



# Viewing pde6b\_sm\_343-446H-multi.table

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All-Atom Contacts	Clashscore, all atoms:	34.99		11 <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	6	6.52%	Goal: <1%
	Ramachandran outliers	4	3.92%	Goal: <0.05%
	Ramachandran favored	86	84.31%	Goal: >98%
	MolProbity score^	3.32		13 <sup>th</sup> percentile* (N=27675, 0Å - 99Å)
	Cβ deviations >0.25Å	0	0.00%	Goal: 0
	Bad backbone bonds:	3 / 844	0.36%	Goal: 0%
	Bad backbone angles:	6 / 1136	0.53%	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: 34.99	Outliers: 4 of 102	Poor rotamers: 6 of 92	Outliers: 0 of 97	Outliers: 2 of 104	Outliers: 5 of 104
A 343	GLY	50	-	-	-	-	-	-
A 344	LEU	50	0.515Å HD11 with A 366 PHE N	Favored (20.28%) Pre-proline / -48.2,-55.0	9.1% ( <i>mp</i> ) chi angles: 284.4,63.8	0.138Å	-	-
A 345	PRO	50	0.415Å HD2 with A 344 LEU N	Favored (5.05%) Trans-proline / -65.7,-46.5	96.3% ( <i>Cg_endo</i> ) chi angles: 30.4	0.068Å	-	-
A 346	SER	50	-	Favored (4.58%) General / -44.6,-38.8	33.9% ( <i>t</i> ) chi angles: 175.4	0.058Å	-	-
A 347	TYR	50	0.65Å HA with A 350 GLU HG2	Favored (8.6%) General / -80.2,-51.7	68.2% ( <i>t80</i> ) chi angles: 187,79.6	0.055Å	-	-
Allowed								

A 348	VAL	50	-	(0.44%) Isoleucine or valine / -41.8,-58.3	92.7% ( <i>t</i> ) chi angles: 178.1	0.012Å	-	-
A 349	ALA	50	-	Allowed (1.5%) General / -42.7,-60.6	-	0.038Å	-	-
A 350	GLU	50	0.65Å HG2 with A 347 TYR HA	Favored (63.31%) General / -69.3,-15.2	12.9% ( <i>pt</i> -20) chi angles: 64.1,181,68.1	0.124Å	-	-
A 351	SER	50	-	Favored (9.09%) General / -115.6,-22.7	49.4% ( <i>m</i> ) chi angles: 300.8	0.043Å	-	-
A 352	GLY	50	-	Favored (73.24%) Glycine / 65.7,28.0	-	-	-	-
A 353	PHE	50	-	Favored (53%) General / -118.6,137.8	1.9% ( <i>m</i> -85) chi angles: 290,35.8	0.055Å	-	-
A 354	ILE	50	0.807Å HG22 with A 387 PRO HD2	Favored (2.45%) Isoleucine or valine / -61.6,159.3	27.4% ( <i>pt</i> ) chi angles: 67.1,178.4	0.058Å	-	-
A 355	CYS	50	-	Favored (30.04%) General / -135.1,127.3	78.4% ( <i>m</i> ) chi angles: 299.3	0.012Å	-	-
A 356	ASN	50	0.564Å HD21 with A 410 PHE HB2	Allowed (1.59%) General / -119.6,80.6	0.4% chi angles: 195.3,168.6	0.042Å	-	-
A 357	ILE	50	0.449Å HG13 with A 383 VAL HB	Favored (9.48%) Isoleucine or valine / -77.8,145.7	0% chi angles: 354.6,269.9	0.053Å	-	-
A 358	MET	50	0.51Å HA with A 382 ASN OD1	Favored (7.98%) General / -100.3,-39.5	65.9% ( <i>mtt</i> ) chi angles: 294.6,180.9,178.1	0.053Å	-	-
A 359	ASN	50	-	Favored (9.31%) General / -130.5,107.6	25.8% ( <i>t</i> -20) chi angles: 187.2,298.9	0.042Å	-	-
A			0.726Å HB1 with A	Favored (39.96%)				OUTLIER(S) worst is N-

360	ALA	50	366 PHE CD2	General / -53.6,-30.0	-	0.185Å	-	CA-CB: 4.859 σ
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A 361	SER	50	-	Favored (68.2%) General / -69.8,-30.6	34.2% ( <i>m</i> ) chi angles: 303.7	0.039Å	-	-
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A 362	ALA	50	-	Favored (69.94%) General / -61.3,-29.6	-	0.021Å	-	-
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#	Alt	Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
			Avg: 58.17	Clashscore: 34.99	Outliers: 4 of 102	Poor rotamers: 6 of 92	Outliers: 0 of 97	Outliers: 2 of 104	Outliers: 5 of 104

A 363	ASP	50	0.411Å OD2 with A 357 ILE HD12	Favored (31.12%) General / -73.2,126.9	0.4% chi angles: 227.4,282.4	0.033Å	-	-
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A 364	GLU	50	-	Favored (15.78%) General / -76.8,2.0	12.1% ( <i>pt-20</i> ) chi angles: 65.4,176.7,56.7	0.024Å	-	-
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A 365	MET	50	-	Favored (9.96%) General / -114.2,-22.4	64.8% ( <i>mtt</i> ) chi angles: 292.3,183.2,177.8	0.074Å	-	-
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A 366	PHE	50	0.74Å HE1 with A 368 PHE HA	Favored (32.27%) General / -52.9,130.1	0.5% chi angles: 183,305.7	0.06Å	-	-
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A 367	LYS	99.99	-	Favored (14.57%) General / -106.9,104.8	99% ( <i>mttt</i> ) chi angles: 292.8,183.4,178,180.9	0.008Å	-	-
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A 368	PHE	50	0.74Å HA with A 366 PHE HE1	Favored (27.59%) General / -79.7,1.1	44.4% ( <i>p90</i> ) chi angles: 69.5,270.9	0.157Å	-	OUTLIER(S) worst is CA- CB-CG: 4.063 σ
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A 369	GLN	99.99	-	Favored (72.61%) General / -58.2,-36.0	94% ( <i>mt-30</i> ) chi angles: 298.5,182.2,328.8	0.078Å	-	-
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A 370	GLU	50	1.175Å HA with A 374 ASP HB3	Favored (64.4%) General / -70.7,-45.8	7.2% ( <i>pt-20</i> ) chi angles: 79,170,55.5	0.244Å	-	-
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A 371	GLY	50	-	Favored (96.7%) Glycine / -63.2,-38.6	-	-	-	-
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A 372	ALA	50	-	Allowed (0.51%) General / -64.5,-66.7	-	0.041Å	-	-
A 373	LEU	99.99	-	Favored (4.84%) General / -121.4,-27.3	8.8% ( <i>tt</i> ) chi angles: 185.5,158.6	0.058Å	-	-
A 374	ASP	99.99	1.175Å HB3 with A 370 GLU HA	Favored (75.73%) General / -63.8,-33.5	2.3% ( <i>t70</i> ) chi angles: 165.1,274	0.153Å	-	OUTLIER(S) worst is CA- CB-CG: 5.827 σ
A 375	ASP	99.99	0.546Å CG with A 378 TRP HB2	Favored (12.56%) General / -108.0,24.7	42.7% ( <i>t0</i> ) chi angles: 191.3,331.1	0.038Å	-	-
A 376	SER	99.99	-	Favored (4.08%) General / 53.7,24.1	37.5% ( <i>t</i> ) chi angles: 182.1	0.083Å	-	-
A 377	GLY	50	-	Allowed (0.95%) Glycine / 96.9,61.6	-	-	-	-
A 378	TRP	99.99	0.546Å HB2 with A 375 ASP CG	Favored (21.15%) General / -93.5,149.5	77.1% ( <i>t-105</i> ) chi angles: 181.5,254.5	0.11Å	OUTLIER(S) worst is NE1-- CE2: 4.006 σ	-
A 379	LEU	50	-	Favored (4.13%) General / -111.2,92.7	9.4% ( <i>tt</i> ) chi angles: 186.7,157	0.089Å	-	-
A 380	ILE	99.99	0.529Å HD12 with A 366 PHE HZ	Allowed (1.5%) Isoleucine or valine / -70.7,105.5	47.4% ( <i>mt</i> ) chi angles: 307.7,178.2	0.103Å	-	-
A 381	LYS	50	0.585Å HG3 with A 382 ASN ND2	Allowed (0.3%) General / -88.2,-79.6	27.3% ( <i>tptp</i> ) chi angles: 186.1,63.3,182.9,70.2	0.084Å	-	-
A 382	ASN	50	0.585Å ND2 with A 381 LYS HG3	Favored (34.79%) General / -111.0,147.4	33.1% ( <i>m-80</i> ) chi angles: 294.2,267.3	0.043Å	-	-

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

Avg: Clashscore: 58.17 Outliers: 4 of 102 Poor rotamers: 6 of 92 Outliers: 0 of 97 Outliers: 2 of 104 Outliers: 5 of 104  
Favored

A 383	VAL	99.99	0.449Å HB with A 357 ILE HG13	(54.28%) Isoleucine or valine / -134.0,129.6	92.3% ( <i>t</i> ) chi angles: 177	0.049Å	-	-
A 384	LEU	50	0.586Å O with A 400 THR HA	Favored (14.22%) General / -116.0,106.8	16.8% ( <i>tp</i> ) chi angles: 190.7,50.4	0.027Å	-	-
A 385	SER	50	0.558Å HA with A 400 THR HG22	Favored (5.25%) General / -123.8,97.2	30.7% ( <i>t</i> ) chi angles: 184.8	0.032Å	-	-
A 386	MET	50	0.479Å HE1 with A 415 GLU O	Favored (22.36%) Pre-proline / -113.8,137.6	0.1% chi angles: 312.3,236.2,266	0.022Å	-	-
A 387	PRO	50	0.807Å HD2 with A 354 ILE HG22	Favored (60.38%) Trans-proline / -71.3,151.3	44.5% ( <i>Cg_endo</i> ) chi angles: 35.6	0.034Å	-	-
A 388	ILE	50	0.534Å O with A 395 ILE HD12	Favored (49.97%) Isoleucine or valine / -118.0,115.9	96.6% ( <i>mt</i> ) chi angles: 295.6,172.8	0.08Å	-	-
A 389	VAL	50	0.52Å O with A 426 GLY HA3	Favored (24.57%) Isoleucine or valine / -116.8,144.4	33.6% ( <i>m</i> ) chi angles: 299.6	0.076Å	-	-
A 390	ASN	50	-	Favored (3.97%) General / -73.7,179.8	36.2% ( <i>p30</i> ) chi angles: 59.5,28.4	0.039Å	-	-
A 391	LYS	50	0.687Å HG2 with A 427 TRP HD1	Favored (61.97%) General / -56.0,-30.5	31.9% ( <i>mmmt</i> ) chi angles: 295.9,303,283.7,181.4	0.09Å	-	-
A 392	LYS	50	-	Favored (16.66%) General / -84.3,8.2	56% ( <i>mtpt</i> ) chi angles: 294.8,184.3,66.7,181.9	0.041Å	-	-
A 393	GLU	50	-	Favored (3.48%) General / 72.1,0.2	50.6% ( <i>mt-10</i> ) chi angles: 293,175.2,289.3	0.129Å	-	-
A 394	GLU	50	0.412Å O with A 389 VAL HA	Favored (45.83%) General / -55.4,138.6	68.1% ( <i>mt-10</i> ) chi angles: 297.9,163.1,329	0.104Å	-	-

A 395	ILE	50	0.638Å HD13 with A 387 PRO HB2	Favored (35.29%) Isoleucine or valine / -83.9,120.7	9.2% ( <i>tp</i> ) chi angles: 185.5,60.8	0.108Å	-	-	
A 396	VAL	50	-	Favored (9.68%) Isoleucine or valine / -108.4,-14.8	35% ( <i>m</i> ) chi angles: 298.3	0.091Å	-	-	
A 397	GLY	50	-	Favored (27.91%) Glycine / -175.9,160.1	-	-	-	-	
A 398	VAL	50	-	Favored (40.85%) Isoleucine or valine / -125.9,143.0	26.2% ( <i>t</i> ) chi angles: 186.5	0.04Å	-	-	
A 399	ALA	50	-	Favored (33.85%) General / -135.4,129.8	-	0.042Å	-	-	
A 400	THR	50	0.586Å HA with A 384 LEU O	Favored (47.65%) General / -134.9,144.8	6.5% ( <i>p</i> ) chi angles: 79.5	0.048Å	-	-	
A 401	PHE	50	-	Favored (55.49%) General / -120.4,133.1	1.4% ( <i>m-85</i> ) chi angles: 292.6,37.5	0.04Å	-	-	
A 402	TYR	50	-	Favored (55.46%) General / -115.3,134.1	55.1% ( <i>p90</i> ) chi angles: 62.3,88.4	0.018Å	-	-	
#	Alt	Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
			Avg: 58.17	Clashscore: 34.99	Outliers: 4 of 102	Poor rotamers: 6 of 92	Outliers: 0 of 97	Outliers: 2 of 104	Outliers: 5 of 104
A 403	ASN	50	-	Allowed (0.08%) General / 57.5,86.0	97.5% ( <i>m-20</i> ) chi angles: 292,341.2	0.031Å	-	-	
A 404	ARG	99.99	0.674Å NH1 with A 405 LYS HB3	Favored (3.65%) General / -58.5,116.4	50.1% ( <i>tpt85</i> ) chi angles: 180.5,58.7,182.3,92.3	0.134Å	-	-	
A 405	LYS	99.99	0.674Å HB3 with A 404 ARG	OUTLIER (0.02%) General /	21.3% ( <i>pttp</i> ) chi angles: 61,188.7,179.9,58.3	0.037Å	-	-	

			NH1	42.3,22.6				
A 406	ASP	99.99	-	Favored (25.3%) General / 58.6,38.5	30.9% ( <i>t70</i> ) chi angles: 180.5,76.1	0.136Å	-	-
A 407	GLY	99.99	-	Favored (20.86%) Glycine / 174.5,159.5	-	-	-	-
A 408	LYS	50	0.658Å HB3 with A 405 LYS NZ	Allowed (0.1%) Pre-proline / 62.1,166.7	18.9% ( <i>tptp</i> ) chi angles: 170.8,82,190,61.3	0.109Å	-	OUTLIER(S) worst is CA- CB-CG: 4.745 σ
A 409	PRO	50	0.538Å HD2 with A 408 LYS HD2	Allowed (0.13%) Trans-proline / -90.1,-163.3	65.9% ( <i>Cg_endo</i> ) chi angles: 33.9	0.055Å	-	-
A 410	PHE	50	0.564Å HB2 with A 356 ASN HD21	Favored (45.33%) General / -99.6,125.3	18.1% ( <i>m-85</i> ) chi angles: 281.8,307.7	0.023Å	-	-
A 411	ASP	50	-	Favored (25.89%) General / -63.9,157.0	46.7% ( <i>m-20</i> ) chi angles: 299.7,294.7	0.017Å	-	-
A 412	GLU	50	-	Favored (94.36%) General / -60.2,-42.0	47.5% ( <i>tt0</i> ) chi angles: 195.9,183.8,328.9	0.073Å	-	-
A 413	GLN	50	-	Favored (80.1%) General / -59.0,-38.9	52.2% ( <i>tt0</i> ) chi angles: 182.3,184.9,58.1	0.027Å	-	-
A 414	ASP	50	-	Favored (96.86%) General / -60.6,-42.6	5.5% ( <i>m-20</i> ) chi angles: 265.4,333	0.113Å	-	-
A 415	GLU	50	0.479Å O with A 386 MET HE1	Favored (63.78%) General / -54.0,-51.5	31.1% ( <i>mt-10</i> ) chi angles: 286.7,165.5,280.4	0.06Å	-	-
A 416	VAL	50	0.432Å HA with A 419 GLU HG2	OUTLIER (0.07%) Isoleucine or valine / -51.5,-72.5	58.2% ( <i>t</i> ) chi angles: 180.4	0.099Å	-	-
A 417	LEU	50	-	Favored (3%) General / -41.9,-43.4	92.9% ( <i>mt</i> ) chi angles: 291.8,174.6	0.035Å	-	-
A			0.498Å	Favored (64.99%)	50.8% ( <i>tpp</i> )			

418	MET	50	O with A 422 THR HG23	General / -71.9,-43.7	chi angles: 183.6,68.7,62.2	0.055Å	-	-
A 419	GLU	50	0.432Å HG2 with A 416 VAL HA	Favored (64.8%) General / -72.5,-30.7	12.6% ( <i>pt-20</i> ) chi angles: 65.8,184,64.6	0.103Å	-	-
A 420	SER	50	0.756Å O with A 423 GLN HG2	Favored (2.12%) General / -62.7,-61.9	46.1% ( <i>t</i> ) chi angles: 178.9	0.019Å	-	-
A 421	LEU	50	-	Favored (62.83%) General / -53.7,-37.1	9.4% ( <i>tt</i> ) chi angles: 181.8,155.6	0.08Å	-	-
A 422	THR	50	0.498Å HG23 with A 418 MET O	Favored (82.43%) General / -65.9,-36.1	68.1% ( <i>p</i> ) chi angles: 59.6	0.084Å	-	-
<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: 34.99</div> <div>Outliers: 4 of 102</div> <div>Poor rotamers: 6 of 92</div> <div>Outliers: 0 of 97</div> <div>Outliers: 2 of 104</div> <div>Outliers: 5 of 104</div> </div>								
A 423	GLN	50	0.756Å HG2 with A 420 SER O	Favored (74.24%) General / -60.3,-34.8	10.9% ( <i>pt20</i> ) chi angles: 77.5,186.4,42.2	0.098Å	-	-
A 424	PHE	50	-	Favored (59.07%) General / -67.7,-50.1	43.7% ( <i>m-85</i> ) chi angles: 281.7,286.8	0.049Å	-	-
A 425	LEU	50	0.489Å O with A 429 VAL HG12	Favored (39.67%) General / -49.2,-42.1	90.5% ( <i>mt</i> ) chi angles: 291.8,175.8	0.075Å	-	-
A 426	GLY	50	0.52Å HA3 with A 389 VAL O	Favored (93.47%) Glycine / -58.6,-39.5	-	-	-	-
A 427	TRP	50	0.687Å HD1 with A 391 LYS HG2	Allowed (0.53%) General / -68.6,-66.8	71% ( <i>t90</i> ) chi angles: 185.2,78.1	0.056Å	-	-
A 428	SER	50	-	Favored (60.2%) General / -51.7,-40.5	43.6% ( <i>t</i> ) chi angles: 180.9	0.014Å	-	-
0.489Å				Favored (88.78%)				



A 429	VAL	50	HG12 with A 425 LEU O	Isoleucine or valine / -66.4,-41.4	9.3% ( <i>p</i> ) chi angles: 68.1	0.106Å	-	-
A 430	MET	50	-	Favored (82.04%) General / -63.3,-35.9	15.1% ( <i>tpt</i> ) chi angles: 185.4,58.8,180.7	0.013Å	-	-
A 431	ASN	50	-	Favored (87.03%) General / -67.0,-39.1	96.1% ( <i>m-20</i> ) chi angles: 287.3,333.8	0.025Å	-	-
A 432	THR	50	-	Favored (89.33%) General / -58.9,-42.3	98.4% ( <i>m</i> ) chi angles: 299	0.038Å	-	-
A 433	ASP	50	-	Favored (76.93%) General / -69.7,-38.5	38.8% ( <i>t70</i> ) chi angles: 184.3,62.9	0.052Å	-	-
A 434	THR	50	0.777Å HA with A 438 MET SD	Favored (62.6%) General / -71.9,-27.1	73.1% ( <i>p</i> ) chi angles: 63.5	0.109Å	-	-
A 435	TYR	50	-	Favored (45.31%) General / -77.5,-39.6	43.2% ( <i>t80</i> ) chi angles: 180.3,58.2	0.05Å	-	-
A 436	ASP	99.99	0.471Å O with A 438 MET HG2	Favored (2.07%) General / -114.2,-172.3	25.5% ( <i>p30</i> ) chi angles: 64,29.1	0.084Å	-	-
A 437	LYS	99.99	0.944Å HA with A 441 LEU HD12	OUTLIER (0.04%) General / 47.8,13.5	24.1% ( <i>tptp</i> ) chi angles: 189.4,59.6,189.7,68.1	0.212Å	-	-
A 438	MET	99.99	0.777Å SD with A 434 THR HA	OUTLIER (0.01%) General / -173.3,-79.6	21.8% ( <i>ptp</i> ) chi angles: 65.9,170.8,76.6	0.173Å	-	OUTLIER(S) worst is CA- C-N: 6.579 σ
A 439	ASN	50	0.626Å H with A 438 MET HG3	Favored (28.94%) General / -62.6,-55.2	20% ( <i>m120</i> ) chi angles: 290.3,137.3	0.148Å	-	-
A 440	LYS	50	-	Favored (75.39%) General / -56.2,-41.3	32% ( <i>mmmt</i> ) chi angles: 291.2,294.3,294,180.9	0.016Å	-	-
A	LEU	50	0.944Å HD12 with A	Favored (63.03%)	19.3% ( <i>mt</i> ) chi angles: 282.8,186.2	0.168Å	OUTLIER(S) worst is C--O:	-

441			437 LYS HA		General / -68.6,-48.9		4.694 $\sigma$		
A 442	GLU	50	-		Favored (65.71%) General / -57.0,-32.0	59.7% ( <i>mt-10</i> ) chi angles: 281.5,170.7,321.4	0.048 Å	-	-
#	Alt	Res	High B	Clash > 0.4 Å	Ramachandran	Rotamer	C $\beta$ deviation	Bond lengths	Bond angles
			Avg: 58.17	Clashscore: 34.99	Outliers: 4 of 102	Poor rotamers: 6 of 92	Outliers: 0 of 97	Outliers: 2 of 104	Outliers: 5 of 104
A 443	ASN	50	-		Allowed (0.51%) General / -63.7,-66.7	0.7% chi angles: 254.5,112	0.044 Å	-	-
A 444	ARG	50	-		Favored (5.47%) General / -44.9,-39.5	21.2% ( <i>tpp85</i> ) chi angles: 182.6,60.7,67.3,81.2	0.023 Å	-	-
A 445	LYS	50	-		Favored (96.86%) General / -62.8,-44.2	39% ( <i>ttpt</i> ) chi angles: 185.1,182.64,181.3	0.027 Å	-	-
A 446	ASP	99.99	-		-	34.8% ( <i>t70</i> ) chi angles: 185.5,68.8	0.055 Å	-	-

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