



Viewing TULP1_sm_291-536H-multi.table

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All-Atom Contacts	Clashscore, all atoms:	9.86		72 nd percentile* (N=1784, all resolutions)
	Clashscore is the number of serious steric overlaps (> 0.4 Å) per 1000 atoms.			
Protein Geometry	Poor rotamers	0	0.00%	Goal: <1%
	Ramachandran outliers	3	1.23%	Goal: <0.05%
	Ramachandran favored	228	93.44%	Goal: >98%
	MolProbity score^	1.94		79 th percentile* (N=27675, 0Å - 99Å)
	Cβ deviations >0.25Å	1	0.44%	Goal: 0
	Bad backbone bonds:	5 / 2017	0.25%	Goal: 0%
	Bad backbone angles:	1 / 2727	0.04%	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	Cβ deviation	Bond lengths	Bond angles
		Avg: 54.27	Clashscore: 9.86	Outliers: 3 of 244	Poor rotamers: 0 of 213	Outliers: 1 of 229	Outliers: 4 of 246	Outliers: 1 of 246
A 291	PRO	50	-	-	55.4% (Cg_exo) chi angles: 326.9	0.047Å	-	-
A 292	ARG	50	-	Favored (68.9%) General / -54.4,-41.2	50.3% (ttm-85) chi angles: 190.4,187.3,300.9,290.8	0.073Å	-	-
A 293	GLU	50	-	Favored (3.72%) General / -63.1,-60.2	4.9% (tm-20) chi angles: 167.6,263.4,324	0.058Å	-	-
A 294	PHE	50	-	Favored (43.73%) General / -52.8,-53.7	77.4% (t80) chi angles: 182.3,84.5	0.026Å	-	-
A 295	VAL	50	-	Favored (21.57%) Isoleucine or valine / -59.3,-22.0	32.8% (m) chi angles: 300.3	0.124Å	-	-

A 296	LEU	50	-	Favored (23.16%) General / -94.2,-16.9	87.8% (<i>mt</i>) chi angles: 290.9,175.2	0.046Å	-	-
A 297	ARG	50	-	Favored (59.45%) Pre-proline / -78.8,135.4	90.8% (<i>mtt180</i>) chi angles: 285.3,195.7,181.5,175.3	0.092Å	-	-
A 298	PRO	50	-	Favored (98.09%) Trans-proline / -59.9,142.2	82.2% (<i>Cg_exo</i>) chi angles: 330.8	0.085Å	-	-
A 299	ALA	50	-	Favored (60.28%) Pre-proline / -55.8,143.4	-	0.014Å	-	-
A 300	PRO	50	-	Favored (92.62%) Trans-proline / -60.0,147.5	89.8% (<i>Cg_exo</i>) chi angles: 329	0.067Å	-	-
A 301	GLN	50	-	Favored (36.07%) General / -52.7,134.4	97.1% (<i>mm-40</i>) chi angles: 294.3,299.7,318.9	0.062Å	-	-
A 302	GLY	50	-	Favored (56.78%) Glycine / 66.8,10.9	-	-	-	-
A 303	ARG	50	-	Favored (26.54%) General / -112.8,154.3	51.5% (<i>mtt180</i>) chi angles: 303.5,192.4,207.3,165.4	0.049Å	-	-
A 304	THR	50	-	Favored (48.32%) General / -117.6,124.3	59% (<i>m</i>) chi angles: 304.1	0.068Å	-	-
A 305	VAL	50	-	Favored (34.42%) Isoleucine or valine / -95.5,115.4	47.9% (<i>t</i>) chi angles: 182.9	0.046Å	-	-
A 306	ARG	50	-	Favored (51.33%) General / -103.9,126.9	79.2% (<i>mtt85</i>) chi angles: 293.9,184.4,183.1,102.4	0.016Å	-	-
A 307	CYS	50	-	Favored (38.69%) General / -128.1,158.2	64.6% (<i>m</i>) chi angles: 302.5	0.066Å	-	-
A 308	ARG	50	-	Favored (45.13%) General /	59.2% (<i>ttt85</i>) chi angles:	0.073Å	-	-

-117.9,123.1 182.3,178.6,178.1,90.8

A 309	LEU	50	-	Favored (51.05%) General / -110.5,124.0	6.9% (<i>tt</i>) chi angles: 189.1,164.8	0.063Å	-	-	
A 310	THR	50	-	Favored (42.68%) General / -123.8,152.0	74.4% (<i>p</i>) chi angles: 60	0.052Å	-	-	
#	Alt	Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
			Avg: 54.27	Clashscore: 9.86	Outliers: 3 of 244	Poor rotamers: 0 of 213	Outliers: 1 of 229	Outliers: 4 of 246	Outliers: 1 of 246
A 311	ARG	50	-	Favored (39.61%) General / -130.1,158.4	38.7% (<i>ptt180</i>) chi angles: 64.1,178.9,180.1,190.1	0.013Å	-	-	
A 312	ASP	50	-	Favored (42.76%) General / -53.9,135.0	79.7% (<i>m-20</i>) chi angles: 297.5,331.3	0.045Å	-	-	
A 313	LYS	99.99	-	Favored (48.14%) General / -63.5,131.4	22.6% (<i>pttp</i>) chi angles: 61.4,178.6,182.8,65.3	0.015Å	-	-	
A 314	LYS	99.99	-	Favored (50.77%) General / -130.3,151.5	22.6% (<i>pttp</i>) chi angles: 61.1,181,182.7,64.5	0.029Å	-	-	
A 315	GLY	99.99	-	Favored (43.58%) Glycine / -81.9,-169.8	-	-	-	-	
A 316	MET	99.99	0.43Å HG3 with A 316 MET O	Favored (2.55%) General / -99.8,82.2	24.7% (<i>ptp</i>) chi angles: 58.9,178.4,71	0.045Å	-	-	
A 317	ASP	99.99	-	Favored (10.91%) General / -169.3,164.9	29.7% (<i>p-10</i>) chi angles: 64.6,336.7	0.032Å	-	-	
A 318	ARG	99.99	0.455Å O with A 320 MET HE2	Favored (50.72%) General / -61.2,145.6	30.2% (<i>ptt-85</i>) chi angles: 56.6,191.4,181.8,263.7	0.016Å	-	-	
A 319	GLY	99.99	0.402Å HA3 with A 320 MET CB	Favored (20.01%) Glycine / -179.9,-157.4	-	-	-	OUTLIER(S) worst is C-N- CA: 5.483 σ	

Allowed

A 320	MET	50	0.455Å HE2 with A 318 ARG O	(0.07%) General / 170.9,175.4	2% (<i>mtm</i>) chi angles: 244.1,163.2,290.4	0.111Å	-	-
A 321	TYR	50	-	Favored (62.99%) Pre-proline / -136.1,67.8	53% (<i>m-85</i>) chi angles: 308,274.5	0.042Å	-	-
A 322	PRO	50	-	Favored (26.25%) Trans-proline / -77.5,148.3	68% (<i>Cg_endo</i>) chi angles: 33.7	0.037Å	-	-
A 323	SER	50	-	Favored (31.21%) General / -80.5,146.6	48.7% (<i>m</i>) chi angles: 300.5	0.051Å	-	-
A 324	TYR	50	-	Favored (48.66%) General / -119.7,142.2	88.9% (<i>m-85</i>) chi angles: 299.1,86.4	0.081Å	-	-
A 325	PHE	50	-	Favored (51.84%) General / -130.6,145.2	57.8% (<i>m-85</i>) chi angles: 307,273.8	0.045Å	-	-
A 326	LEU	50	-	Favored (30.18%) General / -128.7,122.2	25% (<i>tp</i>) chi angles: 190.2,68.8	0.053Å	-	-
A 327	HIS	50	-	Favored (39.5%) General / -122.8,153.5	77.5% (<i>m80</i>) chi angles: 295.9,80.8	0.088Å	OUTLIER(S) worst is CG-- ND1: 4.479 σ	-
A 328	LEU	50	0.403Å HD12 with A 334 VAL CG1	Favored (58.4%) General / -62.7,138.0	44% (<i>mt</i>) chi angles: 291,185.2	0.04Å	-	-
A 329	ASP	50	-	Allowed (1.28%) General / -88.1,45.4	29.9% (<i>t0</i>) chi angles: 193.8,32	0.089Å	-	-
A 330	THR	50	0.494Å HG23 with A 332 LYS O	Favored (9.94%) General / -103.5,167.2	6.4% (<i>t</i>) chi angles: 177.8	0.057Å	-	-

#	Alt	Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
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Avg: 54.27	Clashscore: 9.86	Outliers: 3 of 244	Poor rotamers: 0 of 213	Outliers: 1 of 229	Outliers: 4 of 246	Outliers: 1 of 246
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A	GLU	50	-	Favored (71.48%)	2.4% (<i>mm-40</i>) chi angles:	0.052Å	-	-
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331				General / -62.5,-30.7	320.2,319.6,278.4			
A 332	LYS	50	0.494Å O with A 330 THR HG23	Favored (4.1%) General / -94.1,81.3	50.7% (tttt) chi angles: 182.7,209.6,177.5,187.4	0.077Å	-	-
A 333	LYS	50	-	Allowed (0.08%) General / -66.0,80.1	54.8% (mttp) chi angles: 304,171.7,182.2,61.4	0.048Å	-	-
A 334	VAL	50	0.403Å CG1 with A 328 LEU HD12	Favored (26.05%) Isoleucine or valine / -72.9,136.2	8.6% (p) chi angles: 68.5	0.118Å	-	-
A 335	PHE	50	0.447Å CE1 with A 356 PRO HB3	Favored (52.34%) General / -70.3,141.5	84.6% (t80) chi angles: 173.6,78.3	0.077Å	-	-
A 336	LEU	50	-	Allowed (1.77%) General / -118.0,-60.7	90.1% (mt) chi angles: 298.8,179.4	0.025Å	-	-
A 337	LEU	50	-	Favored (33.12%) General / -148.3,150.2	86.1% (mt) chi angles: 293.3,168.6	0.074Å	-	-
A 338	ALA	50	-	Favored (52.21%) General / -132.5,150.1	-	0.045Å	-	-
A 339	GLY	50	-	Favored (23.19%) Glycine / -146.5,150.9	-	-	-	-
A 340	ARG	50	0.673Å HH11 with A 359 LEU CD1	Favored (16.75%) General / -154.6,139.0	34.9% (ttt180) chi angles: 185.4,173.1,178,230.6	0.02Å	-	-
A 341	LYS	50	-	Favored (42.88%) General / -73.3,132.2	87.1% (tttt) chi angles: 188.2,175.1,180.7,176.2	0.095Å	-	-
A 342	ARG	50	0.773Å HH22 with A 344 ARG NH2	Favored (32.35%) General / -80.6,127.3	61.3% (mtp85) chi angles: 295.5,174.3,64.3,67.5	0.104Å	-	-
A 343	LYS	50	-	Favored (60.57%) General / -74.4,-27.4	12.3% (ptmt) chi angles: 53.9,209.8,301,182.7	0.134Å	-	-
			0.773Å	Allowed	27.5% (ptt-85)			

A 344	ARG	50	NH2 with A 342 ARG HH22	(1.27%) General / -94.4,34.7	chi angles: 65.6,171.2,177.8,283.4	0.098Å	-	-
A 345	SER	50	-	Favored (46.41%) General / -115.9,142.7	61.4% (<i>m</i>) chi angles: 292	0.017Å	-	-
A 346	LYS	50	-	Favored (81.37%) General / -63.5,-35.7	83.8% (<i>mttt</i>) chi angles: 308.3,174.9,190.5,181.3	0.049Å	-	-
A 347	THR	50	-	Favored (17.55%) General / -119.2,163.2	81.4% (<i>p</i>) chi angles: 61.1	0.051Å	-	-
A 348	ALA	50	-	Favored (14.89%) General / -55.4,123.7	-	0.021Å	-	-
A 349	ASN	50	-	Favored (4.54%) General / -144.1,107.3	57.7% (<i>t-20</i>) chi angles: 184.1,339.9	0.068Å	-	-
A 350	TYR	50	0.534Å HB2 with A 370 LEU HB3	Favored (48.77%) General / -102.2,131.5	62.4% (<i>m-85</i>) chi angles: 291.3,78.2	0.077Å	-	-
#	Alt Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
		Avg: 54.27	Clashscore: 9.86	Outliers: 3 of 244	Poor rotamers: 0 of 213	Outliers: 1 of 229	Outliers: 4 of 246	Outliers: 1 of 246
A 351	LEU	50	0.724Å HD22 with A 361 ARG HD3	Favored (40.45%) General / -95.9,133.1	74.9% (<i>mt</i>) chi angles: 300.5,183.1	0.04Å	-	-
A 352	ILE	50	-	Favored (53.95%) Isoleucine or valine / -115.8,136.0	61.9% (<i>mt</i>) chi angles: 305.6,171.6	0.073Å	-	-
A 353	SER	50	-	Favored (50.94%) General / -135.0,155.3	46% (<i>t</i>) chi angles: 178.9	0.07Å	-	-
A 354	ILE	50	-	Favored (6.54%) Isoleucine or valine / -101.3,12.7	48.1% (<i>pt</i>) chi angles: 59.5,172.5	0.064Å	-	-
				Favored				

A 355	ASP	50	-	(29.47%) Pre-proline / -124.4,107.8	46.9% (<i>t0</i>) chi angles: 187.4,331.1	0.021Å	-	-
A 356	PRO	50	0.447Å HB3 with A 335 PHE CE1	Favored (63.69%) Trans-proline / -64.9,-22.0	94.7% (<i>Cg_endo</i>) chi angles: 32.2	0.058Å	-	-
A 357	THR	50	-	Favored (56.88%) General / -93.0,-1.2	30.8% (<i>p</i>) chi angles: 69.8	0.006Å	-	-
A 358	ASN	99.99	-	Favored (56.82%) General / -116.5,131.9	53.5% (<i>t30</i>) chi angles: 184.4,26.4	0.056Å	-	-
A 359	LEU	99.99	0.673Å CD1 with A 340 ARG HH11	Favored (11.74%) General / -105.6,-26.7	7.3% (<i>tt</i>) chi angles: 184.6,162.3	0.045Å	-	-
A 360	SER	99.99	-	Favored (29.51%) General / -57.9,147.2	46.3% (<i>t</i>) chi angles: 180.5	0.061Å	-	-
A 361	ARG	99.99	0.883Å HA with A 366 PHE HB2	Allowed (1.39%) General / -117.5,79.7	16.7% (<i>ptt180</i>) chi angles: 68.3,156.6,170.9,198	0.122Å	-	-
A 362	GLY	99.99	-	Favored (23.9%) Glycine / 173.4,161.6	-	-	-	-
A 363	GLY	99.99	-	Allowed (0.64%) Glycine / 64.7,-102.5	-	-	-	-
A 364	GLU	99.99	0.566Å HG2 with A 365 ASN ND2	Favored (34.08%) General / -81.9,-26.5	5.1% (<i>pm0</i>) chi angles: 59.8,291.7,338.6	0.295Å	-	-
A 365	ASN	50	0.566Å ND2 with A 364 GLU HG2	Allowed (0.46%) General / -149.2,-1.8	70.7% (<i>m-80</i>) chi angles: 299.2,293.6	0.176Å	-	-
A 366	PHE	50	0.883Å HB2 with A 361 ARG HA	Favored (26.76%) General / -64.3,126.1	16.2% (<i>t80</i>) chi angles: 175.2,45.6	0.2Å	-	-
A 367	ILE	50	-	Allowed (1.97%) Isoleucine or valine /	9.8% (<i>tp</i>) chi angles: 199,65.4	0.158Å	-	-

-119.0,-28.7

A 368	GLY	50	-	Favored (43.04%) Glycine / -168.8,176.3	-	-	-	-
A 369	LYS	50	-	Favored (24.69%) General / -148.5,141.4	36% (<i>ttpt</i>) chi angles: 173.5,164.3,60.2,180.2	0.053Å	-	-
A 370	LEU	50	0.534Å HB3 with A 350 TYR HB2	Favored (19.52%) General / -114.2,110.2	50.7% (<i>tp</i>) chi angles: 177,68.4	0.044Å	-	-

#	Alt	Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
			Avg: 54.27	Clashscore: 9.86	Outliers: 3 of 244	Poor rotamers: 0 of 213	Outliers: 1 of 229	Outliers: 4 of 246	Outliers: 1 of 246
A 371	ARG	50	-	Favored (56.98%) General / -114.9,130.8	42.7% (<i>ttp180</i>) chi angles: 182.1,199.5,63.1,178.4	0.097Å	-	-	
A 372	SER	50	-	Favored (17.19%) General / -92.8,156.1	59.5% (<i>p</i>) chi angles: 71.5	0.052Å	-	-	
A 373	ASN	50	-	Favored (7.38%) General / -70.2,172.9	41.9% (<i>p-10</i>) chi angles: 65.5,340.6	0.046Å	-	-	
A 374	LEU	50	-	Favored (80.45%) General / -58.4,-39.7	3% (<i>tt</i>) chi angles: 200.2,141.4	0.069Å	-	-	
A 375	LEU	50	-	Favored (93.36%) General / -65.4,-40.3	86.5% (<i>mt</i>) chi angles: 294.6,179.3	0.079Å	-	-	
A 376	GLY	50	-	Favored (42.09%) Glycine / 97.9,13.8	-	-	-	-	
A 377	ASN	50	-	Favored (16.29%) General / -108.0,-7.1	34.1% (<i>p-10</i>) chi angles: 64.9,334.6	0.033Å	-	-	
A 378	ARG	50	-	Favored (51.92%) General / -127.5,140.8	83.6% (<i>mtt180</i>) chi angles: 297.5,187.1,180.2,204.8	0.012Å	-	-	
				Favored					

A 379	PHE	50	-	(49.35%) General / -133.8,145.0	88.5% (<i>m-85</i>) chi angles: 295.8,83.2	0.082Å	-	-
A 380	THR	50	-	Favored (50.59%) General / -121.8,142.1	55.4% (<i>m</i>) chi angles: 304.5	0.038Å	-	-
A 381	VAL	50	-	Favored (67.69%) Isoleucine or valine / -110.4,126.2	46.2% (<i>t</i>) chi angles: 183.5	0.063Å	-	-
A 382	PHE	50	-	Favored (35.61%) General / -116.5,151.7	90.6% (<i>m-85</i>) chi angles: 302.2,276.8	0.098Å	-	-
A 383	ASP	50	0.424Å OD2 with A 401 GLN HG2	OUTLIER (0.03%) General / -71.2,-156.2	50.3% (<i>p-10</i>) chi angles: 67.5,355.7	0.097Å	-	-
A 384	ASN	50	-	Favored (13.32%) General / -97.4,19.4	52.4% (<i>p-10</i>) chi angles: 62.5,359.4	0.062Å	-	-
A 385	GLY	50	0.427Å HA3 with A 400 ARG HA	Favored (54.85%) Glycine / -75.0,168.1	-	-	-	-
A 386	GLN	50	0.421Å HG2 with A 387 ASN N	Favored (42.9%) General / -74.9,145.2	10.2% (<i>tt0</i>) chi angles: 187.1,202.1,108.6	0.06Å	-	-
A 387	ASN	50	0.421Å N with A 386 GLN HG2	Favored (90.28%) Pre-proline / -71.9,127.8	55.2% (<i>t-20</i>) chi angles: 183.1,338	0.049Å	-	-
A 388	PRO	50	-	Favored (40.88%) Trans-proline / -66.0,-33.5	78.1% (<i>Cg_exo</i>) chi angles: 332.1	0.075Å	-	-
A 389	GLN	50	0.455Å HE22 with A 441 ASN HA	Favored (65.04%) General / -62.5,-20.9	2.9% (<i>mp0</i>) chi angles: 270.1,49.4,256.2	0.022Å	-	-
A 390	ARG	50	-	Favored (56.94%) General / -84.5,-11.0	6% (<i>mmp_?</i>) chi angles: 299.3,276.8,109.4,113.8	0.038Å	-	-

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

Avg: Clashscore: 54.27 9.86				Outliers: 3 of 244	Poor rotamers: 0 of 213	Outliers: 1 of 229	Outliers: 4 of 246	Outliers: 1 of 246
A 391	GLY	50	-	Allowed (0.12%) Glycine / 178.9,98.7	-	-	-	-
A 392	TYR	50	-	Favored (64.78%) General / -68.3,-21.3	13.8% (<i>t80</i>) chi angles: 195.7,54.6	0.049Å	-	-
A 393	SER	50	-	Favored (58.85%) General / -87.8,-4.6	61.1% (<i>m</i>) chi angles: 299	0.034Å	-	-
A 394	THR	50	-	Favored (58.82%) General / -64.8,140.0	98.8% (<i>m</i>) chi angles: 298.9	0.09Å	-	-
A 395	ASN	50	-	Favored (44.46%) General / -54.5,136.5	45.8% (<i>t30</i>) chi angles: 182.2,22.6	0.073Å	-	-
A 396	VAL	50	-	Favored (60.25%) Isoleucine or valine / -56.2,-39.6	62% (<i>t</i>) chi angles: 181.5	0.021Å	-	-
A 397	ALA	50	-	Favored (68.36%) General / -60.2,-28.9	-	0.02Å	-	-
A 398	SER	50	-	Favored (57.11%) General / -86.4,-9.1	60.9% (<i>m</i>) chi angles: 299.1	0.04Å	-	-
A 399	LEU	50	-	Favored (49.41%) General / -71.8,140.4	89.1% (<i>mt</i>) chi angles: 298.1,180.2	0.016Å	-	-
A 400	ARG	50	0.427Å HA with A 385 GLY HA3	Favored (57.29%) General / -61.8,142.4	40.1% (<i>ptt180</i>) chi angles: 65.5,184.2,188.6,185.4	0.014Å	-	-
A 401	GLN	50	0.424Å HG2 with A 383 ASP OD2	Favored (20.71%) General / -105.9,154.3	15.9% (<i>pt20</i>) chi angles: 69.8,184.3,285.6	0.043Å	-	-
A 402	GLU	50	-	Favored (38.95%) General /	71.9% (<i>mt-10</i>) chi angles: 295.5,188.6,18.1	0.034Å	-	-

A 403	LEU	50	-	-96.1,122.4 Favored (15.18%) General / -96.3,-26.9	95.9% (<i>mt</i>) chi angles: 295.9,174.2	0.018Å	-	-	
A 404	ALA	50	-	Favored (2.72%) General / -172.4,152.6	-	0.045Å	-	-	
A 405	ALA	50	-	Favored (49.17%) General / -132.7,142.7	-	0.079Å	-	-	
A 406	VAL	50	-	Favored (69.77%) Isoleucine or valine / -127.3,128.1	40.4% (<i>t</i>) chi angles: 184.8	0.037Å	-	-	
A 407	ILE	50	-	Favored (69.59%) Isoleucine or valine / -117.3,122.3	4.2% (<i>mp</i>) chi angles: 305.6,81.2	0.015Å	-	-	
A 408	TYR	50	-	Favored (45.92%) General / -104.7,135.5	91.2% (<i>m-85</i>) chi angles: 291.1,273.5	0.083Å	-	-	
A 409	GLU	50	-	Favored (40.22%) General / -75.7,146.3	67.8% (<i>mt-10</i>) chi angles: 286.2,184.6,23	0.042Å	-	-	
A 410	THR	50	-	Favored (43.99%) General / -97.0,131.2	89.8% (<i>m</i>) chi angles: 297.8	0.08Å	-	-	
#	Alt	Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
			Avg: 54.27	Clashscore: 9.86	Outliers: 3 of 244	Poor rotamers: 0 of 213	Outliers: 1 of 229	Outliers: 4 of 246	Outliers: 1 of 246
A 411	ASN	50		0.812Å ND2 with A 417 GLY HA3	Favored (23.4%) General / -83.3,155.8	87.1% (<i>m-20</i>) chi angles: 296.2,332.7	0.032Å	-	-
A 412	VAL	99.99		-	Favored (43.07%) Isoleucine or valine / -132.2,157.3	14.7% (<i>p</i>) chi angles: 64	0.099Å	-	-
A 413	LEU	99.99		0.408Å C with A 413 LEU HD23	Favored (42.83%) General /	7.1% (<i>tt</i>) chi angles: 184.5,163.3	0.052Å	-	-

A 414	GLY	99.99	-	-55.6,130.4 Favored (33.07%) Glycine / 105.7,-22.0	-	-	-	-
A 415	PHE	99.99	-	Favored (43.48%) General / -116.8,145.5	72.7% (<i>t80</i>) chi angles: 185.5,80.8	0.078Å	-	-
A 416	ARG	99.99	-	Favored (21.54%) General / -90.3,151.3	32.8% (<i>ptt-85</i>) chi angles: 62.3,176.9,178,274.6	0.051Å	-	-
A 417	GLY	99.99	0.812Å HA3 with A 411 ASN ND2	OUTLIER (0.09%) Glycine / -176.1,93.3	-	-	-	-
A 418	PRO	50	0.692Å O with A 417 GLY HA2	OUTLIER (0.07%) Trans-proline / -30.6,127.8	61% (<i>Cg_endo</i>) chi angles: 27.3	0.037Å	OUTLIER(S) worst is C--N: 6.839 σ	-
A 419	ARG	50	-	Favored (26.48%) General / -88.4,144.3	89.6% (<i>mtm180</i>) chi angles: 291.9,177.2,296.2,168.8	0.04Å	-	-
A 420	ARG	50	-	Favored (54.7%) General / -68.3,137.4	98.9% (<i>mtt180</i>) chi angles: 295.4,184,186.9,170.5	0.032Å	-	-
A 421	MET	50	-	Favored (48.9%) General / -119.9,142.2	78.7% (<i>mtp</i>) chi angles: 299.2,177.5,57.1	0.132Å	-	-
A 422	THR	50	-	Favored (53.69%) General / -121.4,130.6	68.8% (<i>m</i>) chi angles: 303.3	0.04Å	-	-
A 423	VAL	50	-	Favored (75.97%) Isoleucine or valine / -120.3,128.3	64.5% (<i>t</i>) chi angles: 179.8	0.05Å	-	-
A 424	ILE	50	-	Favored (73.73%) Isoleucine or valine / -118.5,130.2	40.9% (<i>mm</i>) chi angles: 307.2,299.2	0.044Å	-	-
A 425	ILE	50	-	Favored (66.6%) Pre-proline /	49.9% (<i>pt</i>) chi angles: 61.5,172.1	0.089Å	-	-

-131.1,160.5

A 426	PRO	50	-	Favored (94.48%) Trans-proline / -62.6,144.6	90.4% (<i>Cg_exo</i>) chi angles: 330	0.07Å	-	-
A 427	GLY	50	-	Favored (34.97%) Glycine / -63.6,161.8	-	-	-	-
A 428	MET	50	-	Favored (39.57%) General / -114.8,147.6	86% (<i>mmm</i>) chi angles: 308.2,299.1,286.6	0.089Å	-	-
A 429	SER	50	0.515Å OG with A 431 GLU HB3	Favored (11.79%) General / -77.3,173.6	78.9% (<i>p</i>) chi angles: 59.5	0.05Å	-	-
A 430	ALA	50	-	Favored (66.67%) General / -65.5,-21.8	-	0.021Å	-	-

#	Alt	Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
			Avg: 54.27	Clashscore: 9.86	Outliers: 3 of 244	Poor rotamers: 0 of 213	Outliers: 1 of 229	Outliers: 4 of 246	Outliers: 1 of 246
A 431	GLU	50	0.515Å HB3 with A 429 SER OG	-	Favored (66.44%) General / -66.0,-22.1	14.1% (<i>tp10</i>) chi angles: 178.9,89.7,22.9	0.098Å	-	-
A 432	ASN	50	-	-	Allowed (1.44%) General / 72.9,32.1	9.2% (<i>m120</i>) chi angles: 301.2,158.9	0.097Å	-	-
A 433	GLU	50	-	-	Favored (31.94%) General / -118.3,154.6	69.3% (<i>mt-10</i>) chi angles: 282.7,183.2,325	0.031Å	-	-
A 434	ARG	50	-	-	Favored (48.22%) General / -60.6,145.7	68.4% (<i>mtm-85</i>) chi angles: 276.7,192.5,299.7,291.6	0.082Å	-	-
A 435	VAL	50	-	-	Favored (20.64%) Pre-proline / -102.6,101.5	58.4% (<i>t</i>) chi angles: 180.7	0.04Å	-	-
A 436	PRO	50	-	-	Favored (61.49%) Trans-proline / -69.9,147.1	81% (<i>Cg_exo</i>) chi angles: 330.6	0.073Å	-	-

Favored

A 437	ILE	50	-	(30.23%) Isoleucine or valine / -115.2,110.0	94.9% (<i>mt</i>) chi angles: 297.7,169.1	0.044Å	-	-
A 438	ARG	50	-	Favored (62.01%) Pre-proline / -128.1,84.9	40.4% (<i>tmm-85</i>) chi angles: 198.1,181.5,302.1,259.9	0.127Å	-	-
A 439	PRO	50	-	Favored (79.24%) Trans-proline / -66.6,146.3	78.2% (<i>Cg_exo</i>) chi angles: 328.4	0.064Å	-	-
A 440	ARG	50	-	Favored (33.05%) General / -91.6,-12.9	7.4% (<i>mmm-85</i>) chi angles: 315.4,300.5,265.4,261	0.019Å	-	-
A 441	ASN	50	0.455Å HA with A 389 GLN HE22	Favored (17.71%) General / -166.2,164.9	37.5% (<i>p30</i>) chi angles: 59.3,27.1	0.025Å	-	-
A 442	ALA	50	-	Allowed (0.09%) General / -72.4,18.3	-	0.063Å	-	-
A 443	SER	50	-	Favored (47.74%) General / -97.2,6.8	24.8% (<i>p</i>) chi angles: 78.8	0.029Å	-	-
A 444	ASP	50	-	Favored (43%) General / -146.7,156.2	30.7% (<i>t0</i>) chi angles: 186.7,32.9	0.048Å	-	-
A 445	GLY	50	-	Favored (28.43%) Glycine / 150.8,-178.1	-	-	-	-
A 446	LEU	50	-	Favored (57.51%) General / -63.8,-53.0	85.5% (<i>mt</i>) chi angles: 291.4,177.3	0.043Å	-	-
A 447	LEU	50	-	Favored (86.48%) General / -61.0,-38.5	95.1% (<i>mt</i>) chi angles: 294.3,175.8	0.026Å	-	-
A 448	VAL	50	-	Favored (63.22%) Isoleucine or valine / -61.1,-52.3	95% (<i>t</i>) chi angles: 175.9	0.057Å	-	-
A 449	ARG	50	-	Favored (84.9%) General /	98.3% (<i>mtt180</i>) chi angles: 297.4,183.6,187.4,183.1	0.036Å	-	-

				-65.0,-36.6 Favored (64.39%) General / -57.4,-52.7					57.4% (<i>t</i> -105) chi angles: 168.9,249.9		0.026Å	-	-
#	Alt	Res	High B	Clash > 0.4Å	Ramachandran	Rotamer		Cβ deviation	Bond lengths	Bond angles			
				Avg: 54.27	Clashscore: 9.86	Outliers: 3 of 244		Poor rotamers: 0 of 213	Outliers: 1 of 229	Outliers: 4 of 246	Outliers: 1 of 246		
A 451	GLN	50	-	-	Favored (65.34%) General / -69.7,-27.8	12.8% (<i>pt</i> 20) chi angles: 53.9,186.7,23.1		0.152Å	-	-			
A 452	ASN	50	-	-	Favored (53.06%) General / -80.0,-17.3	90.7% (<i>m</i> -20) chi angles: 291.3,348		0.039Å	-	-			
A 453	LYS	50	-	-	Favored (7.74%) General / 62.0,45.0	75.4% (<i>mmtt</i>) chi angles: 300.6,297.7,177.1,184.4		0.093Å	-	-			
A 454	THR	50	-	-	Allowed (1.66%) General / -111.0,82.8	54.4% (<i>p</i>) chi angles: 56.1		0.05Å	-	-			
A 455	LEU	50	-	-	Favored (18.32%) General / -106.1,20.8	62.2% (<i>mt</i>) chi angles: 306.6,177		0.057Å	-	-			
A 456	GLU	50	-	-	Favored (83.79%) General / -61.4,-47.9	29.4% (<i>tt</i> 0) chi angles: 188.7,168.6,281.9		0.041Å	-	-			
A 457	SER	50	-	-	Favored (12.26%) General / -90.0,14.4	78.6% (<i>p</i>) chi angles: 59.3		0.056Å	-	-			
A 458	LEU	50	-	-	Favored (23.94%) General / -124.4,162.4	36.6% (<i>mt</i>) chi angles: 307.4,185.9		0.027Å	-	-			
A 459	ILE	50	-	-	Favored (69.25%) Isoleucine or valine / -119.5,132.4	86.7% (<i>mt</i>) chi angles: 300.1,173		0.053Å	-	-			
A 460	GLU	50	0.5Å OE2 with A 462 HIS HE1	-	Favored (52.98%) General / -107.3,132.5	65% (<i>tt</i> 0) chi angles: 183.2,183.2,333.9		0.109Å	-	-			

A 461	LEU	50	-	Favored (51.02%) General / -134.5,155.1	66.7% (<i>mt</i>) chi angles: 304.3,174.6	0.093Å	-	-
A 462	HIS	50	0.5Å HE1 with A 460 GLU OE2	Favored (46.25%) General / -140.9,155.7	71.7% (<i>m80</i>) chi angles: 298.9,96.2	0.053Å	OUTLIER(S) worst is CG-- ND1: 4.921 σ	-
A 463	ASN	50	-	Favored (58.79%) General / -63.8,139.7	8.1% (<i>p-10</i>) chi angles: 73.4,291.6	0.019Å	-	-
A 464	LYS	50	-	Favored (75.95%) Pre-proline / -75.5,132.2	86.9% (<i>tttt</i>) chi angles: 184.5,173.2,178.3,173.3	0.055Å	-	-
A 465	PRO	50	-	Favored (42.74%) Trans-proline / -68.0,138.0	90.2% (<i>Cg_exo</i>) chi angles: 329	0.058Å	-	-
A 466	PRO	50	-	Favored (75.37%) Trans-proline / -68.3,152.8	99.6% (<i>Cg_exo</i>) chi angles: 329.5	0.056Å	-	-
A 467	VAL	50	-	Favored (27.63%) Isoleucine or valine / -122.5,156.8	33.4% (<i>m</i>) chi angles: 299.7	0.068Å	-	-
A 468	TRP	50	-	Favored (26.99%) General / -66.8,125.8	68% (<i>t-105</i>) chi angles: 186.3,245.4	0.007Å	-	-
A 469	ASN	50	0.49Å HD22 with A 472 SER H	Favored (9.11%) General / -106.5,99.5	1.6% (<i>t30</i>) chi angles: 194.3,101	0.051Å	-	-
A 470	ASP	50	-	Favored (64.46%) General / -62.2,-20.7	4% (<i>t0</i>) chi angles: 212.8,321.9	0.036Å	-	-

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			Avg: 54.27	Clashscore: 9.86	Outliers: 3 of 244	Poor rotamers: 0 of 213	Outliers: 1 of 229	Outliers: 4 of 246	Outliers: 1 of 246

A 471	ASP	50	-	Favored (30.88%) General / -82.0,-32.0	31% (<i>t70</i>) chi angles: 181.6,76.8	0.063Å	-	-
A			0.49Å	Favored	89.2% (<i>p</i>)			

472	SER	50	H with A 469 ASN HD22	(18.4%) General / -109.1,-2.0 Favored	chi angles: 62.2	0.024Å	-	-
A 473	GLY	50	-	(33.06%) Glycine / 54.3,54.3 Favored	-	-	-	-
A 474	SER	50	-	(18.08%) General / -159.1,147.6 Favored	35% (t) chi angles: 182.9	0.068Å	-	-
A 475	TYR	50	-	(13.7%) General / -82.0,106.1 Favored	27.1% (m-85) chi angles: 276.2,275.3	0.023Å	-	-
A 476	THR	50	-	(3.64%) General / -143.7,-172.0 Favored	13% (t) chi angles: 190.8	0.098Å	-	-
A 477	LEU	50	-	(35.54%) General / -125.9,158.3 Favored	95% (mt) chi angles: 296.5,173	0.047Å	-	-
A 478	ASN	50	-	(9.99%) General / -84.3,98.4 Favored	61.2% (t-20) chi angles: 184.1,344.1	0.015Å	-	-
A 479	PHE	50	-	(53.26%) General / -87.9,1.8 Favored	98.3% (m-85) chi angles: 295.4,276.2	0.029Å	-	-
A 480	GLN	50	-	(13.25%) General / 63.2,34.7 Favored	46.3% (mm-40) chi angles: 302.4,293.6,355.3	0.035Å	-	-
A 481	GLY	50	-	(65.76%) Glycine / 64.0,21.6 Favored	-	-	-	-
A 482	ARG	50	-	(30.55%) General / -84.3,-22.8 Favored	31.4% (mmm180) chi angles: 295.8,293.8,293.4,159.1	0.015Å	-	-
A 483	VAL	50	-	(60.27%) Isoleucine or valine / -128.7,123.9 Favored	64.7% (t) chi angles: 179.8	0.079Å	-	-
A				(10.24%) Favored	82.1% (p)			

484	THR	50	-	General / -117.6,-14.1	chi angles: 60.5	0.063Å	-	-
A 485	GLN	50	-	Favored (52.79%) General / -125.7,140.3	51.4% (<i>mt-30</i>) chi angles: 308.5,192.3,341.2	0.003Å	-	-
A 486	ALA	50	-	Favored (58.45%) General / -62.3,138.5	-	0.052Å	-	-
A 487	SER	50	-	Favored (5.09%) General / -166.4,143.6	40.3% (<i>t</i>) chi angles: 176.7	0.084Å	-	-
A 488	VAL	50	-	Favored (26.75%) Isoleucine or valine / -65.4,-20.0	32% (<i>m</i>) chi angles: 300.6	0.068Å	-	-
A 489	LYS	50	-	Favored (52.15%) General / -79.8,-17.9	32.1% (<i>mtmm</i>) chi angles: 284.4,179.7,281.5,290.6	0.055Å	-	-
A 490	ASN	50	-	Favored (27.04%) General / -66.3,125.9	65% (<i>m-20</i>) chi angles: 298.9,348.6	0.046Å	-	-

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A 491	PHE	50	-		Favored (29%) General / -159.7,157.1	21% (<i>p90</i>) chi angles: 63.8,76.3	0.039Å	-	-
A 492	GLN	50	-		Favored (54.68%) General / -122.7,135.7	97.9% (<i>mt-30</i>) chi angles: 295.9,177.8,328.7	0.09Å	-	-
A 493	ILE	50	-		Favored (63.58%) Isoleucine or valine / -107.9,123.8	51.3% (<i>mm</i>) chi angles: 302.6,300.7	0.042Å	-	-
A 494	VAL	50	-		Favored (42.82%) Isoleucine or valine / -131.4,156.6	34.4% (<i>m</i>) chi angles: 298.8	0.06Å	-	-
A					Favored (25.28%)	59.9% (<i>t-80</i>)	OUTLIER(S)		

495	HIS	50	-	General / -86.0,149.3	chi angles: 190.7,274.8	0.072Å	worst is CG-- ND1: 4.705 σ	-
A 496	ALA	50	-	Favored (61.64%) General / -56.4,-29.6	-	0.016Å	-	-
A 497	ASP	50	-	Favored (61.58%) General / -72.5,-25.8	83.6% (<i>m-20</i>) chi angles: 293.7,350.4	0.126Å	-	-
A 498	ASP	50	-	Favored (3.87%) Pre-proline / -147.8,98.4	50% (<i>t0</i>) chi angles: 192.2,346.5	0.058Å	-	-
A 499	PRO	50	-	Favored (9.86%) Trans-proline / -72.3,-1.3	96.8% (<i>Cg_endo</i>) chi angles: 30.6	0.095Å	-	-
A 500	ASP	50	-	Favored (17.73%) General / -106.7,-6.6	70.7% (<i>m-20</i>) chi angles: 287.9,322.5	0.063Å	-	-
A 501	TYR	50	-	Favored (15.8%) General / -94.3,103.8	55.6% (<i>t80</i>) chi angles: 186.3,270.8	0.065Å	-	-
A 502	ILE	50	-	Favored (5.8%) Isoleucine or valine / -89.2,96.0	25.4% (<i>mm</i>) chi angles: 312.2,304	0.057Å	-	-
A 503	VAL	50	-	Favored (80.17%) Isoleucine or valine / -62.3,-38.1	46% (<i>t</i>) chi angles: 183.5	0.055Å	-	-
A 504	LEU	50	0.458Å HD11 with A 516 LEU HD11	Favored (9.07%) General / -154.1,128.4	39.6% (<i>tp</i>) chi angles: 186.8,63	0.055Å	-	-
A 505	GLN	50	-	Favored (53.28%) General / -124.1,134.8	29.5% (<i>tt0</i>) chi angles: 185.7,175.9,271.1	0.069Å	-	-
A 506	PHE	50	-	Favored (32%) General / -141.1,136.5	37.7% (<i>t80</i>) chi angles: 187.6,59.2	0.085Å	-	-
A 507	GLY	50	-	Favored (31.92%) Glycine / -170.5,159.6	-	-	-	-

A 508	ARG	50	-		Favored (35.53%) General / -81.6,136.4	55.6% (<i>ttm-85</i>) chi angles: 182.8,187.6,288.8,279.9	0.083Å	-	-
A 509	VAL	50	-		Favored (5.6%) Isoleucine or valine / -118.0,-20.0	24.2% (<i>m</i>) chi angles: 293.4	0.112Å	-	-
A 510	ALA	50	0.433Å HB3 with A 513 ALA HB3		Favored (4.49%) General / -155.5,-173.3	-	0.06Å	-	-
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			Avg: 54.27	Clashscore: 9.86	Outliers: 3 of 244	Poor rotamers: 0 of 213	Outliers: 1 of 229	Outliers: 4 of 246	Outliers: 1 of 246
A 511	GLU	50	-		Favored (97.86%) General / -61.2,-42.0	26.2% (<i>tp10</i>) chi angles: 187.6,55.4,42.4	0.018Å	-	-
A 512	ASP	50	-		Favored (5.37%) General / -129.8,24.3	47% (<i>m-20</i>) chi angles: 299.6,294.9	0.067Å	-	-
A 513	ALA	50	0.433Å HB3 with A 510 ALA HB3		Favored (50.65%) General / -130.4,143.3	-	0.023Å	-	-
A 514	PHE	50	-		Favored (43.67%) General / -144.2,155.0	54.9% (<i>m-85</i>) chi angles: 304.8,82.2	0.112Å	-	-
A 515	THR	50	-		Favored (37.3%) General / -104.6,140.9	67.7% (<i>p</i>) chi angles: 59.6	0.019Å	-	-
A 516	LEU	50	0.458Å HD11 with A 504 LEU HD11		Favored (5.15%) General / -136.5,103.2	48.7% (<i>tp</i>) chi angles: 183.1,66.1	0.026Å	-	-
A 517	ASP	50	-		Favored (38.45%) General / -115.8,120.2	21.4% (<i>m-20</i>) chi angles: 309.5,332.2	0.046Å	-	-
A 518	TYR	50	-		Favored (38.18%) General / -119.5,151.7	49% (<i>p90</i>) chi angles: 67.7,273.2	0.038Å	-	-
A	ARG	50	-		Favored (15.78%)	73.5% (<i>mtp180</i>) chi angles:	0.074Å	-	-

519				General / -126.2,167.2	299.4,192.4,65.5,183.4			
A 520	TYR	50	-	Favored (48.21%) Pre-proline / -53.1,128.5	73.4% (<i>t80</i>) chi angles: 182,86.4	0.076Å	-	-
A 521	PRO	50	-	Favored (8.21%) Cis-proline / -106.5,8.3	44.7% (<i>Cg_endo</i>) chi angles: 35.6	0.03Å	-	-
A 522	LEU	50	-	Favored (38.26%) General / -76.1,147.8	77.5% (<i>mt</i>) chi angles: 295.7,182.1	0.025Å	-	-
A 523	CYS	50	-	Favored (6.84%) General / -104.8,172.3	26.9% (<i>p</i>) chi angles: 66.9	0.043Å	-	-
A 524	ALA	50	-	Favored (88.86%) General / -61.8,-38.6	-	0.011Å	-	-
A 525	LEU	50	-	Favored (98.96%) General / -63.1,-43.2	42.8% (<i>tp</i>) chi angles: 182.5,56.1	0.074Å	-	-
A 526	GLN	50	-	Favored (92.22%) General / -63.6,-45.0	89.1% (<i>mt-30</i>) chi angles: 290,173.4,305.5	0.052Å	-	-
A 527	ALA	50	-	Favored (88.48%) General / -64.5,-45.1	-	0.048Å	-	-
A 528	PHE	50	-	Favored (90.37%) General / -64.6,-44.5	35.2% (<i>t80</i>) chi angles: 184.7,56.1	0.039Å	-	-
A 529	ALA	50	-	Favored (81.59%) General / -68.3,-38.5	-	0.05Å	-	-
A 530	ILE	50	-	Favored (93.9%) Isoleucine or valine / -63.7,-41.8	95.2% (<i>mt</i>) chi angles: 297.7,169.1	0.036Å	-	-

#	Alt	Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
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		Avg: Clashscore: 54.27 9.86		Outliers: 3 of 244	Poor rotamers: 0 of 213	Outliers: 1 of 229	Outliers: 4 of 246	Outliers: 1 of 246
A 531	ALA	50	-	Favored (92.44%) General / -65.2,-39.2	-	0.026Å	-	-
A 532	LEU	50	-	Favored (78.97%) General / -62.6,-35.3	60.9% (<i>mt</i>) chi angles: 287.8,178.8	0.054Å	-	-
A 533	SER	50	-	Favored (66.7%) General / -63.9,-21.9	52.4% (<i>p</i>) chi angles: 74.9	0.071Å	-	-
A 534	SER	50	-	Favored (45.77%) General / -78.5,-24.8	61.7% (<i>p</i>) chi angles: 71.4	0.104Å	-	-
A 535	PHE	50	-	Favored (33.91%) General / -71.2,159.8	97.6% (<i>m-85</i>) chi angles: 296.2,270.7	0.051Å	-	-
A 536	ASP	99.99	-	-	24.3% (<i>p30</i>) chi angles: 54.4,24.9	0.085Å	-	-

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