



# Viewing pde6b\_sm\_343-446-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	4	4.35%	Goal: <1%
	Ramachandran outliers	3	2.94%	Goal: <0.05%
	Ramachandran favored	91	89.22%	Goal: >98%
	MolProbity score <sup>^</sup>	1.55		94 <sup>th</sup> percentile* (N=27675, 0Å - 99Å)
	Cβ deviations >0.25Å	2	2.06%	Goal: 0
	Bad backbone bonds:	0 / 844	0.00%	Goal: 0%
	Bad backbone angles:	13 / 1136	1.14%	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: 58.17	Clashscore: 0	Outliers: 3 of 102	Poor rotamers: 4 of 92	Outliers: 2 of 97	Outliers: 0 of 104	Outliers: 13 of 104
A 343	GLY	50	-	-	-	-	-	-
A 344	LEU	50	-	Favored (17.48%) Pre-proline / -46.1,-54.4	39.9% (tp) chi angles: 186.5,63.8	0.134Å	-	-
A 345	PRO	50	-	Favored (13.44%) Trans-proline / -74.1,-25.8	92% (Cg_endo) chi angles: 30.2	0.091Å	-	-
A 346	SER	50	-	Favored (32.24%) General / -67.4,-53.1	8.4% (t) chi angles: 194.2	0.054Å	-	-

A 347	TYR	50	-	Favored (81.46%) General / -56.9,-43.6	81.3% ( <i>t80</i> ) chi angles: 177.3,85.1	0.102Å	-	-
A 348	VAL	50	-	Favored (43.91%) Isoleucine or valine / -71.3,-31.4	86.7% ( <i>t</i> ) chi angles: 177.7	0.192Å	-	-
A 349	ALA	50	-	Favored (33.88%) General / -81.9,-26.6	-	0.086Å	-	-
A 350	GLU	50	-	Favored (12.85%) General / -97.9,-30.3	9.6% ( <i>pt-20</i> ) chi angles: 72.5,200,122.5	0.142Å	-	-
A 351	SER	50	-	Favored (12.97%) General / -96.2,-31.4	26.4% ( <i>p</i> ) chi angles: 78.2	0.104Å	-	-
A 352	GLY	50	-	Favored (84.73%) Glycine / 84.4,-4.1	-	-	-	-
A 353	PHE	50	-	Favored (29.53%) General / -80.8,149.5	17.5% ( <i>m-85</i> ) chi angles: 281.5,66.1	0.044Å	-	-
A 354	ILE	50	-	Favored (4.52%) Isoleucine or valine / -75.8,162.0	32% ( <i>pt</i> ) chi angles: 65.3,165.2	0.087Å	-	-
A 355	CYS	50	-	Favored (36.38%) General / -134.7,130.5	14.2% ( <i>m</i> ) chi angles: 277.7	0.069Å	-	-
A 356	ASN	50	-	Favored (3.08%) General / -128.9,90.7	60.7% ( <i>t-20</i> ) chi angles: 180.9,354	0.07Å	-	-
A 357	ILE	50	-	Favored (2.13%) Isoleucine or valine / -73.3,104.0	1.9% ( <i>mp</i> ) chi angles: 281.8,68.4	0.081Å	-	-
A 358	MET	50	-	Favored (57.7%) General / -77.4,-18.0	4.1% ( <i>mtt</i> ) chi angles: 307.3,217.7,165.4	0.124Å	-	-
A 359	ASN	50	-	Favored (3.24%) General / -158.1,117.7	9.8% ( <i>t30</i> ) chi angles: 183.7,86.1	0.062Å	-	-
A	ALA	50	-	Favored (68.88%)	-	0.127Å	-	-

360				General / -69.4,-30.8					
A 361	SER	50	-	Favored (4.33%) General / -85.6,57.2	56.3% ( <i>p</i> ) chi angles: 73.2	0.075Å	-	-	
A 362	ALA	50	-	OUTLIER (0.01%) General / -174.4,15.2	-	0.037Å	-	-	
#	Alt	Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
			Avg: 58.17	Clashscore: 0	Outliers: 3 of 102	Poor rotamers: 4 of 92	Outliers: 2 of 97	Outliers: 0 of 104	Outliers: 13 of 104
A 363	ASP	50	-	Favored (31.31%) General / -138.0,163.5	32.9% ( <i>t0</i> ) chi angles: 183.8,29.4	0.116Å	-		OUTLIER(S) worst is C-N- CA: 5.047 σ
A 364	GLU	50	-	Favored (8.4%) General / -105.1,-33.1	8.7% ( <i>tm-20</i> ) chi angles: 174.8,288.4,327.4	0.034Å	-	-	
A 365	MET	50	-	Favored (76.49%) General / -64.7,-47.9	18.5% ( <i>mmt</i> ) chi angles: 296,284.3,165	0.093Å	-	-	
A 366	PHE	50	-	Favored (21.85%) General / -80.2,118.4	22.7% ( <i>t80</i> ) chi angles: 163.8,243.8	0.048Å	-	-	
A 367	LYS	99.99	-	Favored (6.14%) General / -77.3,101.0	20.9% ( <i>pttp</i> ) chi angles: 58.7,164.1,173.2,64.4	0.174Å	-	-	
A 368	PHE	50	-	Allowed (0.9%) General / -63.9,0.3	28.8% ( <i>p90</i> ) chi angles: 53.9,260.1	0.176Å	-	-	
A 369	GLN	99.99	-	Favored (56.8%) General / -54.1,-33.1	19.6% ( <i>tp60</i> ) chi angles: 174.3,61,91	0.088Å	-	-	
A 370	GLU	50	-	Favored (84.87%) General / -66.5,-37.3	87.1% ( <i>mt-10</i> ) chi angles: 295.2,167.1,7.3	0.067Å	-	-	
A 371	GLY	50	-	Favored (76.82%) Glycine / -74.7,-22.6	-	-	-	-	
A 372	ALA	50	-	Favored (57.53%) General /	-	0.086Å	-	-	

A 373	LEU	99.99	-	-76.5,-36.7 OUTLIER (0.03%) General / -165.1,-35.1	0.9% chi angles: 198.7,129.7	0.075Å	-	-
A 374	ASP	99.99	-	Favored (88.53%) General / -61.0,-39.1	0% chi angles: 324.6,3.8	0.233Å	-	OUTLIER(S) worst is CA-CB- CG: 7.011 σ
A 375	ASP	99.99	-	Allowed (1.08%) General / -95.6,43.5	36.6% ( <i>t0</i> ) chi angles: 197.9,12.5	0.071Å	-	-
A 376	SER	99.99	-	Favored (3.24%) General / 64.5,6.7	8.5% ( <i>t</i> ) chi angles: 194	0.15Å	-	-
A 377	GLY	50	-	Favored (62.37%) Glycine / 86.3,16.5	-	-	-	-
A 378	TRP	99.99	-	Favored (47.3%) General / -70.0,149.9	41.5% ( <i>t-105</i> ) chi angles: 165.8,243.3	0.069Å	-	OUTLIER(S) worst is CE3- CD2-CG: 4.204 σ
A 379	LEU	50	-	Favored (7.14%) General / -82.0,83.9	35.4% ( <i>mt</i> ) chi angles: 310.2,183.1	0.057Å	-	-
A 380	ILE	99.99	-	Favored (28.78%) Isoleucine or valine / -70.4,125.5	89.6% ( <i>mt</i> ) chi angles: 294.1,165.9	0.064Å	-	-
A 381	LYS	50	-	Favored (5.94%) General / -122.1,-21.4	39.4% ( <i>mtmt</i> ) chi angles: 287.6,163.1,280.3,182.5	0.045Å	-	-
A 382	ASN	50	-	Favored (24.59%) General / -156.9,150.7	31.2% ( <i>m120</i> ) chi angles: 291.9,105.6	0.125Å	-	-
#	Alt Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
		Avg: 58.17	Clashscore: 0	Outliers: 3 of 102	Poor rotamers: 4 of 92	Outliers: 2 of 97	Outliers: 0 of 104	Outliers: 13 of 104
A 383	VAL	99.99	-	Favored (21.87%) Isoleucine or valine / -144.3,145.2	5.9% ( <i>t</i> ) chi angles: 194.1	0.048Å	-	-
A 384	LEU	50	-	Favored (49.91%) General /	60.1% ( <i>tp</i> ) chi angles: 174.8,61.3	0.09Å	-	-

				-123.7,144.0				
A 385	SER	50	-	Favored (23.05%) General / -146.2,135.7	26.4% ( <i>t</i> ) chi angles: 185.7	0.04Å	-	-
A 386	MET	50	-	Favored (66.21%) Pre-proline / -140.9,152.7	53.5% ( <i>mtp</i> ) chi angles: 307.2,190,83.7	0.064Å	-	-
A 387	PRO	50	-	Favored (5.07%) Trans-proline / -85.8,136.0	28% ( <i>Cg_endo</i> ) chi angles: 37.5	0.04Å	-	-
A 388	ILE	50	-	Favored (16.46%) Isoleucine or valine / -102.1,104.5	82.1% ( <i>mt</i> ) chi angles: 293.7,175.5	0.084Å	-	-
A 389	VAL	50	-	Favored (8.67%) Isoleucine or valine / -113.0,164.6	31% ( <i>m</i> ) chi angles: 300.8	0.082Å	-	-
A 390	ASN	50	-	Allowed (0.07%) General / -88.3,-131.1	45.8% ( <i>p30</i> ) chi angles: 58.9,21.1	0.291Å	-	OUTLIER(S) worst is C-CA- CB: 5.048 $\sigma$
A 391	LYS	50	-	Favored (5.08%) General / -130.6,24.9	52.4% ( <i>mmtt</i> ) chi angles: 298.7,295.7,154.5,182.1	0.125Å	-	-
A 392	LYS	50	-	Favored (10.86%) General / -120.3,8.7	28.2% ( <i>mtpt</i> ) chi angles: 297.1,158.9,63.3,205.4	0.068Å	-	OUTLIER(S) worst is C-N- CA: 4.928 $\sigma$
A 393	GLU	50	-	Favored (16.6%) General / 49.0,40.2	1.9% ( <i>mm-40</i> ) chi angles: 307.5,319.6,259.3	0.266Å	-	-
A 394	GLU	50	-	Favored (37.2%) General / -95.0,134.8	68.6% ( <i>mt-10</i> ) chi angles: 295.2,163.7,326.5	0.09Å	-	-
A 395	ILE	50	-	Favored (30.62%) Isoleucine or valine / -65.0,130.9	4.3% ( <i>tp</i> ) chi angles: 197.2,82.9	0.099Å	-	-
A 396	VAL	50	-	Favored (4.49%) Isoleucine or valine / -124.4,-16.3	21.7% ( <i>m</i> ) chi angles: 303	0.197Å	-	-
A 397	GLY	50	-	Favored (33.1%) Glycine / -165.2,-172.8	-	-	-	-
A				Favored (28.41%)	40.8% ( <i>t</i> )			

398	VAL	50	-	Isoleucine or valine / -139.4,144.7	chi angles: 166.7	0.095Å	-	-
A 399	ALA	50	-	Favored (29.28%) General / -108.2,148.9	-	0.094Å	-	-
A 400	THR	50	-	Favored (30.2%) General / -152.6,151.1	13.6% ( <i>t</i> ) chi angles: 186.5	0.125Å	-	-
A 401	PHE	50	-	Favored (43.2%) General / -148.6,160.3	7.2% ( <i>m-85</i> ) chi angles: 317.2,87.3	0.097Å	-	-
A 402	TYR	50	-	Favored (32.33%) General / -148.5,165.1	11.4% ( <i>p90</i> ) chi angles: 71.3,109.8	0.067Å	-	-
<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: 58.17</div> <div>Clashscore: 0</div> <div>Outliers: 3 of 102</div> <div>Poor rotamers: 4 of 92</div> <div>Outliers: 2 of 97</div> <div>Outliers: 0 of 104</div> <div>Outliers: 13 of 104</div> </div>								
A 403	ASN	50	-	Favored (4.03%) General / 51.9,60.2	8% ( <i>m-20</i> ) chi angles: 284.4,24.5	0.153Å	-	-
A 404	ARG	99.99	-	Allowed (0.18%) General / -53.0,106.8	45.8% ( <i>tpt85</i> ) chi angles: 179.4,60.7,171.6,91.1	0.065Å	-	OUTLIER(S) worst is CD-NE-CZ: 5.096 σ
A 405	LYS	99.99	-	Favored (8.17%) General / 48.4,37.2	11.3% ( <i>pttp</i> ) chi angles: 67,155,197.4,60.2	0.194Å	-	-
A 406	ASP	99.99	-	Favored (19.61%) General / 61.1,31.9	10.2% ( <i>t0</i> ) chi angles: 206,35.1	0.186Å	-	-
A 407	GLY	99.99	-	Favored (2.57%) Glycine / 132.6,124.7	-	-	-	OUTLIER(S) worst is C-N-CA: 6.396 σ
A 408	LYS	50	-	OUTLIER (0%) Pre-proline / 139.9,138.5	22.7% ( <i>tptp</i> ) chi angles: 166.9,62.2,185.1,52.6	0.042Å	-	-
A 409	PRO	50	-	Favored (36.86%) Trans-proline / -60.8,157.7	1.4% ( <i>Cg_endo</i> ) chi angles: 2.8	0.079Å	-	-
A 410	PHE	50	-	Favored (19.47%) General / -67.0,163.6	52.9% ( <i>m-85</i> ) chi angles: 293.6,256.1	0.084Å	-	-

A 411	ASP	50	-	Favored (14.63%) General / -131.8,170.6	37% ( <i>m-20</i> ) chi angles: 298,288.9	0.05Å	-	-
A 412	GLU	50	-	Favored (12.65%) General / -45.3,-45.9	2.8% ( <i>tm-20</i> ) chi angles: 161.9,287.9,313.3	0.103Å	-	-
A 413	GLN	50	-	Favored (60.43%) General / -53.2,-35.8	10.8% ( <i>mm-40</i> ) chi angles: 293.1,285.9,260.2	0.1Å	-	-
A 414	ASP	50	-	Favored (5.91%) General / -82.0,-53.7	1.3% ( <i>m-20</i> ) chi angles: 322.2,329.5	0.108Å	-	OUTLIER(S) worst is CA-CB- CG: 5.101 $\sigma$
A 415	GLU	50	-	Favored (39.06%) General / -79.2,-37.2	43.1% ( <i>mt-10</i> ) chi angles: 294.3,170.5,281.6	0.087Å	-	-
A 416	VAL	50	-	Favored (81.94%) Isoleucine or valine / -68.7,-40.6	47.1% ( <i>t</i> ) chi angles: 168.1	0.131Å	-	-
A 417	LEU	50	-	Favored (80.15%) General / -68.8,-38.8	43.4% ( <i>mt</i> ) chi angles: 307,184.8	0.116Å	-	-
A 418	MET	50	-	Favored (75.38%) General / -69.6,-35.5	57.4% ( <i>tpp</i> ) chi angles: 188.8,58.2,71	0.121Å	-	-
A 419	GLU	50	-	Favored (90.25%) General / -64.1,-45.1	4.1% ( <i>tm-20</i> ) chi angles: 197,302.3,311.3	0.09Å	-	-
A 420	SER	50	-	Favored (60.21%) General / -51.5,-40.7	7.3% ( <i>t</i> ) chi angles: 196.6	0.104Å	-	-
A 421	LEU	50	-	Favored (44.54%) General / -67.2,-52.1	37.1% ( <i>tp</i> ) chi angles: 184,55.4	0.1Å	-	-
A 422	THR	50	-	Favored (79.11%) General / -66.3,-34.9	39.7% ( <i>p</i> ) chi angles: 53.5	0.132Å	-	OUTLIER(S) worst is C-N- CA: 5.007 $\sigma$

High Clash &gt;

C $\beta$  Bond

#	Alt Res	B	0.4Å	Ramachandran	Rotamer	deviation	lengths	Bond angles	
			Avg: 58.17	Clashscore: 0	Outliers: 3 of 102	Poor rotamers: 4 of 92	Outliers: 2 of 97	Outliers: 0 of 104	Outliers: 13 of 104
A 423	GLN	50	-	Favored (37.66%) General / -53.0,-30.8	11.5% ( <i>tp-100</i> ) chi angles: 182.9,52.4,231.5	0.041Å	-	OUTLIER(S) worst is NE2-CD-OE1: 4.517σ	
A 424	PHE	50	-	Favored (13.21%) General / -110.9,-17.9	80.1% ( <i>m-85</i> ) chi angles: 288.9,265.6	0.14Å	-	-	
A 425	LEU	50	-	Favored (98.99%) General / -62.5,-41.7	75.8% ( <i>mt</i> ) chi angles: 288.9,176.3	0.118Å	-	-	
A 426	GLY	50	-	Favored (58.65%) Glycine / -75.7,-29.9	-	-	-	-	
A 427	TRP	50	-	Favored (84.24%) General / -58.3,-41.4	63.8% ( <i>t90</i> ) chi angles: 169.9,78.4	0.081Å	-	OUTLIER(S) worst is CE3-CD2-CG: 4.155σ	
A 428	SER	50	-	Favored (91.43%) General / -65.5,-39.1	41.1% ( <i>m</i> ) chi angles: 302.9	0.079Å	-	-	
A 429	VAL	50	-	Favored (92.22%) Isoleucine or valine / -59.4,-46.9	75.6% ( <i>t</i> ) chi angles: 172.9	0.092Å	-	-	
A 430	MET	50	-	Favored (75%) General / -61.1,-34.5	10.4% ( <i>tpt</i> ) chi angles: 201.2,71.2,191.2	0.106Å	-	-	
A 431	ASN	50	-	Favored (87.59%) General / -59.0,-41.5	24.7% ( <i>m-80</i> ) chi angles: 279.3,268.2	0.074Å	-	-	
A 432	THR	50	-	Favored (79.59%) General / -65.9,-35.1	4.9% ( <i>m</i> ) chi angles: 317	0.126Å	-	-	
A 433	ASP	50	-	Favored (73.72%) General / -57.3,-38.3	0.9% chi angles: 293.2,52.4	0.204Å	-	-	
				Favored					



A 434	THR	50	-	(19.11%) General / -87.6,-32.8	14.1% ( <i>p</i> ) chi angles: 45.8	0.125Å	-	-
A 435	TYR	50	-	Favored (14.86%) General / -94.0,-30.1	6.3% ( <i>m-30</i> ) chi angles: 311.5,331	0.143Å	-	-
A 436	ASP	99.99	-	Allowed (0.33%) General / -121.9,-141.3	1.3% ( <i>m-20</i> ) chi angles: 288.4,243.3	0.172Å	-	-
A 437	LYS	99.99	-	Allowed (0.21%) General / 42.1,-113.3	61% ( <i>mtpt</i> ) chi angles: 292.1,174.7,62.6,181.3	0.2Å	-	-
A 438	MET	99.99	-	Favored (89.17%) General / -63.1,-37.9	11.5% ( <i>ptp</i> ) chi angles: 83.6,183.9,81.4	0.18Å	-	-
A 439	ASN	50	-	Favored (31.41%) General / -83.8,-23.5	91.6% ( <i>m-20</i> ) chi angles: 294.1,327	0.182Å	-	-
A 440	LYS	50	-	Favored (49.84%) General / -78.1,-21.8	54.1% ( <i>mttp</i> ) chi angles: 280.7,187.9,176.6,69.9	0.192Å	-	-
A 441	LEU	50	-	Favored (80.21%) General / -68.0,-42.7	89.9% ( <i>mt</i> ) chi angles: 294.3,170.4	0.123Å	-	-
A 442	GLU	50	-	Favored (84.63%) General / -61.0,-38.1	22.5% ( <i>mm-40</i> ) chi angles: 267.7,293.3,303.8	0.079Å	-	-
#	Alt Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	C $\beta$ deviation	Bond lengths	Bond angles
		Avg: 58.17	Clashscore: 0	Outliers: 3 of 102	Poor rotamers: 4 of 92	Outliers: 2 of 97	Outliers: 0 of 104	Outliers: 13 of 104
A 443	ASN	50	-	Favored (5.82%) General / -84.5,13.2	5.2% ( <i>m120</i> ) chi angles: 303.8,167.4	0.079Å	-	OUTLIER(S) worst is CA-CB- CG: 7.532 $\sigma$
A 444	ARG	50	-	Allowed (0.97%) General / -149.3,45.0	1.3% ( <i>tpm_?</i> ) chi angles: 182.7,46.6,276.5,131.5	0.118Å	-	-
				Allowed				

A 445	LYS	50	-	(0.58%) General / -108.0,-79.3	35.4% ( <i>ttpt</i> ) chi angles: 170.7,183.7,59.1,175.5	0.157Å	-	-
A 446	ASP	99.99	-	-	0.5% chi angles: 307,40.1	0.048Å	-	OUTLIER(S) worst is CA-CB- CG: 4.649 $\sigma$

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