

DYNAMIC STRUCUTRES: AVERAGE DISTANCES AND RESTRAINT VIOLATIONS

Distance	restraint	r^6	avg	reg Avg	# viol's	# viol's	Avg viol
						>.32A	nrg
HN1-HN2							
HN13_HN14	5.0	2.91	3.08	0	0	#DIV/0!	
HN14_HN15	4.0	2.22	2.38	0	0	#DIV/0!	
HN15_HN16	4.0	2.71	2.84	0	0	#DIV/0!	
HN16_HN17	4.0	2.68	2.85	4	0	0.11	
HN17_HN18		2.95	3.07	0	0	#DIV/0!	
HN18_HN19	4.0	2.91	3.04	2	0	0.03	
HN19_HN20	4.0	2.72	2.85	1	0	0.03	
HN20_HN21	4.0	3.06	3.15	12	0	0.06	
HA21_HN22	4.0	3.54	3.57	28	0	0.06	
HN24_HN25	5.0	2.86	3.37	0	0	#DIV/0!	
HA1-NH1							
HA12_HN12	5.0	2.81	2.87	0	0	#DIV/0!	
HA13_HN13	4.0	2.75	2.80	0	0	#DIV/0!	
HA14_HN14	4.0	2.94	2.96	0	0	#DIV/0!	
HA15_HN15	4.0	2.84	2.87	0	0	#DIV/0!	
HA16_HN16	4.0	2.94	2.96	0	0	#DIV/0!	
HA17_HN17	4.0	2.86	2.89	0	0	#DIV/0!	
HA18_HN18	4.0	2.86	2.88	0	0	#DIV/0!	
HA19_HN19	4.0	2.85	2.88	0	0	#DIV/0!	
HA20_HN20	4.0	2.83	2.87	0	0	#DIV/0!	
HA21_HN21	4.0	2.94	2.96	0	0	#DIV/0!	
HA22_HN22	4.0	2.88	2.91	0	0	#DIV/0!	
HA24_HN24	4.0	2.28	2.35	0	0	#DIV/0!	
X25_HN25	4.0	2.64	2.67	0	0	#DIV/0!	
HA1-HN2							
HA11_HN12	5.0	2.25	2.45	0	0	#DIV/0!	
HA12_HN13	4.0	2.94	3.04	0	0	#DIV/0!	
HA13_HN14		3.49	3.52	5482	0	#DIV/0!	
HA14_HN15	4.0	3.43	3.46	6	0	0.02	
HA15_HN16	4.0	3.60	3.63	63	0	0.05	
HA16_HN17	4.0	3.52	3.55	23	0	0.02	
HA17_HN18	4.0	3.60	3.63	56	0	0.05	
HA18_HN19	4.0	3.62	3.65	93	0	0.04	
HA19_HN20	4.0	3.46	3.49	7	0	0.09	
HA20_HN21	4.0	3.59	3.61	45	0	0.03	
HA21_HN22	4.0	3.54	3.57	28	0	0.06	
HA23_HN24	3.2	3.31	3.37	4582	1395	0.83	
HA24_HN25	4.0	2.71	3.11	17	0	0.05	
HA1-HN4							
HA12_HN15	5.0	5.16	5.19	4663	1590	1.00	
HA13_HN16	4.0	3.73	3.80	1351	105	0.32	
HA14_HN17	4.0	2.95	3.12	63	1	0.17	
HA15_HN18	4.0	3.79	3.85	1698	212	0.42	
HA16_HN19	4.0	3.09	3.19	22	0	0.10	
HA17_HN20	5.0	3.52	3.61	0	0	#DIV/0!	
HA18_HN21	5.0	3.36	3.44	0	0	#DIV/0!	
HA19_HN22	5.0	2.67	2.79	0	0	#DIV/0!	
HA1-HN3							
HA12_HN14	5.0	5.38	5.42	5400	3727	2.52	
HA17_HN19	5.0	4.68	4.76	1448	218	0.47	
HA18_HN20	5.0	4.50	4.58	608	39	0.28	
HA19_HN21	5.0	4.23	4.31	55	0	0.14	
HA20_HN22	5.0	4.80	4.87	1930	278	0.48	
HA23_HN25	5.0	4.76	4.91	2550	967	1.26	
HA1-HN5							
HA15_HN19	5.0	3.91	3.97	1	0	0.02	
HA16_HN20	4.0	3.37	3.44	65	2	0.09	
HA18_HN22	5.0	4.01	4.07	3	0	0.01	

Phipsi viol's

Lwr B

Uppr B

Avg val

viol's

viol's

Avg viol

>8.1d nrg

PHI13

-70

-50

-61.95

2595

716

0.85

PHI14

-70

-50

-66.85

2387

488

0.60

PHI15

-70

-50

-53.53

2307

410

0.55

PHI16

-70

-50

-68.22

2693

629

0.70

PHI17

-70

-50

-61.29

1587

169

0.36

PHI18

-70

-50

-59.91

1536

156

0.37

PHI19

-70

-50

-62.21

1609

180

0.39

PHI20

-70

-50

-49.65

3167

799

0.73

PHI21

-70

-50

-74.00

4130

1712

1.27

PHI22

-70

-50

-72.37

3790

1501

1.18

PSI13

-55

-35

-60.67

4569

2173

1.50

PSI14

-55

-35

-35.32

3001

835

0.82

PSI15

-55

-35

-47.87

1586

175

0.39

PSI16

-55

-35

-35.15

3119

856

0.80

PSI17

-55

-35

-48.30

1703

217

0.42

PSI18

-55

-35

-46.53

1703

206

0.38

PSI19

-55

-35

-35.04

2981

775

0.78

PSI20

-55

-35

-44.99

1350

131

0.35

PSI21

-55

-35

-42.68

1702

227

0.45

PSI22

-55

-35

-63.05

4910

2925

2.09

restraint

r^6

avg

reg Avg

viol's

viol's

Avg viol

>.32A nrg

O-HN

2

2.14

2.20

4925

1419

0.82

O13_NH17

2

1.88

1.94

2029

126

0.27

O14_NH18

2

1.96

2.02

3029

250

0.35

O15_NH19

2

1.96

2.02

3026

272

0.37

O16_NH20

2

2.30

2.35

5577

3183

1.58

O17_NH21

2

1.87

1.93

1931

98

0.25

O18_NH22

INTERRESIDUE	restraint	r ⁶	avg	reg	Avg	# viol's	# viol's >.32A	Avg viol nrg		restraint	r ⁶	avg	reg	Avg	# viol's	# viol's >.32A	Avg viol nrg
HN-Xother									X-Xother								
HN13_HB112	4.0	1.86	2.01		0	0	#DIV/0!		HB112_X13	4.5	3.96	4.03		235	10	0.23	
HN13_HB212	5.0	3.34	3.39		0	0	#DIV/0!		HB212_X13	5.5	5.61	5.65		4343	1236	0.81	
HN13_X112	5.5	3.39	3.56		0	0	#DIV/0!		X112_X13	5.5	5.32	5.51		3508	998	0.87	
HN14_X13	4.5	2.73	2.82		0	0	#DIV/0!		X212_X13	5.5	3.71	3.95		26	3	0.49	
HN15_X13	5.5	4.84	4.88	34	0	0.11			X212_HG1215	5.5	5.54	5.61		3831	1512	1.26	
HN15_HB214	5.5	3.00	3.43		0	0	#DIV/0!		X13_X214	5.5	6.08	6.16		5470	4587	6.12	
HN15_X114	5.5	5.10	5.25	1856	310	0.52			X13_HB15	5.5	6.08	6.10		5695	5228	4.05	
HN16_X13	5.5	5.49	5.51	3033	370	0.45			X13_X115	5.5	5.88	5.93		5354	3812	2.82	
HN16_HB15	4.0	2.62	2.73		0	0	#DIV/0!		X114_HB217	5.5	5.28	5.48		3131	1282	1.34	
HN16_X215	5.5	4.14	4.22		0	0	#DIV/0!		X114_HG1118	5.5	4.14	4.71		1285	431	1.01	
HN17_HB116	4.0	3.23	3.32	62	0	0.10			X214_HG1118	5.5	5.93	6.01		5280	4088	4.07	
HN17_HB216	4.0	3.68	3.77	1239	80	0.30			HG1115_X118	5.5	5.61	5.67		4205	1827	1.37	
HN17_X20	5.5	5.49	5.52	3061	373	0.45			X215_HG119	4.5	4.67	4.75		4596	2520	1.84	
HN18_X114	5.5	4.98	5.24	2195	831	1.11			X215_HE2119	5.5	3.68	4.52		786	204	0.76	
HN19_X118	5.5	3.13	3.27		0	0	#DIV/0!		X215_HE2219	5.5	3.33	4.12		484	132	0.79	
HN19_X218	5.5	5.15	5.18	412	1	0.13			X216_X118	5.5	6.31	6.35		5701	5606	7.90	
HN20_HB216	5.0	4.66	4.74	1301	140	0.41			HB217_X20	5.5	5.65	5.71		4470	2161	1.44	
HN20_HB219	4.0	3.73	3.81	1524	136	0.36			X217_X20	5.5	5.51	5.64		3809	1993	1.95	
HN20_HG119	5.0	4.86	4.90	1959	165	0.34			X118_HE2219	5.5	4.40	4.85		1329	452	1.04	
HN20_HG219	4.0	4.39	4.43	5525	3966	2.42			X118_X222	4.5	5.07	5.13		5627	4953	4.80	
HN21_X20	4.5	3.24	3.29		0	0	#DIV/0!		HG119_X222	4.5	4.45	4.57		3536	1428	1.31	
HN21_X122	5.5	5.21	5.31	1989	530	0.80			X20_HG121	4.5	4.50	4.58		3553	1164	0.99	
HN22_HB121	5.0	2.70	2.86		0	0	#DIV/0!		HB121_X122	4.5	3.28	3.52		76	4	0.23	
HN22_D223	5.0	3.17	3.31		0	0	#DIV/0!		HG221_X122	5.5	5.07	5.26		1921	599	0.95	
HN24_HB219	4.0	3.75	3.98	3047	1279	1.48			HB22_X424	5.5	5.67	5.73		4464	2176	1.60	
HN24_B223	5.0	4.22	4.31	25	0	0.07			B223_X324	5.5	5.65	5.71		4376	2138	1.66	
HN24_G223	5.0	4.19	4.37	464	33	0.30			D123_HB22	4	3.76	3.84		1775	222	0.42	
HN25_X124	5.5	4.19	5.03	1010	95	0.37			D223_HB22	4	2.37	2.46		0	0	#DIV/0!	
HN25_X24	5.5	2.91	3.59		0	0	#DIV/0!		D223_X122	5.5	5.26	5.30		1155	71	0.27	
									D223_X222	5.5	2.75	2.80		0	0	#DIV/0!	
HA-Xothr																	
HA12_X13	5.5	5.30	5.34	1492	77	0.26											
HA12_HB15	4.0	3.92	3.96	2524	231	0.37											
HA12_X115	5.5	5.05	5.11	655	65	0.39											
HA12_X215	5.5	5.63	5.68	4359	1878	1.30											
HA13_HB112	4.0	4.12	4.16	4491	1239	0.81											
HA13_X212	5.5	4.97	5.09	1007	209	0.66											
HA13_HB216	5.0	4.92	5.03	3253	1199	1.16											
HA13_X116	5.5	5.07	5.25	1844	528	0.92											
HA14_HB217	4.0	2.66	3.11	782	152	0.63											
HA14_X217	4.5	4.61	4.74	4496	2533	2.02											
HA15_HG1118	5.0	2.60	2.75		0	0	#DIV/0!										
HA15_X118	4.5	3.15	3.22		0	0	#DIV/0!										
HA16_X215	5.5	4.86	4.91	62	0	0.10											
HA16_HB119	4.0	2.53	2.71	6	1	0.30											
HA16_HB219	5.0	4.26	4.37	280	16	0.28											
HA16_HG119	5.0	4.43	4.59	1031	126	0.41											
HA16_X20	5.5	5.56	5.61	3877	1154	0.88											
HA17_X20	4.5	2.99	3.07		0	0	#DIV/0!										
HA18_HB121	4.0	2.95	3.16	196	35	0.59											
HA18_HG121	5.0	3.56	4.05	446	83	0.56											
HA18_HG221	5.0	3.35	3.85	199	28	0.47											
HA19_HB22	4.0	2.35	2.45		0	0	#DIV/0!										
HA19_HG1222	5.5	5.13	5.22	1201	107	0.34											
HA19_X122	4.5	4.83	4.88	5312	3401	2.20											
HA19_X222	5.5	3.88	3.98		0	0	#DIV/0!										
HA20_X424	4.5	4.26	4.45	2905	1048	1.11											
HA21_X20	5.5	5.17	5.20	405	3	0.12											
HA22_HB121	5.5	4.37	4.45	3	0	0.30											
HA22_B223	5.0	4.97	5.02	3057	841	0.86											
HA22_G223	5.0	5.07	5.14	4072	1575	1.15											
HA22_D123	4.0	4.61	4.63	5697	5432	4.34											
HA22_D223	3.2	3.65	3.66	5702	4868	2.35											
HA23_X222	5.5	5.34	5.43	2615	626	0.72											
HA23_X24	5.5	5.28	5.35	1870	415	0.72											

HNRESIDUE:	restraint	r ⁶	avg	reg	Avg	# viol's	# viol's	Avg viol		restraint	r ⁶	avg	reg	Avg	# viol's	# viol's	Avg viol
						>.32A	>.32A	nrg							>.32A	>.32A	nrg
HN-X																	
HN12_HB112	5.0	4.08	4.13		0	0	0	#DIV/0!									
HN13_X13	4.5	2.49	2.54		0	0	0	#DIV/0!									
HN14_HB114	3.2	2.71	3.10	2847	2058	2.39	X1-X1										
HN14_HB214	4.0	2.48	2.66		0	0	0	#DIV/0!	HB111_HB211	3.2	1.73	1.76		0	0	0	#DIV/0!
HN14_X114	5.5	5.38	5.42	2121	117	0.27	HB112_HB212	3.2	1.69	1.72		0	0	0	0	0	#DIV/0!
HN14_X214	5.5	3.85	4.26	10	0	0.05	HB112_X112	3.2	2.57	2.62		0	0	0	0	0	#DIV/0!
HN15_HB15	3.2	2.32	2.39	1	0	0.24	HB112_X212	3.2	2.94	3.06	1966	483	0.72				
HN15_HG1115	4.0	3.86	3.90	1951	159	0.34	HB112_HE12	5	3.44	4.28	479	39	0.31				
HN15_HG1215	4.0	2.92	3.09	20	2	0.21	HB212_X212	4.5	3.70	3.76		0	0	0	0	0	#DIV/0!
HN15_X115	5.5	2.68	2.79	0	0	#DIV/0!	HB212_HE12	5	4.35	4.63	1181	196	0.51				
HN15_X215	4.5	4.43	4.46	2382	94	0.23	X112_X212	4	2.48	2.51		0	0	0	0	0	#DIV/0!
HN16_HB116	4.0	2.44	2.55	0	0	#DIV/0!	X212_HE12	4.5	2.65	2.68		0	0	0	0	0	#DIV/0!
HN16_HB216	4.0	3.65	3.69	315	1	0.09	X212_X312	4.5	2.90	2.99		0	0	0	0	0	#DIV/0!
HN16_X116	4.5	3.72	3.86	227	3	0.17	X212_X412	4.5	4.04	4.16	544	10	0.15				
HN17_X117	4.5	3.72	4.15	1723	149	0.34	HB214_X114	5.5	3.23	3.34		0	0	0	0	0	#DIV/0!
HN17_X217	5.5	3.52	4.32	90	1	0.15	HB214_X214	5.5	2.98	3.22		0	0	0	0	0	#DIV/0!
HN18_HB18	4.0	3.81	3.83	881	5	0.11	X114_X214	4	3.26	3.28		0	0	0	0	0	#DIV/0!
HN18_HG1118	4.0	3.47	3.57	492	39	0.30	HB15_HG1115	4	2.74	2.79		0	0	0	0	0	#DIV/0!
HN18_HG1218	3.2	2.27	2.37	12	0	0.09	HB15_X215	3.2	2.52	2.54		0	0	0	0	0	#DIV/0!
HN18_X118	5.5	4.53	4.58	0	0	#DIV/0!	HG1115_HG1215	3.2	1.70	1.73		0	0	0	0	0	#DIV/0!
HN18_X218	4.5	3.37	3.48	10	0	0.03	HG1115_X115	4.5	2.52	2.54		0	0	0	0	0	#DIV/0!
HN19_HG119	4.0	2.87	3.08	65	3	0.20	HG1115_X215	4.5	2.81	2.85		0	0	0	0	0	#DIV/0!
HN21_HG121	5.0	2.42	2.59	0	0	#DIV/0!	HG1215_X115	3.2	2.49	2.51		0	0	0	0	0	#DIV/0!
HN21_HG221	4.0	3.16	3.56	905	49	0.27	HG1215_X215	4.5	3.39	3.44		0	0	0	0	0	#DIV/0!
HN22_HB22	4.0	2.13	2.20	0	0	#DIV/0!	HB116_X116	4.5	2.39	2.43		0	0	0	0	0	#DIV/0!
HN22_HG1222	4.0	3.17	3.51	1250	232	0.57	HB216_X116	4.5	2.38	2.43		0	0	0	0	0	#DIV/0!
HN22_X122	5.5	3.48	3.66	0	0	#DIV/0!	X216_HE116	4.5	2.49	2.57		0	0	0	0	0	#DIV/0!
HN22_X222	5.5	4.36	4.39	0	0	#DIV/0!	X216_HE216	4.5	2.54	2.62		0	0	0	0	0	#DIV/0!
HN24_X24	5.5	3.80	3.88	0	0	#DIV/0!	HB217_X217	3.2	2.82	3.07	2476	1404	1.52				
HN24_X224	5.5	4.60	4.83	305	14	0.24	HB217_HE17	5	3.80	4.51	728	80	0.39				
							HB117_X217	4	2.91	3.28	164	1	0.09				
							HB117_HE17	5	4.31	4.62	1009	119	0.42				
HA1-X1																	
HA11_X11	5.5	2.48	2.56	0	0	#DIV/0!	X117_X217	4.5	2.48	2.50		0	0	0	0	0	#DIV/0!
HA12_HB112	4.0	2.43	2.49	0	0	#DIV/0!	X117_HE17	4.5	2.70	2.87		0	0	0	0	0	#DIV/0!
HA12_HB212	4.0	2.26	2.31	0	0	#DIV/0!	X217_X317	4.5	3.17	3.36		1	0	0	0	0.00	
HA12_X112	4.5	3.91	3.93	1	0	0.00	X217_X417	5.5	3.68	3.85		0	0	0	0	0	#DIV/0!
HA12_X212	4.5	4.30	4.35	1533	196	0.43	X217_HE17	4.5	2.64	2.68		0	0	0	0	0	#DIV/0!
HA13_X13	3.2	2.56	2.59	0	0	#DIV/0!	HG1118_HG1218	3.2	1.67	1.70		0	0	0	0	0	#DIV/0!
HA14_B214	4.0	2.79	2.88	0	0	#DIV/0!	HG1218_X118	3.2	2.48	2.51		0	0	0	0	0	#DIV/0!
HA14_X114	4.5	3.94	4.18	1892	239	0.44	HG1118_X118	3.2	2.59	2.62		0	0	0	0	0	#DIV/0!
HA14_X214	4.5	3.17	3.99	3186	929	0.82	HG1118_X218	4	2.81	2.84		0	0	0	0	0	#DIV/0!
HA15_HB15	3.2	3.02	3.04	484	0	0.05	HB119_HB219	3.2	1.72	1.75		0	0	0	0	0	#DIV/0!
HA15_HG1115	4.0	3.47	3.52	46	0	0.07	HB219_HG119	4	2.70	2.76		0	0	0	0	0	#DIV/0!
HA15_HG1215	4.0	2.40	2.47	0	0	#DIV/0!	HB219_HE2219	5	3.65	4.19	73	0	0	0	0	0.10	
HA15_X115	4.5	4.16	4.20	563	12	0.17	HG119_HG219	3.2	1.72	1.74		0	0	0	0	0	#DIV/0!
HA15_X215	4.5	3.13	3.16	0	0	#DIV/0!	HG119_HE2119	5	2.81	3.37		0	0	0	0	0	#DIV/0!
HA16_HB116	4.0	3.01	3.03	0	0	#DIV/0!	HG119_HE2219	4	2.51	2.90	61	0	0	0	0	0.13	
HA16_HB216	4.0	2.52	2.58	0	0	#DIV/0!	HG219_HE2219	4	2.56	2.96	117	0	0	0	0	0.12	
HA16_X116	5.5	3.26	3.30	0	0	#DIV/0!	HG121_X221	5.5	3.24	3.45		0	0	0	0	0	#DIV/0!
HA17_X117	4.5	2.98	3.11	0	0	#DIV/0!	HG221_HG121	3.2	1.74	1.77		0	0	0	0	0	#DIV/0!
HA17_X217	4.5	3.09	3.42	52	0	0.11	HG221_X221	5.5	3.23	3.42		0	0	0	0	0	#DIV/0!
HA18_HB18	4.0	2.39	2.44	0	0	#DIV/0!	HB22_X122	3.2	2.88	2.93	604	36	0.26				
HA18_HG1218	4.0	3.64	3.67	212	1	0.08	HB22_X222	3.2	2.38	2.41		0	0	0	0	0	#DIV/0!
HA18_HG1118	4.0	4.22	4.24	5460	1588	0.79	HG1222_X222	4.5	3.48	3.61		0	0	0	0	0	#DIV/0!
HA18_X118	5.5	4.71	4.74	0	0	#DIV/0!	X122_X222	4.5	4.09	4.20	1475	83	0.30				
HA18_X218	4.5	2.87	2.90	0	0	#DIV/0!	B223_G223	4	2.28	2.33		0	0	0	0	0	#DIV/0!
HA19_HB219	4.0	2.39	2.45	0	0	#DIV/0!	B223_D123	4	3.85	3.87	1140	3	0.10				
HA19_HG119	4.0	2.54	2.63	0	0	#DIV/0!	B223_D223	4	3.57	3.65	478	7	0.15				
HA20_X20	3.2	2.53	2.56	0	0	#DIV/0!	G223_D123	4	2.96	2.98		0	0	0	0	0	#DIV/0!
HA21_HG121	4.0	2.92	3.07	6	0	0.03	G223_D223	4	2.32	2.37		0	0	0	0	0	#DIV/0!
HA21_HG221	4.0	3.77	3.81	993	11	0.16	D123_D223	3.2	1.70	1.72		0	0	0	0	0	#DIV/0!
HA21_X221	5.5	4.00	4.58	543	140	0.80	X124_X324	4.5	3.51	3.59		0	0	0	0	0	#DIV/0!
HA22_HB22	4.0	2.88	2.90	0	0	#DIV/0!	X124_X424	4.5	3.71	3.86	696	52	0.33				
HA22_HG1222	5.5	2.25	2.32	0	0	#DIV/0!	X324_X424	4.5	2.26	2.28		0	0	0	0	0	#DIV/0!
HA22_X122	4.5	3.81	4.00	541	7	0.14											
HA22_X222	4.5	3.55	3.59	0	0	#DIV/0!											
HA23_B223	3.2	2.24	2.29	0	0	#DIV/0!											
HA23_G223	5.0	3.94	3.98	0	0	#DIV/0!											
HA23_D123	5.0	3.82	3.84	0	0	#DIV/0!											
HA23_X24	5.5	5.28	5.35	1870	415	0.72											
HA24_X124	4.5	2.89	3.06	0	0	#DIV/0!											
HA24_X224	5.5	4.08	4.41	9	0	0.10											