (C-C disulfide bond)	2629.4191	2629.4204	-0.5
5	58-65	HVAKVIEE	924.5147	924.5149	-0.2
6	66-88	AKALAEHGIVFGEPKTDIDKI RT	2509.3824	2509.3773	2.0
7	89-125	WKEKVINQLTGGLAGMAK GRKVKVVNGLGKFTGANTL	3884.2073	3884.2055	0.5
8	126-138	EVEGENGKTVINF	1435.7070	1435.7063	0.5
9	139-152	DNAIIAAGSRPIQL	1438.8016	1438.8013	0.3
10	153-169	PFIPHEDPRIWDSTDAL	2008.9769	2008.9763	0.3
11	170-178	ELKEVPERL	1112.6317	1112.6310	0.6
12	179-187	LVMGGGIIG	816.4640	816.4648	-1.0
13	188-200	LEMGTVYHALGSQ	1405.6783	1405.6780	0.2
14	201-206	IDVVEM	705.3491	705.3488	0.5
15	207-221	FDQVIPAADKDIVKV	1657.9168	1657.9160	0.5
16	222-234	FTKRISKKFNLML	1625.9574	1625.9560	0.8
17	235-249	ETKVTAVEAKEDGIY	1652.8385	1652.8378	0.4
18	250-268	VTMEGKKAPAEPQRYDAVL	2103.0902	2103.0903	0.0
19	269-288	VAIGRVPNGKNLDAGKAGV E	1965.0878	1965.0876	0.1
20	294-310	FIRVDKQLRTNVPHIFA	2054.1673	2054.1658	0.8
21	311-332	IGDIVGQPMLAHKGVHEGH VAA	2236.1652	2236.1655	-0.2
22	333-351	EVIAGKKHYFDPKVIPSIA	2112.1868	2112.1852	0.7
23	352-359	YTEPEVAW	994.4518	994.4516	0.1
24	400-421	IFDKESHRVIGGAIVGTNGG EL	2269.1957	2269.1935	1.0
25	422-427	LGEIGL	601.3558	601.3556	0.5
26	458-474	VFEGSITDLPNPKAKKK	1872.0592	1872.0589	0.1

SD Table S3. Part 1: Sequence-specific resonance assignments on the E2-didomain from *Escherichia coli* PDHc.

Backbone chemical shifts of assigned residues of E2 didomain					
	Atom Type				
Residue	H	N	CA	CB	C
Met0	8.67	121.35	54.63	34.69	173.63
Ala1	8.29	126.50	50.53	19.43	177.04
Ile2	9.23	122.59	59.22	41.30	174.53
Glu3	8.51	125.80	56.83	30.54	174.88
Ile4	8.47	123.76	57.71	35.46	174.79
Lys5	8.59	127.84	53.18	35.49	175.61
Val6	8.48	123.12	61.43	32.16	-
Pro7	-	-	62.38	32.10	172.49
Asp8	7.90	113.46	54.56	39.30	177.38
Ile9	8.17	125.68	59.91	38.25	176.71
Gly10	8.44	112.33	44.58	-	-
Ala11	8.00	124.60	51.68	19.54	-
Val14	-	-	58.83	35.40	173.20
Glu15	8.28	121.45	54.29	33.18	176.47
Ile16	8.79	124.31	61.80	37.42	177.10
Thr17	9.11	123.14	62.07	68.66	175.10
Glu18	7.48	120.29	56.35	33.70	174.38
Ile19	8.88	125.12	61.80	38.50	175.85
Leu20	8.16	126.60	55.87	41.83	176.01
Val21	7.02	109.95	58.14	35.55	173.04
Lys22	8.55	119.50	53.41	35.40	175.93
Val23	8.31	120.25	65.54	31.10	177.25
Gly24	9.15	117.41	44.28	-	174.29
Asp25	8.02	122.36	54.93	40.33	175.14
Lys26	8.37	122.80	55.53	32.07	175.76
Val27	8.91	125.85	59.61	33.97	-
Ser32	-	-	59.89	63.06	173.50
Leu33	9.06	121.54	55.86	45.42	177.18
Ile34	6.93	108.06	58.00	43.07	172.88
Thr35	8.78	119.93	61.33	69.10	174.45
Val36	9.01	117.74	57.11	34.63	174.13
Glu37	9.02	121.20	55.77	33.66	-
Asp39	-	-	56.23	40.44	176.74
Lys40	8.42	116.25	55.85	32.88	175.63
Ala41	7.47	121.53	51.74	21.43	175.95
Ser42	8.23	116.10	57.08	64.59	173.74
Met43	8.89	121.80	54.87	35.86	173.71
Glu44	8.44	121.44	54.41	30.58	176.34
Val45	8.32	124.04	59.11	33.24	-
Pro46	-	-	60.84	32.60	176.31

SD Table S3. Part 2: Sequence-specific resonance assignments on the E2-didomain from *Escherichia coli* PDHc.

Backbone chemical shifts of assigned residues of E2 didomain					
	Atom Type				
Residue	H	N	CA	CB	C
Ala47	8.69	123.37	49.59	17.69	-
Pro48	-	-	63.35	31.05	174.75
Phe49	6.86	113.12	53.97	40.56	175.22
Ala50	8.42	119.83	51.46	20.23	178.04
Gly51	7.96	105.71	45.61	-	169.95
Val52	8.05	119.69	59.58	34.41	176.48
Val53	8.42	126.39	64.42	31.04	175.39
Lys54	9.26	133.47	56.59	34.71	175.65
Glu55	7.58	115.41	55.76	34.10	174.68
Leu56	9.15	127.53	54.29	43.69	176.55
Lys57	7.89	118.85	53.67	31.79	174.53
Val58	6.89	109.37	58.21	36.80	173.01
Asn59	8.70	118.47	51.17	42.46	174.92
Val60	8.61	121.75	65.71	31.17	177.03
Gly61	8.96	118.04	44.31	42.11	174.26
Asp62	7.80	121.71	54.89	40.97	-
Lys63	-	-	53.98	32.80	177.36
Val64	8.99	115.36	58.68	36.39	172.34
Lys65	8.30	117.19	53.71	36.87	175.31
Thr66	8.82	119.07	65.23	69.85	175.78
Gly67	8.78	117.12	45.19	-	174.53
Ser68	8.53	119.38	60.86	62.75	173.59
Leu69	8.67	126.69	55.69	42.00	176.16
Ile70	8.73	117.42	61.47	40.56	175.85
Met71	7.67	115.83	54.94	36.33	171.33
Ile72	8.70	119.26	58.68	39.30	176.17
Phe73	9.37	129.52	53.04	41.87	175.38
Glu74	9.35	121.85	55.43	32.07	-
Val75	8.87	123.55	59.88	34.61	174.96
Glu76	8.49	124.39	56.16	30.29	176.63
Gly77	8.18	111.88	44.66	-	172.81
Ala78	8.00	123.98	51.48	19.56	176.94
Ala79	8.19	125.64	50.19	18.03	-
Pro92	-	-	60.66	32.69	176.24
Ala93	8.68	123.24	49.31	17.64	-
Lys112	-	-	55.96	32.96	175.78
Ser113	7.96	123.99	59.59	64.41	-
Pro179	-	-	63.28	31.81	-
Gly180	7.88	116.19	45.86	-	-

SD Table S4. Co-ordinates of the model of the *E.coli* E3-PSBD Interface. Please see text for details.

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REMARK   A MODEL OF THE ESCHERICHIA COLI E3-PSBD INTERFACE PREPARED
REMARK   ON THE BASIS OF THE CRYSTAL STRUCTURE OF THE E3b-PSBDp
REMARK   COMPLEX FROM THERMUS THERMOPHILUS (PDB CODE 2EQ8) REPORTED
REMARK   BY NAKAI ET AL. (2008) J. BIOCHEM. 143, 747-758 AND KNOWN
REMARK   SEQUENCES OF THE E. COLI E3 AND PSBD.
REMARK
JRNL        AUTH   K.CHANDRASEKHAR,J.WANG,P.ARJUNAN,M.SAX,Y-H.PARK,
JRNL        AUTH   N.S.NEMERIA,S.KUMARAN,J.SONG,F.JORDAN,W.FUREY
JRNL        TITL   INSIGHT TO THE INTERACTION OF THE E2 CORE WITH THE
JRNL        TITL 2 PERIPHERAL COMPONENTS IN THE ESCHERICHIA COLI
JRNL        TITL 3 PYRUVATE DEHYDROGENASE COMPLEX VIA MULTIFACETED
JRNL        TITL 4 STRUCTURAL APPROACHES.
JRNL        REF    SUBMITTED TO J. BIOL. CHEM.
JRNL        REFN   ASTM
CRYST1    1.000    1.000    1.000  90.00  90.00  90.00 P 1           1
ORIGX1      1.000000  0.000000  0.000000        0.00000
ORIGX2      0.000000  1.000000  0.000000        0.00000
ORIGX3      0.000000  0.000000  1.000000        0.00000
SCALE1      1.000000  0.000000  0.000000        0.00000
SCALE2      0.000000  0.000000  0.000000        0.00000
SCALE3      0.000000  0.000000  0.000000        0.00000
ATOM      1  N   ILE A 335      47.640   4.732  31.309  1.00 20.00
ATOM      2  CA  ILE A 335      47.312   5.943  30.566  1.00 20.00
ATOM      3  C   ILE A 335      48.602   6.508  29.983  1.00 20.00
ATOM      4  O   ILE A 335      48.587   7.194  28.958  1.00 20.00
ATOM      5  CB  ILE A 335      46.615   6.981  31.466  1.00 20.00
ATOM      6  CG1 ILE A 335      47.544   7.409  32.604  1.00 20.00
ATOM      7  CG2 ILE A 335      45.314   6.421  32.017  1.00 20.00
ATOM      8  CD1 ILE A 335      47.171   8.734  33.230  1.00 20.00
ATOM      9  N   ALA A 336      49.716   6.215  30.649  1.00 20.00
ATOM     10  CA  ALA A 336      51.021   6.697  30.219  1.00 20.00
ATOM     11  C   ALA A 336      51.658   5.797  29.162  1.00 20.00
ATOM     12  O   ALA A 336      52.803   6.016  28.772  1.00 20.00
ATOM     13  CB  ALA A 336      51.949   6.833  31.424  1.00 20.00
ATOM     14  N   GLY A 337      50.922   4.784  28.710  1.00 20.00
ATOM     15  CA  GLY A 337      51.440   3.894  27.684  1.00 20.00
ATOM     16  C   GLY A 337      52.058   2.589  28.155  1.00 20.00
ATOM     17  O   GLY A 337      52.473   1.769  27.332  1.00 20.00
ATOM     18  N   LYS A 338      52.131   2.387  29.468  1.00 20.00
ATOM     19  CA  LYS A 338      52.703   1.156  30.000  1.00 20.00
ATOM     20  C   LYS A 338      51.659   0.051  29.937  1.00 20.00
ATOM     21  O   LYS A 338      50.581   0.239  29.377  1.00 20.00
ATOM     22  CB  LYS A 338      53.156   1.356  31.449  1.00 20.00
ATOM     23  CG  LYS A 338      54.370   2.256  31.617  1.00 20.00
ATOM     24  CD  LYS A 338      54.755   2.368  33.086  1.00 20.00
ATOM     25  CE  LYS A 338      56.084   3.082  33.270  1.00 20.00
ATOM     26  NZ  LYS A 338      57.210   2.318  32.656  1.00 20.00
ATOM     27  N   LYS A 339      51.982  -1.108  30.494  1.00 20.00
ATOM     28  CA  LYS A 339      51.043  -2.218  30.506  1.00 20.00
ATOM     29  C   LYS A 339      51.030  -2.842  31.894  1.00 20.00
ATOM     30  O   LYS A 339      51.709  -3.839  32.148  1.00 20.00
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ATOM     31  CB  LYS A 339      51.411  -3.260  29.449  1.00 20.00
ATOM     32  CG  LYS A 339      50.432  -4.420  29.352  1.00 20.00
ATOM     33  CD  LYS A 339      50.830  -5.390  28.253  1.00 20.00
ATOM     34  CE  LYS A 339      49.865  -6.561  28.172  1.00 20.00
ATOM     35  NZ  LYS A 339      50.244  -7.520  27.098  1.00 20.00
ATOM     36  N   HIS A 340      50.261  -2.240  32.795  1.00 20.00
ATOM     37  CA  HIS A 340      50.156  -2.738  34.160  1.00 20.00
ATOM     38  C   HIS A 340      48.797  -3.380  34.391  1.00 20.00
ATOM     39  O   HIS A 340      47.814  -3.031  33.734  1.00 20.00
ATOM     40  CB  HIS A 340      50.387  -1.609  35.166  1.00 20.00
ATOM     41  CG  HIS A 340      51.734  -0.967  35.055  1.00 20.00
ATOM     42  ND1 HIS A 340      52.901  -1.618  35.397  1.00 20.00
ATOM     43  CD2 HIS A 340      52.102   0.268  34.640  1.00 20.00
ATOM     44  CE1 HIS A 340      53.928  -0.811  35.198  1.00 20.00
ATOM     45  NE2 HIS A 340      53.472   0.339  34.739  1.00 20.00
ATOM     46  N   TYR A 341      48.744  -4.321  35.328  1.00 20.00
ATOM     47  CA  TYR A 341      47.503  -5.015  35.649  1.00 20.00
ATOM     48  C   TYR A 341      47.386  -5.269  37.148  1.00 20.00
ATOM     49  O   TYR A 341      48.381  -5.533  37.822  1.00 20.00
ATOM     50  CB  TYR A 341      47.414  -6.336  34.883  1.00 20.00
ATOM     51  CG  TYR A 341      48.468  -7.346  35.278  1.00 20.00
ATOM     52  CD1 TYR A 341      49.625  -6.949  35.936  1.00 20.00
ATOM     53  CD2 TYR A 341      48.306  -8.695  34.995  1.00 20.00
ATOM     54  CE1 TYR A 341      50.590  -7.869  36.300  1.00 20.00
ATOM     55  CE2 TYR A 341      49.266  -9.622  35.354  1.00 20.00
ATOM     56  CZ  TYR A 341      50.406  -9.203  36.007  1.00 20.00
ATOM     57  OH  TYR A 341      51.365 -10.122  36.367  1.00 20.00
ATOM     58  N   PHE A 342      46.163  -5.189  37.663  1.00 20.00
ATOM     59  CA  PHE A 342      45.914  -5.410  39.082  1.00 20.00
ATOM     60  C   PHE A 342      45.696  -6.890  39.381  1.00 20.00
ATOM     61  O   PHE A 342      44.616  -7.429  39.141  1.00 20.00
ATOM     62  CB  PHE A 342      44.704  -4.596  39.547  1.00 20.00
ATOM     63  CG  PHE A 342      44.557  -4.528  41.040  1.00 20.00
ATOM     64  CD1 PHE A 342      44.156  -5.640  41.761  1.00 20.00
ATOM     65  CD2 PHE A 342      44.819  -3.352  41.722  1.00 20.00
ATOM     66  CE1 PHE A 342      44.019  -5.581  43.135  1.00 20.00
ATOM     67  CE2 PHE A 342      44.684  -3.285  43.096  1.00 20.00
ATOM     68  CZ  PHE A 342      44.284  -4.401  43.804  1.00 20.00
ATOM     69  N   ASP A 343      46.729  -7.541  39.905  1.00 20.00
ATOM     70  CA  ASP A 343      46.653  -8.958  40.238  1.00 20.00
ATOM     71  C   ASP A 343      47.205  -9.230  41.633  1.00 20.00
ATOM     72  O   ASP A 343      47.646 -10.340  41.931  1.00 20.00
ATOM     73  CB  ASP A 343      47.408  -9.793  39.202  1.00 20.00
ATOM     74  CG  ASP A 343      48.894  -9.490  39.181  1.00 20.00
ATOM     75  OD1 ASP A 343      49.368  -8.769  40.083  1.00 20.00
ATOM     76  OD2 ASP A 343      49.587  -9.973  38.261  1.00 20.00
ATOM     77  N   PRO A 344      47.178  -8.210  42.485  1.00 20.00
ATOM     78  CA  PRO A 344      47.677  -8.340  43.858  1.00 20.00
ATOM     79  C   PRO A 344      46.759  -9.206  44.714  1.00 20.00
ATOM     80  O   PRO A 344      45.553  -8.962  44.730  1.00 20.00
ATOM     81  CB  PRO A 344      47.666  -6.898  44.368  1.00 20.00
ATOM     82  CG  PRO A 344      47.837  -6.069  43.141  1.00 20.00
ATOM     83  CD  PRO A 344      47.110  -6.804  42.050  1.00 20.00
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ATOM    148  N   GLY A 426      50.786 -10.500  53.405  1.00 20.00
ATOM    149  CA  GLY A 426      50.534 -10.084  52.023  1.00 20.00
ATOM    150  C   GLY A 426      51.766 -10.354  51.169  1.00 20.00
ATOM    151  O   GLY A 426      51.666 -10.878  50.052  1.00 20.00
ATOM    152  N   LEU A 427      52.930  -9.985  51.697  1.00 20.00
ATOM    153  CA  LEU A 427      54.183 -10.199  50.988  1.00 20.00
ATOM    154  C   LEU A 427      54.413 -11.691  50.795  1.00 20.00
ATOM    155  O   LEU A 427      54.804 -12.134  49.716  1.00 20.00
ATOM    156  CB  LEU A 427      55.359  -9.595  51.765  1.00 20.00
ATOM    157  CG  LEU A 427      56.721  -9.894  51.127  1.00 20.00
ATOM    158  CD1 LEU A 427      56.747  -9.334  49.720  1.00 20.00
ATOM    159  CD2 LEU A 427      57.842  -9.298  51.963  1.00 20.00
ATOM    160  N   ALA A 428      54.175 -12.461  51.850  1.00 20.00
ATOM    161  CA  ALA A 428      54.348 -13.908  51.799  1.00 20.00
ATOM    162  C   ALA A 428      53.541 -14.463  50.623  1.00 20.00
ATOM    163  O   ALA A 428      54.060 -15.227  49.811  1.00 20.00
ATOM    164  CB  ALA A 428      53.885 -14.540  53.117  1.00 20.00
ATOM    165  N   ILE A 429      52.275 -14.069  50.524  1.00 20.00
ATOM    166  CA  ILE A 429      51.435 -14.543  49.425  1.00 20.00
ATOM    167  C   ILE A 429      51.955 -14.067  48.068  1.00 20.00
ATOM    168  O   ILE A 429      52.018 -14.846  47.117  1.00 20.00
ATOM    169  CB  ILE A 429      49.980 -14.077  49.622  1.00 20.00
ATOM    170  CG1 ILE A 429      49.371 -14.739  50.860  1.00 20.00
ATOM    171  CG2 ILE A 429      49.150 -14.384  48.386  1.00 20.00
ATOM    172  CD1 ILE A 429      48.045 -14.145  51.280  1.00 20.00
ATOM    173  N   GLU A 430      52.334 -12.794  47.978  1.00 20.00
ATOM    174  CA  GLU A 430      52.845 -12.255  46.724  1.00 20.00
ATOM    175  C   GLU A 430      54.085 -13.008  46.253  1.00 20.00
ATOM    176  O   GLU A 430      54.287 -13.189  45.053  1.00 20.00
ATOM    177  CB  GLU A 430      53.174 -10.768  46.869  1.00 20.00
ATOM    178  CG  GLU A 430      51.960  -9.876  47.072  1.00 20.00
ATOM    179  CD  GLU A 430      51.039  -9.841  45.859  1.00 20.00
ATOM    180  OE1 GLU A 430      49.983  -9.176  45.934  1.00 20.00
ATOM    181  OE2 GLU A 430      51.370 -10.474  44.834  1.00 20.00
ATOM    182  N   MET A 431      54.910 -13.445  47.203  1.00 20.00
ATOM    183  CA  MET A 431      56.135 -14.173  46.883  1.00 20.00
ATOM    184  C   MET A 431      55.908 -15.676  46.758  1.00 20.00
ATOM    185  O   MET A 431      56.861 -16.431  46.581  1.00 20.00
ATOM    186  CB  MET A 431      57.200 -13.925  47.957  1.00 20.00
ATOM    187  CG  MET A 431      57.610 -12.472  48.133  1.00 20.00
ATOM    188  SD  MET A 431      58.261 -11.730  46.625  1.00 20.00
ATOM    189  CE  MET A 431      59.744 -12.682  46.390  1.00 20.00
ATOM    190  N   GLY A 432      54.657 -16.112  46.860  1.00 20.00
ATOM    191  CA  GLY A 432      54.364 -17.533  46.753  1.00 20.00
ATOM    192  C   GLY A 432      55.033 -18.362  47.836  1.00 20.00
ATOM    193  O   GLY A 432      55.539 -19.454  47.582  1.00 20.00
ATOM    194  N   CYS A 433      55.031 -17.846  49.058  1.00 20.00
ATOM    195  CA  CYS A 433      55.650 -18.549  50.171  1.00 20.00
ATOM    196  C   CYS A 433      54.875 -19.787  50.606  1.00 20.00
ATOM    197  O   CYS A 433      53.652 -19.860  50.456  1.00 20.00
ATOM    198  CB  CYS A 433      55.812 -17.602  51.361  1.00 20.00
ATOM    199  SG  CYS A 433      56.932 -16.215  51.065  1.00 20.00
TER     200      CYS A 433
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ATOM    309  N   ASP B 437      59.321  -6.030  44.234  1.00 20.00
ATOM    310  CA  ASP B 437      58.404  -6.965  44.889  1.00 20.00
ATOM    311  C   ASP B 437      57.779  -6.289  46.106  1.00 20.00
ATOM    312  O   ASP B 437      56.579  -6.412  46.363  1.00 20.00
ATOM    313  CB  ASP B 437      59.140  -8.222  45.365  1.00 20.00
ATOM    314  CG  ASP B 437      59.551  -9.127  44.223  1.00 20.00
ATOM    315  OD1 ASP B 437      58.796  -9.197  43.233  1.00 20.00
ATOM    316  OD2 ASP B 437      60.612  -9.776  44.326  1.00 20.00
ATOM    317  N   ILE B 438      58.616  -5.587  46.862  1.00 20.00
ATOM    318  CA  ILE B 438      58.172  -4.894  48.062  1.00 20.00
ATOM    319  C   ILE B 438      57.247  -3.730  47.713  1.00 20.00
ATOM    320  O   ILE B 438      56.195  -3.546  48.334  1.00 20.00
ATOM    321  CB  ILE B 438      59.380  -4.386  48.872  1.00 20.00
ATOM    322  CG1 ILE B 438      60.189  -5.564  49.419  1.00 20.00
ATOM    323  CG2 ILE B 438      58.920  -3.479  50.003  1.00 20.00
ATOM    324  CD1 ILE B 438      61.528  -5.167  49.999  1.00 20.00
ATOM    325  N   ALA B 439      57.634  -2.949  46.711  1.00 20.00
ATOM    326  CA  ALA B 439      56.828  -1.813  46.283  1.00 20.00
ATOM    327  C   ALA B 439      55.480  -2.270  45.731  1.00 20.00
ATOM    328  O   ALA B 439      54.477  -1.567  45.878  1.00 20.00
ATOM    329  CB  ALA B 439      57.581  -1.005  45.213  1.00 20.00
ATOM    330  N   LEU B 440      55.454  -3.442  45.097  1.00 20.00
ATOM    331  CA  LEU B 440      54.219  -3.960  44.513  1.00 20.00
ATOM    332  C   LEU B 440      53.337  -4.761  45.461  1.00 20.00
ATOM    333  O   LEU B 440      52.260  -5.211  45.079  1.00 20.00
ATOM    334  CB  LEU B 440      54.518  -4.797  43.260  1.00 20.00
ATOM    335  CG  LEU B 440      55.087  -4.008  42.069  1.00 20.00
ATOM    336  CD1 LEU B 440      55.141  -4.920  40.842  1.00 20.00
ATOM    337  CD2 LEU B 440      54.215  -2.789  41.781  1.00 20.00
ATOM    338  N   THR B 441      53.788  -4.966  46.689  1.00 20.00
ATOM    339  CA  THR B 441      52.954  -5.678  47.644  1.00 20.00
ATOM    340  C   THR B 441      52.000  -4.611  48.172  1.00 20.00
ATOM    341  O   THR B 441      52.422  -3.501  48.510  1.00 20.00
ATOM    342  CB  THR B 441      53.791  -6.287  48.784  1.00 20.00
ATOM    343  OG1 THR B 441      54.604  -7.338  48.250  1.00 20.00
ATOM    344  CG2 THR B 441      52.885  -6.867  49.877  1.00 20.00
ATOM    345  N   ILE B 442      50.713  -4.931  48.217  1.00 20.00
ATOM    346  CA  ILE B 442      49.731  -3.966  48.681  1.00 20.00
ATOM    347  C   ILE B 442      49.619  -3.921  50.197  1.00 20.00
ATOM    348  O   ILE B 442      48.944  -4.758  50.806  1.00 20.00
ATOM    349  CB  ILE B 442      48.352  -4.278  48.069  1.00 20.00
ATOM    350  CG1 ILE B 442      48.386  -4.086  46.552  1.00 20.00
ATOM    351  CG2 ILE B 442      47.279  -3.403  48.698  1.00 20.00
ATOM    352  CD1 ILE B 442      47.162  -4.619  45.842  1.00 20.00
TER     353      ILE B 442
ATOM    354  N   HIS C 123      52.737 -19.005  43.152  1.00 20.00
ATOM    355  CA  HIS C 123      52.730 -18.048  42.063  1.00 20.00
ATOM    356  C   HIS C 123      54.045 -17.335  41.959  1.00 20.00
ATOM    357  O   HIS C 123      54.963 -17.562  42.776  1.00 20.00
ATOM    358  CB  HIS C 123      51.600 -17.041  42.244  1.00 20.00
ATOM    359  CG  HIS C 123      50.225 -17.665  42.259  1.00 20.00
ATOM    360  ND1 HIS C 123      49.662 -18.203  41.162  1.00 20.00
ATOM    361  CD2 HIS C 123      49.302 -17.821  43.291  1.00 20.00
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ATOM    362  CE1 HIS C 123      48.442 -18.680  41.472  1.00 20.00
ATOM    363  NE2 HIS C 123      48.223 -18.445  42.776  1.00 20.00
ATOM    364  N   ALA C 124      54.163 -16.465  40.961  1.00 20.00
ATOM    365  CA  ALA C 124      55.391 -15.708  40.746  1.00 20.00
ATOM    366  C   ALA C 124      55.346 -14.366  41.470  1.00 20.00
ATOM    367  O   ALA C 124      54.271 -13.842  41.759  1.00 20.00
ATOM    368  CB  ALA C 124      55.633 -15.503  39.258  1.00 20.00
ATOM    369  N   THR C 125      56.521 -13.816  41.758  1.00 20.00
ATOM    370  CA  THR C 125      56.619 -12.536  42.448  1.00 20.00
ATOM    371  C   THR C 125      56.072 -11.403  41.586  1.00 20.00
ATOM    372  O   THR C 125      56.043 -11.502  40.359  1.00 20.00
ATOM    373  CB  THR C 125      58.073 -12.214  42.838  1.00 20.00
ATOM    374  OG1 THR C 125      58.899 -12.226  41.667  1.00 20.00
ATOM    375  CG2 THR C 125      58.596 -13.239  43.833  1.00 20.00
ATOM    376  N   PRO C 126      55.639 -10.327  42.236  1.00 20.00
ATOM    377  CA  PRO C 126      55.088  -9.168  41.526  1.00 20.00
ATOM    378  C   PRO C 126      56.061  -8.628  40.483  1.00 20.00
ATOM    379  O   PRO C 126      55.643  -8.251  39.388  1.00 20.00
ATOM    380  CB  PRO C 126      54.892  -8.141  42.643  1.00 20.00
ATOM    381  CG  PRO C 126      54.680  -8.962  43.868  1.00 20.00
ATOM    382  CD  PRO C 126      55.543 -10.180  43.699  1.00 20.00
ATOM    383  N   LEU C 127      57.344  -8.595  40.825  1.00 20.00
ATOM    384  CA  LEU C 127      58.370  -8.114  39.908  1.00 20.00
ATOM    385  C   LEU C 127      58.434  -8.987  38.660  1.00 20.00
ATOM    386  O   LEU C 127      58.502  -8.481  37.539  1.00 20.00
ATOM    387  CB  LEU C 127      59.735  -8.081  40.598  1.00 20.00
ATOM    388  CG  LEU C 127      60.952  -7.918  39.686  1.00 20.00
ATOM    389  CD1 LEU C 127      61.265  -6.447  39.464  1.00 20.00
ATOM    390  CD2 LEU C 127      62.157  -8.647  40.262  1.00 20.00
ATOM    391  N   ILE C 128      58.410 -10.300  38.862  1.00 20.00
ATOM    392  CA  ILE C 128      58.449 -11.246  37.753  1.00 20.00
ATOM    393  C   ILE C 128      57.185 -11.141  36.907  1.00 20.00
ATOM    394  O   ILE C 128      57.245 -11.172  35.677  1.00 20.00
ATOM    395  CB  ILE C 128      58.604 -12.695  38.252  1.00 20.00
ATOM    396  CG1 ILE C 128      60.004 -12.913  38.829  1.00 20.00
ATOM    397  CG2 ILE C 128      58.328 -13.678  37.125  1.00 20.00
ATOM    398  CD1 ILE C 128      60.146 -14.195  39.619  1.00 20.00
ATOM    399  N   ARG C 129      56.042 -11.016  37.574  1.00 20.00
ATOM    400  CA  ARG C 129      54.764 -10.888  36.885  1.00 20.00
ATOM    401  C   ARG C 129      54.712  -9.595  36.079  1.00 20.00
ATOM    402  O   ARG C 129      54.182  -9.564  34.969  1.00 20.00
ATOM    403  CB  ARG C 129      53.608 -10.931  37.887  1.00 20.00
ATOM    404  CG  ARG C 129      53.672 -12.099  38.857  1.00 20.00
ATOM    405  CD  ARG C 129      52.316 -12.368  39.488  1.00 20.00
ATOM    406  NE  ARG C 129      51.760 -11.174  40.118  1.00 20.00
ATOM    407  CZ  ARG C 129      51.870 -10.892  41.412  1.00 20.00
ATOM    408  NH1 ARG C 129      52.518 -11.719  42.221  1.00 20.00
ATOM    409  NH2 ARG C 129      51.332  -9.782  41.899  1.00 20.00
ATOM    410  N   ARG C 130      55.267  -8.529  36.647  1.00 20.00
ATOM    411  CA  ARG C 130      55.299  -7.234  35.978  1.00 20.00
ATOM    412  C   ARG C 130      56.262  -7.260  34.796  1.00 20.00
ATOM    413  O   ARG C 130      55.992  -6.672  33.749  1.00 20.00
ATOM    414  CB  ARG C 130      55.701  -6.133  36.961  1.00 20.00
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ATOM    415  CG  ARG C 130      54.721  -5.935  38.106  1.00 20.00
ATOM    416  CD  ARG C 130      53.398  -5.374  37.610  1.00 20.00
ATOM    417  NE  ARG C 130      52.460  -5.137  38.703  1.00 20.00
ATOM    418  CZ  ARG C 130      51.670  -6.070  39.225  1.00 20.00
ATOM    419  NH1 ARG C 130      50.847  -5.765  40.219  1.00 20.00
ATOM    420  NH2 ARG C 130      51.702  -7.309  38.754  1.00 20.00
ATOM    421  N   LEU C 131      57.386  -7.947  34.972  1.00 20.00
ATOM    422  CA  LEU C 131      58.384  -8.066  33.916  1.00 20.00
ATOM    423  C   LEU C 131      57.824  -8.840  32.728  1.00 20.00
ATOM    424  O   LEU C 131      58.077  -8.494  31.574  1.00 20.00
ATOM    425  CB  LEU C 131      59.645  -8.752  34.444  1.00 20.00
ATOM    426  CG  LEU C 131      60.974  -8.275  33.854  1.00 20.00
ATOM    427  CD1 LEU C 131      62.011  -9.387  33.896  1.00 20.00
ATOM    428  CD2 LEU C 131      60.780  -7.771  32.432  1.00 20.00
ATOM    429  N   ALA C 132      57.060  -9.888  33.019  1.00 20.00
ATOM    430  CA  ALA C 132      56.449 -10.703  31.977  1.00 20.00
ATOM    431  C   ALA C 132      55.545  -9.856  31.088  1.00 20.00
ATOM    432  O   ALA C 132      55.605  -9.944  29.862  1.00 20.00
ATOM    433  CB  ALA C 132      55.666 -11.853  32.593  1.00 20.00
ATOM    434  N   ARG C 133      54.708  -9.037  31.715  1.00 20.00
ATOM    435  CA  ARG C 133      53.787  -8.175  30.983  1.00 20.00
ATOM    436  C   ARG C 133      54.540  -7.140  30.154  1.00 20.00
ATOM    437  O   ARG C 133      54.039  -6.664  29.135  1.00 20.00
ATOM    438  CB  ARG C 133      52.825  -7.478  31.947  1.00 20.00
ATOM    439  CG  ARG C 133      51.941  -8.428  32.737  1.00 20.00
ATOM    440  CD  ARG C 133      50.885  -7.672  33.527  1.00 20.00
ATOM    441  NE  ARG C 133      50.004  -6.896  32.659  1.00 20.00
ATOM    442  CZ  ARG C 133      48.904  -7.378  32.088  1.00 20.00
ATOM    443  NH1 ARG C 133      48.546  -8.638  32.293  1.00 20.00
ATOM    444  NH2 ARG C 133      48.162  -6.599  31.313  1.00 20.00
ATOM    445  N   GLU C 134      55.744  -6.796  30.597  1.00 20.00
ATOM    446  CA  GLU C 134      56.566  -5.815  29.898  1.00 20.00
ATOM    447  C   GLU C 134      57.290  -6.445  28.712  1.00 20.00
ATOM    448  O   GLU C 134      57.477  -5.807  27.677  1.00 20.00
ATOM    449  CB  GLU C 134      57.578  -5.184  30.856  1.00 20.00
ATOM    450  CG  GLU C 134      58.459  -4.123  30.217  1.00 20.00
ATOM    451  CD  GLU C 134      59.693  -3.815  31.043  1.00 20.00
ATOM    452  OE1 GLU C 134      59.563  -3.672  32.277  1.00 20.00
ATOM    453  OE2 GLU C 134      60.792  -3.716  30.458  1.00 20.00
ATOM    454  N   PHE C 135      57.694  -7.701  28.872  1.00 20.00
ATOM    455  CA  PHE C 135      58.400  -8.418  27.816  1.00 20.00
ATOM    456  C   PHE C 135      57.428  -9.180  26.921  1.00 20.00
ATOM    457  O   PHE C 135      57.828  -9.781  25.924  1.00 20.00
ATOM    458  CB  PHE C 135      59.427  -9.380  28.416  1.00 20.00
ATOM    459  CG  PHE C 135      60.580  -8.692  29.091  1.00 20.00
ATOM    460  CD1 PHE C 135      60.635  -7.310  29.159  1.00 20.00
ATOM    461  CD2 PHE C 135      61.608  -9.428  29.657  1.00 20.00
ATOM    462  CE1 PHE C 135      61.693  -6.674  29.779  1.00 20.00
ATOM    463  CE2 PHE C 135      62.669  -8.798  30.278  1.00 20.00
ATOM    464  CZ  PHE C 135      62.712  -7.419  30.340  1.00 20.00
ATOM    465  N   GLY C 136      56.150  -9.151  27.283  1.00 20.00
ATOM    466  CA  GLY C 136      55.124  -9.833  26.517  1.00 20.00
ATOM    467  C   GLY C 136      55.192 -11.340  26.667  1.00 20.00
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ATOM    468  O   GLY C 136      54.752 -12.081  25.788  1.00 20.00
ATOM    469  N   VAL C 137      55.746 -11.794  27.786  1.00 20.00
ATOM    470  CA  VAL C 137      55.877 -13.222  28.051  1.00 20.00
ATOM    471  C   VAL C 137      54.677 -13.752  28.828  1.00 20.00
ATOM    472  O   VAL C 137      54.085 -13.039  29.638  1.00 20.00
ATOM    473  CB  VAL C 137      57.164 -13.534  28.838  1.00 20.00
ATOM    474  CG1 VAL C 137      57.186 -14.995  29.261  1.00 20.00
ATOM    475  CG2 VAL C 137      58.390 -13.195  28.004  1.00 20.00
ATOM    476  N   ASN C 138      54.323 -15.008  28.576  1.00 20.00
ATOM    477  CA  ASN C 138      53.195 -15.637  29.252  1.00 20.00
ATOM    478  C   ASN C 138      53.666 -16.693  30.246  1.00 20.00
ATOM    479  O   ASN C 138      53.929 -17.836  29.874  1.00 20.00
ATOM    480  CB  ASN C 138      52.230 -16.252  28.237  1.00 20.00
ATOM    481  CG  ASN C 138      50.969 -16.791  28.884  1.00 20.00
ATOM    482  OD1 ASN C 138      50.937 -17.051  30.087  1.00 20.00
ATOM    483  ND2 ASN C 138      49.921 -16.961  28.087  1.00 20.00
ATOM    484  N   LEU C 139      53.772 -16.301  31.511  1.00 20.00
ATOM    485  CA  LEU C 139      54.213 -17.211  32.561  1.00 20.00
ATOM    486  C   LEU C 139      53.430 -18.519  32.524  1.00 20.00
ATOM    487  O   LEU C 139      53.953 -19.578  32.871  1.00 20.00
ATOM    488  CB  LEU C 139      54.073 -16.553  33.935  1.00 20.00
ATOM    489  CG  LEU C 139      54.683 -15.158  34.084  1.00 20.00
ATOM    490  CD1 LEU C 139      54.417 -14.601  35.475  1.00 20.00
ATOM    491  CD2 LEU C 139      56.175 -15.189  33.791  1.00 20.00
ATOM    492  N   ALA C 140      52.172 -18.437  32.101  1.00 20.00
ATOM    493  CA  ALA C 140      51.314 -19.613  32.019  1.00 20.00
ATOM    494  C   ALA C 140      51.843 -20.612  30.995  1.00 20.00
ATOM    495  O   ALA C 140      51.378 -21.750  30.925  1.00 20.00
ATOM    496  CB  ALA C 140      49.889 -19.206  31.678  1.00 20.00
ATOM    497  N   LYS C 141      52.819 -20.179  30.203  1.00 20.00
ATOM    498  CA  LYS C 141      53.413 -21.034  29.182  1.00 20.00
ATOM    499  C   LYS C 141      54.925 -21.132  29.358  1.00 20.00
ATOM    500  O   LYS C 141      55.674 -21.134  28.381  1.00 20.00
ATOM    501  CB  LYS C 141      53.079 -20.512  27.784  1.00 20.00
ATOM    502  CG  LYS C 141      51.607 -20.195  27.575  1.00 20.00
ATOM    503  CD  LYS C 141      51.375 -19.504  26.241  1.00 20.00
ATOM    504  CE  LYS C 141      49.906 -19.533  25.853  1.00 20.00
ATOM    505  NZ  LYS C 141      49.561 -20.755  25.075  1.00 20.00
ATOM    506  N   VAL C 142      55.367 -21.213  30.609  1.00 20.00
ATOM    507  CA  VAL C 142      56.789 -21.310  30.914  1.00 20.00
ATOM    508  C   VAL C 142      57.034 -22.212  32.120  1.00 20.00
ATOM    509  O   VAL C 142      56.189 -22.321  33.007  1.00 20.00
ATOM    510  CB  VAL C 142      57.404 -19.925  31.188  1.00 20.00
ATOM    511  CG1 VAL C 142      58.775 -20.071  31.829  1.00 20.00
ATOM    512  CG2 VAL C 142      57.492 -19.120  29.900  1.00 20.00
ATOM    513  N   LYS C 143      58.197 -22.855  32.144  1.00 20.00
ATOM    514  CA  LYS C 143      58.557 -23.747  33.240  1.00 20.00
ATOM    515  C   LYS C 143      59.695 -23.165  34.073  1.00 20.00
ATOM    516  O   LYS C 143      60.837 -23.098  33.619  1.00 20.00
ATOM    517  CB  LYS C 143      58.948 -25.125  32.704  1.00 20.00
ATOM    518  CG  LYS C 143      59.270 -26.144  33.785  1.00 20.00
ATOM    519  CD  LYS C 143      58.029 -26.517  34.579  1.00 20.00
ATOM    520  CE  LYS C 143      58.352 -27.536  35.660  1.00 20.00
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ATOM    521  NZ  LYS C 143      58.794 -28.836  35.083  1.00 20.00
ATOM    522  N   GLY C 144      59.374 -22.746  35.292  1.00 20.00
ATOM    523  CA  GLY C 144      60.363 -22.170  36.185  1.00 20.00
ATOM    524  C   GLY C 144      61.472 -23.143  36.530  1.00 20.00
ATOM    525  O   GLY C 144      61.213 -24.280  36.924  1.00 20.00
ATOM    526  N   THR C 145      62.714 -22.694  36.381  1.00 20.00
ATOM    527  CA  THR C 145      63.872 -23.528  36.681  1.00 20.00
ATOM    528  C   THR C 145      64.464 -23.179  38.042  1.00 20.00
ATOM    529  O   THR C 145      65.584 -23.576  38.363  1.00 20.00
ATOM    530  CB  THR C 145      64.964 -23.384  35.605  1.00 20.00
ATOM    531  OG1 THR C 145      65.489 -22.051  35.627  1.00 20.00
ATOM    532  CG2 THR C 145      64.394 -23.677  34.225  1.00 20.00
ATOM    533  N   GLY C 146      63.704 -22.435  38.839  1.00 20.00
ATOM    534  CA  GLY C 146      64.150 -22.032  40.160  1.00 20.00
ATOM    535  C   GLY C 146      64.197 -23.191  41.135  1.00 20.00
ATOM    536  O   GLY C 146      64.463 -24.330  40.750  1.00 20.00
ATOM    537  N   ARG C 147      63.937 -22.900  42.406  1.00 20.00
ATOM    538  CA  ARG C 147      63.948 -23.924  43.444  1.00 20.00
ATOM    539  C   ARG C 147      62.953 -25.070  43.292  1.00 20.00
ATOM    540  O   ARG C 147      63.340 -26.210  43.036  1.00 20.00
ATOM    541  CB  ARG C 147      63.664 -23.302  44.813  1.00 20.00
ATOM    542  CG  ARG C 147      64.796 -22.440  45.349  1.00 20.00
ATOM    543  CD  ARG C 147      64.406 -21.767  46.655  1.00 20.00
ATOM    544  NE  ARG C 147      65.455 -20.880  47.148  1.00 20.00
ATOM    545  CZ  ARG C 147      65.352 -20.138  48.246  1.00 20.00
ATOM    546  NH1 ARG C 147      64.242 -20.175  48.971  1.00 20.00
ATOM    547  NH2 ARG C 147      66.358 -19.359  48.620  1.00 20.00
ATOM    548  N   LYS C 148      61.671 -24.760  43.453  1.00 20.00
ATOM    549  CA  LYS C 148      60.619 -25.762  43.333  1.00 20.00
ATOM    550  C   LYS C 148      59.794 -25.397  42.103  1.00 20.00
ATOM    551  O   LYS C 148      58.566 -25.346  42.161  1.00 20.00
ATOM    552  CB  LYS C 148      59.715 -25.856  44.563  1.00 20.00
ATOM    553  CG  LYS C 148      60.408 -26.395  45.804  1.00 20.00
ATOM    554  CD  LYS C 148      59.468 -26.414  46.998  1.00 20.00
ATOM    555  CE  LYS C 148      60.137 -27.027  48.217  1.00 20.00
ATOM    556  NZ  LYS C 148      59.232 -27.038  49.400  1.00 20.00
ATOM    557  N   GLY C 149      60.478 -25.143  40.992  1.00 20.00
ATOM    558  CA  GLY C 149      59.814 -24.782  39.754  1.00 20.00
ATOM    559  C   GLY C 149      59.466 -23.308  39.692  1.00 20.00
ATOM    560  O   GLY C 149      58.732 -22.870  38.806  1.00 20.00
ATOM    561  N   ARG C 150      59.996 -22.540  40.639  1.00 20.00
ATOM    562  CA  ARG C 150      59.740 -21.106  40.694  1.00 20.00
ATOM    563  C   ARG C 150      60.333 -20.393  39.483  1.00 20.00
ATOM    564  O   ARG C 150      61.489 -20.617  39.123  1.00 20.00
ATOM    565  CB  ARG C 150      60.307 -20.510  41.984  1.00 20.00
ATOM    566  CG  ARG C 150      60.472 -18.999  41.950  1.00 20.00
ATOM    567  CD  ARG C 150      61.082 -18.482  43.243  1.00 20.00
ATOM    568  NE  ARG C 150      60.361 -18.960  44.418  1.00 20.00
ATOM    569  CZ  ARG C 150      59.210 -18.450  44.847  1.00 20.00
ATOM    570  NH1 ARG C 150      58.645 -17.443  44.196  1.00 20.00
ATOM    571  NH2 ARG C 150      58.624 -18.948  45.927  1.00 20.00
ATOM    572  N   ILE C 151      59.534 -19.533  38.859  1.00 20.00
ATOM    573  CA  ILE C 151      59.978 -18.787  37.687  1.00 20.00
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ATOM    574  C   ILE C 151      60.907 -17.644  38.081  1.00 20.00
ATOM    575  O   ILE C 151      60.528 -16.759  38.849  1.00 20.00
ATOM    576  CB  ILE C 151      58.786 -18.218  36.896  1.00 20.00
ATOM    577  CG1 ILE C 151      57.880 -19.351  36.408  1.00 20.00
ATOM    578  CG2 ILE C 151      59.275 -17.379  35.726  1.00 20.00
ATOM    579  CD1 ILE C 151      56.553 -18.877  35.857  1.00 20.00
ATOM    580  N   LEU C 152      62.125 -17.668  37.550  1.00 20.00
ATOM    581  CA  LEU C 152      63.110 -16.634  37.843  1.00 20.00
ATOM    582  C   LEU C 152      63.097 -15.542  36.779  1.00 20.00
ATOM    583  O   LEU C 152      62.529 -15.719  35.701  1.00 20.00
ATOM    584  CB  LEU C 152      64.509 -17.242  37.955  1.00 20.00
ATOM    585  CG  LEU C 152      64.705 -18.296  39.047  1.00 20.00
ATOM    586  CD1 LEU C 152      66.018 -19.038  38.849  1.00 20.00
ATOM    587  CD2 LEU C 152      64.649 -17.657  40.426  1.00 20.00
ATOM    588  N   ARG C 153      63.727 -14.413  37.089  1.00 20.00
ATOM    589  CA  ARG C 153      63.798 -13.295  36.156  1.00 20.00
ATOM    590  C   ARG C 153      64.421 -13.729  34.834  1.00 20.00
ATOM    591  O   ARG C 153      63.960 -13.338  33.761  1.00 20.00
ATOM    592  CB  ARG C 153      64.600 -12.142  36.762  1.00 20.00
ATOM    593  CG  ARG C 153      64.705 -10.920  35.864  1.00 20.00
ATOM    594  CD  ARG C 153      65.492  -9.807  36.536  1.00 20.00
ATOM    595  NE  ARG C 153      65.602  -8.625  35.686  1.00 20.00
ATOM    596  CZ  ARG C 153      66.546  -8.453  34.766  1.00 20.00
ATOM    597  NH1 ARG C 153      67.468  -9.388  34.574  1.00 20.00
ATOM    598  NH2 ARG C 153      66.569  -7.346  34.036  1.00 20.00
ATOM    599  N   GLU C 154      65.470 -14.541  34.918  1.00 20.00
ATOM    600  CA  GLU C 154      66.151 -15.039  33.730  1.00 20.00
ATOM    601  C   GLU C 154      65.208 -15.878  32.875  1.00 20.00
ATOM    602  O   GLU C 154      65.271 -15.843  31.646  1.00 20.00
ATOM    603  CB  GLU C 154      67.380 -15.861  34.120  1.00 20.00
ATOM    604  CG  GLU C 154      68.564 -15.027  34.580  1.00 20.00
ATOM    605  CD  GLU C 154      68.630 -13.678  33.890  1.00 20.00
ATOM    606  OE1 GLU C 154      67.865 -12.771  34.281  1.00 20.00
ATOM    607  OE2 GLU C 154      69.446 -13.525  32.957  1.00 20.00
ATOM    608  N   ASP C 155      64.333 -16.632  33.534  1.00 20.00
ATOM    609  CA  ASP C 155      63.368 -17.472  32.836  1.00 20.00
ATOM    610  C   ASP C 155      62.483 -16.637  31.918  1.00 20.00
ATOM    611  O   ASP C 155      62.243 -17.004  30.768  1.00 20.00
ATOM    612  CB  ASP C 155      62.507 -18.244  33.838  1.00 20.00
ATOM    613  CG  ASP C 155      63.256 -19.388  34.491  1.00 20.00
ATOM    614  OD1 ASP C 155      62.857 -19.807  35.598  1.00 20.00
ATOM    615  OD2 ASP C 155      64.245 -19.868  33.898  1.00 20.00
ATOM    616  N   VAL C 156      62.002 -15.510  32.433  1.00 20.00
ATOM    617  CA  VAL C 156      61.155 -14.613  31.657  1.00 20.00
ATOM    618  C   VAL C 156      61.946 -13.962  30.528  1.00 20.00
ATOM    619  O   VAL C 156      61.450 -13.823  29.410  1.00 20.00
ATOM    620  CB  VAL C 156      60.538 -13.514  32.541  1.00 20.00
ATOM    621  CG1 VAL C 156      59.635 -12.613  31.713  1.00 20.00
ATOM    622  CG2 VAL C 156      59.769 -14.133  33.698  1.00 20.00
ATOM    623  N   GLN C 157      63.177 -13.564  30.828  1.00 20.00
ATOM    624  CA  GLN C 157      64.038 -12.924  29.840  1.00 20.00
ATOM    625  C   GLN C 157      64.424 -13.897  28.731  1.00 20.00
ATOM    626  O   GLN C 157      64.492 -13.523  27.560  1.00 20.00
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ATOM    627  CB  GLN C 157      65.295 -12.362  30.508  1.00 20.00
ATOM    628  CG  GLN C 157      65.160 -10.919  30.968  1.00 20.00
ATOM    629  CD  GLN C 157      66.422 -10.399  31.628  1.00 20.00
ATOM    630  OE1 GLN C 157      67.113 -11.130  32.338  1.00 20.00
ATOM    631  NE2 GLN C 157      66.729  -9.127  31.397  1.00 20.00
ATOM    632  N   ALA C 158      64.676 -15.146  29.107  1.00 20.00
ATOM    633  CA  ALA C 158      65.058 -16.174  28.146  1.00 20.00
ATOM    634  C   ALA C 158      63.913 -16.487  27.189  1.00 20.00
ATOM    635  O   ALA C 158      64.130 -16.715  25.999  1.00 20.00
ATOM    636  CB  ALA C 158      65.509 -17.434  28.869  1.00 20.00
ATOM    637  N   TYR C 159      62.693 -16.498  27.717  1.00 20.00
ATOM    638  CA  TYR C 159      61.512 -16.785  26.911  1.00 20.00
ATOM    639  C   TYR C 159      61.090 -15.567  26.095  1.00 20.00
ATOM    640  O   TYR C 159      60.391 -15.694  25.090  1.00 20.00
ATOM    641  CB  TYR C 159      60.356 -17.248  27.799  1.00 20.00
ATOM    642  CG  TYR C 159      59.061 -17.476  27.051  1.00 20.00
ATOM    643  CD1 TYR C 159      58.873 -18.620  26.284  1.00 20.00
ATOM    644  CD2 TYR C 159      58.031 -16.549  27.113  1.00 20.00
ATOM    645  CE1 TYR C 159      57.692 -18.832  25.600  1.00 20.00
ATOM    646  CE2 TYR C 159      56.844 -16.754  26.431  1.00 20.00
ATOM    647  CZ  TYR C 159      56.681 -17.896  25.677  1.00 20.00
ATOM    648  OH  TYR C 159      55.504 -18.104  24.994  1.00 20.00
ATOM    649  N   VAL C 160      61.520 -14.389  26.534  1.00 20.00
ATOM    650  CA  VAL C 160      61.187 -13.147  25.847  1.00 20.00
ATOM    651  C   VAL C 160      61.774 -13.121  24.439  1.00 20.00
ATOM    652  O   VAL C 160      61.128 -12.667  23.495  1.00 20.00
ATOM    653  CB  VAL C 160      61.692 -11.918  26.625  1.00 20.00
ATOM    654  CG1 VAL C 160      61.510 -10.655  25.798  1.00 20.00
ATOM    655  CG2 VAL C 160      60.967 -11.800  27.957  1.00 20.00
ATOM    656  N   LYS C 161      63.002 -13.612  24.306  1.00 20.00
ATOM    657  CA  LYS C 161      63.678 -13.646  23.015  1.00 20.00
ATOM    658  C   LYS C 161      64.682 -14.792  22.948  1.00 20.00
ATOM    659  O   LYS C 161      64.759 -15.505  21.947  1.00 20.00
ATOM    660  CB  LYS C 161      64.381 -12.314  22.743  1.00 20.00
ATOM    661  CG  LYS C 161      63.461 -11.105  22.792  1.00 20.00
ATOM    662  CD  LYS C 161      64.246  -9.809  22.677  1.00 20.00
ATOM    663  CE  LYS C 161      63.320  -8.604  22.642  1.00 20.00
ATOM    664  NZ  LYS C 161      64.077  -7.324  22.572  1.00 20.00
TER     665      LYS C 161
END
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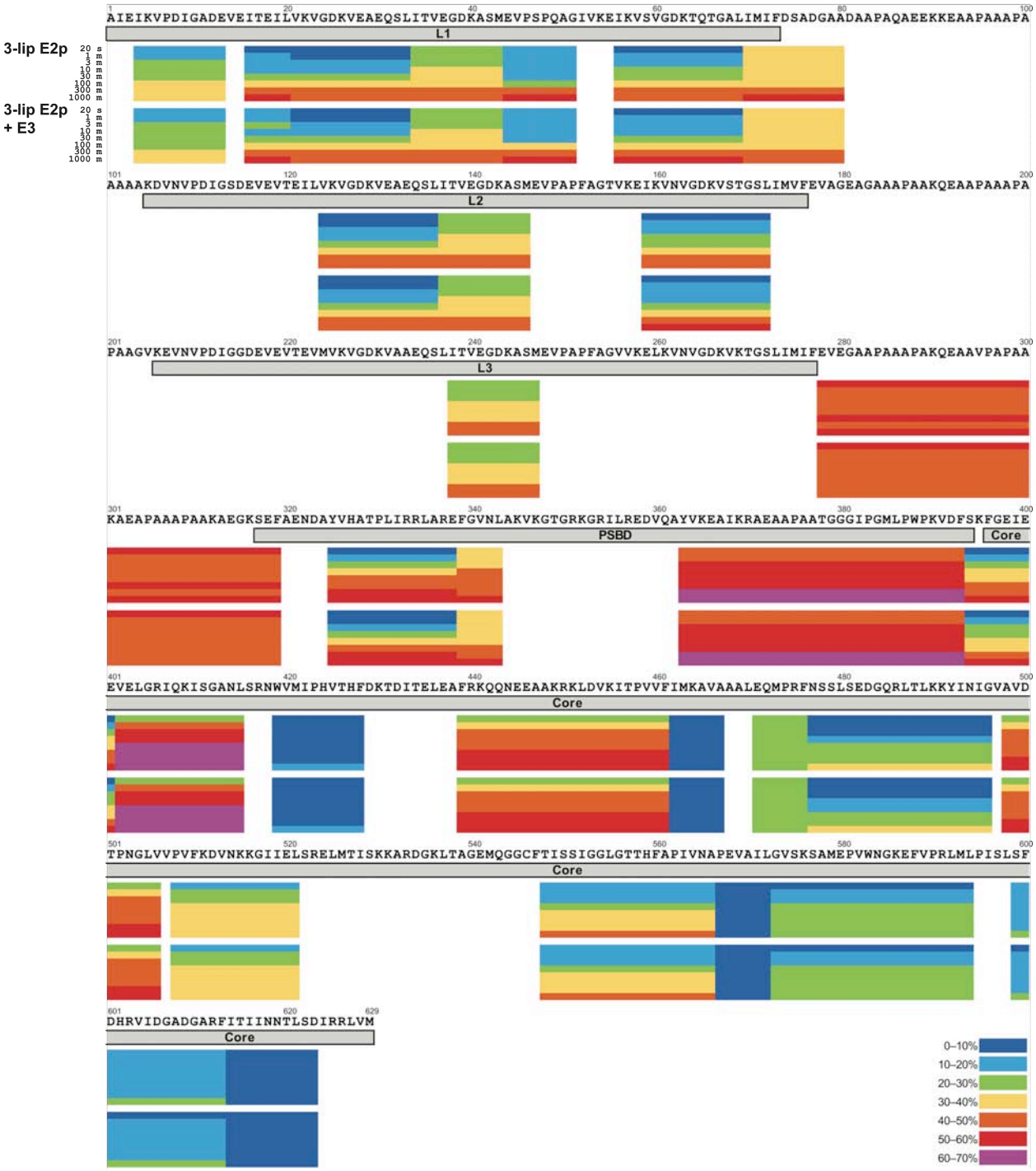
SD Figure S1. Heat map representation of deuterium exchange results for E2 in the presence and absence of E3.



SI Figure S2. Heat map representation of deuterium exchange results for E3 in the presence and absence of E2