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All-Atom Contacts	Clashscore, all atoms:	0	100 th percentile* (N=1784, all resolutions)	
	Clashscore is the number of serious steric overlaps (> 0.4 Å) per 1000 atoms.			
Protein Geometry	Poor rotamers	2	2.20%	Goal: <1%
	Ramachandran outliers	6	5.77%	Goal: <0.05%
	Ramachandran favored	86	82.69%	Goal: >98%
	MolProbity score [^]	1.46		96 th percentile* (N=27675, 0Å - 99Å)
	Cβ deviations >0.25Å	0	0.00%	Goal: 0
	Bad backbone bonds:	0 / 815	0.00%	Goal: 0%
	Bad backbone angles:	13 / 1106	1.18%	Goal: <0.1%

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	C β deviation	Bond lengths	Bond angles
		Avg: 55.19	Clashscore: 0	Outliers: 6 of 104	Poor rotamers: 2 of 91	Outliers: 0 of 95	Outliers: 0 of 106	Outliers: 13 of 106
A1145	SER	50	-	-	43.7% (t) chi angles: 180.9	0.079Å	-	-
A1146	ASN	50	-	Favored (93.83%) Pre-proline / -67.2,136.9	52.3% (t-20) chi angles: 192.9,350	0.089Å	-	-
A1147	PRO	50	-	Favored (10.34%) Trans-proline / -82.8,-11.1	64.4% (Cg_endo) chi angles: 34.1	0.05Å	-	-
A1148	CYS	50	-	Favored (17.88%) General / -92.9,155.0	3.7% (m) chi angles: 320.9	0.081Å	-	-

A1149	LEU	50	-	Favored (6.18%) General / -112.3,173.8	50.1% (<i>mt</i>) chi angles: 306.9,183.4	0.042Å	-	-
A1150	HIS	50	-	Favored (11.34%) General / 56.9,26.2	71.5% (<i>m80</i>) chi angles: 300.2,93.9	0.097Å	-	-
A1151	GLY	50	-	Favored (83.22%) Glycine / 83.8,9.2	-	-	-	-
A1152	GLY	50	-	Favored (36.97%) Glycine / -58.9,149.8	-	-	-	-
A1153	ASN	50	-	Favored (36.91%) General / -78.9,134.4	65.6% (<i>t30</i>) chi angles: 190.6,31.2	0.098Å	-	-
A1154	CYS	50	-	Favored (28.46%) General / -93.7,116.0	41.3% (<i>t</i>) chi angles: 177.8	0.043Å	-	-
A1155	GLU	50	-	Favored (3.44%) General / -142.8,99.3	21.4% (<i>tt0</i>) chi angles: 202.9,181,267.1	0.234Å	-	OUTLIER(S) worst is N-CA- CB: 4.195 σ
A1156	ASP	50	-	Favored (4.91%) General / -108.1,177.1	2.6% (<i>t0</i>) chi angles: 214.6,315.7	0.135Å	-	OUTLIER(S) worst is C-N- CA: 6.603 σ
A1157	ILE	50	-	OUTLIER (0.01%) Isoleucine or valine / -149.7,-131.6	12% (<i>pt</i>) chi angles: 46.6,175.6	0.189Å	-	-
A1158	TYR	50	-	Favored (7.39%) General / -86.5,84.6	70% (<i>t80</i>) chi angles: 185,84.1	0.052Å	-	-
A1159	SER	50	-	Favored (22.18%) General / 58.1,42.6	30% (<i>t</i>) chi angles: 184.9	0.084Å	-	-
A1160	SER	50	-	Allowed (0.86%) General / -151.8,62.9	7.7% (<i>t</i>) chi angles: 195.9	0.058Å	-	-
A1161	TYR	50	-	Favored (14.55%)	28.7% (<i>p90</i>)	0.062Å	-	-

				General / -52.6,124.8	chi angles: 68.4,102.4			
A1162	HIS	50	-	Favored (17.57%) General / -101.4,156.2	1.2% (<i>p80</i>) chi angles: 28.7,103.4	0.1Å	-	OUTLIER(S) worst is CA- CB-CG: 5.281 σ
A1163	CYS	50	-	Favored (15.82%) General / -132.5,115.7	61.2% (<i>m</i>) chi angles: 303.8	0.072Å	-	-
A1164	SER	50	-	Favored (12.73%) General / -90.8,99.8	59.2% (<i>m</i>) chi angles: 299.3	0.095Å	-	-
#	Alt Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
		Avg: 55.19	Clashscore: 0	Outliers: 6 of 104	Poor rotamers: 2 of 91	Outliers: 0 of 95	Outliers: 0 of 106	Outliers: 13 of 106
A1165	CYS	50	-	Favored (89.15%) Pre-proline / -63.6,126.2	76.2% (<i>m</i>) chi angles: 298.9	0.052Å	-	-
A1166	PRO	50	-	Favored (4.44%) Trans-proline / -90.5,158.0	27.8% (<i>Cg_endo</i>) chi angles: 37.6	0.052Å	-	-
A1167	LEU	99.99	-	Favored (8.12%) General / -47.8,138.9	45.5% (<i>mt</i>) chi angles: 306.2,185	0.048Å	-	-
A1168	GLY	50	-	Favored (56.51%) Glycine / 93.8,-18.5	-	-	-	-
A1169	TRP	99.99	-	Favored (50.17%) General / -129.5,151.4	13.4% (<i>m95</i>) chi angles: 316.6,90.2	0.049Å	-	OUTLIER(S) worst is CE3- CD2-CG: 4.98 σ
A1170	SER	50	-	Allowed (1.21%) General / -145.5,-160.9	10% (<i>t</i>) chi angles: 192.3	0.132Å	-	-
A1171	GLY	50	-	Favored (45.63%) Glycine / 85.6,-171.6	-	-	-	-
				Favored				

A1172	LYS	50	-	(47.3%) General / -78.8,-21.6	18% (<i>tptp</i>) chi angles: 173.7,59.9,201.5,68.3	0.136Å	-	-
A1173	HIS	50	-	Favored (9.26%) General / -123.9,14.9	44.7% (<i>m80</i>) chi angles: 305.4,76.5	0.049Å	-	-
A1174	CYS	50	-	Favored (15.4%) General / 62.9,33.1	2.4% (<i>m</i>) chi angles: 326.2	0.094Å	-	-
A1175	GLU	50	-	Favored (8.92%) General / -100.9,-36.8	3% (<i>pm0</i>) chi angles: 71.4,286,54.7	0.113Å	-	-
A1176	LEU	50	-	Favored (47.21%) General / -69.9,150.0	70.4% (<i>mt</i>) chi angles: 304.5,180.2	0.043Å	-	-
A1177	ASN	50	-	Favored (33.82%) General / -93.2,136.1	1.9% (<i>t30</i>) chi angles: 195.2,99.5	0.131Å	-	-
A1178	ILE	50	-	Favored (12.5%) Isoleucine or valine / -100.3,101.7	2.5% (<i>tp</i>) chi angles: 215.1,76.1	0.167Å	-	-
A1179	ASP	50	-	Favored (10.66%) General / -69.7,116.9	17.8% (<i>t0</i>) chi angles: 175.1,30.6	0.035Å	-	-
A1180	GLU	50	-	Favored (30.53%) General / -86.3,6.3	71.3% (<i>mt-10</i>) chi angles: 296.2,162.6,14.1	0.146Å	-	-
A1181	CYS	50	-	Favored (22.31%) General / -92.0,-19.5	48.6% (<i>m</i>) chi angles: 283.4	0.096Å	-	-
A1182	PHE	50	-	Favored (71.67%) General / -63.6,-30.6	75.7% (<i>t80</i>) chi angles: 183.2,84.1	0.127Å	-	-
A1183	SER	50	-	Favored (60.37%) General / -75.6,-14.1	78.5% (<i>p</i>) chi angles: 59.2	0.088Å	-	-
								OUTLIER(S) worst is CA-
				Allowed (0.36%)	3.1% (<i>m120</i>)			

A1184	ASN	50	-	Pre-proline / 67.2,45.2	chi angles: 315.2,153	0.085Å	-	CB-CG: 6.082 σ
#	Alt Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
		Avg: 55.19	Clashscore: 0	Outliers: 6 of 104	Poor rotamers: 2 of 91	Outliers: 0 of 95	Outliers: 0 of 106	Outliers: 13 of 106
A1185	PRO	50	-	Allowed (0.41%) Trans-proline / -76.7,32.8	0.4% chi angles: 43.4	0.048Å	-	-
A1186	CYS	50	-	Favored (23.48%) General / -130.4,119.9	53.3% (<i>m</i>) chi angles: 284.1	0.084Å	-	-
A1187	ILE	99.99	-	Favored (5.81%) Isoleucine or valine / -86.8,-28.6	26.2% (<i>mm</i>) chi angles: 310.5,307.3	0.111Å	-	-
A1188	HIS	99.99	-	Allowed (1.32%) General / -152.7,87.9	10.1% (<i>m80</i>) chi angles: 316.7,79.1	0.06Å	-	OUTLIER(S) worst is CA- CB-CG: 6.267 σ
A1189	GLY	99.99	-	Favored (32.17%) Glycine / 153.4,-173.6	-	-	-	-
A1190	ASN	50	-	Favored (31.71%) General / -107.3,146.3	7.9% (<i>t-20</i>) chi angles: 163,252	0.096Å	-	-
A1191	CYS	50	-	Favored (17.27%) General / -110.0,159.4	16.5% (<i>t</i>) chi angles: 192.7	0.036Å	-	-
A1192	SER	50	-	Favored (51.86%) General / -127.1,141.1	48.4% (<i>t</i>) chi angles: 179.5	0.068Å	-	-
A1193	ASP	50	-	Favored (11.36%) General / -56.5,152.6	49.6% (<i>t0</i>) chi angles: 188.9,16.2	0.077Å	-	-
A1194	ARG	50	-	Allowed (0.13%) General / -142.5,-101.2	4.2% (<i>mmp_?</i>) chi angles: 285.1,293.8,90.8,169.2	0.146Å	-	OUTLIER(S) worst is C-N- CA: 4.382 σ

A1195	VAL	50	-	OUTLIER (0%) Isoleucine or valine / 154.0,69.9	9.5% (<i>p</i>) chi angles: 60.6	0.224Å	-	OUTLIER(S) worst is C-N- CA: 5.256 σ
A1196	ALA	50	-	OUTLIER (0.01%) General / 108.3,5.5	-	0.205Å	-	-
A1197	ALA	50	-	Allowed (0.06%) General / -179.8,117.4	-	0.079Å	-	-
A1198	TYR	50	-	Favored (27.22%) General / -56.1,145.0	22.4% (<i>p90</i>) chi angles: 52.2,78.1	0.031Å	-	-
A1199	HIS	50	-	Favored (6.85%) General / -103.6,96.6	60.9% (<i>t-80</i>) chi angles: 184.5,278.3	0.07Å	-	-
A1200	CYS	50	-	Favored (57.76%) General / -62.1,136.0	58.9% (<i>m</i>) chi angles: 305	0.077Å	-	-
A1201	THR	50	-	Favored (2.49%) General / -130.8,87.4	1.4% (<i>m</i>) chi angles: 325	0.054Å	-	-
A1202	CYS	50	-	Favored (29.94%) General / -53.9,140.6	60.8% (<i>m</i>) chi angles: 304.1	0.089Å	-	-
A1203	GLU	50	-	Favored (92.16%) Pre-proline / -60.9,133.1	5.5% (<i>tp10</i>) chi angles: 161.7,39.7,46.9	0.08Å	-	-
A1204	PRO	50	-	OUTLIER (0.02%) Trans-proline / -50.2,71.2	0.1% chi angles: 317.9	0.02Å	-	-
<div> <div>#</div> <div>Alt Res</div> <div>High B</div> <div>Clash > 0.4Å</div> <div>Ramachandran</div> <div>Rotamer</div> <div>Cβ deviation</div> <div>Bond lengths</div> <div>Bond angles</div> </div> <div> <div>Avg: 55.19</div> <div>Clashscore: 0</div> <div>Outliers: 6 of 104</div> <div>Poor rotamers: 2 of 91</div> <div>Outliers: 0 of 95</div> <div>Outliers: 0 of 106</div> <div>Outliers: 13 of 106</div> </div>								
A1205	GLY	50	-	Allowed (0.1%) Glycine / 159.5,-3.8	-	-	-	-
A1206	TYR	50	-	Favored (32.44%)	96.7% (<i>m-85</i>)	0.037Å	-	-

				General / -119.3,155.1	chi angles: 297.8,269.4			
A1207	THR	50	-	Allowed (1.27%) General / -141.5,-161.7	11.3% (<i>t</i>) chi angles: 192	0.196Å	-	-
A1208	GLY	50	-	Favored (21.87%) Glycine / 97.1,-162.5	-	-	-	-
A1209	VAL	50	-	Favored (9.14%) Isoleucine or valine / -83.5,-20.6	77.8% (<i>t</i>) chi angles: 174.3	0.133Å	-	-
A1210	ASN	50	-	Allowed (1.14%) General / -144.8,34.6	19.2% (<i>m120</i>) chi angles: 295.2,90.6	0.022Å	-	-
A1211	CYS	50	-	Favored (16.97%) General / 47.7,49.0	14.7% (<i>p</i>) chi angles: 53.4	0.209Å	-	OUTLIER(S) worst is C-N- CA: 5.128 σ
A1212	GLU	50	-	Favored (7.72%) General / -104.3,-36.1	13.2% (<i>pm0</i>) chi angles: 76,293.2,20.1	0.069Å	-	OUTLIER(S) worst is CB- CG-CD: 4.942 σ
A1213	VAL	50	-	Favored (36.18%) Isoleucine or valine / -75.3,130.4	91.4% (<i>t</i>) chi angles: 175.4	0.056Å	-	-
A1214	ASP	50	-	Favored (31.81%) General / -80.4,127.0	22.2% (<i>t0</i>) chi angles: 200.5,29.4	0.039Å	-	-
A1215	ILE	50	-	Favored (18.88%) Isoleucine or valine / -57.7,138.2	44.7% (<i>pt</i>) chi angles: 59.9,169.3	0.179Å	-	-
A1216	ASP	50	-	Favored (22.94%) General / -94.7,147.8	29.5% (<i>t70</i>) chi angles: 176.7,62	0.025Å	-	-
A1217	ASN	50	-	Favored (4.73%) General / -129.5,-5.5	5.6% (<i>m120</i>) chi angles: 314.3,141.7	0.042Å	-	OUTLIER(S) worst is CA- CB-CG: 5.629 σ
A1218	CYS	50	-	Favored (79.05%) General /	97.2% (<i>m</i>) chi angles: 294.1	0.077Å	-	-

A1219	GLN	50	-	-69.0,-38.3 Favored (52.99%) General / -77.2,-22.0	7% (<i>tp-100</i>) chi angles: 193.4,63,261.9	0.102Å	-	-
A1220	SER	50	-	Favored (72.46%) General / -71.0,-36.4	3.3% (<i>p</i>) chi angles: 90.4	0.149Å	-	-
A1221	HIS	50	-	Allowed (0.09%) General / 75.6,47.5	64.5% (<i>m80</i>) chi angles: 303.3,83.5	0.159Å	-	-
A1222	GLN	99.99	-	Favored (70.21%) General / -59.0,-33.0	22.3% (<i>mm-40</i>) chi angles: 298.7,295.2,266.3	0.109Å	-	-
A1223	CYS	50	-	Favored (9.96%) General / -88.3,94.8	57.3% (<i>m</i>) chi angles: 305.7	0.047Å	-	-
A1224	ALA	50	-	Favored (7.68%) General / -54.7,151.9	-	0.05Å	-	-
#	Alt Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
		Avg: 55.19	Clashscore: 0	Outliers: 6 of 104	Poor rotamers: 2 of 91	Outliers: 0 of 95	Outliers: 0 of 106	Outliers: 13 of 106
A1225	ASN	99.99	-	Favored (4.02%) General / 73.8,14.9	24% (<i>m-80</i>) chi angles: 313.9,294.8	0.103Å	-	-
A1226	GLY	50	-	Favored (77.48%) Glycine / 89.0,2.8	-	-	-	-
A1227	ALA	50	-	Favored (48.54%) General / -59.2,143.7	-	0.042Å	-	-
A1228	THR	50	-	Favored (48.17%) General / -71.9,138.4	24.5% (<i>m</i>) chi angles: 309	0.035Å	-	-
A1229	CYS	50	-	Favored (42.74%) General / -113.2,144.4	45.1% (<i>t</i>) chi angles: 183	0.094Å	-	-
				Allowed (1.5%)	4.5% (<i>mp</i>)			

A1230	ILE	50	-	Isoleucine or valine /-138.9,100.6	chi angles: 305,96	0.032Å	-	-
A1231	SER	50	-	Favored (12.14%) General / -55.3,150.0	55.5% (<i>m</i>) chi angles: 299.7	0.079Å	-	-
A1232	HIS	50	-	Favored (27.46%) General / -159.1,168.1	26.2% (<i>m80</i>) chi angles: 312.2,88.3	0.121Å	-	-
A1233	THR	50	-	OUTLIER (0.03%) General / -42.1,103.7	9.4% (<i>m</i>) chi angles: 313.5	0.056Å	-	-
A1234	ASN	50	-	Favored (13.45%) General / 47.7,41.2	11.3% (<i>t-20</i>) chi angles: 210.5,349.8	0.094Å	-	-
A1235	GLY	50	-	OUTLIER (0.05%) Glycine / 173.2,82.2	-	-	-	-
A1236	TYR	99.99	-	Favored (46.15%) General / -62.1,147.8	36.9% (<i>p90</i>) chi angles: 67.6,279.5	0.05Å	-	-
A1237	SER	50	-	Favored (11.4%) General / -104.2,164.9	69.5% (<i>p</i>) chi angles: 57.5	0.079Å	-	-
A1238	CYS	50	-	Favored (37.39%) General / -124.0,155.9	31.5% (<i>m</i>) chi angles: 309.9	0.096Å	-	-
A1239	LEU	50	-	Favored (4.66%) General / -129.2,97.7	2.9% (<i>tt</i>) chi angles: 206.5,174	0.034Å	-	-
A1240	CYS	50	-	Favored (9.56%) General / -65.6,118.5	83.2% (<i>m</i>) chi angles: 300	0.06Å	-	-
A1241	PHE	99.99	-	Favored (38.88%) General / -68.3,155.9	56% (<i>t80</i>) chi angles: 188.8,85.7	0.035Å	-	-
A1242	GLY	50	-	Favored (31.01%) Glycine /	-	-	-	OUTLIER(S) worst is C-N-

-58.4,122.8

CA: 5.502 σ

A1243	ASN	50	-	Favored (2.23%) General / -127.0,48.1	78.2% (<i>m</i> -20) chi angles: 297.3,344.6	0.049Å	-	-
A1244	PHE	50	-	Favored (27.63%) General / -79.3,157.8	40.2% (<i>m</i> -85) chi angles: 309,295.5	0.026Å	-	-
#	Alt Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	C β deviation	Bond lengths	Bond angles
		Avg: 55.19	Clashscore: 0	Outliers: 6 of 104	Poor rotamers: 2 of 91	Outliers: 0 of 95	Outliers: 0 of 106	Outliers: 13 of 106
A1245	THR	50	-	Favored (40.01%) General / -153.0,163.3	12% (<i>t</i>) chi angles: 191.5	0.114Å	-	OUTLIER(S) worst is C-N-CA: 4.302 σ
A1246	GLY	50	-	Favored (2.2%) Glycine / -122.6,-24.1	-	-	-	-
A1247	LYS	50	-	Favored (3.17%) General / -127.0,-26.3	26.5% (<i>tptp</i>) chi angles: 194.8,66.6,177.3,64.4	0.077Å	-	-
A1248	PHE	99.99	-	Favored (17.22%) General / -108.6,-4.3	88.4% (<i>m</i> -85) chi angles: 302.9,97.3	0.056Å	-	-
A1249	CYS	50	-	Favored (16.4%) General / 62.2,34.1	35.4% (<i>m</i>) chi angles: 308.5	0.144Å	-	-
A1250	ARG	99.99	-	-	43.1% (<i>tpt85</i>) chi angles: 185.5,63.1,195.3,79	0.046Å	-	-

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