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All-Atom Contacts	Clashscore, all atoms:	117.31		0 th percentile* (N=1784, all resolutions)
	Clashscore is the number of serious steric overlaps (> 0.4 Å) per 1000 atoms.			
Protein Geometry	Poor rotamers	3	3.66%	Goal: <1%
	Ramachandran outliers	3	2.86%	Goal: <0.05%
	Ramachandran favored	93	88.57%	Goal: >98%
	MolProbity score^	3.55		8 th percentile* (N=27675, 0Å - 99Å)
	Cβ deviations >0.25Å	0	0.00%	Goal: 0
	Bad backbone bonds:	0 / 791	0.00%	Goal: 0%
	Bad backbone angles:	16 / 1074	1.49%	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: 110.61	Clashscore: 117.31	Outliers: 3 of 105	Poor rotamers: 3 of 82	Outliers: 0 of 94	Outliers: 0 of 107	Outliers: 16 of 107
252	SER	26.76	0.659Å OG with 287 PRO HB2	-	54.7% (m) chi angles: 299.8	0.087Å	-	-
253	VAL	48.83	0.88Å HB with 294 LEU HD12	Favored (52.28%) Isoleucine or valine / -104.0,119.1	56.1% (t) chi angles: 169.5	0.129Å	-	-
254	VAL	95.83	0.491Å O with 254 VAL HG13	Favored (47.91%) Isoleucine or valine / -98.7,130.2	7.5% (p) chi angles: 59	0.076Å	-	-
255	CYS	87.38	0.738Å HB3 with 265 VAL HG21	Favored (25.05%) General / -92.3,112.9	25.5% (p) chi angles: 57.7	0.07Å	-	-

256	VAL	59.76	0.914Å HA with 297 ILE HG22	Favored (15.53%) Isoleucine or valine / -99.5,104.0	27.3% (<i>m</i>) chi angles: 296	0.032Å	-	-
257	GLY	33.58	1.039Å HA2 with 299 ALA HB3	Favored (34.41%) Glycine / 157.9,-168.1	-	-	-	-
258	GLY	34.43	-	Favored (43.89%) Glycine / -83.1,-168.9	-	-	-	-
259	ASP	89.91	-	Favored (86.26%) General / -60.1,-39.4	43.1% (<i>t0</i>) chi angles: 193.1,19.6	0.086Å	-	OUTLIER(S) worst is CA-CB- CG: 4.607 σ
260	GLY	23.54	-	Favored (98.15%) Glycine / -64.2,-41.9	-	-	-	-
261	SER	72.22	-	Favored (90.67%) General / -64.0,-45.0	47.6% (<i>t</i>) chi angles: 180	0.071Å	-	-
262	ALA	40.77	0.55Å O with 265 VAL HG22	Favored (96.45%) General / -61.6,-40.9	-	0.084Å	-	-
263	SER	80.26	-	Favored (93.25%) General / -63.4,-39.0	73.9% (<i>m</i>) chi angles: 295.2	0.083Å	-	-
264	GLU	46.22	-	Favored (88.2%) General / -64.1,-45.5	52.2% (<i>mt-10</i>) chi angles: 290.5,192.7,312.4	0.087Å	-	-
265	VAL	108.33	0.738Å HG21 with 255 CYS HB3	Favored (94.33%) Isoleucine or valine / -65.2,-45.3	30.4% (<i>m</i>) chi angles: 294.3	0.076Å	-	-
266	ALA	45.98	0.565Å N with 265 VAL HG23	Favored (96.9%) General / -61.9,-44.4	-	0.092Å	-	-
267	HIS	81.91	0.519Å HD2 with 343 ARG HB3	Favored (97.41%) General / -64.0,-40.9	57.7% (<i>t-80</i>) chi angles: 187.9,267.8	0.076Å	-	OUTLIER(S) worst is CD2- NE2-CE1: 4.455 σ

268	ALA	40.77	1.122Å HB1 with 277 ALA HB1	Favored (95.76%) General / -60.5,-44.6	-	0.072Å	-	OUTLIER(S) worst is C-N- CA: 4.163 σ
269	LEU	81.86	0.953Å HD12 with 294 LEU HD21	Favored (13.52%) General / -65.2,-56.3	25.8% (<i>mt</i>) chi angles: 290.6,189.7	0.098Å	-	-
270	LEU	140.79	0.804Å HD22 with 271 LEU HD12	Favored (11.29%) General / -70.9,-54.5	4.4% (<i>tt</i>) chi angles: 190.8,176.1	0.049Å	-	-
271	LEU	231.07	0.804Å HD12 with 270 LEU HD22	Favored (9.36%) General / -99.7,169.3	5.9% (<i>mp</i>) chi angles: 292.8,64.9	0.093Å	-	-
#	Alt Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
Avg: 110.61			Clashscore: 117.31	Outliers: 3 of 105	Poor rotamers: 3 of 82	Outliers: 0 of 94	Outliers: 0 of 107	Outliers: 16 of 107
272	ARG	254.22	0.588Å HA with 278 GLY CA	Favored (49.59%) General / -66.7,150.1	0% chi angles: 307.8,226.4,101.8,260	0.098Å	-	-
273	ALA	227.12	0.782Å HB3 with 277 ALA HB3	Favored (31.98%) General / -125.0,159.1	-	0.102Å	-	-
274	GLN	129.03	-	Favored (85.84%) General / -63.3,-46.6	64.7% (<i>tt0</i>) chi angles: 179.8,180.2,31.4	0.1Å	-	-
275	LYS	293.87	-	Favored (36.34%) General / -139.9,139.8	37.3% (<i>ttpt</i>) chi angles: 183,173,81.4,174.1	0.117Å	-	-
276	ASN	239.14	-	Favored (10.01%) General / 45.3,46.1	73% (<i>m-20</i>) chi angles: 289.2,303	0.07Å	-	OUTLIER(S) worst is CA-CB- CG: 5.456 σ
277	ALA	283.13	1.122Å HB1 with 268 ALA HB1	Favored (2.34%) General / -175.0,175.3	-	0.096Å	-	-
278	GLY	272.41	0.749Å HA2 with 271 LEU O	Favored (2.25%) Glycine / 113.2,-41.3	-	-	-	-

279	MET	144.44	-		Favored (24.66%) General / -161.4,168.0	96.9% (<i>mtp</i>) chi angles: 293.9,180.9,75.1	0.121Å	-	-
280	GLU	103.55	1.119Å HG2 with 285 LEU H		Allowed (1.15%) General / -153.4,-160.8	5.3% (<i>tp10</i>) chi angles: 209.3,79.5,50.7	0.079Å	-	-
281	THR	131.82	-		Allowed (0.11%) General / -77.2,-158.5	61.6% (<i>p</i>) chi angles: 62.7	0.073Å	-	-
282	ASP	56.98	-		Favored (50.13%) General / -58.0,-54.2	56.9% (<i>m-20</i>) chi angles: 292.9,300.7	0.065Å	-	OUTLIER(S) worst is CA-CB- CG: 5.67 σ
283	ARG	143.69	-		Favored (51.48%) General / -104.0,127.8	0.1% chi angles: 276.2,87.7,94.4,140.2	0.138Å	-	-
284	ILE	88.89	0.763Å HA with 280 GLU HB3		Favored (15.6%) Isoleucine or valine / -60.3,142.4	93.4% (<i>mt</i>) chi angles: 297.9,168.3	0.09Å	-	-
285	LEU	143.86	1.119Å H with 280 GLU HG2		Favored (78.5%) General / -55.9,-45.2	2.8% (<i>tm?</i>) chi angles: 180.1,291	0.089Å	-	-
286	THR	228.94	0.765Å OG1 with 253 VAL HG23		Favored (43.48%) Pre-proline / -83.0,137.1	11.1% (<i>t</i>) chi angles: 184.6	0.124Å	-	-
287	PRO	113.13	0.664Å HD3 with 285 LEU O		Favored (28.71%) Trans-proline / -78.5,158.2	76.5% (<i>Cg_exo</i>) chi angles: 333.2	0.086Å	-	-
288	VAL	167.56	0.98Å HA with 294 LEU HD22		Allowed (1.6%) Isoleucine or valine / -97.5,168.6	28.5% (<i>m</i>) chi angles: 295.3	0.107Å	-	-
289	ARG	302.22	0.834Å CZ with 323 ILE HA		Favored (3.74%) General / -148.8,-170.9	32.1% (<i>mtm105</i>) chi angles: 292.4,188.4,297.4,87.8	0.131Å	-	-
290	ALA	240.95	0.653Å HB2 with 326 HIS O		Favored (27.44%) General / -59.8,150.7	-	0.089Å	-	-
			0.668Å		OUTLIER	27.1% (<i>mm-40</i>)			

291	GLN	271.8	OE1 with 309 LEU HD11	(0.02%) General / 93.4,169.6	chi angles: 297.1,300.7,8.5	0.107Å	-	-
#	Alt Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
		Avg: 110.61	Clashscore: 117.31	Outliers: 3 of 105	Poor rotamers: 3 of 82	Outliers: 0 of 94	Outliers: 0 of 107	Outliers: 16 of 107
292	LEU	60.04	0.523Å HB2 with 293 PRO CD	Favored (76.55%) Pre-proline / -62.5,-41.9	66.9% (<i>mt</i>) chi angles: 298.3,184.6	0.041Å	-	-
293	PRO	69.76	0.523Å CD with 292 LEU HB2	Favored (21.95%) Trans-proline / -80.2,164.3	9.6% (<i>Cg_endo</i>) chi angles: 12.9	0.113Å	-	-
294	LEU	255.97	0.98Å HD22 with 288 VAL HA	Favored (25.18%) General / -58.6,-56.2	56.2% (<i>mt</i>) chi angles: 307.6,179	0.212Å	-	-
295	GLY	55.38	0.71Å HA3 with 289 ARG NH2	Favored (9.16%) Glycine / -152.9,142.3	-	-	-	-
296	LEU	151.76	0.993Å HD21 with 306 ALA HB2	Favored (43.09%) General / -134.4,136.1	55.8% (<i>tp</i>) chi angles: 172.5,63.3	0.12Å	-	-
297	ILE	165.66	0.914Å HG22 with 256 VAL HA	Favored (28.52%) Pre-proline / -121.8,120.5	0% chi angles: 192.8,294.4	0.045Å	-	-
298	PRO	117.73	0.737Å HD2 with 297 ILE HD13	OUTLIER (0.1%) Trans-proline / -62.1,74.8	95% (<i>Cg_endo</i>) chi angles: 30.4	0.052Å	-	-
299	ALA	82.49	1.039Å HB3 with 257 GLY HA2	Favored (48.07%) General / -78.5,-33.5	-	0.083Å	-	-
300	GLY	45.76	-	Favored (48.53%) Glycine / -80.0,-175.6	-	-	-	-
301	SER	89.25	-	Allowed (0.14%) General / -68.9,-74.0	65.3% (<i>p</i>) chi angles: 56.9	0.044Å	-	-

302	THR	117.84	0.59Å HG23 with 303 ASN N	Favored (74.37%) General / -65.1,-48.2	9% (<i>t</i>) chi angles: 183.4	0.049Å	-	-
303	ASN	50.89	0.59Å N with 302 THR HG23	Favored (30.81%) General / 54.3,43.3	92.4% (<i>m-20</i>) chi angles: 292.9,324	0.094Å	-	OUTLIER(S) worst is CA-CB- CG: 4.092 σ
304	VAL	98.1	0.608Å HG13 with 305 LEU N	Favored (83.85%) Isoleucine or valine / -60.9,-49.6	7.6% (<i>p</i>) chi angles: 59.1	0.041Å	-	-
305	LEU	103.45	0.63Å HD23 with 346 PHE HD1	Favored (83.27%) General / -64.8,-46.2	3.1% (<i>tm?</i>) chi angles: 180.4,287.4	0.064Å	-	-
306	ALA	35.54	0.993Å HB2 with 296 LEU HD21	Favored (87.98%) General / -60.9,-47.1	-	0.098Å	-	-
307	HIS	73.04	-	Favored (73.92%) General / -69.5,-43.0	56.3% (<i>t-80</i>) chi angles: 193.6,275.5	0.084Å	-	OUTLIER(S) worst is CD2- NE2-CE1: 4.371 σ
308	SER	32.31	-	Favored (70.69%) General / -59.3,-51.3	92% (<i>p</i>) chi angles: 62.9	0.083Å	-	-
309	LEU	126.26	0.683Å HD22 with 311 GLY CA	Favored (83.81%) General / -62.5,-36.8	3.2% (<i>tt</i>) chi angles: 187.2,179.8	0.091Å	-	-
310	HIS	257.37	-	Favored (11.51%) General / 64.3,18.8	20.1% (<i>t60</i>) chi angles: 196.6,89.2	0.095Å	-	OUTLIER(S) worst is CD2- NE2-CE1: 4.44 σ
311	GLY	126.77	0.683Å CA with 309 LEU HD22	Favored (79.02%) Glycine / -68.4,-43.4	-	-	-	-
<div> <div>#</div> <div>Alt Res</div> <div>High B</div> <div>Clash > 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:</div> <div>Clashscore:</div> <div>Outliers: 3 of</div> <div>Poor rotamers: 3 of</div> <div>Outliers:</div> <div>Outliers:</div> <div>Outliers: 16</div> </div>								
<div> <div>110.61</div> <div>117.31</div> <div>105</div> <div>82</div> <div>0 of 94</div> <div>0 of 107</div> <div>of 107</div> </div>								
312	VAL	127.62	0.738Å HG21 with 306 ALA HB1	Favored (50.84%) Pre-proline / -82.1,133.5	35.2% (<i>m</i>) chi angles: 298.2	0.095Å	-	-

313	PRO	143.88	0.439Å HD2 with 312 VAL HA	Favored (22.13%) Trans-proline / -80.1,154.0	11.4% (<i>Cg_endo</i>) chi angles: 14.6	0.089Å	-	-
314	HIS	101.61	-	Favored (72.1%) General / -71.2,-37.7	42.8% (<i>t60</i>) chi angles: 198.3,69.3	0.095Å	-	OUTLIER(S) worst is CD2- NE2-CE1: 4.401 σ
315	VAL	92.08	0.72Å HG13 with 318 ALA HB3	Favored (23.28%) Isoleucine or valine / -58.9,131.6	9.3% (<i>p</i>) chi angles: 60.5	0.046Å	-	-
316	ILE	91.53	0.705Å HG13 with 317 THR N	Favored (94.2%) Isoleucine or valine / -65.4,-45.1	42.2% (<i>pt</i>) chi angles: 62.2,166.7	0.054Å	-	-
317	THR	30.17	0.705Å N with 316 ILE HG13	Favored (85.86%) General / -65.2,-45.2	71.2% (<i>p</i>) chi angles: 61.9	0.062Å	-	-
318	ALA	33.81	0.72Å HB3 with 315 VAL HG13	Favored (93.43%) General / -63.4,-44.9	-	0.071Å	-	-
319	THR	105.68	0.836Å HA with 322 ILE HD13	Favored (86.09%) General / -62.0,-37.8	12.9% (<i>t</i>) chi angles: 185.9	0.057Å	-	-
320	LEU	93.53	0.674Å O with 320 LEU HD23	Favored (88.6%) General / -62.1,-38.4	3.2% (<i>tt</i>) chi angles: 187.4,180	0.083Å	-	-
321	HIS	111.84	-	Favored (76.74%) General / -62.0,-34.8	29.1% (<i>t60</i>) chi angles: 189,94.5	0.091Å	-	OUTLIER(S) worst is CD2- NE2-CE1: 4.442 σ
322	ILE	88.05	0.836Å HD13 with 319 THR HA	Favored (37.34%) Isoleucine or valine / -56.8,-32.2	3.5% (<i>mp</i>) chi angles: 294.4,76.6	0.108Å	-	-
323	ILE	53.31	0.834Å HA with 289 ARG CZ	Favored (57.14%) Isoleucine or valine / -56.9,-38.0	71.4% (<i>mt</i>) chi angles: 301.8,166.7	0.071Å	-	-
324	MET	129.23	-	Favored (74.59%) General / -63.4,-33.0	6.1% (<i>tpt</i>) chi angles: 205.1,73.9,171.5	0.107Å	-	-

325	GLY	37.06	-	Favored (24.71%) Glycine / -62.3,164.3	-	-	-	-
326	HIS	84.92	0.653Å O with 290 ALA HB2	Favored (34.99%) General / -72.6,158.8	75.4% (<i>m80</i>) chi angles: 293.8,77.5	0.069Å	-	OUTLIER(S) worst is CD2- NE2-CE1: 4.439 σ
327	VAL	111.69	0.794Å HG23 with 289 ARG CA	Favored (4.23%) Isoleucine or valine / -85.7,149.5	12.4% (<i>p</i>) chi angles: 62.3	0.089Å	-	-
328	GLN	75.72	0.585Å H with 290 ALA HA	Favored (35.18%) General / -134.0,128.8	8.8% (<i>tt0</i>) chi angles: 185.6,174.3,183.4	0.105Å	-	-
329	LEU	119.8	0.741Å H with 329 LEU HD23	Favored (53.84%) General / -105.5,129.2	1.3% (<i>pt?</i>) chi angles: 66.1,180.2	0.103Å	-	-
330	VAL	49.65	0.739Å HG12 with 331 ASP O	Favored (22.56%) Isoleucine or valine / -141.9,146.6	75.7% (<i>t</i>) chi angles: 174.1	0.085Å	-	-
331	ASP	98.59	0.739Å O with 330 VAL HG12	Favored (3.25%) General / -90.8,-172.1	48.6% (<i>t0</i>) chi angles: 191.4,9.1	0.112Å	-	OUTLIER(S) worst is C-N- CA: 5.018 σ
#	Alt Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	C β deviation	Bond lengths	Bond angles
		Avg: 110.61	Clashscore: 117.31	Outliers: 3 of 105	Poor rotamers: 3 of 82	Outliers: 0 of 94	Outliers: 0 of 107	Outliers: 16 of 107
332	VAL	86.06	0.727Å HG22 with 345 GLY HA2	Allowed (1.19%) Isoleucine or valine / -71.2,103.4	84.1% (<i>t</i>) chi angles: 174.8	0.12Å	-	-
333	CYS	104.41	0.403Å SG with 334 THR N	Allowed (1.69%) General / -64.7,-62.3	16.6% (<i>p</i>) chi angles: 53.9	0.052Å	-	-
334	THR	124.14	0.841Å HG23 with 335 PHE CD2	Favored (69.99%) General / -71.6,-40.3	10.1% (<i>t</i>) chi angles: 181.2	0.051Å	-	-
335	PHE	210.72	0.841Å CD2 with 334 THR HG23	Allowed (0.65%) General /	68.6% (<i>m-85</i>) chi angles: 285.5,273.6	0.066Å	-	OUTLIER(S) worst is CA-CB- CG: 7.39 σ

336	SER	100.48	0.449Å HB3 with 335 PHE O	-111.7,-158.7 OUTLIER (0.01%) General / 177.3,-144.0	99.1% (<i>p</i>) chi angles: 64.6	0.116Å	-	-
337	THR	110.72	0.742Å CG2 with 340 LYS HA	Favored (28.92%) General / -101.1,145.3	14.9% (<i>t</i>) chi angles: 188.7	0.097Å	-	-
338	ALA	31.16	-	Favored (54.14%) General / -111.9,125.5	-	0.108Å	-	-
339	GLY	22.82	0.412Å C with 341 LEU H	Favored (74.66%) Glycine / 77.7,0.7	-	-	-	-
340	LYS	102.5	0.742Å HA with 337 THR CG2	Allowed (1.15%) General / 69.2,-5.0	37.8% (<i>mtmt</i>) chi angles: 293.8,165,298.3,170.2	0.06Å	-	-
341	LEU	155.23	0.412Å H with 339 GLY C	Favored (5.98%) General / -75.8,-55.1	62.7% (<i>tp</i>) chi angles: 179.4,63.8	0.11Å	-	-
342	LEU	170.71	0.775Å HD23 with 343 ARG N	Favored (47.87%) General / -118.2,142.0	5.6% (<i>tt</i>) chi angles: 181.9,167.6	0.059Å	-	-
343	ARG	161.92	0.775Å N with 342 LEU HD23	Favored (29.46%) General / -116.9,155.2	44.9% (<i>ttt180</i>) chi angles: 160.1,185.5,164.8,181	0.11Å	-	-
344	PHE	103.11	0.58Å O with 332 VAL HG11	Favored (23.13%) General / -146.8,136.5	21.9% (<i>p90</i>) chi angles: 59.1,284.3	0.118Å	-	-
345	GLY	70.57	0.727Å HA2 with 332 VAL HG22	Favored (51.04%) Glycine / -74.5,-35.8	-	-	-	-
346	PHE	140.71	0.63Å HD1 with 305 LEU HD23	Allowed (0.15%) General / -98.0,-113.3	48.8% (<i>t80</i>) chi angles: 191.4,72.2	0.076Å	-	OUTLIER(S) worst is CA-CB- CG: 6.473 σ
347	SER	100.17	0.48Å N with 346 PHE CD2	Favored (22.67%) General / -129.4,164.9	68.4% (<i>m</i>) chi angles: 296.2	0.093Å	-	-

348	ALA	32.37	-	Favored (54.43%) General / -121.9,138.3	-	0.097Å	-	-
349	MET	94.34	-	Favored (47.53%) General / -111.9,139.3	1.8% (<i>mpt?</i>) chi angles: 285.2,74.6,159.7	0.152Å	-	-
350	PHE	99.52	0.411Å CD2 with 351 GLY O	Favored (51.01%) General / -129.6,150.3	30.6% (<i>t80</i>) chi angles: 196.3,73.4	0.067Å	-	OUTLIER(S) worst is CA-CB- CG: 4.546 σ
351	GLY	18.76	0.411Å O with 350 PHE CD2	Favored (12.4%) Glycine / -110.7,166.9	-	-	-	-
#	Alt Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
		Avg: 110.61	Clashscore: 117.31	Outliers: 3 of 105	Poor rotamers: 3 of 82	Outliers: 0 of 94	Outliers: 0 of 107	Outliers: 16 of 107
352	PHE	37.33	-	Favored (49.82%) General / -104.0,132.8	89.5% (<i>m-85</i>) chi angles: 299.7,88.6	0.073Å	-	OUTLIER(S) worst is CA-CB- CG: 6.343 σ
353	GLY	17.5	-	Favored (16.22%) Glycine / 141.1,177.4	-	-	-	-
354	GLY	18.52	-	Favored (30.05%) Glycine / -97.5,-155.4	-	-	-	-
355	ARG	154.09	-	Favored (7.77%) General / -110.0,170.9	16.2% (<i>mtp85</i>) chi angles: 282.9,165.9,27.6,89.9	0.148Å	-	-
356	THR	116.03	-	Favored (18.04%) General / -74.3,169.2	15.3% (<i>t</i>) chi angles: 187.7	0.08Å	-	-
357	LEU	216.07	0.798Å HD23 with 358 ALA N	Favored (48.8%) General / -105.4,134.3	3.4% (<i>tt</i>) chi angles: 188.6,179.3	0.046Å	-	-
358	ALA	33.4	0.798Å N with 357 LEU HD23	-	-	0.109Å	-	-

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