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All-Atom	Clashscore, all atoms:	50.29		4 th percentile* (N=1784, all resolutions)
Contacts	Clashscore is the number	of serious	steric ove	rlaps (> 0.4 Å) per 1000 atoms.
	Poor rotamers	0	0.00%	Goal: <1%
	Ramachandran outliers	3	2.21%	Goal: <0.05%
	Ramachandran favored	121 88.97%		Goal: >98%
Protein Geometry	MolProbity score [^]	2.75		34 th percentile* (N=27675, 0Å - 99Å)
acometry	Cβ deviations >0.25Å	3	2.42%	Goal: 0
	Bad backbone bonds:	16 / 1060 1.51%		Goal: 0%
	Bad backbone angles:	22 / 1443	1.52%	Goal: <0.1%

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

[^] 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: 62.68		Outliers: 3 of 136	Poor rotamers: 0 of 120	Outliers: 3 of 124	Outliers: 9 of 138	Outliers: 12 of 138
A 262		ASN	50	-	-	47.7% (<i>t30</i>) chi angles: 181.5,32	0.057Å	-	-
A 263		THR	50	-	Favored (53.81%) General / -108.0,132.2	94% (<i>m</i>) chi angles: 298.1	0.052Å	-	-
A 264		ASP	50	0.694Å HA with A 279 ASP OD2	Favored (5.69%) General / -79.2,95.6	52.2% (<i>t0</i>) chi angles: 191.5,347	0.037Å	-	-
A 265		GLU	50	0.547Å O with A 269 GLN HB3	Favored (68.48%) General / -64.3,-26.4	51.5% (mp0) chi angles: 288.5,75.9,16.6	0.118Å	-	-

^{* 100&}lt;sup>th</sup> 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.

A 266	CYS	50	-	Favored (72.71%) General / -70.9,-36.4	85.3% (<i>m</i>) chi angles: 300.3	0.03Å	-	-
A 267	ALA	50	-	Favored (62.71%) General / -70.6,-24.2	-	0.014Å	-	-
A 268	SER	99.99	-	Favored (6.61%) General / -120.7,-21.6	31.8% (<i>t</i>) chi angles: 184.5	0.017Å	-	-
A 269	GLN	99.99	0.547Å HB3 with A 265 GLU O	Favored (68.85%) Pre-proline / -125.4,76.4	46.7% (tt0) chi angles: 176.8,186.9,66	0.078Å	-	-
A 270	PRO	99.99	-	Favored (42.04%) Trans-proline / -73.5,148.1	85.1% (<i>Cg_endo</i>) chi angles: 31.6	0.013Å	-	-
A 271	CYS	99.99	0.558Å O with A 272 LEU HD23	Favored (26.94%) General / -141.8,165.6	42.6% (t) chi angles: 177	0.114Å	-	-
A 272	LEU	99.99	0.958Å HD22 with A 274 GLY HA2	Allowed (0.23%) General / -133.0,-110.2	25.1% (<i>mt</i>) chi angles: 288,187.6	0.375Å	-	OUTLIER(S) worst is C-CA- CB: 5.42 σ
	LEU HIS	99.99 50	HD22 with A 274 GLY HA2 0.495Å O with A 289 THR HG21	(0.23%) General /	, ,	0.375Å 0.077Å	- OUTLIER(S) worst is CG ND1: 4.597 σ	worst is C-CA-CB: 5.42σ
272 A			HD22 with A 274 GLY HA2 0.495Å O with A 289	(0.23%) General / -133.0,-110.2 OUTLIER (0%) General /	chi angles: 288,187.6 30.4% (<i>m80</i>)		worst is CG	worst is C-CA-CB: 5.42σ
272 A 273 A	HIS	50	HD22 with A 274 GLY HA2 0.495Å O with A 289 THR HG21 0.958Å HA2 with A 272 LEU	(0.23%) General / -133.0,-110.2 OUTLIER (0%) General / 19.4,36.5 Favored (79.56%) Glycine /	chi angles: 288,187.6 30.4% (<i>m80</i>)		worst is CG	worst is C-CA-CB: 5.42σ
272 A 273 A 274	HIS	50 50	HD22 with A 274 GLY HA2 0.495Å O with A 289 THR HG21 0.958Å HA2 with A 272 LEU	(0.23%) General / -133.0,-110.2 OUTLIER (0%) General / 19.4,36.5 Favored (79.56%) Glycine / 74.2,16.9 Favored (30.12%) Glycine / -74.8,142.7 Favored (36.06%) General / -79.2,131.1	chi angles: 288,187.6 30.4% (<i>m80</i>)		worst is CG	worst is C-CA-CB: 5.42σ
272 A 273 A 274 A 275	HIS GLY GLY	50 50	HD22 with A 274 GLY HA2 0.495Å O with A 289 THR HG21 0.958Å HA2 with A 272 LEU	(0.23%) General / -133.0,-110.2 OUTLIER (0%) General / 19.4,36.5 Favored (79.56%) Glycine / 74.2,16.9 Favored (30.12%) Glycine / -74.8,142.7 Favored (36.06%) General /	chi angles: 288,187.6 30.4% (<i>m80</i>) chi angles: 285.5,116.1 - 8.5% (<i>tt</i>)	0.077Å - -	worst is CG	worst is C-CA-CB: 5.42σ

A 278	VAL	50	0.59Å HG23 with A 285 SER OG	(50.66%) Isoleucine or valine / -119.7,116.5	33% (<i>m</i>) chi angles: 300.1	0.047Å	-	OUTLIER(S) worst is CG1- CB-CG2: 5.503 σ
A 279	ASP	50	0.694Å OD2 with A 264 ASP HA	Favored (44.9%) General / -73.1,136.2	45.3% (<i>t0</i>) chi angles: 188,330.1	0.057Å	-	-
A 280	GLY	50	-	Favored (14.41%) Glycine / -120.4,162.2	-	-	-	-
A 281	GLU	50	-	Favored (7.67%) General / -76.5,105.5	52.7% (<i>mt-10</i>) chi angles: 296.4,182.3,293.3	0.084Å	-	-
# A	It Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	$\begin{array}{c} C\beta \\ \text{deviation} \end{array}$	Bond lengths	Bond angles
		Avg: 62.68	Clashscore: 50.29	Outliers: 3 of 136	Poor rotamers: 0 of 120	Outliers: 3 of 124	Outliers: 9 of 138	Outliers: 12 of 138
A 282	ASN	50	-	OUTLIER (0.01%) General / 111.7,-30.4	24% (<i>t-20</i>) chi angles: 184.7,298	0.06Å	-	OUTLIER(S) worst is CA- CB-CG: 4.477 σ
A 283	ARG	50	0.959Å HG2 with A 284 TYR H	Allowed (0.21%) General / -145.3,-147.4	52.9% (ttm-85) chi angles: 188.2,188.6,286.6,279.4	0.109Å	-	-
A 284	TYR	50	0.959Å H with A 283 ARG HG2	Favored (22.85%) General / -162.8,158.4	53.1% (<i>p90</i>) chi angles: 64.4,89.6	0.063Å	-	-
A 285	SER	50	0.59Å OG with A 278 VAL HG23	Favored (48.86%) General / -131.7,154.6	14.7% (<i>p</i>) chi angles: 48.8	0.057Å	-	-
A 286	CYS	50	-	Favored (55.77%) General / -113.4,132.0	80.3% (<i>m</i>) chi angles: 296	0.042Å	-	-
A 287	ASN	50	-	Favored (6.38%) General / -99.4,94.3	25.4% (<i>t-20</i>) chi angles: 186.1,298.9	0.075Å	-	-
A 288	CYS	99.99	0.911Å SG with A 293 PHE HB2	Favored (28.1%) General /	45.2% (<i>t</i>) chi angles: 184.9	0.127Å	-	-

A 289	THR 9	99.99	0.516Å C with A 291 SER H	-54.9,142.8 Favored (33.61%) General / -85.3,126.3	9.4% (<i>t</i>) chi angles: 182.1	0.018Å	-	-
A 290	GLY 9	99.99) -	Allowed (0.23%) Glycine / 67.9,-32.1	-	-	-	-
A 291	SER 9	99.99	0.516Å H with A 289 THR C	Favored (19.25%) General / 60.3,29.7	26% (<i>t</i>) chi angles: 185.8	0.054Å	-	-
A 292	GLY	50	0.684Å O with A 302 MET HG2	Favored (34.7%) Glycine / -65.2,-8.0	-	-	-	-
A 293	PHE	50	0.911Å HB2 with A 288 CYS SG	Favored (50.31%) General / -127.0,146.5	63.1% (<i>m-85</i>) chi angles: 305.4,270.5	0.063Å	-	OUTLIER(S) worst is CB- CG-CD1: 4.194 σ
A 294	THR	50	-	Favored (13.14%) General / -141.2,172.1	13.9% (<i>t</i>) chi angles: 186.7	0.076Å	-	-
A 295	GLY	50	-	Favored (15.63%) Glycine / 111.6,159.8	-	-	-	-
A 296	THR	50	-	Favored (66.46%) General / -60.0,-26.9	71.8% (p) chi angles: 59.8	0.028Å	-	-
A 297	HIS	50	-	Favored (11.68%) General / -121.0,17.3	58.3% (<i>m170</i>) chi angles: 297.2,160.4	0.008Å	OUTLIER(S) worst is CD2 NE2: 4.767 σ	
A 298	CYS	50	0.433Å SG with A 288 CYS HA	Favored (24.65%) General / 58.3,35.1	47.5% (<i>m</i>) chi angles: 307	0.039Å	-	-
A 299	GLU	50	-	Favored (58.95%) General / -87.5,-5.0	1.6% (<i>pm0</i>) chi angles: 60.5,272.5,79.3	0.114Å	-	-
A 300	THR	50	-	Favored (40.6%) General /	99.1% (<i>m</i>) chi angles: 298.8	0.022Å	-	-

				-104.3,120.2				
A 301	LEU	50	0.427Å HD13 with A 293 PHE CE1	Favored (9.82%) General / -85.3,97.2	58.3% (<i>tp</i>) chi angles: 182.2,63.3	0.037Å	-	-
#	Alt Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
		Avg: 62.68	Clashscore: 50.29	Outliers: 3 of 136	Poor rotamers: 0 of 120	Outliers: 3 of 124	Outliers: 9 of 138	Outliers: 12 of 138
A 302	MET	50	0.684Å HG2 with A 292 GLY O	Favored (35.45%) Pre-proline / -52.8,124.3	13.5% (<i>ptp</i>) chi angles: 60.3,186.4,49.6	0.08Å	-	-
A 303	PRO	50	-	Allowed (1.01%) Trans-proline / -81.5,98.7	79.9% (<i>Cg_endo</i>) chi angles: 33.1	0.011Å	-	-
A 304	LEU	50	0.601Å HD22 with A 322 ASN CA	Favored (23.04%) General / -73.4,-2.6	8% (<i>mp</i>) chi angles: 278.5,75.3	0.022Å	-	-
A 305	CYS	50	-	Favored (24.52%) General / -108.0,3.9	88.5% (<i>m</i>) chi angles: 292	0.062Å	-	-
A 306	TRP	50	-	Favored (69.49%) General / -65.5,-28.9	76.3% (<i>t-105</i>) chi angles: 183.2,256.6	0.033Å	-	-
A 307	SER	50	-	Favored (33.84%) General / -97.8,12.5	79.8% (<i>p</i>) chi angles: 59.9	0.023Å	-	-
A 308	LYS	50	-	Favored (4.38%) Pre-proline / 50.1,67.5	32% (<i>mmmt</i>) chi angles: 296.9,292.8,296.2,181.2	0.037Å	-	-
A 309	PRO	50	-	Favored (12.61%) Trans-proline / -71.9,-31.5	91.2% (<i>Cg_endo</i>) chi angles: 32	0.053Å	-	-
A 310	CYS	50	0.464Å HB3 with A 314 ALA HB3	Favored (35.18%) General / -78.3,129.6	61.8% (<i>m</i>) chi angles: 303.5	0.046Å	-	-
A	HIS	50	-	Favored (15.88%)	59.1% (<i>m170</i>)	0.046Å	OUTLIER(S)	-

			0.601Å	Favored	/			
		Avg: 62.68		Outliers: 3 of 136	Poor rotamers: 0 of 120	Outliers: 3 of 124	Outliers: 9 of 138	Outliers: 12 of 138
# .	Alt Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	C β deviation	Bond lengths	Bond angles
A 321	ASP	50	0.411Å HB3 with A 320 VAL O	Favored (6.2%) General / 71.6,14.4	31.2% (<i>t70</i>) chi angles: 177.1,70.9	0.043Å	-	-
A 320	VAL	. 50	0.411Å O with A 321 ASP HB3	Allowed (1.13%) Isoleucine or valine / -70.7,103.7	10.9% (<i>p</i>) chi angles: 61.3	0.084Å	-	-
A 319	SER	50	-	Favored (6.42%) General / -110.7,173.2	66.5% (<i>m</i>) chi angles: 298.4	0.032Å	-	-
A 318	ASP	50	-	Favored (2.13%) General / -72.1,98.7	42.6% (<i>t0</i>) chi angles: 188.2,24.6	0.038Å	-	-
A 317	GLU	J 50	-	Favored (16.69%) General / -107.9,106.4	56.7% (<i>mm-40</i>) chi angles: 291.5,290.7,359	0.063Å	-	-
A 316	CYS	5 50	-	Favored (50.68%) General / -108.7,135.0	22.7% (<i>t</i>) chi angles: 191	0.057Å	-	-
A 315	THR	2 50	-	Favored (32.9%) General / -95.0,138.3	12.9% (<i>m</i>) chi angles: 312.3	0.068Å	-	-
A 314	ALA	50	0.464Å HB3 with A 310 CYS HB3	Favored (40.39%) General / -73.6,153.1	-	0.04Å	-	-
A 313	ASN	1 50	-	Favored (7.93%) General / 57.1,22.9	96% (<i>m-20</i>) chi angles: 293,337	0.03Å	-	-
A 312	ASN	J 50	-	Allowed (1.57%) General / 64.0,55.3	80.4% (<i>m-20</i>) chi angles: 301,314	0.029Å	-	-
311				Generai / -106.2,159.7	cni angles: 29/.5,161		worst is CG ND1: 4.511 σ	

A 322	ASN	50	CA WIUI A 304 LEU HD22	(22./%) General / -162.0,156.8	53.4% (<i>t30</i>) chi angles: 185.8,57.3	0.145Å	-	-
A 323	TYR	50	-	Favored (43.14%) General / -122.0,149.7	54.8% (<i>p90</i>) chi angles: 63.1,89.7	0.037Å	-	-
A 324	THR	50	-	Favored (50.24%) General / -131.0,141.1	80.6% (p) chi angles: 60.4	0.026Å	-	-
A 325	CYS	50	-	Favored (54.76%) General / -107.2,130.2	74.1% (<i>m</i>) chi angles: 298.5	0.048Å	-	-
A 326	HIS	50	-	Favored (8.22%) General / -102.9,98.2	22.1% (<i>t-160</i>) chi angles: 181.6,201.4	0.053Å	OUTLIER(S) worst is CG ND1: 4.426 σ	-
A 327	CYS	50	-	Favored (58.26%) General / -65.9,141.3	60.3% (<i>m</i>) chi angles: 304.3	0.01Å	-	-
A 328	TRP	50	0.447Å CD2 with A 329 PRO HD2	Favored (80.31%) Pre-proline / -72.7,138.6	77% (<i>t-105</i>) chi angles: 182.8,255.2	0.059Å	-	-
A 329	PRO	50	0.447Å HD2 with A 328 TRP CD2	Favored (12.37%) Trans-proline / -46.0,129.5	62.6% (<i>Cg_exo</i>) chi angles: 327.3	0.062Å	-	-
A 330	GLY	50	-	Favored (35.74%) Glycine / 108.3,-15.5	-	-	-	-
A 331	TYR	50	-	Favored (42.2%) General / -118.8,149.0	99% (<i>m</i> -85) chi angles: 296.7,275.1	0.038Å	-	-
A 332	THR	50	0.544Å O with A 338 ILE HG22	Favored (10.43%) General / -140.6,174.5	55.6% (<i>p</i>) chi angles: 56.2	0.108Å	-	-
A 333	GLY	50	-	Favored (19.78%) Glycine / 110.2,169.7	-	-	-	-

A 334	ALA	50	-	Favored (75.5%) General / -63.6,-33.4	-	0.02Å	-	-
A 335	GLN	50	-	Favored (17.47%) General / -114.0,9.9	26.7% (<i>mp0</i>) chi angles: 298.2,80.8,1.5	0.049Å	-	-
A 336	CYS	50	0.48Å HA with A 332 THR O	Favored (28.79%) General / 57.1,38.0	57.8% (<i>m</i>) chi angles: 305.5	0.022Å	-	-
A 337	GLU	50	-	Favored (30.83%) General / -84.0,-23.9	18.8% (<i>pm0</i>) chi angles: 68.7,285.2,360	0.088Å	-	-
A 338	ILE	50	0.544Å HG22 with A 332 THR O	Favored (42.74%) Isoleucine or valine / -89.8,126.3	6.3% (<i>tp</i>) chi angles: 179.4,70.6	0.131Å	-	-
A 339	ASP	50	-	Favored (11.06%) General / -85.4,99.2	45.3% (<i>t0</i>) chi angles: 188,330.1	0.047Å	-	-
A 340	LEU	50	0.595Å HD22 with A 342 GLU OE2	Favored (9.68%) General / -47.0,126.9	7% (tt) chi angles: 189.5,163.8	0.056Å	-	-
A 341	ASN	50	-	Favored (9.58%) General / -85.1,96.8	53% (<i>t30</i>) chi angles: 184,53.5	0.037Å	-	-
341	ASN Alt Res	50 High B	- Clash > 0.4Å	(9.58%) General /		0.037Å Cβ deviation	- Bond lengths	- Bond angles
341	Alt Res	High B	0.4Å Clashscore:	(9.58%) General / -85.1,96.8	chi angles: 184,53.5 Rotamer Poor rotamers: 0 of	Cβ deviation Outliers:	lengths Outliers: 9	angles Outliers: 12
341	Alt Res	High B Avg:	0.4Å Clashscore:	(9.58%) General / -85.1,96.8 Ramachandran Outliers: 3 of 136 Favored (62.64%) General / -64.5,-16.5	chi angles: 184,53.5 Rotamer	Cβ deviation	lengths	angles
341 # A	Alt Res	High B Avg: 62.68	0.4Å Clashscore: 50.29 0.595Å OE2 with A 340 LEU	(9.58%) General / -85.1,96.8 Ramachandran Outliers: 3 of 136 Favored (62.64%) General / -64.5,-16.5 Favored (59.14%) General / -81.9,-11.0	Rotamer Poor rotamers: 0 of 120 20.1% (mp0) chi angles:	Cβ deviation Outliers: 3 of 124	lengths Outliers: 9	angles Outliers: 12
341 # A A 342	Alt Res GLU	High B Avg: 62.68	0.4Å Clashscore: 50.29 0.595Å OE2 with A 340 LEU	(9.58%) General / -85.1,96.8 Ramachandran Outliers: 3 of 136 Favored (62.64%) General / -64.5,-16.5 Favored (59.14%) General /	chi angles: 184,53.5 Rotamer Poor rotamers: 0 of 120 20.1% (<i>mp0</i>) chi angles: 279.8,70.5,36.2 88.9% (<i>m</i>)	Cβ deviation Outliers: 3 of 124 0.066Å	lengths Outliers: 9	angles Outliers: 12

344				-62.5,-37.5	CIII aligico. 107.3,430.4			
A 345	SER	50	-	Favored (34.44%) General / -82.5,2.1	76% (p) chi angles: 58.3	0.013Å	-	-
A 346	ASN	50	-	Allowed (1.32%) Pre-proline / 51.6,72.0	30.8% (<i>t-20</i>) chi angles: 184.4,304.7	0.018Å	-	-
A 347	PRO	50	0.872Å HG3 with A 361 LYS HD2	Favored (4.56%) Trans-proline / -78.4,-28.4	16.2% (<i>Cg_endo</i>) chi angles: 39.2	0.107Å	-	OUTLIER(S) worst is N-CA- CB: 4.384 σ
A 348	CYS	50	-	Favored (6.94%) General / -72.8,110.1	64.4% (<i>m</i>) chi angles: 302.6	0.038Å	-	-
A 349	GLN	50	0.517Å OE1 with A 395 GLU HB3	Favored (37.9%) General / -71.2,157.6	84.3% (<i>mt-30</i>) chi angles: 295.4,181.4,296.7	0.031Å	-	-
A 350	SER	50	-	Favored (16.59%) General / 62.4,33.0	66.4% (<i>m</i>) chi angles: 296.6	0.029Å	-	-
A 351	ASN	50	-	Favored (3.61%) General / 56.7,59.3	23.9% (<i>m120</i>) chi angles: 295.8,136.5	0.019Å	-	-
A 352	GLY	50	-	Favored (18.16%) Glycine / -93.5,146.5	-	-	-	OUTLIER(S) worst is C-N- CA: 4.058 σ
A 353	GLU 9	99.99	0.855Å HA with A 364 GLY O	Favored (37.38%) General / -53.1,135.4	19.2% (<i>mt-10</i>) chi angles: 316.6,197.4,326.7	0.382Å		OUTLIER(S) worst is C-CA-CB: 7.911 σ
A 354	CYS	50	0.546Å N with A 364 GLY O	Favored (51.36%) General / -109.6,124.6	23.7% (<i>t</i>) chi angles: 190.8	0.093Å	OUTLIER(S) worst is CA C: 6.007 σ	-
A 355	VAL 9	99.99	0.845Å HG23 with A 379 SER HB2	Favored (5.28%) Isoleucine or valine / -103.5,156.8	13.6% (<i>p</i>) chi angles: 65	0.065Å	-	OUTLIER(S) worst is CG1- CB-CG2: 5.858 σ
٨	CHI	20.00		Favored	Q7 70/ (++∩\	0 110 Å		
٨	<i>i</i> 1116	1(1)(1)		1/111 6 30/ 1	Q / /U/ [##]\	A 110A		

7356	ULU	ઝઝ. ઝઝ	-	(49.03 /o) General / -103.2,132.2	07 .7 /ο (ιιυ) chi angles: 187.9,179.5,354.8	U.IIYA	-	-
A 357	LEU	99.99	-	Allowed (0.59%) General / -120.6,-154.5	72.4% (<i>mt</i>) chi angles: 293.9,182	0.067Å	-	-
A 358	SER	50	-	Favored (23.48%) General / -105.2,110.9	35% (<i>t</i>) chi angles: 182.9	0.05Å	-	-
A 359	SER	50	-	Favored (23.59%) General / 56.0,34.4	30.2% (<i>t</i>) chi angles: 184.9	0.02Å	-	-
A 360	GLU	50	-	Favored (8.38%) General / -165.1,148.3	10.7% (<i>tp10</i>) chi angles: 191.3,65.3,73.2	0.101Å	-	-
A 361	LYS	99.99	0.872Å HD2 with A 347 PRO HG3	Favored (40.32%) General / -128.4,157.7	21.1% (pttp) chi angles: 62.7,190.5,183,70.1	0.066Å	-	-
	la Daa	High	Clash >	Damachanduan	Rotamer	Сβ	Bond	Bond
# A	It Res	B	0.4Å	Ramachandran	Kotamer	deviation	lengths	angles
# A	it kes	В	Clashscore:	Outliers: 3 of	Poor rotamers: 0 of	deviation Outliers:	Outliers: 9	
# A	it kes	В		Outliers: 3 of 136				Outliers: 12 of 138
# A A 362	gen GLN	B Avg: 62.68	Clashscore:	Outliers: 3 of	Poor rotamers: 0 of	Outliers:	Outliers: 9	Outliers: 12
A	GLN	B Avg: 62.68	Clashscore: 50.29 0.922Å HG3 with A	Outliers: 3 of 136 Allowed (0.29%) General /	Poor rotamers: 0 of 120 12.3% (mm-40) chi angles:	Outliers: 3 of 124	Outliers: 9	Outliers: 12 of 138 OUTLIER(S) worst is CB- CG-CD: 5.388
A 362 A	GLN TYR	B Avg: 62.68 50 99.99	Clashscore: 50.29 0.922Å HG3 with A 381 TYR HA 1.095Å HB2 with A	Outliers: 3 of 136 Allowed (0.29%) General / -132.5,-98.4 Favored (6.56%) General /	Poor rotamers: 0 of 120 12.3% (<i>mm-40</i>) chi angles: 317,266,342.8 31.2% (<i>t80</i>)	Outliers: 3 of 124 0.055Å	Outliers: 9 of 138 - OUTLIER(S)	Outliers: 12 of 138 OUTLIER(S) worst is CB- CG-CD: 5.388 OUTLIER(S) worst is C-N-
A 362 A 363	GLN TYR GLY	B Avg: 62.68 50 99.99	Clashscore: 50.29 0.922Å HG3 with A 381 TYR HA 1.095Å HB2 with A 383 CYS HA 0.855Å O with A 353	Outliers: 3 of 136 Allowed (0.29%) General / -132.5,-98.4 Favored (6.56%) General / -147.4,115.6 Favored (21.03%) Glycine / -151.0,149.2 Favored (51.21%) General / -131.6,151.9	Poor rotamers: 0 of 120 12.3% (<i>mm-40</i>) chi angles: 317,266,342.8 31.2% (<i>t80</i>)	Outliers: 3 of 124 0.055Å	Outliers: 9 of 138 - OUTLIER(S) worst is CA	Outliers: 12 of 138 OUTLIER(S) worst is CB- CG-CD: 5.388 σ OUTLIER(S) worst is C-N- CA: 12.529 σ OUTLIER(S) worst is CA-C-
A 362 A 363 A 364	GLN TYR GLY	B Avg: 62.68 50 99.99	Clashscore: 50.29 0.922Å HG3 with A 381 TYR HA 1.095Å HB2 with A 383 CYS HA 0.855Å O with A 353 GLU HA 0.791Å HB2 with A	Outliers: 3 of 136 Allowed (0.29%) General / -132.5,-98.4 Favored (6.56%) General / -147.4,115.6 Favored (21.03%) Glycine / -151.0,149.2 Favored (51.21%) General /	Poor rotamers: 0 of 120 12.3% (mm-40)	Outliers: 3 of 124 0.055Å 0.066Å	Outliers: 9 of 138 - OUTLIER(S) worst is CA	Outliers: 12 of 138 OUTLIER(S) worst is CB- CG-CD: 5.388 σ OUTLIER(S) worst is C-N- CA: 12.529 σ OUTLIER(S) worst is CA-C- O: 9.33 σ OUTLIER(S) worst is CA-C-

			,				
A 367	THR 99.99	-	Favored (25.81%) General / -155.3,149.4	46% (<i>m</i>) chi angles: 305.2	0.067Å	-	-
A 368	GLY 99.99	0.963Å HA3 with A 375 TYR CD1	Favored (30.7%) Glycine / -175.6,161.7	-	-	-	-
A 369	LEU 99.99	-	Favored (42.81%) Pre-proline / -123.7,96.8	88.7% (<i>mt</i>) chi angles: 299.4,174.6	0.04Å	-	-
A 370	PRO 99.99	-	Favored (45.01%) Trans-proline / -49.8,-37.2	97.6% (<i>Cg_exo</i>) chi angles: 329.4	0.067Å	-	-
A 371	SER 99.99	-	Favored (71.28%) General / -63.8,-30.1	88.9% (p) chi angles: 62	0.03Å	-	-
A 372	SER 99.99	-	Favored (28.08%) General / -107.8,7.2	94% (p) chi angles: 63.3	0.014Å	-	-
A 373	PHE 99.99	-	Favored (17.54%) General / 59.3,28.3	97.4% (<i>m</i> -85) chi angles: 296.2,270.1	0.05Å	-	-
A 374	SER 99.99	-	Favored (49.22%) General / -125.5,147.5	93.5% (p) chi angles: 63.2	0.026Å	-	-
A 375	TYR 99.99	0.963Å CD1 with A 368 GLY HA3	Favored (35.42%) General / -156.6,165.7	97.2% (<i>m-85</i>) chi angles: 294,272.8	0.07Å	-	-
A 376	HIS 99.99	-	Favored (22.94%) General / -149.2,140.2	99.3% (<i>m-70</i>) chi angles: 297.5,282.7	0.028Å	OUTLIER(S) worst is CG ND1: 4.331 σ	-
A 377	GLU 99.99	-	Favored (52.61%) General / -125.4,130.8	79.3% (tt0) chi angles: 177.8,178.4,14.5	0.092Å	-	-
A 378	ALA 99.99	0.556Å O with A 364 GIY HA2	Favored (5.61%) General / -133.3.102.6	-	0.034Å	-	-

				,				
A 379	SER	99.99	0.845Å HB2 with A 355 VAL HG23	Favored (32.36%) General / -110.3,116.9	92.2% (p) chi angles: 63	0.077Å	-	-
A 380	GLY	99.99	0.665Å O with A 355 VAL HG11	Favored (16.8%) Glycine / -122.6,146.8	-	-	-	-
A 381	TYR	99.99	0.922Å HA with A 362 GLN HG3	Allowed (0.99%) General / -91.5,39.1	49.6% (<i>p90</i>) chi angles: 67.2,89.9	0.167Å	-	-
#	Alt Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
		Avg: 62.68	Clashscore: 50.29	Outliers: 3 of 136	Poor rotamers: 0 of 120	Outliers: 3 of 124	Outliers: 9 of 138	Outliers: 12 of 138
A 382	₂ VAL	99.99	0.46Å HA with A 362 GLN OE1	Favored (2.13%) Isoleucine or valine / -155.9,132.7	75.3% (<i>t</i>) chi angles: 179.3	0.061Å	-	-
A 383	CYS	50	1.095Å HA with A 363 TYR HB2	Favored (8.11%) General / -80.7,99.2	3.8% (<i>m</i>) chi angles: 320.7	0.131Å	-	-
A 384	4 ILE	50	-	Favored (9.18%) Isoleucine or valine / -96.3,-9.4	69.9% (<i>mt</i>) chi angles: 296.2,178.9	0.197Å	-	-
A 385	S CYS	50	0.83Å HA with A 363 TYR CE1	OUTLIER (0.01%) General / 55.2,161.2	34.5% (<i>m</i>) chi angles: 309	0.091Å	-	-
A 386	GLN	50	0.461Å HB2 with A 387 PRO HD2	Favored (45.13%) Pre-proline / -73.8,166.3	12.3% (<i>pt20</i>) chi angles: 64.5,173.7,22.4	0.069Å	-	-
A 387	₇ PRO	50	0.461Å HD2 with A 386 GLN HB2	Favored (8.02%) Trans-proline / -73.9,122.8	95.7% (<i>Cg_endo</i>) chi angles: 32.6	0.037Å	-	-
A 388	GLY	50	0.656Å O with A 398 VAL HG12	Allowed (0.48%) Glycine / -122.7,92.7	-	-	-	-
				Favored				
Δ				(22 49%)	07 60/ (m 05)	^		

389	PHE	50	-	General / -128.3,164.5	97 .076 (111-09) chi angles: 295.2,272	0.007Å	-	-
A 390	THR	50	0.603Å HG22 with A 396 GLU OE1	Favored (9.16%) General / -165.5,151.0	10.6% (t) chi angles: 184.3	0.058Å	-	-
A 391	GLY	50	0.844Å O with A 383 CYS HB2	Allowed (0.13%) Glycine / -138.5,-38.0	-	-	-	-
A 392	ILE	50	-	Favored (5.13%) Isoleucine or valine / -99.9,-36.2	48.7% (<i>pt</i>) chi angles: 61.8,170.9	0.056Å	-	-
A 393	HIS	50	-	Favored (12.04%) General / -115.9,-5.2	62.9% (<i>m170</i>) chi angles: 296.4,162.7	0.013Å	OUTLIER(S) worst is CGND1: 4.586σ	-
A 394	CYS	50	-	Favored (10.83%) General / 63.2,37.9	51.2% (<i>m</i>) chi angles: 306.8	0.034Å	-	-
A 395	GLU	50	0.517Å HB3 with A 349 GLN OE1	Favored (17.76%) General / -90.1,-30.3	11.6% (<i>pt-20</i>) chi angles: 56.8,180.1,69.9	0.039Å	-	-
A 396	GLU	50	0.603Å OE1 with A 390 THR HG22	Favored (14.09%) General / -71.0,118.7	10.8% (<i>tm-20</i>) chi angles: 181.2,290.8,330.5	0.079Å	-	-
A 397	ASP	50	-	Favored (26.26%) General / -96.1,114.5	41.1% (<i>t0</i>) chi angles: 184.3,24.2	0.037Å	-	-
A 398	VAL	50	0.656Å HG12 with A 388 GLY O	Favored (14.74%) Isoleucine or valine / -76.5,-13.9	8.1% (<i>p</i>) chi angles: 70.2	0.09Å	-	-
A 399	ASN 9	99.99) -	- -	35.8% (<i>m120</i>) chi angles: 298.8,116.4	0.031Å	-	-

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