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All-Atom Contacts	Clashscore, all atoms:	0	100 th percentile* (N=1784, all resolutions)	
	Clashscore is the number of serious steric overlaps (> 0.4 Å) per 1000 atoms.			
Protein Geometry	Poor rotamers	13	8.67%	Goal: <1%
	Ramachandran outliers	3	1.76%	Goal: <0.05%
	Ramachandran favored	138	81.18%	Goal: >98%
	MolProbity score [^]	1.93		79 th percentile* (N=27675, 0Å - 99Å)
	Cβ deviations >0.25Å	4	2.53%	Goal: 0
	Bad backbone bonds:	0 / 1382	0.00%	Goal: 0%
	Bad backbone angles:	11 / 1868	0.59%	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	C β deviation	Bond lengths	Bond angles
Avg: Clashscore: 100.32 0 Outliers: 3 of 170 Poor rotamers: 13 of 150 Outliers: 4 of 158 Outliers: 0 of 172 Outliers: 11 of 172								
465	TYR	76.46	-	-	29.1% (<i>m-85</i>) chi angles: 312.9,293.2	0.17Å	-	-
466	MET	32.81	-	Favored (68.84%) General / -61.4,-27.9	36.6% (<i>mtm</i>) chi angles: 295.6,209.5,284.9	0.195Å	-	-
467	ASN	93.52	-	Allowed (1.69%) General / -47.8,-26.7	14.9% (<i>p-10</i>) chi angles: 65,298.2	0.098Å	-	-
468	ASN	80.76	-	Favored (4.34%) General / -132.9,12.8	7.1% (<i>p-10</i>) chi angles: 68.5,282.4	0.063Å	-	-

469	TYR	97.41	-	Favored (2.79%) General / -129.9,-23.6	22.2% (<i>m-30</i>) chi angles: 299.4,323.1	0.109Å	-	-
470	SER	240.49	-	Allowed (0.9%) General / -165.6,111.6	22.3% (<i>t</i>) chi angles: 187.9	0.053Å	-	-
471	ILE	220.1	-	Allowed (0.3%) Pre-proline / -94.4,-38.5	37.8% (<i>mm</i>) chi angles: 305,306.5	0.11Å	-	-
472	PRO	191.85	-	Favored (23.29%) Trans-proline / -74.3,137.3	28.2% (<i>Cg_endo</i>) chi angles: 37.5	0.031Å	-	-
473	LYS	117.13	-	Favored (74.46%) General / -58.9,-36.4	28.3% (<i>mmmt</i>) chi angles: 311.2,308.7,295.2,177.1	0.139Å	-	-
474	LEU	133.42	-	Favored (92.3%) General / -64.6,-38.8	3% (<i>mm?</i>) chi angles: 293.2,312.2	0.11Å	-	-
475	VAL	55.27	-	Favored (21.15%) Isoleucine or valine / -77.7,-35.3	43.6% (<i>t</i>) chi angles: 184	0.106Å	-	-
476	GLN	91.11	-	Favored (77.63%) General / -59.6,-37.1	96.6% (<i>mt-30</i>) chi angles: 289.8,177.9,339	0.128Å	-	-
477	LYS	60.2	-	Favored (20.21%) General / -86.5,-34.0	49.7% (<i>tptt</i>) chi angles: 177.2,53.8,170.4,169.2	0.182Å	-	-
478	ARG	121.87	-	Favored (79.71%) General / -65.3,-35.0	52.7% (<i>mtp180</i>) chi angles: 277.6,184.3,65.6,169.8	0.223Å	-	-
479	VAL	94.56	-	Favored (70.34%) Isoleucine or valine / -66.4,-34.5	5.2% (<i>p</i>) chi angles: 76	0.199Å	-	-
480	ARG	159.42	-	Favored (63.38%) General / -73.1,-30.1	19.6% (<i>tpt180</i>) chi angles: 171.3,59.4,192.7,188	0.185Å	-	-
481	THR	98.79	-	Favored (66.37%)	22.7% (<i>p</i>)	0.208Å	-	-

				General / -69.4,-28.7	chi angles: 49.4			
482	TRP	94.31	-	Favored (84.16%) General / -58.0,-47.1	35.8% (<i>t90</i>) chi angles: 195,97.8	0.057Å	-	OUTLIER(S) worst is CE3- CD2-CG: 4.067 σ
483	TYR	46.03	-	Favored (93.1%) General / -61.4,-40.1	0.3% chi angles: 189.9,324.4	0.075Å	-	OUTLIER(S) worst is CA-CB- CG: 5.785 σ
484	GLU	41.96	-	Allowed (1%) General / -77.3,14.3	85.5% (<i>mt-10</i>) chi angles: 294,161.8,348.1	0.102Å	-	-
#	Alt Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
Avg: 100.32				Clashscore: 0	Outliers: 3 of 170	Poor rotamers: 13 of 150	Outliers: 4 of 158	Outliers: 0 of 172
485	TYR	59.78	-	Favored (3.28%) General / -136.0,22.4	96.5% (<i>m-85</i>) chi angles: 294.1,269.9	0.101Å	-	OUTLIER(S) worst is C-N- CA: 4.232 σ
486	THR	53.46	-	Allowed (0.65%) General / -124.5,-73.0	1.8% (<i>m</i>) chi angles: 323.3	0.108Å	-	-
487	TRP	110.19	-	Favored (13.13%) General / -112.2,-15.9	2.6% (<i>m-90</i>) chi angles: 315.3,292.5	0.119Å	-	-
488	ASP	55.74	-	Favored (15.93%) General / 50.6,51.9	6.8% (<i>m-20</i>) chi angles: 306.9,0.4	0.165Å	-	-
489	SER	109.81	-	Allowed (0.36%) General / 88.3,-15.4	0.8% chi angles: 211.7	0.278Å	-	-
490	GLN	220.23	-	Favored (39.58%) General / -64.7,153.5	7% (<i>tp-100</i>) chi angles: 179.2,57,266.1	0.053Å	-	-
491	ARG	188.01	-	Favored (44.5%) General / -54.3,135.6	66.6% (<i>ttp85</i>) chi angles: 190.8,184.1,69.8,87.3	0.075Å	-	-
492	MET	50.74	-	Favored (19.49%) General /	4.3% (<i>ttp</i>) chi angles: 177.3,220.3,82.3	0.097Å	-	-

				-49.1,131.6 Favored (26.85%) General / -86.6,145.2	80.9% (<i>mt</i>) chi angles: 302.1,180.6	0.026Å	-	-
493	LEU	54.95	-	Allowed (1.48%) General / -88.7,47.3	0.8% chi angles: 325.4,275.8	0.063Å	-	-
494	ASP	86.32	-	Favored (66.02%) General / -57.0,-32.3	65.4% (<i>mt-10</i>) chi angles: 294.3,175.6,29.6	0.064Å	-	-
495	GLU	104.66	-	Favored (68.11%) General / -55.5,-37.6	45.1% (<i>p</i>) chi angles: 54.1	0.105Å	-	-
496	SER	75.85	-	Favored (9.46%) General / -93.0,-42.4	18.3% (<i>t70</i>) chi angles: 183.3,270.1	0.073Å	-	-
497	ASP	46.22	-	Favored (91.44%) General / -61.3,-39.7	85.7% (<i>mt</i>) chi angles: 297.8,171.2	0.165Å	-	-
498	LEU	50.73	-	Favored (85.53%) General / -60.1,-39.2	9.1% (<i>mp</i>) chi angles: 268.1,63.6	0.13Å	-	-
499	LEU	101.96	-	Favored (84.73%) General / -65.3,-45.4	14.5% (<i>tpp</i>) chi angles: 166.4,192.9,56.3,54.3	0.039Å	-	-
500	LYS	118.13	-	Favored (58.31%) General / -75.8,-20.4	21.7% (<i>m</i>) chi angles: 309.9	0.15Å	-	-
501	THR	106.65	-	Favored (88.09%) Pre-proline / -59.7,130.4	32.2% (<i>mt</i>) chi angles: 291.6,188	0.071Å	-	-
502	LEU	112.83	-	Favored (99.36%) Trans-proline / -59.3,144.5	1.3% (<i>Cg_exo</i>) chi angles: 321.4	0.078Å	-	-
503	PRO	148.8	-	Favored (50.73%) General /	25.4% (<i>m</i>) chi angles: 308.7	0.216Å	-	-
504	THR	32.08	-					

-53.1,-33.1

#	Alt	Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
Avg: 100.32				Clashscore: 0	Outliers: 3 of 170	Poor rotamers: 13 of 150	Outliers: 4 of 158	Outliers: 0 of 172	Outliers: 11 of 172
505	THR	89.44	-	Favored (89.21%) General / -59.6,-41.0	21.7% (<i>p</i>) chi angles: 49	0.106Å	-	-	
506	VAL	92.54	-	Favored (9.08%) Isoleucine or valine / -89.0,-15.1	1.4% (<i>p</i>) chi angles: 85.3	0.245Å	-	-	
507	GLN	83.39	-	Favored (93.36%) General / -63.3,-39.0	96.6% (<i>mt-30</i>) chi angles: 291.4,171,338.3	0.112Å	-	-	
508	LEU	104.53	-	Favored (82.62%) General / -67.3,-37.0	0.6% chi angles: 276.3,29.9	0.1Å	-	-	
509	ALA	56.74	-	Favored (5.92%) General / -82.8,-53.4	-	0.057Å	-	-	
510	LEU	190.57	-	Allowed (0.18%) General / -100.8,-114.0	1.4% (<i>tt</i>) chi angles: 212.3,178.2	0.209Å	-	OUTLIER(S) worst is C-CA- CB: 4.303 σ	
511	ALA	221.96	-	Favored (17.79%) General / 50.3,50.9	-	0.128Å	-	-	
512	ILE	201.22	-	Allowed (0.39%) Isoleucine or valine / 48.8,52.7	12.5% (<i>tt</i>) chi angles: 201.3,164.3	0.401Å	-	-	
513	ASP	201.63	-	OUTLIER (0.04%) General / 80.8,78.6	4.2% (<i>m-20</i>) chi angles: 319.8,311.2	0.147Å	-	-	
514	VAL	121.88	-	Allowed (0.1%) Isoleucine or valine / -92.3,-87.9	99.4% (<i>t</i>) chi angles: 176.5	0.212Å	-	-	
515	ASN	77.09	-	Favored (48.07%) General / -77.7,-38.0	83.5% (<i>m-20</i>) chi angles: 292.9,350.1	0.147Å	-	-	

516	PHE	195.07	-	Favored (9.32%) General / -82.5,77.2	81.5% (<i>t80</i>) chi angles: 179.8,84.2	0.033Å	-	-
517	SER	268.21	-	Allowed (0.17%) General / -155.7,-145.9	8.2% (<i>t</i>) chi angles: 195	0.121Å	-	OUTLIER(S) worst is C-N- CA: 4.884 σ
518	ILE	233.12	-	Allowed (1.44%) Isoleucine or valine / -67.4,-1.8	40.2% (<i>pt</i>) chi angles: 62.2,166.1	0.153Å	-	-
519	ILE	122.5	-	Allowed (0.2%) Isoleucine or valine / -35.6,-53.7	20.9% (<i>tt</i>) chi angles: 187.4,169.6	0.176Å	-	-
520	SER	74.62	-	Favored (20.94%) General / -91.6,-21.2	93.1% (<i>p</i>) chi angles: 66	0.126Å	-	-
521	LYS	123.2	-	Favored (17.05%) General / -82.8,-43.1	17% (<i>mmtm</i>) chi angles: 333.7,301,172.1,293.5	0.138Å	-	-
522	VAL	105.96	-	Allowed (0.7%) Isoleucine or valine / -72.8,175.2	1.4% (<i>p</i>) chi angles: 84.6	0.122Å	-	-
523	ASP	40.14	-	Favored (5%) General / -129.5,-0.4	3.7% (<i>m-20</i>) chi angles: 320.6,286.2	0.15Å	-	-
524	LEU	114.03	-	Favored (5.16%) General / -86.4,-53.2	51.1% (<i>tp</i>) chi angles: 175.1,58	0.053Å	-	-

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Avg: 100.32				Clashscore: 0	Outliers: 3 of 170	Poor rotamers: 13 of 150	Outliers: 4 of 158	Outliers: 0 of 172	Outliers: 11 of 172
525	PHE	86.76	-	Allowed (0.54%) General / -81.0,40.6	9.2% (<i>m-30</i>) chi angles: 310.8,323.5	0.123Å	-	-	
526	LYS	143.12	-	Favored (7.79%) General / -122.4,-14.7	12.2% (<i>ptpt</i>) chi angles: 52.8,184.5,54.5,151.8	0.178Å	-	-	
527	GLY	39.91	-	Favored (10.64%)	-	-	-	-	

528	CYS	101.26	-	Glycine / -107.6,-18.0 Favored (22.3%) General / -66.2,161.3	20.2% (<i>p</i>) chi angles: 69.9	0.043Å	-	-
529	ASP	97.16	-	Favored (19.73%) General / -69.3,165.8	9.1% (<i>p-10</i>) chi angles: 66.2,292.1	0.068Å	-	-
530	THR	110.26	-	Favored (59.91%) General / -74.7,-10.8	6.9% (<i>t</i>) chi angles: 194.3	0.221Å	-	-
531	GLN	77.03	-	Favored (14.2%) General / -88.7,-39.1	7.9% (<i>tt0</i>) chi angles: 204.9,205.6,11.9	0.126Å	-	-
532	MET	77.62	-	Favored (90.95%) General / -59.2,-42.4	15.6% (<i>ttt</i>) chi angles: 180.6,172.8,147.5	0.086Å	-	-
533	ILE	102.85	-	Favored (85.33%) Isoleucine or valine / -61.9,-39.9	11.6% (<i>tt</i>) chi angles: 203,170.8	0.263Å	-	-
534	TYR	182.02	-	Favored (32.77%) General / -81.0,-34.5	2.5% (<i>p90</i>) chi angles: 78.8,71.8	0.25Å	-	-
535	ASP	51.36	-	Favored (56.83%) General / -68.7,-49.7	38.8% (<i>t0</i>) chi angles: 187.4,28	0.114Å	-	-
536	MET	172.35	-	Favored (21.27%) General / -57.3,-56.5	47.5% (<i>tpp</i>) chi angles: 181.5,75.8,82.7	0.092Å	-	-
537	LEU	114.98	-	Favored (66.25%) General / -70.7,-29.9	8.9% (<i>mp</i>) chi angles: 280.6,55.5	0.226Å	-	-
538	LEU	143.31	-	Favored (73.19%) General / -67.6,-32.5	36.4% (<i>tp</i>) chi angles: 182.4,54.4	0.096Å	-	-
				Favored (36.61%)	13.6% (<i>mtm-85</i>)			

539	ARG	153.25	-	General / -80.6,-31.8	chi angles: 302.7,229.1,291,281.5	0.181Å	-	-
540	LEU	63.35	-	Favored (4.89%) General / -54.8,154.6	36% (<i>mt</i>) chi angles: 297.9,189.9	0.072Å	-	-
541	LYS	89.03	-	Favored (37.01%) General / -139.9,144.2	36.6% (<i>mmtm</i>) chi angles: 298.2,294.7,162.1,292.8	0.05Å	-	-
542	SER	84.28	-	Favored (31.48%) General / -73.9,126.9	66.2% (<i>m</i>) chi angles: 298.5	0.071Å	-	-
543	VAL	40.74	-	Favored (19.26%) Isoleucine or valine / -143.6,132.0	51.2% (<i>t</i>) chi angles: 182.3	0.057Å	-	-
544	LEU	156.28	-	Favored (15.37%) General / -95.5,158.6	6.5% (<i>mp</i>) chi angles: 279.2,81.3	0.073Å	-	-
#	Alt Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
Avg: 100.32			Clashscore: 0	Outliers: 3 of 170	Poor rotamers: 13 of 150	Outliers: 4 of 158	Outliers: 0 of 172	Outliers: 11 of 172
545	TYR	113.97	-	Favored (38.73%) General / -142.1,161.2	98.7% (<i>m-85</i>) chi angles: 296.9,93	0.073Å	-	-
546	LEU	95.02	-	Favored (40.73%) Pre-proline / -123.4,162.3	18.6% (<i>mt</i>) chi angles: 314.5,171.8	0.108Å	-	-
547	PRO	144.95	-	Allowed (0.89%) Trans-proline / -67.2,104.5	70.3% (<i>Cg_endo</i>) chi angles: 28.2	0.03Å	-	-
548	GLY	31.08	-	Favored (3.34%) Glycine / 106.2,33.9	-	-	-	-
549	ASP	106.62	-	Favored (52.55%) General / -131.8,148.2	0.8% chi angles: 37.2,52.6	0.149Å	-	-

550	PHE	63.85	-	Favored (49.11%) General / -104.2,124.4	29.7% (<i>m-85</i>) chi angles: 287.1,250.5	0.038Å	-	-
551	VAL	100.78	-	Favored (14.57%) Isoleucine or valine / -87.7,-49.4	0.2% chi angles: 272.4	0.181Å	-	-
552	CYS	51.07	-	Favored (44.48%) General / -102.2,122.6	19.6% (<i>m</i>) chi angles: 279.3	0.044Å	-	-
553	LYS	145.27	-	Favored (46.38%) General / -122.3,125.6	21.9% (<i>mtmm</i>) chi angles: 295.7,155.4,298.1,305.5	0.116Å	-	-
554	LYS	216.98	-	Favored (71.07%) General / -55.9,-39.0	9.7% (<i>tttm</i>) chi angles: 224.2,190.8,191.3,307.8	0.197Å	-	-
555	GLY	131.1	-	Favored (70.55%) Glycine / -87.6,-10.2	-	-	-	-
556	GLU	109.62	-	Favored (53.67%) General / -63.7,133.5	26.3% (<i>tt0</i>) chi angles: 165.4,189.7,46.5	0.088Å	-	-
557	ILE	123.96	-	Allowed (1.78%) Isoleucine or valine / -79.0,94.6	5.3% (<i>mm</i>) chi angles: 306.4,323.8	0.062Å	-	-
558	GLY	61.45	-	OUTLIER (0.05%) Glycine / -60.9,91.5	-	-	-	-
559	LYS	164.69	-	Favored (80.26%) General / -64.0,-35.3	19% (<i>pttp</i>) chi angles: 47.7,170.5,174,59.4	0.137Å	-	-
560	GLU	108.99	-	Favored (35.65%) General / -136.6,161.5	0.3% chi angles: 74.9,278.7,293.1	0.08Å	-	OUTLIER(S) worst is C-N- CA: 4.554 σ
561	MET	100.93	-	Favored (4.96%) General / -107.7,177.0	26.6% (<i>ptm</i>) chi angles: 70.3,180.8,279.3	0.029Å	-	-

562	TYR	71.19	-	Favored (32.78%) General / -142.4,143.7	0.9% chi angles: 324.3,80.3	0.037Å	-	-	
563	ILE	89.67	-	Favored (61.31%) Isoleucine or valine / -113.5,132.8	4.3% (<i>mp</i>) chi angles: 299.2,97.7	0.081Å	-	-	
564	ILE	122.09	-	Favored (14.36%) Isoleucine or valine / -75.2,113.8	11.4% (<i>mm</i>) chi angles: 317,307.3	0.056Å	-	-	
#	Alt	Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
		Avg: 100.32	Clashscore: 0	Outliers: 3 of 170	Poor rotamers: 13 of 150	Outliers: 4 of 158	Outliers: 0 of 172	Outliers: 11 of 172	
565	LYS	87.15	-	Favored (8.81%) General / -97.3,-40.3	74% (<i>tttt</i>) chi angles: 202.7,174.7,181.7,180.1	0.073Å	-	-	
566	HIS	57.87	-	Allowed (0.32%) General / -172.2,114.2	0.2% chi angles: 135.3,73.6	0.045Å	-	OUTLIER(S) worst is CA-CB-CG: 7.465 σ	
567	GLY	29.33	-	Favored (20.3%) Glycine / 135.2,-176.0	-	-	-	-	
568	GLU	63.51	-	Favored (41.12%) General / -107.4,139.9	7.9% (<i>mm-40</i>) chi angles: 267.9,290.9,274.5	0.084Å	-	-	
569	VAL	52.11	-	Favored (11.84%) Isoleucine or valine / -136.1,174.8	14.7% (<i>m</i>) chi angles: 289.3	0.035Å	-	-	
570	GLN	100.11	-	Favored (15.58%) General / -163.6,153.9	13% (<i>pt20</i>) chi angles: 66.4,176.3,114.3	0.058Å	-	-	
571	VAL	110.02	-	Favored (3.11%) Isoleucine or valine / -81.6,163.8	4.6% (<i>p</i>) chi angles: 77.1	0.134Å	-	-	
572	LEU	57.36	-	Favored (13.26%) General /	47.3% (<i>mt</i>) chi angles: 284.2,176.4	0.096Å	-	-	

				-162.0,147.7 Favored (13.07%) Glycine / 158.4,-146.3					
573	GLY	65.73	-		-	-	-	-	-
				Favored (67.93%) Glycine / -70.5,-35.0					
574	GLY	60.33	-		-	-	-	-	-
				Favored (8.44%) Trans-proline / -72.9,176.9	37.4% (<i>Cg_endo</i>) chi angles: 23	0.023Å	-	-	-
575	PRO	82.65	-						
				OUTLIER (0.02%) General / -56.4,-177.0	8.9% (<i>p-10</i>) chi angles: 65.1,289.5	0.077Å	-	-	-
576	ASP	129.42	-						
				Favored (12.88%) Glycine / -118.3,11.1	-	-	-	-	-
577	GLY	40.63	-						
				Allowed (0.21%) General / -83.2,-157.1	6.3% (<i>p</i>) chi angles: 79.7	0.194Å	-	-	-
578	THR	136.38	-						
				Favored (3.65%) General / -132.6,34.9	48.8% (<i>mtmt</i>) chi angles: 303.3,186.2,298.4,192.5	0.029Å	-	-	-
579	LYS	149.2	-						
				Allowed (1.6%) Isoleucine or valine / -129.8,28.9	4.9% (<i>p</i>) chi angles: 76.5	0.193Å	-	-	-
580	VAL	127.33	-						
				Allowed (0.29%) General / -120.5,-130.7	6.6% (<i>tp</i>) chi angles: 205,79.6	0.168Å	-	-	-
581	LEU	289.52	-						
				Favored (57.86%) Isoleucine or valine / -61.4,-33.7	4.1% (<i>p</i>) chi angles: 78.2	0.243Å	-	-	-
582	VAL	184.77	-						
				Favored (26.5%) General / -113.0,154.4	1.6% (<i>t</i>) chi angles: 204.1	0.102Å	-	-	-
583	THR	251.32	-						
				Allowed (0.1%) General / -142.4,-123.4	3.9% (<i>mp</i>) chi angles: 302.9,97.9	0.226Å	-	-	-
584	LEU	179.05	-						

#	Alt	Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
Avg: 100.32				Clashscore: 0	Outliers: 3 of 170	Poor rotamers: 13 of 150	Outliers: 4 of 158	Outliers: 0 of 172	Outliers: 11 of 172
585	LYS	120.81	-	Favored (4.86%) General / -93.8,-179.0	19.8% (<i>pttp</i>) chi angles: 63.2,161.7,175.2,71.5	0.05Å	-	-	
586	ALA	42.77	-	Favored (20.04%) General / -64.1,123.8	-	0.028Å	-	-	
587	GLY	26.55	-	Favored (3.41%) Glycine / 84.2,53.0	-	-	-	-	
588	SER	83.88	-	Favored (30.65%) General / -146.0,164.9	45.3% (<i>m</i>) chi angles: 289.1	0.034Å	-	-	
589	VAL	43.83	-	Favored (3.78%) Isoleucine or valine / -111.8,170.5	16.6% (<i>m</i>) chi angles: 305.3	0.058Å	-	-	
590	PHE	70.55	-	Allowed (0.38%) General / -174.9,135.7	26.8% (<i>p90</i>) chi angles: 68.8,103	0.056Å	-	-	
591	GLY	40.75	-	Favored (26.81%) Glycine / 112.3,-5.2	-	-	-	OUTLIER(S) worst is C-N- CA: 4.594 σ	
592	GLU	156.88	-	Allowed (0.72%) General / -35.9,-56.1	0% chi angles: 57.8,317.2,280.7	0.071Å	-	-	
593	ILE	55.51	-	Favored (36.37%) Isoleucine or valine / -58.6,-28.3	9.8% (<i>mt</i>) chi angles: 286.9,145.6	0.162Å	-	-	
594	SER	93.85	-	Favored (88.25%) General / -62.0,-46.7	25.4% (<i>m</i>) chi angles: 304.5	0.105Å	-	-	
595	LEU	112	-	Favored (61.41%) General / -74.1,-41.6	0.3% chi angles: 296.7,342	0.115Å	-	-	

596	LEU	57.19	-	Allowed (1.83%) General / -56.6,-62.3	15.4% (<i>mt</i>) chi angles: 313.1,188.9	0.115Å	-	-
597	ALA	37.72	-	Favored (35.09%) General / -82.5,-22.1	-	0.144Å	-	-
598	ALA	45.17	-	Allowed (0.28%) General / 65.0,-40.4	-	0.156Å	-	-
599	GLY	61.1	-	Allowed (1.2%) Glycine / -38.5,135.4	-	-	-	-
600	GLY	102.85	-	Favored (3.33%) Glycine / -81.8,45.6	-	-	-	-
601	GLY	144.49	-	Favored (9.29%) Glycine / -110.6,-142.6	-	-	-	-
602	ASN	182.57	-	Allowed (1.1%) General / -52.9,113.5	0.7% chi angles: 156.1,97.5	0.066Å	-	-
603	ARG	267.67	-	Favored (7.76%) General / -119.5,-20.6	7.2% (<i>tpm_?</i>) chi angles: 188.2,65.4,287.2,164.4	0.118Å	-	-
604	ARG	116.08	-	Favored (23.7%) General / -102.6,150.2	21.8% (<i>mmt180</i>) chi angles: 309.2,298.2,199.3,163.2	0.056Å	-	-
#	Alt Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	C β deviation	Bond lengths	Bond angles
		Avg: 100.32	Clashscore: 0	Outliers: 3 of 170	Poor rotamers: 13 of 150	Outliers: 4 of 158	Outliers: 0 of 172	Outliers: 11 of 172
605	THR	49.55	-	Favored (57.81%) General / -62.0,-53.3	12.3% (<i>p</i>) chi angles: 45.2	0.04Å	-	-
606	ALA	53	-	Allowed (1.31%) General / -142.2,-161.8	-	0.095Å	-	-

Favored

607	ASN	51.03	-	(21.8%) General / -100.5,151.2	38.3% (<i>m-80</i>) chi angles: 306.7,281.1	0.066Å	-	-
608	VAL	56.3	-	Favored (44.07%) Isoleucine or valine / -136.9,129.2	94.7% (<i>t</i>) chi angles: 175.8	0.029Å	-	-
609	VAL	96.47	-	Favored (15.94%) Isoleucine or valine / -113.8,150.2	8.4% (<i>p</i>) chi angles: 70.4	0.096Å	-	-
610	ALA	46.76	-	Favored (18.46%) General / -76.5,117.7	-	0.05Å	-	-
611	HIS	111.19	-	Favored (23.01%) General / -87.5,-26.8	85.7% (<i>t60</i>) chi angles: 178.2,68.7	0.073Å	-	-
612	GLY	24.29	-	Favored (11.22%) Glycine / -135.8,-167.3	-	-	-	-
613	PHE	54.53	-	Favored (55.18%) General / -67.2,145.5	73% (<i>m-85</i>) chi angles: 305,101.3	0.037Å	-	-
614	ALA	44.01	-	Favored (9.54%) General / -162.2,141.6	-	0.106Å	-	-
615	ASN	101.06	-	Favored (44.46%) General / -99.4,132.8	30.8% (<i>p-10</i>) chi angles: 65.9,330.7	0.139Å	-	OUTLIER(S) worst is CA-CB- CG: 5.711 σ
616	LEU	70.34	-	Favored (8.57%) General / -120.1,171.3	11% (<i>mt</i>) chi angles: 319.9,180	0.045Å	-	-
617	LEU	93.1	-	Favored (54.24%) General / -111.4,125.8	1.9% (<i>mp</i>) chi angles: 304.7,108.6	0.029Å	-	-
618	THR	111.56	-	Favored (29.65%) General / -83.2,144.7	6.6% (<i>p</i>) chi angles: 42.5	0.044Å	-	-

619	LEU	59.31	-	Favored (3.7%) General / -145.0,102.0	15.9% (<i>tp</i>) chi angles: 172.4,49	0.082Å	-	-
620	ASP	41.12	-	Favored (13.87%) General / -86.7,168.2	9.7% (<i>p-10</i>) chi angles: 66.2,294.9	0.047Å	-	-
621	LYS	63.02	-	Favored (56.08%) General / -75.8,-22.6	54.8% (<i>tttp</i>) chi angles: 193.6,182.4,177.7,68.7	0.161Å	-	-
622	LYS	89.66	-	Favored (60.14%) General / -73.5,-22.6	8.3% (<i>tptp</i>) chi angles: 190.2,63.5,222.5,68.4	0.155Å	-	-
623	THR	47.38	-	Favored (2.86%) General / -77.5,-59.2	19.7% (<i>m</i>) chi angles: 289.8	0.033Å	-	-
624	LEU	46.92	-	Favored (90.31%) General / -63.9,-45.2	35.8% (<i>tp</i>) chi angles: 186.9,58.9	0.115Å	-	-
#	Alt Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
		Avg: 100.32	Clashscore: 0	Outliers: 3 of 170	Poor rotamers: 13 of 150	Outliers: 4 of 158	Outliers: 0 of 172	Outliers: 11 of 172
625	GLN	111.94	-	Favored (75.57%) General / -63.1,-33.5	21.6% (<i>tp60</i>) chi angles: 189.3,58.2,89.8	0.136Å	-	-
626	GLU	70.8	-	Favored (35.02%) General / -81.4,-27.1	6% (<i>mm-40</i>) chi angles: 319.1,314.6,351.8	0.126Å	-	-
627	ILE	88.89	-	Favored (16.05%) Isoleucine or valine / -75.8,-22.2	1.6% (<i>tt</i>) chi angles: 222.9,169.8	0.246Å	-	-
628	LEU	47.32	-	Favored (78.04%) General / -68.4,-35.7	11.7% (<i>mt</i>) chi angles: 309.7,195.8	0.138Å	-	-
629	VAL	23.88	-	Favored (79.58%) Isoleucine or valine / -63.5,-37.5	84% (<i>t</i>) chi angles: 177.5	0.095Å	-	-

630	HIS	76.13	-	Favored (74.26%) General / -70.5,-38.1	8.5% (<i>t-160</i>) chi angles: 198.3,170.8	0.081Å	-	-
631	TYR	72.75	-	Favored (3.63%) Pre-proline / -149.9,117.7	4.8% (<i>m-85</i>) chi angles: 320.1,270.9	0.098Å	-	-
632	PRO	69.95	-	Favored (18.72%) Trans-proline / -60.6,-11.8	80.2% (<i>Cg_exo</i>) chi angles: 332	0.052Å	-	OUTLIER(S) worst is C-N- CA: 5.406 σ
633	ASP	79.73	-	Favored (58.55%) General / -80.2,-14.3	0.1% chi angles: 329.5,57.7	0.04Å	-	OUTLIER(S) worst is CA-CB- CG: 4.388 σ
634	SER	90.68	-	Favored (20.11%) General / -84.4,7.3	3.6% (<i>m</i>) chi angles: 276.2	0.114Å	-	-
635	GLU	37.55	-	Favored (5.86%) General / -125.2,30.4	40.1% (<i>tt0</i>) chi angles: 185.1,183.1,63.5	0.088Å	-	-
636	ARG	66.46	-	-	3.8% (<i>mmt180</i>) chi angles: 324.1,297.8,152,222.2	0.049Å	-	-

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