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All-Atom Contacts	Clashscore, all atoms:	18.63		36 th 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	2.68%	Goal: <0.05%
	Ramachandran favored	102	91.07%	Goal: >98%
	MolProbity score^	2.28		60 th percentile* (N=27675, 0Å - 99Å)
	Cβ deviations >0.25Å	0	0.00%	Goal: 0
	Bad backbone bonds:	8 / 858	0.93%	Goal: 0%
	Bad backbone angles:	3 / 1167	0.26%	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: 54.82	Clashscore: 18.63	Outliers: 3 of 112	Poor rotamers: 0 of 95	Outliers: 0 of 102	Outliers: 5 of 114	Outliers: 2 of 114
A 186	GLU	50	0.507Å HG3 with A 205 ILE HA	-	11.6% (<i>tm</i> -20) chi angles: 179.1,287.4,331.1	0.097Å	-	-
A 187	VAL	50	-	Favored (67.4%) Isoleucine or valine / -110.2,126.0	7.5% (<i>p</i>) chi angles: 57.2	0.065Å	-	-
A 188	ASP	50	-	Favored (4.59%) General / -76.5,98.4	60% (<i>t0</i>) chi angles: 188.9,348.1	0.05Å	-	-
A 189	GLU	50	-	Favored (69.85%) General /	50.8% (<i>mp0</i>) chi angles: 288.9,76.7,17.6	0.095Å	-	-

A 190	CYS	50	-	-62.6,-28.4 Favored (78.31%) General / -69.3,-38.2	83.1% (<i>m</i>) chi angles: 300.7	0.024Å	-	-
A 191	ALA	50	-	Favored (62.18%) General / -71.1,-22.0	-	0.011Å	-	-
A 192	SER	99.99	-	Favored (10.56%) General / -91.3,-42.1	39.2% (<i>t</i>) chi angles: 181.7	0.022Å	-	-
A 193	ASP	99.99	-	Favored (12.05%) Pre-proline / -149.8,138.0	18.2% (<i>p30</i>) chi angles: 58.7,35	0.076Å	-	-
A 194	PRO	99.99	-	Favored (19.04%) Trans-proline / -81.5,163.8	67.8% (<i>Cg_endo</i>) chi angles: 33.7	0.006Å	-	-
A 195	CYS	99.99	-	Favored (54.09%) General / -114.9,125.8	51.8% (<i>t</i>) chi angles: 179.9	0.056Å	-	-
A 196	LYS	99.99	-	OUTLIER (0.04%) General / -75.5,-154.2	23.2% (<i>pttp</i>) chi angles: 61.2,184,178.4,64.7	0.203Å	-	-
A 197	ASN	50	0.54Å O with A 198 GLU HG2	OUTLIER (0%) General / 20.5,38.9	22.7% (<i>m120</i>) chi angles: 287.3,126.5	0.097Å	-	-
A 198	GLU	50	0.54Å HG2 with A 197 ASN O	Favored (9.01%) General / 52.8,30.4	14.2% (<i>pt-20</i>) chi angles: 71.3,185.6,45.4	0.116Å	-	-
A 199	ALA	50	-	Favored (49.58%) General / -70.5,147.3	-	0.122Å	-	-
A 200	THR	50	0.723Å OG1 with A 211 ILE HB	Favored (35.42%) General / -80.1,130.7	64% (<i>p</i>) chi angles: 62.9	0.026Å	-	-
A 201	CYS	50	-	Favored (40.78%) General / -96.8,124.4	43.5% (<i>t</i>) chi angles: 184.6	0.066Å	-	-

A 202	LEU	50	-	Favored (23.82%) General / -117.4,114.6	77.6% (<i>mt</i>) chi angles: 295,181.6	0.032Å	-	-	
A 203	ASN	50	-	Favored (46.64%) General / -72.3,137.3	56% (<i>t30</i>) chi angles: 184.9,38	0.051Å	-	-	
A 204	GLU	50	0.51Å OE2 with A 207 ARG HB3	Favored (17.64%) General / -125.2,165.8	13% (<i>pt-20</i>) chi angles: 68.9,179.4,53.5	0.051Å	-	-	
A 205	ILE	50	0.507Å HA with A 186 GLU HG3	Allowed (1.79%) Isoleucine or valine / -73.9,102.1	39.3% (<i>pt</i>) chi angles: 61.5,166.1	0.097Å	-	-	
#	Alt	Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
			Avg: 54.82	Clashscore: 18.63	Outliers: 3 of 112	Poor rotamers: 0 of 95	Outliers: 0 of 102	Outliers: 5 of 114	Outliers: 2 of 114
A 206	GLY	50	-	Favored (8.76%) Glycine / 111.2,-29.5	-	-	-	-	
A 207	ARG	50	0.939Å HG2 with A 208 TYR H	Allowed (0.14%) General / -145.9,-143.2	51.1% (<i>ttm-85</i>) chi angles: 186.3,190.4,286.1,281.8	0.132Å	-	-	
A 208	TYR	50	0.939Å H with A 207 ARG HG2	Favored (17.06%) General / -165.1,158.9	54% (<i>p90</i>) chi angles: 63.8,89.9	0.062Å	-	-	
A 209	THR	50	0.492Å HG23 with A 204 GLU OE1	Favored (47.66%) General / -129.3,153.6	45.2% (<i>p</i>) chi angles: 55.1	0.028Å	-	-	
A 210	CYS	50	-	Favored (55.43%) General / -115.2,134.1	72.5% (<i>m</i>) chi angles: 297.1	0.051Å	-	-	
A 211	ILE	50	0.723Å HB with A 200 THR OG1	Favored (6.65%) Isoleucine or valine / -102.7,98.3	50% (<i>mm</i>) chi angles: 303,299.6	0.03Å	-	-	
				Favored					

A 212	CYS	50	-	(88.11%) Pre-proline / -71.4,143.6	56.7% (<i>m</i>) chi angles: 306	0.017Å	-	-
A 213	PRO	50	0.56Å HG2 with A 216 TYR CD2	Favored (56.39%) Trans-proline / -70.3,158.4	61.5% (<i>Cg_endo</i>) chi angles: 27.5	0.045Å	-	-
A 214	HIS	50	-	Favored (4%) General / -59.3,116.6	22% (<i>t-160</i>) chi angles: 181.1,200.8	0.077Å	OUTLIER(S) worst is CD2-- NE2: 4.414 σ	-
A 215	ASN	50	0.73Å O with A 225 ILE HG22	OUTLIER (0.01%) General / 118.1,-15.5	61.9% (<i>t30</i>) chi angles: 191.9,46.8	0.175Å	-	-
A 216	TYR	50	0.56Å CD2 with A 213 PRO HG2	Favored (53.06%) General / -116.8,136.3	81.6% (<i>m-85</i>) chi angles: 303.3,282	0.045Å	-	-
A 217	SER	50	-	Favored (21.22%) General / -132.3,166.7	25.9% (<i>t</i>) chi angles: 185.8	0.024Å	-	-
A 218	GLY	50	-	Favored (14.26%) Glycine / 113.1,160.4	-	-	-	-
A 219	VAL	50	-	Favored (34.05%) Isoleucine or valine / -56.8,-30.8	14.3% (<i>p</i>) chi angles: 63.2	0.096Å	-	-
A 220	ASN	50	-	Favored (12.34%) General / -120.1,18.4	34.5% (<i>m120</i>) chi angles: 294.4,114.4	0.017Å	-	-
A 221	CYS	50	-	Favored (26.7%) General / 56.6,35.9	18.1% (<i>m</i>) chi angles: 312.6	0.023Å	-	-
A 222	GLU	50	-	Favored (58.69%) General / -86.3,-7.2	1.5% (<i>pm0</i>) chi angles: 60.5,272.4,80.5	0.121Å	-	-
A 223	LEU	50	-	Favored (32.39%) General / -102.7,116.3	96% (<i>mt</i>) chi angles: 294.7,174.7	0.023Å	-	-

A 224	GLU	50	-	Favored (9.37%) General / -82.1,99.8	10.8% (<i>tm-20</i>) chi angles: 180.8,286.8,321.7	0.06Å	-	-
A 225	ILE	50	0.73Å HG22 with A 215 ASN O	Favored (10.06%) Isoleucine or valine / -52.8,127.1	7.1% (<i>tp</i>) chi angles: 181.7,70.1	0.126Å	-	-
#	Alt Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
		Avg: 54.82	Clashscore: 18.63	Outliers: 3 of 112	Poor rotamers: 0 of 95	Outliers: 0 of 102	Outliers: 5 of 114	Outliers: 2 of 114
A 226	ASP	50	-	Favored (11.34%) General / -87.9,98.2	49.6% (<i>t0</i>) chi angles: 188.6,334.7	0.055Å	-	-
A 227	GLU	50	0.6Å OE2 with A 225 ILE HG23	Favored (20.28%) General / -71.3,-3.4	49.8% (<i>mp0</i>) chi angles: 288.2,77,18	0.076Å	-	-
A 228	CYS	50	-	Favored (25.96%) General / -107.8,4.8	84.3% (<i>m</i>) chi angles: 292.5	0.068Å	-	-
A 229	TRP	50	-	Favored (69.64%) General / -66.0,-29.3	76.4% (<i>t-105</i>) chi angles: 182.9,257.4	0.044Å	-	-
A 230	SER	50	-	Favored (31.6%) General / -96.8,12.6	78.7% (<i>p</i>) chi angles: 59.4	0.018Å	-	-
A 231	GLN	50	-	Favored (4.38%) Pre-proline / 49.6,67.5	19.6% (<i>mm100</i>) chi angles: 296.7,294.6,99.8	0.045Å	-	-
A 232	PRO	50	-	Favored (14.2%) Trans-proline / -71.5,-31.2	87.4% (<i>Cg_endo</i>) chi angles: 31.8	0.061Å	-	-
A 233	CYS	50	0.454Å HB3 with A 237 ALA HB3	Favored (33.35%) General / -78.6,128.3	62.3% (<i>m</i>) chi angles: 303.3	0.039Å	-	-
A 234	LEU	50	-	Favored (18.21%) General / -82.1,99.8	95.8% (<i>mt</i>) chi angles: 294.1,174.9	0.023Å	-	-

A 235	ASN	50	0.647Å HB3 with A 254 PHE CE2	General / -103.2,155.8 Allowed (1.41%) General / 64.1,56.3	80.2% (<i>m</i> -20) chi angles: 298.7,306.5	0.153Å	-	-
A 236	GLY	50	-	Favored (48.93%) Glycine / 57.0,24.1	-	-	-	-
A 237	ALA	50	0.454Å HB3 with A 233 CYS HB3	Favored (40.32%) General / -73.6,153.0	-	0.042Å	-	-
A 238	THR	50	-	Favored (34.1%) General / -94.8,137.3	11.1% (<i>m</i>) chi angles: 312.9	0.061Å	-	-
A 239	CYS	50	-	Favored (49.54%) General / -107.5,135.1	19.8% (<i>t</i>) chi angles: 191.6	0.055Å	-	-
A 240	GLN	50	-	Favored (17.86%) General / -108.3,107.3	20.1% (<i>mm</i> 100) chi angles: 294.1,296.2,99.1	0.039Å	-	-
A 241	ASP	50	-	Favored (2.07%) General / -72.5,97.4	40.9% (<i>t</i> 0) chi angles: 188.4,26	0.037Å	-	-
A 242	ALA	50	-	Favored (7.3%) General / -110.7,171.7	-	0.049Å	-	-
A 243	LEU	50	0.687Å HA with A 215 ASN ND2	Allowed (0.66%) General / -69.0,94.8	72.3% (<i>mt</i>) chi angles: 304.8,178.4	0.09Å	-	-
A 244	GLY	50	0.43Å N with A 215 ASN HB2	Favored (64.54%) Glycine / 80.5,21.4	-	-	-	-
A 245	ALA	50	-	Favored (5.33%) General / -171.4,158.7	-	0.036Å	-	-

#	Alt	Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
Avg:			Clashscore:	Outliers: 3 of	Poor rotamers: 0 of	Outliers:	Outliers: 5	Outliers: 2	
54.00			10.00	110	05	0.1100	0.111	0.111	

		54.82	18.63	112	95	0 of 102	0 of 114	0 of 114
A 246	TYR	50	0.486Å C with A 247 PHE HD1	Favored (50.7%) General / -130.1,141.5	45.5% (<i>p90</i>) chi angles: 66.4,86	0.102Å	-	-
A 247	PHE	50	0.486Å HD1 with A 246 TYR C	Favored (53.31%) General / -126.6,139.3	1.6% (<i>m-30</i>) chi angles: 292.7,32.4	0.064Å	-	-
A 248	CYS	50	-	Favored (54.33%) General / -106.6,128.7	74.3% (<i>m</i>) chi angles: 298.5	0.046Å	-	-
A 249	ASP	50	-	Favored (9.71%) General / -101.5,99.4	47.6% (<i>t0</i>) chi angles: 187.8,331.8	0.04Å	-	-
A 250	CYS	50	-	Favored (58.33%) General / -66.0,141.0	60.3% (<i>m</i>) chi angles: 304.3	0.01Å	-	-
A 251	ALA	50	-	Favored (88.41%) Pre-proline / -70.0,140.1	-	0.052Å	-	-
A 252	PRO	50	-	Favored (15.11%) Trans-proline / -47.3,128.9	72.1% (<i>Cg_exo</i>) chi angles: 328	0.055Å	-	-
A 253	GLY	50	-	Favored (16.75%) Glycine / 113.2,-21.8	-	-	-	-
A 254	PHE	50	0.647Å CE2 with A 235 ASN HB3	Favored (38.75%) General / -115.5,149.0	1.3% (<i>m-30</i>) chi angles: 293.9,34.2	0.03Å	-	-
A 255	LEU	50	0.453Å HG with A 256 GLY N	Favored (37.23%) General / -145.7,162.6	43.5% (<i>tp</i>) chi angles: 186.1,62.6	0.048Å	-	-
A 256	GLY	50	0.453Å N with A 255 LEU HG	Favored (14.71%) Glycine / 119.7,171.4	-	-	-	-
A 257	ASP	50	-	Favored (78.9%) General / -62.5,35.0	39.1% (<i>t0</i>) chi angles: 190.3,326.7	0.02Å	-	-

A 258	HIS	50	-	-65.5,-55.0 Favored (21.94%) General / -111.0,8.5	58.6% (<i>m80</i>) chi angles: 305,91.1	0.066Å	OUTLIER(S) worst is CG-- ND1: 4.101 σ	OUTLIER(S) worst is CB- CG-CD2: 4.046 σ
A 259	CYS	50	-	Favored (29.5%) General / 56.8,38.5	55.4% (<i>m</i>) chi angles: 306.5	0.024Å	-	-
A 260	GLU	50	-	Favored (31.36%) General / -83.8,-23.8	17.8% (<i>pm0</i>) chi angles: 69.1,286,358.9	0.079Å	-	-
A 261	LEU	50	-	Favored (35.31%) General / -92.0,123.4	9.1% (<i>tt</i>) chi angles: 184,157.6	0.079Å	-	-
A 262	ASN	50	-	Favored (9.89%) General / -84.5,98.0	47.9% (<i>t-20</i>) chi angles: 190.3,329.5	0.066Å	-	-
A 263	THR	50	-	Favored (4.8%) General / -44.1,126.1	57.4% (<i>m</i>) chi angles: 304.3	0.033Å	-	-
A 264	ASP	50	-	Favored (10.22%) General / -86.0,97.4	36.1% (<i>t0</i>) chi angles: 184.4,27.8	0.049Å	-	-
A 265	GLU	50	-	Favored (63.48%) General / -64.3,-17.3	18.7% (<i>mp0</i>) chi angles: 280.3,69.5,39.8	0.074Å	-	-
#	Alt Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
		Avg: 54.82	Clashscore: 18.63	Outliers: 3 of 112	Poor rotamers: 0 of 95	Outliers: 0 of 102	Outliers: 5 of 114	Outliers: 2 of 114
A 266	CYS	50	-	Favored (59.53%) General / -81.2,-10.8	72.7% (<i>m</i>) chi angles: 297	0.017Å	-	-
A 267	ALA	50	-	Favored (84.07%) General / -62.6,-36.8	-	0.009Å	-	-
A 268	SER	50	-	Favored (40.47%) General /	68.3% (<i>p</i>) chi angles: 57.4	0.016Å	-	-

A 269	GLN	50	-	-62.5,11.2 Allowed (1.52%) Pre-proline / 53.2,71.1	51.1% (<i>tt0</i>) chi angles: 181.1,185.9,61.6	0.096Å	-	-
A 270	PRO	50	-	Favored (10.4%) Trans-proline / -72.2,-32.6	86.1% (<i>Cg_endo</i>) chi angles: 31.7	0.057Å	-	-
A 271	CYS	50	-	Favored (10.43%) General / -76.1,110.3	23.7% (<i>m</i>) chi angles: 311.3	0.031Å	-	-
A 272	LEU	50	-	Favored (34.83%) General / -69.3,158.6	8.2% (<i>mp</i>) chi angles: 283.5,73.6	0.039Å	-	-
A 273	HIS	50	-	Favored (20.1%) General / 60.8,31.9	51% (<i>m80</i>) chi angles: 305.6,101.4	0.042Å	OUTLIER(S) worst is CG-- ND1: 4.152 σ	-
A 274	GLY	50	-	Favored (7.81%) Glycine / 57.0,61.2	-	-	-	-
A 275	GLY	50	-	Favored (18.21%) Glycine / -93.5,146.6	-	-	-	-
A 276	LEU	50	0.511Å HB3 with A 287 ASN HB3	Favored (42.34%) General / -68.3,130.2	51.6% (<i>tp</i>) chi angles: 183.8,63.5	0.039Å	-	-
A 277	CYS	50	-	Favored (55.84%) General / -113.4,131.8	46.7% (<i>t</i>) chi angles: 182.8	0.069Å	-	-
A 278	VAL	50	0.718Å HG13 with A 285 SER HB3	Favored (72.06%) Isoleucine or valine / -119.4,123.9	3.3% (<i>p</i>) chi angles: 51.8	0.184Å	-	-
A 279	ASP	50	-	Favored (46.59%) General / -72.4,137.6	32.7% (<i>t70</i>) chi angles: 187.8,50.6	0.061Å	-	-
A	GLY	50	-	Favored (8.55%)				

A 280	GLU	50	-	(0.55%) Glycine / -125.2,-153.6	-	-	-	-	
A 281	GLU	50	-	Favored (21.51%) General / -104.9,109.5	10.6% (<i>pt-20</i>) chi angles: 56.5,176.3,70.7	0.045Å	-	-	
A 282	ASN	50	-	Favored (23.85%) General / 54.1,36.0	62.1% (<i>t30</i>) chi angles: 197.4,27.5	0.048Å	-	-	
A 283	ARG	50	-	Favored (8.67%) General / -164.6,147.3	28.3% (<i>tpt180</i>) chi angles: 185,60.3,182.6,183	0.079Å	-	-	
A 284	TYR	99.99	0.451Å OH with A 297 HIS CE1	Favored (39.99%) General / -126.2,156.5	55.6% (<i>p90</i>) chi angles: 62.5,269.7	0.014Å	OUTLIER(S) worst is CZ-- OH: 4.168 σ	-	
A 285	SER	50	0.718Å HB3 with A 278 VAL HG13	Favored (8.32%) General / -128.6,105.5	27.2% (<i>t</i>) chi angles: 171.2	0.105Å	-	-	
#	Alt	Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
			Avg: 54.82	Clashscore: 18.63	Outliers: 3 of 112	Poor rotamers: 0 of 95	Outliers: 0 of 102	Outliers: 5 of 114	Outliers: 2 of 114
A 286	CYS	50	-	Favored (30.61%) General / -82.8,124.8	85.6% (<i>m</i>) chi angles: 292.3	0.02Å	-	-	
A 287	ASN	50	0.511Å HB3 with A 276 LEU HB3	Favored (3.75%) General / -103.7,90.8	26.1% (<i>t-20</i>) chi angles: 186.6,299.4	0.075Å	-	-	
A 288	CYS	50	-	Favored (51.93%) General / -65.8,148.3	61.8% (<i>m</i>) chi angles: 303.5	0.019Å	-	-	
A 289	THR	99.99	0.553Å HG23 with A 293 PHE HD2	Favored (48.22%) General / -63.9,131.6	7% (<i>t</i>) chi angles: 178.4	0.101Å	-	-	
A 290	GLY	99.99	-	Favored (48.31%) Glycine / -72.6,152.8	-	-	-	-	

A 291	SER	99.99	0.406Å N with A 292 GLY CA	Favored (11.85%) General / 45.9,45.6	23.1% (t) chi angles: 187.6	0.09Å	-	-
A 292	GLY	50	0.406Å CA with A 291 SER N	Allowed (0.2%) Glycine / 156.6,103.5	-	-	-	-
A 293	PHE	50	0.553Å HD2 with A 289 THR HG23	Favored (23.13%) General / -127.0,163.7	97.2% (m-85) chi angles: 295.2,270.8	0.033Å	-	-
A 294	THR	50	-	Favored (10.81%) General / -163.7,148.7	13.1% (t) chi angles: 186.1	0.065Å	-	-
A 295	GLY	50	-	Allowed (0.12%) Glycine / -138.3,-39.0	-	-	-	-
A 296	THR	50	-	Favored (10.81%) General / -97.7,-34.8	77.1% (p) chi angles: 58.4	0.021Å	-	-
A 297	HIS	99.99	0.591Å HB2 with A 299 GLU OE1	Favored (10.91%) General / -119.1,-1.4	85.5% (m-70) chi angles: 297.8,266.6	0.029Å	OUTLIER(S) worst is CG-- CD2: 5.692 σ	OUTLIER(S) worst is ND1- CG-CD2: 5.865 σ
A 298	CYS	50	-	Favored (23.33%) General / 59.4,36.6	34.4% (m) chi angles: 309	0.023Å	-	-
A 299	GLU	99.99	0.591Å OE1 with A 297 HIS HB2	-	14.2% (pm0) chi angles: 68.5,289.5,354.9	0.055Å	-	-

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