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Viewing spiderAK- ARG_refine_47FH-multi.table

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All-Atom Contacts	Clashscore, all atoms:	2.93	99 th percentile* (N=715, 2.000Å ± 0.25Å)	
	Clashscore is the number of serious steric overlaps (> 0.4 Å) per 1000 atoms.			
Protein Geometry	Poor rotamers	2	0.68%	Goal: <0.3%
	Favored rotamers	270	91.84%	Goal: >98%
	Ramachandran outliers	0	0.00%	Goal: <0.05%
	Ramachandran favored	334	98.24%	Goal: >98%
	MolProbity score [^]	1.08	100 th percentile* (N=12522, 2.000Å ± 0.25Å)	
	Cβ deviations >0.25Å	0	0.00%	Goal: 0
	Bad bonds:	0 / 2800	0.00%	Goal: 0%
Bad angles:	1 / 3778	0.03%	Goal: <0.1%	
Peptide Omegas	Cis Prolines:	1 / 15	6.67%	Expected: ≤1 per chain, or ≤5%

In the two column results, the left column gives the raw count, right column gives the percentage.

* 100th percentile is the best among structures of comparable resolution; 0th percentile is the worst. For clashscore the comparative set of structures was selected in 2004, for MolProbity score in 2006.

[^] MolProbity score combines the clashscore, rotamer, and Ramachandran evaluations into a single score, normalized to be on the same scale as X-ray resolution.

#	Alt Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles	Cis Peptides
		Avg: Clashscore: 34.13		Outliers: 0 of 340	Poor rotamers: 2 of 294	Outliers: 0 of 323	Outliers: 0 of 348	Outliers: 1 of 348	Non-Trans: 1 of 345
A 1	ALA 39.83	0.47Å N with S 251 HOH O	-	Favored (24.63%) Ile or Val / -78.1,136.2	Favored (83.8%) t chi angles: 177	0.01Å	-	-	-
A 2	VAL 36.16	-	-	Favored (37.17%) General / -75.4,154.3	Favored (46%) p0 chi angles: 65.9,348.1	0.04Å	-	-	-
A 3	ASP 45.67	-	-	Favored (71.05%) General / -62.8,-29.9	Favored (77.3%) tp40 chi angles: 184,68.3,41.7	0.05Å	-	-	-

A 5	ALA 35.34	-	Favored (97.9%) General / -63.7,-42.5	-	0.02Å	-	-	-
A 6	THR 34.43	-	Favored (86.6%) General / -67.2,-40.2	Favored (47.6%) <i>m</i> chi angles: 304.4	0.03Å	-	-	-
A 7	LEU 36.01	-	Favored (88.36%) General / -61.5,-38.8	Favored (93.8%) <i>mt</i> chi angles: 294.2,171.6	0.04Å	-	-	-
A 8	ASP 38.21	-	Favored (85.1%) General / -67.0,-42.4	Favored (51.3%) <i>m-30</i> chi angles: 278.6,340.8	0.02Å	-	-	-
A 9	LYS 41.09	-	Favored (98.32%) General / -63.3,-40.8	Allowed (0.9%) <i>mttt</i> chi angles: 270.7,146.3,201.5,136.9	0.02Å	-	-	-
A 10	LEU 36.56	-	Favored (81.3%) General / -59.0,-48.5	Favored (28.4%) <i>mt</i> chi angles: 282.2,171	0.03Å	-	-	-
A 11	GLU 38.06	-	Favored (83.59%) General / -62.7,-36.6	Favored (52.4%) <i>mm-30</i> chi angles: 287.5,283.9,358.4	0.02Å	-	-	-
A 12	ALA 37.73	-	Favored (75.25%) General / -69.7,-35.8	-	0.02Å	-	-	-
A 13	GLY 37.35	-	Favored (70.47%) Glycine / -66.5,-47.3	-	-	-	-	-
A 14	PHE 39.36	0.41Å O with A 18 GLN HG2	Favored (77.63%) General / -56.4,-48.1	Favored (72.9%) <i>t80</i> chi angles: 174.8,85.7	0.01Å	-	-	-
A 15	LYS 41.89	-	Favored (91.82%) General / -60.8,-40.2	Allowed (1.3%) <i>tttm</i> chi angles: 154.1,146.4,198.7,293.3	0.01Å	-	-	-
A 16	LYS 41.8	-	Favored (75.82%) General / -62.6,-33.8	Favored (18.2%) <i>tttt</i> chi angles: 175.7,172.2,182.6,212.8	0.02Å	-	-	-
A 17	LEU 38.38	-	Favored (63.13%) General / -74.3,-33.4	Favored (28.9%) <i>mt</i> chi angles: 285.6,159.9	0.02Å	-	-	-
A 18	GLN 44.72	0.41Å HG2 with A 14 PHE O	Favored (62.9%) General /	Favored (14.6%) <i>mm-40</i> chi angles:	0.04Å	-	-	-

#	Alt Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles	Cis Peptides
A 19	ASP 44.62	-	-	Favored (58.06%) General / -82.5,-12.0	Favored (79.5%) <i>m-30</i> chi angles: 294,349.8	0.02Å	-	-	-
A 20	ALA 43.88	-	-	Favored (6.29%) General / -90.8,76.8	-	0.03Å	-	-	-
Avg: Clashscore: 34.13 Outliers: 0 of 340 Poor rotamers: 2 of 294 Outliers: 0 of 323 Outliers: 0 of 348 Outliers: 1 of 348 Non-Trans: 1 of 345									
A 21	THR 46.84	-	-	Favored (65.73%) General / -59.0,-27.7	Favored (70.9%) <i>p</i> chi angles: 59.3	0.06Å	-	-	-
A 22	ASP 47.1	-	-	-	Favored (59.5%) <i>m-30</i> chi angles: 288.7,319.7	0.01Å	-	-	-
A 23	CSO 41.03	-	-	-	-	0.06Å	-	-	-
A 24	LYS 57.67	-	-	-	Allowed (1.2%) <i>mttp</i> chi angles: 280.1,130.3,163.7,51	0.03Å	-	-	-
A 25	SER 30.41	-	-	Favored (32.8%) General / -74.6,158.9	Favored (75.6%) <i>p</i> chi angles: 59.9	0.04Å	-	-	-
A 26	LEU 26.73	-	-	Favored (73.62%) General / -62.2,-32.9	Favored (76.3%) <i>mt</i> chi angles: 299.7,181.4	0.04Å	-	-	-
A 27	LEU 25.22	-	-	Favored (75.87%) General / -55.7,-48.0	Favored (75.5%) <i>tp</i> chi angles: 177.3,62.4	0.01Å	-	-	-
A 28	LYS 39.43	-	-	Favored (77.36%) General / -68.5,-35.3	Allowed (0.6%) <i>tttm</i> chi angles: 181.7,225.7,205.5,324.4	0.02Å	-	-	-
A 29	LYS 28.74	-	-	Favored (99.69%) General / -62.4,-42.8	Favored (65.1%) <i>tttt</i> chi angles: 175.9,167.9,192.7,183.3	0.03Å	-	-	-
A 30	TYR 27.59	-	-	Favored (16.49%) General / -106.4,-9.9	Favored (75.7%) <i>m-80</i> chi angles: 297,290.3	0.04Å	-	-	-
A 31	LEU 32.73	-	-	Favored (10.23%) General / -86.5,72.7	Favored (32.6%) <i>tp</i> chi angles: 186,66.1	0.04Å	-	-	-

A	ASN	36.58	-	Favored (7.11%) General / -84.4,-179.2	Favored (34.8%) <i>p0</i> chi angles: 62.8,39.9	0.06Å	-	-	-
A	ARG	30	-	Favored (92.14%) General / -65.4,-39.5	Favored (3.9%) <i>tpt170</i> chi angles: 182.3,74.9,217.1,185.7	0.02Å	-	-	-
A	GLU	36.53	-	Favored (69.73%) General / -71.8,-39.9	Favored (3.9%) <i>tp30</i> chi angles: 198.1,45.9,67.9	0.01Å	-	-	-
A	VAL	31.29	-	Favored (95.62%) Ile or Val / -63.9,-42.4	Favored (51.9%) <i>t</i> chi angles: 169.7	0.06Å	-	-	-
A	PHE	32.71	-	Favored (95.02%) General / -60.6,-45.2	Favored (85.5%) <i>t80</i> chi angles: 181.3,76.1	0.03Å	-	-	-
A	ASP	35.85	-	Favored (67.97%) General / -69.8,-30.4	Favored (4.6%) <i>m-30</i> chi angles: 274.5,304.8	0.03Å	-	-	-
A	GLN	33.08	-	Favored (84.94%) General / -59.1,-40.3	Favored (35.4%) <i>mt0</i> chi angles: 284.1,183.9,261.8	0.06Å	-	-	-
A	CYS	31.11	-	Favored (13.58%) General / -102.0,-26.0	Favored (94.9%) <i>m</i> chi angles: 292	0.05Å	-	-	-
A	LYS	34.66	-	Favored (67.72%) General / -64.7,-24.9	Favored (8.2%) <i>pttm</i> chi angles: 65.7,181.1,205,289.8	0.01Å	-	-	-
#	Alt Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles	Cis Peptides
		Avg: 34.13	Clashscore: 2.93	Outliers: 0 of 340	Poor rotamers: 2 of 294	Outliers: 0 of 323	Outliers: 0 of 348	Outliers: 1 of 348	Non-Trans: 1 of 345
A	SER	37.81	-	Favored (36.8%) General / -102.6,12.1	Allowed (0.9%) <i>m</i> chi angles: 272.6	0.04Å	-	-	-
A	LEU	31.51	-	Favored (17.19%) General / -92.9,156.0	Favored (54.6%) <i>mt</i> chi angles: 303.9,173.1	0.02Å	-	-	-
A	LYS	34.53	-	Favored (9.36%) General / -153.7,128.3	Favored (20%) <i>ttmt</i> chi angles: 180.6,187.1,271.5,177.8	0.01Å	-	-	-

A 44	THR 31.89	-	Favored (9.13%) General / -67.2,169.1	Favored (50.5%) <i>p</i> chi angles: 65.6	0.05Å	-	-	-
A 45	ALA 33.83	-	Favored (67.24%) General / -66.7,-26.9	-	0.03Å	-	-	-
A 46	LEU 34.85	-	Favored (57.83%) General / -87.4,-1.3	Favored (79.2%) <i>mt</i> chi angles: 293.5,167	0.02Å	-	-	-
A 47	GLY 32.06	-	Favored (44.64%) Glycine / 104.2,1.0	-	-	-	-	-
A 48	ALA 28.96	-	Favored (44.94%) General / -73.1,137.1	-	0.03Å	-	-	-
A 49	THR 27.09	-	Favored (4.71%) General / -110.4,177.4	Favored (2.3%) <i>p</i> chi angles: 81.2	0.05Å	-	-	-
A 50	LEU 28.53	-	Favored (71.46%) General / -63.4,-30.3	Favored (69.6%) <i>tp</i> chi angles: 176.3,62.9	0.03Å	-	-	-
A 51	LEU 29.62	-	Favored (89.72%) General / -63.6,-38.1	Favored (24.7%) <i>tp</i> chi angles: 189.6,61.8	0.01Å	-	-	-
A 52	ASP 24.33	-	Favored (23.96%) General / -65.8,-8.9	Favored (60.6%) <i>m-30</i> chi angles: 302.4,309.2	0.01Å	-	-	-
A 53	CYS 25.9	-	Favored (5.28%) General / -94.0,-50.5	Favored (50.4%) <i>m</i> chi angles: 303.5	0.03Å	-	-	-
A 54	ILE 24.47	-	Favored (9.73%) Ile or Val / -102.2,-2.0	Favored (7.7%) <i>pt</i> chi angles: 71.4,183.5	0.05Å	-	-	-
A 55	GLN 25.37	-	Favored (84.92%) General / -61.5,-37.8	Favored (6.5%) <i>pt0</i> chi angles: 53.5,195.4,346.8	0.03Å	-	-	-
A 56	SER 26.46	-	Favored (84.72%) General / -66.0,-37.0	Favored (38.1%) <i>t</i> chi angles: 181.2	0.01Å	-	-	-
A 57	GLY 27.65	-	Favored (79.71%) Glycine / -77.7,-16.8	-	-	-	-	-

A 58	VAL	31.56	-	Favored (27.4%) Ile or Val / -77.5,-39.3	Favored (18.2%) <i>t</i> chi angles: 164.3	0.09Å	-	-	-
A 59	GLU	36.09	-	Favored (40.14%) General / -79.9,-33.0	Favored (48.8%) <i>mm-30</i> chi angles: 295.4,303.9,293.6	0.03Å	-	-	-
A 60	ASN	29.84	-	Favored (3.48%) General / -112.4,91.0	Favored (51.1%) <i>m-40</i> chi angles: 302.8,285.1	0.04Å	-	-	-
#	Alt Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles	Cis Peptides
		Avg: 34.13	Clashscore: 2.93	Outliers: 0 of 340	Poor rotamers: 2 of 294	Outliers: 0 of 323	Outliers: 0 of 348	Outliers: 1 of 348	Non-Trans: 1 of 345
A 61	LEU	34.62	-	Favored (61.62%) General / -71.2,-12.7	Favored (31.5%) <i>mt</i> chi angles: 296.3,162.7	0.03Å	-	-	-
A 62	ASP	29.43	-	Favored (28.14%) General / -87.1,7.4	Favored (24.9%) <i>p0</i> chi angles: 58.9,335	0.04Å	-	-	-
A 63	SER	27.1	-	Favored (48.5%) General / -57.8,141.5	Favored (59.7%) <i>m</i> chi angles: 299.1	0.02Å	-	-	-
A 64	GLY	26.54	-	Favored (30.58%) Glycine / -76.1,-40.1	-	-	-	-	-
A 65	VAL	26.06	-	Allowed (0.8%) Ile or Val / -105.7,-70.2	Favored (89.4%) <i>t</i> chi angles: 176.1	0.09Å	-	-	-
A 66	GLY	22.04	-	Favored (55.33%) Glycine / 97.5,9.3	-	-	-	-	-
A 67	ILE	21.83	-	Favored (25.35%) Ile or Val / -138.4,147.6	Favored (6.6%) <i>tt</i> chi angles: 199.3,176.8	0.07Å	-	-	-
A 68	TYR	26.17	-	Favored (42.98%) General / -138.3,159.1	Favored (89.2%) <i>m-80</i> chi angles: 290.9,273.3	0.07Å	-	-	-
A 69	ALA	21.3	-	Favored (46.35%) Pre-Pro / -98.8,124.3	-	0.03Å	-	-	-
A 70	PRO	23.71	-	Favored (3.58%) Trans-Pro / -84.8,-20.7	Favored (65.2%) <i>Cg_endo</i> chi angles: 31.4,319.6,33.2	0.02Å	-	-	-

A 71	ASP	26.26	-	Favored (11.41%) General / -159.3,177.1	Favored (43.6%) <i>p0</i> chi angles: 62,22.1	0.05Å	-	-	-	
A 72	ALA	28.73	-	Favored (77.64%) General / -69.2,-40.9	-	0.04Å	-	-	-	
A 73	GLU	29.74	-	Favored (71.99%) General / -57.5,-36.9	Favored (74.6%) <i>tt0</i> chi angles: 184.5,186.4,347.1	0.03Å	-	-	-	
A 74	ALA	24.48	-	Favored (21.25%) General / -51.6,-30.5	-	0.02Å	-	-	-	
A 75	TYR	24.73	-	Favored (94.93%) General / -64.9,-40.4	Favored (9.3%) <i>m-80</i> chi angles: 272.3,299.8	0.02Å	-	-	-	
A 76	THR	24.31	-	Favored (10%) General / -80.8,-50.3	Favored (39.6%) <i>m</i> chi angles: 305.2	0.10Å	-	-	-	
A 77	LEU	27.21	-	Favored (83.45%) General / -58.9,-40.1	Favored (47.7%) <i>tp</i> chi angles: 173.9,65.7	0.03Å	-	-	-	
A 78	PHE	26.23	-	Favored (5.32%) General / -100.7,28.2	Favored (85.8%) <i>m-80</i> chi angles: 297.5,286.3	0.04Å	-	-	-	
A 79	ALA	24.82	-	Favored (6.74%) Pre-Pro / -50.5,-32.7	-	0.04Å	-	-	-	
A 80	PRO	27.03	-	Favored (86.13%) Trans-Pro / -61.1,-28.9	Favored (55.2%) <i>Cg_exo</i> chi angles: 328.1,39,329.8	0.02Å	-	-	-	
#	Alt	Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles	Cis Peptides
			Avg: 34.13	Clashscore: 2.93	Outliers: 0 of 340	Poor rotamers: 2 of 294	Outliers: 0 of 323	Outliers: 0 of 348	Outliers: 1 of 348	Non-Trans: 1 of 345
A 81	ILE	25.74	-	Favored (4.82%) Ile or Val / -99.1,-35.3	Favored (4.2%) <i>tp</i> chi angles: 181.5,56.1	0.06Å	-	-	-	
A 82	PHE	22.64	-	Favored (79.56%) General / -66.0,-46.0	Favored (14.2%) <i>m-80</i> chi angles: 275.2,299.6	0.02Å	-	-	-	
A 83	ASN	23.76	-	Favored (96.43%) Pre-Pro /	Favored (63.8%) <i>m-40</i> chi angles: 280.6,353.1	0.06Å	-	-	-	

A 84	PRO 22.33	-	-57.4,-49.0 Favored (47.54%) Trans-Pro / -66.1,-30.1	Favored (29.9%) <i>Cg_endo</i> chi angles: 21.3,328.7,28.4	0.03Å	-	-	-
A 85	ILE 24.36	-	Favored (65.53%) Ile or Val / -72.3,-40.6	Favored (49.3%) <i>mt</i> chi angles: 295.3,180.1	0.06Å	-	-	-
A 86	ILE 22.59	-	Favored (85.58%) Ile or Val / -60.3,-49.1	Favored (59.8%) <i>mt</i> chi angles: 286.9,166.2	0.07Å	-	-	-
A 87	GLU 27.94	-	Favored (51.77%) General / -52.7,-53.1	Favored (12.2%) <i>tm-30</i> chi angles: 190.8,287,318.5	0.04Å	-	-	-
A 88	ASP 25.84	-	Favored (26.61%) General / -59.0,-56.1	Favored (16.2%) <i>t0</i> chi angles: 195.4,316.1	0.04Å	-	-	-
A 89	TYR 28.28	-	Favored (99.43%) General / -61.7,-42.8	Favored (79.9%) <i>t80</i> chi angles: 182.2,85.3	0.05Å	-	-	-
A 90	HIS 24.21	-	Favored (14.3%) General / -90.0,13.7	Favored (89.1%) <i>m-70</i> chi angles: 294.7,274.2	0.08Å	-	-	-
A 91	GLU 34.06	-	Favored (2.82%) General / 58.5,59.8	Favored (64.6%) <i>mt-10</i> chi angles: 281,182.1,3.3	0.06Å	-	-	-
A 92	GLY 27.32	-	Favored (10.38%) Glycine / 109.8,16.8	-	-	-	-	-
A 93	PHE 22.42	-	Favored (8.57%) General / -88.5,90.9	Favored (38.3%) <i>t80</i> chi angles: 193.4,85.7	0.04Å	-	-	-
A 94	LYS 35.48	-	Favored (80.57%) Pre-Pro / -70.8,160.9	Favored (6.1%) <i>mmtm</i> chi angles: 319.9,299.4,175.8,320.6	0.03Å	-	-	-
A 95	PRO 26.18	-	Favored (55.83%) Trans-Pro / -56.5,-25.1	Favored (82.1%) <i>Cg_exo</i> chi angles: 334.5,30,338	0.03Å	-	-	-
A 96	THR 33.41	-	Favored (49.72%) General / -94.2,-4.0	Favored (14.4%) <i>p</i> chi angles: 47.6	0.03Å	-	-	-
A 97	ASP 24.78	-	Favored (23.56%) General / -79.0,165.3	Favored (35%) <i>m-30</i> chi angles: 276.7,338.2	0.01Å	-	-	-

A 98	LYS	30.46	-	Favored (29.74%) General / -141.1,134.5	Favored (75.9%) <i>tttt</i> chi angles: 170.7,178.5,181.9,176.8	0.03Å	-	-	-
A 99	HIS	21.01	-	Favored (43.26%) Pre-Pro / -83.6,142.8	Favored (82.6%) <i>t70</i> chi angles: 178.4,79.8	0.06Å	-	-	-
A 100	PRO	21.45	-	Favored (46.72%) Trans-Pro / -66.8,160.4	Favored (35%) <i>Cg_endo</i> chi angles: 22.3,323.2,36.7	0.04Å	-	-	-
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A 101	PRO	23.51	-	Favored (41.16%) Trans-Pro / -63.3,159.1	Favored (3%) <i>Cg_exo</i> chi angles: 354.7,17.7,337.3	0.05Å	-	-	-
A 102	THR	24.09	-	Favored (55.61%) General / -58.0,133.5	Favored (13.7%) <i>m</i> chi angles: 311.1	0.05Å	-	-	-
A 103	ASP	27.25	-	Favored (3.03%) General / -155.3,110.6	Favored (42%) <i>t0</i> chi angles: 186.9,12.5	0.03Å	-	-	-
A 104	PHE	30.83	-	Favored (56.07%) General / -83.0,-13.4	Favored (71.9%) <i>m-80</i> chi angles: 300.7,289.8	0.03Å	-	-	-
A 105	GLY	31.92	-	Favored (53.74%) Glycine / 77.9,-167.7	-	-	-	-	-
A 106	ASP	36.32	-	Favored (11.16%) General / -87.6,98.0	Favored (41.6%) <i>t0</i> chi angles: 190.7,2.8	0.05Å	-	-	-
A 107	ILE	33.02	-	Favored (35.67%) Ile or Val / -60.7,-25.7	Favored (3.1%) <i>tp</i> chi angles: 185.2,51.8	0.08Å	-	-	-
A 108	ASN	38.05	-	Favored (59%) General / -77.3,-9.8	Favored (10.2%) <i>m-40</i> chi angles: 275.5,262.8	0.04Å	-	-	-
A 109	THR	33.28	-	Favored (58.02%) General / -84.3,-3.1	Favored (16.9%) <i>p</i> chi angles: 73.9	0.03Å	-	-	-
A 110	ILE	29.73	-	Favored (15.89%) Ile or Val / -83.9,140.6	Favored (45.6%) <i>mm</i> chi angles: 298,299.4	0.05Å	-	-	-

A 111	VAL	31.07	-	Favored (21.98%) Ile or Val / -125.9,166.4	Favored (3.4%) <i>m</i> chi angles: 309.6	0.04Å	-	-	-
A 112	ASN	31.67	-	Favored (24.09%) General / -73.2,123.7	Favored (38.3%) <i>t0</i> chi angles: 188.9,310.8	0.04Å	-	-	-
A 113	VAL	27.75	-	Favored (14.23%) Ile or Val / -77.6,-14.2	Favored (6.4%) <i>m</i> chi angles: 288.4	0.05Å	-	-	-
A 114	ASP	28.88	-	Favored (5.11%) Pre-Pro / -156.0,73.8	Favored (25.2%) <i>t0</i> chi angles: 179.2,27.4	0.03Å	-	-	-
A 115	PRO	35.7	-	Favored (43.02%) Trans-Pro / -58.9,-18.6	Favored (7.8%) <i>Cg_exo</i> chi angles: 348.5,26.3,329.9	0.03Å	-	-	-
A 116	SER	34.05	-	Favored (68.93%) General / -68.8,-30.4	Favored (6.8%) <i>p</i> chi angles: 84	0.01Å	-	-	-
A 117	GLY	30.05	-	Favored (61.65%) Glycine / 74.2,2.0	-	-	-	-	-
A 118	LYS	32.39	-	Favored (41.11%) General / -80.3,-23.0	Favored (36.5%) <i>mtmt</i> chi angles: 302.3,199.4,285.1,180.1	0.04Å	-	-	-
A 119	TYR	27.77	-	Allowed (1.76%) General / -124.1,-52.3	Favored (66.5%) <i>m-80</i> chi angles: 303.8,287.9	0.04Å	-	-	-
A 120	VAL	25.09	-	Favored (32.77%) Ile or Val / -86.2,118.5	Favored (94.7%) <i>t</i> chi angles: 174.8	0.03Å	-	-	-

#	Alt	Res	<u>High</u> <u>B</u>	<u>Clash ></u> <u>0.4Å</u>	<u>Ramachandran</u>	<u>Rotamer</u>	<u>Cβ</u> <u>deviation</u>	<u>Bond</u> <u>lengths</u>	<u>Bond angles</u>	<u>Cis</u> <u>Peptides</u>
			Avg: Clashscore:	Outliers: 0 of	Poor rotamers: 2 of	Outliers: 0 of	Outliers: 0 of	Outliers: 1 of	Non-Trans: 1 of	
			34.13	340	294	323	348	348	345	

A 121	VAL	27.64	-	Favored (26.97%) Ile or Val / -75.7,-49.3	Favored (84.2%) <i>t</i> chi angles: 173.4	0.07Å	-	-	-
A 122	SER	24.65	-	Favored (35.96%) General / -151.2,154.0	Favored (7.6%) <i>p</i> chi angles: 49.4	0.05Å	-	-	-
A 123	THR	24.23	-	Favored (47.48%)	Favored (88.4%) <i>m</i> chi angles: 301.3	0.04Å	-	-	-

A 124	HIS	26.21	-	General / -122.7,146.4 Favored (25.83%) General / -146.6,140.1	Allowed (1.3%) <i>m-70</i> chi angles: 323.6,260.5	0.07Å	-	-	-
A 125	VAL	24.51	-	Favored (33.97%) Ile or Val / -131.0,116.5	Favored (32.7%) <i>t</i> chi angles: 185.5	0.06Å	-	-	-
A 126	ARG	30	-	Favored (46.52%) General / -109.4,137.9	Favored (26.4%) <i>ttm170</i> chi angles: 173.7,197.9,296.1,172.2	0.06Å	-	-	-
A 127	CYS	25.49	-	Favored (15.38%) General / -135.7,170.8	Favored (11.4%) <i>p</i> chi angles: 74.5	0.04Å	-	-	-
A 128	GLY	20.71	-	Favored (21.29%) Glycine / -135.1,153.8	-	-	-	-	-
A 129	ARG	30	-	Favored (23.31%) General / -147.4,137.8	Favored (86.5%) <i>mmt-90</i> chi angles: 294.2,286.8,189.4,267.3	0.06Å	-	-	-
A 130	SER	21.3	-	Favored (30.16%) General / -99.0,142.7	Favored (63.3%) <i>m</i> chi angles: 297.8	0.02Å	-	-	-
A 131	LEU	27.18	-	Favored (35.26%) General / -90.0,132.7	Favored (33.3%) <i>mt</i> chi angles: 306.4,171.8	0.01Å	-	-	-
A 132	LYS	34.18	0.67Å NZ with S 213 HOH O	Favored (57.93%) General / -62.3,136.4	Allowed (1.5%) <i>tttt</i> chi angles: 186.7,142.7,147.1,215.2	0.01Å	-	-	-
A 133	GLY	28.12	-	Favored (64.46%) Glycine / 96.5,-14.3	-	-	-	-	-
A 134	TYR	34.53	-	Favored (22.58%) Pre-Pro / -102.7,141.5	Favored (77.4%) <i>m-80</i> chi angles: 288.3,274	0.04Å	-	-	-
A 135	PRO	29.35	-	Favored (10.76%) Trans-Pro / -65.2,170.3	Allowed (1%) <i>Cg_exo</i> chi angles: 359.5,13.5,339.4	0.02Å	-	-	-
A 136	PHE	24.47	-	Favored (7.27%) General / -89.1,175.7	Favored (10.1%) <i>m-10</i> chi angles: 297.2,353.7	0.06Å	-	-	-

#	Alt	Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles	Cis Peptides
A 137	ASN	25.47	0.60Å HA with A 140 LEU HD12	-	Favored (7.58%) Pre-Pro / -55.1,-30.6	Favored (9.5%) <i>m-40</i> chi angles: 268.6,275.4	0.08Å	-	-	-
A 138	PRO	26.17	-	-	Favored (68.73%) Trans-Pro / -61.4,-20.5	Favored (85.5%) <i>Cg_exo</i> chi angles: 333.9,35.6,329.4	0.03Å	-	-	-
A 139	CYS	27.99	-	-	Favored (5%) General / -131.4,12.7	Favored (93.1%) <i>m</i> chi angles: 291.8	0.01Å	-	-	-
A 140	LEU	26.81	0.60Å HD12 with A 137 ASN HA	-	Favored (41.72%) General / -76.1,142.2	Favored (17.8%) <i>mt</i> chi angles: 286.1,157.5	0.05Å	-	-	-
<p>Avg: Clashscore: 34.13 Clashes: 2.93 Outliers: 0 of 340 Poor rotamers: 2 of 294 Outliers: 0 of 323 Outliers: 0 of 348 Outliers: 1 of 348 Non-Trans: 1 of 345</p>										
A 141	THR	32.2	-	-	Favored (13.43%) General / -91.2,165.5	Favored (60.2%) <i>p</i> chi angles: 64	0.07Å	-	-	-
A 142	GLU	33.44	-	-	Favored (72.36%) General / -54.4,-44.6	Favored (4.5%) <i>tt0</i> chi angles: 192.9,147.8,30.1	0.03Å	-	-	-
A 143	ALA	28.9	-	-	Favored (99.06%) General / -63.3,-42.4	-	0.01Å	-	-	-
A 144	ASN	27.56	-	-	Favored (8.74%) General / -52.7,-57.9	Favored (7.3%) <i>m110</i> chi angles: 290.6,153.3	0.06Å	-	-	-
A 145	TYR	25.75	-	-	Favored (36.23%) General / -48.8,-50.1	Favored (26.3%) <i>m-80</i> chi angles: 278.3,289.8	0.02Å	-	-	-
A 146	LYS	43.7	-	-	Favored (75%) General / -58.7,-50.1	Favored (69.7%) <i>mttt</i> chi angles: 277.7,188,180.4,172.7	0.02Å	-	-	-
A 147	GLU	37.46	0.64Å OE1 with S 77 HOH O	-	Favored (97.17%) General / -64.0,-42.4	Favored (14.7%) <i>tt0</i> chi angles: 168.6,198.6,358.7	0.03Å	-	-	-
A 148	MET	26.65	-	-	Favored (97.5%) General / -61.0,-44.4	Favored (41.8%) <i>ttm</i> chi angles: 184.7,189,298.5	0.02Å	-	-	-
A 149	GLU	29.3	-	-	Favored (88.28%) General /	Favored (59.3%) <i>tt0</i> chi angles:	0.02Å	-	-	-

A 150	ASP	34.89	-	-61.8,-38.5 Favored (99.05%) General / -61.6,-42.5	179.4,183,26.1 Favored (36.7%) <i>t0</i> chi angles: 193.6,7.4	0.05Å	-	-	-
A 151	LYS	33.94	-	Favored (68.59%) General / -71.5,-42.1	Favored (12.7%) <i>mttm</i> chi angles: 300.2,176.8,180.5,326.4	0.03Å	-	-	-
A 152	VAL	29.35	-	Favored (82.4%) Ile or Val / -66.7,-47.7	Allowed (1.8%) <i>t</i> chi angles: 158.1	0.10Å	-	-	-
A 153	SER	31.43	-	Favored (81.89%) General / -61.7,-36.8	Favored (65.4%) <i>p</i> chi angles: 58.3	0.03Å	-	-	-
A 154	ALA	31.59	-	Favored (77.72%) General / -56.0,-47.5	-	0.04Å	-	-	-
A 155	ILE	31.37	-	Favored (96.35%) Ile or Val / -61.6,-46.5	Favored (70.1%) <i>mt</i> chi angles: 292.3,160.7	0.05Å	-	-	-
A 156	PHE	30.05	-	Favored (67.68%) General / -56.7,-34.7	Favored (22.6%) <i>m-10</i> chi angles: 294.2,344.5	0.02Å	-	-	-
A 157	GLY	34.44	-	Favored (60.69%) Glycine / -59.6,-25.1	-	-	-	-	-
A 158	THR	34.53	-	Favored (56.27%) General / -85.7,-10.1	Favored (24.8%) <i>p</i> chi angles: 71	0.02Å	-	-	-
A 159	PHE	32.37	0.41Å O with A 164 LYS HD3	Favored (46.44%) General / -58.4,130.4	Favored (7.5%) <i>m-10</i> chi angles: 282.1,350.2	0.04Å	-	-	-
A 160	GLU	43.26	-	Favored (5.14%) General / -126.4,179.8	Allowed (0.6%) <i>mp0</i> chi angles: 324.9,108.8,302.1	0.03Å	-	-	-

Alt Res High B Clash > 0.4Å Ramachandran Rotamer Cβ deviation Bond lengths Bond angles Cis Peptides

Avg: Clashscore: 34.13 Outliers: 0 of 340 Poor rotamers: 2 of 294 Outliers: 0 of 323 Outliers: 0 of 348 Outliers: 1 of 348 Non-Trans: 1 of 345

A 161	GLY	32.73	-	Favored (36.66%) Glycine / 71.7,-144.3	-	-	-	-	-
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A 162	GLU 32.22	0.72Å OE1 with S 237 HOH O	Favored (64.55%) General / -66.8,-16.9	Favored (12.5%) <i>pt0</i> chi angles: 72.3,172.8,160.9	0.01Å	-	-	-
A 163	LEU 29.75	-	Favored (53.99%) General / -85.6,-11.4	Favored (14.8%) <i>mt</i> chi angles: 290.6,189.4	0.04Å	-	-	-
A 164	LYS 30.76	0.41Å HD3 with A 159 PHE O	Favored (44.33%) General / -66.1,130.8	Favored (2.2%) <i>tptp</i> chi angles: 185.5,36.2,189.4,52.1	0.03Å	-	-	-
A 165	GLY 27.82	-	Favored (3.89%) Glycine / -164.2,-144.0	-	-	-	-	-
A 166	LYS 28.59	-	Favored (36.9%) General / -139.6,139.8	Favored (38.6%) <i>ttm</i> chi angles: 193.4,168.8,191.4,297.2	0.03Å	-	-	-
A 167	TYR 28.31	-	Favored (37.69%) General / -95.0,134.5	Favored (70.2%) <i>t80</i> chi angles: 180.3,68.2	0.01Å	-	-	-
A 168	TYR 27.85	-	Favored (52.26%) Pre-Pro / -116.2,104.2	Favored (34.6%) <i>m-80</i> chi angles: 305.4,80.7	0.03Å	-	-	-
A 169	PRO 27.17	-	Favored (63.96%) Trans-Pro / -64.8,139.7	Allowed (1.7%) <i>Cg_exo</i> chi angles: 358.3,9.5,346.8	0.04Å	-	-	-
A 170	LEU 26.2	-	Favored (66.64%) General / -70.1,-29.6	Favored (2.5%) <i>mp</i> chi angles: 259.7,54.3	0.05Å	-	-	-
A 171	THR 25.77	-	Favored (15.12%) General / -67.2,121.2	Favored (95.3%) <i>m</i> chi angles: 300.8	0.03Å	-	-	-
A 172	GLY 25.06	-	Favored (79.48%) Glycine / 74.0,17.5	-	-	-	-	-
A 173	MET 23.43	-	Favored (41.6%) General / -72.7,130.9	Favored (59.9%) <i>ttm</i> chi angles: 183.5,175.3,287.7	0.05Å	-	-	-
A 174	ASP 24.47	-	Favored (19.02%) General / -87.0,159.4	Favored (2.8%) <i>p0</i> chi angles: 66.8,71.9	0.04Å	-	-	-
A 175	LYS 28.89	-	Favored (69.94%) General / -63.6,-28.4	Favored (4.7%) <i>tttp</i> chi angles: 212.7,176.6,169.7,89.4	0.03Å	-	-	-

A 176	ALA	24.84	-	Favored (63.51%) General / -72.2,-44.1	-	0.03Å	-	-	-
A 177	THR	24.8	-	Favored (77.62%) General / -56.3,-47.9	Favored (99.5%) <i>m</i> chi angles: 300.5	0.07Å	-	-	-
A 178	GLN	28.55	-	Favored (74.14%) General / -54.8,-47.4	Favored (80.1%) <i>mt0</i> chi angles: 283,174.8,347.9	0.02Å	-	-	-
A 179	GLN	31.95	-	Favored (91.28%) General / -63.6,-38.5	Favored (85.9%) <i>tp40</i> chi angles: 186.6,61,43.5	0.01Å	-	-	-
A 180	GLN	35.19	-	Favored (80.89%) General / -57.2,-42.4	Favored (36.5%) <i>tt0</i> chi angles: 172.8,186.4,336.2	0.07Å	-	-	-
#	Alt Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles	Cis Peptides
			Avg: Clashscore: 34.13	Outliers: 0 of 340	Poor rotamers: 2 of 294	Outliers: 0 of 323	Outliers: 0 of 348	Outliers: 1 of 348	Non-Trans: 1 of 345
A 181	LEU	25.24	-	Favored (54.44%) General / -77.4,-34.9	Favored (96.3%) <i>mt</i> chi angles: 291.9,172.4	0.06Å	-	-	-
A 182	ILE	29.21	-	Favored (85.72%) Ile or Val / -57.8,-44.2	Favored (70.5%) <i>mt</i> chi angles: 292.8,160.7	0.07Å	-	-	-
A 183	ASP	33.87	-	Favored (69.42%) General / -60.5,-30.0	Favored (83.2%) <i>m-30</i> chi angles: 289.9,333.6	0.02Å	-	-	-
A 184	ASP	30.13	-	Favored (59.19%) General / -86.6,-5.3	Favored (73.1%) <i>m-30</i> chi angles: 296.4,316.2	0.02Å	-	-	-
A 185	HIS	30.54	-	Favored (18.9%) General / 60.5,29.3	Favored (65.7%) <i>m-70</i> chi angles: 302.1,265.3	0.04Å	-	-	-
A 186	PHE	26.33	-	Favored (29.31%) General / -102.8,-1.7	Favored (20.9%) <i>m-10</i> chi angles: 291.3,345.6	0.04Å	-	-	-
A 187	LEU	24.96	-	Favored (31.48%) General / -94.5,139.2	Favored (10.8%) <i>tp</i> chi angles: 189.5,76.8	0.03Å	-	-	-
A 188	PHE	23.45	-	Favored (26.75%) General /	Favored (55.7%) <i>p90</i> chi angles: 65.3,270	0.06Å	-	-	-

A 189	LYS 37.97	-	-118.3,157.6 Favored (4.74%) General / -122.3,178.9	Favored (4.2%) <i>ptpp</i> chi angles: 66,171.2,89,56	0.01Å	-	-	-
A 190	GLU 34.21	-	Favored (47.13%) General / -60.6,146.0	Favored (12.3%) <i>tt0</i> chi angles: 207.1,180.7,344.6	0.01Å	-	-	-
A 191	GLY 28.29	-	Favored (46.17%) Glycine / -66.0,159.8	-	-	-	-	-
A 192	ASP 25.23	-	Favored (2.21%) General / -78.2,-171.0	Favored (52%) <i>p0</i> chi angles: 62.9,14.7	0.06Å	-	-	-
A 193	ARG 30	-	Favored (66.66%) General / -67.0,-26.1	Favored (20.7%) <i>ptt90</i> chi angles: 67.1,193.3,159.3,91.3	0.03Å	-	-	-
A 194	PHE 26.67	-	Favored (79.18%) General / -66.7,-45.3	Favored (93%) <i>m-80</i> chi angles: 296.7,282.4	0.01Å	-	-	-
A 195	LEU 26.12	-	Favored (73.32%) General / -70.8,-37.8	Favored (34.9%) <i>mt</i> chi angles: 292.8,185	0.03Å	-	-	-
A 196	GLN 26.98	-	Favored (78.94%) General / -60.7,-49.1	Favored (69.3%) <i>mm-40</i> chi angles: 297.8,286.9,330.1	0.03Å	-	-	-
A 197	ALA 26.25	-	Favored (63.92%) General / -64.6,-17.4	-	0.07Å	-	-	-
A 198	ALA 23.52	-	Favored (56.61%) General / -86.8,-0.5	-	0.05Å	-	-	-
A 199	ASN 28.07	-	Favored (17.66%) General / 62.2,31.5	Favored (49.4%) <i>m-40</i> chi angles: 276.2,341.3	0.05Å	-	-	-
A 200	ALA 24.5	-	Favored (47.43%) General / -88.8,-10.7	-	0.05Å	-	-	-

Alt Res High B Clash > 0.4Å Ramachandran Rotamer Cβ deviation Bond lengths Bond angles Cis Peptides

Avg: Clashscore: 34.13 Outliers: 0 of 340 Poor rotamers: 2 of 294 Outliers: 0 of 323 Outliers: 0 of 348 Outliers: 1 of 348 Non-Trans: 1 of 345

A 201	CYS 29.26	-	Favored (13.98%) General / -116.9,20.2	Favored (34.5%) <i>m</i> chi angles: 306	0.04Å	-	-	-
A 202	ARG 30	-	Favored (56.05%) General / -61.9,143.7	Favored (36.9%) <i>mtt180</i> chi angles: 288.8,159.2,154.9,170.2	0.09Å	-	-	-
A 203	TYR 33.41	-	Favored (17.66%) General / 62.0,29.2	Favored (3.7%) <i>m-80</i> chi angles: 322,291.8	0.05Å	-	-	-
A 204	TRP 27.82	-	Favored (96.01%) Pre-Pro / -62.5,136.8	Favored (28.7%) <i>t-100</i> chi angles: 196.9,269	0.04Å	-	-	-
A 205	PRO 26.04	-	Favored (15.35%) Cis-Pro / -101.5,25.5	Favored (49.5%) <i>Cg_endo</i> chi angles: 33.1,335.6,5.9	0.03Å	-	-	Cis PRO omega= 2.36
A 206	THR 25.1	-	Favored (39.21%) General / -61.7,129.1	Favored (96.5%) <i>m</i> chi angles: 300.8	0.06Å	-	-	-
A 207	GLY 25.57	-	Favored (83.49%) Glycine / 80.3,-0.8	-	-	-	-	-
A 208	ARG 30	-	Favored (33.64%) General / -100.5,141.2	Favored (5.5%) <i>mpt180</i> chi angles: 282.5,70.9,163,203	0.06Å	-	-	-
A 209	GLY 23.13	-	Favored (42.38%) Glycine / -170.8,169.4	-	-	-	-	-
A 210	ILE 23.97	-	Favored (67.91%) Ile or Val / -128.0,133.1	Favored (8%) <i>mt</i> chi angles: 297.7,148.3	0.03Å	-	-	-
A 211	TYR 26.64	-	Favored (49.78%) General / -122.3,143.2	Favored (63.2%) <i>t80</i> chi angles: 181.9,272.1	0.01Å	-	-	-
A 212	HIS 26.91	-	Favored (26.7%) General / -153.3,148.4	Favored (8%) <i>p90</i> chi angles: 77.1,72.5	0.08Å	-	-	-
A 213	ASN 26.3	-	Favored (21.82%) General / -82.8,162.1	Favored (40.2%) <i>p0</i> chi angles: 69.8,341.2	0.07Å	-	-	-
A 214	ASP 30.75	-	Favored (73.74%) General / -58.5,-36.4	Favored (81%) <i>m-30</i> chi angles: 295,332.6	0.03Å	-	-	-

#	Alt Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles	Cis Peptides
A 215	ALA 25.9	-	-	Favored (56.41%) General / -70.7,-9.1	-	0.02Å	-	-	-
A 216	LYS 30.76	-	-	Favored (29.74%) General / 53.8,39.0	Favored (93.4%) <i>mttt</i> chi angles: 297.1,176.8,182.2,172	0.05Å	-	-	-
A 217	THR 24.04	-	-	Favored (17.23%) General / -114.4,11.4	Favored (33.7%) <i>p</i> chi angles: 53.8	0.04Å	-	-	-
A 218	PHE 25.34	-	-	Favored (12.75%) General / -151.5,130.7	Favored (82%) <i>t80</i> chi angles: 176.8,71.9	0.03Å	-	-	-
A 219	LEU 23.52	-	-	Favored (29.48%) General / -143.7,139.3	Favored (2.5%) <i>tp</i> chi angles: 169.5,83.6	0.02Å	-	-	-
A 220	VAL 22.35	0.41Å HA with A 229 ARG O	-	Favored (67.23%) Ile or Val / -129.5,131.4	Favored (58.3%) <i>t</i> chi angles: 180.2	0.02Å	-	-	-
<p>Avg: Clashscore: 34.13 Outliers: 0 of 340 Poor rotamers: 2 of 294 Outliers: 0 of 323 Outliers: 0 of 348 Outliers: 1 of 348 Non-Trans: 1 of 345</p>									
A 221	TRP 23.44	-	-	Favored (52.44%) General / -104.6,127.8	Favored (46.8%) <i>m-10</i> chi angles: 287.5,356.1	0.02Å	-	-	-
A 222	VAL 20.89	-	-	Favored (43.22%) Ile or Val / -102.5,114.9	Favored (36.6%) <i>t</i> chi angles: 184.2	0.03Å	-	-	-
A 223	ASN 21.25	-	-	Favored (7.97%) General / 65.6,34.2	Favored (62%) <i>m-40</i> chi angles: 283.6,313.5	0.11Å	-	-	-
A 224	GLU 25.14	-	-	Favored (30.47%) General / -78.7,-41.8	Favored (9.4%) <i>tm-30</i> chi angles: 177.2,267,335.6	0.03Å	-	-	-
A 225	GLU 27.26	0.41Å HG3 with A 270 PHE HD2	-	Allowed (0.24%) General / -146.3,-53.1	Favored (6.9%) <i>tt0</i> chi angles: 163.4,168.9,296.5	0.04Å	-	-	-
A 226	ASP 21.9	-	-	Favored (11.67%) General / -97.2,166.2	Favored (13.5%) <i>m-30</i> chi angles: 281.1,306.1	0.01Å	-	-	-
A 227	HIS 21.52	-	-	Favored (62.28%) General /	Favored (53.8%) <i>m170</i> chi angles: 297.1,159.7	0.02Å	-	-	-

A 228	LEU	23.53	-	-51.3,-48.7 Favored (30.61%) General / -132.7,125.6	Favored (95.7%) <i>mt</i> chi angles: 296.9,176	0.08Å	-	-	-
A 229	ARG	30	0.41Å O with A 220 VAL HA	Favored (45.28%) General / -111.3,121.5	Favored (3.7%) <i>ttm-80</i> chi angles: 173.4,199.5,293.3,232.4	0.02Å	-	-	-
A 230	ILE	24.45	-	Favored (59.06%) Ile or Val / -119.1,118.9	Favored (17.6%) <i>mt</i> chi angles: 311.2,165.3	0.06Å	-	-	-
A 231	ILE	27.58	-	Favored (63.08%) Ile or Val / -124.1,135.6	Allowed (1.8%) <i>mt</i> chi angles: 312.4,194.6	0.04Å	-	-	-
A 232	SER	24.17	-	Favored (54.46%) General / -118.5,135.3	Favored (38.2%) <i>t</i> chi angles: 177.3	0.01Å	-	-	-
A 233	MET	31.71	-	Favored (26.48%) General / -162.6,164.8	Allowed (0.3%) <i>pmt</i> chi angles: 68.7,292,176	0.03Å	-	-	-
A 234	GLN	29.75	0.59Å HG2 with A 242 ILE HD11	Favored (2.16%) General / -177.4,165.1	Favored (18.7%) <i>pt0</i> chi angles: 62.6,188.1,51.5	0.06Å	-	-	-
A 235	LYS	32.92	-	Favored (49.96%) General / -67.8,149.3	Favored (4.4%) <i>mmtt</i> chi angles: 300.1,265.7,215.6,188.5	0.04Å	-	-	-
A 236	GLY	24.57	-	Favored (27.68%) Glycine / 89.5,-158.6	-	-	-	-	-
A 237	GLY	27.21	-	Favored (4.21%) Glycine / -129.3,27.5	-	-	-	-	-
A 238	ASP	33.45	-	Favored (7.01%) General / -80.3,71.0	Favored (53%) <i>t0</i> chi angles: 187.5,0.9	0.02Å	-	-	-
A 239	LEU	27.27	-	Favored (66.8%) General / -57.9,-31.6	Favored (41.8%) <i>tp</i> chi angles: 185.4,62.7	0.04Å	-	-	-
A 240	LYS	35.53	-	Favored (17.83%) General / -62.8,-56.4	Favored (54.7%) <i>tttt</i> chi angles: 181.7,166.3,162.8,186.9	0.01Å	-	-	-

[Alt Res](#) [High B](#) [Clash > 0.4Å](#) [Ramachandran](#) [Rotamer](#) [Cβ deviation](#) [Bond lengths](#) [Bond angles](#) [Cis Peptides](#)

		Avg: Clashscore: 34.13	2.93	Outliers: 0 of 340	Poor rotamers: 2 of 294	Outliers: 0 of 323	Outliers: 0 of 348	Outliers: 1 of 348	Non- Trans: 1 of 345
A 241	THR 29.42	-		Favored (75.1%) General / -57.9,-38.1	Favored (44.6%) <i>m</i> chi angles: 304.6	0.05Å	-	-	-
A 242	ILE 24.55	0.59Å HD11 with A 234 GLN HG2		Favored (70.6%) Ile or Val / -67.3,-49.6	Favored (71%) <i>mt</i> chi angles: 289.8,163.1	0.07Å	-	-	-
A 243	PHE 24.46	-		Favored (90.13%) General / -65.4,-38.5	Favored (7.7%) <i>t80</i> chi angles: 186.3,34.8	0.06Å	-	-	-
A 244	GLN 32.81	-		Favored (75.65%) General / -67.7,-33.8	Favored (51.5%) <i>tp40</i> chi angles: 181.9,56.6,70.2	0.01Å	-	-	-
A 245	ARG 30	-		Favored (92.9%) General / -62.5,-45.5	Favored (15.4%) <i>ttp-110</i> chi angles: 186.9,159.3,49.1,235.9	0.03Å	-	-	-
A 246	LEU 27.25	-		Favored (85.88%) General / -58.9,-47.1	Favored (45.5%) <i>tp</i> chi angles: 184.4,63.4	0.03Å	-	-	-
A 247	VAL 30	-		Favored (85.7%) Ile or Val / -63.1,-48.9	Favored (70.3%) <i>t</i> chi angles: 172.1	0.05Å	-	-	-
A 248	ASN 32.67	-		Favored (61.43%) General / -51.1,-44.9	Favored (92.8%) <i>m-40</i> chi angles: 290.7,346.2	0.04Å	-	-	-
A 249	ALA 27.17	-		Favored (63.41%) General / -66.4,-50.4	-	0.01Å	-	-	-
A 250	VAL 26.35	-		Favored (92.26%) Ile or Val / -59.0,-44.8	Favored (89.3%) <i>t</i> chi angles: 174.1	0.08Å	-	-	-
A 251	ASN 32.2	-		Favored (94.1%) General / -60.4,-41.6	Favored (82.5%) <i>m-40</i> chi angles: 283.1,345.1	0.02Å	-	-	-
A 252	THR 31.5	-		Favored (90.56%) General / -60.9,-46.5	Favored (99.3%) <i>m</i> chi angles: 300.3	0.08Å	-	-	-
A 253	ILE 25.98	-		Favored (87.47%) Ile or Val / -61.2,-48.8	Favored (31.2%) <i>mt</i> chi angles: 290,155.5	0.08Å	-	-	-

A 254	GLU	28.7	-	Favored (70.48%) General / -58.1,-34.7	Favored (57.1%) <i>tt0</i> chi angles: 186.4,180.4,27.9	0.03Å	-	-	-
A 255	SER	32	-	Favored (61.92%) General / -58.4,-25.4	Favored (8.3%) <i>p</i> chi angles: 83.2	0.02Å	-	-	-
A 256	LYS	36.72	0.40Å HA with A 256 LYS HD3	Favored (9.18%) General / -106.3,-30.4	Favored (6.3%) <i>mmtp</i> chi angles: 295.8,311.5,154.3,67.3	0.03Å	-	-	-
A 257	LEU	30.57	-	Favored (15.88%) Pre-Pro / -131.8,116.4	Allowed (1.1%) <i>mt</i> chi angles: 273.3,200.2	0.01Å	-	-	-
A 258	PRO	29.7	-	Favored (49.32%) Trans-Pro / -72.5,149.0	Allowed (1.1%) <i>Cg_exo</i> chi angles: 359.2,15.4,336.5	0.03Å	-	-	-
A 259	PHE	25.7	-	Favored (15.06%) General / -94.1,159.7	Favored (23.2%) <i>m-10</i> chi angles: 301.2,321	0.04Å	-	-	-
A 260	SER	25.64	-	Favored (31.13%) General / -89.7,120.6	Favored (6.6%) <i>t</i> chi angles: 163.6	0.02Å	-	-	-
#	Alt Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles	Cis Peptides
		Avg: 34.13	Clashscore: 2.93	Outliers: 0 of 340	Poor rotamers: 2 of 294	Outliers: 0 of 323	Outliers: 0 of 348	Outliers: 1 of 348	Non-Trans: 1 of 345
A 261	ARG	30	-	Favored (34.46%) General / -140.9,140.6	Favored (35.3%) <i>ttt-90</i> chi angles: 202.4,185.9,184.5,280.8	0.02Å	-	-	-
A 262	ASP	27.58	-	Favored (49.43%) General / -114.1,139.3	Favored (27.4%) <i>t70</i> chi angles: 179,78.5	0.02Å	-	-	-
A 263	ASP	33.48	-	Favored (77.67%) General / -63.7,-34.4	Favored (85.3%) <i>m-30</i> chi angles: 283.5,345	0.02Å	-	-	-
A 264	ARG	30	-	Favored (22.39%) General / -81.4,-41.1	Favored (4.2%) <i>ttp80</i> chi angles: 190.5,173.2,102.4,70.5	0.04Å	-	-	-
A 265	LEU	23.83	-	Favored (21.51%) General / -101.9,-8.5	Favored (78.7%) <i>mt</i> chi angles: 300.1,180.5	0.04Å	-	-	-

A 266	GLY 21.77	-	Favored (39.17%) Glycine / 73.6,-147.7	-	-	-	-	-
A 267	PHE 23.94	-	Favored (28.66%) General / -66.9,126.3	Favored (51.2%) <i>m-80</i> chi angles: 287.1,292.4	0.03Å	-	-	-
A 268	LEU 24.63	-	Favored (33.67%) General / -88.2,134.9	Favored (70.1%) <i>mt</i> chi angles: 300.2,182.8	0.04Å	-	-	-
A 269	THR 23.15	-	Favored (40.5%) General / -133.9,159.5	Favored (17.5%) <i>p</i> chi angles: 49.3	0.04Å	-	-	-
A 270	PHE 22.61	0.41Å HD2 with A 225 GLU HG3	Favored (96.39%) General / -64.5,-41.4	Favored (25%) <i>t80</i> chi angles: 163.9,67.4	0.12Å	-	-	-
A 271	CYS 25.73	0.63Å SG with B 1 ARG NE	Favored (20.54%) Pre-Pro / -99.3,136.2	Favored (46.4%) <i>t</i> chi angles: 185.1	0.06Å	-	-	-
A 272	PRO 22.46	-	Favored (44.35%) Trans-Pro / -62.9,-15.0	Favored (10%) <i>Cg_endo</i> chi angles: 15.2,335.6,23.1	0.02Å	-	-	-
A 273	THR 23.59	-	Favored (61.79%) General / -72.3,-18.5	Favored (57.9%) <i>p</i> chi angles: 64.5	0.05Å	-	-	-
A 274	ASN 24.83	-	Favored (19.43%) General / -103.0,19.5	Favored (35.3%) <i>m110</i> chi angles: 294.9,127.9	0.03Å	-	-	-
A 275	LEU 23.62	-	Favored (3.31%) General / -76.8,-175.1	Favored (65.3%) <i>mt</i> chi angles: 287.1,173.1	0.06Å	-	-	-
A 276	GLY 22.37	-	Favored (3.52%) Glycine / 71.4,-111.1	-	-	-	-	-
A 277	THR 22.25	-	Favored (60.75%) General / -74.5,-27.8	Favored (36%) <i>p</i> chi angles: 68.5	0.05Å	-	-	-
A 278	THR 23.74	-	Allowed (1.5%) General / 65.5,0.8	Favored (2.8%) <i>p</i> chi angles: 80.7	0.07Å	-	-	-
A 279	ILE 24.06	-	Favored (33.35%) Ile or Val / -76.8,132.2	Allowed (1.4%) <i>mm</i> chi angles: 295.8,272.2	0.04Å	-	-	-

#	Alt	Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles	Cis Peptides
A 280	ARG	30		0.41Å NH2 with A 324 ASP OD2	Favored (5.93%) General / -128.7,101.0	Favored (46.1%) <i>ttt-90</i> chi angles: 177.6,185.8,194.8,284.3	0.03Å	-	-	-
			Avg: Clashscore:	Outliers: 0 of	Poor rotamers: 2 of	Outliers: 0 of	Outliers: 0 of	Outliers: 1 of	Non-Trans: 1 of	
			34.13	2.93	340	294	323	348	348	345
A 281	ALA	22.44	-		Favored (48.35%) General / -101.6,127.5	-	0.03Å	-	-	-
A 282	SER	24.79	-		Favored (43.03%) General / -149.4,160.9	Favored (75.5%) <i>p</i> chi angles: 71.2	0.03Å	-	-	-
A 283	VAL	27.26	-		Favored (28.51%) Ile or Val / -124.1,147.4	Favored (17.4%) <i>m</i> chi angles: 293.2	0.01Å	-	-	-
A 284	HIS	30	-		Favored (30.32%) General / -92.2,117.9	Favored (54.5%) <i>m170</i> chi angles: 297,171.3	0.06Å	-	-	-
A 285	ILE	29.68	-		Favored (25.52%) Ile or Val / -143.2,142.6	Favored (6.2%) <i>tt</i> chi angles: 190.9,179.2	0.04Å	-	-	-
A 286	ALA	31.69	-		Favored (49.97%) General / -111.1,123.3	-	0.02Å	-	-	-
A 287	LEU	35.22	-		Favored (66.14%) Pre-Pro / -124.9,76.9	Favored (55.8%) <i>mt</i> chi angles: 302.9,171.9	0.05Å	-	-	-
A 288	PRO	37.7	-		Favored (26.3%) Trans-Pro / -56.0,-47.1	Favored (27.3%) <i>Cg_exo</i> chi angles: 340.4,30.5,331.4	0.01Å	-	-	-
A 289	LYS	41.58	-		Favored (28.64%) General / -63.9,-54.8	Favored (2.2%) <i>mttm</i> chi angles: 300.6,212.4,215.9,317.3	0.04Å	-	-	-
A 290	LEU	41.93	-		Favored (69.97%) General / -63.4,-28.4	Favored (11.4%) <i>mt</i> chi angles: 302.9,194.1	0.03Å	-	-	-
A 291	ALA	45.19	C with A 293	0.42Å ASP H	Favored (58.14%) General / -84.9,-9.4	-	0.01Å	-	-	-
A 292	LYS	47.44	-		Allowed (0.11%)	Allowed (0.9%) <i>tttp</i>	0.02Å	-	-	-

#	Alt Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles	Cis Peptides
A 293	ASP 51.65	0.42Å H with A 291 ALA C	-	General / -73.3,18.5 Allowed (0.27%) General / -161.3,65.0	Favored (42.4%) <i>t0</i> chi angles: 190.9,359.6	0.03Å	-	-	-
A 294	LYS 50.31	-	-	Favored (29.09%) General / -52.8,-29.7	Allowed (0.7%) <i>tptt</i> chi angles: 165.5,105.1,140.9,152.5	0.04Å	-	-	-
A 295	LYS 73.29	-	-	Favored (76.94%) General / -66.0,-33.9	Allowed (0.3%) <i>mptt</i> chi angles: 258.9,31.5,186.1,145.3	0.03Å	-	-	-
A 296	GLN 52.52	-	-	Favored (27.39%) General / -83.1,-31.3	Favored (23.4%) <i>tp40</i> chi angles: 206.7,63.3,42.4	0.02Å	-	-	-
A 297	LEU 45.05	-	-	Favored (74.92%) General / -59.2,-50.2	Favored (17.8%) <i>tp</i> chi angles: 172.4,72.2	0.01Å	-	-	-
A 298	GLU 44.64	-	-	Favored (85.02%) General / -61.8,-37.6	OUTLIER (0.3%) chi angles: 277.4,249.3,147.1	0.01Å	-	-	-
A 299	ALA 45.13	0.46Å O with A 303 LYS HG3	-	Favored (95.23%) General / -63.4,-39.7	-	0.02Å	-	-	-
A 300	ILE 44.14	-	-	Favored (32.81%) Ile or Val / -67.4,-53.4	Favored (49.4%) <i>mt</i> chi angles: 290.9,158.2	0.04Å	-	-	-
<p>Avg: Clashscore: 34.13 Clashes: 2.93 Outliers: 0 of 340 Poor rotamers: 2 of 294 Outliers: 0 of 323 Outliers: 0 of 348 Outliers: 1 of 348 Non-Trans: 1 of 345</p>									
A 301	ALA 37.48	-	-	Favored (56.55%) General / -50.5,-46.0	-	0.04Å	-	-	-
A 302	ALA 36.31	-	-	Favored (64.15%) General / -56.7,-31.2	-	0.03Å	-	-	-
A 303	LYS 47.65	0.46Å HG3 with A 299 ALA O	-	Favored (65.59%) General / -72.4,-31.6	Favored (3.9%) <i>mttm</i> chi angles: 316.4,149.9,186.9,281.8	0.03Å	-	-	-
A 304	PHE 33.45	-	-	Favored (16.21%) General / -90.6,13.4	Favored (62.9%) <i>m-80</i> chi angles: 298.9,294.8	0.03Å	-	-	-

A 305	ASN 29.19	-	Favored (5.85%) General / 65.5,37.8	Favored (77.8%) <i>m-40</i> chi angles: 282.1,335.4	0.05Å	-	-	-
A 306	LEU 29.42	-	Favored (25.98%) General / -114.0,155.4	Favored (30.7%) <i>mt</i> chi angles: 298.9,188	0.01Å	-	-	-
A 307	GLN 35.8	-	Favored (53.67%) General / -122.7,131.2	OUTLIER (0.2%) chi angles: 98.8,153.3,63.3	0.04Å	-	OUTLIER(S) worst is CA- CB-CG: 4.1 σ	-
A 308	VAL 35.01	-	Favored (32.51%) Ile or Val / -99.6,136.0	Favored (14.5%) <i>t</i> chi angles: 188.3	0.02Å	-	-	-
A 309	ALA 34.51	-	Favored (3.17%) General / -143.7,-169.8	-	0.03Å	-	-	-
A 310	GLY 42.64	0.73Å O with S 334 HOH O	-	-	-	-	-	-
A 321	GLY 35.67	-	-	-	-	-	-	-
A 322	VAL 34.53	-	Favored (35.82%) Ile or Val / -86.8,120.2	Favored (63.2%) <i>t</i> chi angles: 171.2	0.03Å	-	-	-
A 323	TYR 41.45	-	Favored (17.9%) General / -107.8,157.7	Favored (68.1%) <i>m-80</i> chi angles: 286.8,278	0.02Å	-	-	-
A 324	ASP 30.02	0.41Å OD2 with A 280 ARG NH2	Favored (25.13%) General / -98.4,113.2	Favored (21.6%) <i>t70</i> chi angles: 189,82.7	0.06Å	-	-	-
A 325	ILE 27.22	-	Favored (68.18%) Ile or Val / -111.0,127.3	Favored (6.6%) <i>mt</i> chi angles: 306.5,190.6	0.04Å	-	-	-
A 326	SER 27.34	-	Favored (38.86%) General / -139.4,160.9	Favored (72.4%) <i>p</i> chi angles: 59.3	0.04Å	-	-	-
A 327	ASN 23.44	-	Favored (35.26%) General / -65.7,128.3	Favored (10.2%) <i>p0</i> chi angles: 64.6,287.6	0.01Å	-	-	-
A 328	LYS 33.24	-	Favored (44.58%) General / -78.8,-28.1	Allowed (0.8%) <i>tmtt</i> chi angles: 222.8,285.7,169.5,187	0.01Å	-	-	-
A 329	ARG 30	-	Favored (33.65%) General /	Favored (74.9%) <i>mtp180</i> chi angles:	0.03Å	-	-	-

#	Alt Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles	Cis Peptides
A 330	ARG 30	-	-	Favored (3.94%) General / -116.7,-36.4	Favored (44.1%) <i>mmt-90</i> chi angles: 307.9,273.6,188.4,271.1	0.07Å	-	-	-
		Avg: Clashscore: 34.13	Clashscore: 2.93	Outliers: 0 of 340	Poor rotamers: 2 of 294	Outliers: 0 of 323	Outliers: 0 of 348	Outliers: 1 of 348	Non-Trans: 1 of 345
A 331	MET 24.79	-	-	Favored (33.05%) General / -113.3,150.1	Favored (81%) <i>mtp</i> chi angles: 300.6,184.6,76.1	0.03Å	-	-	-
A 332	GLY 24.01	-	-	Favored (73.68%) Glycine / 90.8,1.2	-	-	-	-	-
A 333	LEU 23.79	-	-	Favored (46.11%) General / -140.7,156.8	Favored (2.1%) <i>pt</i> chi angles: 76.1,175.1	0.01Å	-	-	-
A 334	THR 22.95	-	-	Favored (17.39%) General / -81.5,169.3	Favored (62.5%) <i>p</i> chi angles: 63.6	0.06Å	-	-	-
A 335	GLU 23.85	-	-	Favored (86.47%) General / -58.5,-46.5	Favored (59.9%) <i>mp0</i> chi angles: 290.6,79.7,358.4	0.01Å	-	-	-
A 336	TYR 27.1	-	-	Favored (14.84%) General / -51.6,-56.2	Favored (86.9%) <i>t80</i> chi angles: 180.4,82	0.02Å	-	-	-
A 337	GLN 27.66	-	-	Favored (75.11%) General / -58.5,-37.2	Favored (85%) <i>mt0</i> chi angles: 286.8,165.7,334.7	0.04Å	-	-	-
A 338	ALA 22.17	-	-	Favored (71.1%) General / -64.2,-49.7	-	0.03Å	-	-	-
A 339	VAL 23.16	-	-	Favored (91.11%) Ile or Val / -63.2,-41.0	Favored (70%) <i>t</i> chi angles: 172.1	0.05Å	-	-	-
A 340	LYS 32.17	-	-	Favored (70.52%) General / -65.7,-29.9	Favored (12.3%) <i>tptp</i> chi angles: 175.2,65.7,152.8,46.5	0.03Å	-	-	-
A 341	GLU 30.3	-	-	Favored (70.69%) General / -69.1,-45.3	Allowed (0.7%) <i>tt0</i> chi angles: 230.9,164.9,60.7	0.04Å	-	-	-

A 342	MET 24.33	-	Favored (73.11%) General / -56.4,-49.9	Favored (20.2%) <i>tmm</i> chi angles: 187.9,271.8,282.8	0.03Å	-	-	-
A 343	GLN 28.93	-	Favored (74.29%) General / -57.8,-50.1	Favored (9.9%) <i>tt0</i> chi angles: 168.1,195.5,283.8	0.04Å	-	-	-
A 344	ASP 27.75	-	Favored (87.65%) General / -66.9,-39.7	Favored (87.3%) <i>m-30</i> chi angles: 291.7,350.6	0.04Å	-	-	-
A 345	GLY 25.78	-	Favored (97.97%) Glycine / -62.7,-44.1	-	-	-	-	-
A 346	ILE 24.96	-	Favored (86.6%) Ile or Val / -67.8,-43.2	Favored (24.9%) <i>mm</i> chi angles: 295.1,305.4	0.07Å	-	-	-
A 347	LEU 28.61	-	Favored (70.2%) General / -54.2,-42.9	Favored (73.5%) <i>mt</i> chi angles: 287.4,170.4	0.02Å	-	-	-
A 348	GLU 30.82	-	Favored (75.99%) General / -69.2,-42.4	Favored (79.6%) <i>mm-30</i> chi angles: 291.1,296.8,129.1	0.02Å	-	-	-
A 349	MET 32.34	-	Favored (77.49%) General / -63.9,-34.2	Favored (73.7%) <i>mtp</i> chi angles: 299.1,186.2,66.1	0.04Å	-	-	-
A 350	ILE 26.48	-	Favored (81.85%) Ile or Val / -68.9,-41.0	Favored (29%) <i>mt</i> chi angles: 283.4,169.3	0.06Å	-	-	-

Alt Res High B Clash > 0.4Å Ramachandran Rotamer Cβ deviation Bond lengths Bond angles Cis Peptides

Avg: Clashscore: 34.13 Clashes: 2.93 Outliers: 0 of 340 Poor rotamers: 2 of 294 Outliers: 0 of 323 Outliers: 0 of 348 Outliers: 1 of 348 Non-Trans: 1 of 345

A 351	LYS 27.76	-	Favored (73.53%) General / -54.8,-44.1	Favored (86.5%) <i>mttt</i> chi angles: 288.2,183.3,187.6,171.9	0.03Å	-	-	-
A 352	MET 34.59	-	Favored (84.92%) General / -65.4,-45.2	Favored (85%) <i>mtp</i> chi angles: 295.9,176.1,62.3	0.02Å	-	-	-
A 353	GLU 38.05	-	Favored (98.67%) General / -62.4,-41.4	Favored (43.3%) <i>tp30</i> chi angles: 177.1,74.3,203.4	0.04Å	-	-	-

A 354	GLU 34.72	-	Favored (63.27%) General / -70.1,-24.9	Allowed (0.8%) <i>tp30</i> chi angles: 203,88.6,94.7	0.02Å	-	-	-
A 355	ALA 36.54	-	Favored (27.33%) General / -95.9,-11.0	-	0.01Å	-	-	-
A 356	ALA 39.12	-	Favored (89.43%) Pre-Pro / -73.1,156.4	-	0.01Å	-	-	-
A 357	PRO 42.77	-	-	Favored (40.7%) <i>Cg_endo</i> chi angles: 23.5,327,28.5	0.02Å	-	-	-
B 1	ARG 29.32	0.63Å NE with A 271 CYS SG	-	Favored (2.5%) <i>ptp-110</i> chi angles: 87.2,189.6,51.1,230.9	0.05Å	-	-	-
D 3	NA 38.65	-	-	-	-	-	-	-
D 5	NA 48.85	-	-	-	-	-	-	-
S 1	HOH 23.41	-	-	-	-	-	-	-
S 2	HOH 23.54	-	-	-	-	-	-	-
S 3	HOH 27.26	-	-	-	-	-	-	-
S 4	HOH 26.02	-	-	-	-	-	-	-
S 5	HOH 25.17	-	-	-	-	-	-	-
S 6	HOH 23.45	-	-	-	-	-	-	-
S 7	HOH 19.68	-	-	-	-	-	-	-
S 8	HOH 22.08	-	-	-	-	-	-	-
S 9	HOH 25.07	-	-	-	-	-	-	-
S 10	HOH 20.82	-	-	-	-	-	-	-

Alt Res High B Clash > 0.4Å Ramachandran Rotamer Cβ deviation Bond lengths Bond angles Cis Peptides

Avg: Clashscore: 34.13 Outliers: 0 of 340 Poor rotamers: 2 of 294 Outliers: 0 of 323 Outliers: 0 of 348 Outliers: 1 of 348 Non-Trans: 1 of 345

S 11	HOH 22.54	-	-	-	-	-	-	-
S 12	HOH 30.7	-	-	-	-	-	-	-
S 13	HOH 27.36	-	-	-	-	-	-	-
S 14	HOH 23.39	-	-	-	-	-	-	-
S 15	HOH 27.81	-	-	-	-	-	-	-

S	16	HOH	30.4	-	-	-	-	-	-	-
S	17	HOH	28.57	-	-	-	-	-	-	-
S	18	HOH	25.55	-	-	-	-	-	-	-
S	19	HOH	25.28	-	-	-	-	-	-	-
S	20	HOH	28.12	-	-	-	-	-	-	-
S	21	HOH	23.54	-	-	-	-	-	-	-
S	22	HOH	25.01	-	-	-	-	-	-	-
S	23	HOH	30.2	-	-	-	-	-	-	-
S	24	HOH	33.57	-	-	-	-	-	-	-
S	25	HOH	28.38	-	-	-	-	-	-	-
S	26	HOH	26.31	-	-	-	-	-	-	-
S	27	HOH	21.41	-	-	-	-	-	-	-
S	28	HOH	25.99	-	-	-	-	-	-	-
S	29	HOH	30.37	-	-	-	-	-	-	-
S	30	HOH	31.76	-	-	-	-	-	-	-

Alt Res High B Clash > 0.4Å Ramachandran Rotamer Cβ deviation Bond lengths Bond angles Cis Peptides

Avg: Clashscore: 34.13 Outliers: 0 of 340 Poor rotamers: 2 of 294 Outliers: 0 of 323 Outliers: 0 of 348 Outliers: 1 of 348 Non-Trans: 1 of 345

S	31	HOH	26.43	-	-	-	-	-	-	-
S	32	HOH	29.23	-	-	-	-	-	-	-
S	33	HOH	25.06	-	-	-	-	-	-	-
S	34	HOH	24.84	-	-	-	-	-	-	-
S	35	HOH	17.91	-	-	-	-	-	-	-
S	36	HOH	30.8	-	-	-	-	-	-	-

S										
37	HOH	27.29	-	-	-	-	-	-	-	-
S										
38	HOH	31.24	-	-	-	-	-	-	-	-
S										
39	HOH	32.03	-	-	-	-	-	-	-	-
S										
40	HOH	30.51	-	-	-	-	-	-	-	-
S										
41	HOH	29.88	-	-	-	-	-	-	-	-
S										
42	HOH	28.83	-	-	-	-	-	-	-	-
S										
43	HOH	24.48	-	-	-	-	-	-	-	-
S										
44	HOH	25.96	-	-	-	-	-	-	-	-
S										
45	HOH	25.14	-	-	-	-	-	-	-	-
S										
46	HOH	26.79	-	-	-	-	-	-	-	-
S										
47	HOH	29.46	-	-	-	-	-	-	-	-
S										
48	HOH	27.52	-	-	-	-	-	-	-	-
S										
49	HOH	24.04	-	-	-	-	-	-	-	-
S										
50	HOH	23.26	-	-	-	-	-	-	-	-

**Alt** **Res** **High** **Clash >** **Ramachandran** **Rotamer** **Cβ** **Bond** **Bond angles** **Cis**
B **0.4Å**

Avg: Clashscore: 34.13 Outliers: 0 of 340 Poor rotamers: 2 of 294 Outliers: 0 of 323 Outliers: 0 of 348 Outliers: 1 of 348 Non-Trans: 1 of 345

S										
51	HOH	28.19	-	-	-	-	-	-	-	-
S										
52	HOH	27	-	-	-	-	-	-	-	-
S										
53	HOH	27.17	-	-	-	-	-	-	-	-
S										
54	HOH	28.85	-	-	-	-	-	-	-	-
S										
55	HOH	36.58	-	-	-	-	-	-	-	-
S										
56	HOH	27.48	-	-	-	-	-	-	-	-
S										
57	HOH	23.42	-	-	-	-	-	-	-	-

S	HOH	26	-	-	-	-	-	-	-
58									
S	HOH	32.04	-	-	-	-	-	-	-
59									
S	HOH	21.63	-	-	-	-	-	-	-
60									
S	HOH	25.84	-	-	-	-	-	-	-
61									
S	HOH	29.82	-	-	-	-	-	-	-
62									
S	HOH	32.54	-	-	-	-	-	-	-
63									
S	HOH	25.69	-	-	-	-	-	-	-
64									
S	HOH	26.91	-	-	-	-	-	-	-
65									
S	HOH	29.26	-	-	-	-	-	-	-
66									
S	HOH	27.33	-	-	-	-	-	-	-
67									
S	HOH	33.39	-	-	-	-	-	-	-
68									
S	HOH	27.24	-	-	-	-	-	-	-
69									
S	HOH	33.31	-	-	-	-	-	-	-
70									

#	Alt	Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles	Cis Peptides
			Avg: Clashscore:	Outliers: 0 of	Poor rotamers: 2 of	Outliers: 0 of	Outliers: 0 of	Outliers: 1 of	Non-Trans: 1 of 345	
			34.13	340	294	323	348	348		

S	HOH	28.41	-	-	-	-	-	-	-
71									
S	HOH	28.55	-	-	-	-	-	-	-
72									
S	HOH	34.31	-	-	-	-	-	-	-
73									
S	HOH	27.01	-	-	-	-	-	-	-
74									
S	HOH	29.95	-	-	-	-	-	-	-
75									
S	HOH	37.28	-	-	-	-	-	-	-
76									
S	HOH	30.25	-	-	-	-	-	-	-
77									
S	HOH	29.02	-	-	-	-	-	-	-
78									

0.64Å
O with A 147
GLU OE1

S										
79	HOH	32.72	-	-	-	-	-	-	-	-
S										
80	HOH	29.66	-	-	-	-	-	-	-	-
S										
81	HOH	31.1	-	-	-	-	-	-	-	-
S										
82	HOH	32.14	-	-	-	-	-	-	-	-
S										
83	HOH	32.03	-	-	-	-	-	-	-	-
S										
84	HOH	27.41	-	-	-	-	-	-	-	-
S										
85	HOH	27.77	-	-	-	-	-	-	-	-
S										
86	HOH	23.9	-	-	-	-	-	-	-	-
S										
87	HOH	30.08	-	-	-	-	-	-	-	-
S										
88	HOH	30.39	-	-	-	-	-	-	-	-
S										
89	HOH	32.92	-	-	-	-	-	-	-	-
S										
90	HOH	30.04	-	-	-	-	-	-	-	-

Alt Res High B Clash > 0.4Å Ramachandran Rotamer Cβ deviation Bond lengths Bond angles Cis Peptides

Avg: Clashscore: 34.13 Outliers: 0 of 340 Poor rotamers: 2 of 294 Outliers: 0 of 323 Outliers: 0 of 348 Outliers: 1 of 348 Non-Trans: 1 of 345

S										
91	HOH	32.99	-	-	-	-	-	-	-	-
S										
92	HOH	35.07	-	-	-	-	-	-	-	-
S										
93	HOH	33.02	-	-	-	-	-	-	-	-
S										
94	HOH	24.03	-	-	-	-	-	-	-	-
S										
95	HOH	29.91	-	-	-	-	-	-	-	-
S										
96	HOH	26.01	-	-	-	-	-	-	-	-
S										
97	HOH	36.55	-	-	-	-	-	-	-	-
S										
98	HOH	30.99	-	-	-	-	-	-	-	-
S										
99	HOH	28.07	-	-	-	-	-	-	-	-

S	HOH 26.96	-	-	-	-	-	-	-	-
100									
S	HOH 33.91	-	-	-	-	-	-	-	-
101									
S	HOH 35.07	-	-	-	-	-	-	-	-
102									
S	HOH 36.17	-	-	-	-	-	-	-	-
103									
S	HOH 29.11	-	-	-	-	-	-	-	-
104									
S	HOH 32.7	-	-	-	-	-	-	-	-
105									
S	HOH 22.9	-	-	-	-	-	-	-	-
106									
S	HOH 31.01	-	-	-	-	-	-	-	-
107									
S	HOH 38.95	-	-	-	-	-	-	-	-
108									
S	HOH 38.32	-	-	-	-	-	-	-	-
109									
S	HOH 38.34	-	-	-	-	-	-	-	-
110									

**Alt Res** **High B** **Clash > 0.4Å** **Ramachandran** **Rotamer** **Cβ deviation** **Bond lengths** **Bond angles** **Cis Peptides**

Avg: Clashscore: 34.13 Outliers: 0 of 340 Poor rotamers: 2 of 294 Outliers: 0 of 323 Outliers: 0 of 348 Outliers: 1 of 348 Non-Trans: 1 of 345

S	HOH 31.17	-	-	-	-	-	-	-	-
111									
S	HOH 24.21	-	-	-	-	-	-	-	-
112									
S	HOH 35.38	-	-	-	-	-	-	-	-
113									
S	HOH 31.08	-	-	-	-	-	-	-	-
114									
S	HOH 27.97	-	-	-	-	-	-	-	-
115									
S	HOH 28.31	-	-	-	-	-	-	-	-
116									
S	HOH 25.92	-	-	-	-	-	-	-	-
117									
S	HOH 35.67	-	-	-	-	-	-	-	-
118									
S	HOH 27.95	-	-	-	-	-	-	-	-
119									
S	HOH 38.91	-	-	-	-	-	-	-	-
120									

S	121	HOH	37.34	-	-	-	-	-	-	-
S	122	HOH	32.65	-	-	-	-	-	-	-
S	123	HOH	36.27	-	-	-	-	-	-	-
S	124	HOH	47.54	-	-	-	-	-	-	-
S	125	HOH	35.54	-	-	-	-	-	-	-
S	126	HOH	31.37	-	-	-	-	-	-	-
S	127	HOH	32.59	-	-	-	-	-	-	-
S	128	HOH	25.42	-	-	-	-	-	-	-
S	129	HOH	40.11	-	-	-	-	-	-	-
S	130	HOH	27.11	-	-	-	-	-	-	-

**Alt** **Res** **High B** **Clash > 0.4Å** **Ramachandran** **Rotamer** **Cβ deviation** **Bond lengths** **Bond angles** **Cis Peptides**

Avg: Clashscore: 34.13 Outliers: 0 of 340 Poor rotamers: 2 of 294 Outliers: 0 of 323 Outliers: 0 of 348 Outliers: 1 of 348 Non-Trans: 1 of 345

S	131	HOH	33.95	-	-	-	-	-	-	-
S	132	HOH	28.57	-	-	-	-	-	-	-
S	133	HOH	47.03	-	-	-	-	-	-	-
S	134	HOH	31.47	-	-	-	-	-	-	-
S	135	HOH	32.21	-	-	-	-	-	-	-
S	136	HOH	29.37	-	-	-	-	-	-	-
S	137	HOH	31.43	-	-	-	-	-	-	-
S	138	HOH	35.44	-	-	-	-	-	-	-
S	139	HOH	24.94	-	-	-	-	-	-	-
S	140	HOH	34.87	-	-	-	-	-	-	-
S	141	HOH	34.4	-	-	-	-	-	-	-

S	HOH	33.6	-	-	-	-	-	-	-
142									
S	HOH	23.72	-	-	-	-	-	-	-
143									
S	HOH	39.85	-	-	-	-	-	-	-
144									
S	HOH	37.96	-	-	-	-	-	-	-
145									
S	HOH	31.37	-	-	-	-	-	-	-
146									
S	HOH	37.17	-	-	-	-	-	-	-
147									
S	HOH	26.28	-	-	-	-	-	-	-
148									
S	HOH	37.92	-	-	-	-	-	-	-
149									
S	HOH	33.88	-	-	-	-	-	-	-
150									

#	<u>Alt</u>	<u>Res</u>	<u>High</u> <u>B</u>	<u>Clash ></u> <u>0.4Å</u>	<u>Ramachandran</u>	<u>Rotamer</u>	<u>Cβ</u> <u>deviation</u>	<u>Bond</u> <u>lengths</u>	<u>Bond angles</u>	<u>Cis</u> <u>Peptides</u>
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			Avg: Clashscore:	Outliers: 0 of	Poor rotamers: 2 of	Outliers: 0 of 323	Outliers: 0 of 348	Outliers: 1 of 348	Non-Trans: 1 of 345
			34.13	340	294				

S	HOH	27.31	-	-	-	-	-	-	-
151									
S	HOH	34.95	-	-	-	-	-	-	-
152									
S	HOH	48.92	-	-	-	-	-	-	-
153									
S	HOH	28.55	-	-	-	-	-	-	-
154									
S	HOH	35.85	-	-	-	-	-	-	-
155									
S	HOH	37.35	-	-	-	-	-	-	-
156									
S	HOH	22.01	-	-	-	-	-	-	-
157									
S	HOH	38.28	-	-	-	-	-	-	-
158									
S	HOH	29.06	-	-	-	-	-	-	-
159									
S	HOH	31.8	-	-	-	-	-	-	-
160									
S	HOH	31.74	-	-	-	-	-	-	-
161									
S	HOH	34.27	-	-	-	-	-	-	-
162									

S										
163	HOH	36.35	-	-	-	-	-	-	-	-
S										
164	HOH	30.88	-	-	-	-	-	-	-	-
S										
165	HOH	33.09	-	-	-	-	-	-	-	-
S										
166	HOH	30.64	-	-	-	-	-	-	-	-
S										
167	HOH	51.47	-	-	-	-	-	-	-	-
S										
168	HOH	35.98	-	-	-	-	-	-	-	-
S										
169	HOH	39.07	-	-	-	-	-	-	-	-
S										
170	HOH	52.01	-	-	-	-	-	-	-	-

#	<u>Alt</u>	<u>Res</u>	<u>High</u> <u>B</u>	<u>Clash ></u> <u>0.4Å</u>	<u>Ramachandran</u>	<u>Rotamer</u>	<u>Cβ</u> <u>deviation</u>	<u>Bond</u> <u>lengths</u>	<u>Bond angles</u>	<u>Cis</u> <u>Peptides</u>
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			Avg: Clashscore:	Outliers: 0 of	Poor rotamers: 2 of	Outliers: 0 of 323	Outliers: 0 of 348	Outliers: 1 of 348	Non-Trans: 1 of 345
			34.13	340	294				

S										
171	HOH	26.97	-	-	-	-	-	-	-	-
S										
172	HOH	40.49	-	-	-	-	-	-	-	-
S										
173	HOH	38.27	-	-	-	-	-	-	-	-
S										
174	HOH	38.47	-	-	-	-	-	-	-	-
S										
175	HOH	49.04	-	-	-	-	-	-	-	-
S										
176	HOH	45.91	-	-	-	-	-	-	-	-
S										
177	HOH	33.34	-	-	-	-	-	-	-	-
S										
178	HOH	30.88	-	-	-	-	-	-	-	-
S										
179	HOH	33.5	-	-	-	-	-	-	-	-
S										
180	HOH	35.1	-	-	-	-	-	-	-	-
S										
181	HOH	31.59	-	-	-	-	-	-	-	-
S										
182	HOH	43.12	-	-	-	-	-	-	-	-
S										
183	HOH	45.14	-	-	-	-	-	-	-	-

S										
184	HOH	35.07	-	-	-	-	-	-	-	-
S										
185	HOH	40.72	-	-	-	-	-	-	-	-
S										
186	HOH	41.63	-	-	-	-	-	-	-	-
S										
187	HOH	42.6	-	-	-	-	-	-	-	-
S										
188	HOH	49.56	-	-	-	-	-	-	-	-
S										
189	HOH	46.35	-	-	-	-	-	-	-	-
S										
190	HOH	30.12	-	-	-	-	-	-	-	-
#	Alt	Res	High	Clash >	Ramachandran	Rotamer	Cβ	Bond	Bond angles	Cis
			B	0.4Å			deviation	lengths		Peptides
			Avg: Clashscore:	Outliers: 0 of	Poor rotamers: 2 of	Outliers: 0 of 323	Outliers: 0 of 348	Outliers: 1 of 348	Non-Trans: 1 of 345	
			34.13	2.93	340	294				
S										
191	HOH	34.72	-	-	-	-	-	-	-	-
S										
192	HOH	37.77	-	-	-	-	-	-	-	-
S										
193	HOH	41.16	-	-	-	-	-	-	-	-
S										
194	HOH	39.97	-	-	-	-	-	-	-	-
S										
195	HOH	41.94	-	-	-	-	-	-	-	-
S										
196	HOH	39.03	-	-	-	-	-	-	-	-
S										
197	HOH	51.01	-	-	-	-	-	-	-	-
S										
198	HOH	49.96	-	-	-	-	-	-	-	-
S										
199	HOH	33.98	-	-	-	-	-	-	-	-
S										
200	HOH	38.64	-	-	-	-	-	-	-	-
S										
201	HOH	37.79	-	-	-	-	-	-	-	-
S										
202	HOH	51.04	-	-	-	-	-	-	-	-
S										
203	HOH	45.05	-	-	-	-	-	-	-	-
S										
204	HOH	47.8	-	-	-	-	-	-	-	-

S	HOH	33.44	-	-	-	-	-	-	-
205									
S	HOH	33.71	-	-	-	-	-	-	-
206									
S	HOH	49.62	-	-	-	-	-	-	-
207									
S	HOH	43.7	-	-	-	-	-	-	-
208									
S	HOH	43.78	-	-	-	-	-	-	-
209									
S	HOH	49.24	-	-	-	-	-	-	-
210									

#	Alt	Res	<u>High</u> <u>B</u>	<u>Clash ></u> <u>0.4Å</u>	<u>Ramachandran</u>	<u>Rotamer</u>	<u>Cβ</u> <u>deviation</u>	<u>Bond</u> <u>lengths</u>	<u>Bond angles</u>	<u>Cis</u> <u>Peptides</u>
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Avg: Clashscore:	Outliers: 0 of	Poor rotamers: 2 of	Outliers:	Outliers:	Outliers: 1 of	Non- Trans: 1
34.13	340	294	0 of 323	0 of 348	348	of 345

S	HOH	50.3	-	-	-	-	-	-	-
211									
S	HOH	44.22	-	-	-	-	-	-	-
212									
S	HOH	46.01	0.67Å O with A 132 LYS NZ	-	-	-	-	-	-
213									
S	HOH	37.38	-	-	-	-	-	-	-
214									
S	HOH	36.44	-	-	-	-	-	-	-
215									
S	HOH	43.41	-	-	-	-	-	-	-
216									
S	HOH	39.5	-	-	-	-	-	-	-
217									
S	HOH	55.22	-	-	-	-	-	-	-
218									
S	HOH	27.22	-	-	-	-	-	-	-
219									
S	HOH	30.68	-	-	-	-	-	-	-
220									
S	HOH	49.24	-	-	-	-	-	-	-
221									
S	HOH	53.87	-	-	-	-	-	-	-
222									
S	HOH	43.36	-	-	-	-	-	-	-
223									
S	HOH	51.51	-	-	-	-	-	-	-
224									
S	HOH	41.35	-	-	-	-	-	-	-
225									

S												
226	HOH	30.88	-	-	-	-	-	-	-	-	-	-
S												
227	HOH	45.5	-	-	-	-	-	-	-	-	-	-
S												
228	HOH	49.58	-	-	-	-	-	-	-	-	-	-
S												
229	HOH	37.84	-	-	-	-	-	-	-	-	-	-
S												
230	HOH	37.74	-	-	-	-	-	-	-	-	-	-
#	Alt Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles	Cis Peptides			
Avg: Clashscore:			Outliers: 0 of	Poor rotamers: 2 of	Outliers: 0 of	Outliers: 0 of	Outliers: 0 of	Outliers: 1 of	Non-Trans: 1			
34.13			340	294	0 of 323	0 of 348	348	of 345				
S												
231	HOH	46.62	-	-	-	-	-	-	-	-	-	-
S												
232	HOH	46.52	-	-	-	-	-	-	-	-	-	-
S												
233	HOH	41.89	-	-	-	-	-	-	-	-	-	-
S												
234	HOH	45.05	-	-	-	-	-	-	-	-	-	-
S												
235	HOH	42.62	-	-	-	-	-	-	-	-	-	-
S												
236	HOH	48.18	-	-	-	-	-	-	-	-	-	-
S												
237	HOH	38.77	0.72Å O with A 162 GLU OE1	-	-	-	-	-	-	-	-	-
S												
238	HOH	53.71	-	-	-	-	-	-	-	-	-	-
S												
239	HOH	44.46	-	-	-	-	-	-	-	-	-	-
S												
240	HOH	48.85	-	-	-	-	-	-	-	-	-	-
S												
241	HOH	40.03	-	-	-	-	-	-	-	-	-	-
S												
242	HOH	38.87	-	-	-	-	-	-	-	-	-	-
S												
243	HOH	40.68	-	-	-	-	-	-	-	-	-	-
S												
244	HOH	58.94	-	-	-	-	-	-	-	-	-	-
S												
245	HOH	46.87	-	-	-	-	-	-	-	-	-	-
S												
246	HOH	49.76	-	-	-	-	-	-	-	-	-	-

S	HOH	48.41	-	-	-	-	-	-	-	-
247										
S	HOH	42.06	-	-	-	-	-	-	-	-
248										
S	HOH	31.2	-	-	-	-	-	-	-	-
249										
S	HOH	39.91	-	-	-	-	-	-	-	-
250										
#	Alt Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles	Cis Peptides	
			Avg: Clashscore: 34.13	Outliers: 0 of 340	Poor rotamers: 2 of 294	Outliers: 0 of 323	Outliers: 0 of 348	Outliers: 1 of 348	Non-Trans: 1 of 345	
S	HOH	47.73	0.47Å O with A 1 ALA N	-	-	-	-	-	-	-
251										
S	HOH	52.67	-	-	-	-	-	-	-	-
252										
S	HOH	43.01	-	-	-	-	-	-	-	-
253										
S	HOH	49.13	-	-	-	-	-	-	-	-
254										
S	HOH	53.62	-	-	-	-	-	-	-	-
255										
S	HOH	33.34	-	-	-	-	-	-	-	-
256										
S	HOH	45.97	-	-	-	-	-	-	-	-
257										
S	HOH	48.12	-	-	-	-	-	-	-	-
258										
S	HOH	41.11	-	-	-	-	-	-	-	-
259										
S	HOH	42.95	-	-	-	-	-	-	-	-
260										
S	HOH	46.83	-	-	-	-	-	-	-	-
261										
S	HOH	32.81	-	-	-	-	-	-	-	-
262										
S	HOH	43.66	-	-	-	-	-	-	-	-
263										
S	HOH	46.28	-	-	-	-	-	-	-	-
264										
S	HOH	24.79	-	-	-	-	-	-	-	-
265										
S	HOH	44.96	-	-	-	-	-	-	-	-
266										
S	HOH	51.72	-	-	-	-	-	-	-	-
267										

S												
268		HOH 47.41	-	-	-	-	-	-	-	-	-	-
S												
269		HOH 44.83	-	-	-	-	-	-	-	-	-	-
S												
270		HOH 33.25	-	-	-	-	-	-	-	-	-	-
#	Alt	Res	High	Clash >	Ramachandran	Rotamer	Cβ	Bond	Bond angles	Cis		
			B	0.4Å			deviation	lengths		Peptides		
			Avg: Clashscore:	Outliers: 0 of	Poor rotamers: 2 of	Outliers: 0 of	Outliers: 0 of	Outliers: 0 of	Outliers: 1 of	Non-		
			34.13	340	294	0 of 323	0 of 348	0 of 348	348	Trans: 1		
										of 345		
S												
271		HOH 35.34	-	-	-	-	-	-	-	-	-	-
S												
272		HOH 52.47	-	-	-	-	-	-	-	-	-	-
S												
273		HOH 42.62	-	-	-	-	-	-	-	-	-	-
S												
274		HOH 46.72	-	-	-	-	-	-	-	-	-	-
S												
275		HOH 45.46	-	-	-	-	-	-	-	-	-	-
S												
276		HOH 39.97	-	-	-	-	-	-	-	-	-	-
S												
277		HOH 60.45	-	-	-	-	-	-	-	-	-	-
S												
278		HOH 54.7	-	-	-	-	-	-	-	-	-	-
S												
279		HOH 48.2	-	-	-	-	-	-	-	-	-	-
S												
280		HOH 55.15	-	-	-	-	-	-	-	-	-	-
S												
281		HOH 49.64	-	-	-	-	-	-	-	-	-	-
S												
282		HOH 49.24	-	-	-	-	-	-	-	-	-	-
S												
283		HOH 58.09	-	-	-	-	-	-	-	-	-	-
S												
284		HOH 50.01	-	-	-	-	-	-	-	-	-	-
S												
285		HOH 39.72	-	-	-	-	-	-	-	-	-	-
S												
286		HOH 38.76	-	-	-	-	-	-	-	-	-	-
S												
287		HOH 35.23	-	-	-	-	-	-	-	-	-	-
S												
288		HOH 38.55	-	-	-	-	-	-	-	-	-	-

#	Alt Res	<u>High B</u>	<u>Clash > 0.4Å</u>	<u>Ramachandran</u>	<u>Rotamer</u>	<u>Cβ deviation</u>	<u>Bond lengths</u>	<u>Bond angles</u>	<u>Cis Peptides</u>
S 289	HOH 50	-	-	-	-	-	-	-	-
S 290	HOH 45.97	-	-	-	-	-	-	-	-
		Avg: Clashscore:	Outliers: 0 of	Poor rotamers: 2 of	Outliers: 0 of	Outliers: 0 of	Outliers: 1 of	Non-Trans: 1 of	
		34.13	340	294	323	348	348	345	
S 291	HOH 48.69	-	-	-	-	-	-	-	-
S 292	HOH 52.11	-	-	-	-	-	-	-	-
S 293	HOH 44.85	-	-	-	-	-	-	-	-
S 294	HOH 45.8	-	-	-	-	-	-	-	-
S 295	HOH 41.12	-	-	-	-	-	-	-	-
S 296	HOH 35.27	-	-	-	-	-	-	-	-
S 297	HOH 46.71	-	-	-	-	-	-	-	-
S 298	HOH 36.49	-	-	-	-	-	-	-	-
S 299	HOH 44.13	-	-	-	-	-	-	-	-
S 300	HOH 39.32	-	-	-	-	-	-	-	-
S 301	HOH 57.19	-	-	-	-	-	-	-	-
S 302	HOH 52.23	-	-	-	-	-	-	-	-
S 303	HOH 43.31	-	-	-	-	-	-	-	-
S 304	HOH 54.17	-	-	-	-	-	-	-	-
S 305	HOH 44.2	-	-	-	-	-	-	-	-
S 306	HOH 48.59	-	-	-	-	-	-	-	-
S 307	HOH 53.15	-	-	-	-	-	-	-	-
S 308	HOH 36.2	-	-	-	-	-	-	-	-
S 309	HOH 41.84	-	-	-	-	-	-	-	-

<u>#</u>	<u>Alt Res</u>	<u>High B</u>	<u>Clash > 0.4Å</u>	<u>Ramachandran</u>	<u>Rotamer</u>	<u>Cβ deviation</u>	<u>Bond lengths</u>	<u>Bond angles</u>	<u>Cis Peptides</u>
S 310	HOH 51.07	-	-	-	-	-	-	-	-
		Avg: Clashscore:	Outliers: 0 of	Poor rotamers: 2 of	Outliers: 0 of	Outliers: 0 of	Outliers: 1 of	Non-Trans: 1 of 345	
		34.13	2.93	340	294	323	348	348	
S 311	HOH 54.41	-	-	-	-	-	-	-	-
S 312	HOH 59.45	-	-	-	-	-	-	-	-
S 313	HOH 74.24	-	-	-	-	-	-	-	-
S 314	HOH 54.57	-	-	-	-	-	-	-	-
S 315	HOH 50.96	-	-	-	-	-	-	-	-
S 316	HOH 43.59	-	-	-	-	-	-	-	-
S 317	HOH 47.83	-	-	-	-	-	-	-	-
S 318	HOH 64.92	-	-	-	-	-	-	-	-
S 319	HOH 52.51	-	-	-	-	-	-	-	-
S 320	HOH 33.38	-	-	-	-	-	-	-	-
S 321	HOH 42.54	-	-	-	-	-	-	-	-
S 322	HOH 49.21	-	-	-	-	-	-	-	-
S 324	HOH 53.69	-	-	-	-	-	-	-	-
S 325	HOH 57.61	-	-	-	-	-	-	-	-
S 326	HOH 47.38	-	-	-	-	-	-	-	-
S 327	HOH 61.96	-	-	-	-	-	-	-	-
S 328	HOH 53.77	-	-	-	-	-	-	-	-
S 329	HOH 54.33	-	-	-	-	-	-	-	-
S 330	HOH 58.56	-	-	-	-	-	-	-	-
S 331	HOH 66.5	-	-	-	-	-	-	-	-

#	Alt Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles	Cis Peptides
		Avg: 34.13	Clashscore: 2.93	Outliers: 0 of 340	Poor rotamers: 2 of 294	Outliers: 0 of 323	Outliers: 0 of 348	Outliers: 1 of 348	Non-Trans: 1 of 345
S 332	HOH	56.58	-	-	-	-	-	-	-
S 333	HOH	58.82	-	-	-	-	-	-	-
S 334	HOH	51.01	0.73Å O with A 310 GLY O	-	-	-	-	-	-
S 335	HOH	70.34	-	-	-	-	-	-	-
S 336	HOH	54.01	-	-	-	-	-	-	-
S 337	HOH	56.09	-	-	-	-	-	-	-
S 338	HOH	49.21	-	-	-	-	-	-	-
S 339	HOH	61.24	-	-	-	-	-	-	-
S 340	HOH	59.04	-	-	-	-	-	-	-
S 341	HOH	68.85	-	-	-	-	-	-	-

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