Viewing ndp_sm_1-133H-multi.table

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All-Atom Contacts	Clashscore, all atoms:	14.91		50th percentile* (N=1784, all resolutions)
	Clashscore is the number of serious steric overlaps (> 0.4 Å) per 1000 atoms.			
Protein Geometry	Poor rotamers	7	5.69%	Goal: <1%
	Ramachandran outliers	0	0.00%	Goal: <0.05%
	Ramachandran favored	122	93.13%	Goal: >98%
	MolProbity score^	2.69		37th percentile* (N=27675, 0Å - 99Å)
	Cβ deviations >0.25Å	0	0.00%	Goal: 0
	Bad backbone bonds:	17 / 1059	1.61%	Goal: 0%
	Bad backbone angles:	5 / 1420	0.35%	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: 52.26	Clashscore: 14.91	Outliers: 0 of 131	Poor rotamers: 7 of 123	Outliers: 0 of 129	Outliers: 9 of 133	Outliers: 5 of 133
A 1		MET	50	-	-	25.7% (*ptp*) chi angles: 61.7,180.4,67.2	0.044Å	-	-
A 2		ARG	50	-	Favored (87.7%) General / -66.4,-42.5	43.2% (*ttm105*) chi angles: 181.6,180.9,293.5,106.4	0.009Å	-	-
A 3		LYS	50	-	Favored (90.14%) General / -63.8,-45.4	28.8% (*tptp*) chi angles: 184.5,63.4,180.5,65.1	0.042Å	-	-
A 4		HIS	99.99	1.062Å HB2 with A 22 THR HG21	Favored (2.25%) General / -49.8,-61.2	22.1% (*t-160*) chi angles: 189.3,196.7	0.077Å	OUTLIER(S) worst is CG-- ND1: 5.272 σ	OUTLIER(S) worst is CD2- NE2-CE1: 4.251 σ
A 5		VAL	50	-	Favored (94.02%) Isoleucine or valine / -64.9,-45.7	87.4% (*t*) chi angles: 177.3	0.088Å	-	-
					Favored				

A 6	LEU	50	0.407Å O with A 10 PHE HD2	(93.02%) General / -63.4,-45.0	97.7% (*mt*) chi angles: 297,176.3	0.034Å	OUTLIER(S) worst is C--N: 5.88 σ	-
A 7	ALA	50	0.452Å HB3 with A 18 ILE HG21	Favored (92.87%) General / -62.8,-39.0	-	0.106Å	-	-
A 8	ALA	50	0.652Å HB2 with A 18 ILE HD12	Favored (61.79%) General / -75.1,-34.4	-	0.064Å	-	-
A 9	SER	50	-	Favored (57.32%) General / -75.5,-40.3	23.9% (*t*) chi angles: 186.2	0.04Å	-	-
A 10	PHE	99.99	0.407Å HD2 with A 6 LEU O	Favored (18.28%) General / -88.6,11.1	98.7% (*m-85*) chi angles: 296.2,275.3	0.017Å	-	-
A 11	SER	50	-	Allowed (0.87%) General / 74.3,-12.6	39.8% (*t*) chi angles: 176.5	0.052Å	-	-
A 12	MET	99.99	-	Favored (10.85%) General / -47.9,-35.5	93.9% (*mmm*) chi angles: 287.6,298.5,293.7	0.029Å	-	-
A 13	LEU	50	0.657Å HB2 with A 18 ILE HG12	Favored (44.04%) General / -141.9,158.2	64.8% (*mt*) chi angles: 300.5,169.8	0.068Å	-	-
A 14	SER	50	0.699Å O with A 17 VAL HG12	Favored (51.7%) General / -67.2,148.5	38.2% (*t*) chi angles: 181.9	0.039Å	-	-
A 15	LEU	50	0.456Å HD23 with A 16 LEU N	Favored (31.05%) General / -57.0,145.3	9.2% (*tt*) chi angles: 186.4,157.6	0.064Å	-	-
A 16	LEU	50	0.456Å N with A 15 LEU HD23	Allowed (1.22%) General / 78.4,-11.3	54.6% (*tp*) chi angles: 179.4,66.8	0.066Å	-	-
A 17	VAL	50	0.699Å HG12 with A 14 SER O	Favored (6.93%) Isoleucine or valine / -97.6,-16.9	4.2% (*p*) chi angles: 77.9	0.135Å	-	-
A 18	ILE	99.99	0.802Å HB with A 4	Favored (4.04%) Isoleucine or	4.2% (*mt*) chi angles: 323.6,170.6	0.069Å	-	-

#	Alt	Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
						valine / -102.3,-35.4	HIS CD2		
A 19		MET	99.99	0.507Å HB2 with A 4 HIS CE1	Favored (67.1%) General / -69.5,-29.5	41.3% (*ttm*) chi angles: 193.2,172,274.7	0.09Å	-	-
A 20		GLY	50	-	Favored (98.97%) Glycine / -60.6,-41.8	-	-	-	-

#	Alt	Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
			Avg: 52.26	Clashscore: 14.91	Outliers: 0 of 131	Poor rotamers: 7 of 123	Outliers: 0 of 129	Outliers: 9 of 133	Outliers: 5 of 133
A 21		ASP	50	-	Favored (64.65%) General / -72.6,-42.3	13.7% (*m-20*) chi angles: 286.2,19	0.024Å	-	-
A 22		THR	50	1.062Å HG21 with A 4 HIS HB2	Favored (71.65%) General / -65.5,-30.8	47.5% (*p*) chi angles: 55.5	0.077Å	-	-
A 23		ASP	50	-	Favored (88.57%) General / -58.8,-42.2	96.4% (*m-20*) chi angles: 292,341	0.031Å	-	-
A 24		SER	50	-	Favored (16.71%) General / -86.0,-39.6	23.1% (*t*) chi angles: 187.2	0.028Å	-	-
A 25		LYS	50	-	Favored (72.56%) General / -57.2,-37.7	30.1% (*mtpp*) chi angles: 291,179.6,66.2,62.6	0.043Å	-	-
A 26		THR	50	-	Favored (67.07%) General / -66.5,-26.3	40.7% (*p*) chi angles: 53.9	0.1Å	-	-
A 27		ASP	50	-	Favored (26.78%) General / -106.1,2.1	34.3% (*t0*) chi angles: 195.3,334.2	0.038Å	-	-
A 28		SER	50	-	Favored (50.84%) General / -70.5,145.4	30.1% (*t*) chi angles: 184.9	0.03Å	-	-
A 29		SER	50	-	Favored (58.29%) General / -63.5,142.7	66.6% (*m*) chi angles: 298.4	0.057Å	-	-
					Favored				

#	Alt	Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
A 30		PHE	50	-	(47.03%) General / -126.0,151.5	17.4% (*p90*) chi angles: 50.6,279.7	0.039Å	-	-
A 31		ILE	50	-	Favored (28.3%) Isoleucine or valine / -62.7,133.7	49.6% (*mt*) chi angles: 298.9,158	0.1Å	-	-
A 32		MET	50	0.429Å HG2 with A 33 ASP N	Favored (18.7%) General / -100.7,154.3	46.5% (*ttp*) chi angles: 184.2,185.3,58.8	0.017Å	-	-
A 33		ASP	50	0.429Å N with A 32 MET HG2	Favored (22.16%) General / -61.3,125.0	2% (*m-20*) chi angles: 319.7,335.8	0.118Å	-	-
A 34		SER	50	-	Favored (23.17%) General / -60.5,153.4	0.1% chi angles: 225.6	0.04Å	-	-
A 35		ASP	50	-	Favored (78.25%) Pre-proline / -82.4,124.2	13.6% (*t0*) chi angles: 174.3,41.9	0.073Å	-	-
A 36		PRO	50	-	Favored (88.53%) Trans-proline / -58.0,-30.0	74.9% (*Cg_exo*) chi angles: 333	0.08Å	-	-
A 37		ARG	50	-	Favored (66.61%) General / -66.0,-23.5	14% (*mtp-105*) chi angles: 294.2,184.5,99.9,247.5	0.07Å	-	-
A 38		ARG	50	0.429Å HG2 with A 40 MET HE2	Favored (25.83%) General / -60.0,151.7	2% (*ptm180*) chi angles: 82.4,193.5,316.4,208.8	0.059Å	-	-
A 39		CYS	50	-	Favored (38.54%) General / -58.7,128.7	42.9% (*t*) chi angles: 176.1	0.061Å	-	-
A 40		MET	50	0.429Å HE2 with A 38 ARG HG2	Favored (10.29%) General / -165.2,174.4	19% (*ptp*) chi angles: 71.6,176.6,82.9	0.063Å	-	-
#	Alt	Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
			Avg: 52.26	Clashscore: 14.91	Outliers: 0 of 131	Poor rotamers: 7 of 123	Outliers: 0 of 129	Outliers: 9 of 133	Outliers: 5 of 133
A		ARG	50	-	Favored (39.9%)	26.2% (*ttt-85*) chi angles:	0.195Å	-	OUTLIER(S) worst is N-

41				General / -100.1,136.5	179.9,169,157.5,248.3			CA-CB: 4.069 σ
A 42	HIS	50	0.412Å O with A 63 ALA HA	Favored (50.11%) General / -120.5,141.6	89.7% (*m-70*) chi angles: 292.8,268.9	0.046Å	OUTLIER(S) worst is CG-- ND1: 4.413 σ	-
A 43	HIS	50	-	Favored (52.69%) General / -104.6,129.8	70.1% (*m80*) chi angles: 301.9,85.3	0.088Å	OUTLIER(S) worst is CG-- ND1: 4.348 σ	-
A 44	TYR	50	-	Favored (43.5%) General / -144.4,158.9	35.7% (*p90*) chi angles: 66.6,280.1	0.033Å	-	-
A 45	VAL	50	-	Favored (65.36%) Isoleucine or valine / -111.7,130.4	95% (*t*) chi angles: 178.7	0.048Å	-	-
A 46	ASP	50	-	Favored (48.6%) General / -136.9,151.1	46.8% (*t0*) chi angles: 189.9,18.9	0.076Å	-	-
A 47	SER	50	0.593Å HA with A 58 LYS O	Favored (40.21%) General / -96.5,123.7	90.3% (*p*) chi angles: 65.3	0.046Å	-	-
A 48	ILE	50	-	Favored (40.82%) Isoleucine or valine / -86.8,125.0	96.4% (*mt*) chi angles: 294.8,167.7	0.1Å	-	-
A 49	SER	50	-	Favored (41.82%) General / -126.7,156.0	50.2% (*m*) chi angles: 301.1	0.09Å	-	-
A 50	HIS	50	-	Favored (71.24%) Pre-proline / -75.5,136.6	59.8% (*t-80*) chi angles: 192.6,276.1	0.008Å	OUTLIER(S) worst is CG-- ND1: 4.127 σ	OUTLIER(S) worst is CB-CG-CD2: 4.247 σ
A 51	PRO	50	-	Favored (69.53%) Trans-proline / -63.6,-27.6	73.2% (*Cg_endo*) chi angles: 28.4	0.073Å	-	-
A 52	LEU	50	-	Allowed (0.79%) General / -113.9,-70.7	2.3% (*tm?*) chi angles: 192.4,294.4	0.066Å	-	-
A 53	TYR	50	-	Favored (58.9%) General / -65.0,140.9	48.4% (*m-85*) chi angles: 304.8,297.6	0.031Å	-	-

A 54		LYS	50	-	Favored (10.73%) General / -74.8,112.2	73.8% (*tttt*) chi angles: 190.1,191.8,178.7,194.3	0.058Å	-	-
A 55		CYS	50	-	Favored (37.17%) General / -139.2,161.5	59.1% (*m*) chi angles: 304.9	0.078Å	-	-
A 56		SER	50	-	Favored (58.02%) General / -65.3,138.2	58.1% (*m*) chi angles: 291.2	0.073Å	-	-
A 57		SER	50	-	Favored (50.02%) General / -107.4,134.8	69.1% (*p*) chi angles: 57.5	0.028Å	-	-
A 58		LYS	50	0.593Å O with A 47 SER HA	Favored (28.65%) General / -101.4,145.6	0.2% chi angles: 266.4,83.9,201.9,283.3	0.068Å	-	-
A 59		MET	50	-	Favored (25.31%) General / -87.9,115.4	36.1% (*mmm*) chi angles: 289,270,280	0.09Å	-	-
A 60		VAL	50	-	Favored (39.07%) Isoleucine or valine / -125.3,143.4	17.2% (*t*) chi angles: 162.1	0.112Å	-	-

#	Alt	Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
			Avg: 52.26	Clashscore: 14.91	Outliers: 0 of 131	Poor rotamers: 7 of 123	Outliers: 0 of 129	Outliers: 9 of 133	Outliers: 5 of 133
A 61		LEU	50	-	Favored (22.95%) General / -72.5,123.4	6.4% (*mt*) chi angles: 324.1,170.9	0.151Å	-	-
A 62		LEU	50	-	Favored (40.2%) General / -125.1,155.3	92.1% (*mt*) chi angles: 298.6,174.8	0.019Å	-	-
A 63		ALA	50	0.412Å HA with A 42 HIS O	Favored (51.69%) General / -122.9,141.6	-	0.035Å	-	-
A 64		ARG	50	-	Favored (34.84%) General / -129.3,159.8	23.8% (*ptt-85*) chi angles: 71.4,187.9,200.2,263.9	0.039Å	-	-
A					Favored (37.13%)	75.4% (*m*)			

65	CYS	50	-	General / -103.9,140.8	chi angles: 296.5	0.071Å	-	-
A 66	GLU	50	-	Favored (4.5%) General / -165.5,138.9	27.8% (tt0) chi angles: 197.3,178.9,273.1	0.049Å	-	-
A 67	GLY	50	-	Favored (39.35%) Glycine / 166.0,-167.7	-	-	-	-
A 68	HIS	50	-	Favored (6.07%) General / -126.0,99.8	73.7% (m-70) chi angles: 296,260.7	0.077Å	OUTLIER(S) worst is CG-- ND1: 4.548 σ	-
A 69	CYS	50	-	Favored (51.59%) General / -60.8,131.7	72.2% (m) chi angles: 297.9	0.041Å	-	-
A 70	SER	50	-	Favored (61.5%) General / -74.4,-29.3	81.1% (p) chi angles: 60.5	0.079Å	-	-
A 71	GLN	50	-	Favored (54.6%) General / -64.7,134.6	19.5% (mp0) chi angles: 305.4,92.9,328.8	0.076Å	-	-
A 72	ALA	50	-	Favored (55.86%) General / -67.6,137.7	-	0.063Å	-	-
A 73	SER	50	-	Favored (31.02%) General / -83.9,141.8	72.1% (p) chi angles: 57.9	0.006Å	-	-
A 74	ARG	50	-	Favored (44.47%) General / -142.6,154.5	6.2% (ptp85) chi angles: 57,176.3,59.2,68.5	0.018Å	-	-
A 75	SER	50	-	Favored (24.22%) General / -145.3,135.8	22.9% (t) chi angles: 187.7	0.04Å	-	-
A 76	GLU	50	-	Favored (25.03%) Pre-proline / -142.3,142.8	7.9% (tt0) chi angles: 213.3,175.6,285.8	0.16Å	-	-
A 77	PRO	50	-	Favored (37.68%) Trans-proline / -71.0,140.2	83.7% (Cg_endo) chi angles: 31.5	0.027Å	-	-
A	LEU	50	-	Favored (23.58%)	74.9% (mt)	0.057Å	-	-

#	Alt	Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
78					General / -98.0,148.3	chi angles: 287.2,170.5			
A 79		VAL	50	-	Favored (49.32%) Isoleucine or valine / -103.3,132.5	48.7% (*t*) chi angles: 182.6	0.05Å	-	-
A 80		SER	50	-	Favored (50.65%) General / -131.4,152.4	89.9% (*p*) chi angles: 62.5	0.024Å	-	-

#	Alt	Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
			Avg: 52.26	Clashscore: 14.91	Outliers: 0 of 131	Poor rotamers: 7 of 123	Outliers: 0 of 129	Outliers: 9 of 133	Outliers: 5 of 133
A 81		PHE	50	0.409Å CD1 with A 81 PHE N	Favored (2.77%) General / -119.3,-40.8	9.5% (*m-85*) chi angles: 314.1,78.8	0.118Å	-	-
A 82		SER	50	0.57Å HB2 with A 84 VAL HG23	Allowed (0.65%) General / -44.0,114.4	3.3% (*p*) chi angles: 40.1	0.077Å	-	-
A 83		THR	50	-	Favored (5.63%) General / -63.5,-7.0	40.5% (*p*) chi angles: 53.8	0.06Å	-	-
A 84		VAL	50	0.57Å HG23 with A 82 SER HB2	Allowed (1.47%) Isoleucine or valine / -58.4,158.6	2.9% (*t*) chi angles: 198.6	0.059Å	-	-
A 85		LEU	50	0.468Å O with A 86 LYS HG3	Favored (3.95%) General / -59.8,164.2	0.2% chi angles: 286.7,266.1	0.162Å	-	-
A 86		LYS	50	0.468Å HG3 with A 85 LEU O	Allowed (0.31%) General / 177.5,155.4	0.8% chi angles: 259.6,175.8,262,53.4	0.085Å	-	-
A 87		GLN	50	-	Favored (22.42%) Pre-proline / -62.8,116.2	23.6% (*mm-40*) chi angles: 295.9,271.5,21.7	0.106Å	-	-
A 88		PRO	50	-	Favored (40.49%) Trans-proline / -69.0,-18.3	88.3% (*Cg_endo*) chi angles: 31.2	0.052Å	-	-
A					Favored (53.5%)	38.4% (*m-85*)			

#	Alt	Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
89		PHE	50	-	General / -125.0,139.8	chi angles: 300.2,303.9	0.029Å	-	-
A 90		ARG	50	-	Favored (25.98%) General / -102.4,113.0	53.1% (*ttp85*) chi angles: 177.9,173.7,57.2,99.5	0.079Å	-	-
A 91		SER	50	-	Favored (50.59%) General / -130.0,151.4	74% (*p*) chi angles: 58.1	0.026Å	-	-
A 92		SER	50	-	Favored (48.66%) General / -128.3,132.6	46.9% (*t*) chi angles: 180.4	0.104Å	OUTLIER(S) worst is C--O: 4.432 σ	-
A 93		CYS	50	-	Favored (12.43%) General / -153.2,132.0	51.8% (*t*) chi angles: 181.6	0.146Å	-	-
A 94		HIS	50	-	Favored (49.05%) General / -106.0,134.5	62.6% (*m80*) chi angles: 283.7,81.7	0.009Å	OUTLIER(S) worst is CG--ND1: 4.344 σ	OUTLIER(S) worst is CB-CG-CD2: 4.34 σ
A 95		CYS	50	-	Favored (49.57%) General / -124.7,145.7	63.6% (*m*) chi angles: 302.9	0.079Å	-	-
A 96		CYS	50	-	Favored (11.19%) General / -83.2,101.4	39.1% (*t*) chi angles: 187.5	0.045Å	-	-
A 97		ARG	50	-	Favored (52.53%) Pre-proline / -125.6,161.1	79.7% (*mtt180*) chi angles: 285.7,189.9,182.7,149.9	0.041Å	-	-
A 98		PRO	50	-	Favored (26.62%) Trans-proline / -58.5,128.0	73.2% (*Cg_exo*) chi angles: 332.4	0.108Å	-	-
A 99		GLN	50	-	Favored (10.5%) General / -91.0,-42.5	63.8% (*tt0*) chi angles: 185.4,178,30.6	0.101Å	-	-
A 100		THR	50	-	Favored (37.39%) General / -139.8,144.6	73.4% (*p*) chi angles: 63.5	0.037Å	-	-
			Avg: 52.26	Clashscore: 14.91	Outliers: 0 of 131	Poor rotamers: 7 of 123	Outliers: 0 of 129	Outliers: 9 of 133	Outliers: 5 of 133

A 101	SER	50	-	Favored (37.98%) General / -156.6,159.0	96.4% (*p*) chi angles: 64.8	0.025Å	-	-
A 102	LYS	50	-	Favored (44.08%) General / -122.8,149.5	64.2% (*pttt*) chi angles: 65,183.7,182.5,186.5	0.04Å	-	-
A 103	LEU	50	-	Favored (38.91%) General / -78.2,141.1	24.1% (*tp*) chi angles: 191.9,64.3	0.05Å	-	-
A 104	LYS	50	-	Favored (52.28%) General / -131.7,146.6	0.5% chi angles: 233,90.6,155.2,63.9	0.142Å	-	-
A 105	ALA	50	-	Favored (49.87%) General / -131.8,143.0	-	0.028Å	-	-
A 106	LEU	50	0.571Å HD21 with A 58 LYS HB2	Favored (29.61%) General / -139.9,133.1	41.9% (*tp*) chi angles: 185.1,66.2	0.066Å	-	-
A 107	ARG	50	-	Favored (36.45%) General / -90.5,128.1	0% chi angles: 316.2,65.4,40.2,188.2	0.127Å	-	-
A 108	LEU	50	-	Favored (46.99%) General / -113.0,141.3	71.3% (*mt*) chi angles: 296.3,183.5	0.05Å	-	-
A 109	ARG	50	-	Favored (29.07%) General / -99.6,115.3	37.5% (*ttm180*) chi angles: 179.6,187,287.9,140.3	0.085Å	-	-
A 110	CYS	50	-	Favored (39.75%) General / -110.7,144.4	59.5% (*m*) chi angles: 304.7	0.063Å	-	-
A 111	SER	50	0.431Å HA with A 112 GLY HA2	Favored (15.1%) General / -100.2,103.6	55.2% (*p*) chi angles: 55.2	0.039Å	-	-
A 112	GLY	50	0.431Å HA2 with A 111 SER HA	Favored (4.28%) Glycine / -129.8,26.3	-	-	-	-
A 113	GLY	50	-	Allowed (0.83%) Glycine / -167.0,119.1	-	-	-	-

# Alt Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
A 114 MET	50	-	Favored (5.02%) General / -132.0,-178.7	4% (*tmm?*) chi angles: 214.9,287.8,301.2	0.108Å	-	-
A 115 ARG	50	-	Allowed (1.41%) General / -58.5,111.9	9.7% (*mmm180*) chi angles: 292.9,260.7,288.3,178.6	0.039Å	-	-
A 116 LEU	50	-	Favored (26.29%) General / -103.6,148.2	64.7% (*mt*) chi angles: 303.9,173.4	0.064Å	-	-
A 117 THR	50	-	Favored (41.96%) General / -113.6,120.7	75.1% (*p*) chi angles: 58.7	0.014Å	-	-
A 118 ALA	50	-	Favored (50.98%) General / -103.7,129.1	-	0.056Å	-	-
A 119 THR	50	-	Favored (29.44%) General / -110.7,150.2	72.8% (*p*) chi angles: 63.5	0.018Å	-	-
A 120 TYR	50	-	Favored (18.87%) General / -160.8,151.9	53.8% (*p90*) chi angles: 61,88.2	0.062Å	-	-

#	Alt	Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
			Avg: 52.26	Clashscore: 14.91	Outliers: 0 of 131	Poor rotamers: 7 of 123	Outliers: 0 of 129	Outliers: 9 of 133	Outliers: 5 of 133
A 121		ARG	50	-	Favored (31%) General / -92.5,139.0	51.3% (*mtp85*) chi angles: 304,196.9,73.5,80.8	0.016Å	-	-
A 122		TYR	50	-	Favored (22.46%) General / -102.3,110.5	43.7% (*t80*) chi angles: 180.2,276.2	0.067Å	-	-
A 123		ILE	50	-	Favored (32.61%) Isoleucine or valine / -66.8,131.3	72.7% (*mt*) chi angles: 303.4,172.7	0.075Å	-	-
A 124		LEU	50	-	Favored (12.33%) General / -100.8,-29.3	96.6% (*mt*) chi angles: 294.6,173.5	0.003Å	-	-
A					Favored (8.07%)	88% (*p*)			

125	SER	50	-	General / -166.0,150.3	chi angles: 61.7	0.028Å	-	-
A 126	CYS	50	-	Favored (35.75%) General / -118.0,152.3	62.4% (*m*) chi angles: 303.3	0.104Å	-	-
A 127	HIS	50	-	Favored (36%) General / -151.8,164.9	0% chi angles: 71.6,338.9	0.027Å	OUTLIER(S) worst is CD2--NE2: 4.192 σ	OUTLIER(S) worst is CB-CG-CD2: 4.38 σ
A 128	CYS	50	-	Favored (13.49%) General / -89.1,100.8	32.9% (*m*) chi angles: 281.6	0.018Å	-	-
A 129	GLU	50	-	Favored (24.78%) General / -113.8,155.9	14.4% (*pt-20*) chi angles: 68.3,173.5,295.9	0.089Å	-	-
A 130	GLU	50	-	Favored (35.92%) General / -54.5,140.0	7.4% (*tp10*) chi angles: 202.8,64.8,68.9	0.138Å	-	-
A 131	CYS	50	-	Allowed (0.05%) General / -54.5,-73.3	20.5% (*t*) chi angles: 171.5	0.038Å	-	-
A 132	ASN	50	-	Favored (6.72%) General / -82.1,85.7	2.3% (*m120*) chi angles: 266.5,54	0.044Å	-	-
A 133	SER	99.99	-	-	90.4% (*p*) chi angles: 65.8	0.035Å	-	-

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