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All-Atom Contacts	Clashscore, all atoms:	0.63	99 th percentile* (N=1784, all resolutions)	
	Clashscore is the number of serious steric overlaps (> 0.4 Å) per 1000 atoms.			
Protein Geometry	Poor rotamers	4	4.88%	Goal: <1%
	Ramachandran outliers	2	1.90%	Goal: <0.05%
	Ramachandran favored	88	83.81%	Goal: >98%
	MolProbity score [^]	1.91		80 th percentile* (N=27675, 0Å - 99Å)
	Cβ deviations >0.25Å	3	3.19%	Goal: 0
	Bad backbone bonds:	0 / 791	0.00%	Goal: 0%
	Bad backbone angles:	7 / 1074	0.65%	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: 0.63	Outliers: 2 of 105	Poor rotamers: 4 of 82	Outliers: 3 of 94	Outliers: 0 of 107	Outliers: 7 of 107
252	SER	26.76	0.651Å N with 286 THR HG1	-	95% (p) chi angles: 66.2	0.024Å	-	-
253	VAL	48.83	-	Favored (18.39%) Isoleucine or valine / -62.3,125.3	88.6% (t) chi angles: 177.2	0.046Å	-	-
254	VAL	95.83	-	Favored (24.07%) Isoleucine or valine / -75.7,119.7	10.5% (p) chi angles: 61.2	0.124Å	-	-
255	CYS	87.38	-	Favored (7.48%) General / -89.0,78.3 Favored (27.8%)	1.8% (p) chi angles: 40.9	0.127Å	-	-

256	VAL	59.76	-	Isoleucine or valine / -70.9,135.6	27.9% (<i>m</i>) chi angles: 294	0.084Å	-	-
257	GLY	33.58	-	Favored (4.46%) Glycine / 114.8,-118.8	-	-	-	-
258	GLY	34.43	-	Favored (8.43%) Glycine / -130.6,-155.9	-	-	-	-
259	ASP	89.91	-	Favored (77.4%) General / -61.5,-35.4	8.7% (<i>m-20</i>) chi angles: 307.8,93.8	0.074Å	-	-
260	GLY	23.54	-	Favored (98.88%) Glycine / -63.9,-41.0	-	-	-	-
261	SER	72.22	-	Favored (96.72%) General / -60.4,-42.8	2.7% (<i>m</i>) chi angles: 318.5	0.081Å	-	-
262	ALA	40.77	-	Favored (98.72%) General / -62.2,-41.8	-	0.068Å	-	-
263	SER	80.26	-	Favored (99.6%) General / -61.5,-43.0	72.9% (<i>m</i>) chi angles: 293.7	0.079Å	-	-
264	GLU	46.22	-	Favored (14.56%) General / -58.5,-57.1	1.5% (<i>tm-20</i>) chi angles: 190.5,306.1,299.7	0.053Å	-	-
265	VAL	108.33	-	Favored (74.67%) Isoleucine or valine / -64.1,-35.7	16.4% (<i>m</i>) chi angles: 305.4	0.233Å	-	-
266	ALA	45.98	-	Favored (70.82%) General / -67.1,-30.8	-	0.086Å	-	-
267	HIS	81.91	-	Favored (34.54%) General / -79.7,-37.9	21.8% (<i>t-80</i>) chi angles: 202,301.2	0.031Å	-	-
268	ALA	40.77	-	Favored (72.3%) General / -60.5,-33.2	-	0.062Å	-	-
269	LEU	81.86	-	Favored (31.75%) General /	86% (<i>mt</i>)	0.134Å	-	-

-88.0,-17.2 chi angles: 301.9,178.3

270	LEU	140.79	-	Favored (2.19%) General / -131.4,-25.2	0.6% chi angles: 211.4,142	0.117Å	-	-
271	LEU	231.07	-	Favored (50.99%) General / -128.4,143.4	5.6% (<i>mp</i>) chi angles: 283.8,87	0.029Å	-	-
#	Alt Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	C β deviation	Bond lengths	Bond angles
Avg:			Clashscore:	Outliers: 2 of	Poor rotamers: 4 of	Outliers:	Outliers:	Outliers:
110.61			0.63	105	82	3 of 94	0 of 107	7 of 107
272	ARG	254.22	-	Allowed (1.88%) General / -40.9,134.7	3% (<i>mmp_?</i>) chi angles: 284.4,282.9,78.6,246.7	0.057Å	-	-
273	ALA	227.12	-	Favored (19.14%) General / -135.9,168.5	-	0.054Å	-	-
274	GLN	129.03	-	Favored (66.77%) General / -67.8,-48.2	50.7% (<i>tt0</i>) chi angles: 192.6,187,18.9	0.067Å	-	-
275	LYS	293.87	-	Favored (2.96%) General / -153.7,107.1	3.8% (<i>tpp</i>) chi angles: 183,208,54.8,41.4	0.076Å	-	-
276	ASN	239.14	-	Allowed (1.18%) General / 73.1,33.4	14.2% (<i>m120</i>) chi angles: 313.8,109.7	0.112Å	-	-
277	ALA	283.13	-	Favored (6.89%) General / -159.7,-178.2	-	0.057Å	-	-
278	GLY	272.41	-	Favored (34.08%) Glycine / 108.4,-17.2	-	-	-	OUTLIER(S) worst is C-N- CA: 4.776 σ
279	MET	144.44	-	Favored (21.53%) General / -163.8,166.8	1.4% (<i>mtp</i>) chi angles: 281.9,125.3,69.5	0.088Å	-	-
280	GLU	103.55	-	Favored (3.74%) General / -146.6,-171.4	5% (<i>tt0</i>) chi angles: 219.9,178.5,98.3	0.085Å	-	-
281	THR	131.82	-	Favored (29.4%) General /	1.6% (<i>p</i>) chi angles: 37	0.07Å	-	-

282	ASP	56.98	-	-63.8,155.7 Favored (26.35%) General / -55.4,-55.9	0% chi angles: 139.2,85.7	0.161Å	-	-
283	ARG	143.69	-	Favored (5.72%) General / -80.5,91.0	5.7% (<i>mmt-85</i>) chi angles: 301.9,292.8,143.3,283.1	0.055Å	-	-
284	ILE	88.89	-	Favored (5.26%) Isoleucine or valine / -51.1,125.9	70.1% (<i>mt</i>) chi angles: 288.2,171.5	0.106Å	-	-
285	LEU	143.86	-	Favored (73.42%) General / -70.4,-35.5	2.6% (<i>tm?</i>) chi angles: 191.2,274.5	0.092Å	-	-
286	THR	228.94	0.651Å HG1 with 252 SER N	Allowed (0.17%) Pre-proline / -101.9,75.9	10.1% (<i>t</i>) chi angles: 181.1	0.158Å	-	-
287	PRO	113.13	-	Favored (32.08%) Trans-proline / -50.4,141.6	79.6% (<i>Cg_exo</i>) chi angles: 330.5	0.073Å	-	-
288	VAL	167.56	-	Favored (9.92%) Isoleucine or valine / -58.8,145.8	15.6% (<i>m</i>) chi angles: 289.9	0.065Å	-	-
289	ARG	302.22	-	Allowed (0.48%) General / -118.0,-96.1	30.6% (<i>mtm105</i>) chi angles: 286.6,187.5,302.3,88.3	0.163Å	-	-
290	ALA	240.95	-	Favored (26.04%) General / -126.3,162.2	-	0.065Å	-	-
291	GLN	271.8	-	Allowed (0.07%) General / 57.9,-175.8	55% (<i>mm-40</i>) chi angles: 296.6,295.2,350	0.119Å	-	-
<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: 110.61</div> <div>Clashscore: 0.63</div> <div>Outliers: 2 of 105</div> <div>Poor rotamers: 4 of 82</div> <div>Outliers: 3 of 94</div> <div>Outliers: 0 of 107</div> <div>Outliers: 7 of 107</div> </div>								
292	LEU	60.04	-	Allowed (0.63%) Pre-proline / -84.1,-36.6 Favored (3.43%)	0.2% chi angles: 33.4,154.7 75.7% (<i>Cg_endo</i>)	0.283Å	-	-

293	PRO	69.76	-	Trans-proline / -83.8,124.1	chi angles: 29.7	0.058Å	-	-
294	LEU	255.97	-	Favored (74.11%) General / -59.9,-35.1	23.3% (<i>mt</i>) chi angles: 313.4,175	0.127Å	-	-
295	GLY	55.38	-	Allowed (0.1%) Glycine / -170.8,76.1	-	-	-	-
296	LEU	151.76	-	Favored (13.38%) General / -72.5,116.8	46.9% (<i>tp</i>) chi angles: 176.1,56.4	0.052Å	-	-
297	ILE	165.66	-	Favored (13.71%) Pre-proline / -96.8,103.1	7.7% (<i>mt</i>) chi angles: 297.6,196.4	0.04Å	-	-
298	PRO	117.73	-	Allowed (0.92%) Trans-proline / -74.5,94.2	88.1% (<i>Cg_endo</i>) chi angles: 31.8	0.064Å	-	-
299	ALA	82.49	-	Favored (7.26%) General / -126.0,4.4	-	0.04Å	-	-
300	GLY	45.76	-	Favored (52.94%) Glycine / -82.5,180.0	-	-	-	-
301	SER	89.25	-	Favored (71.06%) General / -71.2,-34.7	51.4% (<i>p</i>) chi angles: 54.6	0.096Å	-	-
302	THR	117.84	-	Allowed (0.14%) General / -91.1,-92.5	20% (<i>p</i>) chi angles: 48.3	0.134Å	-	-
303	ASN	50.89	-	Allowed (0.43%) General / 73.7,41.6	7.6% (<i>m-80</i>) chi angles: 318.8,290	0.11Å	-	-
304	VAL	98.1	-	Favored (37.35%) Isoleucine or valine / -71.4,-29.9	10.9% (<i>p</i>) chi angles: 67.2	0.276Å	-	-
305	LEU	103.45	-	Favored (89.13%) General / -65.6,-38.3	9.9% (<i>tt</i>) chi angles: 188.4,153.6	0.06Å	-	-
				Favored				

306	ALA	35.54	-	(78.26%) General / -62.3,-35.2	-	0.099Å	-	-
307	HIS	73.04	-	Favored (75.7%) General / -65.3,-47.7	32.4% (<i>t</i> -80) chi angles: 189.8,300.1	0.052Å	-	OUTLIER(S) worst is CA- CB-CG: 5.699 σ
308	SER	32.31	-	Favored (5.26%) General / -86.3,-53.0	89.5% (<i>p</i>) chi angles: 62.3	0.128Å	-	-
309	LEU	126.26	-	Favored (86.34%) General / -63.3,-37.2	2.3% (<i>tt</i>) chi angles: 210,170.9	0.089Å	-	-
310	HIS	257.37	-	Favored (2.37%) General / 71.6,30.6	5.5% (<i>t</i> 60) chi angles: 211,81.8	0.081Å	-	-
311	GLY	126.77	-	Favored (16.59%) Glycine / -117.2,-4.0	-	-	-	-
#	Alt Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
Avg: 110.61			Clashscore: 0.63	Outliers: 2 of 105	Poor rotamers: 4 of 82	Outliers: 3 of 94	Outliers: 0 of 107	Outliers: 7 of 107
312	VAL	127.62	-	Favored (19.95%) Pre-proline / -129.9,121.6	12.8% (<i>m</i>) chi angles: 288.5	0.074Å	-	-
313	PRO	143.88	-	Favored (5.65%) Trans-proline / -89.2,164.5	2.1% (<i>Cg_endo</i>) chi angles: 42	0.079Å	-	-
314	HIS	101.61	-	Favored (56.77%) General / -77.1,-19.7	57% (<i>t</i> 60) chi angles: 195.4,62.7	0.126Å	-	-
315	VAL	92.08	-	Favored (13.51%) Isoleucine or valine / -70.4,117.5	8.5% (<i>p</i>) chi angles: 70.5	0.149Å	-	-
316	ILE	91.53	-	Favored (79.66%) Isoleucine or valine / -62.4,-37.8	28% (<i>pt</i>) chi angles: 62,180.6	0.215Å	-	-
317	THR	30.17	-	Favored (59.54%) General / -58.4,-53.3	14.9% (<i>p</i>) chi angles: 46	0.077Å	-	-

318	ALA	33.81	-	Favored (93.31%) General / -64.8,-39.3	-	0.112Å	-	-
319	THR	105.68	-	Favored (75.13%) General / -66.1,-33.1	0.6% chi angles: 214.7	0.255Å	-	-
320	LEU	93.53	-	Favored (74.47%) General / -69.3,-34.3	2.7% (<i>tt</i>) chi angles: 208.6,160.5	0.072Å	-	-
321	HIS	111.84	-	Favored (63.25%) General / -70.0,-24.4	34.9% (<i>t60</i>) chi angles: 198.4,54.1	0.146Å	-	-
322	ILE	88.05	-	Favored (17.94%) Isoleucine or valine / -75.5,-25.7	53% (<i>mt</i>) chi angles: 291.8,157.8	0.152Å	-	-
323	ILE	53.31	-	Favored (22.03%) Isoleucine or valine / -71.6,-22.6	97.1% (<i>mt</i>) chi angles: 293.1,168.9	0.152Å	-	-
324	MET	129.23	-	Favored (59.81%) General / -78.1,-13.6	64.6% (<i>mtt</i>) chi angles: 300,181.1,188.9	0.099Å	-	-
325	GLY	37.06	-	Favored (49.18%) Glycine / -58.9,138.8	-	-	-	-
326	HIS	84.92	-	Allowed (1.9%) General / -67.8,178.0	12.2% (<i>p80</i>) chi angles: 69.9,65.4	0.128Å	-	OUTLIER(S) worst is CA- CB-CG: 4.764 σ
327	VAL	111.69	-	Favored (9.67%) Isoleucine or valine / -53.1,140.1	8.4% (<i>p</i>) chi angles: 70.4	0.115Å	-	OUTLIER(S) worst is C-N- CA: 4.684 σ
328	GLN	75.72	-	OUTLIER (0%) General / -178.8,41.7	9.2% (<i>tp60</i>) chi angles: 178.4,46.4,91.1	0.065Å	-	-
329	LEU	119.8	-	Favored (41.66%) General / -60.3,147.1	1.6% (<i>pt?</i>) chi angles: 78,179.1	0.056Å	-	-
				Favored				

330	VAL	49.65	-	(36.99%) Isoleucine or valine / -140.3,138.3	46.7% (t) chi angles: 183.3	0.079Å	-	-
331	ASP	98.59	-	Favored (3.32%) General / -89.5,-171.7	2.1% (t70) chi angles: 209.3,273.1	0.144Å	-	-
#	Alt Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
Avg: 110.61				Clashscore: 0.63	Outliers: 2 of 105	Poor rotamers: 4 of 82	Outliers: 3 of 94	Outliers: 0 of 107
332	VAL	86.06	-	Allowed (0.88%) Isoleucine or valine / -88.0,72.4	38.3% (t) chi angles: 185.5	0.098Å	-	-
333	CYS	104.41	-	Favored (67.59%) General / -57.9,-32.4	26.6% (p) chi angles: 59.2	0.166Å	-	-
334	THR	124.14	-	Favored (49.12%) General / -82.5,-16.3	12.6% (p) chi angles: 45.4	0.11Å	-	-
335	PHE	210.72	-	Allowed (0.11%) General / -142.3,-137.9	47.2% (m-85) chi angles: 308.9,288.5	0.152Å	-	-
336	SER	100.48	-	OUTLIER (0%) General / 175.0,-99.7	72.1% (p) chi angles: 57.9	0.199Å	-	-
337	THR	110.72	-	Favored (4.08%) General / -153.3,114.2	2.4% (t) chi angles: 170.9	0.078Å	-	-
338	ALA	31.16	-	Favored (23.56%) General / -62.0,125.3	-	0.026Å	-	-
339	GLY	22.82	-	Favored (33.42%) Glycine / 66.0,6.8	-	-	-	-
340	LYS	102.5	-	Favored (2.34%) General / 76.3,14.7	48% (mtmt) chi angles: 302.4,172.7,290.5,182.5	0.166Å	-	-
341	LEU	155.23	-	Favored (2.11%) General / -129.7,-30.1	40.4% (tp) chi angles: 184.3,56.8	0.045Å	-	-
342	LEU	170.71	-	Allowed (1.35%)	1.9% (tt)	0.052Å	-	-

			General / -108.8,80.7	chi angles: 209.3,177.1				
343	ARG	161.92	-	Favored (50.13%) General / -71.0,138.7	54.8% (<i>ttt180</i>) chi angles: 178.5,165.6,175.5,157.1	0.032Å	-	-
344	PHE	103.11	-	Favored (24.81%) General / -140.2,166.4	37.1% (<i>p90</i>) chi angles: 52.9,266.2	0.059Å	-	-
345	GLY	70.57	-	Favored (10.93%) Glycine / -109.3,-16.6	-	-	-	-
346	PHE	140.71	-	Allowed (0.35%) General / -104.5,-137.6	34.3% (<i>t80</i>) chi angles: 188.4,58.5	0.22Å	-	OUTLIER(S) worst is C-CA- CB: 4.734 σ
347	SER	100.17	-	Favored (12.41%) General / -98.4,164.1	32.9% (<i>t</i>) chi angles: 183.9	0.067Å	-	-
348	ALA	32.37	-	Favored (5.97%) General / -95.8,176.9	-	0.044Å	-	-
349	MET	94.34	-	Favored (43.87%) General / -145.8,158.2	1.1% (<i>mpt?</i>) chi angles: 295,84.8,201.1	0.076Å	-	-
350	PHE	99.52	-	Favored (6.42%) General / -169.4,155.8	70.1% (<i>t80</i>) chi angles: 178.1,67.1	0.064Å	-	-
351	GLY	18.76	-	Favored (20.28%) Glycine / -133.4,152.0	-	-	-	-
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352	PHE	37.33	-	Favored (29.03%) General / -55.8,127.2	35.5% (<i>m-85</i>) chi angles: 310.2,116.2	0.052Å	-	-
353	GLY	17.5	-	Favored (23.06%) Glycine /	-	-	-	-

354	GLY	18.52	-	151.5,175.2 Favored (13.4%) Glycine / -119.5,-166.6	-	-	-	-
355	ARG	154.09	-	Favored (22.26%) General / -89.7,150.5	59.9% (<i>ttp85</i>) chi angles: 192.1,182.9,72,94.6	0.101Å	-	-
356	THR	116.03	-	Favored (4.91%) General / -72.9,177.4	68.8% (<i>p</i>) chi angles: 63.2	0.039Å	-	-
357	LEU	216.07	-	Favored (38.04%) General / -69.4,156.9	24.3% (<i>tp</i>) chi angles: 191.8,60.6	0.059Å	-	OUTLIER(S) worst is C-N- CA: 5.202 σ
358	ALA	33.4	-	-	-	0.157Å	-	OUTLIER(S) worst is N-CA- CB: 4.154 σ

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