



# Viewing pde6b\_sm\_484-813-FFX1H-multi.table

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All-Atom Contacts	Clashscore, all atoms:	0		100 <sup>th</sup> percentile* (N=1784, all resolutions)
	Clashscore is the number of serious steric overlaps (> 0.4 Å) per 1000 atoms.			
Protein Geometry	Poor rotamers	8	7.55%	Goal: <1%
	Ramachandran outliers	3	2.65%	Goal: <0.05%
	Ramachandran favored	97	85.84%	Goal: >98%
	MolProbity score <sup>^</sup>	1.81		85 <sup>th</sup> percentile* (N=27675, 0Å - 99Å)
	Cβ deviations >0.25Å	3	2.65%	Goal: 0
	Bad backbone bonds:	0 / 970	0.00%	Goal: 0%
	Bad backbone angles:	10 / 1311	0.76%	Goal: <0.1%

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

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

<sup>^</sup> 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
		Avg: 109.32	Clashscore: 0	Outliers: 3 of 113	Poor rotamers: 8 of 106	Outliers: 3 of 113	Outliers: 0 of 115	Outliers: 9 of 115
77	GLU	50.66	-	-	4.5% ( <i>mp0</i> ) chi angles: 281,57,352.9	0.243Å	-	OUTLIER(S) worst is CB-CG-CD: 6.609 σ
78	ARG	160.75	-	Allowed (0.89%) General / -73.5,10.9	18% ( <i>mtm180</i> ) chi angles: 309.3,186.5,305.8,230.7	0.037Å	-	-
79	LEU	235.06	-	Favored (20.63%) General / -85.6,156.6	5.7% ( <i>mp</i> ) chi angles: 295.9,83.5	0.035Å	-	-
80	GLN	173.91	-	Favored (65.62%) General /	7.7% ( <i>tp-100</i> ) chi angles: 171.8,49,230.5	0.136Å	-	-

81	LEU	57.9	-	-57.8,-30.4 Favored (76.42%) General / -59.3,-36.9	37.5% ( <i>mt</i> ) chi angles: 310,182.7	0.105Å	-	-
82	GLU	94.21	-	Favored (76.29%) General / -69.9,-38.4	10.1% ( <i>tm-20</i> ) chi angles: 173.7,283.1,332.7	0.125Å	-	-
83	ASP	89.21	-	Favored (71.32%) General / -64.7,-30.3	32.1% ( <i>t70</i> ) chi angles: 181.3,54.1	0.153Å	-	-
84	VAL	34.28	-	Favored (91.31%) Isoleucine or valine / -63.9,-47.3	43.8% ( <i>t</i> ) chi angles: 167.6	0.104Å	-	-
85	CYS	83.13	-	Favored (69.93%) General / -59.5,-32.1	65.6% ( <i>m</i> ) chi angles: 287.2	0.171Å	-	-
86	VAL	40.64	-	Favored (81.58%) Isoleucine or valine / -56.8,-44.4	53.2% ( <i>t</i> ) chi angles: 170.4	0.083Å	-	-
87	LYS	85.68	-	Favored (15.96%) General / -92.4,-30.1	34.4% ( <i>mtmm</i> ) chi angles: 292.5,173.7,285.6,297.2	0.137Å	-	-
88	ILE	101.11	-	Favored (9.06%) Isoleucine or valine / -92.9,-12.0	21% ( <i>pt</i> ) chi angles: 71.2,166.7	0.189Å	-	-
89	HIS	72.47	-	Favored (2.12%) Pre-proline / -140.6,50.5	38.8% ( <i>m-70</i> ) chi angles: 298.4,318.3	0.037Å	-	OUTLIER(S) worst is CA- CB-CG: 5.251 σ
90	PRO	84.27	-	Allowed (0.39%) Trans-proline / -72.7,-46.9	60.4% ( <i>Cg_endo</i> ) chi angles: 27.2	0.128Å	-	-
91	SER	84.26	-	Favored (59.88%) General / -75.8,-36.1	57% ( <i>p</i> ) chi angles: 55.5	0.083Å	-	-
92	TYR	83.32	-	Favored (92.91%) General /	1.9% ( <i>t80</i> ) chi angles: 174.2,114.7	0.096Å	-	-

				-63.5,-38.9				
93	CYS	72.4	-	Favored (18.7%) General / -86.7,-36.4	99.1% ( <i>m</i> ) chi angles: 290.5	0.12Å	-	-
94	GLY	101.99	-	Favored (28.85%) Glycine / 53.2,-124.6	-	-	-	-
95	PRO	73.9	-	Favored (15.87%) Trans-proline / -53.0,-21.4	34.1% ( <i>Cg_exo</i> ) chi angles: 325.5	0.071Å	-	-
96	ALA	42.56	-	Favored (61.6%) General / -72.3,-13.8	-	0.089Å	-	-
#	Alt Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
		Avg: 109.32	Clashscore: 0	Outliers: 3 of 113	Poor rotamers: 8 of 106	Outliers: 3 of 113	Outliers: 0 of 115	Outliers: 9 of 115
97	ILE	59.59	-	Favored (49.07%) Isoleucine or valine / -58.9,-33.2	81.7% ( <i>mt</i> ) chi angles: 296.8,164.7	0.096Å	-	-
98	LEU	129.14	-	Favored (81%) General / -58.1,-40.4	2.7% ( <i>tm?</i> ) chi angles: 186.9,273.7	0.069Å	-	-
99	ARG	149.8	-	Favored (58.6%) General / -72.1,-46.0	5.9% ( <i>tpt85</i> ) chi angles: 174.1,66.2,213.5,116.2	0.097Å	-	-
100	PHE	60.42	-	Favored (82.87%) General / -60.7,-37.8	29% ( <i>m-85</i> ) chi angles: 290.9,308.2	0.123Å	-	-
101	ARG	78.31	-	Favored (56%) General / -84.4,-11.6	24.5% ( <i>mmm180</i> ) chi angles: 303.2,312.6,304.6,154.4	0.158Å	-	-
102	GLN	251.23	-	Favored (9.23%) General / -82.2,74.2	85.5% ( <i>mt-30</i> ) chi angles: 284.1,168.2,341.1	0.051Å	-	-
103	LEU	261.05	-	Favored (57.3%) General / -59.1,139.1	25.4% ( <i>mt</i> ) chi angles: 308.5,188.2	0.053Å	-	-

104	LEU	145.2	-	Favored (33.46%) General / -69.6,127.6	56.6% ( <i>mt</i> ) chi angles: 307.1,176.1	0.031Å	-	-
105	ALA	47.21	-	Favored (21.44%) General / -111.5,14.1	-	0.04Å	-	-
106	GLU	120.37	-	Favored (94.05%) General / -63.7,-39.3	0% chi angles: 30.2,43.6,283.8	0.165Å	-	-
107	GLN	186.21	-	Allowed (0.76%) General / -106.3,51.1	79.4% ( <i>mt-30</i> ) chi angles: 294.2,162.7,343.2	0.056Å	-	-
108	GLU	87.13	-	Favored (72.1%) Pre-proline / -59.5,-39.5	6.3% ( <i>tm-20</i> ) chi angles: 183.6,298,318.3	0.189Å	-	-
109	PRO	129.3	-	Favored (30.81%) Trans-proline / -57.6,-17.9	0.4% chi angles: 319.9	0.041Å	-	-
110	GLU	76.26	-	Favored (11.21%) General / -92.9,-39.3	68.8% ( <i>mm-40</i> ) chi angles: 304,288.2,336.2	0.075Å	-	-
111	VAL	51.45	-	Favored (59.01%) Isoleucine or valine / -72.3,-37.5	62.6% ( <i>t</i> ) chi angles: 180	0.156Å	-	-
112	GLN	103.7	-	Favored (88.65%) General / -59.1,-41.7	5% ( <i>pt20</i> ) chi angles: 67.3,177,241.8	0.112Å	-	-
113	GLU	124.08	-	Favored (92.26%) General / -65.6,-40.2	76.7% ( <i>mt-10</i> ) chi angles: 298.2,195.1,354.5	0.065Å	-	-
114	VAL	114.59	-	Favored (14.21%) Isoleucine or valine / -77.4,-19.2	0.3% chi angles: 98.2	0.206Å	-	-
115	SER	84	-	Favored (56.25%) General / -73.9,-8.5	7.3% ( <i>t</i> ) chi angles: 196.6	0.141Å	-	-

116	GLN	108.9	-	Favored (34.15%) General / -85.1,-18.5	5.7% ( <i>tp-100</i> ) chi angles: 177.7,48.5,207.7	0.11Å	-	OUTLIER(S) worst is CB- CG-CD: 4.642 σ
#	Alt Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
		Avg: 109.32	Clashscore: 0	Outliers: 3 of 113	Poor rotamers: 8 of 106	Outliers: 3 of 113	Outliers: 0 of 115	Outliers: 9 of 115
117	LEU	232.16	-	Allowed (0.21%) General / -169.9,91.6	2.5% ( <i>tm?</i> ) chi angles: 196.7,282	0.037Å	-	-
118	PHE	331.89	-	Favored (8.84%) General / -61.3,119.6	78.2% ( <i>m-85</i> ) chi angles: 288.1,277.3	0.048Å	-	-
119	ARG	355.68	-	Favored (2.05%) General / -132.6,-168.4	10.8% ( <i>ttp180</i> ) chi angles: 219.6,194.5,72.8,199.9	0.073Å	-	-
120	SER	77.46	-	Favored (63.88%) General / -51.8,-45.7	67.3% ( <i>p</i> ) chi angles: 57.2	0.028Å	-	OUTLIER(S) worst is C-N- CA: 7.576 σ
121	VAL	45.65	-	OUTLIER (0%) Isoleucine or valine / -7.6,-38.7	9.5% ( <i>t</i> ) chi angles: 160.1	0.233Å	-	-
122	LEU	153.19	-	Favored (53.6%) General / -76.8,-22.6	2.1% ( <i>mm?</i> ) chi angles: 301.1,310.2	0.14Å	-	-
123	GLN	48.27	-	Favored (64.98%) General / -71.3,-44.6	8.6% ( <i>tp60</i> ) chi angles: 177.6,63.1,100.5	0.079Å	-	-
124	GLU	62.5	-	Favored (72.23%) General / -61.7,-32.1	3.4% ( <i>mp0</i> ) chi angles: 303.9,94.7,298.3	0.147Å	-	-
125	VAL	99.92	-	Favored (63.44%) Isoleucine or valine / -70.5,-35.8	0.3% chi angles: 97.3	0.221Å	-	-
126	LEU	126.04	-	Favored (76.52%) General / -68.8,-35.0	61.9% ( <i>mt</i> ) chi angles: 305.7,181.8	0.128Å	-	-

127	GLU	82.41	-	Favored (60.19%) General / -76.2,-13.4	55.4% ( <i>mm-40</i> ) chi angles: 291.2,302.1,291.1	0.114Å	-	-
128	ARG	111.84	-	Favored (59.84%) General / -77.0,-11.7	10.1% ( <i>ttp-105</i> ) chi angles: 206.6,173.4,94.2,254.6	0.208Å	-	-
129	MET	52.7	-	Allowed (1.9%) General / -67.9,2.6	59.1% ( <i>mtm</i> ) chi angles: 289.3,174.8,274.5	0.108Å	-	-
130	LYS	79.49	-	Favored (3.26%) General / -135.3,5.6	44.1% ( <i>mtmt</i> ) chi angles: 294.8,167.4,283.2,174.7	0.042Å	-	-
131	GLN	116.43	-	Favored (6.65%) General / -149.8,-178.8	2.2% ( <i>pt20</i> ) chi angles: 78.7,196.5,237.5	0.131Å	-	-
132	GLU	80.52	-	Favored (14.17%) General / -65.7,164.6	1.2% ( <i>tm-20</i> ) chi angles: 201.5,260.8,282.1	0.078Å	-	-
133	GLU	132.72	-	Allowed (1.04%) General / -64.7,0.7	53% ( <i>mm-40</i> ) chi angles: 277.5,296.6,123.7	0.065Å	-	-
134	GLU	110.54	-	Favored (68.95%) General / -58.3,-32.9	15% ( <i>tp10</i> ) chi angles: 186.7,42.2,43.7	0.122Å	-	-
135	ALA	56.37	-	Favored (61.62%) General / -72.0,-24.7	-	0.174Å	-	-
136	HIS	49.22	-	Favored (52.23%) General / -77.8,-32.7	33% ( <i>t-80</i> ) chi angles: 198.2,268.7	0.045Å	-	-
<div> <div>#</div> <div>Alt Res</div> <div>High B</div> <div>Clash &gt; 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: 109.32</div> <div>Clashscore: 0</div> <div>Outliers: 3 of 113</div> <div>Poor rotamers: 8 of 106</div> <div>Outliers: 3 of 113</div> <div>Outliers: 0 of 115</div> <div>Outliers: 9 of 115</div> </div>								
137	LYS	75.5	-	Favored (71.71%) General / -64.4,-30.7	5.7% ( <i>mtmt</i> ) chi angles: 292.4,173.3,255.9,132.9	0.124Å	-	-
Favored								

138	LEU	46.43	-	(63.09%) General / -53.8,-37.0 Favored	92.1% ( <i>mt</i> ) chi angles: 290.9,172	0.203Å	-	-
139	THR	44.46	-	(3.19%) General / -75.5,-58.6 Favored	0.3% chi angles: 330.8	0.123Å	-	-
140	ARG	141.27	-	(10.4%) General / -74.5,-53.0 Favored	38% ( <i>mmt180</i> ) chi angles: 290.5,287.1,183.3,175.9	0.098Å	-	OUTLIER(S) worst is CD- NE-CZ: 4.387 σ
141	GLN	79.06	-	(27.61%) General / -85.4,-24.1 Favored	59.3% ( <i>mm-40</i> ) chi angles: 301.2,290.8,347.7	0.079Å	-	-
142	TRP	119.1	-	(9.91%) General / -118.4,-12.3 Favored	56.8% ( <i>m95</i> ) chi angles: 310.2,110.8	0.195Å	-	-
143	SER	95.53	-	(4.45%) General / -105.9,-45.1 Favored	42.2% ( <i>m</i> ) chi angles: 302.8	0.089Å	-	-
144	LEU	141.71	-	(10.82%) General / -85.7,-46.3 Favored	32.9% ( <i>tp</i> ) chi angles: 178.8,53.2	0.062Å	-	-
145	ARG	157.59	-	(92.88%) Pre-proline / -61.6,-47.4 Favored	36.3% ( <i>ttp180</i> ) chi angles: 174.9,180.3,63,160.3	0.159Å	-	-
146	PRO	153.21	-	(4.99%) Trans-proline / -78.6,121.0 Favored	14.2% ( <i>Cg_exo</i> ) chi angles: 347.7	0.048Å	-	-
147	ARG	112.31	-	(60.55%) General / -75.1,-14.3 Favored	22.9% ( <i>mmt180</i> ) chi angles: 304.2,312.4,198.7,185.8	0.188Å	-	-
148	GLY	33.79	-	(67.11%) Glycine / -70.6,-34.1 Favored	-	-	-	-
149	SER	95.93	-	(74.96%) General / -68.5,-33.9	7.4% ( <i>m</i> ) chi angles: 312.5	0.092Å	-	-

150	LEU	139.49	-	Favored (43.64%) General / -80.7,-20.2	12.3% ( <i>tp</i> ) chi angles: 203.5,67.2	0.042Å	-	-
151	ALA	55.07	-	Favored (55.37%) General / -68.0,144.0	-	0.056Å	-	-
152	THR	129.4	-	Favored (58.24%) General / -61.6,137.3	19.7% ( <i>m</i> ) chi angles: 310.5	0.028Å	-	-
153	PHE	120.33	-	Favored (10.79%) General / -69.4,117.2	27.4% ( <i>t80</i> ) chi angles: 186.6,102.3	0.032Å	-	-
154	LYS	189.06	-	Allowed (1.51%) General / -143.5,27.8	52.9% ( <i>tttm</i> ) chi angles: 199.4,177.3,187.9,288.6	0.113Å	-	-
155	THR	145.73	-	Favored (4.73%) General / -83.6,-173.5	8% ( <i>t</i> ) chi angles: 193.4	0.276Å	-	-
156	ARG	163.42	-	Favored (38.26%) General / -74.8,154.6	0.4% chi angles: 86.7,171.7,292.2,83.6	0.108Å	-	-
#	Alt Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
Avg: 109.32			Clashscore: 0	Outliers: 3 of 113	Poor rotamers: 8 of 106	Outliers: 3 of 113	Outliers: 0 of 115	Outliers: 9 of 115
157	ALA	54.82	-	Allowed (0.37%) General / -148.5,-9.5	-	0.051Å	-	-
158	ARG	232.54	-	Favored (5.63%) General / -88.2,60.2	38.4% ( <i>ttm180</i> ) chi angles: 190.9,190.8,293.9,126.2	0.076Å	-	-
159	ILE	194.89	-	OUTLIER (0.03%) Isoleucine or valine / 47.2,-136.1	6.9% ( <i>mm</i> ) chi angles: 321.8,298.7	0.282Å	-	OUTLIER(S) worst is C-CA- CB: 4.188 σ
160	SER	131.43	-	Allowed (1.19%) Pre-proline /	31.6% ( <i>t</i> ) chi angles: 184.6	0.114Å	-	-



161	PRO	73.63	-	-178.3,161.2 Favored (77.48%) Trans-proline / -66.7,146.1	82.9% ( <i>Cg_exo</i> ) chi angles: 330.3	0.07Å	-	-
162	PHE	92.3	-	Favored (59.21%) General / -75.6,-29.5	18.3% ( <i>m-85</i> ) chi angles: 312.7,303.9	0.12Å	-	-
163	ALA	29.58	-	Favored (22.84%) General / -88.9,-23.2	-	0.081Å	-	-
164	SER	89.35	-	Favored (2.3%) General / -97.7,72.7	99.2% ( <i>p</i> ) chi angles: 64.6	0.041Å	-	-
165	ASP	183.88	-	Favored (43.17%) General / -75.4,140.7	25.7% ( <i>t0</i> ) chi angles: 185.2,36.8	0.066Å	-	OUTLIER(S) worst is C-N- CA: 4.281 $\sigma$
166	ILE	142.5	-	OUTLIER (0.03%) Isoleucine or valine / 175.0,160.4	9.8% ( <i>tp</i> ) chi angles: 196.3,59.8	0.11Å	-	-
167	ARG	107.6	-	Favored (44.65%) General / -86.7,-13.7	8.4% ( <i>mmt-85</i> ) chi angles: 307.3,293.5,145.3,258.5	0.133Å	-	-
168	THR	111	-	Favored (3.78%) General / -148.8,107.3	32.6% ( <i>p</i> ) chi angles: 51.7	0.079Å	-	-
169	ILE	103.88	-	Favored (44.81%) Isoleucine or valine / -120.1,140.2	96.7% ( <i>mt</i> ) chi angles: 294.4,170.4	0.049Å	-	-
170	SER	80.43	-	Favored (7.28%) General / -57.3,156.7	6.7% ( <i>t</i> ) chi angles: 197.2	0.071Å	-	-
171	GLU	81.97	-	Allowed (1.94%) General / -129.9,-31.3	2.7% ( <i>tp10</i> ) chi angles: 213.8,69.5,98.7	0.029Å	-	OUTLIER(S) worst is C-N- CA: 4.003 $\sigma$
172	ASP	95.87	-	Favored (4.24%) General / -94.6,-177.5	5.6% ( <i>p-10</i> ) chi angles: 58.9,275.4	0.054Å	-	-

173	VAL	102.72	-	Favored (6.81%) Isoleucine or valine / -118.6,7.3	4% ( <i>p</i> ) chi angles: 78.4	0.144Å	-	-
174	GLU	60.06	-	Favored (97.29%) General / -63.3,-43.7	6.6% ( <i>mt-10</i> ) chi angles: 306.2,142.7,40.4	0.118Å	-	-
175	ARG	132.11	-	Favored (2.33%) General / -65.9,-0.5	0% chi angles: 70.4,97.9,213.4,209.9	0.094Å	-	OUTLIER(S) worst is CD- NE-CZ: 4.021 σ
176	ASP	51.12	-	Favored (23.91%) General / -98.9,-9.6	1.8% ( <i>m-20</i> ) chi angles: 305.2,244.3	0.118Å	-	-
#	Alt Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
Avg: 109.32			Clashscore: 0	Outliers: 3 of 113	Poor rotamers: 8 of 106	Outliers: 3 of 113	Outliers: 0 of 115	Outliers: 9 of 115
177	THR	136.17	-	Allowed (0.17%) Pre-proline / -102.5,-15.6	0.6% chi angles: 217.9	0.324Å	-	-
178	PRO	132.66	-	Favored (47.69%) Trans-proline / -67.7,-17.8	43.7% ( <i>Cg_exo</i> ) chi angles: 326.2	0.096Å	-	-
179	PRO	146.25	-	Favored (54.51%) Trans-proline / -61.6,155.2	1.2% ( <i>Cg_exo</i> ) chi angles: 321.3	0.07Å	-	-
180	PRO	168.87	-	Favored (32.96%) Trans-proline / -77.0,161.5	43.7% ( <i>Cg_endo</i> ) chi angles: 35.8	0.036Å	-	-
181	LEU	201.83	-	Allowed (0.16%) General / 69.7,157.6	37% ( <i>mt</i> ) chi angles: 311,177.9	0.099Å	-	-
182	ARG	99.52	-	Favored (5.25%) General / -140.8,107.1	31.9% ( <i>mmm180</i> ) chi angles: 304.8,299.2,294.1,168.9	0.078Å	-	-
183	SER	36.49	-	Favored (74.16%) General / -60.8,-34.2	40.2% ( <i>m</i> ) chi angles: 303.1	0.086Å	-	-

184	TRP	72.73	-	Allowed (0.78%) General / -64.1,1.0	5.3% ( <i>m-90</i> ) chi angles: 313.6,276.7	0.068Å	-	-
185	SER	88.42	-	Favored (9.44%) General / -121.3,-4.2	19.7% ( <i>m</i> ) chi angles: 306.1	0.062Å	-	-
186	MET	152.75	-	Favored (56.08%) Pre-proline / -56.1,145.3	15.2% ( <i>tpt</i> ) chi angles: 187.9,64.1,178	0.108Å	-	-
187	PRO	66.37	-	Favored (34.8%) Trans-proline / -49.4,-44.3	19.6% ( <i>Cg_exo</i> ) chi angles: 324.1	0.102Å	-	-
188	GLU	76.78	-	Favored (37.46%) General / -77.2,-42.5	2.5% ( <i>mp0</i> ) chi angles: 314.6,88.5,292.3	0.075Å	-	-
189	PHE	61.1	-	Favored (7.75%) General / -89.0,77.2	3.8% ( <i>m-30</i> ) chi angles: 315.4,327.9	0.088Å	-	-
190	ARG	135.36	-	Favored (3.44%) General / -135.1,19.8	97.2% ( <i>mtt180</i> ) chi angles: 298.8,183.6,179.2,189.8	0.063Å	-	-
191	ALA	11.72	-	-	-	0.032Å	-	-

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