SUPPORTING INFORMATION

The periplasmic domain of TolR forms a large hydrophobic groove and may contact TolQ through its C-terminus: NMR solution structure and comparison to SAXS data

Lisa M. Parsons, Alexander Grishaev, and Ad Bax

Supplemental Table I. Chemical Shift Assignments for TolR39-139

Group	Atom	Shift
S39	C	174.618
S39	CA	57.998
S39	CB	63.449
S39	HA	4.434
S39	HB#	3.873
V40	C	176.195
V40	CA	61.968
V40	CB	32.214
V40	CG1	19.702
V40	HA	4.136
V40	HB	2.08
V40	HG1#	0.936
V40	HN	8.057
V40	N	121.427
Q41	CA	56.858
Q41	CB	29.982
Q41	HN	7.936
Q41	N	128.539
V42	C	175.402
V42	CA	61.955
V42	CB	32.43
V42	CG1	20.087
V42	HA	4.139
V42	HB	2.062
E43	C	175.874
E43	CA	55.809
E43	CB	29.774
E43	CG	35.638
E43	HA	4.312
E43	HB1	1.985
E43	HB2	1.898
E43	HG#	2.217
E43	HN	8.444
E43	N	124.533
L44	C	175.302
L44	CA	52.579
L44	CB	41.362
L44	HA	4.635
L44	HB#	1.611
L44	HN	8.325
L44	N	124.807
P45	C	176.747
P45	CA	62.835
P45	CB	31.561
P45	CD	50.428
P45	CG	26.899

P45	HA	4.423
P45	HB1	2.293
P45	HB2	1.917
P45	HD1	3.808
P45	HD2	3.598
P45	HG#	1.983
D46	C	176.435
D46	CA	54.427
D46	CB	40.722
D46	HA	4.579
D46	HB#	2.638
D46	HN	8.349
D46	N	119.52
S47	C	174.441
S47	CA	58.236
S47	CB	63.739
S47	HA	4.53
S47	HB#	3.845
S47	HN	8.116
S47	N	115.163
V48	C	176.265
V48	CA	62.12
V48	CB	32.168
V48	CG1	20.272
V48	HA	4.105
V48	HB	2.083
V48	HG1#	0.908
V48	HN	8.222
V48	N	121.463
Q49	C	176.044
Q49	CA	55.636
Q49	CB	28.837
Q49	CG	33.226
Q49	HA	4.36
Q49	HB1	2.126
Q49	HB2	2.033
Q49	HE21	7.5
Q49	HE22	6.807
Q49	HG#	2.342
Q49	HN	8.368
Q49	N	123.289
Q49	NE2	112.056
S50	C	175.841
S50	CA	58.284
S50	CB	63.708
S50	HA	4.369
S50	HB#	3.836
S50	HN	8.314
S50	N	116.975
Q51	C	174.567

Q51	CA	55.449
Q51	CB	28.77
Q51	CG	33.21
Q51	HA	3.865
Q51	HB1	2.122
Q51	HB2	1.987
Q51	HG#	2.369
Q51	HN	8.369
Q51	N	121.937
E52	C	176.353
E52	CA	56.449
E52	CB	29.646
E52	CG	35.647
E52	HA	4.292
E52	HB1	2.036
E52	HB2	1.907
E52	HG#	2.229
E52	HN	8.359
E52	N	121.931
V53	C	176.001
V53	CA	61.967
V53	CB	32.335
V53	CG1	20.183
V53	HA	4.143
V53	HB	2.076
V53	HG1#	0.919
V53	HN	8.145
V53	N	121.049
S54	C	174.386
S54	CA	57.845
S54	CB	63.793
S54	HA	4.563
S54	HB#	3.848
S54	HN	8.404
S54	N	119.452
N55	C	175.201
N55	CA	53.155
N55	CB	38.32
N55	CG	180.477
N55	HA	4.706
N55	HB#	2.802
N55	HD21	7.578
N55	HD22	6.876
N55	HN	8.508
N55	N	121.267
N55	ND2	112.586
E56	C	175.993
E56	CA	56.499
E56	CB	29.467
E56	CG	35.643

E56	HA	4.24
E56	HB1	2.063
E56	HB2	1.893
E56	HG#	2.221
E56	HN	8.351
E18	N	120.631
D19	C	175.832
D19	CA	54.337
D19	CB	40.67
D19	HA	4.555
D19	HB#	2.617
D19	HN	8.244
D19	N	120.613
K20	C	175.94
K20	CA	55.225
K20	CB	32.646
K20	CD	28.06
K20	CG	23.793
K20	HA	4.363
K20	HB1	1.801
K20	HB2	1.664
K20	HG#	1.376
K20	HN	7.941
K20	N	121.059
V21	C	174.556
V21	CA	59.239
V21	CB	32.055
V21	CG1	20.832
V21	HA	4.388
V21	HB	2.061
V21	HG1#	0.95
V21	HG2#	0.9
V21	HN	8.324
V21	N	123.764
P22	C	175.889
P22	CA	55.589
P22	CB	32.685
P22	CD	50.572
P22	CG	26.036
P22	HA	4.388
P22	HB#	2.338
P22	HD#	3.702
P22	HD1	3.819
P22	HD2	3.724
P22	HG#	1.95
V23	C	175.084
V23	CA	61.806
V23	CB	31.377
V23	CG1	21.823
V23	HA	4.399

V23	HB	1.261
V23	HG1#	0.683
V23	HG2#	0.811
V23	HN	8.532
V23	N	122.481
I24	C	175.074
I24	CA	59.888
I24	CB	39.719
I24	CD1	13.124
I24	CG1	26.89
I24	CG2	16.778
I24	HA	4.879
I24	HB	1.807
I24	HD1#	0.811
I24	HN	8.343
I24	N	125.535
L25	C	173.76
L25	CA	53.402
L25	CB	43.697
L25	CD1	24.109
L25	CD2	26.51
L25	CG	26.125
L25	HA	5.168
L25	HB1	2.126
L25	HB2	1.293
L25	HD1#	0.977
L25	HD2#	0.803
L25	HN	9.499
L25	N	130.917
E26	CA	53.711
E26	CB	31.942
E26	HN	9.406
E26	N	125.487
V27	CB	33.213
V27	CG2	21.951
V27	HG2#	0.962
A28	C	176.904
A28	CA	52.184
A28	CB	19.444
A28	HA	4.384
A28	HB#	1.219
A28	HN	8.163
A28	N	128.566
G29	C	171.651
G29	CA	43.856
G29	HA#	3.847
G29	HN	7.917
G29	N	105.556
G31	C	172.929
G31	CA	46.14

G31	HA1	3.89
G31	HA2	3.626
G31	HN	8.622
G31	N	116.555
K32	CA	54.263
K32	CB	33.343
K32	HN	6.873
K32	N	119.506
Y33	C	174.814
Y33	CA	55.295
Y33	CB	42.404
Y33	CE#	117.65
Y33	HB1	2.932
Y33	HB2	2.464
Y33	HD#	6.95
Y33	HE#	6.664
Y33	HN	8.348
Y33	N	120.823
A34	C	175.093
A34	CA	50.354
A34	CB	22.513
A34	HA	5.27
A34	HB#	1.358
A34	HN	8.886
A34	N	123.035
I35	C	173.582
I35	CA	58.189
I35	CB	42.59
I35	CD1	13.394
I35	CG1	28.712
I35	CG2	16.59
I35	HA	5.655
I35	HB	1.47
I35	HD1#	0.819
I35	HG11	1.632
I35	HG12	1.083
I35	HG2#	0.867
I35	HN	8.783
I35	N	120.522
S36	C	173.539
S36	CA	56.201
S36	CB	64.178
S36	HA	5.346
S36	HB1	3.669
S36	HB2	3.508
S36	HN	9.097
S36	N	121.97
I37	C	178.019
I37	CA	60.133
I37	CB	40.195

I37	CD1	13.381
I37	CG1	27.567
I37	CG2	16.831
I37	HA	4.413
I37	HB	1.733
I37	HD1#	0.857
I37	HG11	0.492
I37	HG12	0.343
I37	HG2#	0.781
I37	HN	8.156
I37	N	125.454
G38	C	175.236
G38	CA	46.617
G38	HA1	3.723
G38	HA2	3.886
G38	HN	9.985
G38	N	120.172
G39	C	173.267
G39	CA	44.605
G39	HA1	3.532
G39	HA2	4.126
G39	HN	8.538
G39	N	106.316
E40	C	175.206
E40	CA	54.975
E40	CB	29.89
E40	CG	35.436
E40	HA	4.56
E40	HG1	2.24
E40	HG2	2.078
E40	HN	7.661
E40	N	121.029
R41	C	175.926
R41	CA	55.56
R41	CB	32.103
R41	CD	42.931
R41	CG	27.476
R41	HA	5.112
R41	HB1	1.669
R41	HB2	1.607
R41	HD1	3.159
R41	HD2	3.03
R41	HN	8.734
R41	N	127.945
Q42	C	174.233
Q42	CA	54.872
Q42	CB	31.047
Q42	CD	179.84
Q42	CG	33.298
Q42	HA	4.68

Q42	HB1	2.113
Q42	HB2	1.933
Q42	HE21	7.693
Q42	HE22	6.565
Q42	HG1	2.385
Q42	HG2	2.333
Q42	HN	9.211
Q42	N	125.447
Q42	NE2	110.638
E43	C	176.174
E43	CA	54.428
E43	CB	31.983
E43	CG	35.616
E43	HA	4.834
E43	HB#	2.023
E43	HG#	2.174
E43	HN	8.677
E43	N	120.982
G44	C	175.492
G44	CA	46.535
G44	HA1	3.965
G44	HA2	3.851
G44	HN	8.648
G44	N	108.491
L45	C	177.924
L45	CA	54.604
L45	CB	43.036
L45	CD1	26.667
L45	CD2	23.359
L45	HB#	1.601
L45	HD1#	0.744
L45	HD2#	0.737
T46	C	175.787
T46	CA	59.899
T46	CB	71.195
T46	CG2	21.762
T46	HA	4.771
T46	HB	4.863
T46	HG2#	1.448
T46	HN	7.551
T46	N	110.758
E47	C	178.138
E47	CA	60.054
E47	CB	28.782
E47	CG	36.549
E47	HA	3.636
E47	HB1	2.14
E47	HB2	2.066
E47	HG#	2.433
E47	HN	9.404

E47	N	119.786
E48	C	179.379
E48	CA	58.959
E48	CB	28.52
E48	CG	36.256
E48	HA	4.089
E48	HB#	2.066
E48	HG#	2.315
E48	HN	8.612
E48	N	117.357
M49	C	178.385
M49	CA	57.654
M49	CB	32.185
M49	CE	16.681
M49	CG	32.709
M49	HA	4.309
M49	HB1	2.729
M49	HB2	2.663
M49	HE#	2.177
M49	HG#	2.167
M49	HN	7.591
M49	N	118.73
V50	C	179.085
V50	CA	66.889
V50	CB	30.429
V50	CG1	23.149
V50	CG2	21.862
V50	HA	3.385
V50	HB	2.099
V50	HG1#	0.629
V50	HG2#	0.557
V50	HN	8.115
V50	N	119.026
T51	CA	67.57
T51	CB	68.567
T51	CG2	21.52
T51	HA	3.542
T51	HB	4.082
T51	HG2#	1.133
Q52	C	178.978
Q52	CA	59.144
Q52	CB	27.905
Q52	CD	179.659
Q52	CG	32.705
Q52	HA	4
Q52	HB2	2.153
Q52	HE21	7.405
Q52	HE22	6.745
Q52	NE2	111.094
L53	C	180.056

L53	CA	57.665
L53	CB	41.575
L53	CD1	25.733
L53	CD2	22.227
L53	CG	27.158
L53	HA	4.107
L53	HB1	1.829
L53	HB2	1.389
L53	HD1#	0.851
L53	HD2#	0.886
L53	HG	1.888
L53	HN	8.698
L53	N	118.977
S54	C	175.907
S54	CA	63.485
S54	CB	61.495
S54	HA	4.19
S54	HB1	3.675
S54	HB2	3.458
S54	HN	8.004
S54	N	114.908
R55	C	177.71
R55	CA	58.638
R55	CB	28.914
R55	CD	42.933
R55	CG	26.451
R55	HA	4.032
R55	HB1	2.058
R55	HB2	1.942
R55	HD#	3.282
R55	HG#	1.8
R55	HN	8.342
R55	N	122.76
Q56	C	179.42
Q56	CA	58.529
Q56	CB	28.314
Q56	CD	180.475
Q56	CG	34.135
Q56	HA	4.197
Q56	HB1	2.392
Q56	HB2	2.291
Q56	HE21	7.81
Q56	HE22	6.912
Q56	HG1	2.42
Q56	HG2	2.584
Q56	HN	7.973
Q56	N	116.807
Q56	NE2	111.24
E57	C	178.295
E57	CA	58.389

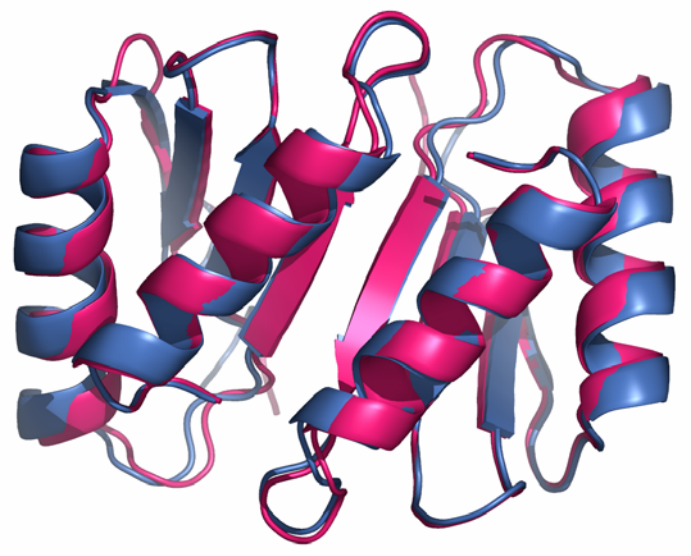
E57	CB	28.749
E57	CG	35.704
E57	HA	4.169
E57	HN	7.737
E57	N	117.04
F58	C	177.096
F58	CA	60.344
F58	CB	39.466
F58	HA	4.364
F58	HB#	3.175
F58	HD#	7.274
F58	HE#	7.354
F58	HN	8.697
F58	HZ	7.45
F58	N	121.782
D59	C	178.953
D59	CA	56.437
D59	CB	39.759
D59	HA	4.176
D59	HB1	2.751
D59	HB2	2.585
D59	HN	8.922
D59	N	117.781
E59	C	178.959
K60	C	177.209
K60	CA	58.519
K60	CB	32.177
K60	CG	24.755
K60	HA	3.988
K60	HB#	1.912
K60	HG1	1.671
K60	HG2	1.425
K60	HN	7.296
K60	N	118.998
D61	C	176.49
D61	CA	53.686
D61	CB	40.503
D61	HA	4.493
D61	HB#	2.69
D61	HN	7.406
D61	N	115.507
N62	C	175.602
N62	CA	54.209
N62	CB	37.745
N62	CG	176.345
N62	HA	3.988
N62	HB1	2.65
N62	HB2	2.546
N62	HD21	7.086
N62	HD22	7.007

N62	HN	9.356
N62	N	125.684
N62	ND2	114.5
N63	C	174.936
N63	CA	52.766
N63	CB	38.208
N63	CG	177.702
N63	HA	4.924
N63	HB1	2.773
N63	HB2	2.958
N63	HD21	7.791
N63	HD22	6.925
N63	HN	8.868
N63	N	117.541
N63	ND2	114.233
T64	C	172.318
T64	CA	65.086
T64	CB	70.291
T64	CG2	21.985
T64	HA	3.721
T64	HB	4.021
T64	HG2#	0.728
T64	HN	7.584
T64	N	119.274
L65	C	173.694
L65	CA	53.931
L65	CB	42.539
L65	CD1	22.774
L65	CD2	24.348
L65	CG	26.944
L65	HB1	1.587
L65	HB2	1.416
L65	HG	1.418
L65	HN	8.587
L65	N	129.659
F66	C	174.87
F66	CA	56.778
F66	CB	41.497
F66	HA	5.34
F66	HB1	3.112
F66	HB2	2.632
F66	HD#	7.24
F66	HE#	7.373
F66	HN	8.707
F66	HZ	7.117
F66	N	124.423
L67	CA	52.271
L67	CB	45.711
L67	HB1	1.693
L67	HB2	1.255

L67	HN	9.166
L67	N	122.341
A71	CB	18.96
A71	HA	4.616
A71	HB#	1.522
V74	CB	30.397
V74	CG2	20.347
V74	HB	1.908
V74	HG2#	0.145
V79	CA	66.238
V79	CG1	20.589
V79	CG2	19.61
V79	HA	3.488
V79	HG1#	0.971
V79	HG2#	0.637
A82	CA	55.04
A82	CB	17.961
A82	HA	3.844
A82	HB#	1.486
N84	C	177.204
L85	C	179.876
L85	CA	57.639
L85	CB	40.322
L85	CD2	24.599
L85	CG	55.594
L85	HA	3.873
L85	HB1	1.902
L85	HB2	1.228
L85	HD1#	0.696
L85	HD2#	0.562
L85	HG	1.919
L85	HN	7.863
L85	N	119.09
L86	C	178.919
L86	CA	57.286
L86	CB	39.664
L86	CD1	21.978
L86	CD2	26.473
L86	CG	25.972
L86	HA	3.844
L86	HB1	1.776
L86	HB2	0.857
L86	HD1#	0.479
L86	HD2#	0.649
L86	HG	1.611
L86	HN	7.314
L86	N	117.263
L88	C	178.139
L88	CA	57.315
L88	CB	41.504

L88	CD1	22.38
L88	CD2	24.832
L88	HA	3.867
L88	HB1	1.811
L88	HB2	1.426
L88	HD1#	0.847
L88	HD2#	0.841
A89	C	175.611
A89	CA	52.115
A89	CB	18.761
A89	HA	4.082
A89	HB#	1.412
A89	HN	7.258
A89	N	120.277
G90	C	171.71
G90	CA	43.827
G90	HA1	3.828
G90	HA2	3.248
G90	HN	7.389
G90	N	103.51
I91	CA	62.157
I91	CB	36.235
I91	CD1	13.293
I91	CG1	28.829
I91	CG2	19.006
I91	HB	1.086
I91	HD1#	-0.038
I91	HG11	0.49
I91	HG12	0.317
I91	HG2#	0.499
I91	HN	8.568
I91	N	120.051
M97	CE	16.623
M97	HE#	2.027

* errors are 0.03 ppm for ^{1}H shifts and 0.3 ppm for ^{13}C and ^{15}N shifts



Supplemental Figure 1.

The NMR-only (blue) and NMR-SAXS refined (magenta) structures are shown with β-sheets superimposed.