APPENDIX

Table A.1. Estimation of Molecular Weights of EnvZ Fragments

Protein	Calculated M.W. (kDa)	Measured M.W. (kDa)		Form
		Gel Filtration	Light Scattering	
Cytoplasmic Region (223 - 450)	24.9	not done	57 - 59	Dimer
Domain A (223 - 289)	7.6	15	19 - 21	Dimer
Domain B (290 - 450)	17.6	19	25 - 28	Monomer

Table A.2. Distance Constraints Used for Structure Calculation of Domain B

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! Intramolecular NOEs in Domain B
assign (resid 292 and name HA  )(resid 292 and name HB#  ) 0.0 1.0 3.9
assign (resid 292 and name HA  )(resid 292 and name HG#  ) 0.0 1.0 3.9
assign (resid 293 and name HA  )(resid 293 and name HB#  ) 0.0 1.0 3.9
assign (resid 293 and name HA  )(resid 293 and name HG#  ) 0.0 1.0 3.9
assign (resid 293 and name HA  )(resid 293 and name HN   ) 0.0 0.0 5.0
assign (resid 293 and name HB#  )(resid 293 and name HN   ) 0.0 0.6 4.1
assign (resid 293 and name HG#  )(resid 293 and name HN   ) 0.0 1.0 6.0
assign (resid 294 and name HA  )(resid 294 and name HB#  ) 0.0 1.0 4.5
assign (resid 294 and name HA  )(resid 294 and name HG#  ) 0.0 1.0 3.9
assign (resid 294 and name HB#  )(resid 294 and name HN   ) 0.0 0.6 4.1
assign (resid 294 and name HG#  )(resid 294 and name HN   ) 0.0 1.0 6.0
assign (resid 295 and name HA  )(resid 295 and name HB#  ) 0.0 1.0 3.9
assign (resid 295 and name HA  )(resid 295 and name HD#  ) 0.0 1.0 6.0
assign (resid 295 and name HA  )(resid 295 and name HG#  ) 0.0 1.0 4.5
assign (resid 295 and name HB#  )(resid 295 and name HD#  ) 0.0 2.0 5.5
assign (resid 296 and name HA  )(resid 296 and name HB#  ) 0.0 1.0 3.9
assign (resid 296 and name HA  )(resid 296 and name HE#  ) 0.0 1.5 4.4
assign (resid 296 and name HA  )(resid 296 and name HG#  ) 0.0 1.0 3.9
assign (resid 296 and name HB#  )(resid 296 and name HE#  ) 0.0 2.5 5.0
assign (resid 296 and name HB#  )(resid 296 and name HN   ) 0.0 0.6 3.1
assign (resid 296 and name HE#  )(resid 296 and name HG#  ) 0.0 2.5 5.0
assign (resid 296 and name HG#  )(resid 296 and name HN   ) 0.0 1.0 3.9
assign (resid 297 and name HA  )(resid 297 and name HB#  ) 0.0 1.0 3.9
assign (resid 297 and name HA  )(resid 297 and name HG#  ) 0.0 1.0 6.0
assign (resid 297 and name HA  )(resid 297 and name HN   ) 0.0 0.0 3.5
assign (resid 297 and name HB#  )(resid 297 and name HN   ) 0.0 0.6 3.5
assign (resid 297 and name HG#  )(resid 297 and name HN   ) 0.0 1.0 3.9
assign (resid 298 and name HA  )(resid 298 and name HE#  ) 0.0 1.5 4.4
assign (resid 298 and name HA  )(resid 298 and name HG#  ) 0.0 1.0 4.5
assign (resid 298 and name HA  )(resid 298 and name HN   ) 0.0 0.0 2.9
assign (resid 298 and name HB#  )(resid 298 and name HN   ) 0.0 0.6 3.1
assign (resid 298 and name HE#  )(resid 298 and name HG#  ) 0.0 2.5 5.0
assign (resid 298 and name HG#  )(resid 298 and name HN   ) 0.0 1.0 3.9
assign (resid 299 and name HA  )(resid 299 and name HN   ) 0.0 0.0 2.9
assign (resid 299 and name HB#  )(resid 299 and name HN   ) 0.0 1.1 4.0
assign (resid 300 and name HA  )(resid 300 and name HN   ) 0.0 0.0 2.9
assign (resid 300 and name HB#  )(resid 300 and name HN   ) 0.0 0.6 3.5
assign (resid 301 and name HA  )(resid 301 and name HD1# ) 0.0 1.5 5.0
assign (resid 301 and name HA  )(resid 301 and name HD2# ) 0.0 1.5 4.4
assign (resid 301 and name HA  )(resid 301 and name HN   ) 0.0 0.0 5.0
assign (resid 301 and name HD1# )(resid 301 and name HN   ) 0.0 1.5 5.0
assign (resid 301 and name HD2# )(resid 301 and name HN   ) 0.0 1.5 5.0
assign (resid 301 and name HG  )(resid 301 and name HN   ) 0.0 0.0 3.5
assign (resid 302 and name HA  )(resid 302 and name HB#  ) 0.0 1.0 4.5
assign (resid 302 and name HA  )(resid 302 and name HN   ) 0.0 0.0 3.5
assign (resid 302 and name HB#  )(resid 302 and name HD2# ) 0.0 2.0 5.5
assign (resid 302 and name HB#  )(resid 302 and name HN   ) 0.0 0.6 3.5
assign (resid 302 and name HD2# )(resid 302 and name HN   ) 0.0 1.0 6.0
assign (resid 303 and name HA  )(resid 303 and name HN   ) 0.0 0.0 2.9
assign (resid 303 and name HB#  )(resid 303 and name HN   ) 0.0 1.1 3.6
assign (resid 304 and name HA  )(resid 304 and name HB   ) 0.0 0.0 3.5
assign (resid 304 and name HA  )(resid 304 and name HG1# ) 0.0 1.5 4.4
assign (resid 304 and name HA  )(resid 304 and name HG2# ) 0.0 1.5 4.0
assign (resid 304 and name HA  )(resid 304 and name HN   ) 0.0 0.0 2.9
assign (resid 304 and name HB  )(resid 304 and name HN   ) 0.0 0.0 2.9
assign (resid 304 and name HG1# )(resid 304 and name HN   ) 0.0 1.5 4.4
assign (resid 304 and name HG2# )(resid 304 and name HN   ) 0.0 1.5 4.4
assign (resid 305 and name HA  )(resid 305 and name HB#  ) 0.0 1.0 6.0
assign (resid 305 and name HA  )(resid 305 and name HD1# ) 0.0 1.5 4.4
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Table A.2. *(continued)*

```
assign (resid 305 and name HA   )(resid 305 and name HD2# ) 0.0 1.5 4.4
assign (resid 305 and name HA   )(resid 305 and name HN   ) 0.0 0.0 3.5
assign (resid 305 and name HB#  )(resid 305 and name HN   ) 0.0 0.6 4.1
assign (resid 305 and name HD1# )(resid 305 and name HN   ) 0.0 1.5 5.0
assign (resid 305 and name HD2# )(resid 305 and name HN   ) 0.0 1.5 5.0
assign (resid 305 and name HG   )(resid 305 and name HN   ) 0.0 0.0 2.9
assign (resid 306 and name HA#  )(resid 306 and name HN   ) 0.0 0.6 3.5
assign (resid 307 and name HA   )(resid 307 and name HB#  ) 0.0 1.0 3.9
assign (resid 307 and name HA   )(resid 307 and name HG#  ) 0.0 1.0 3.9
assign (resid 307 and name HA   )(resid 307 and name HN   ) 0.0 0.0 2.9
assign (resid 307 and name HB#  )(resid 307 and name HN   ) 0.0 0.6 3.5
assign (resid 307 and name HG#  )(resid 307 and name HN   ) 0.0 1.0 3.9
assign (resid 308 and name HA   )(resid 308 and name HB   ) 0.0 0.0 3.5
assign (resid 308 and name HA   )(resid 308 and name HG1# ) 0.0 1.5 4.0
assign (resid 308 and name HA   )(resid 308 and name HG2# ) 0.0 1.5 4.0
assign (resid 308 and name HA   )(resid 308 and name HN   ) 0.0 0.0 2.9
assign (resid 308 and name HG1# )(resid 308 and name HN   ) 0.0 1.5 4.4
assign (resid 308 and name HG2# )(resid 308 and name HN   ) 0.0 1.5 4.4
assign (resid 309 and name HA   )(resid 309 and name HB   ) 0.0 0.0 3.5
assign (resid 309 and name HA   )(resid 309 and name HD1# ) 0.0 1.5 4.4
assign (resid 309 and name HA   )(resid 309 and name HG2# ) 0.0 1.5 4.4
assign (resid 309 and name HA   )(resid 309 and name HN   ) 0.0 0.0 3.5
assign (resid 309 and name HB   )(resid 309 and name HD1# ) 0.0 1.5 4.4
assign (resid 309 and name HB   )(resid 309 and name HN   ) 0.0 0.0 2.9
assign (resid 309 and name HD1# )(resid 309 and name HG2# ) 0.0 3.0 5.5
assign (resid 309 and name HG1# )(resid 309 and name HN   ) 0.0 1.0 3.9
assign (resid 310 and name HA   )(resid 310 and name HN   ) 0.0 0.0 2.9
assign (resid 310 and name HB#  )(resid 310 and name HN   ) 0.0 1.1 3.6
assign (resid 311 and name HA   )(resid 311 and name HN   ) 0.0 0.0 2.9
assign (resid 311 and name HB#  )(resid 311 and name HN   ) 0.0 1.1 3.6
assign (resid 312 and name HA   )(resid 312 and name HB#  ) 0.0 1.0 4.5
assign (resid 312 and name HA   )(resid 312 and name HN   ) 0.0 0.0 2.9
assign (resid 312 and name HB#  )(resid 312 and name HN   ) 0.0 0.6 4.1
assign (resid 312 and name HG#  )(resid 312 and name HN   ) 0.0 1.0 3.9
assign (resid 313 and name HA   )(resid 313 and name HB#  ) 0.0 1.0 3.9
assign (resid 313 and name HA   )(resid 313 and name HN   ) 0.0 0.0 2.9
assign (resid 313 and name HB#  )(resid 313 and name HN   ) 0.0 0.6 3.5
assign (resid 314 and name HA#  )(resid 314 and name HN   ) 0.0 0.6 3.1
assign (resid 315 and name HA   )(resid 315 and name HB#  ) 0.0 1.0 3.9
assign (resid 315 and name HA   )(resid 315 and name HD#  ) 0.0 2.0 4.9
assign (resid 315 and name HA   )(resid 315 and name HN   ) 0.0 0.0 3.5
assign (resid 315 and name HB#  )(resid 315 and name HD#  ) 0.0 3.0 5.9
assign (resid 315 and name HB#  )(resid 315 and name HN   ) 0.0 0.6 4.1
assign (resid 315 and name HD#  )(resid 315 and name HN   ) 0.0 2.0 7.0
assign (resid 316 and name HA   )(resid 316 and name HN   ) 0.0 0.0 2.9
assign (resid 316 and name HB#  )(resid 316 and name HN   ) 0.0 0.6 3.5
assign (resid 317 and name HA   )(resid 317 and name HB#  ) 0.0 1.0 3.9
assign (resid 317 and name HA   )(resid 317 and name HD#  ) 0.0 1.0 4.5
assign (resid 317 and name HA   )(resid 317 and name HG#  ) 0.0 1.0 3.9
assign (resid 317 and name HA   )(resid 317 and name HN   ) 0.0 0.0 2.9
assign (resid 317 and name HB#  )(resid 317 and name HD#  ) 0.0 2.0 4.9
assign (resid 317 and name HB#  )(resid 317 and name HN   ) 0.0 0.6 3.5
assign (resid 317 and name HG#  )(resid 317 and name HN   ) 0.0 1.0 3.9
assign (resid 318 and name HA   )(resid 318 and name HN   ) 0.0 0.0 2.9
assign (resid 318 and name HB#  )(resid 318 and name HN   ) 0.0 0.6 3.5
assign (resid 318 and name HG#  )(resid 318 and name HN   ) 0.0 1.0 3.9
assign (resid 319 and name HA   )(resid 319 and name HD1# ) 0.0 1.5 4.4
assign (resid 319 and name HA   )(resid 319 and name HG1# ) 0.0 1.0 6.0
assign (resid 319 and name HA   )(resid 319 and name HG2# ) 0.0 1.5 4.4
assign (resid 319 and name HA   )(resid 319 and name HN   ) 0.0 0.0 3.5
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Table A.2. *(continued)*

```
assign (resid 319 and name HB   )(resid 319 and name HN   ) 0.0 0.0 2.9
assign (resid 319 and name HD1# )(resid 319 and name HN   ) 0.0 1.5 4.4
assign (resid 319 and name HG2# )(resid 319 and name HN   ) 0.0 1.5 4.4
assign (resid 320 and name HA   )(resid 320 and name HB#  ) 0.0 1.0 3.9
assign (resid 320 and name HA   )(resid 320 and name HG#  ) 0.0 1.0 3.9
assign (resid 320 and name HA   )(resid 320 and name HN   ) 0.0 0.0 2.9
assign (resid 320 and name HB#  )(resid 320 and name HN   ) 0.0 0.6 3.5
assign (resid 320 and name HG#  )(resid 320 and name HN   ) 0.0 1.0 6.0
assign (resid 321 and name HA   )(resid 321 and name HB   ) 0.0 0.0 2.5
assign (resid 321 and name HA   )(resid 321 and name HG2# ) 0.0 1.5 4.0
assign (resid 321 and name HA   )(resid 321 and name HN   ) 0.0 0.0 2.9
assign (resid 321 and name HB   )(resid 321 and name HN   ) 0.0 0.0 3.5
assign (resid 321 and name HG2# )(resid 321 and name HN   ) 0.0 1.5 4.4
assign (resid 322 and name HA   )(resid 322 and name HN   ) 0.0 0.0 3.5
assign (resid 322 and name HB#  )(resid 322 and name HN   ) 0.0 1.1 4.0
assign (resid 323 and name HA   )(resid 323 and name HB#  ) 0.0 1.0 4.5
assign (resid 323 and name HA   )(resid 323 and name HD1# ) 0.0 1.5 4.4
assign (resid 323 and name HA   )(resid 323 and name HD2# ) 0.0 1.5 4.4
assign (resid 323 and name HA   )(resid 323 and name HN   ) 0.0 0.0 3.5
assign (resid 323 and name HB#  )(resid 323 and name HD1# ) 0.0 2.5 5.4
assign (resid 323 and name HB#  )(resid 323 and name HD2# ) 0.0 2.5 5.4
assign (resid 323 and name HB#  )(resid 323 and name HN   ) 0.0 0.6 3.1
assign (resid 323 and name HD1# )(resid 323 and name HN   ) 0.0 1.5 4.4
assign (resid 323 and name HD2# )(resid 323 and name HN   ) 0.0 1.5 4.4
assign (resid 324 and name HA   )(resid 324 and name HB#  ) 0.0 1.0 4.5
assign (resid 324 and name HA   )(resid 324 and name HD#  ) 0.0 2.0 4.9
assign (resid 324 and name HA   )(resid 324 and name HE#  ) 0.0 2.0 5.5
assign (resid 324 and name HA   )(resid 324 and name HN   ) 0.0 0.0 3.5
assign (resid 324 and name HB#  )(resid 324 and name HD#  ) 0.0 3.0 5.9
assign (resid 324 and name HB#  )(resid 324 and name HE#  ) 0.0 3.0 8.0
assign (resid 324 and name HB#  )(resid 324 and name HN   ) 0.0 0.6 4.1
assign (resid 324 and name HD#  )(resid 324 and name HN   ) 0.0 2.0 7.0
assign (resid 325 and name HA   )(resid 325 and name HB#  ) 0.0 1.0 3.9
assign (resid 325 and name HA   )(resid 325 and name HG#  ) 0.0 1.0 4.5
assign (resid 325 and name HB#  )(resid 325 and name HD#  ) 0.0 2.0 5.5
assign (resid 326 and name HA#  )(resid 326 and name HN   ) 0.0 0.6 3.1
assign (resid 327 and name HA   )(resid 327 and name HB#  ) 0.0 1.0 3.5
assign (resid 327 and name HA   )(resid 327 and name HN   ) 0.0 0.0 3.5
assign (resid 327 and name HB#  )(resid 327 and name HN   ) 0.0 0.6 3.5
assign (resid 328 and name HA   )(resid 328 and name HB   ) 0.0 0.0 6.0
assign (resid 328 and name HA   )(resid 328 and name HD1# ) 0.0 1.5 4.4
assign (resid 328 and name HA   )(resid 328 and name HG1# ) 0.0 1.0 4.5
assign (resid 328 and name HA   )(resid 328 and name HG2# ) 0.0 1.5 4.4
assign (resid 328 and name HA   )(resid 328 and name HN   ) 0.0 0.0 3.5
assign (resid 328 and name HB   )(resid 328 and name HD1# ) 0.0 1.5 4.4
assign (resid 328 and name HB   )(resid 328 and name HN   ) 0.0 0.0 3.5
assign (resid 328 and name HD1# )(resid 328 and name HG2# ) 0.0 3.0 5.5
assign (resid 328 and name HD1# )(resid 328 and name HN   ) 0.0 1.5 5.0
assign (resid 328 and name HG1# )(resid 328 and name HN   ) 0.0 1.0 4.5
assign (resid 328 and name HG2# )(resid 328 and name HN   ) 0.0 1.5 5.0
assign (resid 329 and name HA   )(resid 329 and name HB#  ) 0.0 1.0 3.9
assign (resid 329 and name HA   )(resid 329 and name HG#  ) 0.0 1.0 4.5
assign (resid 329 and name HA   )(resid 329 and name HN   ) 0.0 0.0 2.9
assign (resid 329 and name HB#  )(resid 329 and name HN   ) 0.0 0.6 3.1
assign (resid 329 and name HG#  )(resid 329 and name HN   ) 0.0 1.0 3.9
assign (resid 330 and name HA   )(resid 330 and name HB   ) 0.0 0.0 2.9
assign (resid 330 and name HA   )(resid 330 and name HG1# ) 0.0 1.5 4.0
assign (resid 330 and name HA   )(resid 330 and name HG2# ) 0.0 1.5 4.4
assign (resid 330 and name HA   )(resid 330 and name HN   ) 0.0 0.0 3.5
assign (resid 330 and name HB   )(resid 330 and name HN   ) 0.0 0.0 5.0
```

Table A.2. *(continued)*

```
assign (resid 330 and name HG1# )(resid 330 and name HN   ) 0.0 1.5 5.0
assign (resid 330 and name HG2# )(resid 330 and name HN   ) 0.0 1.5 4.4
assign (resid 331 and name HA   )(resid 331 and name HB#  ) 0.0 1.0 4.5
assign (resid 331 and name HA   )(resid 331 and name HD#  ) 0.0 1.0 4.5
assign (resid 331 and name HA   )(resid 331 and name HG#  ) 0.0 1.0 6.0
assign (resid 331 and name HA   )(resid 331 and name HN   ) 0.0 0.0 2.9
assign (resid 331 and name HB#  )(resid 331 and name HE#  ) 0.0 2.0 4.9
assign (resid 331 and name HB#  )(resid 331 and name HN   ) 0.0 0.6 3.5
assign (resid 331 and name HD#  )(resid 331 and name HN   ) 0.0 1.0 3.9
assign (resid 331 and name HE#  )(resid 331 and name HG#  ) 0.0 2.0 4.5
assign (resid 331 and name HE#  )(resid 331 and name HN   ) 0.0 1.0 7.0
assign (resid 331 and name HG#  )(resid 331 and name HN   ) 0.0 1.0 4.5
assign (resid 332 and name HA   )(resid 332 and name HE#  ) 0.0 1.5 5.0
assign (resid 332 and name HA   )(resid 332 and name HN   ) 0.0 0.0 5.0
assign (resid 332 and name HB#  )(resid 332 and name HN   ) 0.0 0.6 4.1
assign (resid 333 and name HA   )(resid 333 and name HB#  ) 0.0 1.0 4.5
assign (resid 333 and name HA   )(resid 333 and name HD2  ) 0.0 0.0 2.9
assign (resid 333 and name HA   )(resid 333 and name HN   ) 0.0 0.0 5.0
assign (resid 333 and name HB#  )(resid 333 and name HD2  ) 0.0 1.0 6.0
assign (resid 333 and name HB#  )(resid 333 and name HN   ) 0.0 0.6 5.6
assign (resid 334 and name HA   )(resid 334 and name HB#  ) 0.0 1.0 4.5
assign (resid 335 and name HA   )(resid 335 and name HB#  ) 0.0 1.0 3.9
assign (resid 335 and name HA   )(resid 335 and name HD#  ) 0.0 1.7 4.2
assign (resid 335 and name HA   )(resid 335 and name HG   ) 0.0 0.0 3.5
assign (resid 335 and name HA   )(resid 335 and name HN   ) 0.0 0.0 2.9
assign (resid 335 and name HB#  )(resid 335 and name HD#  ) 0.0 3.4 5.9
assign (resid 335 and name HB#  )(resid 335 and name HN   ) 0.0 0.6 3.5
assign (resid 335 and name HD#  )(resid 335 and name HN   ) 0.0 1.7 4.6
assign (resid 336 and name HA   )(resid 336 and name HB#  ) 0.0 1.0 4.5
assign (resid 336 and name HA   )(resid 336 and name HN   ) 0.0 0.0 3.5
assign (resid 336 and name HB#  )(resid 336 and name HN   ) 0.0 0.6 5.6
assign (resid 337 and name HA   )(resid 337 and name HB   ) 0.0 0.0 5.0
assign (resid 337 and name HA   )(resid 337 and name HD1# ) 0.0 1.5 4.4
assign (resid 337 and name HA   )(resid 337 and name HG2# ) 0.0 1.5 4.4
assign (resid 337 and name HA   )(resid 337 and name HN   ) 0.0 0.0 5.0
assign (resid 337 and name HB   )(resid 337 and name HN   ) 0.0 0.0 2.9
assign (resid 337 and name HD1# )(resid 337 and name HG2# ) 0.0 3.0 5.5
assign (resid 337 and name HD1# )(resid 337 and name HN   ) 0.0 1.5 5.0
assign (resid 337 and name HG2# )(resid 337 and name HN   ) 0.0 1.5 5.0
assign (resid 338 and name HA   )(resid 338 and name HB#  ) 0.0 1.0 4.5
assign (resid 338 and name HA   )(resid 338 and name HD#  ) 0.0 1.0 6.0
assign (resid 338 and name HA   )(resid 338 and name HG#  ) 0.0 1.0 4.5
assign (resid 338 and name HA   )(resid 338 and name HN   ) 0.0 0.0 2.9
assign (resid 338 and name HB#  )(resid 338 and name HN   ) 0.0 0.6 3.5
assign (resid 338 and name HE#  )(resid 338 and name HG#  ) 0.0 2.0 7.0
assign (resid 338 and name HE#  )(resid 338 and name HN   ) 0.0 1.0 7.0
assign (resid 338 and name HG#  )(resid 338 and name HN   ) 0.0 1.0 3.9
assign (resid 339 and name HA   )(resid 339 and name HD#  ) 0.0 1.0 3.9
assign (resid 339 and name HA   )(resid 339 and name HN   ) 0.0 0.0 2.9
assign (resid 339 and name HD#  )(resid 339 and name HN   ) 0.0 1.0 6.0
assign (resid 340 and name HA   )(resid 340 and name HN   ) 0.0 0.0 2.9
assign (resid 340 and name HB#  )(resid 340 and name HN   ) 0.0 1.1 4.0
assign (resid 341 and name HA   )(resid 341 and name HB   ) 0.0 0.0 3.5
assign (resid 341 and name HA   )(resid 341 and name HG1# ) 0.0 1.5 4.4
assign (resid 341 and name HA   )(resid 341 and name HG2# ) 0.0 1.5 4.4
assign (resid 341 and name HA   )(resid 341 and name HN   ) 0.0 0.0 2.9
assign (resid 341 and name HB   )(resid 341 and name HN   ) 0.0 0.0 2.9
assign (resid 341 and name HG1# )(resid 341 and name HN   ) 0.0 1.5 4.4
assign (resid 341 and name HG2# )(resid 341 and name HN   ) 0.0 1.5 4.4
assign (resid 342 and name HA   )(resid 342 and name HN   ) 0.0 0.0 2.9
```


Table A.2. *(continued)*

```
assign (resid 342 and name HB#  )(resid 342 and name HN   ) 0.0 1.1 3.6
assign (resid 343 and name HA   )(resid 343 and name HB#  ) 0.0 1.0 6.0
assign (resid 343 and name HA   )(resid 343 and name HN   ) 0.0 0.0 3.5
assign (resid 343 and name HB#  )(resid 343 and name HN   ) 0.0 0.6 4.1
assign (resid 345 and name HA   )(resid 345 and name HG#  ) 0.0 1.7 4.6
assign (resid 345 and name HA   )(resid 345 and name HN   ) 0.0 0.0 5.0
assign (resid 345 and name HG#  )(resid 345 and name HN   ) 0.0 1.7 5.2
assign (resid 346 and name HA   )(resid 346 and name HB   ) 0.0 0.0 3.5
assign (resid 346 and name HA   )(resid 346 and name HG#  ) 0.0 1.7 4.6
assign (resid 347 and name HA   )(resid 347 and name HB#  ) 0.0 1.0 4.5
assign (resid 348 and name HA   )(resid 348 and name HN   ) 0.0 0.0 5.0
assign (resid 348 and name HB#  )(resid 348 and name HN   ) 0.0 1.1 6.1
assign (resid 349 and name HA   )(resid 349 and name HN   ) 0.0 0.0 2.9
assign (resid 349 and name HB#  )(resid 349 and name HN   ) 0.0 1.1 3.6
assign (resid 350 and name HA   )(resid 350 and name HD#  ) 0.0 1.0 4.5
assign (resid 350 and name HA   )(resid 350 and name HG#  ) 0.0 1.0 4.5
assign (resid 350 and name HA   )(resid 350 and name HN   ) 0.0 0.0 3.5
assign (resid 350 and name HD#  )(resid 350 and name HN   ) 0.0 1.0 6.0
assign (resid 350 and name HG#  )(resid 350 and name HN   ) 0.0 1.0 6.0
assign (resid 353 and name HA   )(resid 353 and name HB#  ) 0.0 1.0 3.9
assign (resid 353 and name HA   )(resid 353 and name HD2# ) 0.0 1.0 6.0
assign (resid 353 and name HB#  )(resid 353 and name HD2# ) 0.0 2.0 5.5
assign (resid 354 and name HA#  )(resid 354 and name HN   ) 0.0 0.6 4.1
assign (resid 355 and name HA   )(resid 355 and name HB#  ) 0.0 1.0 3.9
assign (resid 355 and name HA   )(resid 355 and name HD1  ) 0.0 0.0 3.5
assign (resid 355 and name HA   )(resid 355 and name HN   ) 0.0 0.0 5.0
assign (resid 355 and name HB#  )(resid 355 and name HD1  ) 0.0 1.0 4.5
assign (resid 355 and name HB#  )(resid 355 and name HE1  ) 0.0 1.0 6.0
assign (resid 355 and name HB#  )(resid 355 and name HN   ) 0.0 0.6 5.6
assign (resid 355 and name HD1  )(resid 355 and name HN   ) 0.0 0.0 6.0
assign (resid 356 and name HA   )(resid 356 and name HG2# ) 0.0 1.5 4.4
assign (resid 356 and name HA   )(resid 356 and name HN   ) 0.0 0.0 3.5
assign (resid 356 and name HB   )(resid 356 and name HN   ) 0.0 0.0 2.9
assign (resid 356 and name HG2# )(resid 356 and name HN   ) 0.0 1.5 4.4
assign (resid 357 and name HA   )(resid 357 and name HN   ) 0.0 0.0 5.0
assign (resid 358 and name HA   )(resid 358 and name HB   ) 0.0 0.0 2.9
assign (resid 358 and name HA   )(resid 358 and name HG1# ) 0.0 1.5 4.4
assign (resid 358 and name HA   )(resid 358 and name HG2# ) 0.0 1.5 4.4
assign (resid 358 and name HB   )(resid 358 and name HN   ) 0.0 0.0 3.5
assign (resid 358 and name HG2# )(resid 358 and name HN   ) 0.0 1.5 4.4
assign (resid 359 and name HA   )(resid 359 and name HB#  ) 0.0 1.0 4.5
assign (resid 359 and name HA   )(resid 359 and name HN   ) 0.0 0.0 5.0
assign (resid 359 and name HB#  )(resid 359 and name HN   ) 0.0 0.6 5.6
assign (resid 360 and name HA   )(resid 360 and name HN   ) 0.0 0.0 2.9
assign (resid 361 and name HA#  )(resid 361 and name HN   ) 0.0 0.6 4.1
assign (resid 362 and name HA   )(resid 362 and name HB   ) 0.0 0.0 2.9
assign (resid 362 and name HA   )(resid 362 and name HG2# ) 0.0 1.5 4.4
assign (resid 362 and name HA   )(resid 362 and name HN   ) 0.0 0.0 3.5
assign (resid 362 and name HB   )(resid 362 and name HN   ) 0.0 0.0 5.0
assign (resid 362 and name HG2# )(resid 362 and name HN   ) 0.0 1.5 4.4
assign (resid 363 and name HA   )(resid 363 and name HG#  ) 0.0 1.0 3.9
assign (resid 363 and name HG#  )(resid 363 and name HN   ) 0.0 1.0 4.5
assign (resid 364 and name HA   )(resid 364 and name HB#  ) 0.0 1.0 3.9
assign (resid 364 and name HA   )(resid 364 and name HG#  ) 0.0 1.0 4.5
assign (resid 365 and name HA   )(resid 365 and name HB#  ) 0.0 1.0 3.9
assign (resid 365 and name HB#  )(resid 365 and name HD2# ) 0.0 2.0 5.5
assign (resid 365 and name HB#  )(resid 365 and name HN   ) 0.0 0.6 5.6
assign (resid 366 and name HA   )(resid 366 and name HB#  ) 0.0 1.0 4.5
assign (resid 366 and name HA   )(resid 366 and name HG#  ) 0.0 1.0 6.0
assign (resid 366 and name HA   )(resid 366 and name HN   ) 0.0 0.0 3.5
```

Table A.2. *(continued)*

```
assign (resid 366 and name HB# )(resid 366 and name HN  ) 0.0 0.6 4.1
assign (resid 366 and name HG# )(resid 366 and name HN  ) 0.0 1.0 4.5
assign (resid 367 and name HA  )(resid 367 and name HN  ) 0.0 0.0 5.0
assign (resid 367 and name HB# )(resid 367 and name HN  ) 0.0 1.1 4.0
assign (resid 368 and name HA  )(resid 368 and name HE3 ) 0.0 0.0 5.0
assign (resid 368 and name HA  )(resid 368 and name HN  ) 0.0 0.0 5.0
assign (resid 368 and name HD1 )(resid 368 and name HN  ) 0.0 0.0 5.0
assign (resid 368 and name HE1 )(resid 368 and name HN  ) 0.0 0.0 5.0
assign (resid 369 and name HA  )(resid 369 and name HB# ) 0.0 1.0 4.5
assign (resid 369 and name HA  )(resid 369 and name HD# ) 0.0 2.0 5.5
assign (resid 369 and name HB# )(resid 369 and name HD# ) 0.0 3.0 5.9
assign (resid 369 and name HB# )(resid 369 and name HN  ) 0.0 0.6 5.6
assign (resid 369 and name HD# )(resid 369 and name HN  ) 0.0 2.0 7.0
assign (resid 370 and name HA  )(resid 370 and name HN  ) 0.0 0.0 5.0
assign (resid 371 and name HA  )(resid 371 and name HB  ) 0.0 0.0 2.9
assign (resid 371 and name HA  )(resid 371 and name HG1# ) 0.0 1.5 4.4
assign (resid 371 and name HA  )(resid 371 and name HG2# ) 0.0 1.5 4.4
assign (resid 371 and name HA  )(resid 371 and name HN  ) 0.0 0.0 5.0
assign (resid 371 and name HB  )(resid 371 and name HN  ) 0.0 0.0 3.5
assign (resid 371 and name HG1# )(resid 371 and name HN  ) 0.0 1.5 5.0
assign (resid 371 and name HG2# )(resid 371 and name HN  ) 0.0 1.5 5.0
assign (resid 372 and name HA  )(resid 372 and name HN  ) 0.0 0.0 5.0
assign (resid 373 and name HA  )(resid 373 and name HB# ) 0.0 1.0 4.5
assign (resid 374 and name HA  )(resid 374 and name HN  ) 0.0 0.0 5.0
assign (resid 374 and name HB# )(resid 374 and name HN  ) 0.0 0.6 4.1
assign (resid 378 and name HA  )(resid 378 and name HB  ) 0.0 0.0 3.5
assign (resid 378 and name HA  )(resid 378 and name HD1# ) 0.0 1.5 6.5
assign (resid 378 and name HA  )(resid 378 and name HG1# ) 0.0 1.0 6.0
assign (resid 378 and name HB  )(resid 378 and name HD1# ) 0.0 1.5 6.5
assign (resid 378 and name HB  )(resid 378 and name HN  ) 0.0 0.0 3.5
assign (resid 378 and name HD1# )(resid 378 and name HG2# ) 0.0 3.0 5.9
assign (resid 378 and name HG1# )(resid 378 and name HN  ) 0.0 1.0 7.0
assign (resid 378 and name HG2# )(resid 378 and name HN  ) 0.0 1.5 5.0
assign (resid 379 and name HA  )(resid 379 and name HN  ) 0.0 0.0 3.5
assign (resid 379 and name HB# )(resid 379 and name HN  ) 0.0 1.1 4.0
assign (resid 380 and name HA  )(resid 380 and name HB# ) 0.0 1.0 3.9
assign (resid 381 and name HA  )(resid 381 and name HB# ) 0.0 1.0 3.5
assign (resid 381 and name HA  )(resid 381 and name HG# ) 0.0 1.0 3.9
assign (resid 381 and name HA  )(resid 381 and name HN  ) 0.0 0.0 3.5
assign (resid 381 and name HB# )(resid 381 and name HN  ) 0.0 0.6 3.5
assign (resid 381 and name HG# )(resid 381 and name HN  ) 0.0 1.0 4.5
assign (resid 382 and name HA  )(resid 382 and name HB# ) 0.0 1.0 3.9
assign (resid 382 and name HA  )(resid 382 and name HG# ) 0.0 1.0 3.9
assign (resid 382 and name HA  )(resid 382 and name HN  ) 0.0 0.0 3.5
assign (resid 382 and name HB# )(resid 382 and name HN  ) 0.0 0.6 3.5
assign (resid 382 and name HG# )(resid 382 and name HN  ) 0.0 1.0 4.5
assign (resid 383 and name HA  )(resid 383 and name HG# ) 0.0 1.0 4.5
assign (resid 383 and name HA  )(resid 383 and name HN  ) 0.0 0.0 3.5
assign (resid 383 and name HD# )(resid 383 and name HN  ) 0.0 1.0 6.0
assign (resid 383 and name HG# )(resid 383 and name HN  ) 0.0 1.0 6.0
assign (resid 384 and name HA  )(resid 384 and name HB# ) 0.0 1.0 3.9
assign (resid 384 and name HA  )(resid 384 and name HD# ) 0.0 1.0 3.9
assign (resid 384 and name HA  )(resid 384 and name HG# ) 0.0 1.0 3.9
assign (resid 384 and name HA  )(resid 384 and name HN  ) 0.0 0.0 3.5
assign (resid 384 and name HB# )(resid 384 and name HE# ) 0.0 2.0 5.5
assign (resid 384 and name HB# )(resid 384 and name HN  ) 0.0 0.6 3.5
assign (resid 384 and name HE# )(resid 384 and name HG# ) 0.0 2.0 4.9
assign (resid 384 and name HE# )(resid 384 and name HN  ) 0.0 1.0 7.0
assign (resid 384 and name HG# )(resid 384 and name HN  ) 0.0 1.0 4.5
assign (resid 385 and name HA  )(resid 385 and name HB# ) 0.0 1.0 3.9
```


Table A.2. *(continued)*

```
assign (resid 385 and name HA  )(resid 385 and name HD2 ) 0.0 0.0 5.0
assign (resid 385 and name HB# )(resid 385 and name HD2 ) 0.0 1.0 4.5
assign (resid 386 and name HA  )(resid 386 and name HB# ) 0.0 1.0 3.9
assign (resid 386 and name HA  )(resid 386 and name HD# ) 0.0 1.7 4.2
assign (resid 386 and name HA  )(resid 386 and name HG  ) 0.0 0.0 3.5
assign (resid 386 and name HA  )(resid 386 and name HN  ) 0.0 0.0 3.5
assign (resid 386 and name HB# )(resid 386 and name HD# ) 0.0 3.4 6.3
assign (resid 386 and name HB# )(resid 386 and name HN  ) 0.0 0.6 3.5
assign (resid 386 and name HD# )(resid 386 and name HN  ) 0.0 1.7 4.6
assign (resid 387 and name HA  )(resid 387 and name HB# ) 0.0 1.0 4.5
assign (resid 387 and name HA  )(resid 387 and name HD# ) 0.0 2.0 5.5
assign (resid 387 and name HA  )(resid 387 and name HN  ) 0.0 0.0 2.9
assign (resid 387 and name HB# )(resid 387 and name HD# ) 0.0 3.0 5.9
assign (resid 387 and name HB# )(resid 387 and name HN  ) 0.0 0.6 3.5
assign (resid 387 and name HD# )(resid 387 and name HN  ) 0.0 2.0 4.9
assign (resid 388 and name HA  )(resid 388 and name HB# ) 0.0 1.0 3.9
assign (resid 388 and name HA  )(resid 388 and name HG# ) 0.0 1.0 3.9
assign (resid 388 and name HB# )(resid 388 and name HN  ) 0.0 0.6 3.5
assign (resid 388 and name HG# )(resid 388 and name HN  ) 0.0 1.0 3.9
assign (resid 389 and name HA  )(resid 389 and name HB# ) 0.0 1.0 3.9
assign (resid 389 and name HA  )(resid 389 and name HD# ) 0.0 1.0 6.0
assign (resid 389 and name HB# )(resid 389 and name HD# ) 0.0 2.0 5.5
assign (resid 390 and name HA  )(resid 390 and name HB# ) 0.0 1.0 3.9
assign (resid 390 and name HA  )(resid 390 and name HD# ) 0.0 2.0 4.9
assign (resid 390 and name HB# )(resid 390 and name HD# ) 0.0 3.0 5.9
assign (resid 390 and name HB# )(resid 390 and name HN  ) 0.0 0.6 4.1
assign (resid 390 and name HD# )(resid 390 and name HN  ) 0.0 2.0 7.0
assign (resid 391 and name HA  )(resid 391 and name HB  ) 0.0 0.0 2.9
assign (resid 391 and name HA  )(resid 391 and name HG# ) 0.0 1.7 4.2
assign (resid 391 and name HA  )(resid 391 and name HN  ) 0.0 0.0 3.5
assign (resid 391 and name HB  )(resid 391 and name HN  ) 0.0 0.0 2.9
assign (resid 391 and name HG# )(resid 391 and name HN  ) 0.0 1.7 4.6
assign (resid 392 and name HA  )(resid 392 and name HB# ) 0.0 1.0 3.9
assign (resid 392 and name HA  )(resid 392 and name HD# ) 0.0 1.0 3.9
assign (resid 392 and name HA  )(resid 392 and name HG# ) 0.0 1.0 3.9
assign (resid 392 and name HA  )(resid 392 and name HN  ) 0.0 0.0 3.5
assign (resid 392 and name HB# )(resid 392 and name HN  ) 0.0 0.6 4.1
assign (resid 392 and name HD# )(resid 392 and name HN  ) 0.0 1.0 7.0
assign (resid 394 and name HA  )(resid 394 and name HB# ) 0.0 1.0 3.9
assign (resid 394 and name HB# )(resid 394 and name HN  ) 0.0 0.6 5.6
assign (resid 395 and name HA  )(resid 395 and name HB# ) 0.0 1.0 3.5
assign (resid 396 and name HB# )(resid 396 and name HN  ) 0.0 1.1 6.1
assign (resid 397 and name HA  )(resid 397 and name HN  ) 0.0 0.0 3.5
assign (resid 399 and name HA  )(resid 399 and name HB  ) 0.0 0.0 2.9
assign (resid 399 and name HA  )(resid 399 and name HD1# ) 0.0 1.5 4.4
assign (resid 399 and name HA  )(resid 399 and name HG1# ) 0.0 1.0 3.9
assign (resid 399 and name HA  )(resid 399 and name HG2# ) 0.0 1.5 4.0
assign (resid 399 and name HA  )(resid 399 and name HN  ) 0.0 0.0 3.5
assign (resid 399 and name HB  )(resid 399 and name HD1# ) 0.0 1.5 4.0
assign (resid 399 and name HB  )(resid 399 and name HN  ) 0.0 0.0 3.5
assign (resid 399 and name HG1# )(resid 399 and name HG2# ) 0.0 2.5 5.0
assign (resid 399 and name HG1# )(resid 399 and name HN  ) 0.0 1.0 4.5
assign (resid 399 and name HG2# )(resid 399 and name HN  ) 0.0 1.5 5.0
assign (resid 400 and name HA  )(resid 400 and name HB# ) 0.0 1.0 3.5
assign (resid 408 and name HA  )(resid 408 and name HB  ) 0.0 0.0 3.5
assign (resid 408 and name HA  )(resid 408 and name HD1# ) 0.0 1.5 4.4
assign (resid 408 and name HA  )(resid 408 and name HG1# ) 0.0 1.0 4.5
assign (resid 408 and name HA  )(resid 408 and name HG2# ) 0.0 1.5 4.4
assign (resid 408 and name HB  )(resid 408 and name HD1# ) 0.0 1.5 4.4
assign (resid 408 and name HG1# )(resid 408 and name HG2# ) 0.0 2.5 5.4
```

Table A.2. *(continued)*

```
assign (resid 409 and name HA  )(resid 409 and name HG#  ) 0.0 1.7 4.6
assign (resid 410 and name HA  )(resid 410 and name HE2# ) 0.0 1.0 6.0
assign (resid 410 and name HA  )(resid 410 and name HG#  ) 0.0 1.0 3.9
assign (resid 410 and name HA  )(resid 410 and name HN   ) 0.0 0.0 3.5
assign (resid 410 and name HE2# )(resid 410 and name HG#  ) 0.0 2.0 4.9
assign (resid 410 and name HG#  )(resid 410 and name HN   ) 0.0 1.0 4.5
assign (resid 411 and name HA  )(resid 411 and name HD#  ) 0.0 1.0 3.9
assign (resid 411 and name HA  )(resid 411 and name HG#  ) 0.0 1.0 3.9
assign (resid 411 and name HA  )(resid 411 and name HN   ) 0.0 0.0 2.9
assign (resid 411 and name HD#  )(resid 411 and name HN   ) 0.0 1.0 6.0
assign (resid 411 and name HG#  )(resid 411 and name HN   ) 0.0 1.0 4.5
assign (resid 412 and name HA  )(resid 412 and name HB   ) 0.0 0.0 3.5
assign (resid 412 and name HA  )(resid 412 and name HD1# ) 0.0 1.5 5.0
assign (resid 412 and name HA  )(resid 412 and name HG2# ) 0.0 1.5 4.4
assign (resid 412 and name HA  )(resid 412 and name HN   ) 0.0 0.0 3.5
assign (resid 412 and name HB  )(resid 412 and name HD1# ) 0.0 1.5 5.0
assign (resid 412 and name HB  )(resid 412 and name HN   ) 0.0 0.0 2.9
assign (resid 412 and name HD1# )(resid 412 and name HG2# ) 0.0 3.0 5.5
assign (resid 412 and name HD1# )(resid 412 and name HN   ) 0.0 1.5 5.0
assign (resid 412 and name HG2# )(resid 412 and name HN   ) 0.0 1.5 5.0
assign (resid 413 and name HA  )(resid 413 and name HB   ) 0.0 0.0 3.5
assign (resid 413 and name HA  )(resid 413 and name HG1# ) 0.0 1.5 4.4
assign (resid 413 and name HA  )(resid 413 and name HG2# ) 0.0 1.5 4.0
assign (resid 413 and name HA  )(resid 413 and name HN   ) 0.0 0.0 5.0
assign (resid 413 and name HB  )(resid 413 and name HN   ) 0.0 0.0 5.0
assign (resid 413 and name HG1# )(resid 413 and name HN   ) 0.0 1.5 5.0
assign (resid 413 and name HG2# )(resid 413 and name HN   ) 0.0 1.5 5.0
assign (resid 414 and name HA  )(resid 414 and name HB#  ) 0.0 1.0 3.9
assign (resid 414 and name HA  )(resid 414 and name HN   ) 0.0 0.0 2.9
assign (resid 414 and name HB#  )(resid 414 and name HN   ) 0.0 0.6 3.5
assign (resid 415 and name HA  )(resid 415 and name HB#  ) 0.0 1.0 3.9
assign (resid 415 and name HA  )(resid 415 and name HD2# ) 0.0 1.0 6.0
assign (resid 415 and name HA  )(resid 415 and name HN   ) 0.0 0.0 2.9
assign (resid 415 and name HB#  )(resid 415 and name HD2# ) 0.0 2.0 5.5
assign (resid 415 and name HB#  )(resid 415 and name HN   ) 0.0 0.6 3.5
assign (resid 415 and name HD2# )(resid 415 and name HN   ) 0.0 1.0 6.0
assign (resid 416 and name HA  )(resid 416 and name HB#  ) 0.0 1.0 4.5
assign (resid 416 and name HA  )(resid 416 and name HD2  ) 0.0 0.0 3.5
assign (resid 416 and name HA  )(resid 416 and name HN   ) 0.0 0.0 2.9
assign (resid 416 and name HB#  )(resid 416 and name HN   ) 0.0 0.6 3.5
assign (resid 416 and name HD2  )(resid 416 and name HN   ) 0.0 0.0 6.0
assign (resid 417 and name HA  )(resid 417 and name HB#  ) 0.0 1.0 3.9
assign (resid 417 and name HA  )(resid 417 and name HN   ) 0.0 0.0 2.5
assign (resid 417 and name HB#  )(resid 417 and name HN   ) 0.0 0.6 4.1
assign (resid 418 and name HA#  )(resid 418 and name HN   ) 0.0 0.6 3.5
assign (resid 419 and name HA  )(resid 419 and name HB#  ) 0.0 1.0 3.9
assign (resid 419 and name HA  )(resid 419 and name HE#  ) 0.0 1.5 5.0
assign (resid 419 and name HA  )(resid 419 and name HG#  ) 0.0 1.0 3.9
assign (resid 419 and name HB#  )(resid 419 and name HE#  ) 0.0 2.5 5.4
assign (resid 419 and name HB#  )(resid 419 and name HN   ) 0.0 0.6 4.1
assign (resid 419 and name HE#  )(resid 419 and name HG#  ) 0.0 2.5 5.0
assign (resid 419 and name HG#  )(resid 419 and name HN   ) 0.0 1.0 4.5
assign (resid 420 and name HA  )(resid 420 and name HD1# ) 0.0 1.5 4.4
assign (resid 420 and name HA  )(resid 420 and name HN   ) 0.0 0.0 3.5
assign (resid 420 and name HB#  )(resid 420 and name HN   ) 0.0 0.6 3.5
assign (resid 420 and name HD#  )(resid 420 and name HN   ) 0.0 1.7 5.2
assign (resid 421 and name HA  )(resid 421 and name HN   ) 0.0 0.0 3.5
assign (resid 422 and name HA  )(resid 422 and name HB#  ) 0.0 1.0 4.5
assign (resid 422 and name HA  )(resid 422 and name HD#  ) 0.0 1.7 4.6
assign (resid 422 and name HA  )(resid 422 and name HN   ) 0.0 0.0 3.5
```


Table A.2. *(continued)*

```
assign (resid 422 and name HB#  )(resid 422 and name HD#  ) 0.0 3.4 5.9
assign (resid 422 and name HB#  )(resid 422 and name HN   ) 0.0 0.6 3.5
assign (resid 422 and name HD#  )(resid 422 and name HN   ) 0.0 1.7 4.6
assign (resid 423 and name HA#  )(resid 423 and name HN   ) 0.0 0.6 4.1
assign (resid 424 and name HA  )(resid 424 and name HB   ) 0.0 0.0 2.9
assign (resid 424 and name HA  )(resid 424 and name HG2# ) 0.0 1.5 4.0
assign (resid 424 and name HA  )(resid 424 and name HN   ) 0.0 0.0 5.0
assign (resid 424 and name HB  )(resid 424 and name HN   ) 0.0 0.0 3.5
assign (resid 424 and name HG2# )(resid 424 and name HN   ) 0.0 1.5 6.5
assign (resid 425 and name HA  )(resid 425 and name HB#  ) 0.0 1.0 4.5
assign (resid 425 and name HA  )(resid 425 and name HN   ) 0.0 0.0 5.0
assign (resid 425 and name HB#  )(resid 425 and name HN   ) 0.0 0.6 5.6
assign (resid 426 and name HA  )(resid 426 and name HB#  ) 0.0 1.0 3.9
assign (resid 426 and name HA  )(resid 426 and name HG#  ) 0.0 1.0 3.9
assign (resid 426 and name HA  )(resid 426 and name HN   ) 0.0 0.0 3.5
assign (resid 426 and name HB#  )(resid 426 and name HN   ) 0.0 0.6 4.1
assign (resid 426 and name HG#  )(resid 426 and name HN   ) 0.0 1.0 4.5
assign (resid 427 and name HA  )(resid 427 and name HB#  ) 0.0 1.0 4.5
assign (resid 427 and name HA  )(resid 427 and name HD#  ) 0.0 1.0 6.0
assign (resid 427 and name HA  )(resid 427 and name HG#  ) 0.0 1.0 4.5
assign (resid 427 and name HA  )(resid 427 and name HN   ) 0.0 0.0 3.5
assign (resid 427 and name HB#  )(resid 427 and name HN   ) 0.0 0.6 5.6
assign (resid 427 and name HG#  )(resid 427 and name HN   ) 0.0 1.0 6.0
assign (resid 428 and name HA#  )(resid 428 and name HN   ) 0.0 0.6 3.5
assign (resid 429 and name HA#  )(resid 429 and name HN   ) 0.0 0.6 4.1
assign (resid 430 and name HA  )(resid 430 and name HD#  ) 0.0 1.7 4.6
assign (resid 430 and name HD#  )(resid 430 and name HN   ) 0.0 1.7 6.7
assign (resid 431 and name HA  )(resid 431 and name HB#  ) 0.0 1.0 4.5
assign (resid 431 and name HB#  )(resid 431 and name HN   ) 0.0 0.6 5.6
assign (resid 432 and name HA  )(resid 432 and name HD1# ) 0.0 1.5 6.5
assign (resid 432 and name HA  )(resid 432 and name HN   ) 0.0 0.0 2.9
assign (resid 433 and name HA  )(resid 433 and name HN   ) 0.0 0.0 5.0
assign (resid 434 and name HA  )(resid 434 and name HN   ) 0.0 0.0 3.5
assign (resid 434 and name HB#  )(resid 434 and name HN   ) 0.0 1.1 4.0
assign (resid 435 and name HA  )(resid 435 and name HD1  ) 0.0 0.0 5.0
assign (resid 435 and name HA  )(resid 435 and name HE3  ) 0.0 0.0 3.5
assign (resid 435 and name HB#  )(resid 435 and name HD1  ) 0.0 1.0 3.9
assign (resid 435 and name HB#  )(resid 435 and name HE3  ) 0.0 1.0 6.0
assign (resid 435 and name HB#  )(resid 435 and name HN   ) 0.0 0.6 4.1
assign (resid 435 and name HD1  )(resid 435 and name HN   ) 0.0 0.0 3.5
assign (resid 435 and name HE1  )(resid 435 and name HN   ) 0.0 0.0 5.0
assign (resid 435 and name HE3  )(resid 435 and name HN   ) 0.0 0.0 6.0
assign (resid 436 and name HA  )(resid 436 and name HD1# ) 0.0 1.5 5.0
assign (resid 436 and name HA  )(resid 436 and name HD2# ) 0.0 1.5 4.4
assign (resid 436 and name HA  )(resid 436 and name HN   ) 0.0 0.0 3.5
assign (resid 436 and name HB#  )(resid 436 and name HN   ) 0.0 0.6 4.1
assign (resid 436 and name HD1# )(resid 436 and name HN   ) 0.0 1.5 5.0
assign (resid 436 and name HD2# )(resid 436 and name HN   ) 0.0 1.5 5.0
assign (resid 436 and name HG  )(resid 436 and name HN   ) 0.0 0.0 3.5
assign (resid 437 and name HA  )(resid 437 and name HB#  ) 0.0 1.0 3.9
assign (resid 437 and name HA  )(resid 437 and name HD#  ) 0.0 1.0 7.0
assign (resid 437 and name HA  )(resid 437 and name HG#  ) 0.0 1.0 4.5
assign (resid 438 and name HA  )(resid 438 and name HB   ) 0.0 0.0 2.9
assign (resid 438 and name HA  )(resid 438 and name HG#  ) 0.0 1.7 4.6
assign (resid 438 and name HB  )(resid 438 and name HN   ) 0.0 0.0 2.9
assign (resid 438 and name HG#  )(resid 438 and name HN   ) 0.0 1.7 4.6
assign (resid 439 and name HA  )(resid 439 and name HB#  ) 0.0 1.0 3.5
assign (resid 439 and name HA  )(resid 439 and name HD#  ) 0.0 1.0 4.5
assign (resid 439 and name HA  )(resid 439 and name HG#  ) 0.0 1.0 3.9
assign (resid 439 and name HB#  )(resid 439 and name HD#  ) 0.0 2.0 5.5
```

Table A.2. *(continued)*

```
assign (resid 440 and name HA  )(resid 440 and name HB  ) 0.0 0.0 2.9
assign (resid 440 and name HA  )(resid 440 and name HG# ) 0.0 1.7 4.2
assign (resid 440 and name HA  )(resid 440 and name HN  ) 0.0 0.0 2.9
assign (resid 440 and name HB  )(resid 440 and name HN  ) 0.0 0.0 2.5
assign (resid 440 and name HG# )(resid 440 and name HN  ) 0.0 1.7 4.2
assign (resid 441 and name HA  )(resid 441 and name HB  ) 0.0 0.0 2.5
assign (resid 441 and name HA  )(resid 441 and name HG2# ) 0.0 1.5 4.0
assign (resid 441 and name HA  )(resid 441 and name HN  ) 0.0 0.0 5.0
assign (resid 442 and name HA  )(resid 442 and name HB# ) 0.0 1.0 3.5
assign (resid 442 and name HA  )(resid 442 and name HD# ) 0.0 1.0 3.5
assign (resid 442 and name HA  )(resid 442 and name HG# ) 0.0 1.0 3.5
assign (resid 442 and name HB# )(resid 442 and name HD# ) 0.0 2.0 4.9
assign (resid 443 and name HB# )(resid 443 and name HN  ) 0.0 1.1 6.1
assign (resid 444 and name HA  )(resid 444 and name HB# ) 0.0 1.0 3.9
assign (resid 444 and name HA  )(resid 444 and name HG# ) 0.0 1.0 3.9
assign (resid 446 and name HA  )(resid 446 and name HB  ) 0.0 0.0 2.5
assign (resid 447 and name HA  )(resid 447 and name HB  ) 0.0 0.0 2.5
assign (resid 447 and name HA  )(resid 447 and name HG2# ) 0.0 1.5 4.0
assign (resid 292 and name HA  )(resid 293 and name HN  ) 0.0 0.0 3.5
assign (resid 293 and name HA  )(resid 294 and name HN  ) 0.0 0.0 2.9
assign (resid 293 and name HB# )(resid 294 and name HN  ) 0.0 1.0 6.0
assign (resid 294 and name HA  )(resid 295 and name HD# ) 0.0 1.0 3.9
assign (resid 294 and name HA  )(resid 295 and name HG# ) 0.0 1.0 4.5
assign (resid 294 and name HN  )(resid 295 and name HD# ) 0.0 1.0 7.0
assign (resid 295 and name HA  )(resid 296 and name HN  ) 0.0 0.0 2.5
assign (resid 296 and name HA  )(resid 297 and name HN  ) 0.0 0.0 2.9
assign (resid 296 and name HB# )(resid 297 and name HA  ) 0.0 1.0 6.0
assign (resid 296 and name HB# )(resid 297 and name HN  ) 0.0 1.0 3.9
assign (resid 296 and name HG# )(resid 297 and name HN  ) 0.0 1.0 4.5
assign (resid 296 and name HN  )(resid 297 and name HN  ) 0.0 0.0 5.0
assign (resid 297 and name HA  )(resid 298 and name HG# ) 0.0 1.0 6.0
assign (resid 297 and name HA  )(resid 298 and name HN  ) 0.0 0.0 2.9
assign (resid 297 and name HB# )(resid 298 and name HN  ) 0.0 1.0 3.5
assign (resid 297 and name HG# )(resid 298 and name HN  ) 0.0 1.0 6.0
assign (resid 297 and name HN  )(resid 298 and name HA  ) 0.0 0.0 6.0
assign (resid 297 and name HN  )(resid 298 and name HN  ) 0.0 0.0 5.0
assign (resid 298 and name HA  )(resid 299 and name HA  ) 0.0 0.0 5.0
assign (resid 298 and name HA  )(resid 299 and name HB# ) 0.0 1.5 5.0
assign (resid 298 and name HA  )(resid 299 and name HN  ) 0.0 0.0 2.5
assign (resid 298 and name HB# )(resid 299 and name HN  ) 0.0 1.0 3.9
assign (resid 298 and name HB# )(resid 299 and name HA  ) 0.0 1.5 6.5
assign (resid 298 and name HG# )(resid 299 and name HN  ) 0.0 1.0 4.5
assign (resid 298 and name HN  )(resid 299 and name HB# ) 0.0 1.5 6.5
assign (resid 298 and name HN  )(resid 299 and name HN  ) 0.0 0.0 5.0
assign (resid 299 and name HA  )(resid 300 and name HN  ) 0.0 0.0 2.5
assign (resid 299 and name HB# )(resid 300 and name HN  ) 0.0 1.5 4.0
assign (resid 299 and name HN  )(resid 300 and name HN  ) 0.0 0.0 5.0
assign (resid 300 and name HA  )(resid 301 and name HN  ) 0.0 0.0 2.9
assign (resid 300 and name HB# )(resid 301 and name HN  ) 0.0 1.0 6.0
assign (resid 300 and name HN  )(resid 301 and name HN  ) 0.0 0.0 5.0
assign (resid 301 and name HA  )(resid 302 and name HN  ) 0.0 0.0 5.0
assign (resid 301 and name HN  )(resid 302 and name HA  ) 0.0 0.0 6.0
assign (resid 301 and name HN  )(resid 302 and name HN  ) 0.0 0.0 3.5
assign (resid 302 and name HA  )(resid 303 and name HN  ) 0.0 0.0 3.5
assign (resid 302 and name HB# )(resid 303 and name HN  ) 0.0 1.0 4.5
assign (resid 302 and name HN  )(resid 303 and name HA  ) 0.0 0.0 5.0
assign (resid 302 and name HN  )(resid 303 and name HN  ) 0.0 0.0 2.9
assign (resid 303 and name HA  )(resid 304 and name HN  ) 0.0 0.0 3.5
assign (resid 303 and name HB# )(resid 304 and name HA  ) 0.0 1.5 5.0
assign (resid 303 and name HB# )(resid 304 and name HN  ) 0.0 1.5 4.4
```


Table A.2. *(continued)*

```
assign (resid 303 and name HN  )(resid 304 and name HA  ) 0.0 0.0 5.0
assign (resid 303 and name HN  )(resid 304 and name HG2# ) 0.0 1.5 5.0
assign (resid 304 and name HB  )(resid 305 and name HD2# ) 0.0 1.5 4.4
assign (resid 304 and name HB  )(resid 305 and name HN  ) 0.0 0.0 3.5
assign (resid 304 and name HG2# )(resid 305 and name HN  ) 0.0 1.5 5.0
assign (resid 304 and name HN  )(resid 305 and name HD2# ) 0.0 1.5 7.5
assign (resid 304 and name HN  )(resid 305 and name HN  ) 0.0 0.0 2.9
assign (resid 305 and name HB# )(resid 306 and name HN  ) 0.0 1.0 4.5
assign (resid 305 and name HD2# )(resid 306 and name HN  ) 0.0 1.5 6.5
assign (resid 306 and name HA# )(resid 307 and name HN  ) 0.0 1.0 3.9
assign (resid 306 and name HN  )(resid 307 and name HB# ) 0.0 1.0 6.0
assign (resid 306 and name HN  )(resid 307 and name HG# ) 0.0 1.0 7.0
assign (resid 306 and name HN  )(resid 307 and name HN  ) 0.0 0.0 2.9
assign (resid 307 and name HA  )(resid 308 and name HN  ) 0.0 0.0 3.5
assign (resid 307 and name HB# )(resid 308 and name HN  ) 0.0 1.0 3.9
assign (resid 307 and name HG# )(resid 308 and name HN  ) 0.0 1.0 6.0
assign (resid 307 and name HN  )(resid 308 and name HG1# ) 0.0 1.5 6.5
assign (resid 307 and name HN  )(resid 308 and name HG2# ) 0.0 1.5 5.0
assign (resid 307 and name HN  )(resid 308 and name HN  ) 0.0 0.0 2.9
assign (resid 308 and name HA  )(resid 309 and name HN  ) 0.0 0.0 5.0
assign (resid 308 and name HB  )(resid 309 and name HN  ) 0.0 0.0 3.5
assign (resid 308 and name HG1# )(resid 309 and name HA  ) 0.0 1.5 5.0
assign (resid 308 and name HG2# )(resid 309 and name HN  ) 0.0 1.5 5.0
assign (resid 308 and name HN  )(resid 309 and name HA  ) 0.0 0.0 5.0
assign (resid 308 and name HN  )(resid 309 and name HB  ) 0.0 0.0 5.0
assign (resid 308 and name HN  )(resid 309 and name HN  ) 0.0 0.0 2.9
assign (resid 309 and name HA  )(resid 310 and name HN  ) 0.0 0.0 3.5
assign (resid 309 and name HB  )(resid 310 and name HN  ) 0.0 0.0 2.9
assign (resid 309 and name HG2# )(resid 310 and name HA  ) 0.0 1.5 4.4
assign (resid 309 and name HG2# )(resid 310 and name HB# ) 0.0 3.0 5.9
assign (resid 309 and name HG2# )(resid 310 and name HN  ) 0.0 1.5 4.4
assign (resid 309 and name HN  )(resid 310 and name HA  ) 0.0 0.0 5.0
assign (resid 309 and name HN  )(resid 310 and name HB# ) 0.0 1.5 6.5
assign (resid 309 and name HN  )(resid 310 and name HN  ) 0.0 0.0 2.9
assign (resid 310 and name HA  )(resid 311 and name HN  ) 0.0 0.0 3.5
assign (resid 310 and name HB# )(resid 311 and name HN  ) 0.0 1.5 4.0
assign (resid 310 and name HN  )(resid 311 and name HA  ) 0.0 0.0 5.0
assign (resid 310 and name HN  )(resid 311 and name HN  ) 0.0 0.0 2.9
assign (resid 311 and name HA  )(resid 312 and name HN  ) 0.0 0.0 3.5
assign (resid 311 and name HB# )(resid 312 and name HG# ) 0.0 2.5 6.0
assign (resid 311 and name HB# )(resid 312 and name HN  ) 0.0 1.5 5.0
assign (resid 311 and name HN  )(resid 312 and name HA  ) 0.0 0.0 5.0
assign (resid 311 and name HN  )(resid 312 and name HB# ) 0.0 1.0 6.0
assign (resid 311 and name HN  )(resid 312 and name HG# ) 0.0 1.0 6.0
assign (resid 311 and name HN  )(resid 312 and name HN  ) 0.0 0.0 2.9
assign (resid 312 and name HA  )(resid 313 and name HN  ) 0.0 0.0 2.9
assign (resid 312 and name HB# )(resid 313 and name HN  ) 0.0 1.0 4.5
assign (resid 312 and name HG# )(resid 313 and name HN  ) 0.0 1.0 6.0
assign (resid 312 and name HN  )(resid 313 and name HA  ) 0.0 0.0 6.0
assign (resid 312 and name HN  )(resid 313 and name HB# ) 0.0 1.0 6.0
assign (resid 312 and name HN  )(resid 313 and name HN  ) 0.0 0.0 2.9
assign (resid 313 and name HA  )(resid 314 and name HN  ) 0.0 0.0 2.9
assign (resid 313 and name HN  )(resid 314 and name HN  ) 0.0 0.0 3.5
assign (resid 314 and name HA# )(resid 315 and name HN  ) 0.0 1.0 4.5
assign (resid 314 and name HN  )(resid 315 and name HA  ) 0.0 0.0 5.0
assign (resid 314 and name HN  )(resid 315 and name HD# ) 0.0 2.0 8.0
assign (resid 315 and name HA  )(resid 316 and name HN  ) 0.0 0.0 2.9
assign (resid 315 and name HB# )(resid 316 and name HN  ) 0.0 1.0 4.5
assign (resid 315 and name HD# )(resid 316 and name HN  ) 0.0 2.0 7.0
assign (resid 315 and name HN  )(resid 316 and name HN  ) 0.0 0.0 5.0
```

Table A.2. *(continued)*

```
assign (resid 316 and name HA   )(resid 317 and name HN   ) 0.0 0.0 2.9
assign (resid 316 and name HB#  )(resid 317 and name HN   ) 0.0 1.0 3.9
assign (resid 316 and name HN   )(resid 317 and name HB#  ) 0.0 1.0 6.0
assign (resid 316 and name HN   )(resid 317 and name HN   ) 0.0 0.0 2.9
assign (resid 317 and name HA   )(resid 318 and name HN   ) 0.0 0.0 2.9
assign (resid 317 and name HB#  )(resid 318 and name HN   ) 0.0 1.0 3.9
assign (resid 317 and name HD#  )(resid 318 and name HN   ) 0:0 1.0 6.0
assign (resid 317 and name HG#  )(resid 318 and name HN   ) 0:0 1.0 3.9
assign (resid 317 and name HN   )(resid 318 and name HN   ) 0.0 0.0 3.5
assign (resid 318 and name HA   )(resid 319 and name HN   ) 0.0 0.0 2.5
assign (resid 318 and name HB#  )(resid 319 and name HN   ) 0.0 1.0 4.5
assign (resid 318 and name HG#  )(resid 319 and name HN   ) 0.0 1.0 4.5
assign (resid 318 and name HN   )(resid 319 and name HN   ) 0.0 0.0 3.5
assign (resid 319 and name HA   )(resid 320 and name HN   ) 0.0 0.0 2.9
assign (resid 319 and name HB   )(resid 320 and name HN   ) 0.0 0.0 5.0
assign (resid 319 and name HG2# )(resid 320 and name HN   ) 0.0 1.5 4.4
assign (resid 319 and name HN   )(resid 320 and name HN   ) 0.0 0.0 5.0
assign (resid 320 and name HA   )(resid 321 and name HG2# ) 0.0 1.5 5.0
assign (resid 320 and name HA   )(resid 321 and name HN   ) 0.0 0.0 2.5
assign (resid 320 and name HB#  )(resid 321 and name HN   ) 0.0 1.0 4.5
assign (resid 320 and name HG#  )(resid 321 and name HN   ) 0.0 1.0 3.9
assign (resid 320 and name HN   )(resid 321 and name HG2# ) 0.0 1.5 7.5
assign (resid 320 and name HN   )(resid 321 and name HN   ) 0.0 0.0 5.0
assign (resid 321 and name HA   )(resid 322 and name HB#  ) 0.0 1.5 7.5
assign (resid 321 and name HA   )(resid 322 and name HN   ) 0.0 0.0 2.9
assign (resid 321 and name HB   )(resid 322 and name HN   ) 0.0 0.0 3.5
assign (resid 321 and name HG2# )(resid 322 and name HN   ) 0.0 1.5 5.0
assign (resid 321 and name HN   )(resid 322 and name HB#  ) 0.0 1.5 7.5
assign (resid 322 and name HA   )(resid 323 and name HN   ) 0.0 0.0 2.5
assign (resid 322 and name HB#  )(resid 323 and name HN   ) 0.0 1.5 4.4
assign (resid 322 and name HN   )(resid 323 and name HA   ) 0.0 0.0 5.0
assign (resid 322 and name HN   )(resid 323 and name HB#  ) 0.0 1.0 6.0
assign (resid 322 and name HN   )(resid 323 and name HD1# ) 0.0 1.5 5.0
assign (resid 322 and name HN   )(resid 323 and name HD2# ) 0.0 1.5 6.5
assign (resid 323 and name HB#  )(resid 324 and name HN   ) 0.0 1.0 6.0
assign (resid 323 and name HD1# )(resid 324 and name HN   ) 0.0 1.5 5.0
assign (resid 323 and name HD2# )(resid 324 and name HN   ) 0.0 1.5 6.5
assign (resid 323 and name HN   )(resid 324 and name HN   ) 0.0 0.0 5.0
assign (resid 324 and name HA   )(resid 325 and name HD#  ) 0.0 1.0 3.9
assign (resid 324 and name HN   )(resid 325 and name HD#  ) 0.0 1.0 6.0
assign (resid 325 and name HA   )(resid 326 and name HN   ) 0.0 0.0 2.5
assign (resid 325 and name HB#  )(resid 326 and name HN   ) 0.0 1.0 4.5
assign (resid 325 and name HD#  )(resid 326 and name HN   ) 0.0 1.0 6.0
assign (resid 325 and name HG#  )(resid 326 and name HN   ) 0.0 1.0 6.0
assign (resid 326 and name HA#  )(resid 327 and name HN   ) 0.0 1.0 3.9
assign (resid 326 and name HN   )(resid 327 and name HA   ) 0.0 0.0 5.0
assign (resid 326 and name HN   )(resid 327 and name HB#  ) 0.0 1.0 6.0
assign (resid 326 and name HN   )(resid 327 and name HN   ) 0.0 0.0 3.5
assign (resid 327 and name HA   )(resid 328 and name HD1# ) 0.0 1.5 6.5
assign (resid 327 and name HA   )(resid 328 and name HN   ) 0.0 0.0 2.9
assign (resid 327 and name HB#  )(resid 328 and name HN   ) 0.0 1.0 3.9
assign (resid 327 and name HN   )(resid 328 and name HD1# ) 0.0 1.5 7.5
assign (resid 327 and name HN   )(resid 328 and name HN   ) 0.0 0.0 3.5
assign (resid 328 and name HA   )(resid 329 and name HN   ) 0.0 0.0 2.5
assign (resid 328 and name HB   )(resid 329 and name HN   ) 0.0 0.0 5.0
assign (resid 328 and name HD1# )(resid 329 and name HN   ) 0.0 1.5 5.0
assign (resid 328 and name HG1# )(resid 329 and name HN   ) 0.0 1.0 4.5
assign (resid 328 and name HG2# )(resid 329 and name HN   ) 0.0 1.5 4.4
assign (resid 329 and name HA   )(resid 330 and name HN   ) 0.0 0.0 2.5
assign (resid 329 and name HB#  )(resid 330 and name HN   ) 0.0 1.0 3.9
```


Table A.2. *(continued)*

```
assign (resid 329 and name HG#  )(resid 330 and name HN   ) 0.0 1.0 4.5
assign (resid 329 and name HN   )(resid 330 and name HA   ) 0.0 0.0 6.0
assign (resid 329 and name HN   )(resid 330 and name HG1# ) 0.0 1.5 6.5
assign (resid 329 and name HN   )(resid 330 and name HG2# ) 0.0 1.5 6.5
assign (resid 329 and name HN   )(resid 330 and name HN   ) 0.0 0.0 3.5
assign (resid 330 and name HA   )(resid 331 and name HN   ) 0.0 0.0 2.5
assign (resid 330 and name HB   )(resid 331 and name HN   ) 0.0 0.0 2.9
assign (resid 330 and name HG1# )(resid 331 and name HN   ) 0.0 1.5 4.4
assign (resid 330 and name HG2# )(resid 331 and name HN   ) 0.0 1.5 5.0
assign (resid 330 and name HN   )(resid 331 and name HN   ) 0.0 0.0 5.0
assign (resid 331 and name HA   )(resid 332 and name HN   ) 0.0 0.0 2.9
assign (resid 331 and name HB#  )(resid 332 and name HN   ) 0.0 1.0 4.5
assign (resid 331 and name HG#  )(resid 332 and name HN   ) 0.0 1.0 4.5
assign (resid 331 and name HN   )(resid 332 and name HN   ) 0.0 0.0 5.0
assign (resid 332 and name HA   )(resid 333 and name HN   ) 0.0 0.0 3.5
assign (resid 332 and name HB#  )(resid 333 and name HN   ) 0.0 1.0 4.5
assign (resid 332 and name HN   )(resid 333 and name HN   ) 0.0 0.0 6.0
assign (resid 333 and name HA   )(resid 334 and name HD#  ) 0.0 1.0 3.9
assign (resid 333 and name HN   )(resid 334 and name HD#  ) 0.0 1.0 7.0
assign (resid 334 and name HA   )(resid 335 and name HN   ) 0.0 0.0 3.5
assign (resid 334 and name HB#  )(resid 335 and name HN   ) 0.0 1.0 4.5
assign (resid 334 and name HD#  )(resid 335 and name HN   ) 0.0 1.0 6.0
assign (resid 335 and name HA   )(resid 336 and name HN   ) 0.0 0.0 3.5
assign (resid 335 and name HB#  )(resid 336 and name HN   ) 0.0 1.0 4.5
assign (resid 335 and name HD#  )(resid 336 and name HA   ) 0.0 2.4 5.9
assign (resid 335 and name HD#  )(resid 336 and name HN   ) 0.0 2.4 5.9
assign (resid 335 and name HN   )(resid 336 and name HN   ) 0.0 0.0 3.5
assign (resid 336 and name HA   )(resid 337 and name HN   ) 0.0 0.0 5.0
assign (resid 336 and name HB#  )(resid 337 and name HN   ) 0.0 1.0 6.0
assign (resid 336 and name HN   )(resid 337 and name HA   ) 0.0 0.0 6.0
assign (resid 336 and name HN   )(resid 337 and name HD1# ) 0.0 1.5 7.5
assign (resid 336 and name HN   )(resid 337 and name HG2# ) 0.0 1.5 7.5
assign (resid 336 and name HN   )(resid 337 and name HN   ) 0.0 0.0 3.5
assign (resid 337 and name HA   )(resid 338 and name HN   ) 0.0 0.0 5.0
assign (resid 337 and name HB   )(resid 338 and name HN   ) 0.0 0.0 3.5
assign (resid 337 and name HD1# )(resid 338 and name HN   ) 0.0 1.5 6.5
assign (resid 337 and name HG2# )(resid 338 and name HA   ) 0.0 1.5 5.0
assign (resid 337 and name HG2# )(resid 338 and name HN   ) 0.0 1.5 5.0
assign (resid 337 and name HN   )(resid 338 and name HA   ) 0.0 0.0 6.0
assign (resid 337 and name HN   )(resid 338 and name HB#  ) 0.0 1.0 6.0
assign (resid 337 and name HN   )(resid 338 and name HN   ) 0.0 0.0 3.5
assign (resid 338 and name HA   )(resid 339 and name HN   ) 0.0 0.0 5.0
assign (resid 338 and name HB#  )(resid 339 and name HN   ) 0.0 1.0 4.5
assign (resid 338 and name HG#  )(resid 339 and name HN   ) 0.0 1.0 4.5
assign (resid 338 and name HN   )(resid 339 and name HN   ) 0.0 0.0 3.5
assign (resid 339 and name HD#  )(resid 340 and name HN   ) 0.0 1.0 6.0
assign (resid 339 and name HN   )(resid 340 and name HN   ) 0.0 0.0 3.5
assign (resid 340 and name HA   )(resid 341 and name HG2# ) 0.0 1.5 6.5
assign (resid 340 and name HA   )(resid 341 and name HN   ) 0.0 0.0 5.0
assign (resid 340 and name HB#  )(resid 341 and name HG2# ) 0.0 3.0 5.9
assign (resid 340 and name HB#  )(resid 341 and name HN   ) 0.0 1.5 4.4
assign (resid 340 and name HN   )(resid 341 and name HG2# ) 0.0 1.5 6.5
assign (resid 340 and name HN   )(resid 341 and name HN   ) 0.0 0.0 2.9
assign (resid 341 and name HB   )(resid 342 and name HN   ) 0.0 0.0 2.9
assign (resid 341 and name HG1# )(resid 342 and name HN   ) 0.0 1.5 5.0
assign (resid 341 and name HG2# )(resid 342 and name HN   ) 0.0 1.5 5.0
assign (resid 341 and name HN   )(resid 342 and name HB#  ) 0.0 1.5 5.0
assign (resid 341 and name HN   )(resid 342 and name HN   ) 0.0 0.0 2.9
assign (resid 342 and name HA   )(resid 343 and name HN   ) 0.0 0.0 5.0
assign (resid 342 and name HB#  )(resid 343 and name HN   ) 0.0 1.5 4.4
```

Table A.2. *(continued)*

```
assign (resid 342 and name HN  )(resid 343 and name HN  ) 0.0 0.0 3.5
assign (resid 343 and name HA  )(resid 344 and name HN  ) 0.0 0.0 5.0
assign (resid 343 and name HB#  )(resid 344 and name HN  ) 0.0 1.0 6.0
assign (resid 343 and name HN  )(resid 344 and name HN  ) 0.0 0.0 5.0
assign (resid 345 and name HA  )(resid 346 and name HN  ) 0.0 0.0 6.0
assign (resid 348 and name HA  )(resid 349 and name HN  ) 0.0 0.0 3.5
assign (resid 348 and name HB#  )(resid 349 and name HB#  ) 0.0 3.0 6.5
assign (resid 348 and name HB#  )(resid 349 and name HN  ) 0.0 1.5 4.4
assign (resid 348 and name HN  )(resid 349 and name HN  ) 0.0 0.0 3.5
assign (resid 349 and name HA  )(resid 350 and name HN  ) 0.0 0.0 5.0
assign (resid 349 and name HB#  )(resid 350 and name HN  ) 0.0 1.5 4.4
assign (resid 349 and name HN  )(resid 350 and name HN  ) 0.0 0.0 3.5
assign (resid 350 and name HA  )(resid 351 and name HN  ) 0.0 0.0 5.0
assign (resid 350 and name HN  )(resid 351 and name HN  ) 0.0 0.0 3.5
assign (resid 351 and name HN  )(resid 352 and name HN  ) 0.0 0.0 3.5
assign (resid 353 and name HA  )(resid 354 and name HN  ) 0.0 0.0 3.5
assign (resid 353 and name HB#  )(resid 354 and name HN  ) 0.0 1.0 6.0
assign (resid 354 and name HA#  )(resid 355 and name HN  ) 0.0 1.0 6.0
assign (resid 354 and name HN  )(resid 355 and name HN  ) 0.0 0.0 3.5
assign (resid 355 and name HA  )(resid 356 and name HN  ) 0.0 0.0 2.5
assign (resid 355 and name HB#  )(resid 356 and name HN  ) 0.0 1.0 4.5
assign (resid 355 and name HD1  )(resid 356 and name HN  ) 0.0 0.0 3.5
assign (resid 355 and name HE1  )(resid 356 and name HN  ) 0.0 0.0 5.0
assign (resid 355 and name HN  )(resid 356 and name HN  ) 0.0 0.0 5.0
assign (resid 356 and name HA  )(resid 357 and name HN  ) 0.0 0.0 2.9
assign (resid 356 and name HB  )(resid 357 and name HN  ) 0.0 0.0 5.0
assign (resid 356 and name HG2#  )(resid 357 and name HN  ) 0.0 1.5 4.4
assign (resid 356 and name HN  )(resid 357 and name HA  ) 0.0 0.0 6.0
assign (resid 357 and name HA  )(resid 358 and name HN  ) 0.0 0.0 3.5
assign (resid 357 and name HN  )(resid 358 and name HN  ) 0.0 0.0 6.0
assign (resid 358 and name HA  )(resid 359 and name HN  ) 0.0 0.0 2.9
assign (resid 358 and name HG1#  )(resid 359 and name HN  ) 0.0 1.5 5.0
assign (resid 358 and name HG2#  )(resid 359 and name HN  ) 0.0 1.5 6.5
assign (resid 358 and name HN  )(resid 359 and name HN  ) 0.0 0.0 6.0
assign (resid 359 and name HB#  )(resid 360 and name HN  ) 0.0 1.0 4.5
assign (resid 359 and name HN  )(resid 360 and name HN  ) 0.0 0.0 5.0
assign (resid 360 and name HA  )(resid 361 and name HN  ) 0.0 0.0 2.9
assign (resid 360 and name HN  )(resid 361 and name HN  ) 0.0 0.0 6.0
assign (resid 361 and name HA#  )(resid 362 and name HG2#  ) 0.0 2.5 7.5
assign (resid 361 and name HN  )(resid 362 and name HN  ) 0.0 0.0 5.0
assign (resid 362 and name HA  )(resid 363 and name HN  ) 0.0 0.0 2.9
assign (resid 362 and name HB  )(resid 363 and name HN  ) 0.0 0.0 3.5
assign (resid 362 and name HG2#  )(resid 363 and name HN  ) 0.0 1.5 6.5
assign (resid 362 and name HN  )(resid 363 and name HN  ) 0.0 0.0 5.0
assign (resid 363 and name HA  )(resid 364 and name HD#  ) 0.0 1.0 4.5
assign (resid 363 and name HN  )(resid 364 and name HD#  ) 0.0 1.0 7.0
assign (resid 364 and name HA  )(resid 365 and name HN  ) 0.0 0.0 2.9
assign (resid 364 and name HD#  )(resid 365 and name HN  ) 0.0 1.0 7.0
assign (resid 364 and name HG#  )(resid 365 and name HN  ) 0.0 1.0 6.0
assign (resid 365 and name HA  )(resid 366 and name HN  ) 0.0 0.0 2.9
assign (resid 365 and name HB#  )(resid 366 and name HN  ) 0.0 1.0 6.0
assign (resid 365 and name HN  )(resid 366 and name HB#  ) 0.0 1.0 6.0
assign (resid 365 and name HN  )(resid 366 and name HG#  ) 0.0 1.0 6.0
assign (resid 365 and name HN  )(resid 366 and name HN  ) 0.0 0.0 3.5
assign (resid 366 and name HA  )(resid 367 and name HB#  ) 0.0 1.5 5.0
assign (resid 366 and name HA  )(resid 367 and name HN  ) 0.0 0.0 2.9
assign (resid 366 and name HB#  )(resid 367 and name HN  ) 0.0 1.0 4.5
assign (resid 366 and name HG#  )(resid 367 and name HN  ) 0.0 1.0 6.0
assign (resid 366 and name HN  )(resid 367 and name HN  ) 0.0 0.0 5.0
assign (resid 367 and name HA  )(resid 368 and name HD1  ) 0.0 0.0 5.0
```


Table A.2. *(continued)*

```
assign (resid 367 and name HA  )(resid 368 and name HE1  ) 0.0 0.0 5.0
assign (resid 367 and name HA  )(resid 368 and name HN  ) 0.0 0.0 2.9
assign (resid 367 and name HB#  )(resid 368 and name HD1  ) 0.0 1.5 6.5
assign (resid 367 and name HB#  )(resid 368 and name HN  ) 0.0 1.5 4.4
assign (resid 367 and name HN  )(resid 368 and name HN  ) 0.0 0.0 5.0
assign (resid 368 and name HA  )(resid 369 and name HN  ) 0.0 0.0 2.9
assign (resid 368 and name HE1  )(resid 369 and name HA  ) 0.0 0.0 5.0
assign (resid 368 and name HE1  )(resid 369 and name HN  ) 0.0 0.0 5.0
assign (resid 369 and name HA  )(resid 370 and name HN  ) 0.0 0.0 3.5
assign (resid 369 and name HB#  )(resid 370 and name HN  ) 0.0 1.0 6.0
assign (resid 369 and name HD#  )(resid 370 and name HN  ) 0.0 2.0 7.0
assign (resid 369 and name HN  )(resid 370 and name HN  ) 0.0 0.0 6.0
assign (resid 370 and name HA  )(resid 371 and name HG2#  ) 0.0 1.5 6.5
assign (resid 370 and name HA  )(resid 371 and name HN  ) 0.0 0.0 3.5
assign (resid 370 and name HN  )(resid 371 and name HN  ) 0.0 0.0 5.0
assign (resid 371 and name HA  )(resid 372 and name HN  ) 0.0 0.0 3.5
assign (resid 371 and name HG1#  )(resid 372 and name HA  ) 0.0 1.5 6.5
assign (resid 371 and name HG1#  )(resid 372 and name HN  ) 0.0 1.5 5.0
assign (resid 371 and name HG2#  )(resid 372 and name HN  ) 0.0 1.5 6.5
assign (resid 372 and name HA  )(resid 373 and name HN  ) 0.0 0.0 3.5
assign (resid 372 and name HN  )(resid 373 and name HN  ) 0.0 0.0 6.0
assign (resid 373 and name HA  )(resid 374 and name HN  ) 0.0 0.0 3.5
assign (resid 373 and name HN  )(resid 374 and name HN  ) 0.0 0.0 5.0
assign (resid 374 and name HN  )(resid 375 and name HN  ) 0.0 0.0 5.0
assign (resid 377 and name HA#  )(resid 378 and name HN  ) 0.0 1.0 4.5
assign (resid 378 and name HA  )(resid 379 and name HN  ) 0.0 0.0 2.9
assign (resid 378 and name HB  )(resid 379 and name HN  ) 0.0 0.0 5.0
assign (resid 378 and name HG2#  )(resid 379 and name HN  ) 0.0 1.5 4.4
assign (resid 378 and name HN  )(resid 379 and name HN  ) 0.0 0.0 5.0
assign (resid 379 and name HA  )(resid 380 and name HD#  ) 0.0 1.0 3.9
assign (resid 379 and name HB#  )(resid 380 and name HD#  ) 0.0 2.5 5.4
assign (resid 380 and name HA  )(resid 381 and name HN  ) 0.0 0.0 5.0
assign (resid 381 and name HA  )(resid 382 and name HN  ) 0.0 0.0 3.5
assign (resid 381 and name HN  )(resid 382 and name HN  ) 0.0 0.0 5.0
assign (resid 382 and name HA  )(resid 383 and name HN  ) 0.0 0.0 5.0
assign (resid 382 and name HB#  )(resid 383 and name HN  ) 0.0 1.0 4.5
assign (resid 382 and name HG#  )(resid 383 and name HN  ) 0.0 1.0 6.0
assign (resid 382 and name HN  )(resid 383 and name HG#  ) 0.0 1.0 7.0
assign (resid 382 and name HN  )(resid 383 and name HN  ) 0.0 0.0 2.9
assign (resid 383 and name HA  )(resid 384 and name HN  ) 0.0 0.0 6.0
assign (resid 384 and name HA  )(resid 385 and name HN  ) 0.0 0.0 6.0
assign (resid 384 and name HB#  )(resid 385 and name HD2  ) 0.0 1.0 6.0
assign (resid 384 and name HG#  )(resid 385 and name HN  ) 0.0 1.0 6.0
assign (resid 385 and name HB#  )(resid 386 and name HN  ) 0.0 1.0 6.0
assign (resid 386 and name HA  )(resid 387 and name HN  ) 0.0 0.0 2.9
assign (resid 386 and name HB#  )(resid 387 and name HN  ) 0.0 1.0 4.5
assign (resid 386 and name HD#  )(resid 387 and name HN  ) 0.0 2.4 5.9
assign (resid 386 and name HN  )(resid 387 and name HN  ) 0.0 0.0 3.5
assign (resid 387 and name HA  )(resid 388 and name HN  ) 0.0 0.0 2.9
assign (resid 387 and name HB#  )(resid 388 and name HN  ) 0.0 1.0 4.5
assign (resid 387 and name HD#  )(resid 388 and name HN  ) 0.0 2.0 7.0
assign (resid 387 and name HN  )(resid 388 and name HG#  ) 0.0 1.0 6.0
assign (resid 387 and name HN  )(resid 388 and name HN  ) 0.0 0.0 2.9
assign (resid 388 and name HA  )(resid 389 and name HD#  ) 0.0 1.0 3.9
assign (resid 388 and name HA  )(resid 389 and name HG#  ) 0.0 1.0 4.5
assign (resid 388 and name HN  )(resid 389 and name HD#  ) 0.0 1.0 6.0
assign (resid 389 and name HA  )(resid 390 and name HN  ) 0.0 0.0 2.9
assign (resid 389 and name HB#  )(resid 390 and name HN  ) 0.0 1.0 6.0
assign (resid 390 and name HA  )(resid 391 and name HG#  ) 0.0 2.4 5.3
assign (resid 390 and name HA  )(resid 391 and name HN  ) 0.0 0.0 2.9
```

Table A.2. *(continued)*

```
assign (resid 390 and name HB# )(resid 391 and name HN  ) 0.0 1.0 4.5
assign (resid 390 and name HD# )(resid 391 and name HN  ) 0.0 2.0 7.0
assign (resid 390 and name HN  )(resid 391 and name HA  ) 0.0 0.0 6.0
assign (resid 390 and name HN  )(resid 391 and name HG# ) 0.0 2.4 7.4
assign (resid 390 and name HN  )(resid 391 and name HN  ) 0.0 0.0 5.0
assign (resid 391 and name HA  )(resid 392 and name HN  ) 0.0 0.0 2.9
assign (resid 391 and name HB  )(resid 392 and name HN  ) 0.0 0.0 5.0
assign (resid 391 and name HG# )(resid 392 and name HN  ) 0.0 2.4 5.3
assign (resid 391 and name HN  )(resid 392 and name HN  ) 0.0 0.0 6.0
assign (resid 396 and name HB# )(resid 397 and name HN  ) 0.0 1.5 6.5
assign (resid 399 and name HG2# )(resid 400 and name HA  ) 0.0 1.5 6.5
assign (resid 409 and name HG# )(resid 410 and name HN  ) 0.0 2.4 5.9
assign (resid 410 and name HG# )(resid 411 and name HN  ) 0.0 1.0 3.9
assign (resid 410 and name HN  )(resid 411 and name HN  ) 0.0 0.0 3.5
assign (resid 411 and name HA  )(resid 412 and name HN  ) 0.0 0.0 5.0
assign (resid 411 and name HG# )(resid 412 and name HN  ) 0.0 1.0 6.0
assign (resid 411 and name HN  )(resid 412 and name HN  ) 0.0 0.0 3.5
assign (resid 412 and name HB  )(resid 413 and name HN  ) 0.0 0.0 5.0
assign (resid 412 and name HD1# )(resid 413 and name HN  ) 0.0 1.5 6.5
assign (resid 412 and name HN  )(resid 413 and name HN  ) 0.0 0.0 5.0
assign (resid 413 and name HA  )(resid 414 and name HN  ) 0.0 0.0 5.0
assign (resid 413 and name HB  )(resid 414 and name HN  ) 0.0 0.0 2.9
assign (resid 413 and name HG1# )(resid 414 and name HN  ) 0.0 1.5 5.0
assign (resid 413 and name HG2# )(resid 414 and name HN  ) 0.0 1.5 5.0
assign (resid 413 and name HN  )(resid 414 and name HN  ) 0.0 0.0 2.9
assign (resid 414 and name HN  )(resid 415 and name HB# ) 0.0 1.0 6.0
assign (resid 414 and name HN  )(resid 415 and name HN  ) 0.0 0.0 2.9
assign (resid 415 and name HA  )(resid 416 and name HN  ) 0.0 0.0 3.5
assign (resid 415 and name HB# )(resid 416 and name HN  ) 0.0 1.0 4.5
assign (resid 415 and name HN  )(resid 416 and name HA  ) 0.0 0.0 6.0
assign (resid 415 and name HN  )(resid 416 and name HN  ) 0.0 0.0 3.5
assign (resid 416 and name HA  )(resid 417 and name HN  ) 0.0 0.0 3.5
assign (resid 416 and name HB# )(resid 417 and name HN  ) 0.0 1.0 6.0
assign (resid 416 and name HN  )(resid 417 and name HN  ) 0.0 0.0 2.9
assign (resid 417 and name HB# )(resid 418 and name HN  ) 0.0 1.0 6.0
assign (resid 417 and name HN  )(resid 418 and name HA# ) 0.0 1.0 6.0
assign (resid 417 and name HN  )(resid 418 and name HN  ) 0.0 0.0 2.9
assign (resid 418 and name HA# )(resid 419 and name HN  ) 0.0 1.0 3.9
assign (resid 419 and name HB# )(resid 420 and name HN  ) 0.0 1.0 3.9
assign (resid 419 and name HG# )(resid 420 and name HA  ) 0.0 1.0 4.5
assign (resid 419 and name HG# )(resid 420 and name HN  ) 0.0 1.0 4.5
assign (resid 419 and name HN  )(resid 420 and name HN  ) 0.0 0.0 5.0
assign (resid 420 and name HA  )(resid 421 and name HN  ) 0.0 0.0 2.9
assign (resid 420 and name HD# )(resid 421 and name HN  ) 0.0 2.4 5.9
assign (resid 420 and name HN  )(resid 421 and name HN  ) 0.0 0.0 5.0
assign (resid 421 and name HA  )(resid 422 and name HN  ) 0.0 0.0 2.5
assign (resid 421 and name HN  )(resid 422 and name HN  ) 0.0 0.0 5.0
assign (resid 422 and name HA  )(resid 423 and name HN  ) 0.0 0.0 3.5
assign (resid 422 and name HB# )(resid 423 and name HN  ) 0.0 1.0 3.9
assign (resid 422 and name HD# )(resid 423 and name HN  ) 0.0 2.4 5.3
assign (resid 423 and name HA# )(resid 424 and name HN  ) 0.0 1.0 4.5
assign (resid 423 and name HN  )(resid 424 and name HN  ) 0.0 0.0 5.0
assign (resid 424 and name HA  )(resid 425 and name HN  ) 0.0 0.0 3.5
assign (resid 424 and name HG2# )(resid 425 and name HN  ) 0.0 1.5 5.0
assign (resid 425 and name HA  )(resid 426 and name HN  ) 0.0 0.0 2.9
assign (resid 425 and name HB# )(resid 426 and name HN  ) 0.0 1.0 6.0
assign (resid 426 and name HA  )(resid 427 and name HN  ) 0.0 0.0 5.0
assign (resid 426 and name HB# )(resid 427 and name HN  ) 0.0 1.0 6.0
assign (resid 426 and name HG# )(resid 427 and name HG# ) 0.0 2.0 5.5
assign (resid 426 and name HG# )(resid 427 and name HN  ) 0.0 1.0 6.0
```


Table A.2. *(continued)*

```
assign (resid 426 and name HN  )(resid 427 and name HN  ) 0.0 0.0 5.0
assign (resid 427 and name HA  )(resid 428 and name HN  ) 0.0 0.0 3.5
assign (resid 427 and name HB# )(resid 428 and name HN  ) 0.0 1.0 6.0
assign (resid 427 and name HG# )(resid 428 and name HN  ) 0.0 1.0 6.0
assign (resid 427 and name HN  )(resid 428 and name HA# ) 0.0 1.0 6.0
assign (resid 427 and name HN  )(resid 428 and name HN  ) 0.0 0.0 3.5
assign (resid 428 and name HA# )(resid 429 and name HN  ) 0.0 1.0 4.5
assign (resid 428 and name HN  )(resid 429 and name HA# ) 0.0 1.0 7.0
assign (resid 428 and name HN  )(resid 429 and name HN  ) 0.0 0.0 3.5
assign (resid 429 and name HA# )(resid 430 and name HN  ) 0.0 1.0 6.0
assign (resid 429 and name HN  )(resid 430 and name HN  ) 0.0 0.0 6.0
assign (resid 430 and name HA  )(resid 431 and name HN  ) 0.0 0.0 3.5
assign (resid 430 and name HD# )(resid 431 and name HN  ) 0.0 2.4 5.9
assign (resid 431 and name HA  )(resid 432 and name HN  ) 0.0 0.0 3.5
assign (resid 431 and name HN  )(resid 432 and name HN  ) 0.0 0.0 6.0
assign (resid 432 and name HA  )(resid 433 and name HN  ) 0.0 0.0 2.9
assign (resid 433 and name HN  )(resid 434 and name HN  ) 0.0 0.0 5.0
assign (resid 434 and name HA  )(resid 435 and name HE1 ) 0.0 0.0 6.0
assign (resid 434 and name HA  )(resid 435 and name HN  ) 0.0 0.0 2.9
assign (resid 434 and name HB# )(resid 435 and name HN  ) 0.0 1.5 4.4
assign (resid 434 and name HN  )(resid 435 and name HN  ) 0.0 0.0 6.0
assign (resid 435 and name HA  )(resid 436 and name HD1# ) 0.0 1.5 6.5
assign (resid 435 and name HA  )(resid 436 and name HN  ) 0.0 0.0 2.9
assign (resid 435 and name HB# )(resid 436 and name HN  ) 0.0 1.0 4.5
assign (resid 435 and name HE3 )(resid 436 and name HN  ) 0.0 0.0 5.0
assign (resid 435 and name HN  )(resid 436 and name HA  ) 0.0 0.0 6.0
assign (resid 435 and name HN  )(resid 436 and name HN  ) 0.0 0.0 5.0
assign (resid 436 and name HA  )(resid 437 and name HD# ) 0.0 1.0 6.0
assign (resid 436 and name HA  )(resid 437 and name HG# ) 0.0 1.0 6.0
assign (resid 436 and name HD2# )(resid 437 and name HD# ) 0.0 2.5 5.4
assign (resid 436 and name HN  )(resid 437 and name HD# ) 0.0 1.0 6.0
assign (resid 437 and name HB# )(resid 438 and name HN  ) 0.0 1.0 3.9
assign (resid 438 and name HA  )(resid 439 and name HD# ) 0.0 1.0 3.9
assign (resid 438 and name HG# )(resid 439 and name HD# ) 0.0 3.4 6.3
assign (resid 438 and name HN  )(resid 439 and name HD# ) 0.0 1.0 6.0
assign (resid 439 and name HA  )(resid 440 and name HG# ) 0.0 2.4 5.9
assign (resid 439 and name HA  )(resid 440 and name HN  ) 0.0 0.0 2.5
assign (resid 439 and name HB# )(resid 440 and name HG# ) 0.0 3.4 8.4
assign (resid 439 and name HD# )(resid 440 and name HN  ) 0.0 1.0 6.0
assign (resid 439 and name HG# )(resid 440 and name HG# ) 0.0 3.4 6.9
assign (resid 440 and name HG# )(resid 441 and name HN  ) 0.0 2.4 5.9
assign (resid 292 and name HA  )(resid 294 and name HN  ) 0.0 0.0 5.0
assign (resid 295 and name HA  )(resid 297 and name HN  ) 0.0 0.0 5.0
assign (resid 295 and name HD# )(resid 297 and name HN  ) 0.0 1.0 7.0
assign (resid 297 and name HN  )(resid 299 and name HN  ) 0.0 0.0 6.0
assign (resid 299 and name HB# )(resid 301 and name HD2# ) 0.0 3.0 6.5
assign (resid 300 and name HA  )(resid 302 and name HN  ) 0.0 0.0 3.5
assign (resid 300 and name HA  )(resid 303 and name HB# ) 0.0 1.5 5.0
assign (resid 300 and name HA  )(resid 303 and name HN  ) 0.0 0.0 5.0
assign (resid 300 and name HB# )(resid 302 and name HN  ) 0.0 1.0 7.0
assign (resid 300 and name HB# )(resid 303 and name HN  ) 0.0 1.0 4.5
assign (resid 300 and name HB# )(resid 304 and name HN  ) 0.0 1.0 6.0
assign (resid 300 and name HN  )(resid 303 and name HB# ) 0.0 1.5 4.4
assign (resid 300 and name HN  )(resid 303 and name HN  ) 0.0 0.0 5.0
assign (resid 300 and name HN  )(resid 304 and name HG1# ) 0.0 1.5 7.5
assign (resid 300 and name HN  )(resid 304 and name HG2# ) 0.0 1.5 6.5
assign (resid 301 and name HA  )(resid 303 and name HN  ) 0.0 0.0 5.0
assign (resid 301 and name HA  )(resid 304 and name HG2# ) 0.0 1.5 4.4
assign (resid 301 and name HA  )(resid 304 and name HN  ) 0.0 0.0 5.0
assign (resid 301 and name HD2# )(resid 304 and name HB  ) 0.0 1.5 4.4
```

Table A.2. *(continued)*

```
assign (resid 301 and name HD2# )(resid 305 and name HD1# ) 0.0 3.0 6.5
assign (resid 301 and name HD2# )(resid 305 and name HG  ) 0.0 1.5 4.4
assign (resid 301 and name HN   )(resid 303 and name HN  ) 0.0 0.0 5.0
assign (resid 302 and name HA   )(resid 304 and name HN  ) 0.0 0.0 5.0
assign (resid 302 and name HA   )(resid 305 and name HD1# ) 0.0 1.5 4.4
assign (resid 302 and name HA   )(resid 305 and name HN  ) 0.0 0.0 3.5
assign (resid 302 and name HA   )(resid 306 and name HN  ) 0.0 0.0 5.0
assign (resid 303 and name HA   )(resid 305 and name HN  ) 0.0 0.0 6.0
assign (resid 303 and name HA   )(resid 306 and name HN  ) 0.0 0.0 3.5
assign (resid 303 and name HB#  )(resid 305 and name HN  ) 0.0 1.5 6.5
assign (resid 303 and name HB#  )(resid 306 and name HN  ) 0.0 1.5 6.5
assign (resid 303 and name HN   )(resid 305 and name HG  ) 0.0 0.0 5.0
assign (resid 304 and name HA   )(resid 307 and name HB# ) 0.0 1.0 4.5
assign (resid 304 and name HN   )(resid 306 and name HN  ) 0.0 0.0 5.0
assign (resid 304 and name HN   )(resid 307 and name HN  ) 0.0 0.0 6.0
assign (resid 305 and name HA   )(resid 308 and name HB  ) 0.0 0.0 5.0
assign (resid 305 and name HA   )(resid 308 and name HG1# ) 0.0 1.5 5.0
assign (resid 305 and name HD2# )(resid 308 and name HG2# ) 0.0 3.0 5.9
assign (resid 305 and name HD2# )(resid 308 and name HN  ) 0.0 1.5 7.5
assign (resid 305 and name HN   )(resid 307 and name HN  ) 0.0 0.0 6.0
assign (resid 306 and name HA#  )(resid 308 and name HN  ) 0.0 1.0 4.5
assign (resid 306 and name HA#  )(resid 309 and name HB  ) 0.0 1.0 4.5
assign (resid 306 and name HA#  )(resid 309 and name HD1# ) 0.0 2.5 6.0
assign (resid 306 and name HA#  )(resid 309 and name HN  ) 0.0 1.0 6.0
assign (resid 306 and name HA#  )(resid 310 and name HN  ) 0.0 1.0 6.0
assign (resid 306 and name HN   )(resid 308 and name HN  ) 0.0 0.0 5.0
assign (resid 306 and name HN   )(resid 309 and name HN  ) 0.0 0.0 6.0
assign (resid 307 and name HA   )(resid 310 and name HB# ) 0.0 1.5 4.4
assign (resid 307 and name HB#  )(resid 309 and name HN  ) 0.0 1.0 7.0
assign (resid 307 and name HB#  )(resid 310 and name HN  ) 0.0 1.0 7.0
assign (resid 307 and name HN   )(resid 309 and name HB  ) 0.0 0.0 5.0
assign (resid 307 and name HN   )(resid 309 and name HN  ) 0.0 0.0 5.0
assign (resid 307 and name HN   )(resid 310 and name HN  ) 0.0 0.0 5.0
assign (resid 308 and name HA   )(resid 310 and name HN  ) 0.0 0.0 5.0
assign (resid 308 and name HA   )(resid 311 and name HB# ) 0.0 1.5 4.0
assign (resid 308 and name HA   )(resid 311 and name HN  ) 0.0 0.0 3.5
assign (resid 308 and name HA   )(resid 312 and name HN  ) 0.0 0.0 5.0
assign (resid 308 and name HG1# )(resid 311 and name HB# ) 0.0 3.0 5.9
assign (resid 308 and name HG1# )(resid 311 and name HN  ) 0.0 1.5 6.5
assign (resid 308 and name HG1# )(resid 312 and name HN  ) 0.0 1.5 5.0
assign (resid 308 and name HG2# )(resid 310 and name HN  ) 0.0 1.5 6.5
assign (resid 308 and name HG2# )(resid 311 and name HB# ) 0.0 3.0 5.9
assign (resid 308 and name HG2# )(resid 311 and name HN  ) 0.0 1.5 6.5
assign (resid 308 and name HG2# )(resid 312 and name HN  ) 0.0 1.5 7.5
assign (resid 308 and name HN   )(resid 310 and name HN  ) 0.0 0.0 6.0
assign (resid 309 and name HA   )(resid 311 and name HN  ) 0.0 0.0 5.0
assign (resid 309 and name HA   )(resid 312 and name HN  ) 0.0 0.0 5.0
assign (resid 309 and name HA   )(resid 313 and name HN  ) 0.0 0.0 5.0
assign (resid 309 and name HB   )(resid 311 and name HN  ) 0.0 0.0 5.0
assign (resid 309 and name HG2# )(resid 311 and name HN  ) 0.0 1.5 5.0
assign (resid 309 and name HN   )(resid 311 and name HN  ) 0.0 0.0 5.0
assign (resid 310 and name HA   )(resid 312 and name HN  ) 0.0 0.0 5.0
assign (resid 310 and name HA   )(resid 313 and name HB# ) 0.0 1.0 4.5
assign (resid 310 and name HA   )(resid 313 and name HN  ) 0.0 0.0 5.0
assign (resid 310 and name HN   )(resid 312 and name HN  ) 0.0 0.0 5.0
assign (resid 310 and name HN   )(resid 313 and name HN  ) 0.0 0.0 6.0
assign (resid 311 and name HA   )(resid 313 and name HN  ) 0.0 0.0 5.0
assign (resid 311 and name HB#  )(resid 313 and name HN  ) 0.0 1.5 5.0
assign (resid 311 and name HB#  )(resid 314 and name HN  ) 0.0 1.5 7.5
assign (resid 311 and name HN   )(resid 313 and name HN  ) 0.0 0.0 5.0
```


Table A.2. *(continued)*

```
assign (resid 312 and name HB#  )(resid 314 and name HN  ) 0.0 1.0 7.0
assign (resid 312 and name HN   )(resid 314 and name HN  ) 0.0 0.0 6.0
assign (resid 314 and name HA#  )(resid 316 and name HN  ) 0.0 1.0 6.0
assign (resid 314 and name HA#  )(resid 317 and name HN  ) 0.0 1.0 6.0
assign (resid 314 and name HN   )(resid 316 and name HN  ) 0.0 0.0 6.0
assign (resid 314 and name HN   )(resid 317 and name HB# ) 0.0 1.0 6.0
assign (resid 314 and name HN   )(resid 317 and name HN  ) 0.0 0.0 5.0
assign (resid 315 and name HB#  )(resid 317 and name HN  ) 0.0 1.0 6.0
assign (resid 316 and name HA   )(resid 318 and name HN  ) 0.0 0.0 5.0
assign (resid 316 and name HA   )(resid 319 and name HN  ) 0.0 0.0 5.0
assign (resid 316 and name HN   )(resid 319 and name HN  ) 0.0 0.0 6.0
assign (resid 317 and name HB#  )(resid 319 and name HN  ) 0.0 1.0 6.0
assign (resid 317 and name HG#  )(resid 319 and name HD1# ) 0.0 2.5 5.4
assign (resid 319 and name HA   )(resid 321 and name HN  ) 0.0 0.0 6.0
assign (resid 319 and name HB   )(resid 321 and name HN  ) 0.0 0.0 5.0
assign (resid 319 and name HG2# )(resid 321 and name HN  ) 0.0 1.5 6.5
assign (resid 320 and name HB#  )(resid 322 and name HN  ) 0.0 1.0 7.0
assign (resid 321 and name HA   )(resid 323 and name HD1# ) 0.0 1.5 5.0
assign (resid 321 and name HA   )(resid 323 and name HN  ) 0.0 0.0 5.0
assign (resid 321 and name HB   )(resid 323 and name HD1# ) 0.0 1.5 4.4
assign (resid 321 and name HB   )(resid 323 and name HN  ) 0.0 0.0 5.0
assign (resid 321 and name HG2# )(resid 323 and name HD1# ) 0.0 3.0 5.5
assign (resid 323 and name HB#  )(resid 326 and name HN  ) 0.0 1.0 6.0
assign (resid 324 and name HB#  )(resid 326 and name HN  ) 0.0 1.0 6.0
assign (resid 324 and name HB#  )(resid 328 and name HD1# ) 0.0 2.5 6.0
assign (resid 324 and name HD#  )(resid 326 and name HN  ) 0.0 2.0 4.9
assign (resid 324 and name HD#  )(resid 327 and name HN  ) 0.0 2.0 7.0
assign (resid 324 and name HD#  )(resid 328 and name HD1# ) 0.0 3.5 6.4
assign (resid 324 and name HD#  )(resid 328 and name HN  ) 0.0 2.0 8.0
assign (resid 324 and name HE#  )(resid 326 and name HN  ) 0.0 2.0 5.5
assign (resid 324 and name HE#  )(resid 327 and name HN  ) 0.0 2.0 7.0
assign (resid 324 and name HE#  )(resid 328 and name HD1# ) 0.0 3.5 7.0
assign (resid 324 and name HN   )(resid 328 and name HD1# ) 0.0 1.5 6.5
assign (resid 325 and name HB#  )(resid 327 and name HN  ) 0.0 1.0 7.0
assign (resid 326 and name HA#  )(resid 328 and name HN  ) 0.0 1.0 7.0
assign (resid 326 and name HN   )(resid 328 and name HD1# ) 0.0 1.5 6.5
assign (resid 328 and name HB   )(resid 330 and name HN  ) 0.0 0.0 6.0
assign (resid 328 and name HG2# )(resid 330 and name HN  ) 0.0 1.5 6.5
assign (resid 330 and name HB   )(resid 332 and name HN  ) 0.0 0.0 5.0
assign (resid 330 and name HG2# )(resid 332 and name HA  ) 0.0 1.5 5.0
assign (resid 330 and name HG2# )(resid 332 and name HE# ) 0.0 3.0 5.5
assign (resid 330 and name HG2# )(resid 332 and name HN  ) 0.0 1.5 6.5
assign (resid 330 and name HG2# )(resid 333 and name HN  ) 0.0 1.5 6.5
assign (resid 332 and name HE#  )(resid 334 and name HA  ) 0.0 1.5 5.0
assign (resid 333 and name HA   )(resid 335 and name HN  ) 0.0 0.0 5.0
assign (resid 333 and name HA   )(resid 336 and name HN  ) 0.0 0.0 6.0
assign (resid 333 and name HB#  )(resid 336 and name HN  ) 0.0 1.0 6.0
assign (resid 333 and name HD2  )(resid 335 and name HG  ) 0.0 0.0 5.0
assign (resid 333 and name HE1  )(resid 335 and name HB# ) 0.0 1.0 3.9
assign (resid 333 and name HE1  )(resid 335 and name HD# ) 0.0 2.4 5.3
assign (resid 333 and name HE1  )(resid 335 and name HG  ) 0.0 0.0 3.5
assign (resid 333 and name HN   )(resid 337 and name HD1# ) 0.0 1.5 7.5
assign (resid 334 and name HA   )(resid 336 and name HN  ) 0.0 0.0 6.0
assign (resid 334 and name HA   )(resid 337 and name HB  ) 0.0 0.0 3.5
assign (resid 334 and name HA   )(resid 337 and name HG2# ) 0.0 1.5 5.0
assign (resid 334 and name HA   )(resid 337 and name HN  ) 0.0 0.0 5.0
assign (resid 335 and name HA   )(resid 337 and name HN  ) 0.0 0.0 6.0
assign (resid 335 and name HA   )(resid 338 and name HB# ) 0.0 1.0 4.5
assign (resid 335 and name HA   )(resid 338 and name HE# ) 0.0 1.0 4.5
assign (resid 335 and name HA   )(resid 338 and name HN  ) 0.0 0.0 3.5
```

Table A.2. *(continued)*

```
assign (resid 335 and name HA  )(resid 339 and name HN  ) 0.0 0.0 5.0
assign (resid 335 and name HD# )(resid 338 and name HE# ) 0.0 3.4 6.9
assign (resid 335 and name HN  )(resid 338 and name HN  ) 0.0 0.0 6.0
assign (resid 336 and name HA  )(resid 339 and name HN  ) 0.0 0.0 5.0
assign (resid 336 and name HN  )(resid 338 and name HN  ) 0.0 0.0 5.0
assign (resid 337 and name HA  )(resid 340 and name HB# ) 0.0 1.5 4.4
assign (resid 337 and name HA  )(resid 340 and name HN  ) 0.0 0.0 3.5
assign (resid 337 and name HD1# )(resid 340 and name HN  ) 0.0 1.5 6.5
assign (resid 337 and name HD1# )(resid 341 and name HN  ) 0.0 1.5 7.5
assign (resid 337 and name HG2# )(resid 340 and name HB# ) 0.0 3.0 5.9
assign (resid 337 and name HG2# )(resid 340 and name HN  ) 0.0 1.5 6.5
assign (resid 337 and name HG2# )(resid 341 and name HG2# ) 0.0 3.0 5.9
assign (resid 338 and name HA  )(resid 340 and name HN  ) 0.0 0.0 5.0
assign (resid 338 and name HA  )(resid 341 and name HG2# ) 0.0 1.5 5.0
assign (resid 338 and name HA  )(resid 341 and name HN  ) 0.0 0.0 5.0
assign (resid 338 and name HA  )(resid 342 and name HN  ) 0.0 0.0 5.0
assign (resid 339 and name HA  )(resid 342 and name HB# ) 0.0 1.5 4.4
assign (resid 339 and name HA  )(resid 342 and name HN  ) 0.0 0.0 5.0
assign (resid 339 and name HN  )(resid 341 and name HN  ) 0.0 0.0 6.0
assign (resid 339 and name HN  )(resid 342 and name HN  ) 0.0 0.0 6.0
assign (resid 340 and name HA  )(resid 343 and name HB# ) 0.0 1.0 6.0
assign (resid 340 and name HA  )(resid 343 and name HN  ) 0.0 0.0 5.0
assign (resid 340 and name HA  )(resid 344 and name HE# ) 0.0 1.5 6.5
assign (resid 340 and name HB# )(resid 344 and name HE# ) 0.0 3.0 5.9
assign (resid 340 and name HN  )(resid 342 and name HN  ) 0.0 0.0 5.0
assign (resid 341 and name HA  )(resid 344 and name HN  ) 0.0 0.0 5.0
assign (resid 341 and name HG2# )(resid 344 and name HE# ) 0.0 3.0 5.9
assign (resid 341 and name HG2# )(resid 344 and name HN  ) 0.0 1.5 7.5
assign (resid 341 and name HN  )(resid 343 and name HN  ) 0.0 0.0 6.0
assign (resid 342 and name HB# )(resid 344 and name HN  ) 0.0 1.5 6.5
assign (resid 342 and name HN  )(resid 344 and name HN  ) 0.0 0.0 6.0
assign (resid 343 and name HA  )(resid 346 and name HB  ) 0.0 0.0 3.5
assign (resid 343 and name HA  )(resid 346 and name HG# ) 0.0 2.4 5.3
assign (resid 343 and name HA  )(resid 346 and name HN  ) 0.0 0.0 6.0
assign (resid 343 and name HN  )(resid 346 and name HN  ) 0.0 0.0 6.0
assign (resid 344 and name HA  )(resid 347 and name HB# ) 0.0 1.0 4.5
assign (resid 344 and name HN  )(resid 346 and name HN  ) 0.0 0.0 5.0
assign (resid 345 and name HA  )(resid 348 and name HB# ) 0.0 1.5 5.0
assign (resid 345 and name HA  )(resid 348 and name HN  ) 0.0 0.0 6.0
assign (resid 345 and name HG# )(resid 348 and name HB# ) 0.0 3.9 6.8
assign (resid 346 and name HA  )(resid 349 and name HB# ) 0.0 1.5 4.4
assign (resid 346 and name HA  )(resid 349 and name HN  ) 0.0 0.0 3.5
assign (resid 346 and name HA  )(resid 350 and name HN  ) 0.0 0.0 5.0
assign (resid 346 and name HG# )(resid 350 and name HD# ) 0.0 3.4 6.9
assign (resid 346 and name HN  )(resid 349 and name HN  ) 0.0 0.0 6.0
assign (resid 348 and name HA  )(resid 351 and name HN  ) 0.0 0.0 5.0
assign (resid 348 and name HB# )(resid 352 and name HN  ) 0.0 1.5 5.0
assign (resid 349 and name HB# )(resid 352 and name HN  ) 0.0 1.5 7.5
assign (resid 350 and name HA  )(resid 352 and name HN  ) 0.0 0.0 6.0
assign (resid 350 and name HN  )(resid 352 and name HN  ) 0.0 0.0 6.0
assign (resid 355 and name HE1 )(resid 357 and name HA  ) 0.0 0.0 5.0
assign (resid 355 and name HE1 )(resid 358 and name HN  ) 0.0 0.0 6.0
assign (resid 363 and name HN  )(resid 365 and name HN  ) 0.0 0.0 6.0
assign (resid 363 and name HN  )(resid 366 and name HN  ) 0.0 0.0 5.0
assign (resid 363 and name HN  )(resid 367 and name HA  ) 0.0 0.0 3.5
assign (resid 363 and name HN  )(resid 367 and name HB# ) 0.0 1.5 6.5
assign (resid 363 and name HN  )(resid 367 and name HN  ) 0.0 0.0 6.0
assign (resid 364 and name HA  )(resid 366 and name HN  ) 0.0 0.0 5.0
assign (resid 368 and name HE3 )(resid 370 and name HN  ) 0.0 0.0 5.0
assign (resid 369 and name HD# )(resid 371 and name HG2# ) 0.0 3.5 7.0
```


Table A.2. *(continued)*

```
assign (resid 369 and name HE# )(resid 371 and name HG2# ) 0.0 3.5 8.5
assign (resid 369 and name HZ  )(resid 371 and name HG2# ) 0.0 1.5 7.5
assign (resid 371 and name HG1# )(resid 373 and name HN  ) 0.0 1.5 7.5
assign (resid 378 and name HG2# )(resid 382 and name HB# ) 0.0 2.5 5.4
assign (resid 378 and name HG2# )(resid 382 and name HG# ) 0.0 2.5 6.0
assign (resid 378 and name HG2# )(resid 382 and name HN  ) 0.0 1.5 6.5
assign (resid 379 and name HA  )(resid 381 and name HN  ) 0.0 0.0 6.0
assign (resid 379 and name HA  )(resid 382 and name HN  ) 0.0 0.0 6.0
assign (resid 379 and name HB# )(resid 381 and name HB# ) 0.0 2.5 5.4
assign (resid 379 and name HB# )(resid 381 and name HN  ) 0.0 1.5 5.0
assign (resid 379 and name HB# )(resid 382 and name HG# ) 0.0 2.5 5.4
assign (resid 379 and name HB# )(resid 382 and name HN  ) 0.0 1.5 5.0
assign (resid 379 and name HB# )(resid 383 and name HN  ) 0.0 1.5 6.5
assign (resid 380 and name HA  )(resid 382 and name HN  ) 0.0 0.0 6.0
assign (resid 380 and name HA  )(resid 383 and name HN  ) 0.0 0.0 5.0
assign (resid 381 and name HA  )(resid 383 and name HN  ) 0.0 0.0 5.0
assign (resid 381 and name HN  )(resid 383 and name HN  ) 0.0 0.0 6.0
assign (resid 382 and name HA  )(resid 385 and name HB# ) 0.0 1.0 4.5
assign (resid 382 and name HA  )(resid 385 and name HD2 ) 0.0 0.0 2.9
assign (resid 382 and name HA  )(resid 385 and name HE1 ) 0.0 0.0 5.0
assign (resid 383 and name HA  )(resid 386 and name HD# ) 0.0 2.4 5.9
assign (resid 383 and name HA  )(resid 386 and name HN  ) 0.0 0.0 5.0
assign (resid 385 and name HA  )(resid 388 and name HG# ) 0.0 1.0 6.0
assign (resid 386 and name HA  )(resid 388 and name HN  ) 0.0 0.0 5.0
assign (resid 408 and name HA  )(resid 411 and name HN  ) 0.0 0.0 5.0
assign (resid 409 and name HA  )(resid 411 and name HN  ) 0.0 0.0 5.0
assign (resid 409 and name HA  )(resid 412 and name HB  ) 0.0 0.0 3.5
assign (resid 409 and name HA  )(resid 412 and name HD1# ) 0.0 1.5 5.0
assign (resid 409 and name HA  )(resid 412 and name HG1# ) 0.0 1.0 4.5
assign (resid 409 and name HA  )(resid 412 and name HG2# ) 0.0 1.5 4.4
assign (resid 409 and name HA  )(resid 412 and name HN  ) 0.0 0.0 5.0
assign (resid 409 and name HG# )(resid 413 and name HG2# ) 0.0 3.9 6.4
assign (resid 410 and name HA  )(resid 413 and name HN  ) 0.0 0.0 6.0
assign (resid 410 and name HN  )(resid 412 and name HN  ) 0.0 0.0 6.0
assign (resid 411 and name HA  )(resid 414 and name HB# ) 0.0 1.0 4.5
assign (resid 411 and name HA  )(resid 414 and name HN  ) 0.0 0.0 3.5
assign (resid 411 and name HA  )(resid 415 and name HN  ) 0.0 0.0 5.0
assign (resid 411 and name HN  )(resid 415 and name HN  ) 0.0 0.0 6.0
assign (resid 412 and name HA  )(resid 415 and name HB# ) 0.0 1.0 4.5
assign (resid 412 and name HA  )(resid 415 and name HD2# ) 0.0 1.0 6.0
assign (resid 412 and name HA  )(resid 415 and name HN  ) 0.0 0.0 3.5
assign (resid 412 and name HD1# )(resid 414 and name HN  ) 0.0 1.5 6.5
assign (resid 412 and name HG2# )(resid 416 and name HE1 ) 0.0 1.5 4.4
assign (resid 412 and name HN  )(resid 414 and name HN  ) 0.0 0.0 5.0
assign (resid 413 and name HA  )(resid 415 and name HN  ) 0.0 0.0 5.0
assign (resid 413 and name HA  )(resid 416 and name HB# ) 0.0 1.0 4.5
assign (resid 413 and name HA  )(resid 416 and name HN  ) 0.0 0.0 3.5
assign (resid 413 and name HA  )(resid 417 and name HN  ) 0.0 0.0 5.0
assign (resid 413 and name HG1# )(resid 416 and name HN  ) 0.0 1.5 6.5
assign (resid 413 and name HG1# )(resid 417 and name HN  ) 0.0 1.5 7.5
assign (resid 413 and name HG2# )(resid 416 and name HB# ) 0.0 2.5 7.5
assign (resid 414 and name HN  )(resid 416 and name HN  ) 0.0 0.0 5.0
assign (resid 414 and name HN  )(resid 417 and name HN  ) 0.0 0.0 6.0
assign (resid 415 and name HN  )(resid 417 and name HN  ) 0.0 0.0 5.0
assign (resid 415 and name HN  )(resid 418 and name HN  ) 0.0 0.0 6.0
assign (resid 416 and name HN  )(resid 418 and name HN  ) 0.0 0.0 5.0
assign (resid 417 and name HN  )(resid 419 and name HN  ) 0.0 0.0 5.0
assign (resid 424 and name HG2# )(resid 428 and name HA# ) 0.0 2.5 5.4
assign (resid 424 and name HG2# )(resid 428 and name HN  ) 0.0 1.5 4.4
assign (resid 425 and name HB# )(resid 427 and name HN  ) 0.0 1.0 6.0
```

Table A.2. *(continued)*

```
assign (resid 425 and name HB# )(resid 429 and name HN  ) 0.0 1.0 6.0
assign (resid 425 and name HN  )(resid 429 and name HN  ) 0.0 0.0 5.0
assign (resid 426 and name HB# )(resid 428 and name HN  ) 0.0 1.0 7.0
assign (resid 426 and name HG# )(resid 428 and name HN  ) 0.0 1.0 6.0
assign (resid 426 and name HN  )(resid 428 and name HN  ) 0.0 0.0 5.0
assign (resid 427 and name HD# )(resid 430 and name HD# ) 0.0 3.4 6.3
assign (resid 434 and name HB# )(resid 436 and name HN  ) 0.0 1.5 7.5
assign (resid 295 and name HG# )(resid 333 and name HD2 ) 0.0 1.0 4.5
assign (resid 296 and name HA  )(resid 333 and name HA  ) 0.0 0.0 5.0
assign (resid 296 and name HE# )(resid 332 and name HA  ) 0.0 1.5 4.4
assign (resid 296 and name HE# )(resid 333 and name HN  ) 0.0 1.5 6.5
assign (resid 296 and name HE# )(resid 412 and name HA  ) 0.0 1.5 5.0
assign (resid 296 and name HE# )(resid 415 and name HB# ) 0.0 2.5 5.4
assign (resid 296 and name HE# )(resid 415 and name HD2# ) 0.0 2.5 7.5
assign (resid 296 and name HE# )(resid 416 and name HA  ) 0.0 1.5 4.0
assign (resid 296 and name HE# )(resid 416 and name HD2 ) 0.0 1.5 4.4
assign (resid 296 and name HE# )(resid 416 and name HE1 ) 0.0 1.5 5.0
assign (resid 296 and name HE# )(resid 416 and name HN  ) 0.0 1.5 6.5
assign (resid 296 and name HE# )(resid 417 and name HN  ) 0.0 1.5 7.5
assign (resid 296 and name HN  )(resid 333 and name HA  ) 0.0 0.0 6.0
assign (resid 297 and name HA  )(resid 331 and name HG# ) 0.0 1.0 6.0
assign (resid 297 and name HN  )(resid 331 and name HG# ) 0.0 1.0 4.5
assign (resid 297 and name HN  )(resid 332 and name HA  ) 0.0 0.0 6.0
assign (resid 297 and name HN  )(resid 332 and name HN  ) 0.0 0.0 3.5
assign (resid 297 and name HN  )(resid 333 and name HA  ) 0.0 0.0 5.0
assign (resid 297 and name HN  )(resid 334 and name HD# ) 0.0 1.0 6.0
assign (resid 297 and name HN  )(resid 416 and name HD2 ) 0.0 0.0 6.0
assign (resid 298 and name HA  )(resid 331 and name HA  ) 0.0 0.0 2.9
assign (resid 298 and name HA  )(resid 331 and name HD# ) 0.0 1.0 6.0
assign (resid 298 and name HA  )(resid 331 and name HG# ) 0.0 1.0 6.0
assign (resid 298 and name HA  )(resid 331 and name HN  ) 0.0 0.0 5.0
assign (resid 298 and name HA  )(resid 332 and name HN  ) 0.0 0.0 3.5
assign (resid 298 and name HE# )(resid 330 and name HA  ) 0.0 1.5 4.4
assign (resid 298 and name HE# )(resid 331 and name HD# ) 0.0 2.5 5.4
assign (resid 298 and name HE# )(resid 331 and name HE# ) 0.0 2.5 5.4
assign (resid 298 and name HE# )(resid 331 and name HG# ) 0.0 2.5 5.4
assign (resid 298 and name HG# )(resid 331 and name HG# ) 0.0 2.0 5.5
assign (resid 298 and name HN  )(resid 331 and name HD# ) 0.0 1.0 6.0
assign (resid 298 and name HN  )(resid 331 and name HG# ) 0.0 1.0 6.0
assign (resid 298 and name HN  )(resid 332 and name HN  ) 0.0 0.0 6.0
assign (resid 299 and name HB# )(resid 304 and name HG1# ) 0.0 3.0 6.5
assign (resid 299 and name HB# )(resid 304 and name HG2# ) 0.0 3.0 5.5
assign (resid 299 and name HB# )(resid 330 and name HG2# ) 0.0 3.0 5.9
assign (resid 299 and name HB# )(resid 330 and name HN  ) 0.0 1.5 6.5
assign (resid 299 and name HB# )(resid 332 and name HE# ) 0.0 3.0 5.5
assign (resid 299 and name HB# )(resid 334 and name HB# ) 0.0 2.5 7.5
assign (resid 299 and name HB# )(resid 337 and name HG2# ) 0.0 3.0 8.0
assign (resid 299 and name HN  )(resid 330 and name HA  ) 0.0 0.0 6.0
assign (resid 299 and name HN  )(resid 330 and name HG1# ) 0.0 1.5 6.5
assign (resid 299 and name HN  )(resid 330 and name HG2# ) 0.0 1.5 6.5
assign (resid 299 and name HN  )(resid 330 and name HN  ) 0.0 0.0 3.5
assign (resid 299 and name HN  )(resid 331 and name HA  ) 0.0 0.0 3.5
assign (resid 299 and name HN  )(resid 331 and name HD# ) 0.0 1.0 6.0
assign (resid 299 and name HN  )(resid 331 and name HN  ) 0.0 0.0 5.0
assign (resid 299 and name HN  )(resid 332 and name HN  ) 0.0 0.0 5.0
assign (resid 300 and name HB# )(resid 328 and name HN  ) 0.0 1.0 7.0
assign (resid 300 and name HN  )(resid 328 and name HN  ) 0.0 0.0 7.0
assign (resid 300 and name HN  )(resid 329 and name HG# ) 0.0 1.0 6.0
assign (resid 300 and name HN  )(resid 330 and name HN  ) 0.0 0.0 6.0
assign (resid 301 and name HA  )(resid 332 and name HE# ) 0.0 1.5 4.0
```


Table A.2. *(continued)*

```
assign (resid 301 and name HD1# )(resid 326 and name HD1# ) 0.0 3.0 5.9
assign (resid 301 and name HD1# )(resid 332 and name HE# ) 0.0 3.0 5.9
assign (resid 301 and name HD1# )(resid 337 and name HG2# ) 0.0 3.0 6.5
assign (resid 301 and name HD1# )(resid 367 and name HB# ) 0.0 3.0 5.9
assign (resid 301 and name HD1# )(resid 368 and name HN  ) 0.0 1.5 5.0
assign (resid 301 and name HD1# )(resid 369 and name HB# ) 0.0 2.5 7.5
assign (resid 301 and name HD1# )(resid 369 and name HD# ) 0.0 3.5 6.4
assign (resid 301 and name HD1# )(resid 369 and name HE# ) 0.0 3.5 7.0
assign (resid 301 and name HD1# )(resid 436 and name HD1# ) 0.0 3.0 5.9
assign (resid 301 and name HD2# )(resid 330 and name HG2# ) 0.0 3.0 5.9
assign (resid 301 and name HD2# )(resid 332 and name HE# ) 0.0 3.0 5.5
assign (resid 301 and name HD2# )(resid 337 and name HD1# ) 0.0 3.0 6.5
assign (resid 301 and name HD2# )(resid 337 and name HG2# ) 0.0 3.0 5.9
assign (resid 301 and name HD2# )(resid 369 and name HB# ) 0.0 2.5 7.5
assign (resid 301 and name HD2# )(resid 369 and name HD# ) 0.0 3.5 6.4
assign (resid 301 and name HD2# )(resid 369 and name HE# ) 0.0 3.5 7.0
assign (resid 301 and name HD2# )(resid 436 and name HD1# ) 0.0 3.0 5.9
assign (resid 301 and name HG  )(resid 330 and name HG2# ) 0.0 1.5 4.4
assign (resid 301 and name HN  )(resid 328 and name HB  ) 0.0 0.0 5.0
assign (resid 301 and name HN  )(resid 328 and name HD1# ) 0.0 1.5 6.5
assign (resid 301 and name HN  )(resid 328 and name HG1# ) 0.0 1.0 4.5
assign (resid 301 and name HN  )(resid 328 and name HN  ) 0.0 0.0 5.0
assign (resid 301 and name HN  )(resid 329 and name HN  ) 0.0 0.0 5.0
assign (resid 301 and name HN  )(resid 330 and name HG1# ) 0.0 1.5 6.5
assign (resid 301 and name HN  )(resid 330 and name HN  ) 0.0 0.0 5.0
assign (resid 302 and name HA  )(resid 323 and name HD1# ) 0.0 1.5 5.0
assign (resid 302 and name HA  )(resid 323 and name HD2# ) 0.0 1.5 4.4
assign (resid 302 and name HB# )(resid 323 and name HD1# ) 0.0 2.5 7.5
assign (resid 302 and name HB# )(resid 323 and name HD2# ) 0.0 2.5 6.0
assign (resid 302 and name HB# )(resid 326 and name HN  ) 0.0 1.0 6.0
assign (resid 302 and name HB# )(resid 328 and name HN  ) 0.0 1.0 6.0
assign (resid 302 and name HD2# )(resid 323 and name HB# ) 0.0 2.0 7.0
assign (resid 302 and name HD2# )(resid 323 and name HD1# ) 0.0 2.5 8.5
assign (resid 302 and name HD2# )(resid 323 and name HD2# ) 0.0 2.5 7.5
assign (resid 302 and name HD2# )(resid 324 and name HB# ) 0.0 2.0 7.0
assign (resid 302 and name HD2# )(resid 324 and name HN  ) 0.0 1.0 6.0
assign (resid 302 and name HD2# )(resid 326 and name HN  ) 0.0 1.0 4.5
assign (resid 302 and name HD2# )(resid 327 and name HA  ) 0.0 1.0 6.0
assign (resid 302 and name HD2# )(resid 327 and name HB# ) 0.0 2.0 8.0
assign (resid 302 and name HD2# )(resid 328 and name HD1# ) 0.0 2.5 7.5
assign (resid 302 and name HD2# )(resid 328 and name HG1# ) 0.0 2.0 8.0
assign (resid 302 and name HD2# )(resid 328 and name HN  ) 0.0 1.0 6.0
assign (resid 302 and name HN  )(resid 328 and name HD1# ) 0.0 1.5 6.5
assign (resid 302 and name HN  )(resid 328 and name HG1# ) 0.0 1.0 4.5
assign (resid 302 and name HN  )(resid 328 and name HN  ) 0.0 0.0 5.0
assign (resid 303 and name HN  )(resid 328 and name HD1# ) 0.0 1.5 7.5
assign (resid 303 and name HN  )(resid 328 and name HN  ) 0.0 0.0 6.0
assign (resid 304 and name HG1# )(resid 332 and name HE# ) 0.0 3.0 5.5
assign (resid 304 and name HG1# )(resid 334 and name HA  ) 0.0 1.5 5.0
assign (resid 304 and name HG1# )(resid 337 and name HB  ) 0.0 1.5 5.0
assign (resid 304 and name HG1# )(resid 337 and name HD1# ) 0.0 3.0 6.5
assign (resid 304 and name HG1# )(resid 337 and name HG2# ) 0.0 3.0 5.9
assign (resid 304 and name HG1# )(resid 337 and name HN  ) 0.0 1.5 6.5
assign (resid 304 and name HG1# )(resid 338 and name HA  ) 0.0 1.5 4.4
assign (resid 304 and name HG1# )(resid 338 and name HD# ) 0.0 2.5 5.4
assign (resid 304 and name HG1# )(resid 338 and name HE# ) 0.0 2.5 5.4
assign (resid 304 and name HG1# )(resid 338 and name HG# ) 0.0 2.5 5.4
assign (resid 304 and name HG1# )(resid 338 and name HN  ) 0.0 1.5 5.0
assign (resid 304 and name HG1# )(resid 339 and name HN  ) 0.0 1.5 7.5
assign (resid 304 and name HG2# )(resid 334 and name HA  ) 0.0 1.5 4.4
```

Table A.2. *(continued)*

```
assign (resid 304 and name HG2# )(resid 337 and name HG2# ) 0.0 3.0 5.9
assign (resid 304 and name HG2# )(resid 338 and name HE# ) 0.0 2.5 6.0
assign (resid 305 and name HA )(resid 341 and name HG2# ) 0.0 1.5 5.0
assign (resid 305 and name HD1# )(resid 323 and name HD1# ) 0.0 3.0 6.5
assign (resid 305 and name HD1# )(resid 341 and name HG2# ) 0.0 3.0 5.9
assign (resid 305 and name HD1# )(resid 358 and name HG1# ) 0.0 3.0 5.9
assign (resid 305 and name HD1# )(resid 369 and name HA ) 0.0 1.5 6.5
assign (resid 305 and name HD1# )(resid 369 and name HB# ) 0.0 2.5 7.5
assign (resid 305 and name HD1# )(resid 369 and name HD# ) 0.0 3.5 6.4
assign (resid 305 and name HD1# )(resid 369 and name HE# ) 0.0 3.5 8.5
assign (resid 305 and name HD2# )(resid 337 and name HG2# ) 0.0 3.0 5.9
assign (resid 305 and name HD2# )(resid 338 and name HA ) 0.0 1.5 6.5
assign (resid 305 and name HD2# )(resid 341 and name HG1# ) 0.0 3.0 5.9
assign (resid 305 and name HD2# )(resid 341 and name HG2# ) 0.0 3.0 5.9
assign (resid 305 and name HD2# )(resid 341 and name HN ) 0.0 1.5 6.5
assign (resid 305 and name HD2# )(resid 369 and name HB# ) 0.0 2.5 6.0
assign (resid 305 and name HD2# )(resid 369 and name HD# ) 0.0 3.5 6.4
assign (resid 305 and name HD2# )(resid 369 and name HE# ) 0.0 3.5 8.5
assign (resid 305 and name HG )(resid 341 and name HG2# ) 0.0 1.5 5.0
assign (resid 305 and name HN )(resid 323 and name HD2# ) 0.0 1.5 5.0
assign (resid 305 and name HN )(resid 337 and name HG2# ) 0.0 1.5 7.5
assign (resid 306 and name HN )(resid 323 and name HD2# ) 0.0 1.5 4.4
assign (resid 308 and name HB )(resid 341 and name HG1# ) 0.0 1.5 4.4
assign (resid 308 and name HG1# )(resid 338 and name HA ) 0.0 1.5 5.0
assign (resid 308 and name HG1# )(resid 341 and name HG2# ) 0.0 3.0 5.9
assign (resid 308 and name HG1# )(resid 341 and name HN ) 0.0 1.5 5.0
assign (resid 308 and name HG1# )(resid 342 and name HA ) 0.0 1.5 4.4
assign (resid 308 and name HG1# )(resid 342 and name HB# ) 0.0 3.0 5.5
assign (resid 308 and name HG1# )(resid 342 and name HN ) 0.0 1.5 5.0
assign (resid 308 and name HG2# )(resid 338 and name HA ) 0.0 1.5 4.4
assign (resid 308 and name HG2# )(resid 338 and name HB# ) 0.0 2.5 5.4
assign (resid 308 and name HG2# )(resid 338 and name HD# ) 0.0 2.5 5.4
assign (resid 308 and name HG2# )(resid 338 and name HE# ) 0.0 2.5 6.0
assign (resid 308 and name HG2# )(resid 338 and name HG# ) 0.0 2.5 5.4
assign (resid 308 and name HG2# )(resid 341 and name HG1# ) 0.0 3.0 5.5
assign (resid 308 and name HG2# )(resid 341 and name HG2# ) 0.0 3.0 5.9
assign (resid 308 and name HG2# )(resid 341 and name HN ) 0.0 1.5 5.0
assign (resid 308 and name HG2# )(resid 342 and name HN ) 0.0 1.5 5.0
assign (resid 309 and name HA )(resid 319 and name HG2# ) 0.0 1.5 5.0
assign (resid 309 and name HD1# )(resid 321 and name HA ) 0.0 1.5 5.0
assign (resid 309 and name HD1# )(resid 321 and name HB ) 0.0 1.5 5.0
assign (resid 309 and name HD1# )(resid 321 and name HG2# ) 0.0 3.0 5.5
assign (resid 309 and name HD1# )(resid 358 and name HG2# ) 0.0 3.0 5.9
assign (resid 309 and name HG2# )(resid 321 and name HG2# ) 0.0 3.0 5.5
assign (resid 312 and name HG# )(resid 345 and name HG# ) 0.0 3.4 6.9
assign (resid 313 and name HA )(resid 319 and name HD1# ) 0.0 1.5 4.4
assign (resid 313 and name HB# )(resid 319 and name HN ) 0.0 1.0 6.0
assign (resid 313 and name HN )(resid 319 and name HD1# ) 0.0 1.5 5.0
assign (resid 314 and name HN )(resid 319 and name HD1# ) 0.0 1.5 6.5
assign (resid 316 and name HN )(resid 356 and name HD1# ) 0.0 1.5 6.5
assign (resid 317 and name HN )(resid 356 and name HD1# ) 0.0 1.5 6.5
assign (resid 318 and name HN )(resid 355 and name HA ) 0.0 0.0 6.0
assign (resid 318 and name HN )(resid 356 and name HD1# ) 0.0 1.5 6.5
assign (resid 319 and name HA )(resid 356 and name HN ) 0.0 0.0 5.0
assign (resid 319 and name HA )(resid 357 and name HN ) 0.0 0.0 6.0
assign (resid 319 and name HG2# )(resid 357 and name HA ) 0.0 1.5 5.0
assign (resid 319 and name HG2# )(resid 358 and name HG2# ) 0.0 3.0 5.5
assign (resid 319 and name HG2# )(resid 358 and name HN ) 0.0 1.5 5.0
assign (resid 319 and name HG2# )(resid 359 and name HN ) 0.0 1.5 6.5
assign (resid 319 and name HN )(resid 356 and name HN ) 0.0 0.0 6.0
```


Table A.2. *(continued)*

```
assign (resid 320 and name HA )(resid 355 and name HE1 ) 0.0 0.0 5.0
assign (resid 320 and name HA )(resid 358 and name HN ) 0.0 0.0 5.0
assign (resid 320 and name HB# )(resid 355 and name HE1 ) 0.0 1.0 4.5
assign (resid 320 and name HB# )(resid 356 and name HN ) 0.0 1.0 6.0
assign (resid 320 and name HB# )(resid 358 and name HN ) 0.0 1.0 6.0
assign (resid 320 and name HG# )(resid 355 and name HE1 ) 0.0 1.0 4.5
assign (resid 320 and name HG# )(resid 358 and name HN ) 0.0 1.0 7.0
assign (resid 320 and name HN )(resid 355 and name HD1 ) 0.0 0.0 6.0
assign (resid 320 and name HN )(resid 355 and name HE1 ) 0.0 0.0 5.0
assign (resid 320 and name HN )(resid 356 and name HB ) 0.0 0.0 5.0
assign (resid 320 and name HN )(resid 356 and name HN ) 0.0 0.0 5.0
assign (resid 320 and name HN )(resid 357 and name HA ) 0.0 0.0 3.5
assign (resid 320 and name HN )(resid 358 and name HG2# ) 0.0 1.5 5.0
assign (resid 320 and name HN )(resid 358 and name HN ) 0.0 0.0 5.0
assign (resid 321 and name HA )(resid 358 and name HN ) 0.0 0.0 3.5
assign (resid 321 and name HB )(resid 358 and name HB ) 0.0 0.0 5.0
assign (resid 321 and name HG2# )(resid 358 and name HN ) 0.0 1.5 6.5
assign (resid 321 and name HN )(resid 358 and name HB ) 0.0 0.0 6.0
assign (resid 322 and name HB# )(resid 358 and name HN ) 0.0 1.5 6.5
assign (resid 322 and name HB# )(resid 359 and name HA ) 0.0 1.5 5.0
assign (resid 322 and name HB# )(resid 359 and name HB# ) 0.0 2.5 5.4
assign (resid 322 and name HB# )(resid 360 and name HN ) 0.0 1.5 6.5
assign (resid 322 and name HN )(resid 358 and name HB ) 0.0 0.0 5.0
assign (resid 322 and name HN )(resid 358 and name HG1# ) 0.0 1.5 6.5
assign (resid 322 and name HN )(resid 359 and name HA ) 0.0 0.0 3.5
assign (resid 322 and name HN )(resid 359 and name HB# ) 0.0 1.0 7.0
assign (resid 322 and name HN )(resid 360 and name HN ) 0.0 0.0 5.0
assign (resid 323 and name HA )(resid 360 and name HN ) 0.0 0.0 3.5
assign (resid 323 and name HB# )(resid 360 and name HN ) 0.0 1.0 4.5
assign (resid 323 and name HD1# )(resid 360 and name HN ) 0.0 1.5 4.4
assign (resid 323 and name HD1# )(resid 361 and name HN ) 0.0 1.5 6.5
assign (resid 323 and name HD1# )(resid 370 and name HN ) 0.0 1.5 6.5
assign (resid 323 and name HD2# )(resid 360 and name HN ) 0.0 1.5 6.5
assign (resid 323 and name HN )(resid 328 and name HD1# ) 0.0 1.5 7.5
assign (resid 323 and name HN )(resid 358 and name HG1# ) 0.0 1.5 7.5
assign (resid 323 and name HN )(resid 360 and name HN ) 0.0 0.0 6.0
assign (resid 324 and name HA )(resid 362 and name HG2# ) 0.0 1.5 6.5
assign (resid 324 and name HB# )(resid 362 and name HG2# ) 0.0 2.5 7.5
assign (resid 324 and name HB# )(resid 362 and name HN ) 0.0 1.0 6.0
assign (resid 324 and name HD# )(resid 361 and name HN ) 0.0 2.0 8.0
assign (resid 324 and name HD# )(resid 362 and name HG2# ) 0.0 3.5 6.4
assign (resid 324 and name HD# )(resid 362 and name HN ) 0.0 2.0 7.0
assign (resid 324 and name HD# )(resid 368 and name HE1 ) 0.0 2.0 8.0
assign (resid 324 and name HE# )(resid 362 and name HG2# ) 0.0 3.5 6.4
assign (resid 324 and name HE# )(resid 363 and name HG# ) 0.0 3.0 8.0
assign (resid 324 and name HE# )(resid 367 and name HB# ) 0.0 3.5 8.5
assign (resid 324 and name HN )(resid 359 and name HA ) 0.0 0.0 6.0
assign (resid 324 and name HN )(resid 360 and name HN ) 0.0 0.0 5.0
assign (resid 324 and name HN )(resid 361 and name HA# ) 0.0 1.0 6.0
assign (resid 324 and name HN )(resid 361 and name HN ) 0.0 0.0 6.0
assign (resid 324 and name HN )(resid 362 and name HG2# ) 0.0 1.5 5.0
assign (resid 328 and name HA )(resid 362 and name HG2# ) 0.0 1.5 5.0
assign (resid 328 and name HA )(resid 367 and name HB# ) 0.0 1.5 6.5
assign (resid 328 and name HB )(resid 367 and name HB# ) 0.0 1.5 5.0
assign (resid 328 and name HD1# )(resid 361 and name HN ) 0.0 1.5 5.0
assign (resid 328 and name HD1# )(resid 362 and name HA ) 0.0 1.5 6.5
assign (resid 328 and name HD1# )(resid 362 and name HB ) 0.0 1.5 4.4
assign (resid 328 and name HD1# )(resid 362 and name HG2# ) 0.0 3.0 5.5
assign (resid 328 and name HD1# )(resid 367 and name HB# ) 0.0 3.0 5.9
assign (resid 328 and name HG1# )(resid 362 and name HG2# ) 0.0 2.5 6.0
```

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assign (resid 328 and name HG2# )(resid 362 and name HA   ) 0.0 1.5 5.0
assign (resid 328 and name HG2# )(resid 362 and name HB   ) 0.0 1.5 4.4
assign (resid 328 and name HG2# )(resid 362 and name HG2# ) 0.0 3.0 5.5
assign (resid 328 and name HG2# )(resid 367 and name HA   ) 0.0 1.5 5.0
assign (resid 328 and name HG2# )(resid 367 and name HB#  ) 0.0 3.0 5.5
assign (resid 328 and name HG2# )(resid 368 and name HN   ) 0.0 1.5 6.5
assign (resid 329 and name HN   )(resid 362 and name HB   ) 0.0 0.0 5.0
assign (resid 329 and name HN   )(resid 367 and name HB#  ) 0.0 1.5 6.5
assign (resid 330 and name HA   )(resid 367 and name HB#  ) 0.0 1.5 6.5
assign (resid 330 and name HG1# )(resid 367 and name HB#  ) 0.0 3.0 5.5
assign (resid 330 and name HG2# )(resid 416 and name HD2  ) 0.0 1.5 6.5
assign (resid 331 and name HN   )(resid 439 and name HD#  ) 0.0 1.0 6.0
assign (resid 332 and name HA   )(resid 416 and name HD2  ) 0.0 0.0 2.9
assign (resid 332 and name HA   )(resid 436 and name HD2# ) 0.0 1.5 5.0
assign (resid 332 and name HE#  )(resid 337 and name HD1# ) 0.0 3.0 5.9
assign (resid 332 and name HE#  )(resid 337 and name HG2# ) 0.0 3.0 5.5
assign (resid 332 and name HE#  )(resid 436 and name HD1# ) 0.0 3.0 5.9
assign (resid 332 and name HN   )(resid 416 and name HD2  ) 0.0 0.0 5.0
assign (resid 333 and name HB#  )(resid 416 and name HE1  ) 0.0 1.0 6.0
assign (resid 333 and name HN   )(resid 416 and name HD2  ) 0.0 0.0 3.5
assign (resid 333 and name HN   )(resid 416 and name HE1  ) 0.0 0.0 5.0
assign (resid 336 and name HA   )(resid 412 and name HD1# ) 0.0 1.5 5.0
assign (resid 337 and name HA   )(resid 412 and name HG2# ) 0.0 1.5 4.4
assign (resid 337 and name HD1# )(resid 369 and name HD#  ) 0.0 3.5 8.5
assign (resid 337 and name HD1# )(resid 369 and name HE#  ) 0.0 3.5 7.0
assign (resid 337 and name HD1# )(resid 369 and name HZ   ) 0.0 1.5 5.0
assign (resid 337 and name HD1# )(resid 412 and name HG2# ) 0.0 3.0 5.9
assign (resid 337 and name HD1# )(resid 416 and name HD2  ) 0.0 1.5 6.5
assign (resid 337 and name HD1# )(resid 416 and name HE1  ) 0.0 1.5 5.0
assign (resid 337 and name HD1# )(resid 436 and name HD1# ) 0.0 3.0 6.5
assign (resid 337 and name HD1# )(resid 436 and name HD2# ) 0.0 3.0 6.5
assign (resid 337 and name HG2# )(resid 369 and name HE#  ) 0.0 3.5 7.0
assign (resid 337 and name HG2# )(resid 369 and name HZ   ) 0.0 1.5 5.0
assign (resid 337 and name HG2# )(resid 412 and name HG2# ) 0.0 3.0 5.9
assign (resid 337 and name HG2# )(resid 436 and name HD1# ) 0.0 3.0 6.5
assign (resid 337 and name HG2# )(resid 436 and name HD2# ) 0.0 3.0 6.5
assign (resid 339 and name HD#  )(resid 412 and name HD1# ) 0.0 2.5 5.4
assign (resid 340 and name HA   )(resid 409 and name HA   ) 0.0 0.0 5.0
assign (resid 340 and name HA   )(resid 409 and name HG#  ) 0.0 2.4 5.3
assign (resid 340 and name HA   )(resid 412 and name HD1# ) 0.0 1.5 5.0
assign (resid 340 and name HA   )(resid 412 and name HG1# ) 0.0 1.0 4.5
assign (resid 340 and name HB#  )(resid 369 and name HE#  ) 0.0 3.5 7.0
assign (resid 340 and name HB#  )(resid 369 and name HZ   ) 0.0 1.5 5.0
assign (resid 340 and name HB#  )(resid 409 and name HA   ) 0.0 1.5 4.4
assign (resid 340 and name HB#  )(resid 412 and name HD1# ) 0.0 3.0 5.9
assign (resid 340 and name HN   )(resid 412 and name HD1# ) 0.0 1.5 4.4
assign (resid 340 and name HN   )(resid 412 and name HG2# ) 0.0 1.5 5.0
assign (resid 341 and name HG1# )(resid 369 and name HD#  ) 0.0 3.5 8.5
assign (resid 341 and name HG1# )(resid 369 and name HE#  ) 0.0 3.5 8.5
assign (resid 341 and name HG1# )(resid 369 and name HZ   ) 0.0 1.5 7.5
assign (resid 341 and name HG2# )(resid 369 and name HD#  ) 0.0 3.5 6.4
assign (resid 341 and name HG2# )(resid 369 and name HE#  ) 0.0 3.5 6.4
assign (resid 341 and name HG2# )(resid 369 and name HZ   ) 0.0 1.5 5.0
assign (resid 341 and name HN   )(resid 369 and name HE#  ) 0.0 2.0 7.0
assign (resid 341 and name HN   )(resid 369 and name HZ   ) 0.0 0.0 6.0
assign (resid 344 and name HE#  )(resid 369 and name HD#  ) 0.0 3.5 6.4
assign (resid 344 and name HE#  )(resid 369 and name HE#  ) 0.0 3.5 6.4
assign (resid 344 and name HE#  )(resid 369 and name HZ   ) 0.0 1.5 4.4
assign (resid 344 and name HE#  )(resid 371 and name HG2# ) 0.0 3.0 5.5
assign (resid 344 and name HE#  )(resid 413 and name HG2# ) 0.0 3.0 5.9
```



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assign (resid 344 and name HE#  )(resid 420 and name HD1# ) 0.0 3.0 5.5
assign (resid 344 and name HE#  )(resid 432 and name HD1# ) 0.0 3.0 5.9
assign (resid 344 and name HE#  )(resid 434 and name HB#  ) 0.0 3.0 5.9
assign (resid 345 and name HA   )(resid 356 and name HG2# ) 0.0 1.5 5.0
assign (resid 348 and name HB#  )(resid 356 and name HA   ) 0.0 1.5 5.0
assign (resid 348 and name HB#  )(resid 356 and name HG2# ) 0.0 3.0 5.5
assign (resid 348 and name HB#  )(resid 373 and name HA   ) 0.0 1.5 5.0
assign (resid 348 and name HB#  )(resid 373 and name HB#  ) 0.0 2.5 6.0
assign (resid 348 and name HB#  )(resid 374 and name HN   ) 0.0 1.5 6.5
assign (resid 349 and name HA   )(resid 356 and name HD1# ) 0.0 1.5 4.4
assign (resid 349 and name HB#  )(resid 356 and name HD1# ) 0.0 3.0 5.5
assign (resid 355 and name HB#  )(resid 374 and name HN   ) 0.0 1.0 6.0
assign (resid 355 and name HE3  )(resid 373 and name HA   ) 0.0 0.0 3.5
assign (resid 355 and name HE3  )(resid 374 and name HN   ) 0.0 0.0 5.0
assign (resid 355 and name HH2  )(resid 373 and name HA   ) 0.0 0.0 5.0
assign (resid 355 and name HN   )(resid 374 and name HN   ) 0.0 0.0 6.0
assign (resid 355 and name HZ3  )(resid 373 and name HA   ) 0.0 0.0 5.0
assign (resid 356 and name HA   )(resid 372 and name HN   ) 0.0 0.0 5.0
assign (resid 356 and name HA   )(resid 373 and name HA   ) 0.0 0.0 3.5
assign (resid 356 and name HA   )(resid 374 and name HN   ) 0.0 0.0 5.0
assign (resid 356 and name HG2# )(resid 372 and name HN   ) 0.0 1.5 6.5
assign (resid 356 and name HG2# )(resid 373 and name HA   ) 0.0 1.5 6.5
assign (resid 356 and name HG2# )(resid 374 and name HN   ) 0.0 1.5 6.5
assign (resid 356 and name HN   )(resid 373 and name HA   ) 0.0 0.0 6.0
assign (resid 357 and name HN   )(resid 371 and name HA   ) 0.0 0.0 5.0
assign (resid 357 and name HN   )(resid 372 and name HN   ) 0.0 0.0 5.0
assign (resid 357 and name HN   )(resid 373 and name HA   ) 0.0 0.0 5.0
assign (resid 358 and name HA   )(resid 371 and name HA   ) 0.0 0.0 3.5
assign (resid 358 and name HA   )(resid 372 and name HN   ) 0.0 0.0 5.0
assign (resid 359 and name HB#  )(resid 370 and name HN   ) 0.0 1.0 7.0
assign (resid 359 and name HN   )(resid 368 and name HZ3  ) 0.0 0.0 6.0
assign (resid 359 and name HN   )(resid 369 and name HD#  ) 0.0 2.0 8.0
assign (resid 359 and name HN   )(resid 371 and name HA   ) 0.0 0.0 5.0
assign (resid 359 and name HN   )(resid 371 and name HG1# ) 0.0 1.5 6.5
assign (resid 359 and name HN   )(resid 371 and name HG2# ) 0.0 1.5 6.5
assign (resid 360 and name HA   )(resid 369 and name HA   ) 0.0 0.0 2.9
assign (resid 360 and name HA   )(resid 369 and name HN   ) 0.0 0.0 6.0
assign (resid 360 and name HA   )(resid 370 and name HN   ) 0.0 0.0 5.0
assign (resid 361 and name HN   )(resid 367 and name HA   ) 0.0 0.0 6.0
assign (resid 361 and name HN   )(resid 367 and name HB#  ) 0.0 1.5 6.5
assign (resid 361 and name HN   )(resid 368 and name HN   ) 0.0 0.0 3.5
assign (resid 361 and name HN   )(resid 368 and name HZ2  ) 0.0 0.0 6.0
assign (resid 361 and name HN   )(resid 369 and name HA   ) 0.0 0.0 5.0
assign (resid 361 and name HN   )(resid 369 and name HB#  ) 0.0 1.0 6.0
assign (resid 361 and name HN   )(resid 370 and name HN   ) 0.0 0.0 5.0
assign (resid 362 and name HA   )(resid 367 and name HA   ) 0.0 0.0 2.9
assign (resid 362 and name HA   )(resid 367 and name HB#  ) 0.0 1.5 4.4
assign (resid 362 and name HA   )(resid 368 and name HD1  ) 0.0 0.0 3.5
assign (resid 362 and name HA   )(resid 368 and name HE1  ) 0.0 0.0 5.0
assign (resid 362 and name HA   )(resid 368 and name HN   ) 0.0 0.0 3.5
assign (resid 362 and name HB   )(resid 367 and name HA   ) 0.0 0.0 3.5
assign (resid 362 and name HB   )(resid 367 and name HB#  ) 0.0 1.5 4.4
assign (resid 362 and name HB   )(resid 367 and name HN   ) 0.0 0.0 6.0
assign (resid 362 and name HB   )(resid 368 and name HE1  ) 0.0 0.0 6.0
assign (resid 362 and name HB   )(resid 368 and name HN   ) 0.0 0.0 5.0
assign (resid 362 and name HG2# )(resid 367 and name HA   ) 0.0 1.5 5.0
assign (resid 362 and name HG2# )(resid 367 and name HB#  ) 0.0 3.0 5.9
assign (resid 362 and name HG2# )(resid 368 and name HE1  ) 0.0 1.5 6.5
assign (resid 362 and name HN   )(resid 367 and name HA   ) 0.0 0.0 5.0
assign (resid 362 and name HN   )(resid 367 and name HB#  ) 0.0 1.5 7.5
```

Table A.2. *(continued)*

```
assign (resid 362 and name HN   )(resid 368 and name HE1  ) 0.0 0.0 3.5
assign (resid 362 and name HN   )(resid 368 and name HN   ) 0.0 0.0 5.0
assign (resid 363 and name HG#  )(resid 368 and name HD1  ) 0.0 1.0 6.0
assign (resid 363 and name HG#  )(resid 368 and name HE1  ) 0.0 1.0 4.5
assign (resid 363 and name HG#  )(resid 368 and name HZ2  ) 0.0 1.0 6.0
assign (resid 363 and name HN   )(resid 368 and name HE1  ) 0.0 0.0 6.0
assign (resid 363 and name HN   )(resid 368 and name HN   ) 0.0 0.0 5.0
assign (resid 365 and name HA   )(resid 438 and name HG#  ) 0.0 2.4 5.3
assign (resid 365 and name HB#  )(resid 438 and name HG#  ) 0.0 3.4 6.9
assign (resid 365 and name HD2# )(resid 438 and name HG#  ) 0.0 3.4 9.4
assign (resid 365 and name HN   )(resid 438 and name HB   ) 0.0 0.0 5.0
assign (resid 365 and name HN   )(resid 438 and name HG#  ) 0.0 2.4 7.4
assign (resid 366 and name HA   )(resid 436 and name HN   ) 0.0 0.0 5.0
assign (resid 366 and name HA   )(resid 437 and name HA   ) 0.0 0.0 3.5
assign (resid 366 and name HA   )(resid 438 and name HG#  ) 0.0 2.4 5.3
assign (resid 366 and name HA   )(resid 438 and name HN   ) 0.0 0.0 2.9
assign (resid 366 and name HB#  )(resid 436 and name HN   ) 0.0 1.0 6.0
assign (resid 366 and name HB#  )(resid 438 and name HN   ) 0.0 1.0 6.0
assign (resid 366 and name HN   )(resid 438 and name HG#  ) 0.0 2.4 5.9
assign (resid 366 and name HN   )(resid 438 and name HN   ) 0.0 0.0 5.0
assign (resid 367 and name HA   )(resid 438 and name HG#  ) 0.0 2.4 7.4
assign (resid 367 and name HB#  )(resid 436 and name HD1# ) 0.0 3.0 6.5
assign (resid 367 and name HB#  )(resid 436 and name HN   ) 0.0 1.5 6.5
assign (resid 367 and name HB#  )(resid 438 and name HG#  ) 0.0 3.9 6.4
assign (resid 367 and name HB#  )(resid 438 and name HN   ) 0.0 1.5 6.5
assign (resid 367 and name HN   )(resid 437 and name HA   ) 0.0 0.0 3.5
assign (resid 367 and name HN   )(resid 438 and name HG#  ) 0.0 2.4 5.9
assign (resid 367 and name HN   )(resid 438 and name HN   ) 0.0 0.0 3.5
assign (resid 368 and name HA   )(resid 435 and name HA   ) 0.0 0.0 3.5
assign (resid 368 and name HA   )(resid 436 and name HN   ) 0.0 0.0 3.5
assign (resid 368 and name HD1  )(resid 435 and name HE3  ) 0.0 0.0 3.5
assign (resid 368 and name HD1  )(resid 435 and name HH2  ) 0.0 0.0 3.5
assign (resid 368 and name HD1  )(resid 435 and name HZ2  ) 0.0 0.0 5.0
assign (resid 368 and name HD1  )(resid 435 and name HZ3  ) 0.0 0.0 2.9
assign (resid 368 and name HE1  )(resid 435 and name HE3  ) 0.0 0.0 6.0
assign (resid 368 and name HE1  )(resid 435 and name HZ3  ) 0.0 0.0 3.5
assign (resid 368 and name HE3  )(resid 434 and name HN   ) 0.0 0.0 6.0
assign (resid 368 and name HZ3  )(resid 434 and name HN   ) 0.0 0.0 6.0
assign (resid 369 and name HD#  )(resid 434 and name HB#  ) 0.0 3.5 7.0
assign (resid 369 and name HD#  )(resid 436 and name HD1# ) 0.0 3.5 7.0
assign (resid 369 and name HD#  )(resid 436 and name HD2# ) 0.0 3.5 8.5
assign (resid 369 and name HE#  )(resid 413 and name HG2# ) 0.0 3.5 8.5
assign (resid 369 and name HE#  )(resid 434 and name HB#  ) 0.0 3.5 6.4
assign (resid 369 and name HE#  )(resid 436 and name HD1# ) 0.0 3.5 7.0
assign (resid 369 and name HE#  )(resid 436 and name HD2# ) 0.0 3.5 8.5
assign (resid 369 and name HN   )(resid 434 and name HA   ) 0.0 0.0 6.0
assign (resid 369 and name HN   )(resid 434 and name HB#  ) 0.0 1.5 6.5
assign (resid 369 and name HN   )(resid 434 and name HN   ) 0.0 0.0 5.0
assign (resid 369 and name HN   )(resid 435 and name HA   ) 0.0 0.0 3.5
assign (resid 369 and name HN   )(resid 436 and name HD1# ) 0.0 1.5 6.5
assign (resid 369 and name HN   )(resid 436 and name HN   ) 0.0 0.0 5.0
assign (resid 369 and name HZ   )(resid 434 and name HB#  ) 0.0 1.5 5.0
assign (resid 369 and name HZ   )(resid 436 and name HD1# ) 0.0 1.5 6.5
assign (resid 370 and name HA   )(resid 434 and name HN   ) 0.0 0.0 5.0
assign (resid 370 and name HN   )(resid 434 and name HB#  ) 0.0 1.5 6.5
assign (resid 371 and name HB   )(resid 432 and name HN   ) 0.0 0.0 5.0
assign (resid 371 and name HG1# )(resid 432 and name HN   ) 0.0 1.5 6.5
assign (resid 371 and name HN   )(resid 433 and name HA   ) 0.0 0.0 5.0
assign (resid 371 and name HN   )(resid 434 and name HN   ) 0.0 0.0 6.0
assign (resid 372 and name HA   )(resid 431 and name HA   ) 0.0 0.0 2.9
```


Table A.2. *(continued)*

```
assign (resid 372 and name HA   )(resid 432 and name HN   ) 0.0 0.0 5.0
assign (resid 373 and name HN   )(resid 431 and name HA   ) 0.0 0.0 5.0
assign (resid 373 and name HN   )(resid 431 and name HB#  ) 0.0 1.0 7.0
assign (resid 375 and name HN   )(resid 429 and name HA#  ) 0.0 1.0 7.0
assign (resid 375 and name HN   )(resid 430 and name HN   ) 0.0 0.0 6.0
assign (resid 377 and name HA#  )(resid 430 and name HN   ) 0.0 1.0 7.0
assign (resid 378 and name HD1# )(resid 386 and name HD#  ) 0.0 3.9 7.4
assign (resid 378 and name HD1# )(resid 422 and name HD#  ) 0.0 3.9 6.8
assign (resid 378 and name HD1# )(resid 430 and name HD#  ) 0.0 3.9 6.8
assign (resid 378 and name HD1# )(resid 432 and name HD1# ) 0.0 3.0 8.0
assign (resid 378 and name HG2# )(resid 383 and name HA   ) 0.0 1.5 4.4
assign (resid 378 and name HG2# )(resid 383 and name HD#  ) 0.0 2.5 7.5
assign (resid 378 and name HG2# )(resid 383 and name HG#  ) 0.0 2.5 5.4
assign (resid 378 and name HG2# )(resid 383 and name HN   ) 0.0 1.5 5.0
assign (resid 378 and name HN   )(resid 430 and name HD#  ) 0.0 2.4 7.4
assign (resid 387 and name HD#  )(resid 420 and name HD2# ) 0.0 3.5 7.0
assign (resid 387 and name HD#  )(resid 422 and name HD#  ) 0.0 4.4 7.3
assign (resid 387 and name HE#  )(resid 409 and name HG#  ) 0.0 4.4 9.4
assign (resid 387 and name HE#  )(resid 420 and name HD2# ) 0.0 3.5 7.0
assign (resid 387 and name HE#  )(resid 422 and name HD#  ) 0.0 4.4 7.3
assign (resid 387 and name HE#  )(resid 432 and name HD1# ) 0.0 3.5 8.5
assign (resid 387 and name HZ   )(resid 409 and name HG#  ) 0.0 2.4 7.4
assign (resid 387 and name HZ   )(resid 420 and name HD2# ) 0.0 1.5 5.0
assign (resid 387 and name HZ   )(resid 422 and name HD#  ) 0.0 2.4 5.3
assign (resid 387 and name HZ   )(resid 432 and name HD1# ) 0.0 1.5 6.5
assign (resid 410 and name HA   )(resid 420 and name HD2# ) 0.0 1.5 4.4
assign (resid 410 and name HG#  )(resid 420 and name HD2# ) 0.0 2.5 5.4
assign (resid 411 and name HA   )(resid 416 and name HN   ) 0.0 0.0 6.0
assign (resid 413 and name HA   )(resid 418 and name HN   ) 0.0 0.0 5.0
assign (resid 413 and name HA   )(resid 436 and name HD2# ) 0.0 1.5 5.0
assign (resid 413 and name HG1# )(resid 418 and name HA#  ) 0.0 2.5 5.4
assign (resid 413 and name HG1# )(resid 418 and name HN   ) 0.0 1.5 5.0
assign (resid 413 and name HG1# )(resid 419 and name HN   ) 0.0 1.5 4.4
assign (resid 413 and name HG1# )(resid 420 and name HA   ) 0.0 1.5 5.0
assign (resid 413 and name HG1# )(resid 434 and name HB#  ) 0.0 3.0 6.5
assign (resid 413 and name HG1# )(resid 435 and name HN   ) 0.0 1.5 6.5
assign (resid 413 and name HG2# )(resid 420 and name HD2# ) 0.0 3.0 5.5
assign (resid 413 and name HG2# )(resid 434 and name HB#  ) 0.0 3.0 5.9
assign (resid 416 and name HA   )(resid 436 and name HD2# ) 0.0 1.5 5.0
assign (resid 416 and name HB#  )(resid 436 and name HD1# ) 0.0 2.5 7.5
assign (resid 416 and name HB#  )(resid 436 and name HD2# ) 0.0 2.5 5.4
assign (resid 416 and name HD2  )(resid 436 and name HD1# ) 0.0 1.5 6.5
assign (resid 416 and name HD2  )(resid 436 and name HD2# ) 0.0 1.5 5.0
assign (resid 417 and name HB#  )(resid 437 and name HB#  ) 0.0 2.0 8.0
assign (resid 417 and name HB#  )(resid 437 and name HG#  ) 0.0 2.0 5.5
assign (resid 417 and name HN   )(resid 436 and name HD2# ) 0.0 1.5 6.5
assign (resid 418 and name HA#  )(resid 436 and name HD2# ) 0.0 2.5 6.0
assign (resid 418 and name HA#  )(resid 436 and name HN   ) 0.0 1.0 7.0
assign (resid 418 and name HN   )(resid 436 and name HA   ) 0.0 0.0 5.0
assign (resid 418 and name HN   )(resid 436 and name HD2# ) 0.0 1.5 6.5
assign (resid 418 and name HN   )(resid 437 and name HD#  ) 0.0 1.0 6.0
assign (resid 419 and name HB#  )(resid 435 and name HD1  ) 0.0 1.0 4.5
assign (resid 419 and name HB#  )(resid 435 and name HE1  ) 0.0 1.0 4.5
assign (resid 419 and name HB#  )(resid 435 and name HN   ) 0.0 1.0 6.0
assign (resid 419 and name HE#  )(resid 435 and name HD1  ) 0.0 1.5 4.4
assign (resid 419 and name HE#  )(resid 435 and name HE1  ) 0.0 1.5 5.0
assign (resid 419 and name HG#  )(resid 435 and name HD1  ) 0.0 1.0 3.9
assign (resid 419 and name HG#  )(resid 435 and name HE1  ) 0.0 1.0 6.0
assign (resid 419 and name HG#  )(resid 435 and name HN   ) 0.0 1.0 6.0
assign (resid 419 and name HN   )(resid 434 and name HB#  ) 0.0 1.5 6.5
```

Table A.2. *(continued)*

```
assign (resid 419 and name HN  )(resid 435 and name HD1 ) 0.0 0.0 5.0
assign (resid 419 and name HN  )(resid 435 and name HN  ) 0.0 0.0 3.5
assign (resid 419 and name HN  )(resid 436 and name HD2# ) 0.0 1.5 6.5
assign (resid 419 and name HN  )(resid 436 and name HN  ) 0.0 0.0 5.0
assign (resid 419 and name HN  )(resid 437 and name HD# ) 0.0 1.0 6.0
assign (resid 420 and name HA  )(resid 433 and name HN  ) 0.0 0.0 5.0
assign (resid 420 and name HA  )(resid 434 and name HA  ) 0.0 0.0 2.9
assign (resid 420 and name HA  )(resid 434 and name HB# ) 0.0 1.5 5.0
assign (resid 420 and name HA  )(resid 434 and name HN  ) 0.0 0.0 5.0
assign (resid 420 and name HA  )(resid 435 and name HE1 ) 0.0 0.0 6.0
assign (resid 420 and name HA  )(resid 435 and name HN  ) 0.0 0.0 3.5
assign (resid 420 and name HD1# )(resid 434 and name HA  ) 0.0 1.5 4.4
assign (resid 420 and name HD1# )(resid 434 and name HB# ) 0.0 3.0 5.9
assign (resid 420 and name HN  )(resid 434 and name HB# ) 0.0 1.5 7.5
assign (resid 420 and name HN  )(resid 435 and name HB# ) 0.0 1.0 7.0
assign (resid 420 and name HN  )(resid 435 and name HD1 ) 0.0 0.0 6.0
assign (resid 421 and name HN  )(resid 433 and name HN  ) 0.0 0.0 5.0
assign (resid 421 and name HN  )(resid 434 and name HA  ) 0.0 0.0 3.5
assign (resid 421 and name HN  )(resid 434 and name HB# ) 0.0 1.5 6.5
assign (resid 421 and name HN  )(resid 435 and name HD1 ) 0.0 0.0 5.0
assign (resid 421 and name HN  )(resid 435 and name HE1 ) 0.0 0.0 5.0
assign (resid 421 and name HN  )(resid 435 and name HN  ) 0.0 0.0 5.0
assign (resid 422 and name HA  )(resid 430 and name HD# ) 0.0 2.4 5.9
assign (resid 422 and name HA  )(resid 432 and name HA  ) 0.0 0.0 5.0
assign (resid 422 and name HA  )(resid 432 and name HD1# ) 0.0 1.5 6.5
assign (resid 422 and name HA  )(resid 433 and name HN  ) 0.0 0.0 5.0
assign (resid 423 and name HN  )(resid 430 and name HD# ) 0.0 2.4 7.4
assign (resid 423 and name HN  )(resid 431 and name HN  ) 0.0 0.0 5.0
assign (resid 423 and name HN  )(resid 432 and name HA  ) 0.0 0.0 3.5
assign (resid 424 and name HA  )(resid 430 and name HA  ) 0.0 0.0 3.5
assign (resid 424 and name HA  )(resid 430 and name HD# ) 0.0 2.4 5.9
assign (resid 424 and name HA  )(resid 431 and name HN  ) 0.0 0.0 5.0
assign (resid 424 and name HG2# )(resid 429 and name HN  ) 0.0 1.5 6.5
assign (resid 425 and name HN  )(resid 431 and name HN  ) 0.0 0.0 6.0
assign (resid 451 and name H8  )(resid 378 and name HG2# ) 0.0 1.5 5.0
assign (resid 451 and name H8  )(resid 386 and name HD# ) 0.0 2.4 5.9
! Intermolecular NOEs between EnvZ domain B & AMP-PNP
assign (resid 451 and name H1' )(resid 378 and name HA  ) 0.0 0.0 3.5
assign (resid 451 and name H1' )(resid 378 and name HG2# ) 0.0 1.5 4.4
assign (resid 451 and name H1' )(resid 378 and name HD1# ) 0.0 1.5 5.0
assign (resid 451 and name H1' )(resid 386 and name HD# ) 0.0 2.4 5.9
assign (resid 451 and name H1' )(resid 422 and name HD# ) 0.0 2.4 5.9
assign (resid 451 and name H4' )(resid 386 and name HD# ) 0.0 2.4 4.9
assign (resid 451 and name H5' )(resid 386 and name HD# ) 0.0 2.4 4.9
assign (resid 451 and name H2  )(resid 430 and name HD# ) 0.0 2.4 5.9
assign (resid 451 and name H8  )(resid 430 and name HD# ) 0.0 2.4 5.3
assign (resid 451 and name H5' )(resid 430 and name HD# ) 0.0 3.4 5.9
! Intramolecular NOEs in AMP-PNP
assign (resid 451 and name H1' )(resid 451 and name H8  ) 0.0 0.0 5.0
assign (resid 451 and name H1' )(resid 451 and name H3' ) 0.0 0.0 5.0
assign (resid 451 and name H1' )(resid 451 and name H4' ) 0.0 0.0 3.5
assign (resid 451 and name H1' )(resid 451 and name H5' ) 0.0 1.0 5.0
assign (resid 451 and name H3' )(resid 451 and name H8  ) 0.0 0.0 2.9
assign (resid 451 and name H3' )(resid 451 and name H4' ) 0.0 0.0 2.9
assign (resid 451 and name H3' )(resid 451 and name H5' ) 0.0 1.0 2.9
assign (resid 451 and name H4' )(resid 451 and name H8  ) 0.0 0.0 5.0
assign (resid 451 and name H4' )(resid 451 and name H5' ) 0.0 1.0 2.9
assign (resid 451 and name H5' )(resid 451 and name H8  ) 0.0 1.0 2.9
! Hydrogen bond
assign (resid 301 and name O   )(resid 305 and name N   ) 0.0 0.0 3.3
```


Table A.2. *(continued)*

```
assign (resid 301 and name O   )(resid 305 and name HN  ) 0.0 0.0 2.3
assign (resid 336 and name O   )(resid 340 and name N   ) 0.0 0.0 3.3
assign (resid 336 and name O   )(resid 340 and name HN  ) 0.0 0.0 2.3
assign (resid 337 and name O   )(resid 341 and name N   ) 0.0 0.0 3.3
assign (resid 337 and name O   )(resid 341 and name HN  ) 0.0 0.0 2.3
assign (resid 338 and name O   )(resid 342 and name N   ) 0.0 0.0 3.3
assign (resid 338 and name O   )(resid 342 and name HN  ) 0.0 0.0 2.3
assign (resid 300 and name O   )(resid 304 and name N   ) 0.0 0.0 3.3
assign (resid 300 and name O   )(resid 304 and name HN  ) 0.0 0.0 2.3
assign (resid 302 and name O   )(resid 306 and name N   ) 0.0 0.0 3.3
assign (resid 302 and name O   )(resid 306 and name HN  ) 0.0 0.0 2.3
assign (resid 304 and name O   )(resid 308 and name N   ) 0.0 0.0 3.3
assign (resid 304 and name O   )(resid 308 and name HN  ) 0.0 0.0 2.3
assign (resid 305 and name O   )(resid 309 and name N   ) 0.0 0.0 3.3
assign (resid 305 and name O   )(resid 309 and name HN  ) 0.0 0.0 2.3
assign (resid 333 and name O   )(resid 337 and name N   ) 0.0 0.0 3.3
assign (resid 333 and name O   )(resid 337 and name HN  ) 0.0 0.0 2.3
assign (resid 334 and name O   )(resid 338 and name N   ) 0.0 0.0 3.3
assign (resid 334 and name O   )(resid 338 and name HN  ) 0.0 0.0 2.3
assign (resid 335 and name O   )(resid 339 and name N   ) 0.0 0.0 3.3
assign (resid 335 and name O   )(resid 339 and name HN  ) 0.0 0.0 2.3
assign (resid 339 and name O   )(resid 343 and name N   ) 0.0 0.0 3.3
assign (resid 339 and name O   )(resid 343 and name HN  ) 0.0 0.0 2.3
assign (resid 306 and name O   )(resid 310 and name N   ) 0.0 0.0 3.3
assign (resid 306 and name O   )(resid 310 and name HN  ) 0.0 0.0 2.3
assign (resid 410 and name O   )(resid 414 and name N   ) 0.0 0.0 3.3
assign (resid 410 and name O   )(resid 414 and name HN  ) 0.0 0.0 2.3
assign (resid 299 and name O   )(resid 330 and name N   ) 0.0 0.0 3.3
assign (resid 299 and name O   )(resid 330 and name HN  ) 0.0 0.0 2.3
assign (resid 372 and name O   )(resid 357 and name N   ) 0.0 0.0 3.3
assign (resid 372 and name O   )(resid 357 and name HN  ) 0.0 0.0 2.3
assign (resid 320 and name O   )(resid 358 and name N   ) 0.0 0.0 3.3
assign (resid 320 and name O   )(resid 358 and name HN  ) 0.0 0.0 2.3
assign (resid 370 and name O   )(resid 359 and name N   ) 0.0 0.0 3.3
assign (resid 370 and name O   )(resid 359 and name HN  ) 0.0 0.0 2.3
assign (resid 322 and name O   )(resid 360 and name N   ) 0.0 0.0 3.3
assign (resid 322 and name O   )(resid 360 and name HN  ) 0.0 0.0 2.3
assign (resid 368 and name O   )(resid 361 and name N   ) 0.0 0.0 3.3
assign (resid 368 and name O   )(resid 361 and name HN  ) 0.0 0.0 2.3
assign (resid 436 and name O   )(resid 367 and name N   ) 0.0 0.0 3.3
assign (resid 436 and name O   )(resid 367 and name HN  ) 0.0 0.0 2.3
assign (resid 361 and name O   )(resid 368 and name N   ) 0.0 0.0 3.3
assign (resid 361 and name O   )(resid 368 and name HN  ) 0.0 0.0 2.3
assign (resid 434 and name O   )(resid 369 and name N   ) 0.0 0.0 3.3
assign (resid 434 and name O   )(resid 369 and name HN  ) 0.0 0.0 2.3
assign (resid 359 and name O   )(resid 370 and name N   ) 0.0 0.0 3.3
assign (resid 359 and name O   )(resid 370 and name HN  ) 0.0 0.0 2.3
assign (resid 432 and name O   )(resid 371 and name N   ) 0.0 0.0 3.3
assign (resid 432 and name O   )(resid 371 and name HN  ) 0.0 0.0 2.3
assign (resid 357 and name O   )(resid 372 and name N   ) 0.0 0.0 3.3
assign (resid 357 and name O   )(resid 372 and name HN  ) 0.0 0.0 2.3
assign (resid 430 and name O   )(resid 373 and name N   ) 0.0 0.0 3.3
assign (resid 430 and name O   )(resid 373 and name HN  ) 0.0 0.0 2.3
assign (resid 433 and name O   )(resid 421 and name N   ) 0.0 0.0 3.3
assign (resid 433 and name O   )(resid 421 and name HN  ) 0.0 0.0 2.3
assign (resid 371 and name O   )(resid 432 and name N   ) 0.0 0.0 3.3
assign (resid 371 and name O   )(resid 432 and name HN  ) 0.0 0.0 2.3
assign (resid 421 and name O   )(resid 433 and name N   ) 0.0 0.0 3.3
assign (resid 421 and name O   )(resid 433 and name HN  ) 0.0 0.0 2.3
assign (resid 369 and name O   )(resid 434 and name N   ) 0.0 0.0 3.3
```

Table A.2. *(continued)*

```
assign (resid 369 and name O )(resid 434 and name HN ) 0.0 0.0 2.3
assign (resid 419 and name O )(resid 435 and name N ) 0.0 0.0 3.3
assign (resid 419 and name O )(resid 435 and name HN ) 0.0 0.0 2.3
assign (resid 367 and name O )(resid 436 and name N ) 0.0 0.0 3.3
assign (resid 367 and name O )(resid 436 and name HN ) 0.0 0.0 2.3
assign (resid 330 and name O )(resid 299 and name N ) 0.0 0.0 3.3
assign (resid 330 and name O )(resid 299 and name HN ) 0.0 0.0 2.3
assign (resid 356 and name O )(resid 320 and name N ) 0.0 0.0 3.3
assign (resid 356 and name O )(resid 320 and name HN ) 0.0 0.0 2.3
assign (resid 358 and name O )(resid 322 and name N ) 0.0 0.0 3.3
assign (resid 358 and name O )(resid 322 and name HN ) 0.0 0.0 2.3
assign (resid 360 and name O )(resid 324 and name N ) 0.0 0.0 3.3
assign (resid 360 and name O )(resid 324 and name HN ) 0.0 0.0 2.3
assign (resid 297 and name O )(resid 332 and name N ) 0.0 0.0 3.3
assign (resid 297 and name O )(resid 332 and name HN ) 0.0 0.0 2.3
assign (resid 318 and name O )(resid 356 and name N ) 0.0 0.0 3.3
assign (resid 318 and name O )(resid 356 and name HN ) 0.0 0.0 2.3
assign (resid 355 and name O )(resid 374 and name N ) 0.0 0.0 3.3
assign (resid 355 and name O )(resid 374 and name HN ) 0.0 0.0 2.3
assign (resid 431 and name O )(resid 423 and name N ) 0.0 0.0 3.3
assign (resid 431 and name O )(resid 423 and name HN ) 0.0 0.0 2.3
assign (resid 423 and name O )(resid 431 and name N ) 0.0 0.0 3.3
assign (resid 423 and name O )(resid 431 and name HN ) 0.0 0.0 2.3
assign (resid 366 and name O )(resid 363 and name N ) 0.0 0.0 3.3
assign (resid 366 and name O )(resid 363 and name HN ) 0.0 0.0 2.3
assign (resid 435 and name O )(resid 419 and name N ) 0.0 0.0 3.3
assign (resid 435 and name O )(resid 419 and name HN ) 0.0 0.0 2.3
assign (resid 429 and name O )(resid 425 and name N ) 0.0 0.0 3.3
assign (resid 429 and name O )(resid 425 and name HN ) 0.0 0.0 2.3
assign (resid 425 and name O )(resid 429 and name N ) 0.0 0.0 3.3
assign (resid 425 and name O )(resid 429 and name HN ) 0.0 0.0 2.3
```


Table A.3. Dihedral Angle Constraints Used for Structure Calculation of Domain B

```
! dihedral angle constraints from HMQCJ
assign (resid 293 and name c)(resid 294 and name n)
       (resid 294 and name ca)(resid 294 and name c) 1   -120.000   50.0000 2
assign (resid 296 and name c)(resid 297 and name n)
       (resid 297 and name ca)(resid 297 and name c) 1   -120.000   50.0000 2
assign (resid 302 and name c)(resid 303 and name n)
       (resid 303 and name ca)(resid 303 and name c) 1   -60.000   30.0000 2
assign (resid 303 and name c)(resid 304 and name n)
       (resid 304 and name ca)(resid 304 and name c) 1   -60.000   30.0000 2
assign (resid 304 and name c)(resid 305 and name n)
       (resid 305 and name ca)(resid 305 and name c) 1   -60.000   30.0000 2
assign (resid 306 and name c)(resid 307 and name n)
       (resid 307 and name ca)(resid 307 and name c) 1   -60.000   30.0000 2
assign (resid 307 and name c)(resid 308 and name n)
       (resid 308 and name ca)(resid 308 and name c) 1   -60.000   30.0000 2
assign (resid 308 and name c)(resid 309 and name n)
       (resid 309 and name ca)(resid 309 and name c) 1   -60.000   30.0000 2
assign (resid 309 and name c)(resid 310 and name n)
       (resid 310 and name ca)(resid 310 and name c) 1   -60.000   30.0000 2
assign (resid 310 and name c)(resid 311 and name n)
       (resid 311 and name ca)(resid 311 and name c) 1   -60.000   30.0000 2
assign (resid 316 and name c)(resid 317 and name n)
       (resid 317 and name ca)(resid 317 and name c) 1   -120.000   50.0000 2
assign (resid 317 and name c)(resid 318 and name n)
       (resid 318 and name ca)(resid 318 and name c) 1   -120.000   50.0000 2
assign (resid 319 and name c)(resid 320 and name n)
       (resid 320 and name ca)(resid 320 and name c) 1   -120.000   30.0000 2
assign (resid 320 and name c)(resid 321 and name n)
       (resid 321 and name ca)(resid 321 and name c) 1   -120.000   30.0000 2
assign (resid 321 and name c)(resid 322 and name n)
       (resid 322 and name ca)(resid 322 and name c) 1   -120.000   30.0000 2
assign (resid 327 and name c)(resid 328 and name n)
       (resid 328 and name ca)(resid 328 and name c) 1   -120.000   50.0000 2
assign (resid 329 and name c)(resid 330 and name n)
       (resid 330 and name ca)(resid 330 and name c) 1   -120.000   30.0000 2
assign (resid 334 and name c)(resid 335 and name n)
       (resid 335 and name ca)(resid 335 and name c) 1   -60.000   30.0000 2
assign (resid 337 and name c)(resid 338 and name n)
       (resid 338 and name ca)(resid 338 and name c) 1   -60.000   30.0000 2
assign (resid 339 and name c)(resid 340 and name n)
       (resid 340 and name ca)(resid 340 and name c) 1   -60.000   30.0000 2
assign (resid 340 and name c)(resid 341 and name n)
       (resid 341 and name ca)(resid 341 and name c) 1   -60.000   30.0000 2
assign (resid 355 and name c)(resid 356 and name n)
       (resid 356 and name ca)(resid 356 and name c) 1   -120.000   30.0000 2
assign (resid 356 and name c)(resid 357 and name n)
       (resid 357 and name ca)(resid 357 and name c) 1   -120.000   30.0000 2
assign (resid 357 and name c)(resid 358 and name n)
       (resid 358 and name ca)(resid 358 and name c) 1   -120.000   30.0000 2
assign (resid 366 and name c)(resid 367 and name n)
       (resid 367 and name ca)(resid 367 and name c) 1   -120.000   30.0000 2
assign (resid 368 and name c)(resid 369 and name n)
       (resid 369 and name ca)(resid 369 and name c) 1   -120.000   30.0000 2
assign (resid 369 and name c)(resid 370 and name n)
       (resid 370 and name ca)(resid 370 and name c) 1   -120.000   30.0000 2
assign (resid 371 and name c)(resid 372 and name n)
       (resid 372 and name ca)(resid 372 and name c) 1   -120.000   30.0000 2
assign (resid 373 and name c)(resid 374 and name n)
       (resid 374 and name ca)(resid 374 and name c) 1   -120.000   50.0000 2
```

Table A.3. *(continued)*

```
assign (resid 380 and name c)(resid 381 and name n)
       (resid 381 and name ca)(resid 381 and name c) 1   -60.000   30.0000 2
assign (resid 382 and name c)(resid 383 and name n)
       (resid 383 and name ca)(resid 383 and name c) 1   -60.000   30.0000 2
assign (resid 390 and name c)(resid 391 and name n)
       (resid 391 and name ca)(resid 391 and name c) 1   -120.000   50.0000 2
assign (resid 394 and name c)(resid 395 and name n)
       (resid 395 and name ca)(resid 395 and name c) 1   -120.000   50.0000 2
assign (resid 406 and name c)(resid 407 and name n)
       (resid 407 and name ca)(resid 407 and name c) 1   -60.000   50.0000 2
assign (resid 413 and name c)(resid 414 and name n)
       (resid 414 and name ca)(resid 414 and name c) 1   -60.000   30.0000 2
assign (resid 414 and name c)(resid 415 and name n)
       (resid 415 and name ca)(resid 415 and name c) 1   -60.000   50.0000 2
assign (resid 419 and name c)(resid 420 and name n)
       (resid 420 and name ca)(resid 420 and name c) 1   -120.000   30.0000 2
assign (resid 420 and name c)(resid 421 and name n)
       (resid 421 and name ca)(resid 421 and name c) 1   -120.000   30.0000 2
assign (resid 421 and name c)(resid 422 and name n)
       (resid 422 and name ca)(resid 422 and name c) 1   -120.000   30.0000 2
assign (resid 432 and name c)(resid 433 and name n)
       (resid 433 and name ca)(resid 433 and name c) 1   -120.000   30.0000 2
assign (resid 433 and name c)(resid 434 and name n)
       (resid 434 and name ca)(resid 434 and name c) 1   -120.000   30.0000 2
assign (resid 434 and name c)(resid 435 and name n)
       (resid 435 and name ca)(resid 435 and name c) 1   -120.000   30.0000 2
assign (resid 435 and name c)(resid 436 and name n)
       (resid 436 and name ca)(resid 436 and name c) 1   -120.000   30.0000 2
assign (resid 437 and name c)(resid 438 and name n)
       (resid 438 and name ca)(resid 438 and name c) 1   -120.000   50.0000 2
! dihedral angle constraints from CSI
assign (resid  297 and name c) (resid  298 and name n)
(resid  298 and name ca)(resid  298 and name c) 1 -130.0   40.0  2
assign (resid  298 and name c) (resid  299 and name n)
(resid  299 and name ca)(resid  299 and name c) 1 -130.0   40.0  2
assign (resid  300 and name c) (resid  301 and name n)
(resid  301 and name ca)(resid  301 and name c) 1 -60.0   30.0  2
assign (resid  301 and name c) (resid  302 and name n)
(resid  302 and name ca)(resid  302 and name c) 1 -60.0   30.0  2
assign (resid  305 and name c) (resid  306 and name n)
(resid  306 and name ca)(resid  306 and name c) 1 -60.0   30.0  2
assign (resid  318 and name c) (resid  319 and name n)
(resid  319 and name ca)(resid  319 and name c) 1 -130.0   40.0  2
assign (resid  322 and name c) (resid  323 and name n)
(resid  323 and name ca)(resid  323 and name c) 1 -130.0   40.0  2
assign (resid  335 and name c) (resid  336 and name n)
(resid  336 and name ca)(resid  336 and name c) 1 -60.0   30.0  2
assign (resid  336 and name c) (resid  337 and name n)
(resid  337 and name ca)(resid  337 and name c) 1 -60.0   30.0  2
assign (resid  338 and name c) (resid  339 and name n)
(resid  339 and name ca)(resid  339 and name c) 1 -60.0   30.0  2
assign (resid  341 and name c) (resid  342 and name n)
(resid  342 and name ca)(resid  342 and name c) 1 -60.0   30.0  2
assign (resid  342 and name c) (resid  343 and name n)
(resid  343 and name ca)(resid  343 and name c) 1 -60.0   30.0  2
assign (resid  343 and name c) (resid  344 and name n)
(resid  344 and name ca)(resid  344 and name c) 1 -60.0   30.0  2
assign (resid  344 and name c) (resid  345 and name n)
(resid  345 and name ca)(resid  345 and name c) 1 -60.0   30.0  2
```


Table A.3. *(continued)*

```
assign (resid  345 and name c) (resid  346 and name n)
(resid  346 and name ca)(resid  346 and name c) 1 -60.0   30.0  2
assign (resid  346 and name c) (resid  347 and name n)
(resid  347 and name ca)(resid  347 and name c) 1 -60.0   30.0  2
assign (resid  347 and name c) (resid  348 and name n)
(resid  348 and name ca)(resid  348 and name c) 1 -60.0   30.0  2
assign (resid  348 and name c) (resid  349 and name n)
(resid  349 and name ca)(resid  349 and name c) 1 -60.0   30.0  2
assign (resid  349 and name c) (resid  350 and name n)
(resid  350 and name ca)(resid  350 and name c) 1 -60.0   30.0  2
assign (resid  350 and name c) (resid  351 and name n)
(resid  351 and name ca)(resid  351 and name c) 1 -60.0   30.0  2
assign (resid  367 and name c) (resid  368 and name n)
(resid  368 and name ca)(resid  368 and name c) 1 -130.0   40.0  2
assign (resid  370 and name c) (resid  371 and name n)
(resid  371 and name ca)(resid  371 and name c) 1 -130.0   40.0  2
assign (resid  372 and name c) (resid  373 and name n)
(resid  373 and name ca)(resid  373 and name c) 1 -130.0   40.0  2
assign (resid  379 and name c) (resid  380 and name n)
(resid  380 and name ca)(resid  380 and name c) 1 -60.0   30.0  2
assign (resid  381 and name c) (resid  382 and name n)
(resid  382 and name ca)(resid  382 and name c) 1 -60.0   30.0  2
assign (resid  383 and name c) (resid  384 and name n)
(resid  384 and name ca)(resid  384 and name c) 1 -60.0   30.0  2
assign (resid  409 and name c) (resid  410 and name n)
(resid  410 and name ca)(resid  410 and name c) 1 -60.0   30.0  2
assign (resid  410 and name c) (resid  411 and name n)
(resid  411 and name ca)(resid  411 and name c) 1 -60.0   30.0  2
assign (resid  411 and name c) (resid  412 and name n)
(resid  412 and name ca)(resid  412 and name c) 1 -60.0   30.0  2
assign (resid  412 and name c) (resid  413 and name n)
(resid  413 and name ca)(resid  413 and name c) 1 -60.0   30.0  2
assign (resid  430 and name c) (resid  431 and name n)
(resid  431 and name ca)(resid  431 and name c) 1 -130.0   40.0  2
assign (resid  431 and name c) (resid  432 and name n)
(resid  432 and name ca)(resid  432 and name c) 1 -130.0   40.0  2
assign (resid  298 and name n) (resid  298 and name ca)
(resid  298 and name c)(resid  299 and name n) 1 130.0   50.0  2
assign (resid  299 and name n) (resid  299 and name ca)
(resid  299 and name c)(resid  300 and name n) 1 130.0   50.0  2
assign (resid  301 and name n) (resid  301 and name ca)
(resid  301 and name c)(resid  302 and name n) 1 -50.0   30.0  2
assign (resid  302 and name n) (resid  302 and name ca)
(resid  302 and name c)(resid  303 and name n) 1 -50.0   30.0  2
assign (resid  303 and name n) (resid  303 and name ca)
(resid  303 and name c)(resid  304 and name n) 1 -50.0   30.0  2
assign (resid  304 and name n) (resid  304 and name ca)
(resid  304 and name c)(resid  305 and name n) 1 -50.0   30.0  2
assign (resid  305 and name n) (resid  305 and name ca)
(resid  305 and name c)(resid  306 and name n) 1 -50.0   30.0  2
assign (resid  306 and name n) (resid  306 and name ca)
(resid  306 and name c)(resid  307 and name n) 1 -50.0   30.0  2
assign (resid  307 and name n) (resid  307 and name ca)
(resid  307 and name c)(resid  308 and name n) 1 -50.0   30.0  2
assign (resid  308 and name n) (resid  308 and name ca)
(resid  308 and name c)(resid  309 and name n) 1 -50.0   30.0  2
assign (resid  309 and name n) (resid  309 and name ca)
(resid  309 and name c)(resid  310 and name n) 1 -50.0   30.0  2
assign (resid  310 and name n) (resid  310 and name ca)
(resid  310 and name c)(resid  311 and name n) 1 -50.0   30.0  2
```

Table A.3. *(continued)*

```
assign (resid 311 and name n) (resid 311 and name ca)
(resid 311 and name c)(resid 312 and name n) 1 -50.0  30.0  2
assign (resid 319 and name n) (resid 319 and name ca)
(resid 319 and name c)(resid 320 and name n) 1 130.0  50.0  2
assign (resid 320 and name n) (resid 320 and name ca)
(resid 320 and name c)(resid 321 and name n) 1 130.0  50.0  2
assign (resid 321 and name n) (resid 321 and name ca)
(resid 321 and name c)(resid 322 and name n) 1 130.0  50.0  2
assign (resid 322 and name n) (resid 322 and name ca)
(resid 322 and name c)(resid 323 and name n) 1 130.0  50.0  2
assign (resid 323 and name n) (resid 323 and name ca)
(resid 323 and name c)(resid 324 and name n) 1 130.0  50.0  2
assign (resid 334 and name n) (resid 334 and name ca)
(resid 334 and name c)(resid 335 and name n) 1 -50.0  30.0  2
assign (resid 335 and name n) (resid 335 and name ca)
(resid 335 and name c)(resid 336 and name n) 1 -50.0  30.0  2
assign (resid 336 and name n) (resid 336 and name ca)
(resid 336 and name c)(resid 337 and name n) 1 -50.0  30.0  2
assign (resid 337 and name n) (resid 337 and name ca)
(resid 337 and name c)(resid 338 and name n) 1 -50.0  30.0  2
assign (resid 338 and name n) (resid 338 and name ca)
(resid 338 and name c)(resid 339 and name n) 1 -50.0  30.0  2
assign (resid 339 and name n) (resid 339 and name ca)
(resid 339 and name c)(resid 340 and name n) 1 -50.0  30.0  2
assign (resid 340 and name n) (resid 340 and name ca)
(resid 340 and name c)(resid 341 and name n) 1 -50.0  30.0  2
assign (resid 341 and name n) (resid 341 and name ca)
(resid 341 and name c)(resid 342 and name n) 1 -50.0  30.0  2
assign (resid 342 and name n) (resid 342 and name ca)
(resid 342 and name c)(resid 343 and name n) 1 -50.0  30.0  2
assign (resid 343 and name n) (resid 343 and name ca)
(resid 343 and name c)(resid 344 and name n) 1 -50.0  30.0  2
assign (resid 344 and name n) (resid 344 and name ca)
(resid 344 and name c)(resid 345 and name n) 1 -50.0  30.0  2
assign (resid 345 and name n) (resid 345 and name ca)
(resid 345 and name c)(resid 346 and name n) 1 -50.0  30.0  2
assign (resid 346 and name n) (resid 346 and name ca)
(resid 346 and name c)(resid 347 and name n) 1 -50.0  30.0  2
assign (resid 347 and name n) (resid 347 and name ca)
(resid 347 and name c)(resid 348 and name n) 1 -50.0  30.0  2
assign (resid 348 and name n) (resid 348 and name ca)
(resid 348 and name c)(resid 349 and name n) 1 -50.0  30.0  2
assign (resid 349 and name n) (resid 349 and name ca)
(resid 349 and name c)(resid 350 and name n) 1 -50.0  30.0  2
assign (resid 350 and name n) (resid 350 and name ca)
(resid 350 and name c)(resid 351 and name n) 1 -50.0  30.0  2
assign (resid 351 and name n) (resid 351 and name ca)
(resid 351 and name c)(resid 352 and name n) 1 -50.0  30.0  2
assign (resid 367 and name n) (resid 367 and name ca)
(resid 367 and name c)(resid 368 and name n) 1 130.0  50.0  2
assign (resid 368 and name n) (resid 368 and name ca)
(resid 368 and name c)(resid 369 and name n) 1 130.0  50.0  2
assign (resid 369 and name n) (resid 369 and name ca)
(resid 369 and name c)(resid 370 and name n) 1 130.0  50.0  2
assign (resid 370 and name n) (resid 370 and name ca)
(resid 370 and name c)(resid 371 and name n) 1 130.0  50.0  2
assign (resid 371 and name n) (resid 371 and name ca)
(resid 371 and name c)(resid 372 and name n) 1 130.0  50.0  2
assign (resid 372 and name n) (resid 372 and name ca)
(resid 372 and name c)(resid 373 and name n) 1 130.0  50.0  2
```


Table A.3. *(continued)*

```
assign (resid 373 and name n) (resid 373 and name ca)
(resid 373 and name c)(resid 374 and name n) 1 130.0  50.0  2
assign (resid 380 and name n) (resid 380 and name ca)
(resid 380 and name c)(resid 381 and name n) 1 -50.0  30.0  2
assign (resid 381 and name n) (resid 381 and name ca)
(resid 381 and name c)(resid 382 and name n) 1 -50.0  30.0  2
assign (resid 382 and name n) (resid 382 and name ca)
(resid 382 and name c)(resid 383 and name n) 1 -50.0  30.0  2
assign (resid 383 and name n) (resid 383 and name ca)
(resid 383 and name c)(resid 384 and name n) 1 -50.0  30.0  2
assign (resid 384 and name n) (resid 384 and name ca)
(resid 384 and name c)(resid 385 and name n) 1 -50.0  30.0  2
assign (resid 410 and name n) (resid 410 and name ca)
(resid 410 and name c)(resid 411 and name n) 1 -50.0  30.0  2
assign (resid 411 and name n) (resid 411 and name ca)
(resid 411 and name c)(resid 412 and name n) 1 -50.0  30.0  2
assign (resid 412 and name n) (resid 412 and name ca)
(resid 412 and name c)(resid 413 and name n) 1 -50.0  30.0  2
assign (resid 413 and name n) (resid 413 and name ca)
(resid 413 and name c)(resid 414 and name n) 1 -50.0  30.0  2
assign (resid 414 and name n) (resid 414 and name ca)
(resid 414 and name c)(resid 415 and name n) 1 -50.0  30.0  2
assign (resid 420 and name n) (resid 420 and name ca)
(resid 420 and name c)(resid 421 and name n) 1 130.0  50.0  2
assign (resid 421 and name n) (resid 421 and name ca)
(resid 421 and name c)(resid 422 and name n) 1 130.0  50.0  2
assign (resid 422 and name n) (resid 422 and name ca)
(resid 422 and name c)(resid 423 and name n) 1 130.0  50.0  2
assign (resid 431 and name n) (resid 431 and name ca)
(resid 431 and name c)(resid 432 and name n) 1 130.0  50.0  2
assign (resid 432 and name n) (resid 432 and name ca)
(resid 432 and name c)(resid 433 and name n) 1 130.0  50.0  2
assign (resid 433 and name n) (resid 433 and name ca)
(resid 433 and name c)(resid 434 and name n) 1 130.0  50.0  2
assign (resid 434 and name n) (resid 434 and name ca)
(resid 434 and name c)(resid 435 and name n) 1 130.0  50.0  2
assign (resid 435 and name n) (resid 435 and name ca)
(resid 435 and name c)(resid 436 and name n) 1 130.0  50.0  2
assign (resid 436 and name n) (resid 436 and name ca)
(resid 436 and name c)(resid 437 and name n) 1 130.0  50.0  2
```

Table A.4. Distance Constraints Used for Structure Calculation of Domain A

```
assign (segid a and resid 225 and name HA  )(segid a and resid 225 and name HB#  ) 0.0 1.5 5.0
assign (segid a and resid 227 and name HA  )(segid a and resid 227 and name HB   ) 0.0 0.0 3.5
assign (segid a and resid 227 and name HB  )(segid a and resid 227 and name HN   ) 0.0 0.0 5.0
assign (segid a and resid 227 and name HG1# )(segid a and resid 227 and name HN   ) 0.0 1.5 5.0
assign (segid a and resid 228 and name HA  )(segid a and resid 228 and name HB#  ) 0.0 1.0 3.9
assign (segid a and resid 228 and name HA  )(segid a and resid 228 and name HN   ) 0.0 0.0 5.0
assign (segid a and resid 228 and name HD#  )(segid a and resid 228 and name HG#  ) 0.0 2.0 4.9
assign (segid a and resid 228 and name HG#  )(segid a and resid 228 and name HN   ) 0.0 1.0 6.0
assign (segid a and resid 229 and name HA  )(segid a and resid 229 and name HB#  ) 0.0 1.0 3.9
assign (segid a and resid 229 and name HA  )(segid a and resid 229 and name HG#  ) 0.0 1.0 3.9
assign (segid a and resid 229 and name HB#  )(segid a and resid 229 and name HG#  ) 0.0 2.0 4.9
assign (segid a and resid 229 and name HB#  )(segid a and resid 229 and name HN   ) 0.0 0.6 5.6
assign (segid a and resid 229 and name HG#  )(segid a and resid 229 and name HN   ) 0.0 1.0 6.0
assign (segid a and resid 230 and name HA  )(segid a and resid 230 and name HB#  ) 0.0 1.0 4.5
assign (segid a and resid 230 and name HA  )(segid a and resid 230 and name HD2# ) 0.0 1.5 4.4
assign (segid a and resid 230 and name HA  )(segid a and resid 230 and name HN   ) 0.0 0.0 2.9
assign (segid a and resid 230 and name HD1# )(segid a and resid 230 and name HN   ) 0.0 1.5 6.5
assign (segid a and resid 231 and name HA  )(segid a and resid 231 and name HB#  ) 0.0 1.5 4.4
assign (segid a and resid 231 and name HA  )(segid a and resid 231 and name HN   ) 0.0 0.0 2.9
assign (segid a and resid 231 and name HB#  )(segid a and resid 231 and name HN   ) 0.0 1.1 4.0
assign (segid a and resid 232 and name HA  )(segid a and resid 232 and name HB#  ) 0.0 1.0 3.9
assign (segid a and resid 232 and name HA  )(segid a and resid 232 and name HN   ) 0.0 0.0 3.5
assign (segid a and resid 233 and name HA  )(segid a and resid 233 and name HB#  ) 0.0 1.0 3.9
assign (segid a and resid 233 and name HA  )(segid a and resid 233 and name HN   ) 0.0 0.0 2.9
assign (segid a and resid 233 and name HB#  )(segid a and resid 233 and name HN   ) 0.0 0.6 3.5
assign (segid a and resid 234 and name HA  )(segid a and resid 234 and name HB#  ) 0.0 1.0 3.9
assign (segid a and resid 234 and name HA  )(segid a and resid 234 and name HD#  ) 0.0 1.0 6.0
assign (segid a and resid 234 and name HA  )(segid a and resid 234 and name HG#  ) 0.0 1.0 3.9
assign (segid a and resid 234 and name HA  )(segid a and resid 234 and name HN   ) 0.0 0.0 3.5
assign (segid a and resid 234 and name HB#  )(segid a and resid 234 and name HD#  ) 0.0 2.0 5.5
assign (segid a and resid 234 and name HB#  )(segid a and resid 234 and name HG#  ) 0.0 2.0 4.9
assign (segid a and resid 234 and name HB#  )(segid a and resid 234 and name HN   ) 0.0 0.6 3.5
assign (segid a and resid 235 and name HA  )(segid a and resid 235 and name HB   ) 0.0 0.0 6.0
assign (segid a and resid 235 and name HA  )(segid a and resid 235 and name HG2# ) 0.0 1.5 4.4
assign (segid a and resid 235 and name HA  )(segid a and resid 235 and name HN   ) 0.0 0.0 3.5
assign (segid a and resid 235 and name HB  )(segid a and resid 235 and name HG2# ) 0.0 1.5 4.4
assign (segid a and resid 235 and name HB  )(segid a and resid 235 and name HN   ) 0.0 0.0 2.9
assign (segid a and resid 235 and name HG2# )(segid a and resid 235 and name HN   ) 0.0 1.5 5.0
assign (segid a and resid 236 and name HA  )(segid a and resid 236 and name HB#  ) 0.0 1.0 3.9
assign (segid a and resid 236 and name HA  )(segid a and resid 236 and name HD1# ) 0.0 1.5 4.4
assign (segid a and resid 236 and name HA  )(segid a and resid 236 and name HD2# ) 0.0 1.5 4.4
assign (segid a and resid 236 and name HA  )(segid a and resid 236 and name HG   ) 0.0 0.0 2.9
assign (segid a and resid 236 and name HA  )(segid a and resid 236 and name HN   ) 0.0 0.0 2.9
assign (segid a and resid 236 and name HB#  )(segid a and resid 236 and name HD1# ) 0.0 2.5 5.4
assign (segid a and resid 236 and name HB#  )(segid a and resid 236 and name HD2# ) 0.0 2.5 6.0
assign (segid a and resid 236 and name HD#  )(segid a and resid 236 and name HG   ) 0.0 1.7 4.6
assign (segid a and resid 236 and name HD#  )(segid a and resid 236 and name HN   ) 0.0 1.7 6.7
assign (segid a and resid 236 and name HG   )(segid a and resid 236 and name HN   ) 0.0 0.0 3.5
assign (segid a and resid 237 and name HA  )(segid a and resid 237 and name HB#  ) 0.0 1.0 4.5
assign (segid a and resid 237 and name HA  )(segid a and resid 237 and name HD1# ) 0.0 1.5 7.5
assign (segid a and resid 237 and name HA  )(segid a and resid 237 and name HD2# ) 0.0 1.5 4.4
assign (segid a and resid 237 and name HA  )(segid a and resid 237 and name HN   ) 0.0 0.0 2.9
assign (segid a and resid 237 and name HB#  )(segid a and resid 237 and name HN   ) 0.0 0.6 4.1
assign (segid a and resid 237 and name HD1# )(segid a and resid 237 and name HG   ) 0.0 1.5 4.4
assign (segid a and resid 237 and name HD2# )(segid a and resid 237 and name HG   ) 0.0 1.5 7.5
assign (segid a and resid 238 and name HA  )(segid a and resid 238 and name HB#  ) 0.0 1.0 4.5
assign (segid a and resid 238 and name HA  )(segid a and resid 238 and name HG#  ) 0.0 1.0 4.5
assign (segid a and resid 238 and name HB#  )(segid a and resid 238 and name HG#  ) 0.0 2.0 4.9
assign (segid a and resid 238 and name HG#  )(segid a and resid 238 and name HN   ) 0.0 1.0 6.0
assign (segid a and resid 239 and name HA  )(segid a and resid 239 and name HB#  ) 0.0 1.5 4.4
assign (segid a and resid 239 and name HA  )(segid a and resid 239 and name HN   ) 0.0 0.0 2.9
assign (segid a and resid 239 and name HB#  )(segid a and resid 239 and name HN   ) 0.0 1.1 4.0
assign (segid a and resid 240 and name HA#  )(segid a and resid 240 and name HN   ) 0.0 0.6 3.5
assign (segid a and resid 241 and name HA  )(segid a and resid 241 and name HB   ) 0.0 0.0 5.0
assign (segid a and resid 241 and name HA  )(segid a and resid 241 and name HG1# ) 0.0 1.5 5.0
assign (segid a and resid 241 and name HA  )(segid a and resid 241 and name HG2# ) 0.0 1.5 4.4
```


Table A.4. *(continued)*

```
assign (segid a and resid 241 and name HA  )(segid a and resid 241 and name HN   ) 0.0 0.0 3.5
assign (segid a and resid 241 and name HB  )(segid a and resid 241 and name HG#  ) 0.0 1.7 4.6
assign (segid a and resid 241 and name HB  )(segid a and resid 241 and name HN   ) 0.0 0.0 2.9
assign (segid a and resid 241 and name HG#  )(segid a and resid 241 and name HN   ) 0.0 1.7 5.2
assign (segid a and resid 241 and name HG1# )(segid a and resid 241 and name HN   ) 0.0 1.5 6.5
assign (segid a and resid 241 and name HG2# )(segid a and resid 241 and name HN   ) 0.0 1.5 5.0
assign (segid a and resid 242 and name HA  )(segid a and resid 242 and name HB#  ) 0.0 1.0 4.5
assign (segid a and resid 242 and name HA  )(segid a and resid 242 and name HN   ) 0.0 0.0 5.0
assign (segid a and resid 243 and name HA  )(segid a and resid 243 and name HB#  ) 0.0 1.0 4.5
assign (segid a and resid 243 and name HA  )(segid a and resid 243 and name HN   ) 0.0 0.0 5.0
assign (segid a and resid 243 and name HB#  )(segid a and resid 243 and name HN   ) 0.0 0.6 5.6
assign (segid a and resid 244 and name HA  )(segid a and resid 244 and name HB#  ) 0.0 1.0 6.0
assign (segid a and resid 244 and name HA  )(segid a and resid 244 and name HN   ) 0.0 0.0 5.0
assign (segid a and resid 244 and name HB#  )(segid a and resid 244 and name HN   ) 0.0 0.6 6.6
assign (segid a and resid 245 and name HA  )(segid a and resid 245 and name HB#  ) 0.0 1.0 7.0
assign (segid a and resid 245 and name HA  )(segid a and resid 245 and name HD#  ) 0.0 1.7 5.2
assign (segid a and resid 245 and name HA  )(segid a and resid 245 and name HN   ) 0.0 0.0 5.0
assign (segid a and resid 245 and name HB#  )(segid a and resid 245 and name HD#  ) 0.0 3.4 6.9
assign (segid a and resid 245 and name HB#  )(segid a and resid 245 and name HG   ) 0.0 1.0 4.5
assign (segid a and resid 245 and name HB#  )(segid a and resid 245 and name HN   ) 0.0 0.6 5.6
assign (segid a and resid 246 and name HA  )(segid a and resid 246 and name HB#  ) 0.0 1.0 6.0
assign (segid a and resid 246 and name HA  )(segid a and resid 246 and name HN   ) 0.0 0.0 5.0
assign (segid a and resid 246 and name HB#  )(segid a and resid 246 and name HN   ) 0.0 0.6 5.6
assign (segid a and resid 246 and name HG#  )(segid a and resid 246 and name HN   ) 0.0 1.0 7.0
assign (segid a and resid 247 and name HA  )(segid a and resid 247 and name HB   ) 0.0 0.0 3.5
assign (segid a and resid 247 and name HA  )(segid a and resid 247 and name HG2# ) 0.0 1.5 4.4
assign (segid a and resid 247 and name HA  )(segid a and resid 247 and name HN   ) 0.0 0.0 5.0
assign (segid a and resid 247 and name HB  )(segid a and resid 247 and name HG2# ) 0.0 1.5 4.4
assign (segid a and resid 247 and name HB  )(segid a and resid 247 and name HN   ) 0.0 0.0 5.0
assign (segid a and resid 247 and name HG2# )(segid a and resid 247 and name HN   ) 0.0 1.5 6.5
assign (segid a and resid 248 and name HA  )(segid a and resid 248 and name HB#  ) 0.0 1.0 4.5
assign (segid a and resid 248 and name HD#  )(segid a and resid 248 and name HG#  ) 0.0 2.0 7.0
assign (segid a and resid 249 and name HA  )(segid a and resid 249 and name HB#  ) 0.0 1.0 6.0
assign (segid a and resid 249 and name HA  )(segid a and resid 249 and name HD1# ) 0.0 1.5 5.0
assign (segid a and resid 249 and name HA  )(segid a and resid 249 and name HD2# ) 0.0 1.5 4.4
assign (segid a and resid 249 and name HA  )(segid a and resid 249 and name HG   ) 0.0 0.0 3.5
assign (segid a and resid 249 and name HA  )(segid a and resid 249 and name HN   ) 0.0 0.0 3.5
assign (segid a and resid 249 and name HB#  )(segid a and resid 249 and name HD1# ) 0.0 2.5 6.0
assign (segid a and resid 249 and name HB#  )(segid a and resid 249 and name HD2# ) 0.0 2.5 6.0
assign (segid a and resid 249 and name HB#  )(segid a and resid 249 and name HG   ) 0.0 1.0 4.5
assign (segid a and resid 249 and name HB#  )(segid a and resid 249 and name HN   ) 0.0 0.6 5.6
assign (segid a and resid 249 and name HD#  )(segid a and resid 249 and name HN   ) 0.0 1.7 5.2
assign (segid a and resid 250 and name HA  )(segid a and resid 250 and name HB   ) 0.0 0.0 5.0
assign (segid a and resid 250 and name HA  )(segid a and resid 250 and name HG2# ) 0.0 1.5 4.4
assign (segid a and resid 250 and name HA  )(segid a and resid 250 and name HN   ) 0.0 0.0 3.5
assign (segid a and resid 250 and name HB  )(segid a and resid 250 and name HG2# ) 0.0 1.5 4.4
assign (segid a and resid 250 and name HG2# )(segid a and resid 250 and name HN   ) 0.0 1.5 5.0
assign (segid a and resid 251 and name HA  )(segid a and resid 251 and name HB#  ) 0.0 1.0 3.9
assign (segid a and resid 251 and name HA  )(segid a and resid 251 and name HN   ) 0.0 0.0 3.5
assign (segid a and resid 251 and name HB#  )(segid a and resid 251 and name HN   ) 0.0 0.6 4.1
assign (segid a and resid 252 and name HA  )(segid a and resid 252 and name HB   ) 0.0 0.0 5.0
assign (segid a and resid 252 and name HA  )(segid a and resid 252 and name HG2# ) 0.0 1.5 4.4
assign (segid a and resid 252 and name HA  )(segid a and resid 252 and name HN   ) 0.0 0.0 5.0
assign (segid a and resid 252 and name HB  )(segid a and resid 252 and name HG2# ) 0.0 1.5 5.0
assign (segid a and resid 252 and name HB  )(segid a and resid 252 and name HN   ) 0.0 0.0 3.5
assign (segid a and resid 252 and name HG2# )(segid a and resid 252 and name HN   ) 0.0 1.5 5.0
assign (segid a and resid 253 and name HA  )(segid a and resid 253 and name HD#  ) 0.0 1.0 4.5
assign (segid a and resid 253 and name HA  )(segid a and resid 253 and name HG#  ) 0.0 1.0 6.0
assign (segid a and resid 253 and name HA  )(segid a and resid 253 and name HN   ) 0.0 0.0 3.5
assign (segid a and resid 253 and name HD#  )(segid a and resid 253 and name HG#  ) 0.0 2.0 7.0
assign (segid a and resid 253 and name HD#  )(segid a and resid 253 and name HN   ) 0.0 1.0 6.0
assign (segid a and resid 253 and name HG#  )(segid a and resid 253 and name HN   ) 0.0 1.0 4.5
assign (segid a and resid 254 and name HA  )(segid a and resid 254 and name HB#  ) 0.0 1.0 4.5
assign (segid a and resid 254 and name HA  )(segid a and resid 254 and name HD1# ) 0.0 1.5 4.4
assign (segid a and resid 254 and name HA  )(segid a and resid 254 and name HD2# ) 0.0 1.5 6.5
assign (segid a and resid 254 and name HA  )(segid a and resid 254 and name HG   ) 0.0 0.0 5.0
```

Table A.4. *(continued)*

```
assign (segid a and resid 254 and name HA  )(segid a and resid 254 and name HN  ) 0.0 0.0 3.5
assign (segid a and resid 254 and name HB# )(segid a and resid 254 and name HD1# ) 0.0 2.5 5.4
assign (segid a and resid 254 and name HB# )(segid a and resid 254 and name HD2# ) 0.0 2.5 5.4
assign (segid a and resid 254 and name HB# )(segid a and resid 254 and name HG  ) 0.0 1.0 4.5
assign (segid a and resid 254 and name HD1# )(segid a and resid 254 and name HG  ) 0.0 1.5 4.4
assign (segid a and resid 254 and name HD1# )(segid a and resid 254 and name HN  ) 0.0 1.5 7.5
assign (segid a and resid 254 and name HD2# )(segid a and resid 254 and name HG  ) 0.0 1.5 4.4
assign (segid a and resid 254 and name HD2# )(segid a and resid 254 and name HN  ) 0.0 1.5 5.0
assign (segid a and resid 254 and name HG  )(segid a and resid 254 and name HN  ) 0.0 0.0 3.5
assign (segid a and resid 255 and name HA  )(segid a and resid 255 and name HB# ) 0.0 1.5 4.4
assign (segid a and resid 255 and name HA  )(segid a and resid 255 and name HN  ) 0.0 0.0 2.9
assign (segid a and resid 255 and name HB# )(segid a and resid 255 and name HN  ) 0.0 1.1 4.0
assign (segid a and resid 256 and name HA  )(segid a and resid 256 and name HN  ) 0.0 0.0 3.5
assign (segid a and resid 256 and name HB  )(segid a and resid 256 and name HG1 ) 0.0 0.0 5.0
assign (segid a and resid 256 and name HB  )(segid a and resid 256 and name HN  ) 0.0 0.0 5.0
assign (segid a and resid 256 and name HG1 )(segid a and resid 256 and name HN  ) 0.0 0.0 3.5
assign (segid a and resid 256 and name HG2# )(segid a and resid 256 and name HN  ) 0.0 1.5 4.4
assign (segid a and resid 257 and name HA  )(segid a and resid 257 and name HB# ) 0.0 1.0 3.9
assign (segid a and resid 257 and name HA  )(segid a and resid 257 and name HN  ) 0.0 0.0 2.9
assign (segid a and resid 257 and name HB# )(segid a and resid 257 and name HN  ) 0.0 0.6 4.1
assign (segid a and resid 257 and name HG# )(segid a and resid 257 and name HN  ) 0.0 1.0 4.5
assign (segid a and resid 258 and name HA  )(segid a and resid 258 and name HB# ) 0.0 1.0 4.5
assign (segid a and resid 258 and name HA  )(segid a and resid 258 and name HG# ) 0.0 1.0 4.5
assign (segid a and resid 258 and name HA  )(segid a and resid 258 and name HN  ) 0.0 0.0 3.5
assign (segid a and resid 258 and name HB# )(segid a and resid 258 and name HG# ) 0.0 2.0 5.5
assign (segid a and resid 258 and name HG# )(segid a and resid 258 and name HN  ) 0.0 1.0 4.5
assign (segid a and resid 259 and name HA  )(segid a and resid 259 and name HB# ) 0.0 1.0 4.5
assign (segid a and resid 259 and name HA  )(segid a and resid 259 and name HG# ) 0.0 1.0 7.0
assign (segid a and resid 259 and name HB# )(segid a and resid 259 and name HG# ) 0.0 2.0 8.0
assign (segid a and resid 259 and name HB# )(segid a and resid 259 and name HN  ) 0.0 0.6 3.5
assign (segid a and resid 259 and name HG# )(segid a and resid 259 and name HN  ) 0.0 1.0 7.0
assign (segid a and resid 260 and name HA  )(segid a and resid 260 and name HB# ) 0.0 1.0 3.9
assign (segid a and resid 261 and name HA  )(segid a and resid 261 and name HB# ) 0.0 1.0 3.9
assign (segid a and resid 261 and name HA  )(segid a and resid 261 and name HN  ) 0.0 0.0 3.5
assign (segid a and resid 261 and name HB# )(segid a and resid 261 and name HN  ) 0.0 0.6 3.5
assign (segid a and resid 261 and name HG# )(segid a and resid 261 and name HN  ) 0.0 1.0 6.0
assign (segid a and resid 262 and name HA  )(segid a and resid 262 and name HB# ) 0.0 1.0 3.9
assign (segid a and resid 262 and name HA  )(segid a and resid 262 and name HG# ) 0.0 1.0 3.9
assign (segid a and resid 262 and name HA  )(segid a and resid 262 and name HN  ) 0.0 0.0 5.0
assign (segid a and resid 262 and name HG# )(segid a and resid 262 and name HN  ) 0.0 1.0 6.0
assign (segid a and resid 263 and name HA  )(segid a and resid 263 and name HB# ) 0.0 1.0 4.5
assign (segid a and resid 263 and name HA  )(segid a and resid 263 and name HN  ) 0.0 0.0 3.5
assign (segid a and resid 263 and name HB# )(segid a and resid 263 and name HN  ) 0.0 0.6 4.1
assign (segid a and resid 264 and name HA# )(segid a and resid 264 and name HN  ) 0.0 0.6 3.5
assign (segid a and resid 265 and name HA  )(segid a and resid 265 and name HB# ) 0.0 1.0 4.5
assign (segid a and resid 265 and name HB# )(segid a and resid 265 and name HN  ) 0.0 0.6 4.1
assign (segid a and resid 265 and name HD# )(segid a and resid 265 and name HN  ) 0.0 2.0 7.0
assign (segid a and resid 265 and name HE# )(segid a and resid 265 and name HN  ) 0.0 2.0 4.9
assign (segid a and resid 266 and name HA  )(segid a and resid 266 and name HB# ) 0.0 1.0 6.0
assign (segid a and resid 266 and name HA  )(segid a and resid 266 and name HD1# ) 0.0 1.5 5.0
assign (segid a and resid 266 and name HA  )(segid a and resid 266 and name HD2# ) 0.0 1.5 4.4
assign (segid a and resid 266 and name HA  )(segid a and resid 266 and name HN  ) 0.0 0.0 5.0
assign (segid a and resid 266 and name HB# )(segid a and resid 266 and name HD1# ) 0.0 2.5 6.0
assign (segid a and resid 266 and name HB# )(segid a and resid 266 and name HN  ) 0.0 0.6 5.6
assign (segid a and resid 266 and name HD# )(segid a and resid 266 and name HG  ) 0.0 1.7 4.6
assign (segid a and resid 266 and name HD1# )(segid a and resid 266 and name HN  ) 0.0 1.5 6.5
assign (segid a and resid 266 and name HD2# )(segid a and resid 266 and name HN  ) 0.0 1.5 5.0
assign (segid a and resid 267 and name HA  )(segid a and resid 267 and name HB# ) 0.0 1.5 4.4
assign (segid a and resid 267 and name HA  )(segid a and resid 267 and name HN  ) 0.0 0.0 5.0
assign (segid a and resid 267 and name HB# )(segid a and resid 267 and name HN  ) 0.0 1.1 4.0
assign (segid a and resid 268 and name HA  )(segid a and resid 268 and name HB# ) 0.0 1.0 3.9
assign (segid a and resid 268 and name HA  )(segid a and resid 268 and name HG# ) 0.0 1.0 4.5
assign (segid a and resid 268 and name HG# )(segid a and resid 268 and name HN  ) 0.0 1.0 3.9
assign (segid a and resid 269 and name HA  )(segid a and resid 269 and name HB# ) 0.0 1.0 4.5
assign (segid a and resid 270 and name HA  )(segid a and resid 270 and name HB  ) 0.0 0.0 5.0
assign (segid a and resid 270 and name HA  )(segid a and resid 270 and name HD1# ) 0.0 1.5 5.0
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Table A.4. *(continued)*

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assign (segid a and resid 270 and name HA  )(segid a and resid 270 and name HG2# ) 0.0 1.5 5.0
assign (segid a and resid 270 and name HA  )(segid a and resid 270 and name HN  ) 0.0 0.0 6.0
assign (segid a and resid 270 and name HB  )(segid a and resid 270 and name HD1# ) 0.0 1.5 6.5
assign (segid a and resid 270 and name HB  )(segid a and resid 270 and name HG2# ) 0.0 1.5 5.0
assign (segid a and resid 270 and name HD1# )(segid a and resid 270 and name HG2# ) 0.0 3.0 5.9
assign (segid a and resid 270 and name HD1# )(segid a and resid 270 and name HN  ) 0.0 1.5 6.5
assign (segid a and resid 270 and name HG2# )(segid a and resid 270 and name HN  ) 0.0 1.5 6.5
assign (segid a and resid 271 and name HA  )(segid a and resid 271 and name HB# ) 0.0 1.0 4.5
assign (segid a and resid 271 and name HA  )(segid a and resid 271 and name HN  ) 0.0 0.0 6.0
assign (segid a and resid 271 and name HB# )(segid a and resid 271 and name HN  ) 0.0 0.6 4.1
assign (segid a and resid 271 and name HD2# )(segid a and resid 271 and name HN  ) 0.0 1.0 6.0
assign (segid a and resid 272 and name HA  )(segid a and resid 272 and name HB# ) 0.0 1.0 3.9
assign (segid a and resid 272 and name HA  )(segid a and resid 272 and name HD# ) 0.0 1.0 4.5
assign (segid a and resid 272 and name HA  )(segid a and resid 272 and name HG# ) 0.0 1.0 4.5
assign (segid a and resid 272 and name HA  )(segid a and resid 272 and name HN  ) 0.0 0.0 2.9
assign (segid a and resid 272 and name HB# )(segid a and resid 272 and name HD# ) 0.0 2.0 5.5
assign (segid a and resid 272 and name HB# )(segid a and resid 272 and name HG# ) 0.0 2.0 5.5
assign (segid a and resid 272 and name HB# )(segid a and resid 272 and name HN  ) 0.0 0.6 3.5
assign (segid a and resid 272 and name HD# )(segid a and resid 272 and name HE# ) 0.0 2.0 4.9
assign (segid a and resid 272 and name HG# )(segid a and resid 272 and name HN  ) 0.0 1.0 4.5
assign (segid a and resid 273 and name HA  )(segid a and resid 273 and name HB# ) 0.0 1.0 7.0
assign (segid a and resid 273 and name HA  )(segid a and resid 273 and name HN  ) 0.0 0.0 3.5
assign (segid a and resid 273 and name HB# )(segid a and resid 273 and name HN  ) 0.0 0.6 6.6
assign (segid a and resid 274 and name HA  )(segid a and resid 274 and name HB  ) 0.0 0.0 3.5
assign (segid a and resid 274 and name HA  )(segid a and resid 274 and name HD1# ) 0.0 1.5 4.4
assign (segid a and resid 274 and name HA  )(segid a and resid 274 and name HG1# ) 0.0 1.0 6.0
assign (segid a and resid 274 and name HA  )(segid a and resid 274 and name HG2# ) 0.0 1.5 6.5
assign (segid a and resid 274 and name HA  )(segid a and resid 274 and name HN  ) 0.0 0.0 5.0
assign (segid a and resid 274 and name HB  )(segid a and resid 274 and name HD1# ) 0.0 1.5 4.4
assign (segid a and resid 274 and name HB  )(segid a and resid 274 and name HG1# ) 0.0 1.0 6.0
assign (segid a and resid 274 and name HB  )(segid a and resid 274 and name HG2# ) 0.0 1.5 4.4
assign (segid a and resid 274 and name HB  )(segid a and resid 274 and name HN  ) 0.0 0.0 3.5
assign (segid a and resid 274 and name HD1# )(segid a and resid 274 and name HG1# ) 0.0 2.5 5.4
assign (segid a and resid 274 and name HG1# )(segid a and resid 274 and name HG2# ) 0.0 2.5 8.5
assign (segid a and resid 274 and name HG1# )(segid a and resid 274 and name HN  ) 0.0 1.0 6.0
assign (segid a and resid 274 and name HG2# )(segid a and resid 274 and name HN  ) 0.0 1.5 4.4
assign (segid a and resid 275 and name HA  )(segid a and resid 275 and name HB# ) 0.0 1.0 3.9
assign (segid a and resid 275 and name HG# )(segid a and resid 275 and name HN  ) 0.0 1.0 4.5
assign (segid a and resid 276 and name HA  )(segid a and resid 276 and name HB# ) 0.0 1.0 3.9
assign (segid a and resid 276 and name HG# )(segid a and resid 276 and name HN  ) 0.0 1.0 3.9
assign (segid a and resid 277 and name HA  )(segid a and resid 277 and name HB# ) 0.0 1.0 4.5
assign (segid a and resid 277 and name HA  )(segid a and resid 277 and name HN  ) 0.0 0.0 5.0
assign (segid a and resid 277 and name HB# )(segid a and resid 277 and name HN  ) 0.0 0.6 4.1
assign (segid a and resid 278 and name HA  )(segid a and resid 278 and name HB# ) 0.0 1.0 3.9
assign (segid a and resid 278 and name HA  )(segid a and resid 278 and name HN  ) 0.0 0.0 6.0
assign (segid a and resid 278 and name HB# )(segid a and resid 278 and name HN  ) 0.0 0.6 3.5
assign (segid a and resid 279 and name HB# )(segid a and resid 279 and name HN  ) 0.0 1.1 4.0
assign (segid a and resid 280 and name HA  )(segid a and resid 280 and name HB  ) 0.0 0.0 6.0
assign (segid a and resid 280 and name HA  )(segid a and resid 280 and name HG1# ) 0.0 1.0 4.5
assign (segid a and resid 280 and name HA  )(segid a and resid 280 and name HG2# ) 0.0 1.5 4.4
assign (segid a and resid 280 and name HA  )(segid a and resid 280 and name HN  ) 0.0 0.0 5.0
assign (segid a and resid 280 and name HB  )(segid a and resid 280 and name HD1# ) 0.0 1.5 5.0
assign (segid a and resid 280 and name HB  )(segid a and resid 280 and name HG1# ) 0.0 1.0 4.5
assign (segid a and resid 280 and name HB  )(segid a and resid 280 and name HG2# ) 0.0 1.5 4.4
assign (segid a and resid 280 and name HB  )(segid a and resid 280 and name HN  ) 0.0 0.0 3.5
assign (segid a and resid 280 and name HD1# )(segid a and resid 280 and name HG1# ) 0.0 2.5 6.0
assign (segid a and resid 280 and name HD1# )(segid a and resid 280 and name HN  ) 0.0 1.5 7.5
assign (segid a and resid 280 and name HG1# )(segid a and resid 280 and name HG2# ) 0.0 2.5 6.0
assign (segid a and resid 280 and name HG1# )(segid a and resid 280 and name HN  ) 0.0 1.0 4.5
assign (segid a and resid 280 and name HG2# )(segid a and resid 280 and name HN  ) 0.0 1.5 5.0
assign (segid a and resid 281 and name HA  )(segid a and resid 281 and name HB  ) 0.0 0.0 6.0
assign (segid a and resid 281 and name HA  )(segid a and resid 281 and name HD1# ) 0.0 1.5 5.0
assign (segid a and resid 281 and name HA  )(segid a and resid 281 and name HG1# ) 0.0 1.0 4.5
assign (segid a and resid 281 and name HA  )(segid a and resid 281 and name HG2# ) 0.0 1.5 5.0
assign (segid a and resid 281 and name HA  )(segid a and resid 281 and name HN  ) 0.0 0.0 5.0
assign (segid a and resid 281 and name HD1# )(segid a and resid 281 and name HG1# ) 0.0 2.5 5.4
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Table A.4. *(continued)*

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assign (segid a and resid 281 and name HD1# )(segid a and resid 281 and name HN  ) 0.0 1.5 6.5
assign (segid a and resid 281 and name HG1# )(segid a and resid 281 and name HN  ) 0.0 1.0 4.5
assign (segid a and resid 281 and name HG2# )(segid a and resid 281 and name HN  ) 0.0 1.5 4.4
assign (segid a and resid 282 and name HA   )(segid a and resid 282 and name HB# ) 0.0 1.0 3.9
assign (segid a and resid 282 and name HA   )(segid a and resid 282 and name HG# ) 0.0 1.0 4.5
assign (segid a and resid 282 and name HA   )(segid a and resid 282 and name HN  ) 0.0 0.0 3.5
assign (segid a and resid 282 and name HB#  )(segid a and resid 282 and name HN  ) 0.0 0.6 3.5
assign (segid a and resid 282 and name HG#  )(segid a and resid 282 and name HN  ) 0.0 1.0 6.0
assign (segid a and resid 283 and name HA   )(segid a and resid 283 and name HB# ) 0.0 1.0 4.5
assign (segid a and resid 283 and name HA   )(segid a and resid 283 and name HG# ) 0.0 1.0 4.5
assign (segid a and resid 283 and name HA   )(segid a and resid 283 and name HN  ) 0.0 0.0 2.9
assign (segid a and resid 283 and name HE2# )(segid a and resid 283 and name HG# ) 0.0 2.0 5.5
assign (segid a and resid 283 and name HE2# )(segid a and resid 283 and name HN  ) 0.0 1.0 6.0
assign (segid a and resid 283 and name HG#  )(segid a and resid 283 and name HN  ) 0.0 1.0 3.9
assign (segid a and resid 284 and name HA   )(segid a and resid 284 and name HB# ) 0.0 1.0 4.5
assign (segid a and resid 284 and name HB#  )(segid a and resid 284 and name HN  ) 0.0 0.6 4.1
assign (segid a and resid 285 and name HA   )(segid a and resid 285 and name HB  ) 0.0 0.0 3.5
assign (segid a and resid 285 and name HA   )(segid a and resid 285 and name HD1# ) 0.0 1.5 4.4
assign (segid a and resid 285 and name HA   )(segid a and resid 285 and name HG1# ) 0.0 1.0 4.5
assign (segid a and resid 285 and name HA   )(segid a and resid 285 and name HG2# ) 0.0 1.5 4.4
assign (segid a and resid 285 and name HA   )(segid a and resid 285 and name HN  ) 0.0 0.0 3.5
assign (segid a and resid 285 and name HB   )(segid a and resid 285 and name HD1# ) 0.0 1.5 5.0
assign (segid a and resid 285 and name HB   )(segid a and resid 285 and name HG1# ) 0.0 1.0 4.5
assign (segid a and resid 285 and name HB   )(segid a and resid 285 and name HG2# ) 0.0 1.5 4.4
assign (segid a and resid 285 and name HB   )(segid a and resid 285 and name HN  ) 0.0 0.0 3.5
assign (segid a and resid 285 and name HD1# )(segid a and resid 285 and name HG1# ) 0.0 2.5 5.4
assign (segid a and resid 285 and name HG1# )(segid a and resid 285 and name HG2# ) 0.0 2.5 5.4
assign (segid a and resid 285 and name HG1# )(segid a and resid 285 and name HN  ) 0.0 1.0 6.0
assign (segid a and resid 285 and name HG2# )(segid a and resid 285 and name HN  ) 0.0 1.5 4.4
assign (segid a and resid 286 and name HA   )(segid a and resid 286 and name HB# ) 0.0 1.0 3.9
assign (segid a and resid 286 and name HA   )(segid a and resid 286 and name HN  ) 0.0 0.0 2.9
assign (segid a and resid 286 and name HB#  )(segid a and resid 286 and name HN  ) 0.0 0.6 3.5
assign (segid a and resid 287 and name HA   )(segid a and resid 287 and name HB# ) 0.0 1.0 4.5
assign (segid a and resid 287 and name HA   )(segid a and resid 287 and name HN  ) 0.0 0.0 2.9
assign (segid a and resid 287 and name HB#  )(segid a and resid 287 and name HN  ) 0.0 0.6 3.5
assign (segid a and resid 287 and name HD#  )(segid a and resid 287 and name HN  ) 0.0 2.0 8.0
assign (segid a and resid 287 and name HE#  )(segid a and resid 287 and name HN  ) 0.0 2.0 8.0
assign (segid a and resid 288 and name HA   )(segid a and resid 288 and name HB# ) 0.0 1.0 4.5
assign (segid a and resid 288 and name HA   )(segid a and resid 288 and name HD1# ) 0.0 1.5 6.5
assign (segid a and resid 288 and name HA   )(segid a and resid 288 and name HD2# ) 0.0 1.5 4.4
assign (segid a and resid 288 and name HA   )(segid a and resid 288 and name HG  ) 0.0 0.0 2.9
assign (segid a and resid 288 and name HA   )(segid a and resid 288 and name HN  ) 0.0 0.0 3.5
assign (segid a and resid 288 and name HD#  )(segid a and resid 288 and name HG  ) 0.0 1.7 4.6
assign (segid a and resid 288 and name HD1# )(segid a and resid 288 and name HN  ) 0.0 1.5 7.5
assign (segid a and resid 288 and name HD2# )(segid a and resid 288 and name HN  ) 0.0 1.5 7.5
assign (segid a and resid 288 and name HG   )(segid a and resid 288 and name HN  ) 0.0 0.0 5.0
assign (segid a and resid 289 and name HA   )(segid a and resid 289 and name HB# ) 0.0 1.0 4.5
assign (segid a and resid 289 and name HA   )(segid a and resid 289 and name HD# ) 0.0 1.0 4.5
assign (segid a and resid 289 and name HA   )(segid a and resid 289 and name HG# ) 0.0 1.0 4.5
assign (segid a and resid 289 and name HB#  )(segid a and resid 289 and name HN  ) 0.0 0.6 3.5
assign (segid a and resid 289 and name HD#  )(segid a and resid 289 and name HG# ) 0.0 2.0 4.9
assign (segid a and resid 289 and name HG#  )(segid a and resid 289 and name HN  ) 0.0 1.0 4.5
assign (segid b and resid 225 and name HA   )(segid b and resid 225 and name HB# ) 0.0 1.5 5.0
assign (segid b and resid 227 and name HA   )(segid b and resid 227 and name HB  ) 0.0 0.0 3.5
assign (segid b and resid 227 and name HB   )(segid b and resid 227 and name HN  ) 0.0 0.0 5.0
assign (segid b and resid 227 and name HG1# )(segid b and resid 227 and name HN  ) 0.0 1.5 5.0
assign (segid b and resid 228 and name HA   )(segid b and resid 228 and name HB# ) 0.0 1.0 3.9
assign (segid b and resid 228 and name HA   )(segid b and resid 228 and name HN  ) 0.0 0.0 5.0
assign (segid b and resid 228 and name HD#  )(segid b and resid 228 and name HG# ) 0.0 2.0 4.9
assign (segid b and resid 228 and name HG#  )(segid b and resid 228 and name HN  ) 0.0 1.0 6.0
assign (segid b and resid 229 and name HA   )(segid b and resid 229 and name HB# ) 0.0 1.0 3.9
assign (segid b and resid 229 and name HA   )(segid b and resid 229 and name HG# ) 0.0 1.0 3.9
assign (segid b and resid 229 and name HB#  )(segid b and resid 229 and name HG# ) 0.0 2.0 4.9
assign (segid b and resid 229 and name HB#  )(segid b and resid 229 and name HN  ) 0.0 0.6 5.6
assign (segid b and resid 229 and name HG#  )(segid b and resid 229 and name HN  ) 0.0 1.0 6.0
assign (segid b and resid 230 and name HA   )(segid b and resid 230 and name HB# ) 0.0 1.0 4.5
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Table A.4. *(continued)*

```
assign (segid b and resid 230 and name HA   )(segid b and resid 230 and name HD2# ) 0.0 1.5 4.4
assign (segid b and resid 230 and name HA   )(segid b and resid 230 and name HN  ) 0.0 0.0 2.9
assign (segid b and resid 230 and name HD1# )(segid b and resid 230 and name HN  ) 0.0 1.5 6.5
assign (segid b and resid 231 and name HA   )(segid b and resid 231 and name HB# ) 0.0 1.5 4.4
assign (segid b and resid 231 and name HA   )(segid b and resid 231 and name HN  ) 0.0 0.0 2.9
assign (segid b and resid 231 and name HB#  )(segid b and resid 231 and name HN  ) 0.0 1.1 4.0
assign (segid b and resid 232 and name HA   )(segid b and resid 232 and name HB# ) 0.0 1.0 3.9
assign (segid b and resid 232 and name HA   )(segid b and resid 232 and name HN  ) 0.0 0.0 3.5
assign (segid b and resid 233 and name HA   )(segid b and resid 233 and name HB# ) 0.0 1.0 3.9
assign (segid b and resid 233 and name HA   )(segid b and resid 233 and name HN  ) 0.0 0.0 2.9
assign (segid b and resid 233 and name HB#  )(segid b and resid 233 and name HN  ) 0.0 0.6 3.5
assign (segid b and resid 234 and name HA   )(segid b and resid 234 and name HB# ) 0.0 1.0 3.9
assign (segid b and resid 234 and name HA   )(segid b and resid 234 and name HD# ) 0.0 1.0 6.0
assign (segid b and resid 234 and name HA   )(segid b and resid 234 and name HG# ) 0.0 1.0 3.9
assign (segid b and resid 234 and name HA   )(segid b and resid 234 and name HN  ) 0.0 0.0 3.5
assign (segid b and resid 234 and name HB#  )(segid b and resid 234 and name HD# ) 0.0 2.0 5.5
assign (segid b and resid 234 and name HB#  )(segid b and resid 234 and name HG# ) 0.0 2.0 4.9
assign (segid b and resid 234 and name HB#  )(segid b and resid 234 and name HN  ) 0.0 0.6 3.5
assign (segid b and resid 235 and name HA   )(segid b and resid 235 and name HB  ) 0.0 0.0 6.0
assign (segid b and resid 235 and name HA   )(segid b and resid 235 and name HG2# ) 0.0 1.5 4.4
assign (segid b and resid 235 and name HA   )(segid b and resid 235 and name HN  ) 0.0 0.0 3.5
assign (segid b and resid 235 and name HB   )(segid b and resid 235 and name HG2# ) 0.0 1.5 4.4
assign (segid b and resid 235 and name HB   )(segid b and resid 235 and name HN  ) 0.0 0.0 2.9
assign (segid b and resid 235 and name HG2# )(segid b and resid 235 and name HN  ) 0.0 1.5 5.0
assign (segid b and resid 236 and name HA   )(segid b and resid 236 and name HB# ) 0.0 1.0 3.9
assign (segid b and resid 236 and name HA   )(segid b and resid 236 and name HD1# ) 0.0 1.5 4.4
assign (segid b and resid 236 and name HA   )(segid b and resid 236 and name HD2# ) 0.0 1.5 4.4
assign (segid b and resid 236 and name HA   )(segid b and resid 236 and name HG  ) 0.0 0.0 2.9
assign (segid b and resid 236 and name HA   )(segid b and resid 236 and name HN  ) 0.0 0.0 2.9
assign (segid b and resid 236 and name HB#  )(segid b and resid 236 and name HD1# ) 0.0 2.5 5.4
assign (segid b and resid 236 and name HB#  )(segid b and resid 236 and name HD2# ) 0.0 2.5 6.0
assign (segid b and resid 236 and name HD#  )(segid b and resid 236 and name HG  ) 0.0 1.7 4.6
assign (segid b and resid 236 and name HD#  )(segid b and resid 236 and name HN  ) 0.0 1.7 6.7
assign (segid b and resid 236 and name HG   )(segid b and resid 236 and name HN  ) 0.0 0.0 3.5
assign (segid b and resid 237 and name HA   )(segid b and resid 237 and name HB# ) 0.0 1.0 4.5
assign (segid b and resid 237 and name HA   )(segid b and resid 237 and name HD1# ) 0.0 1.5 7.5
assign (segid b and resid 237 and name HA   )(segid b and resid 237 and name HD2# ) 0.0 1.5 4.4
assign (segid b and resid 237 and name HA   )(segid b and resid 237 and name HN  ) 0.0 0.0 2.9
assign (segid b and resid 237 and name HB#  )(segid b and resid 237 and name HN  ) 0.0 0.6 4.1
assign (segid b and resid 237 and name HD1# )(segid b and resid 237 and name HG  ) 0.0 1.5 4.4
assign (segid b and resid 237 and name HD2# )(segid b and resid 237 and name HG  ) 0.0 1.5 7.5
assign (segid b and resid 238 and name HA   )(segid b and resid 238 and name HB# ) 0.0 1.0 4.5
assign (segid b and resid 238 and name HA   )(segid b and resid 238 and name HG# ) 0.0 1.0 4.5
assign (segid b and resid 238 and name HB#  )(segid b and resid 238 and name HG# ) 0.0 2.0 4.9
assign (segid b and resid 238 and name HG#  )(segid b and resid 238 and name HN  ) 0.0 1.0 6.0
assign (segid b and resid 239 and name HA   )(segid b and resid 239 and name HB# ) 0.0 1.5 4.4
assign (segid b and resid 239 and name HA   )(segid b and resid 239 and name HN  ) 0.0 0.0 2.9
assign (segid b and resid 239 and name HB#  )(segid b and resid 239 and name HN  ) 0.0 1.1 4.0
assign (segid b and resid 240 and name HA#  )(segid b and resid 240 and name HN  ) 0.0 0.6 3.5
assign (segid b and resid 241 and name HA   )(segid b and resid 241 and name HB  ) 0.0 0.0 5.0
assign (segid b and resid 241 and name HA   )(segid b and resid 241 and name HG1# ) 0.0 1.5 5.0
assign (segid b and resid 241 and name HA   )(segid b and resid 241 and name HG2# ) 0.0 1.5 4.4
assign (segid b and resid 241 and name HA   )(segid b and resid 241 and name HN  ) 0.0 0.0 3.5
assign (segid b and resid 241 and name HB   )(segid b and resid 241 and name HG# ) 0.0 1.7 4.6
assign (segid b and resid 241 and name HB   )(segid b and resid 241 and name HN  ) 0.0 0.0 2.9
assign (segid b and resid 241 and name HG#  )(segid b and resid 241 and name HN  ) 0.0 1.7 5.2
assign (segid b and resid 241 and name HG1# )(segid b and resid 241 and name HN  ) 0.0 1.5 6.5
assign (segid b and resid 241 and name HG2# )(segid b and resid 241 and name HN  ) 0.0 1.5 5.0
assign (segid b and resid 242 and name HA   )(segid b and resid 242 and name HB# ) 0.0 1.0 4.5
assign (segid b and resid 242 and name HA   )(segid b and resid 242 and name HN  ) 0.0 0.0 5.0
assign (segid b and resid 243 and name HA   )(segid b and resid 243 and name HB# ) 0.0 1.0 4.5
assign (segid b and resid 243 and name HA   )(segid b and resid 243 and name HN  ) 0.0 0.0 5.0
assign (segid b and resid 243 and name HB#  )(segid b and resid 243 and name HN  ) 0.0 0.6 5.6
assign (segid b and resid 244 and name HA   )(segid b and resid 244 and name HB# ) 0.0 1.0 6.0
assign (segid b and resid 244 and name HA   )(segid b and resid 244 and name HN  ) 0.0 0.0 5.0
assign (segid b and resid 244 and name HB#  )(segid b and resid 244 and name HN  ) 0.0 0.6 6.6
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Table A.4. *(continued)*

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assign (segid b and resid 245 and name HA  )(segid b and resid 245 and name HB#  ) 0.0 1.0 7.0
assign (segid b and resid 245 and name HA  )(segid b and resid 245 and name HD#  ) 0.0 1.7 5.2
assign (segid b and resid 245 and name HA  )(segid b and resid 245 and name HN   ) 0.0 0.0 5.0
assign (segid b and resid 245 and name HB# )(segid b and resid 245 and name HD#  ) 0.0 3.4 6.9
assign (segid b and resid 245 and name HB# )(segid b and resid 245 and name HG   ) 0.0 1.0 4.5
assign (segid b and resid 245 and name HB# )(segid b and resid 245 and name HN   ) 0.0 0.6 5.6
assign (segid b and resid 246 and name HA  )(segid b and resid 246 and name HB#  ) 0.0 1.0 6.0
assign (segid b and resid 246 and name HA  )(segid b and resid 246 and name HN   ) 0.0 0.0 5.0
assign (segid b and resid 246 and name HB# )(segid b and resid 246 and name HN   ) 0.0 0.6 5.6
assign (segid b and resid 246 and name HG# )(segid b and resid 246 and name HN   ) 0.0 1.0 7.0
assign (segid b and resid 247 and name HA  )(segid b and resid 247 and name HB   ) 0.0 0.0 3.5
assign (segid b and resid 247 and name HA  )(segid b and resid 247 and name HG2# ) 0.0 1.5 4.4
assign (segid b and resid 247 and name HA  )(segid b and resid 247 and name HN   ) 0.0 0.0 5.0
assign (segid b and resid 247 and name HB  )(segid b and resid 247 and name HG2# ) 0.0 1.5 4.4
assign (segid b and resid 247 and name HB  )(segid b and resid 247 and name HN   ) 0.0 0.0 5.0
assign (segid b and resid 247 and name HG2# )(segid b and resid 247 and name HN   ) 0.0 1.5 6.5
assign (segid b and resid 248 and name HA  )(segid b and resid 248 and name HB#  ) 0.0 1.0 4.5
assign (segid b and resid 248 and name HD# )(segid b and resid 248 and name HG#  ) 0.0 2.0 7.0
assign (segid b and resid 249 and name HA  )(segid b and resid 249 and name HB#  ) 0.0 1.0 6.0
assign (segid b and resid 249 and name HA  )(segid b and resid 249 and name HD1# ) 0.0 1.5 5.0
assign (segid b and resid 249 and name HA  )(segid b and resid 249 and name HD2# ) 0.0 1.5 4.4
assign (segid b and resid 249 and name HA  )(segid b and resid 249 and name HG   ) 0.0 0.0 3.5
assign (segid b and resid 249 and name HA  )(segid b and resid 249 and name HN   ) 0.0 0.0 3.5
assign (segid b and resid 249 and name HB# )(segid b and resid 249 and name HD1# ) 0.0 2.5 6.0
assign (segid b and resid 249 and name HB# )(segid b and resid 249 and name HD2# ) 0.0 2.5 6.0
assign (segid b and resid 249 and name HB# )(segid b and resid 249 and name HG   ) 0.0 1.0 4.5
assign (segid b and resid 249 and name HB# )(segid b and resid 249 and name HN   ) 0.0 0.6 5.6
assign (segid b and resid 249 and name HD# )(segid b and resid 249 and name HN   ) 0.0 1.7 5.2
assign (segid b and resid 250 and name HA  )(segid b and resid 250 and name HB   ) 0.0 0.0 5.0
assign (segid b and resid 250 and name HA  )(segid b and resid 250 and name HG2# ) 0.0 1.5 4.4
assign (segid b and resid 250 and name HA  )(segid b and resid 250 and name HN   ) 0.0 0.0 3.5
assign (segid b and resid 250 and name HB  )(segid b and resid 250 and name HG2# ) 0.0 1.5 4.4
assign (segid b and resid 250 and name HG2# )(segid b and resid 250 and name HN   ) 0.0 1.5 5.0
assign (segid b and resid 251 and name HA  )(segid b and resid 251 and name HB#  ) 0.0 1.0 3.9
assign (segid b and resid 251 and name HA  )(segid b and resid 251 and name HN   ) 0.0 0.0 3.5
assign (segid b and resid 251 and name HB# )(segid b and resid 251 and name HN   ) 0.0 0.6 4.1
assign (segid b and resid 252 and name HA  )(segid b and resid 252 and name HB   ) 0.0 0.0 5.0
assign (segid b and resid 252 and name HA  )(segid b and resid 252 and name HG2# ) 0.0 1.5 4.4
assign (segid b and resid 252 and name HA  )(segid b and resid 252 and name HN   ) 0.0 0.0 5.0
assign (segid b and resid 252 and name HB  )(segid b and resid 252 and name HG2# ) 0.0 1.5 5.0
assign (segid b and resid 252 and name HB  )(segid b and resid 252 and name HN   ) 0.0 0.0 3.5
assign (segid b and resid 252 and name HG2# )(segid b and resid 252 and name HN   ) 0.0 1.5 5.0
assign (segid b and resid 253 and name HA  )(segid b and resid 253 and name HD#  ) 0.0 1.0 4.5
assign (segid b and resid 253 and name HA  )(segid b and resid 253 and name HG#  ) 0.0 1.0 6.0
assign (segid b and resid 253 and name HA  )(segid b and resid 253 and name HN   ) 0.0 0.0 3.5
assign (segid b and resid 253 and name HD# )(segid b and resid 253 and name HG#  ) 0.0 2.0 7.0
assign (segid b and resid 253 and name HD# )(segid b and resid 253 and name HN   ) 0.0 1.0 6.0
assign (segid b and resid 253 and name HG# )(segid b and resid 253 and name HN   ) 0.0 1.0 4.5
assign (segid b and resid 254 and name HA  )(segid b and resid 254 and name HB#  ) 0.0 1.0 4.5
assign (segid b and resid 254 and name HA  )(segid b and resid 254 and name HD1# ) 0.0 1.5 4.4
assign (segid b and resid 254 and name HA  )(segid b and resid 254 and name HD2# ) 0.0 1.5 6.5
assign (segid b and resid 254 and name HA  )(segid b and resid 254 and name HG   ) 0.0 0.0 5.0
assign (segid b and resid 254 and name HA  )(segid b and resid 254 and name HN   ) 0.0 0.0 3.5
assign (segid b and resid 254 and name HB# )(segid b and resid 254 and name HD1# ) 0.0 2.5 5.4
assign (segid b and resid 254 and name HB# )(segid b and resid 254 and name HD2# ) 0.0 2.5 5.4
assign (segid b and resid 254 and name HB# )(segid b and resid 254 and name HG   ) 0.0 1.0 4.5
assign (segid b and resid 254 and name HD1# )(segid b and resid 254 and name HG   ) 0.0 1.5 4.4
assign (segid b and resid 254 and name HD1# )(segid b and resid 254 and name HN   ) 0.0 1.5 7.5
assign (segid b and resid 254 and name HD2# )(segid b and resid 254 and name HG   ) 0.0 1.5 4.4
assign (segid b and resid 254 and name HD2# )(segid b and resid 254 and name HN   ) 0.0 1.5 5.0
assign (segid b and resid 254 and name HG  )(segid b and resid 254 and name HN   ) 0.0 0.0 3.5
assign (segid b and resid 255 and name HA  )(segid b and resid 255 and name HB#  ) 0.0 1.5 4.4
assign (segid b and resid 255 and name HA  )(segid b and resid 255 and name HN   ) 0.0 0.0 2.9
assign (segid b and resid 255 and name HB# )(segid b and resid 255 and name HN   ) 0.0 1.1 4.0
assign (segid b and resid 256 and name HA  )(segid b and resid 256 and name HN   ) 0.0 0.0 3.5
assign (segid b and resid 256 and name HB  )(segid b and resid 256 and name HG1  ) 0.0 0.0 5.0
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Table A.4. *(continued)*

```
assign (segid b and resid 256 and name HB  )(segid b and resid 256 and name HN   ) 0.0 0.0 5.0
assign (segid b and resid 256 and name HG1 )(segid b and resid 256 and name HN   ) 0.0 0.0 3.5
assign (segid b and resid 256 and name HG2# )(segid b and resid 256 and name HN   ) 0.0 1.5 4.4
assign (segid b and resid 257 and name HA  )(segid b and resid 257 and name HB#  ) 0.0 1.0 3.9
assign (segid b and resid 257 and name HA  )(segid b and resid 257 and name HN   ) 0.0 0.0 2.9
assign (segid b and resid 257 and name HB# )(segid b and resid 257 and name HN   ) 0.0 0.6 4.1
assign (segid b and resid 257 and name HG# )(segid b and resid 257 and name HN   ) 0.0 1.0 4.5
assign (segid b and reşid 258 and name HA  )(segid b and resid 258 and name HB#  ) 0.0 1.0 4.5
assign (segid b and resid 258 and name HA  )(segid b and resid 258 and name HG#  ) 0.0 1.0 4.5
assign (segid b and resid 258 and name HA  )(segid b and resid 258 and name HN   ) 0.0 0.0 3.5
assign (segid b and resid 258 and name HB# )(segid b and resid 258 and name HG#  ) 0.0 2.0 5.5
assign (segid b and resid 258 and name HG# )(segid b and resid 258 and name HN   ) 0.0 1.0 4.5
assign (segid b and resid 259 and name HA  )(segid b and resid 259 and name HB#  ) 0.0 1.0 4.5
assign (segid b and resid 259 and name HA  )(segid b and resid 259 and name HG#  ) 0.0 1.0 7.0
assign (segid b and resid 259 and name HB# )(segid b and resid 259 and name HG#  ) 0.0 2.0 8.0
assign (segid b and resid 259 and name HB# )(segid b and resid 259 and name HN   ) 0.0 0.6 3.5
assign (segid b and resid 259 and name HG# )(segid b and resid 259 and name HN   ) 0.0 1.0 7.0
assign (segid b and resid 260 and name HA  )(segid b and resid 260 and name HB#  ) 0.0 1.0 3.9
assign (segid b and resid 261 and name HA  )(segid b and resid 261 and name HB#  ) 0.0 1.0 3.9
assign (segid b and resid 261 and name HA  )(segid b and resid 261 and name HN   ) 0.0 0.0 3.5
assign (segid b and resid 261 and name HB# )(segid b and resid 261 and name HN   ) 0.0 0.6 3.5
assign (segid b and resid 261 and name HG# )(segid b and resid 261 and name HN   ) 0.0 1.0 6.0
assign (segid b and resid 262 and name HA  )(segid b and resid 262 and name HB#  ) 0.0 1.0 3.9
assign (segid b and resid 262 and name HA  )(segid b and resid 262 and name HG#  ) 0.0 1.0 3.9
assign (segid b and resid 262 and name HA  )(segid b and resid 262 and name HN   ) 0.0 0.0 5.0
assign (segid b and resid 262 and name HG# )(segid b and resid 262 and name HN   ) 0.0 1.0 6.0
assign (segid b and resid 263 and name HA  )(segid b and resid 263 and name HB#  ) 0.0 1.0 4.5
assign (segid b and resid 263 and name HA  )(segid b and resid 263 and name HN   ) 0.0 0.0 3.5
assign (segid b and resid 263 and name HB# )(segid b and resid 263 and name HN   ) 0.0 0.6 4.1
assign (segid b and resid 264 and name HA# )(segid b and resid 264 and name HN   ) 0.0 0.6 3.5
assign (segid b and resid 265 and name HA  )(segid b and resid 265 and name HB#  ) 0.0 1.0 4.5
assign (segid b and resid 265 and name HB# )(segid b and resid 265 and name HN   ) 0.0 0.6 4.1
assign (segid b and resid 265 and name HD# )(segid b and resid 265 and name HN   ) 0.0 2.0 7.0
assign (segid b and resid 265 and name HE# )(segid b and resid 265 and name HN   ) 0.0 2.0 4.9
assign (segid b and resid 266 and name HA  )(segid b and resid 266 and name HB#  ) 0.0 1.0 6.0
assign (segid b and resid 266 and name HA  )(segid b and resid 266 and name HD1# ) 0.0 1.5 5.0
assign (segid b and resid 266 and name HA  )(segid b and resid 266 and name HD2# ) 0.0 1.5 4.4
assign (segid b and resid 266 and name HA  )(segid b and resid 266 and name HN   ) 0.0 0.0 5.0
assign (segid b and resid 266 and name HB# )(segid b and resid 266 and name HD1# ) 0.0 2.5 6.0
assign (segid b and resid 266 and name HB# )(segid b and resid 266 and name HN   ) 0.0 0.6 5.6
assign (segid b and resid 266 and name HD# )(segid b and resid 266 and name HG   ) 0.0 1.7 4.6
assign (segid b and resid 266 and name HD1# )(segid b and resid 266 and name HN   ) 0.0 1.5 6.5
assign (segid b and resid 266 and name HD2# )(segid b and resid 266 and name HN   ) 0.0 1.5 5.0
assign (segid b and resid 267 and name HA  )(segid b and resid 267 and name HB#  ) 0.0 1.5 4.4
assign (segid b and resid 267 and name HA  )(segid b and resid 267 and name HN   ) 0.0 0.0 5.0
assign (segid b and resid 267 and name HB# )(segid b and resid 267 and name HN   ) 0.0 1.1 4.0
assign (segid b and resid 268 and name HA  )(segid b and resid 268 and name HB#  ) 0.0 1.0 3.9
assign (segid b and resid 268 and name HA  )(segid b and resid 268 and name HG#  ) 0.0 1.0 4.5
assign (segid b and resid 268 and name HG# )(segid b and resid 268 and name HN   ) 0.0 1.0 3.9
assign (segid b and resid 269 and name HA  )(segid b and resid 269 and name HB#  ) 0.0 1.0 4.5
assign (segid b and resid 270 and name HA  )(segid b and resid 270 and name HB   ) 0.0 0.0 5.0
assign (segid b and resid 270 and name HA  )(segid b and resid 270 and name HD1# ) 0.0 1.5 5.0
assign (segid b and resid 270 and name HA  )(segid b and resid 270 and name HG2# ) 0.0 1.5 5.0
assign (segid b and resid 270 and name HA  )(segid b and resid 270 and name HN   ) 0.0 0.0 6.0
assign (segid b and resid 270 and name HB  )(segid b and resid 270 and name HD1# ) 0.0 1.5 6.5
assign (segid b and resid 270 and name HB  )(segid b and resid 270 and name HG2# ) 0.0 1.5 5.0
assign (segid b and resid 270 and name HD1# )(segid b and resid 270 and name HG2# ) 0.0 3.0 5.9
assign (segid b and resid 270 and name HD1# )(segid b and resid 270 and name HN   ) 0.0 1.5 6.5
assign (segid b and resid 270 and name HG2# )(segid b and resid 270 and name HN   ) 0.0 1.5 6.5
assign (segid b and resid 271 and name HA  )(segid b and resid 271 and name HB#  ) 0.0 1.0 4.5
assign (segid b and resid 271 and name HA  )(segid b and resid 271 and name HN   ) 0.0 0.0 6.0
assign (segid b and resid 271 and name HB# )(segid b and resid 271 and name HN   ) 0.0 0.6 4.1
assign (segid b and resid 271 and name HD2# )(segid b and resid 271 and name HN   ) 0.0 1.0 6.0
assign (segid b and resid 272 and name HA  )(segid b and resid 272 and name HB#  ) 0.0 1.0 3.9
assign (segid b and resid 272 and name HA  )(segid b and resid 272 and name HD#  ) 0.0 1.0 4.5
assign (segid b and resid 272 and name HA  )(segid b and resid 272 and name HG#  ) 0.0 1.0 4.5
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Table A.4. *(continued)*

```
assign (segid b and resid 272 and name HA  )(segid b and resid 272 and name HN  ) 0.0 0.0 2.9
assign (segid b and resid 272 and name HB# )(segid b and resid 272 and name HD# ) 0.0 2.0 5.5
assign (segid b and resid 272 and name HB# )(segid b and resid 272 and name HG# ) 0.0 2.0 5.5
assign (segid b and resid 272 and name HB# )(segid b and resid 272 and name HN  ) 0.0 0.6 3.5
assign (segid b and resid 272 and name HD# )(segid b and resid 272 and name HE# ) 0.0 2.0 4.9
assign (segid b and resid 272 and name HG# )(segid b and resid 272 and name HN  ) 0.0 1.0 4.5
assign (segid b and resid 273 and name HA  )(segid b and resid 273 and name HB# ) 0.0 1.0 7.0
assign (segid b and resid 273 and name HA  )(segid b and resid 273 and name HN  ) 0.0 0.0 3.5
assign (segid b and resid 273 and name HB# )(segid b and resid 273 and name HN  ) 0.0 0.6 6.6
assign (segid b and resid 274 and name HA  )(segid b and resid 274 and name HB  ) 0.0 0.0 3.5
assign (segid b and resid 274 and name HA  )(segid b and resid 274 and name HD1# ) 0.0 1.5 4.4
assign (segid b and resid 274 and name HA  )(segid b and resid 274 and name HG1# ) 0.0 1.0 6.0
assign (segid b and resid 274 and name HA  )(segid b and resid 274 and name HG2# ) 0.0 1.5 6.5
assign (segid b and resid 274 and name HA  )(segid b and resid 274 and name HN  ) 0.0 0.0 5.0
assign (segid b and resid 274 and name HB  )(segid b and resid 274 and name HD1# ) 0.0 1.5 4.4
assign (segid b and resid 274 and name HB  )(segid b and resid 274 and name HG1# ) 0.0 1.0 6.0
assign (segid b and resid 274 and name HB  )(segid b and resid 274 and name HG2# ) 0.0 1.5 4.4
assign (segid b and resid 274 and name HB  )(segid b and resid 274 and name HN  ) 0.0 0.0 3.5
assign (segid b and resid 274 and name HD1# )(segid b and resid 274 and name HG1# ) 0.0 2.5 5.4
assign (segid b and resid 274 and name HG1# )(segid b and resid 274 and name HG2# ) 0.0 2.5 8.5
assign (segid b and resid 274 and name HG1# )(segid b and resid 274 and name HN  ) 0.0 1.0 6.0
assign (segid b and resid 274 and name HG2# )(segid b and resid 274 and name HN  ) 0.0 1.5 4.4
assign (segid b and resid 275 and name HA  )(segid b and resid 275 and name HB# ) 0.0 1.0 3.9
assign (segid b and resid 275 and name HG# )(segid b and resid 275 and name HN  ) 0.0 1.0 4.5
assign (segid b and resid 276 and name HA  )(segid b and resid 276 and name HB# ) 0.0 1.0 3.9
assign (segid b and resid 276 and name HG# )(segid b and resid 276 and name HN  ) 0.0 1.0 3.9
assign (segid b and resid 277 and name HA  )(segid b and resid 277 and name HB# ) 0.0 1.0 4.5
assign (segid b and resid 277 and name HA  )(segid b and resid 277 and name HN  ) 0.0 0.0 5.0
assign (segid b and resid 277 and name HB# )(segid b and resid 277 and name HN  ) 0.0 0.6 4.1
assign (segid b and resid 278 and name HA  )(segid b and resid 278 and name HB# ) 0.0 1.0 3.9
assign (segid b and resid 278 and name HA  )(segid b and resid 278 and name HN  ) 0.0 0.0 6.0
assign (segid b and resid 278 and name HB# )(segid b and resid 278 and name HN  ) 0.0 0.6 3.5
assign (segid b and resid 279 and name HB# )(segid b and resid 279 and name HN  ) 0.0 1.1 4.0
assign (segid b and resid 280 and name HA  )(segid b and resid 280 and name HB  ) 0.0 0.0 6.0
assign (segid b and resid 280 and name HA  )(segid b and resid 280 and name HG1# ) 0.0 1.0 4.5
assign (segid b and resid 280 and name HA  )(segid b and resid 280 and name HG2# ) 0.0 1.5 4.4
assign (segid b and resid 280 and name HA  )(segid b and resid 280 and name HN  ) 0.0 0.0 5.0
assign (segid b and resid 280 and name HB  )(segid b and resid 280 and name HD1# ) 0.0 1.5 5.0
assign (segid b and resid 280 and name HB  )(segid b and resid 280 and name HG1# ) 0.0 1.0 4.5
assign (segid b and resid 280 and name HB  )(segid b and resid 280 and name HG2# ) 0.0 1.5 4.4
assign (segid b and resid 280 and name HB  )(segid b and resid 280 and name HN  ) 0.0 0.0 3.5
assign (segid b and resid 280 and name HD1# )(segid b and resid 280 and name HG1# ) 0.0 2.5 6.0
assign (segid b and resid 280 and name HD1# )(segid b and resid 280 and name HN  ) 0.0 1.5 7.5
assign (segid b and resid 280 and name HG1# )(segid b and resid 280 and name HG2# ) 0.0 2.5 6.0
assign (segid b and resid 280 and name HG1# )(segid b and resid 280 and name HN  ) 0.0 1.0 4.5
assign (segid b and resid 280 and name HG2# )(segid b and resid 280 and name HN  ) 0.0 1.5 5.0
assign (segid b and resid 281 and name HA  )(segid b and resid 281 and name HB  ) 0.0 0.0 6.0
assign (segid b and resid 281 and name HA  )(segid b and resid 281 and name HD1# ) 0.0 1.5 5.0
assign (segid b and resid 281 and name HA  )(segid b and resid 281 and name HG1# ) 0.0 1.0 4.5
assign (segid b and resid 281 and name HA  )(segid b and resid 281 and name HG2# ) 0.0 1.5 5.0
assign (segid b and resid 281 and name HA  )(segid b and resid 281 and name HN  ) 0.0 0.0 5.0
assign (segid b and resid 281 and name HD1# )(segid b and resid 281 and name HG1# ) 0.0 2.5 5.4
assign (segid b and resid 281 and name HD1# )(segid b and resid 281 and name HN  ) 0.0 1.5 6.5
assign (segid b and resid 281 and name HG1# )(segid b and resid 281 and name HN  ) 0.0 1.0 4.5
assign (segid b and resid 281 and name HG2# )(segid b and resid 281 and name HN  ) 0.0 1.5 4.4
assign (segid b and resid 282 and name HA  )(segid b and resid 282 and name HB# ) 0.0 1.0 3.9
assign (segid b and resid 282 and name HA  )(segid b and resid 282 and name HG# ) 0.0 1.0 4.5
assign (segid b and resid 282 and name HA  )(segid b and resid 282 and name HN  ) 0.0 0.0 3.5
assign (segid b and resid 282 and name HB# )(segid b and resid 282 and name HN  ) 0.0 0.6 3.5
assign (segid b and resid 282 and name HG# )(segid b and resid 282 and name HN  ) 0.0 1.0 6.0
assign (segid b and resid 283 and name HA  )(segid b and resid 283 and name HB# ) 0.0 1.0 4.5
assign (segid b and resid 283 and name HA  )(segid b and resid 283 and name HG# ) 0.0 1.0 4.5
assign (segid b and resid 283 and name HA  )(segid b and resid 283 and name HN  ) 0.0 0.0 2.9
assign (segid b and resid 283 and name HE2# )(segid b and resid 283 and name HG# ) 0.0 2.0 5.5
assign (segid b and resid 283 and name HE2# )(segid b and resid 283 and name HN  ) 0.0 1.0 6.0
assign (segid b and resid 283 and name HG# )(segid b and resid 283 and name HN  ) 0.0 1.0 3.9
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Table A.4. *(continued)*

```
assign (segid b and resid 284 and name HA  )(segid b and resid 284 and name HB# ) 0.0 1.0 4.5
assign (segid b and resid 284 and name HB# )(segid b and resid 284 and name HN  ) 0.0 0.6 4.1
assign (segid b and resid 285 and name HA  )(segid b and resid 285 and name HB  ) 0.0 0.0 3.5
assign (segid b and resid 285 and name HA  )(segid b and resid 285 and name HD1# ) 0.0 1.5 4.4
assign (segid b and resid 285 and name HA  )(segid b and resid 285 and name HG1# ) 0.0 1.0 4.5
assign (segid b and resid 285 and name HA  )(segid b and resid 285 and name HG2# ) 0.0 1.5 4.4
assign (segid b and resid 285 and name HA  )(segid b and resid 285 and name HN  ) 0.0 0.0 3.5
assign (segid b and resid 285 and name HB  )(segid b and resid 285 and name HD1# ) 0.0 1.5 5.0
assign (segid b and resid 285 and name HB  )(segid b and resid 285 and name HG1# ) 0.0 1.0 4.5
assign (segid b and resid 285 and name HB  )(segid b and resid 285 and name HG2# ) 0.0 1.5 4.4
assign (segid b and resid 285 and name HB  )(segid b and resid 285 and name HN  ) 0.0 0.0 3.5
assign (segid b and resid 285 and name HD1# )(segid b and resid 285 and name HG1# ) 0.0 2.5 5.4
assign (segid b and resid 285 and name HG1# )(segid b and resid 285 and name HG2# ) 0.0 2.5 5.4
assign (segid b and resid 285 and name HG1# )(segid b and resid 285 and name HN  ) 0.0 1.0 6.0
assign (segid b and resid 285 and name HG2# )(segid b and resid 285 and name HN  ) 0.0 1.5 4.4
assign (segid b and resid 286 and name HA  )(segid b and resid 286 and name HB# ) 0.0 1.0 3.9
assign (segid b and resid 286 and name HA  )(segid b and resid 286 and name HN  ) 0.0 0.0 2.9
assign (segid b and resid 286 and name HB# )(segid b and resid 286 and name HN  ) 0.0 0.6 3.5
assign (segid b and resid 287 and name HA  )(segid b and resid 287 and name HB# ) 0.0 1.0 4.5
assign (segid b and resid 287 and name HA  )(segid b and resid 287 and name HN  ) 0.0 0.0 2.9
assign (segid b and resid 287 and name HB# )(segid b and resid 287 and name HN  ) 0.0 0.6 3.5
assign (segid b and resid 287 and name HD# )(segid b and resid 287 and name HN  ) 0.0 2.0 8.0
assign (segid b and resid 287 and name HE# )(segid b and resid 287 and name HN  ) 0.0 2.0 8.0
assign (segid b and resid 288 and name HA  )(segid b and resid 288 and name HB# ) 0.0 1.0 4.5
assign (segid b and resid 288 and name HA  )(segid b and resid 288 and name HD1# ) 0.0 1.5 6.5
assign (segid b and resid 288 and name HA  )(segid b and resid 288 and name HD2# ) 0.0 1.5 4.4
assign (segid b and resid 288 and name HA  )(segid b and resid 288 and name HG  ) 0.0 0.0 2.9
assign (segid b and resid 288 and name HA  )(segid b and resid 288 and name HN  ) 0.0 0.0 3.5
assign (segid b and resid 288 and name HD# )(segid b and resid 288 and name HG  ) 0.0 1.7 4.6
assign (segid b and resid 288 and name HD1# )(segid b and resid 288 and name HN  ) 0.0 1.5 7.5
assign (segid b and resid 288 and name HD2# )(segid b and resid 288 and name HN  ) 0.0 1.5 7.5
assign (segid b and resid 288 and name HG  )(segid b and resid 288 and name HN  ) 0.0 0.0 5.0
assign (segid b and resid 289 and name HA  )(segid b and resid 289 and name HB# ) 0.0 1.0 4.5
assign (segid b and resid 289 and name HA  )(segid b and resid 289 and name HD# ) 0.0 1.0 4.5
assign (segid b and resid 289 and name HA  )(segid b and resid 289 and name HG# ) 0.0 1.0 4.5
assign (segid b and resid 289 and name HB# )(segid b and resid 289 and name HN  ) 0.0 0.6 3.5
assign (segid b and resid 289 and name HD# )(segid b and resid 289 and name HG# ) 0.0 2.0 4.9
assign (segid b and resid 289 and name HG# )(segid b and resid 289 and name HN  ) 0.0 1.0 4.5
assign (segid a and resid 226 and name HA# )(segid a and resid 227 and name HN  ) 0.0 1.0 4.5
assign (segid a and resid 227 and name HA  )(segid a and resid 228 and name HN  ) 0.0 0.0 3.5
assign (segid a and resid 227 and name HG# )(segid a and resid 228 and name HN  ) 0.0 2.4 8.4
assign (segid a and resid 227 and name HN  )(segid a and resid 228 and name HN  ) 0.0 0.0 6.0
assign (segid a and resid 228 and name HA  )(segid a and resid 229 and name HN  ) 0.0 0.0 3.5
assign (segid a and resid 228 and name HB# )(segid a and resid 229 and name HN  ) 0.0 1.0 7.0
assign (segid a and resid 228 and name HN  )(segid a and resid 229 and name HB# ) 0.0 1.0 6.0
assign (segid a and resid 229 and name HA  )(segid a and resid 230 and name HN  ) 0.0 0.0 2.9
assign (segid a and resid 229 and name HB# )(segid a and resid 230 and name HN  ) 0.0 1.0 7.0
assign (segid a and resid 229 and name HG# )(segid a and resid 230 and name HN  ) 0.0 1.0 6.0
assign (segid a and resid 229 and name HN  )(segid a and resid 230 and name HD# ) 0.0 2.4 8.4
assign (segid a and resid 229 and name HN  )(segid a and resid 230 and name HN  ) 0.0 0.0 5.0
assign (segid a and resid 230 and name HA  )(segid a and resid 231 and name HN  ) 0.0 0.0 2.9
assign (segid a and resid 230 and name HB# )(segid a and resid 231 and name HN  ) 0.0 1.0 6.0
assign (segid a and resid 230 and name HD# )(segid a and resid 231 and name HN  ) 0.0 2.4 7.4
assign (segid a and resid 231 and name HA  )(segid a and resid 232 and name HN  ) 0.0 0.0 2.9
assign (segid a and resid 231 and name HB# )(segid a and resid 232 and name HN  ) 0.0 1.5 5.0
assign (segid a and resid 231 and name HN  )(segid a and resid 232 and name HN  ) 0.0 0.0 6.0
assign (segid a and resid 232 and name HA  )(segid a and resid 233 and name HN  ) 0.0 0.0 2.9
assign (segid a and resid 232 and name HN  )(segid a and resid 233 and name HN  ) 0.0 0.0 5.0
assign (segid a and resid 233 and name HA  )(segid a and resid 234 and name HN  ) 0.0 0.0 3.5
assign (segid a and resid 233 and name HB# )(segid a and resid 234 and name HN  ) 0.0 1.0 6.0
assign (segid a and resid 233 and name HN  )(segid a and resid 234 and name HA  ) 0.0 0.0 6.0
assign (segid a and resid 233 and name HN  )(segid a and resid 234 and name HB# ) 0.0 1.0 7.0
assign (segid a and resid 233 and name HN  )(segid a and resid 234 and name HG# ) 0.0 1.0 6.0
assign (segid a and resid 233 and name HN  )(segid a and resid 234 and name HN  ) 0.0 0.0 6.0
assign (segid a and resid 234 and name HA  )(segid a and resid 235 and name HN  ) 0.0 0.0 5.0
assign (segid a and resid 234 and name HB# )(segid a and resid 235 and name HN  ) 0.0 1.0 4.5
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Table A.4. *(continued)*

```
assign (segid a and resid 234 and name HD# )(segid a and resid 235 and name HN ) 0.0 1.0 7.0
assign (segid a and resid 234 and name HN )(segid a and resid 235 and name HN ) 0.0 0.0 6.0
assign (segid a and resid 235 and name HA )(segid a and resid 236 and name HN ) 0.0 0.0 6.0
assign (segid a and resid 235 and name HB )(segid a and resid 236 and name HN ) 0.0 0.0 3.5
assign (segid a and resid 235 and name HG2# )(segid a and resid 236 and name HN ) 0.0 1.5 6.5
assign (segid a and resid 235 and name HN )(segid a and resid 236 and name HD2# ) 0.0 1.5 6.5
assign (segid a and resid 235 and name HN )(segid a and resid 236 and name HN ) 0.0 0.0 3.5
assign (segid a and resid 236 and name HA )(segid a and resid 237 and name HG ) 0.0 0.0 6.0
assign (segid a and resid 236 and name HB# )(segid a and resid 237 and name HD2# ) 0.0 2.5 5.4
assign (segid a and resid 236 and name HB# )(segid a and resid 237 and name HN ) 0.0 1.0 4.5
assign (segid a and resid 236 and name HN )(segid a and resid 237 and name HN ) 0.0 0.0 3.5
assign (segid a and resid 237 and name HD# )(segid a and resid 238 and name HN ) 0.0 2.4 7.4
assign (segid a and resid 237 and name HG )(segid a and resid 238 and name HN ) 0.0 0.0 5.0
assign (segid a and resid 237 and name HN )(segid a and resid 238 and name HN ) 0.0 0.0 6.0
assign (segid a and resid 238 and name HB# )(segid a and resid 239 and name HN ) 0.0 1.0 7.0
assign (segid a and resid 238 and name HG# )(segid a and resid 239 and name HN ) 0.0 1.0 6.0
assign (segid a and resid 238 and name HN )(segid a and resid 239 and name HB# ) 0.0 1.5 6.5
assign (segid a and resid 238 and name HN )(segid a and resid 239 and name HN ) 0.0 0.0 6.0
assign (segid a and resid 239 and name HA )(segid a and resid 240 and name HN ) 0.0 0.0 5.0
assign (segid a and resid 239 and name HB# )(segid a and resid 240 and name HN ) 0.0 1.5 5.0
assign (segid a and resid 239 and name HN )(segid a and resid 240 and name HN ) 0.0 0.0 5.0
assign (segid a and resid 240 and name HA# )(segid a and resid 241 and name HN ) 0.0 1.0 6.0
assign (segid a and resid 240 and name HN )(segid a and resid 241 and name HG# ) 0.0 2.4 7.4
assign (segid a and resid 240 and name HN )(segid a and resid 241 and name HN ) 0.0 0.0 6.0
assign (segid a and resid 241 and name HA )(segid a and resid 242 and name HN ) 0.0 0.0 5.0
assign (segid a and resid 241 and name HB )(segid a and resid 242 and name HN ) 0.0 0.0 5.0
assign (segid a and resid 241 and name HG# )(segid a and resid 242 and name HN ) 0.0 2.4 7.4
assign (segid a and resid 241 and name HN )(segid a and resid 242 and name HN ) 0.0 0.0 5.0
assign (segid a and resid 242 and name HA )(segid a and resid 243 and name HN ) 0.0 0.0 6.0
assign (segid a and resid 242 and name HB# )(segid a and resid 243 and name HN ) 0.0 1.0 7.0
assign (segid a and resid 242 and name HN )(segid a and resid 243 and name HN ) 0.0 0.0 5.0
assign (segid a and resid 243 and name HA )(segid a and resid 244 and name HN ) 0.0 0.0 5.0
assign (segid a and resid 243 and name HB# )(segid a and resid 244 and name HN ) 0.0 1.0 7.0
assign (segid a and resid 243 and name HN )(segid a and resid 244 and name HB# ) 0.0 1.0 7.0
assign (segid a and resid 243 and name HN )(segid a and resid 244 and name HN ) 0.0 0.0 5.0
assign (segid a and resid 244 and name HA )(segid a and resid 245 and name HN ) 0.0 0.0 5.0
assign (segid a and resid 244 and name HN )(segid a and resid 245 and name HN ) 0.0 0.0 5.0
assign (segid a and resid 246 and name HA )(segid a and resid 247 and name HN ) 0.0 0.0 5.0
assign (segid a and resid 246 and name HB# )(segid a and resid 247 and name HN ) 0.0 1.0 6.0
assign (segid a and resid 246 and name HG# )(segid a and resid 247 and name HN ) 0.0 1.0 7.0
assign (segid a and resid 246 and name HN )(segid a and resid 247 and name HN ) 0.0 0.0 5.0
assign (segid a and resid 247 and name HA )(segid a and resid 248 and name HD# ) 0.0 1.0 7.0
assign (segid a and resid 247 and name HB )(segid a and resid 248 and name HD# ) 0.0 1.0 4.5
assign (segid a and resid 247 and name HG2# )(segid a and resid 248 and name HD# ) 0.0 2.5 6.0
assign (segid a and resid 247 and name HN )(segid a and resid 248 and name HD# ) 0.0 1.0 6.0
assign (segid a and resid 248 and name HA )(segid a and resid 249 and name HN ) 0.0 0.0 5.0
assign (segid a and resid 248 and name HB# )(segid a and resid 249 and name HN ) 0.0 1.0 4.5
assign (segid a and resid 248 and name HD# )(segid a and resid 249 and name HN ) 0.0 1.0 7.0
assign (segid a and resid 248 and name HG# )(segid a and resid 249 and name HN ) 0.0 1.0 7.0
assign (segid a and resid 249 and name HB# )(segid a and resid 250 and name HN ) 0.0 1.0 6.0
assign (segid a and resid 249 and name HD# )(segid a and resid 250 and name HN ) 0.0 2.4 8.4
assign (segid a and resid 249 and name HN )(segid a and resid 250 and name HN ) 0.0 0.0 6.0
assign (segid a and resid 250 and name HA )(segid a and resid 251 and name HN ) 0.0 0.0 6.0
assign (segid a and resid 250 and name HB )(segid a and resid 251 and name HN ) 0.0 0.0 5.0
assign (segid a and resid 250 and name HG2# )(segid a and resid 251 and name HN ) 0.0 1.5 6.5
assign (segid a and resid 250 and name HN )(segid a and resid 251 and name HN ) 0.0 0.0 6.0
assign (segid a and resid 251 and name HA )(segid a and resid 252 and name HN ) 0.0 0.0 5.0
assign (segid a and resid 251 and name HB# )(segid a and resid 252 and name HN ) 0.0 1.0 6.0
assign (segid a and resid 251 and name HN )(segid a and resid 252 and name HG2# ) 0.0 1.5 6.5
assign (segid a and resid 251 and name HN )(segid a and resid 252 and name HN ) 0.0 0.0 5.0
assign (segid a and resid 252 and name HA )(segid a and resid 253 and name HN ) 0.0 0.0 5.0
assign (segid a and resid 252 and name HB )(segid a and resid 253 and name HN ) 0.0 0.0 5.0
assign (segid a and resid 252 and name HG2# )(segid a and resid 253 and name HN ) 0.0 1.5 4.4
assign (segid a and resid 252 and name HN )(segid a and resid 253 and name HN ) 0.0 0.0 6.0
assign (segid a and resid 253 and name HA )(segid a and resid 254 and name HN ) 0.0 0.0 6.0
assign (segid a and resid 253 and name HN )(segid a and resid 254 and name HA ) 0.0 0.0 5.0
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Table A.4. *(continued)*

```
assign (segid a and resid 253 and name HN )(segid a and resid 254 and name HB# ) 0.0 1.0 7.0
assign (segid a and resid 253 and name HN )(segid a and resid 254 and name HN ) 0.0 0.0 5.0
assign (segid a and resid 254 and name HA )(segid a and resid 255 and name HN ) 0.0 0.0 3.5
assign (segid a and resid 254 and name HB# )(segid a and resid 255 and name HN ) 0.0 1.0 7.0
assign (segid a and resid 254 and name HN )(segid a and resid 255 and name HA ) 0.0 0.0 5.0
assign (segid a and resid 254 and name HN )(segid a and resid 255 and name HB# ) 0.0 1.5 5.0
assign (segid a and resid 254 and name HN )(segid a and resid 255 and name HN ) 0.0 0.0 6.0
assign (segid a and resid 255 and name HA )(segid a and resid 256 and name HN ) 0.0 0.0 3.5
assign (segid a and resid 255 and name HB# )(segid a and resid 256 and name HG2# ) 0.0 3.0 5.9
assign (segid a and resid 255 and name HB# )(segid a and resid 256 and name HN ) 0.0 1.5 5.0
assign (segid a and resid 255 and name HN )(segid a and resid 256 and name HN ) 0.0 0.0 6.0
assign (segid a and resid 256 and name HA )(segid a and resid 257 and name HN ) 0.0 0.0 6.0
assign (segid a and resid 256 and name HB )(segid a and resid 257 and name HN ) 0.0 0.0 5.0
assign (segid a and resid 256 and name HG2# )(segid a and resid 257 and name HN ) 0.0 1.5 6.5
assign (segid a and resid 256 and name HN )(segid a and resid 257 and name HN ) 0.0 0.0 6.0
assign (segid a and resid 257 and name HA )(segid a and resid 258 and name HN ) 0.0 0.0 5.0
assign (segid a and resid 257 and name HB# )(segid a and resid 258 and name HN ) 0.0 1.0 3.9
assign (segid a and resid 257 and name HN )(segid a and resid 258 and name HG# ) 0.0 1.0 6.0
assign (segid a and resid 257 and name HN )(segid a and resid 258 and name HN ) 0.0 0.0 3.5
assign (segid a and resid 258 and name HA )(segid a and resid 259 and name HN ) 0.0 0.0 5.0
assign (segid a and resid 258 and name HB# )(segid a and resid 259 and name HN ) 0.0 1.0 6.0
assign (segid a and resid 258 and name HN )(segid a and resid 259 and name HB# ) 0.0 1.0 6.0
assign (segid a and resid 258 and name HN )(segid a and resid 259 and name HN ) 0.0 0.0 2.9
assign (segid a and resid 259 and name HA )(segid a and resid 260 and name HN ) 0.0 0.0 2.9
assign (segid a and resid 259 and name HB# )(segid a and resid 260 and name HN ) 0.0 1.0 4.5
assign (segid a and resid 260 and name HA )(segid a and resid 261 and name HN ) 0.0 0.0 3.5
assign (segid a and resid 260 and name HB# )(segid a and resid 261 and name HN ) 0.0 1.0 7.0
assign (segid a and resid 261 and name HA )(segid a and resid 262 and name HN ) 0.0 0.0 6.0
assign (segid a and resid 261 and name HG# )(segid a and resid 262 and name HN ) 0.0 1.0 6.0
assign (segid a and resid 261 and name HN )(segid a and resid 262 and name HN ) 0.0 0.0 5.0
assign (segid a and resid 262 and name HA )(segid a and resid 263 and name HN ) 0.0 0.0 5.0
assign (segid a and resid 262 and name HB# )(segid a and resid 263 and name HN ) 0.0 1.0 6.0
assign (segid a and resid 262 and name HG# )(segid a and resid 263 and name HN ) 0.0 1.0 4.5
assign (segid a and resid 262 and name HN )(segid a and resid 263 and name HA ) 0.0 0.0 6.0
assign (segid a and resid 262 and name HN )(segid a and resid 263 and name HB# ) 0.0 1.0 7.0
assign (segid a and resid 262 and name HN )(segid a and resid 263 and name HN ) 0.0 0.0 6.0
assign (segid a and resid 263 and name HA )(segid a and resid 264 and name HN ) 0.0 0.0 5.0
assign (segid a and resid 263 and name HB# )(segid a and resid 264 and name HN ) 0.0 1.0 7.0
assign (segid a and resid 263 and name HN )(segid a and resid 264 and name HA# ) 0.0 1.0 6.0
assign (segid a and resid 263 and name HN )(segid a and resid 264 and name HN ) 0.0 0.0 3.5
assign (segid a and resid 264 and name HA# )(segid a and resid 265 and name HN ) 0.0 1.0 7.0
assign (segid a and resid 264 and name HN )(segid a and resid 265 and name HN ) 0.0 0.0 5.0
assign (segid a and resid 265 and name HA )(segid a and resid 266 and name HN ) 0.0 0.0 5.0
assign (segid a and resid 265 and name HB# )(segid a and resid 266 and name HN ) 0.0 1.0 7.0
assign (segid a and resid 265 and name HD# )(segid a and resid 266 and name HD# ) 0.0 4.4 7.9
assign (segid a and resid 265 and name HE# )(segid a and resid 266 and name HN ) 0.0 2.0 7.0
assign (segid a and resid 265 and name HN )(segid a and resid 266 and name HN ) 0.0 0.0 5.0
assign (segid a and resid 266 and name HA )(segid a and resid 267 and name HN ) 0.0 0.0 5.0
assign (segid a and resid 266 and name HB# )(segid a and resid 267 and name HN ) 0.0 1.0 6.0
assign (segid a and resid 266 and name HD# )(segid a and resid 267 and name HN ) 0.0 2.4 7.4
assign (segid a and resid 266 and name HN )(segid a and resid 267 and name HN ) 0.0 0.0 5.0
assign (segid a and resid 267 and name HA )(segid a and resid 268 and name HN ) 0.0 0.0 5.0
assign (segid a and resid 267 and name HB# )(segid a and resid 268 and name HN ) 0.0 1.5 4.4
assign (segid a and resid 267 and name HN )(segid a and resid 268 and name HN ) 0.0 0.0 6.0
assign (segid a and resid 268 and name HA )(segid a and resid 269 and name HN ) 0.0 0.0 5.0
assign (segid a and resid 268 and name HB# )(segid a and resid 269 and name HN ) 0.0 1.0 3.9
assign (segid a and resid 268 and name HN )(segid a and resid 269 and name HN ) 0.0 0.0 3.5
assign (segid a and resid 269 and name HA )(segid a and resid 270 and name HN ) 0.0 0.0 6.0
assign (segid a and resid 269 and name HB# )(segid a and resid 270 and name HN ) 0.0 1.0 4.5
assign (segid a and resid 269 and name HN )(segid a and resid 270 and name HN ) 0.0 0.0 6.0
assign (segid a and resid 270 and name HA )(segid a and resid 271 and name HN ) 0.0 0.0 5.0
assign (segid a and resid 270 and name HB )(segid a and resid 271 and name HN ) 0.0 0.0 5.0
assign (segid a and resid 270 and name HD1# )(segid a and resid 271 and name HN ) 0.0 1.5 6.5
assign (segid a and resid 270 and name HG2# )(segid a and resid 271 and name HN ) 0.0 1.5 6.5
assign (segid a and resid 270 and name HN )(segid a and resid 271 and name HN ) 0.0 0.0 5.0
assign (segid a and resid 271 and name HA )(segid a and resid 272 and name HN ) 0.0 0.0 6.0
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Table A.4. *(continued)*

```
assign (segid a and resid 271 and name HB# )(segid a and resid 272 and name HN  ) 0.0 1.0 6.0
assign (segid a and resid 271 and name HN  )(segid a and resid 272 and name HB# ) 0.0 1.0 6.0
assign (segid a and resid 271 and name HN  )(segid a and resid 272 and name HG# ) 0.0 1.0 6.0
assign (segid a and resid 271 and name HN  )(segid a and resid 272 and name HN  ) 0.0 0.0 3.5
assign (segid a and resid 272 and name HA  )(segid a and resid 273 and name HN  ) 0.0 0.0 6.0
assign (segid a and resid 272 and name HB# )(segid a and resid 273 and name HN  ) 0.0 1.0 3.9
assign (segid a and resid 272 and name HN  )(segid a and resid 273 and name HA  ) 0.0 0.0 6.0
assign (segid a and resid 272 and name HN  )(segid a and resid 273 and name HB# ) 0.0 1.0 7.0
assign (segid a and resid 272 and name HN  )(segid a and resid 273 and name HN  ) 0.0 0.0 5.0
assign (segid a and resid 273 and name HA  )(segid a and resid 274 and name HN  ) 0.0 0.0 6.0
assign (segid a and resid 273 and name HB# )(segid a and resid 274 and name HN  ) 0.0 1.0 7.0
assign (segid a and resid 273 and name HN  )(segid a and resid 274 and name HB  ) 0.0 0.0 5.0
assign (segid a and resid 273 and name HN  )(segid a and resid 274 and name HG2# ) 0.0 1.5 6.5
assign (segid a and resid 273 and name HN  )(segid a and resid 274 and name HN  ) 0.0 0.0 5.0
assign (segid a and resid 274 and name HB  )(segid a and resid 275 and name HN  ) 0.0 0.0 6.0
assign (segid a and resid 274 and name HD1# )(segid a and resid 275 and name HN  ) 0.0 1.5 7.5
assign (segid a and resid 274 and name HG1# )(segid a and resid 275 and name HN  ) 0.0 1.0 6.0
assign (segid a and resid 274 and name HN  )(segid a and resid 275 and name HN  ) 0.0 0.0 6.0
assign (segid a and resid 275 and name HN  )(segid a and resid 276 and name HN  ) 0.0 0.0 6.0
assign (segid a and resid 276 and name HA  )(segid a and resid 277 and name HN  ) 0.0 0.0 3.5
assign (segid a and resid 276 and name HB# )(segid a and resid 277 and name HN  ) 0.0 1.0 6.0
assign (segid a and resid 276 and name HG# )(segid a and resid 277 and name HN  ) 0.0 1.0 3.9
assign (segid a and resid 276 and name HN  )(segid a and resid 277 and name HN  ) 0.0 0.0 6.0
assign (segid a and resid 277 and name HA  )(segid a and resid 278 and name HN  ) 0.0 0.0 5.0
assign (segid a and resid 277 and name HB# )(segid a and resid 278 and name HN  ) 0.0 1.0 6.0
assign (segid a and resid 277 and name HN  )(segid a and resid 278 and name HB# ) 0.0 1.0 6.0
assign (segid a and resid 277 and name HN  )(segid a and resid 278 and name HN  ) 0.0 0.0 5.0
assign (segid a and resid 278 and name HA  )(segid a and resid 279 and name HN  ) 0.0 0.0 6.0
assign (segid a and resid 278 and name HB# )(segid a and resid 279 and name HN  ) 0.0 1.0 4.5
assign (segid a and resid 278 and name HN  )(segid a and resid 279 and name HA  ) 0.0 0.0 5.0
assign (segid a and resid 278 and name HN  )(segid a and resid 279 and name HB# ) 0.0 1.5 6.5
assign (segid a and resid 278 and name HN  )(segid a and resid 279 and name HN  ) 0.0 0.0 3.5
assign (segid a and resid 279 and name HA  )(segid a and resid 280 and name HN  ) 0.0 0.0 5.0
assign (segid a and resid 279 and name HB# )(segid a and resid 280 and name HN  ) 0.0 1.5 7.5
assign (segid a and resid 279 and name HN  )(segid a and resid 280 and name HN  ) 0.0 0.0 6.0
assign (segid a and resid 280 and name HA  )(segid a and resid 281 and name HN  ) 0.0 0.0 5.0
assign (segid a and resid 280 and name HB  )(segid a and resid 281 and name HN  ) 0.0 0.0 3.5
assign (segid a and resid 280 and name HN  )(segid a and resid 281 and name HG1# ) 0.0 1.0 4.5
assign (segid a and resid 280 and name HN  )(segid a and resid 281 and name HN  ) 0.0 0.0 5.0
assign (segid a and resid 281 and name HA  )(segid a and resid 282 and name HN  ) 0.0 0.0 6.0
assign (segid a and resid 281 and name HB  )(segid a and resid 282 and name HN  ) 0.0 0.0 2.9
assign (segid a and resid 281 and name HD1# )(segid a and resid 282 and name HN  ) 0.0 1.5 6.5
assign (segid a and resid 281 and name HG2# )(segid a and resid 282 and name HN  ) 0.0 1.5 5.0
assign (segid a and resid 281 and name HN  )(segid a and resid 282 and name HA  ) 0.0 0.0 5.0
assign (segid a and resid 281 and name HN  )(segid a and resid 282 and name HB# ) 0.0 1.0 6.0
assign (segid a and resid 281 and name HN  )(segid a and resid 282 and name HN  ) 0.0 0.0 6.0
assign (segid a and resid 282 and name HA  )(segid a and resid 283 and name HN  ) 0.0 0.0 5.0
assign (segid a and resid 282 and name HB# )(segid a and resid 283 and name HN  ) 0.0 1.0 6.0
assign (segid a and resid 282 and name HN  )(segid a and resid 283 and name HN  ) 0.0 0.0 3.5
assign (segid a and resid 283 and name HA  )(segid a and resid 284 and name HN  ) 0.0 0.0 6.0
assign (segid a and resid 283 and name HB# )(segid a and resid 284 and name HN  ) 0.0 1.0 6.0
assign (segid a and resid 283 and name HG# )(segid a and resid 284 and name HN  ) 0.0 1.0 6.0
assign (segid a and resid 283 and name HN  )(segid a and resid 284 and name HA  ) 0.0 0.0 6.0
assign (segid a and resid 283 and name HN  )(segid a and resid 284 and name HN  ) 0.0 0.0 3.5
assign (segid a and resid 284 and name HA  )(segid a and resid 285 and name HN  ) 0.0 0.0 5.0
assign (segid a and resid 284 and name HB# )(segid a and resid 285 and name HN  ) 0.0 1.0 6.0
assign (segid a and resid 284 and name HN  )(segid a and resid 285 and name HA  ) 0.0 0.0 5.0
assign (segid a and resid 284 and name HN  )(segid a and resid 285 and name HG1# ) 0.0 1.0 6.0
assign (segid a and resid 284 and name HN  )(segid a and resid 285 and name HG2# ) 0.0 1.5 6.5
assign (segid a and resid 285 and name HA  )(segid a and resid 286 and name HN  ) 0.0 0.0 5.0
assign (segid a and resid 285 and name HB  )(segid a and resid 286 and name HN  ) 0.0 0.0 6.0
assign (segid a and resid 285 and name HG1# )(segid a and resid 286 and name HN  ) 0.0 1.0 6.0
assign (segid a and resid 285 and name HN  )(segid a and resid 286 and name HA  ) 0.0 0.0 6.0
assign (segid a and resid 285 and name HN  )(segid a and resid 286 and name HB# ) 0.0 1.0 6.0
assign (segid a and resid 285 and name HN  )(segid a and resid 286 and name HN  ) 0.0 0.0 3.5
assign (segid a and resid 286 and name HA  )(segid a and resid 287 and name HN  ) 0.0 0.0 3.5
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Table A.4. *(continued)*

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assign (segid a and resid 286 and name HB# )(segid a and resid 287 and name HN  ) 0.0 1.0 4.5
assign (segid a and resid 286 and name HN  )(segid a and resid 287 and name HN  ) 0.0 0.0 6.0
assign (segid a and resid 287 and name HA  )(segid a and resid 288 and name HN  ) 0.0 0.0 3.5
assign (segid a and resid 287 and name HB# )(segid a and resid 288 and name HN  ) 0.0 1.0 6.0
assign (segid a and resid 287 and name HE# )(segid a and resid 288 and name HD1# ) 0.0 3.5 9.5
assign (segid a and resid 287 and name HE# )(segid a and resid 288 and name HN  ) 0.0 2.0 7.0
assign (segid a and resid 287 and name HN  )(segid a and resid 288 and name HA  ) 0.0 0.0 5.0
assign (segid a and resid 287 and name HN  )(segid a and resid 288 and name HD2# ) 0.0 1.5 6.5
assign (segid a and resid 287 and name HN  )(segid a and resid 288 and name HG  ) 0.0 0.0 5.0
assign (segid a and resid 287 and name HN  )(segid a and resid 288 and name HN  ) 0.0 0.0 2.9
assign (segid a and resid 288 and name HA  )(segid a and resid 289 and name HN  ) 0.0 0.0 2.9
assign (segid a and resid 288 and name HD# )(segid a and resid 289 and name HN  ) 0.0 2.4 5.9
assign (segid a and resid 288 and name HN  )(segid a and resid 289 and name HA  ) 0.0 0.0 6.0
assign (segid a and resid 288 and name HN  )(segid a and resid 289 and name HN  ) 0.0 0.0 3.5
assign (segid b and resid 226 and name HA# )(segid b and resid 227 and name HN  ) 0.0 1.0 4.5
assign (segid b and resid 227 and name HA  )(segid b and resid 228 and name HN  ) 0.0 0.0 3.5
assign (segid b and resid 227 and name HG# )(segid b and resid 228 and name HN  ) 0.0 2.4 8.4
assign (segid b and resid 227 and name HN  )(segid b and resid 228 and name HN  ) 0.0 0.0 6.0
assign (segid b and resid 228 and name HA  )(segid b and resid 229 and name HN  ) 0.0 0.0 3.5
assign (segid b and resid 228 and name HB# )(segid b and resid 229 and name HN  ) 0.0 1.0 7.0
assign (segid b and resid 228 and name HN  )(segid b and resid 229 and name HB# ) 0.0 1.0 6.0
assign (segid b and resid 229 and name HA  )(segid b and resid 230 and name HN  ) 0.0 0.0 2.9
assign (segid b and resid 229 and name HB# )(segid b and resid 230 and name HN  ) 0.0 1.0 7.0
assign (segid b and resid 229 and name HG# )(segid b and resid 230 and name HN  ) 0.0 1.0 6.0
assign (segid b and resid 229 and name HN  )(segid b and resid 230 and name HD# ) 0.0 2.4 8.4
assign (segid b and resid 229 and name HN  )(segid b and resid 230 and name HN  ) 0.0 0.0 5.0
assign (segid b and resid 230 and name HA  )(segid b and resid 231 and name HN  ) 0.0 0.0 2.9
assign (segid b and resid 230 and name HB# )(segid b and resid 231 and name HN  ) 0.0 1.0 6.0
assign (segid b and resid 230 and name HD# )(segid b and resid 231 and name HN  ) 0.0 2.4 7.4
assign (segid b and resid 231 and name HA  )(segid b and resid 232 and name HN  ) 0.0 0.0 2.9
assign (segid b and resid 231 and name HB# )(segid b and resid 232 and name HN  ) 0.0 1.5 5.0
assign (segid b and resid 231 and name HN  )(segid b and resid 232 and name HN  ) 0.0 0.0 6.0
assign (segid b and resid 232 and name HA  )(segid b and resid 233 and name HN  ) 0.0 0.0 2.9
assign (segid b and resid 232 and name HN  )(segid b and resid 233 and name HN  ) 0.0 0.0 5.0
assign (segid b and resid 233 and name HA  )(segid b and resid 234 and name HN  ) 0.0 0.0 3.5
assign (segid b and resid 233 and name HB# )(segid b and resid 234 and name HN  ) 0.0 1.0 6.0
assign (segid b and resid 233 and name HN  )(segid b and resid 234 and name HA  ) 0.0 0.0 6.0
assign (segid b and resid 233 and name HN  )(segid b and resid 234 and name HB# ) 0.0 1.0 7.0
assign (segid b and resid 233 and name HN  )(segid b and resid 234 and name HG# ) 0.0 1.0 6.0
assign (segid b and resid 233 and name HN  )(segid b and resid 234 and name HN  ) 0.0 0.0 6.0
assign (segid b and resid 234 and name HA  )(segid b and resid 235 and name HN  ) 0.0 0.0 5.0
assign (segid b and resid 234 and name HB# )(segid b and resid 235 and name HN  ) 0.0 1.0 4.5
assign (segid b and resid 234 and name HD# )(segid b and resid 235 and name HN  ) 0.0 1.0 7.0
assign (segid b and resid 234 and name HN  )(segid b and resid 235 and name HN  ) 0.0 0.0 6.0
assign (segid b and resid 235 and name HA  )(segid b and resid 236 and name HN  ) 0.0 0.0 6.0
assign (segid b and resid 235 and name HB  )(segid b and resid 236 and name HN  ) 0.0 0.0 3.5
assign (segid b and resid 235 and name HG2# )(segid b and resid 236 and name HN  ) 0.0 1.5 6.5
assign (segid b and resid 235 and name HN  )(segid b and resid 236 and name HD2# ) 0.0 1.5 6.5
assign (segid b and resid 235 and name HN  )(segid b and resid 236 and name HN  ) 0.0 0.0 3.5
assign (segid b and resid 236 and name HA  )(segid b and resid 237 and name HG  ) 0.0 0.0 6.0
assign (segid b and resid 236 and name HB# )(segid b and resid 237 and name HD2# ) 0.0 2.5 5.4
assign (segid b and resid 236 and name HB# )(segid b and resid 237 and name HN  ) 0.0 1.0 4.5
assign (segid b and resid 236 and name HN  )(segid b and resid 237 and name HN  ) 0.0 0.0 3.5
assign (segid b and resid 237 and name HD# )(segid b and resid 238 and name HN  ) 0.0 2.4 7.4
assign (segid b and resid 237 and name HG  )(segid b and resid 238 and name HN  ) 0.0 0.0 5.0
assign (segid b and resid 237 and name HN  )(segid b and resid 238 and name HN  ) 0.0 0.0 6.0
assign (segid b and resid 238 and name HB# )(segid b and resid 239 and name HN  ) 0.0 1.0 7.0
assign (segid b and resid 238 and name HG# )(segid b and resid 239 and name HN  ) 0.0 1.0 6.0
assign (segid b and resid 238 and name HN  )(segid b and resid 239 and name HB# ) 0.0 1.5 6.5
assign (segid b and resid 238 and name HN  )(segid b and resid 239 and name HN  ) 0.0 0.0 6.0
assign (segid b and resid 239 and name HA  )(segid b and resid 240 and name HN  ) 0.0 0.0 5.0
assign (segid b and resid 239 and name HB# )(segid b and resid 240 and name HN  ) 0.0 1.5 5.0
assign (segid b and resid 239 and name HN  )(segid b and resid 240 and name HN  ) 0.0 0.0 5.0
assign (segid b and resid 240 and name HA# )(segid b and resid 241 and name HN  ) 0.0 1.0 6.0
assign (segid b and resid 240 and name HN  )(segid b and resid 241 and name HG# ) 0.0 2.4 7.4
assign (segid b and resid 240 and name HN  )(segid b and resid 241 and name HN  ) 0.0 0.0 6.0
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assign (segid b and resid 241 and name HA ) (segid b and resid 242 and name HN ) 0.0 0.0 5.0
assign (segid b and resid 241 and name HB ) (segid b and resid 242 and name HN ) 0.0 0.0 5.0
assign (segid b and resid 241 and name HG# ) (segid b and resid 242 and name HN ) 0.0 2.4 7.4
assign (segid b and resid 241 and name HN ) (segid b and resid 242 and name HN ) 0.0 0.0 5.0
assign (segid b and resid 242 and name HA ) (segid b and resid 243 and name HN ) 0.0 0.0 6.0
assign (segid b and resid 242 and name HB# ) (segid b and resid 243 and name HN ) 0.0 1.0 7.0
assign (segid b and resid 242 and name HN ) (segid b and resid 243 and name HN ) 0.0 0.0 5.0
assign (segid b and resid 243 and name HA ) (segid b and resid 244 and name HN ) 0.0 0.0 5.0
assign (segid b and resid 243 and name HB# ) (segid b and resid 244 and name HN ) 0.0 1.0 7.0
assign (segid b and resid 243 and name HN ) (segid b and resid 244 and name HB# ) 0.0 1.0 7.0
assign (segid b and resid 243 and name HN ) (segid b and resid 244 and name HN ) 0.0 0.0 5.0
assign (segid b and resid 244 and name HA ) (segid b and resid 245 and name HN ) 0.0 0.0 5.0
assign (segid b and resid 244 and name HN ) (segid b and resid 245 and name HN ) 0.0 0.0 5.0
assign (segid b and resid 246 and name HA ) (segid b and resid 247 and name HN ) 0.0 0.0 5.0
assign (segid b and resid 246 and name HB# ) (segid b and resid 247 and name HN ) 0.0 1.0 6.0
assign (segid b and resid 246 and name HG# ) (segid b and resid 247 and name HN ) 0.0 1.0 7.0
assign (segid b and resid 246 and name HN ) (segid b and resid 247 and name HN ) 0.0 0.0 5.0
assign (segid b and resid 247 and name HA ) (segid b and resid 248 and name HD# ) 0.0 1.0 7.0
assign (segid b and resid 247 and name HB ) (segid b and resid 248 and name HD# ) 0.0 1.0 4.5
assign (segid b and resid 247 and name HG2# ) (segid b and resid 248 and name HD# ) 0.0 2.5 6.0
assign (segid b and resid 247 and name HN ) (segid b and resid 248 and name HD# ) 0.0 1.0 6.0
assign (segid b and resid 248 and name HA ) (segid b and resid 249 and name HN ) 0.0 0.0 5.0
assign (segid b and resid 248 and name HB# ) (segid b and resid 249 and name HN ) 0.0 1.0 4.5
assign (segid b and resid 248 and name HD# ) (segid b and resid 249 and name HN ) 0.0 1.0 7.0
assign (segid b and resid 248 and name HG# ) (segid b and resid 249 and name HN ) 0.0 1.0 7.0
assign (segid b and resid 249 and name HB# ) (segid b and resid 250 and name HN ) 0.0 1.0 6.0
assign (segid b and resid 249 and name HD# ) (segid b and resid 250 and name HN ) 0.0 2.4 8.4
assign (segid b and resid 249 and name HN ) (segid b and resid 250 and name HN ) 0.0 0.0 6.0
assign (segid b and resid 250 and name HA ) (segid b and resid 251 and name HN ) 0.0 0.0 6.0
assign (segid b and resid 250 and name HB ) (segid b and resid 251 and name HN ) 0.0 0.0 5.0
assign (segid b and resid 250 and name HG2# ) (segid b and resid 251 and name HN ) 0.0 1.5 6.5
assign (segid b and resid 250 and name HN ) (segid b and resid 251 and name HN ) 0.0 0.0 6.0
assign (segid b and resid 251 and name HA ) (segid b and resid 252 and name HN ) 0.0 0.0 5.0
assign (segid b and resid 251 and name HB# ) (segid b and resid 252 and name HN ) 0.0 1.0 6.0
assign (segid b and resid 251 and name HN ) (segid b and resid 252 and name HG2# ) 0.0 1.5 6.5
assign (segid b and resid 251 and name HN ) (segid b and resid 252 and name HN ) 0.0 0.0 5.0
assign (segid b and resid 252 and name HA ) (segid b and resid 253 and name HN ) 0.0 0.0 5.0
assign (segid b and resid 252 and name HB ) (segid b and resid 253 and name HN ) 0.0 0.0 5.0
assign (segid b and resid 252 and name HG2# ) (segid b and resid 253 and name HN ) 0.0 1.5 4.4
assign (segid b and resid 252 and name HN ) (segid b and resid 253 and name HN ) 0.0 0.0 6.0
assign (segid b and resid 253 and name HA ) (segid b and resid 254 and name HN ) 0.0 0.0 6.0
assign (segid b and resid 253 and name HN ) (segid b and resid 254 and name HA ) 0.0 0.0 5.0
assign (segid b and resid 253 and name HN ) (segid b and resid 254 and name HB# ) 0.0 1.0 7.0
assign (segid b and resid 253 and name HN ) (segid b and resid 254 and name HN ) 0.0 0.0 5.0
assign (segid b and resid 254 and name HA ) (segid b and resid 255 and name HN ) 0.0 0.0 3.5
assign (segid b and resid 254 and name HB# ) (segid b and resid 255 and name HN ) 0.0 1.0 7.0
assign (segid b and resid 254 and name HN ) (segid b and resid 255 and name HA ) 0.0 0.0 5.0
assign (segid b and resid 254 and name HN ) (segid b and resid 255 and name HB# ) 0.0 1.5 5.0
assign (segid b and resid 254 and name HN ) (segid b and resid 255 and name HN ) 0.0 0.0 6.0
assign (segid b and resid 255 and name HA ) (segid b and resid 256 and name HN ) 0.0 0.0 3.5
assign (segid b and resid 255 and name HB# ) (segid b and resid 256 and name HG2# ) 0.0 3.0 5.9
assign (segid b and resid 255 and name HB# ) (segid b and resid 256 and name HN ) 0.0 1.5 5.0
assign (segid b and resid 255 and name HN ) (segid b and resid 256 and name HN ) 0.0 0.0 6.0
assign (segid b and resid 256 and name HA ) (segid b and resid 257 and name HN ) 0.0 0.0 6.0
assign (segid b and resid 256 and name HB ) (segid b and resid 257 and name HN ) 0.0 0.0 5.0
assign (segid b and resid 256 and name HG2# ) (segid b and resid 257 and name HN ) 0.0 1.5 6.5
assign (segid b and resid 256 and name HN ) (segid b and resid 257 and name HN ) 0.0 0.0 6.0
assign (segid b and resid 257 and name HA ) (segid b and resid 258 and name HN ) 0.0 0.0 5.0
assign (segid b and resid 257 and name HB# ) (segid b and resid 258 and name HN ) 0.0 1.0 3.9
assign (segid b and resid 257 and name HN ) (segid b and resid 258 and name HG# ) 0.0 1.0 6.0
assign (segid b and resid 257 and name HN ) (segid b and resid 258 and name HN ) 0.0 0.0 3.5
assign (segid b and resid 258 and name HA ) (segid b and resid 259 and name HN ) 0.0 0.0 5.0
assign (segid b and resid 258 and name HB# ) (segid b and resid 259 and name HN ) 0.0 1.0 6.0
assign (segid b and resid 258 and name HN ) (segid b and resid 259 and name HB# ) 0.0 1.0 6.0
assign (segid b and resid 258 and name HN ) (segid b and resid 259 and name HN ) 0.0 0.0 2.9
assign (segid b and resid 259 and name HA ) (segid b and resid 260 and name HN ) 0.0 0.0 2.9
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assign (segid b and resid 259 and name HB# ) (segid b and resid 260 and name HN ) 0.0 1.0 4.5
assign (segid b and resid 260 and name HA ) (segid b and resid 261 and name HN ) 0.0 0.0 3.5
assign (segid b and resid 260 and name HB# ) (segid b and resid 261 and name HN ) 0.0 1.0 7.0
assign (segid b and resid 261 and name HA ) (segid b and resid 262 and name HN ) 0.0 0.0 6.0
assign (segid b and resid 261 and name HG# ) (segid b and resid 262 and name HN ) 0.0 1.0 6.0
assign (segid b and resid 261 and name HN ) (segid b and resid 262 and name HN ) 0.0 0.0 5.0
assign (segid b and resid 262 and name HA ) (segid b and resid 263 and name HN ) 0.0 0.0 5.0
assign (segid b and resid 262 and name HB# ) (segid b and resid 263 and name HN ) 0.0 1.0 6.0
assign (segid b and resid 262 and name HG# ) (segid b and resid 263 and name HN ) 0.0 1.0 4.5
assign (segid b and resid 262 and name HN ) (segid b and resid 263 and name HA ) 0.0 0.0 6.0
assign (segid b and resid 262 and name HN ) (segid b and resid 263 and name HB# ) 0.0 1.0 7.0
assign (segid b and resid 262 and name HN ) (segid b and resid 263 and name HN ) 0.0 0.0 6.0
assign (segid b and resid 263 and name HA ) (segid b and resid 264 and name HN ) 0.0 0.0 5.0
assign (segid b and resid 263 and name HB# ) (segid b and resid 264 and name HN ) 0.0 1.0 7.0
assign (segid b and resid 263 and name HN ) (segid b and resid 264 and name HA# ) 0.0 1.0 6.0
assign (segid b and resid 263 and name HN ) (segid b and resid 264 and name HN ) 0.0 0.0 3.5
assign (segid b and resid 264 and name HA# ) (segid b and resid 265 and name HN ) 0.0 1.0 7.0
assign (segid b and resid 264 and name HN ) (segid b and resid 265 and name HN ) 0.0 0.0 5.0
assign (segid b and resid 265 and name HA ) (segid b and resid 266 and name HN ) 0.0 0.0 5.0
assign (segid b and resid 265 and name HB# ) (segid b and resid 266 and name HN ) 0.0 1.0 7.0
assign (segid b and resid 265 and name HD# ) (segid b and resid 266 and name HD# ) 0.0 4.4 7.9
assign (segid b and resid 265 and name HE# ) (segid b and resid 266 and name HN ) 0.0 2.0 7.0
assign (segid b and resid 265 and name HN ) (segid b and resid 266 and name HN ) 0.0 0.0 5.0
assign (segid b and resid 266 and name HA ) (segid b and resid 267 and name HN ) 0.0 0.0 5.0
assign (segid b and resid 266 and name HB# ) (segid b and resid 267 and name HN ) 0.0 1.0 6.0
assign (segid b and resid 266 and name HD# ) (segid b and resid 267 and name HN ) 0.0 2.4 7.4
assign (segid b and resid 266 and name HN ) (segid b and resid 267 and name HN ) 0.0 0.0 5.0
assign (segid b and resid 267 and name HA ) (segid b and resid 268 and name HN ) 0.0 0.0 5.0
assign (segid b and resid 267 and name HB# ) (segid b and resid 268 and name HN ) 0.0 1.5 4.4
assign (segid b and resid 267 and name HN ) (segid b and resid 268 and name HN ) 0.0 0.0 6.0
assign (segid b and resid 268 and name HA ) (segid b and resid 269 and name HN ) 0.0 0.0 5.0
assign (segid b and resid 268 and name HB# ) (segid b and resid 269 and name HN ) 0.0 1.0 3.9
assign (segid b and resid 268 and name HN ) (segid b and resid 269 and name HN ) 0.0 0.0 3.5
assign (segid b and resid 269 and name HA ) (segid b and resid 270 and name HN ) 0.0 0.0 6.0
assign (segid b and resid 269 and name HB# ) (segid b and resid 270 and name HN ) 0.0 1.0 4.5
assign (segid b and resid 269 and name HN ) (segid b and resid 270 and name HN ) 0.0 0.0 6.0
assign (segid b and resid 270 and name HA ) (segid b and resid 271 and name HN ) 0.0 0.0 5.0
assign (segid b and resid 270 and name HB ) (segid b and resid 271 and name HN ) 0.0 0.0 5.0
assign (segid b and resid 270 and name HD1# ) (segid b and resid 271 and name HN ) 0.0 1.5 6.5
assign (segid b and resid 270 and name HG2# ) (segid b and resid 271 and name HN ) 0.0 1.5 6.5
assign (segid b and resid 270 and name HN ) (segid b and resid 271 and name HN ) 0.0 0.0 5.0
assign (segid b and resid 271 and name HA ) (segid b and resid 272 and name HN ) 0.0 0.0 6.0
assign (segid b and resid 271 and name HB# ) (segid b and resid 272 and name HN ) 0.0 1.0 6.0
assign (segid b and resid 271 and name HN ) (segid b and resid 272 and name HB# ) 0.0 1.0 6.0
assign (segid b and resid 271 and name HN ) (segid b and resid 272 and name HG# ) 0.0 1.0 6.0
assign (segid b and resid 271 and name HN ) (segid b and resid 272 and name HN ) 0.0 0.0 3.5
assign (segid b and resid 272 and name HA ) (segid b and resid 273 and name HN ) 0.0 0.0 6.0
assign (segid b and resid 272 and name HB# ) (segid b and resid 273 and name HN ) 0.0 1.0 3.9
assign (segid b and resid 272 and name HN ) (segid b and resid 273 and name HA ) 0.0 0.0 6.0
assign (segid b and resid 272 and name HN ) (segid b and resid 273 and name HB# ) 0.0 1.0 7.0
assign (segid b and resid 272 and name HN ) (segid b and resid 273 and name HN ) 0.0 0.0 5.0
assign (segid b and resid 273 and name HA ) (segid b and resid 274 and name HN ) 0.0 0.0 6.0
assign (segid b and resid 273 and name HB# ) (segid b and resid 274 and name HN ) 0.0 1.0 7.0
assign (segid b and resid 273 and name HN ) (segid b and resid 274 and name HB ) 0.0 0.0 5.0
assign (segid b and resid 273 and name HN ) (segid b and resid 274 and name HG2# ) 0.0 1.5 6.5
assign (segid b and resid 273 and name HN ) (segid b and resid 274 and name HN ) 0.0 0.0 5.0
assign (segid b and resid 274 and name HB ) (segid b and resid 275 and name HN ) 0.0 0.0 6.0
assign (segid b and resid 274 and name HD1# ) (segid b and resid 275 and name HN ) 0.0 1.5 7.5
assign (segid b and resid 274 and name HG1# ) (segid b and resid 275 and name HN ) 0.0 1.0 6.0
assign (segid b and resid 274 and name HN ) (segid b and resid 275 and name HN ) 0.0 0.0 6.0
assign (segid b and resid 275 and name HN ) (segid b and resid 276 and name HN ) 0.0 0.0 6.0
assign (segid b and resid 276 and name HA ) (segid b and resid 277 and name HN ) 0.0 0.0 3.5
assign (segid b and resid 276 and name HB# ) (segid b and resid 277 and name HN ) 0.0 1.0 6.0
assign (segid b and resid 276 and name HG# ) (segid b and resid 277 and name HN ) 0.0 1.0 3.9
assign (segid b and resid 276 and name HN ) (segid b and resid 277 and name HN ) 0.0 0.0 6.0
assign (segid b and resid 277 and name HA ) (segid b and resid 278 and name HN ) 0.0 0.0 5.0
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assign (segid b and resid 277 and name HB# )(segid b and resid 278 and name HN  ) 0.0 1.0 6.0
assign (segid b and resid 277 and name HN  )(segid b and resid 278 and name HB# ) 0.0 1.0 6.0
assign (segid b and resid 277 and name HN  )(segid b and resid 278 and name HN  ) 0.0 0.0 5.0
assign (segid b and resid 278 and name HA  )(segid b and resid 279 and name HN  ) 0.0 0.0 6.0
assign (segid b and resid 278 and name HB# )(segid b and resid 279 and name HN  ) 0.0 1.0 4.5
assign (segid b and resid 278 and name HN  )(segid b and resid 279 and name HA  ) 0.0 0.0 5.0
assign (segid b and resid 278 and name HN  )(segid b and resid 279 and name HB# ) 0.0 1.5 6.5
assign (segid b and resid 278 and name HN  )(segid b and resid 279 and name HN  ) 0.0 0.0 3.5
assign (segid b and resid 279 and name HA  )(segid b and resid 280 and name HN  ) 0.0 0.0 5.0
assign (segid b and resid 279 and name HB# )(segid b and resid 280 and name HN  ) 0.0 1.5 7.5
assign (segid b and resid 279 and name HN  )(segid b and resid 280 and name HN  ) 0.0 0.0 6.0
assign (segid b and resid 280 and name HA  )(segid b and resid 281 and name HN  ) 0.0 0.0 5.0
assign (segid b and resid 280 and name HB  )(segid b and resid 281 and name HN  ) 0.0 0.0 3.5
assign (segid b and resid 280 and name HN  )(segid b and resid 281 and name HG1# ) 0.0 1.0 4.5
assign (segid b and resid 280 and name HN  )(segid b and resid 281 and name HN  ) 0.0 0.0 5.0
assign (segid b and resid 281 and name HA  )(segid b and resid 282 and name HN  ) 0.0 0.0 6.0
assign (segid b and resid 281 and name HB  )(segid b and resid 282 and name HN  ) 0.0 0.0 2.9
assign (segid b and resid 281 and name HD1# )(segid b and resid 282 and name HN  ) 0.0 1.5 6.5
assign (segid b and resid 281 and name HG2# )(segid b and resid 282 and name HN  ) 0.0 1.5 5.0
assign (segid b and resid 281 and name HN  )(segid b and resid 282 and name HA  ) 0.0 0.0 5.0
assign (segid b and resid 281 and name HN  )(segid b and resid 282 and name HB# ) 0.0 1.0 6.0
assign (segid b and resid 281 and name HN  )(segid b and resid 282 and name HN  ) 0.0 0.0 6.0
assign (segid b and resid 282 and name HA  )(segid b and resid 283 and name HN  ) 0.0 0.0 5.0
assign (segid b and resid 282 and name HB# )(segid b and resid 283 and name HN  ) 0.0 1.0 6.0
assign (segid b and resid 282 and name HN  )(segid b and resid 283 and name HN  ) 0.0 0.0 3.5
assign (segid b and resid 283 and name HA  )(segid b and resid 284 and name HN  ) 0.0 0.0 6.0
assign (segid b and resid 283 and name HB# )(segid b and resid 284 and name HN  ) 0.0 1.0 6.0
assign (segid b and resid 283 and name HG# )(segid b and resid 284 and name HN  ) 0.0 1.0 6.0
assign (segid b and resid 283 and name HN  )(segid b and resid 284 and name HA  ) 0.0 0.0 6.0
assign (segid b and resid 283 and name HN  )(segid b and resid 284 and name HN  ) 0.0 0.0 3.5
assign (segid b and resid 284 and name HA  )(segid b and resid 285 and name HN  ) 0.0 0.0 5.0
assign (segid b and resid 284 and name HB# )(segid b and resid 285 and name HN  ) 0.0 1.0 6.0
assign (segid b and resid 284 and name HN  )(segid b and resid 285 and name HA  ) 0.0 0.0 5.0
assign (segid b and resid 284 and name HN  )(segid b and resid 285 and name HG1# ) 0.0 1.0 6.0
assign (segid b and resid 284 and name HN  )(segid b and resid 285 and name HG2# ) 0.0 1.5 6.5
assign (segid b and resid 285 and name HA  )(segid b and resid 286 and name HN  ) 0.0 0.0 5.0
assign (segid b and resid 285 and name HB  )(segid b and resid 286 and name HN  ) 0.0 0.0 6.0
assign (segid b and resid 285 and name HG1# )(segid b and resid 286 and name HN  ) 0.0 1.0 6.0
assign (segid b and resid 285 and name HN  )(segid b and resid 286 and name HA  ) 0.0 0.0 6.0
assign (segid b and resid 285 and name HN  )(segid b and resid 286 and name HB# ) 0.0 1.0 6.0
assign (segid b and resid 285 and name HN  )(segid b and resid 286 and name HN  ) 0.0 0.0 3.5
assign (segid b and resid 286 and name HA  )(segid b and resid 287 and name HN  ) 0.0 0.0 3.5
assign (segid b and resid 286 and name HB# )(segid b and resid 287 and name HN  ) 0.0 1.0 4.5
assign (segid b and resid 286 and name HN  )(segid b and resid 287 and name HN  ) 0.0 0.0 6.0
assign (segid b and resid 287 and name HA  )(segid b and resid 288 and name HN  ) 0.0 0.0 3.5
assign (segid b and resid 287 and name HB# )(segid b and resid 288 and name HN  ) 0.0 1.0 6.0
assign (segid b and resid 287 and name HE# )(segid b and resid 288 and name HD1# ) 0.0 3.5 9.5
assign (segid b and resid 287 and name HE# )(segid b and resid 288 and name HN  ) 0.0 2.0 7.0
assign (segid b and resid 287 and name HN  )(segid b and resid 288 and name HA  ) 0.0 0.0 5.0
assign (segid b and resid 287 and name HN  )(segid b and resid 288 and name HD2# ) 0.0 1.5 6.5
assign (segid b and resid 287 and name HN  )(segid b and resid 288 and name HG  ) 0.0 0.0 5.0
assign (segid b and resid 287 and name HN  )(segid b and resid 288 and name HN  ) 0.0 0.0 2.9
assign (segid b and resid 288 and name HA  )(segid b and resid 289 and name HN  ) 0.0 0.0 2.9
assign (segid b and resid 288 and name HD# )(segid b and resid 289 and name HN  ) 0.0 2.4 5.9
assign (segid b and resid 288 and name HN  )(segid b and resid 289 and name HA  ) 0.0 0.0 6.0
assign (segid b and resid 288 and name HN  )(segid b and resid 289 and name HN  ) 0.0 0.0 3.5
assign (segid a and resid 227 and name HA  )(segid a and resid 230 and name HB# ) 0.0 1.0 6.0
assign (segid a and resid 229 and name HA  )(segid a and resid 232 and name HB# ) 0.0 1.0 6.0
assign (segid a and resid 229 and name HN  )(segid a and resid 231 and name HN  ) 0.0 0.0 5.0
assign (segid a and resid 231 and name HA  )(segid a and resid 233 and name HN  ) 0.0 0.0 5.0
assign (segid a and resid 231 and name HA  )(segid a and resid 234 and name HB# ) 0.0 1.0 7.0
assign (segid a and resid 231 and name HB# )(segid a and resid 233 and name HN  ) 0.0 1.5 6.5
assign (segid a and resid 232 and name HA  )(segid a and resid 235 and name HB  ) 0.0 0.0 3.5
assign (segid a and resid 232 and name HB# )(segid a and resid 235 and name HN  ) 0.0 1.0 7.0
assign (segid a and resid 233 and name HA  )(segid a and resid 235 and name HN  ) 0.0 0.0 5.0
assign (segid a and resid 233 and name HA  )(segid a and resid 236 and name HB# ) 0.0 1.0 4.5
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assign (segid a and resid 233 and name HA  )(segid a and resid 236 and name HN  ) 0.0 0.0 5.0
assign (segid a and resid 233 and name HB# )(segid a and resid 235 and name HN  ) 0.0 1.0 6.0
assign (segid a and resid 233 and name HB# )(segid a and resid 236 and name HN  ) 0.0 1.0 7.0
assign (segid a and resid 234 and name HA  )(segid a and resid 237 and name HN  ) 0.0 0.0 6.0
assign (segid a and resid 234 and name HB# )(segid a and resid 236 and name HN  ) 0.0 1.0 6.0
assign (segid a and resid 234 and name HG# )(segid a and resid 236 and name HN  ) 0.0 1.0 3.9
assign (segid a and resid 234 and name HN  )(segid a and resid 236 and name HD2# ) 0.0 1.5 6.5
assign (segid a and resid 234 and name HN  )(segid a and resid 236 and name HN  ) 0.0 0.0 5.0
assign (segid a and resid 235 and name HA  )(segid a and resid 238 and name HN  ) 0.0 0.0 3.5
assign (segid a and resid 235 and name HN  )(segid a and resid 237 and name HN  ) 0.0 0.0 5.0
assign (segid a and resid 236 and name HA  )(segid a and resid 239 and name HB# ) 0.0 1.5 4.4
assign (segid a and resid 236 and name HB# )(segid a and resid 238 and name HN  ) 0.0 1.0 6.0
assign (segid a and resid 236 and name HG  )(segid a and resid 240 and name HN  ) 0.0 0.0 6.0
assign (segid a and resid 237 and name HA  )(segid a and resid 241 and name HN  ) 0.0 0.0 5.0
assign (segid a and resid 237 and name HD# )(segid a and resid 240 and name HA# ) 0.0 3.4 6.3
assign (segid a and resid 237 and name HD# )(segid a and resid 240 and name HN  ) 0.0 2.4 7.4
assign (segid a and resid 237 and name HD1# )(segid a and resid 241 and name HG# ) 0.0 3.9 6.8
assign (segid a and resid 237 and name HD2# )(segid a and resid 241 and name HG# ) 0.0 3.9 6.8
assign (segid a and resid 238 and name HA  )(segid a and resid 241 and name HB  ) 0.0 0.0 5.0
assign (segid a and resid 238 and name HA  )(segid a and resid 241 and name HG1# ) 0.0 1.5 7.5
assign (segid a and resid 238 and name HA  )(segid a and resid 241 and name HG2# ) 0.0 1.5 6.5
assign (segid a and resid 238 and name HA  )(segid a and resid 241 and name HN  ) 0.0 0.0 3.5
assign (segid a and resid 238 and name HB# )(segid a and resid 241 and name HN  ) 0.0 1.0 6.0
assign (segid a and resid 239 and name HA  )(segid a and resid 242 and name HB# ) 0.0 1.0 6.0
assign (segid a and resid 239 and name HA  )(segid a and resid 242 and name HN  ) 0.0 0.0 6.0
assign (segid a and resid 239 and name HB# )(segid a and resid 241 and name HN  ) 0.0 1.5 6.5
assign (segid a and resid 240 and name HA# )(segid a and resid 243 and name HB# ) 0.0 2.0 8.0
assign (segid a and resid 240 and name HA# )(segid a and resid 243 and name HN  ) 0.0 1.0 6.0
assign (segid a and resid 241 and name HA  )(segid a and resid 243 and name HN  ) 0.0 0.0 5.0
assign (segid a and resid 241 and name HA  )(segid a and resid 244 and name HB# ) 0.0 1.0 7.0
assign (segid a and resid 241 and name HA  )(segid a and resid 244 and name HN  ) 0.0 0.0 5.0
assign (segid a and resid 241 and name HG# )(segid a and resid 243 and name HN  ) 0.0 2.4 8.4
assign (segid a and resid 241 and name HN  )(segid a and resid 243 and name HN  ) 0.0 0.0 5.0
assign (segid a and resid 242 and name HN  )(segid a and resid 244 and name HN  ) 0.0 0.0 5.0
assign (segid a and resid 243 and name HA  )(segid a and resid 246 and name HB# ) 0.0 1.0 7.0
assign (segid a and resid 244 and name HA  )(segid a and resid 246 and name HN  ) 0.0 0.0 6.0
assign (segid a and resid 244 and name HA  )(segid a and resid 247 and name HN  ) 0.0 0.0 5.0
assign (segid a and resid 244 and name HN  )(segid a and resid 246 and name HB# ) 0.0 1.0 6.0
assign (segid a and resid 245 and name HN  )(segid a and resid 247 and name HN  ) 0.0 0.0 6.0
assign (segid a and resid 246 and name HA  )(segid a and resid 249 and name HB# ) 0.0 1.0 4.5
assign (segid a and resid 246 and name HA  )(segid a and resid 249 and name HN  ) 0.0 0.0 6.0
assign (segid a and resid 246 and name HN  )(segid a and resid 249 and name HD# ) 0.0 2.4 7.4
assign (segid a and resid 247 and name HA  )(segid a and resid 250 and name HB  ) 0.0 0.0 5.0
assign (segid a and resid 247 and name HA  )(segid a and resid 250 and name HN  ) 0.0 0.0 6.0
assign (segid a and resid 247 and name HB  )(segid a and resid 249 and name HN  ) 0.0 0.0 6.0
assign (segid a and resid 247 and name HG2# )(segid a and resid 249 and name HN  ) 0.0 1.5 6.5
assign (segid a and resid 247 and name HN  )(segid a and resid 249 and name HD# ) 0.0 2.4 8.4
assign (segid a and resid 247 and name HN  )(segid a and resid 249 and name HN  ) 0.0 0.0 5.0
assign (segid a and resid 248 and name HA  )(segid a and resid 251 and name HB# ) 0.0 1.0 4.5
assign (segid a and resid 248 and name HA  )(segid a and resid 251 and name HN  ) 0.0 0.0 3.5
assign (segid a and resid 248 and name HD# )(segid a and resid 251 and name HN  ) 0.0 1.0 6.0
assign (segid a and resid 249 and name HA  )(segid a and resid 252 and name HB  ) 0.0 0.0 3.5
assign (segid a and resid 249 and name HA  )(segid a and resid 252 and name HN  ) 0.0 0.0 6.0
assign (segid a and resid 249 and name HB# )(segid a and resid 251 and name HN  ) 0.0 1.0 6.0
assign (segid a and resid 249 and name HB# )(segid a and resid 252 and name HG2# ) 0.0 2.5 6.0
assign (segid a and resid 249 and name HB# )(segid a and resid 252 and name HN  ) 0.0 1.0 6.0
assign (segid a and resid 249 and name HN  )(segid a and resid 251 and name HN  ) 0.0 0.0 6.0
assign (segid a and resid 250 and name HA  )(segid a and resid 253 and name HN  ) 0.0 0.0 5.0
assign (segid a and resid 250 and name HG2# )(segid a and resid 253 and name HN  ) 0.0 1.5 6.5
assign (segid a and resid 250 and name HG2# )(segid a and resid 254 and name HD# ) 0.0 3.9 6.8
assign (segid a and resid 250 and name HG2# )(segid a and resid 254 and name HG  ) 0.0 1.5 5.0
assign (segid a and resid 250 and name HG2# )(segid a and resid 254 and name HN  ) 0.0 1.5 6.5
assign (segid a and resid 250 and name HN  )(segid a and resid 253 and name HG# ) 0.0 1.0 6.0
assign (segid a and resid 251 and name HA  )(segid a and resid 254 and name HB# ) 0.0 1.0 4.5
assign (segid a and resid 251 and name HA  )(segid a and resid 254 and name HN  ) 0.0 0.0 5.0
assign (segid a and resid 251 and name HN  )(segid a and resid 253 and name HD# ) 0.0 1.0 6.0
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Table A.4. *(continued)*

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assign (segid a and resid 251 and name HN )(segid a and resid 253 and name HN ) 0.0 0.0 6.0
assign (segid a and resid 251 and name HN )(segid a and resid 254 and name HN ) 0.0 0.0 5.0
assign (segid a and resid 252 and name HA )(segid a and resid 255 and name HB# ) 0.0 1.5 5.0
assign (segid a and resid 252 and name HA )(segid a and resid 255 and name HN ) 0.0 0.0 3.5
assign (segid a and resid 252 and name HB )(segid a and resid 255 and name HN ) 0.0 0.0 6.0
assign (segid a and resid 252 and name HD# )(segid a and resid 255 and name HN ) 0.0 1.5 6.5
assign (segid a and resid 252 and name HD# )(segid a and resid 256 and name HN ) 0.0 1.5 6.5
assign (segid a and resid 252 and name HG2# )(segid a and resid 255 and name HB# ) 0.0 3.0 8.0
assign (segid a and resid 252 and name HG2# )(segid a and resid 255 and name HN ) 0.0 1.5 5.0
assign (segid a and resid 252 and name HG2# )(segid a and resid 256 and name HN ) 0.0 1.5 6.5
assign (segid a and resid 253 and name HA )(segid a and resid 255 and name HN ) 0.0 0.0 5.0
assign (segid a and resid 253 and name HA )(segid a and resid 256 and name HN ) 0.0 0.0 5.0
assign (segid a and resid 253 and name HB# )(segid a and resid 256 and name HN ) 0.0 1.0 7.0
assign (segid a and resid 253 and name HG# )(segid a and resid 257 and name HB# ) 0.0 2.0 5.5
assign (segid a and resid 253 and name HN )(segid a and resid 257 and name HB# ) 0.0 1.0 6.0
assign (segid a and resid 254 and name HA )(segid a and resid 257 and name HN ) 0.0 0.0 2.9
assign (segid a and resid 254 and name HB# )(segid a and resid 256 and name HN ) 0.0 1.0 7.0
assign (segid a and resid 254 and name HN )(segid a and resid 256 and name HN ) 0.0 0.0 5.0
assign (segid a and resid 254 and name HN )(segid a and resid 257 and name HN ) 0.0 0.0 6.0
assign (segid a and resid 255 and name HA )(segid a and resid 258 and name HB# ) 0.0 1.0 6.0
assign (segid a and resid 255 and name HA )(segid a and resid 258 and name HN ) 0.0 0.0 6.0
assign (segid a and resid 255 and name HB# )(segid a and resid 257 and name HN ) 0.0 1.5 6.5
assign (segid a and resid 255 and name HB# )(segid a and resid 258 and name HN ) 0.0 1.5 6.5
assign (segid a and resid 255 and name HN )(segid a and resid 257 and name HN ) 0.0 0.0 5.0
assign (segid a and resid 256 and name HA )(segid a and resid 258 and name HN ) 0.0 0.0 6.0
assign (segid a and resid 256 and name HA )(segid a and resid 259 and name HB# ) 0.0 1.0 6.0
assign (segid a and resid 256 and name HA )(segid a and resid 259 and name HN ) 0.0 0.0 5.0
assign (segid a and resid 256 and name HB )(segid a and resid 259 and name HN ) 0.0 0.0 5.0
assign (segid a and resid 256 and name HG2# )(segid a and resid 258 and name HN ) 0.0 1.5 7.5
assign (segid a and resid 256 and name HN )(segid a and resid 258 and name HB# ) 0.0 1.0 6.0
assign (segid a and resid 256 and name HN )(segid a and resid 258 and name HG# ) 0.0 1.0 7.0
assign (segid a and resid 256 and name HN )(segid a and resid 258 and name HN ) 0.0 0.0 5.0
assign (segid a and resid 257 and name HA )(segid a and resid 260 and name HN ) 0.0 0.0 3.5
assign (segid a and resid 257 and name HB# )(segid a and resid 260 and name HN ) 0.0 1.0 6.0
assign (segid a and resid 257 and name HN )(segid a and resid 259 and name HN ) 0.0 0.0 5.0
assign (segid a and resid 258 and name HA )(segid a and resid 261 and name HB# ) 0.0 1.0 4.5
assign (segid a and resid 259 and name HA )(segid a and resid 262 and name HB# ) 0.0 1.0 6.0
assign (segid a and resid 259 and name HB# )(segid a and resid 263 and name HN ) 0.0 1.0 6.0
assign (segid a and resid 260 and name HA )(segid a and resid 262 and name HN ) 0.0 0.0 5.0
assign (segid a and resid 260 and name HA )(segid a and resid 263 and name HN ) 0.0 0.0 6.0
assign (segid a and resid 261 and name HA )(segid a and resid 263 and name HN ) 0.0 0.0 5.0
assign (segid a and resid 261 and name HA )(segid a and resid 264 and name HN ) 0.0 0.0 2.9
assign (segid a and resid 261 and name HG# )(segid a and resid 263 and name HN ) 0.0 1.0 7.0
assign (segid a and resid 261 and name HN )(segid a and resid 264 and name HA# ) 0.0 1.0 6.0
assign (segid a and resid 262 and name HA )(segid a and resid 264 and name HN ) 0.0 0.0 5.0
assign (segid a and resid 262 and name HN )(segid a and resid 264 and name HA# ) 0.0 1.0 6.0
assign (segid a and resid 262 and name HN )(segid a and resid 264 and name HN ) 0.0 0.0 5.0
assign (segid a and resid 263 and name HA )(segid a and resid 265 and name HD# ) 0.0 2.0 5.5
assign (segid a and resid 263 and name HA )(segid a and resid 265 and name HN ) 0.0 0.0 6.0
assign (segid a and resid 263 and name HA )(segid a and resid 266 and name HN ) 0.0 0.0 6.0
assign (segid a and resid 263 and name HN )(segid a and resid 265 and name HN ) 0.0 0.0 6.0
assign (segid a and resid 264 and name HA# )(segid a and resid 267 and name HB# ) 0.0 2.5 6.0
assign (segid a and resid 265 and name HA )(segid a and resid 267 and name HN ) 0.0 0.0 6.0
assign (segid a and resid 265 and name HA )(segid a and resid 268 and name HB# ) 0.0 1.0 4.5
assign (segid a and resid 265 and name HA )(segid a and resid 268 and name HN ) 0.0 0.0 6.0
assign (segid a and resid 265 and name HB# )(segid a and resid 267 and name HN ) 0.0 1.0 6.0
assign (segid a and resid 265 and name HN )(segid a and resid 267 and name HB# ) 0.0 1.5 7.5
assign (segid a and resid 265 and name HN )(segid a and resid 267 and name HN ) 0.0 0.0 6.0
assign (segid a and resid 266 and name HA )(segid a and resid 269 and name HN ) 0.0 0.0 5.0
assign (segid a and resid 266 and name HB# )(segid a and resid 270 and name HD1# ) 0.0 2.5 8.5
assign (segid a and resid 267 and name HA )(segid a and resid 270 and name HB ) 0.0 0.0 3.5
assign (segid a and resid 267 and name HA )(segid a and resid 270 and name HN ) 0.0 0.0 6.0
assign (segid a and resid 267 and name HB# )(segid a and resid 269 and name HN ) 0.0 1.5 6.5
assign (segid a and resid 267 and name HN )(segid a and resid 269 and name HN ) 0.0 0.0 6.0
assign (segid a and resid 267 and name HN )(segid a and resid 270 and name HN ) 0.0 0.0 5.0
assign (segid a and resid 268 and name HA )(segid a and resid 270 and name HN ) 0.0 0.0 3.5
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Table A.4. *(continued)*

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assign (segid a and resid 268 and name HA )(segid a and resid 271 and name HB# ) 0.0 1.0 4.5
assign (segid a and resid 268 and name HA )(segid a and resid 271 and name HN ) 0.0 0.0 3.5
assign (segid a and resid 268 and name HG# )(segid a and resid 272 and name HG# ) 0.0 2.0 7.0
assign (segid a and resid 269 and name HA )(segid a and resid 272 and name HB# ) 0.0 1.0 4.5
assign (segid a and resid 269 and name HA )(segid a and resid 272 and name HN ) 0.0 0.0 5.0
assign (segid a and resid 269 and name HB# )(segid a and resid 271 and name HN ) 0.0 1.0 7.0
assign (segid a and resid 269 and name HB# )(segid a and resid 272 and name HN ) 0.0 1.0 7.0
assign (segid a and resid 269 and name HN )(segid a and resid 271 and name HN ) 0.0 0.0 5.0
assign (segid a and resid 270 and name HA )(segid a and resid 273 and name HB# ) 0.0 1.0 7.0
assign (segid a and resid 270 and name HA )(segid a and resid 273 and name HN ) 0.0 0.0 5.0
assign (segid a and resid 270 and name HG2# )(segid a and resid 272 and name HN ) 0.0 1.5 6.5
assign (segid a and resid 270 and name HG2# )(segid a and resid 274 and name HG1# ) 0.0 2.5 6.0
assign (segid a and resid 270 and name HN )(segid a and resid 272 and name HN ) 0.0 0.0 6.0
assign (segid a and resid 271 and name HA )(segid a and resid 274 and name HB ) 0.0 0.0 3.5
assign (segid a and resid 271 and name HA )(segid a and resid 274 and name HN ) 0.0 0.0 3.5
assign (segid a and resid 271 and name HA )(segid a and resid 275 and name HN ) 0.0 0.0 6.0
assign (segid a and resid 271 and name HN )(segid a and resid 273 and name HN ) 0.0 0.0 6.0
assign (segid a and resid 271 and name HN )(segid a and resid 274 and name HB ) 0.0 0.0 5.0
assign (segid a and resid 271 and name HN )(segid a and resid 274 and name HD1# ) 0.0 1.5 6.5
assign (segid a and resid 271 and name HN )(segid a and resid 274 and name HN ) 0.0 0.0 6.0
assign (segid a and resid 272 and name HA )(segid a and resid 274 and name HN ) 0.0 0.0 5.0
assign (segid a and resid 272 and name HA )(segid a and resid 275 and name HN ) 0.0 0.0 2.9
assign (segid a and resid 272 and name HB# )(segid a and resid 274 and name HN ) 0.0 1.0 6.0
assign (segid a and resid 272 and name HN )(segid a and resid 274 and name HB ) 0.0 0.0 5.0
assign (segid a and resid 272 and name HN )(segid a and resid 274 and name HN ) 0.0 0.0 6.0
assign (segid a and resid 272 and name HN )(segid a and resid 275 and name HN ) 0.0 0.0 5.0
assign (segid a and resid 273 and name HA )(segid a and resid 275 and name HN ) 0.0 0.0 6.0
assign (segid a and resid 273 and name HA )(segid a and resid 276 and name HB# ) 0.0 1.0 6.0
assign (segid a and resid 273 and name HA )(segid a and resid 276 and name HN ) 0.0 0.0 5.0
assign (segid a and resid 273 and name HA )(segid a and resid 277 and name HN ) 0.0 0.0 5.0
assign (segid a and resid 273 and name HB# )(segid a and resid 275 and name HN ) 0.0 1.0 6.0
assign (segid a and resid 273 and name HB# )(segid a and resid 276 and name HN ) 0.0 1.0 6.0
assign (segid a and resid 273 and name HN )(segid a and resid 275 and name HN ) 0.0 0.0 5.0
assign (segid a and resid 274 and name HA )(segid a and resid 277 and name HB# ) 0.0 1.0 6.0
assign (segid a and resid 274 and name HA )(segid a and resid 277 and name HN ) 0.0 0.0 5.0
assign (segid a and resid 274 and name HA )(segid a and resid 278 and name HN ) 0.0 0.0 5.0
assign (segid a and resid 274 and name HD1# )(segid a and resid 277 and name HN ) 0.0 1.5 6.5
assign (segid a and resid 274 and name HN )(segid a and resid 276 and name HN ) 0.0 0.0 5.0
assign (segid a and resid 275 and name HA )(segid a and resid 278 and name HB# ) 0.0 1.0 3.9
assign (segid a and resid 275 and name HA )(segid a and resid 278 and name HN ) 0.0 0.0 3.5
assign (segid a and resid 276 and name HA )(segid a and resid 278 and name HN ) 0.0 0.0 6.0
assign (segid a and resid 276 and name HA )(segid a and resid 279 and name HB# ) 0.0 1.5 4.4
assign (segid a and resid 276 and name HB# )(segid a and resid 278 and name HN ) 0.0 1.0 7.0
assign (segid a and resid 276 and name HG# )(segid a and resid 278 and name HN ) 0.0 1.0 6.0
assign (segid a and resid 276 and name HG# )(segid a and resid 280 and name HD1# ) 0.0 2.5 7.5
assign (segid a and resid 276 and name HN )(segid a and resid 278 and name HN ) 0.0 0.0 5.0
assign (segid a and resid 276 and name HN )(segid a and resid 279 and name HB# ) 0.0 1.5 6.5
assign (segid a and resid 276 and name HN )(segid a and resid 279 and name HN ) 0.0 0.0 5.0
assign (segid a and resid 276 and name HN )(segid a and resid 280 and name HG1# ) 0.0 1.0 6.0
assign (segid a and resid 277 and name HA )(segid a and resid 279 and name HN ) 0.0 0.0 5.0
assign (segid a and resid 277 and name HA )(segid a and resid 280 and name HB ) 0.0 0.0 5.0
assign (segid a and resid 277 and name HA )(segid a and resid 280 and name HD1# ) 0.0 1.5 6.5
assign (segid a and resid 277 and name HA )(segid a and resid 280 and name HN ) 0.0 0.0 5.0
assign (segid a and resid 277 and name HN )(segid a and resid 281 and name HG1# ) 0.0 1.0 6.0
assign (segid a and resid 278 and name HA )(segid a and resid 280 and name HD1# ) 0.0 1.5 5.0
assign (segid a and resid 278 and name HA )(segid a and resid 281 and name HB ) 0.0 0.0 6.0
assign (segid a and resid 278 and name HA )(segid a and resid 281 and name HN ) 0.0 0.0 5.0
assign (segid a and resid 278 and name HA )(segid a and resid 282 and name HN ) 0.0 0.0 5.0
assign (segid a and resid 278 and name HN )(segid a and resid 280 and name HD1# ) 0.0 1.5 6.5
assign (segid a and resid 278 and name HN )(segid a and resid 280 and name HN ) 0.0 0.0 6.0
assign (segid a and resid 278 and name HN )(segid a and resid 281 and name HG1# ) 0.0 1.0 6.0
assign (segid a and resid 279 and name HA )(segid a and resid 282 and name HB# ) 0.0 1.0 3.9
assign (segid a and resid 279 and name HA )(segid a and resid 282 and name HN ) 0.0 0.0 5.0
assign (segid a and resid 279 and name HB# )(segid a and resid 281 and name HN ) 0.0 1.5 6.5
assign (segid a and resid 279 and name HB# )(segid a and resid 282 and name HN ) 0.0 1.5 6.5
assign (segid a and resid 279 and name HB# )(segid a and resid 283 and name HN ) 0.0 1.5 6.5
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Table A.4. *(continued)*

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assign (segid a and resid 279 and name HN )(segid a and resid 281 and name HN ) 0.0 0.0 5.0
assign (segid a and resid 280 and name HA )(segid a and resid 283 and name HB# ) 0.0 1.0 7.0
assign (segid a and resid 280 and name HA )(segid a and resid 283 and name HG# ) 0.0 1.0 7.0
assign (segid a and resid 280 and name HA )(segid a and resid 283 and name HN ) 0.0 0.0 5.0
assign (segid a and resid 280 and name HN )(segid a and resid 282 and name HN ) 0.0 0.0 6.0
assign (segid a and resid 280 and name HN )(segid a and resid 283 and name HG# ) 0.0 1.0 7.0
assign (segid a and resid 280 and name HN )(segid a and resid 283 and name HN ) 0.0 0.0 5.0
assign (segid a and resid 281 and name HA )(segid a and resid 283 and name HN ) 0.0 0.0 6.0
assign (segid a and resid 281 and name HA )(segid a and resid 284 and name HB# ) 0.0 1.0 6.0
assign (segid a and resid 281 and name HA )(segid a and resid 284 and name HN ) 0.0 0.0 5.0
assign (segid a and resid 281 and name HA )(segid a and resid 285 and name HN ) 0.0 0.0 5.0
assign (segid a and resid 281 and name HB )(segid a and resid 283 and name HN ) 0.0 0.0 6.0
assign (segid a and resid 281 and name HD1# )(segid a and resid 284 and name HN ) 0.0 1.5 6.5
assign (segid a and resid 282 and name HA )(segid a and resid 284 and name HN ) 0.0 0.0 6.0
assign (segid a and resid 282 and name HA )(segid a and resid 285 and name HB ) 0.0 0.0 3.5
assign (segid a and resid 282 and name HA )(segid a and resid 285 and name HN ) 0.0 0.0 5.0
assign (segid a and resid 282 and name HN )(segid a and resid 284 and name HN ) 0.0 0.0 5.0
assign (segid a and resid 282 and name HN )(segid a and resid 285 and name HN ) 0.0 0.0 5.0
assign (segid a and resid 283 and name HA )(segid a and resid 285 and name HN ) 0.0 0.0 6.0
assign (segid a and resid 283 and name HA )(segid a and resid 286 and name HB# ) 0.0 1.0 4.5
assign (segid a and resid 283 and name HA )(segid a and resid 286 and name HN ) 0.0 0.0 6.0
assign (segid a and resid 283 and name HA )(segid a and resid 287 and name HN ) 0.0 0.0 6.0
assign (segid a and resid 283 and name HN )(segid a and resid 285 and name HN ) 0.0 0.0 6.0
assign (segid a and resid 283 and name HN )(segid a and resid 286 and name HB# ) 0.0 1.0 7.0
assign (segid a and resid 284 and name HA )(segid a and resid 286 and name HN ) 0.0 0.0 5.0
assign (segid a and resid 284 and name HA )(segid a and resid 287 and name HB# ) 0.0 1.0 7.0
assign (segid a and resid 284 and name HA )(segid a and resid 287 and name HN ) 0.0 0.0 5.0
assign (segid a and resid 284 and name HB# )(segid a and resid 287 and name HN ) 0.0 1.0 7.0
assign (segid a and resid 285 and name HA )(segid a and resid 287 and name HN ) 0.0 0.0 6.0
assign (segid a and resid 285 and name HA )(segid a and resid 288 and name HD1# ) 0.0 1.5 6.5
assign (segid a and resid 285 and name HA )(segid a and resid 288 and name HN ) 0.0 0.0 5.0
assign (segid a and resid 285 and name HB )(segid a and resid 287 and name HN ) 0.0 0.0 6.0
assign (segid a and resid 285 and name HB )(segid a and resid 288 and name HN ) 0.0 0.0 6.0
assign (segid a and resid 285 and name HD1# )(segid a and resid 287 and name HN ) 0.0 1.5 6.5
assign (segid a and resid 285 and name HD1# )(segid a and resid 288 and name HD# ) 0.0 3.9 6.8
assign (segid a and resid 285 and name HG2# )(segid a and resid 288 and name HD# ) 0.0 3.9 6.8
assign (segid a and resid 285 and name HG2# )(segid a and resid 288 and name HN ) 0.0 1.5 6.5
assign (segid a and resid 286 and name HA )(segid a and resid 288 and name HN ) 0.0 0.0 6.0
assign (segid a and resid 286 and name HA )(segid a and resid 289 and name HB# ) 0.0 1.0 6.0
assign (segid a and resid 286 and name HA )(segid a and resid 289 and name HD# ) 0.0 1.0 4.5
assign (segid a and resid 286 and name HA )(segid a and resid 289 and name HG# ) 0.0 1.0 4.5
assign (segid a and resid 286 and name HA )(segid a and resid 289 and name HN ) 0.0 0.0 6.0
assign (segid a and resid 286 and name HB# )(segid a and resid 288 and name HN ) 0.0 1.0 6.0
assign (segid a and resid 286 and name HB# )(segid a and resid 289 and name HN ) 0.0 1.0 7.0
assign (segid a and resid 286 and name HN )(segid a and resid 288 and name HN ) 0.0 0.0 5.0
assign (segid a and resid 287 and name HA )(segid a and resid 289 and name HN ) 0.0 0.0 5.0
assign (segid a and resid 287 and name HB# )(segid a and resid 289 and name HN ) 0.0 1.0 6.0
assign (segid a and resid 287 and name HN )(segid a and resid 289 and name HN ) 0.0 0.0 6.0
assign (segid b and resid 227 and name HA )(segid b and resid 230 and name HB# ) 0.0 1.0 6.0
assign (segid b and resid 229 and name HA )(segid b and resid 232 and name HB# ) 0.0 1.0 6.0
assign (segid b and resid 229 and name HN )(segid b and resid 231 and name HN ) 0.0 0.0 5.0
assign (segid b and resid 231 and name HA )(segid b and resid 233 and name HN ) 0.0 0.0 5.0
assign (segid b and resid 231 and name HA )(segid b and resid 234 and name HB# ) 0.0 1.0 7.0
assign (segid b and resid 231 and name HB# )(segid b and resid 233 and name HN ) 0.0 1.5 6.5
assign (segid b and resid 232 and name HA )(segid b and resid 235 and name HB ) 0.0 0.0 3.5
assign (segid b and resid 232 and name HB# )(segid b and resid 235 and name HN ) 0.0 1.0 7.0
assign (segid b and resid 233 and name HA )(segid b and resid 235 and name HN ) 0.0 0.0 5.0
assign (segid b and resid 233 and name HA )(segid b and resid 236 and name HB# ) 0.0 1.0 4.5
assign (segid b and resid 233 and name HA )(segid b and resid 236 and name HN ) 0.0 0.0 5.0
assign (segid b and resid 233 and name HB# )(segid b and resid 235 and name HN ) 0.0 1.0 6.0
assign (segid b and resid 233 and name HB# )(segid b and resid 236 and name HN ) 0.0 1.0 7.0
assign (segid b and resid 234 and name HA )(segid b and resid 237 and name HN ) 0.0 0.0 6.0
assign (segid b and resid 234 and name HB# )(segid b and resid 236 and name HN ) 0.0 1.0 6.0
assign (segid b and resid 234 and name HG# )(segid b and resid 236 and name HN ) 0.0 1.0 3.9
assign (segid b and resid 234 and name HN )(segid b and resid 236 and name HD2# ) 0.0 1.5 6.5
assign (segid b and resid 234 and name HN )(segid b and resid 236 and name HN ) 0.0 0.0 5.0
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Table A.4. *(continued)*

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assign (segid b and resid 235 and name HA )(segid b and resid 238 and name HN ) 0.0 0.0 3.5
assign (segid b and resid 235 and name HN )(segid b and resid 237 and name HN ) 0.0 0.0 5.0
assign (segid b and resid 236 and name HA )(segid b and resid 239 and name HB# ) 0.0 1.5 4.4
assign (segid b and resid 236 and name HB# )(segid b and resid 238 and name HN ) 0.0 1.0 6.0
assign (segid b and resid 236 and name HG )(segid b and resid 240 and name HN ) 0.0 0.0 6.0
assign (segid b and resid 237 and name HA )(segid b and resid 241 and name HN ) 0.0 0.0 5.0
assign (segid b and resid 237 and name HD# )(segid b and resid 240 and name HA# ) 0.0 3.4 6.3
assign (segid b and resid 237 and name HD# )(segid b and resid 240 and name HN ) 0.0 2.4 7.4
assign (segid b and resid 237 and name HD1# )(segid b and resid 241 and name HG# ) 0.0 3.9 6.8
assign (segid b and resid 237 and name HD2# )(segid b and resid 241 and name HG# ) 0.0 3.9 6.8
assign (segid b and resid 238 and name HA )(segid b and resid 241 and name HB ) 0.0 0.0 5.0
assign (segid b and resid 238 and name HA )(segid b and resid 241 and name HG1# ) 0.0 1.5 7.5
assign (segid b and resid 238 and name HA )(segid b and resid 241 and name HG2# ) 0.0 1.5 6.5
assign (segid b and resid 238 and name HA )(segid b and resid 241 and name HN ) 0.0 0.0 3.5
assign (segid b and resid 238 and name HB# )(segid b and resid 241 and name HN ) 0.0 1.0 6.0
assign (segid b and resid 239 and name HA )(segid b and resid 242 and name HB# ) 0.0 1.0 6.0
assign (segid b and resid 239 and name HA )(segid b and resid 242 and name HN ) 0.0 0.0 6.0
assign (segid b and resid 239 and name HB# )(segid b and resid 241 and name HN ) 0.0 1.5 6.5
assign (segid b and resid 240 and name HA# )(segid b and resid 243 and name HB# ) 0.0 2.0 8.0
assign (segid b and resid 240 and name HA# )(segid b and resid 243 and name HN ) 0.0 1.0 6.0
assign (segid b and resid 241 and name HA )(segid b and resid 243 and name HN ) 0.0 0.0 5.0
assign (segid b and resid 241 and name HA )(segid b and resid 244 and name HB# ) 0.0 1.0 7.0
assign (segid b and resid 241 and name HA )(segid b and resid 244 and name HN ) 0.0 0.0 5.0
assign (segid b and resid 241 and name HG# )(segid b and resid 243 and name HN ) 0.0 2.4 8.4
assign (segid b and resid 241 and name HN )(segid b and resid 243 and name HN ) 0.0 0.0 5.0
assign (segid b and resid 242 and name HN )(segid b and resid 244 and name HN ) 0.0 0.0 5.0
assign (segid b and resid 243 and name HA )(segid b and resid 246 and name HB# ) 0.0 1.0 7.0
assign (segid b and resid 244 and name HA )(segid b and resid 246 and name HN ) 0.0 0.0 6.0
assign (segid b and resid 244 and name HA )(segid b and resid 247 and name HN ) 0.0 0.0 5.0
assign (segid b and resid 244 and name HN )(segid b and resid 246 and name HB# ) 0.0 1.0 6.0
assign (segid b and resid 245 and name HN )(segid b and resid 247 and name HN ) 0.0 0.0 6.0
assign (segid b and resid 246 and name HA )(segid b and resid 249 and name HB# ) 0.0 1.0 4.5
assign (segid b and resid 246 and name HA )(segid b and resid 249 and name HN ) 0.0 0.0 6.0
assign (segid b and resid 246 and name HN )(segid b and resid 249 and name HD# ) 0.0 2.4 7.4
assign (segid b and resid 247 and name HA )(segid b and resid 250 and name HB ) 0.0 0.0 5.0
assign (segid b and resid 247 and name HA )(segid b and resid 250 and name HN ) 0.0 0.0 6.0
assign (segid b and resid 247 and name HB )(segid b and resid 249 and name HN ) 0.0 0.0 6.0
assign (segid b and resid 247 and name HG2# )(segid b and resid 249 and name HN ) 0.0 1.5 6.5
assign (segid b and resid 247 and name HN )(segid b and resid 249 and name HD# ) 0.0 2.4 8.4
assign (segid b and resid 247 and name HN )(segid b and resid 249 and name HN ) 0.0 0.0 5.0
assign (segid b and resid 248 and name HA )(segid b and resid 251 and name HB# ) 0.0 1.0 4.5
assign (segid b and resid 248 and name HA )(segid b and resid 251 and name HN ) 0.0 0.0 3.5
assign (segid b and resid 248 and name HD# )(segid b and resid 251 and name HN ) 0.0 1.0 6.0
assign (segid b and resid 249 and name HA )(segid b and resid 252 and name HB ) 0.0 0.0 3.5
assign (segid b and resid 249 and name HA )(segid b and resid 252 and name HN ) 0.0 0.0 6.0
assign (segid b and resid 249 and name HB# )(segid b and resid 251 and name HN ) 0.0 1.0 6.0
assign (segid b and resid 249 and name HB# )(segid b and resid 252 and name HG2# ) 0.0 2.5 6.0
assign (segid b and resid 249 and name HB# )(segid b and resid 252 and name HN ) 0.0 1.0 6.0
assign (segid b and resid 249 and name HN )(segid b and resid 251 and name HN ) 0.0 0.0 6.0
assign (segid b and resid 250 and name HA )(segid b and resid 253 and name HN ) 0.0 0.0 5.0
assign (segid b and resid 250 and name HG2# )(segid b and resid 253 and name HN ) 0.0 1.5 6.5
assign (segid b and resid 250 and name HG2# )(segid b and resid 254 and name HD# ) 0.0 3.9 6.8
assign (segid b and resid 250 and name HG2# )(segid b and resid 254 and name HG ) 0.0 1.5 5.0
assign (segid b and resid 250 and name HG2# )(segid b and resid 254 and name HN ) 0.0 1.5 6.5
assign (segid b and resid 250 and name HN )(segid b and resid 253 and name HG# ) 0.0 1.0 6.0
assign (segid b and resid 251 and name HA )(segid b and resid 254 and name HB# ) 0.0 1.0 4.5
assign (segid b and resid 251 and name HA )(segid b and resid 254 and name HN ) 0.0 0.0 5.0
assign (segid b and resid 251 and name HN )(segid b and resid 253 and name HD# ) 0.0 1.0 6.0
assign (segid b and resid 251 and name HN )(segid b and resid 253 and name HN ) 0.0 0.0 6.0
assign (segid b and resid 251 and name HN )(segid b and resid 254 and name HN ) 0.0 0.0 5.0
assign (segid b and resid 252 and name HA )(segid b and resid 255 and name HB# ) 0.0 1.5 5.0
assign (segid b and resid 252 and name HA )(segid b and resid 255 and name HN ) 0.0 0.0 3.5
assign (segid b and resid 252 and name HB )(segid b and resid 255 and name HN ) 0.0 0.0 6.0
assign (segid b and resid 252 and name HD# )(segid b and resid 255 and name HN ) 0.0 1.5 6.5
assign (segid b and resid 252 and name HD# )(segid b and resid 256 and name HN ) 0.0 1.5 6.5
assign (segid b and resid 252 and name HG2# )(segid b and resid 255 and name HB# ) 0.0 3.0 8.0
```

Table A.4. *(continued)*

```
assign (segid b and resid 252 and name HG2# )(segid b and resid 255 and name HN  ) 0.0 1.5 5.0
assign (segid b and resid 252 and name HG2# )(segid b and resid 256 and name HN  ) 0.0 1.5 6.5
assign (segid b and resid 253 and name HA   )(segid b and resid 255 and name HN  ) 0.0 0.0 5.0
assign (segid b and resid 253 and name HA   )(segid b and resid 256 and name HN  ) 0.0 0.0 5.0
assign (segid b and resid 253 and name HB#  )(segid b and resid 256 and name HN  ) 0.0 1.0 7.0
assign (segid b and resid 253 and name HG#  )(segid b and resid 257 and name HB#  ) 0.0 2.0 5.5
assign (segid b and resid 253 and name HN   )(segid b and resid 257 and name HB#  ) 0.0 1.0 6.0
assign (segid b and resid 254 and name HA   )(segid b and resid 257 and name HN  ) 0.0 0.0 2.9
assign (segid b and resid 254 and name HB#  )(segid b and resid 256 and name HN  ) 0.0 1.0 7.0
assign (segid b and resid 254 and name HN   )(segid b and resid 256 and name HN  ) 0.0 0.0 5.0
assign (segid b and resid 254 and name HN   )(segid b and resid 257 and name HN  ) 0.0 0.0 6.0
assign (segid b and resid 255 and name HA   )(segid b and resid 258 and name HB#  ) 0.0 1.0 6.0
assign (segid b and resid 255 and name HA   )(segid b and resid 258 and name HN  ) 0.0 0.0 6.0
assign (segid b and resid 255 and name HB#  )(segid b and resid 257 and name HN  ) 0.0 1.5 6.5
assign (segid b and resid 255 and name HB#  )(segid b and resid 258 and name HN  ) 0.0 1.5 6.5
assign (segid b and resid 255 and name HN   )(segid b and resid 257 and name HN  ) 0.0 0.0 5.0
assign (segid b and resid 256 and name HA   )(segid b and resid 258 and name HN  ) 0.0 0.0 6.0
assign (segid b and resid 256 and name HA   )(segid b and resid 259 and name HB#  ) 0.0 1.0 6.0
assign (segid b and resid 256 and name HA   )(segid b and resid 259 and name HN  ) 0.0 0.0 5.0
assign (segid b and resid 256 and name HB   )(segid b and resid 259 and name HN  ) 0.0 0.0 5.0
assign (segid b and resid 256 and name HG2# )(segid b and resid 258 and name HN  ) 0.0 1.5 7.5
assign (segid b and resid 256 and name HN   )(segid b and resid 258 and name HB#  ) 0.0 1.0 6.0
assign (segid b and resid 256 and name HN   )(segid b and resid 258 and name HG#  ) 0.0 1.0 7.0
assign (segid b and resid 256 and name HN   )(segid b and resid 258 and name HN  ) 0.0 0.0 5.0
assign (segid b and resid 257 and name HA   )(segid b and resid 260 and name HN  ) 0.0 0.0 3.5
assign (segid b and resid 257 and name HB#  )(segid b and resid 260 and name HN  ) 0.0 1.0 6.0
assign (segid b and resid 257 and name HN   )(segid b and resid 259 and name HN  ) 0.0 0.0 5.0
assign (segid b and resid 258 and name HA   )(segid b and resid 261 and name HB#  ) 0.0 1.0 4.5
assign (segid b and resid 259 and name HA   )(segid b and resid 262 and name HB#  ) 0.0 1.0 6.0
assign (segid b and resid 259 and name HB#  )(segid b and resid 263 and name HN  ) 0.0 1.0 6.0
assign (segid b and resid 260 and name HA   )(segid b and resid 262 and name HN  ) 0.0 0.0 5.0
assign (segid b and resid 260 and name HA   )(segid b and resid 263 and name HN  ) 0.0 0.0 6.0
assign (segid b and resid 261 and name HA   )(segid b and resid 263 and name HN  ) 0.0 0.0 5.0
assign (segid b and resid 261 and name HA   )(segid b and resid 264 and name HN  ) 0.0 0.0 2.9
assign (segid b and resid 261 and name HG#  )(segid b and resid 263 and name HN  ) 0.0 1.0 7.0
assign (segid b and resid 261 and name HN   )(segid b and resid 264 and name HA#  ) 0.0 1.0 6.0
assign (segid b and resid 262 and name HA   )(segid b and resid 264 and name HN  ) 0.0 0.0 5.0
assign (segid b and resid 262 and name HN   )(segid b and resid 264 and name HA#  ) 0.0 1.0 6.0
assign (segid b and resid 262 and name HN   )(segid b and resid 264 and name HN  ) 0.0 0.0 5.0
assign (segid b and resid 263 and name HA   )(segid b and resid 265 and name HD#  ) 0.0 2.0 5.5
assign (segid b and resid 263 and name HA   )(segid b and resid 265 and name HN  ) 0.0 0.0 6.0
assign (segid b and resid 263 and name HA   )(segid b and resid 266 and name HN  ) 0.0 0.0 6.0
assign (segid b and resid 263 and name HN   )(segid b and resid 265 and name HN  ) 0.0 0.0 6.0
assign (segid b and resid 264 and name HA#  )(segid b and resid 267 and name HB#  ) 0.0 2.5 6.0
assign (segid b and resid 265 and name HA   )(segid b and resid 267 and name HN  ) 0.0 0.0 6.0
assign (segid b and resid 265 and name HA   )(segid b and resid 268 and name HB#  ) 0.0 1.0 4.5
assign (segid b and resid 265 and name HA   )(segid b and resid 268 and name HN  ) 0.0 0.0 6.0
assign (segid b and resid 265 and name HB#  )(segid b and resid 267 and name HN  ) 0.0 1.0 6.0
assign (segid b and resid 265 and name HN   )(segid b and resid 267 and name HB#  ) 0.0 1.5 7.5
assign (segid b and resid 265 and name HN   )(segid b and resid 267 and name HN  ) 0.0 0.0 6.0
assign (segid b and resid 266 and name HA   )(segid b and resid 269 and name HN  ) 0.0 0.0 5.0
assign (segid b and resid 266 and name HB#  )(segid b and resid 270 and name HD1# ) 0.0 2.5 8.5
assign (segid b and resid 267 and name HA   )(segid b and resid 270 and name HB  ) 0.0 0.0 3.5
assign (segid b and resid 267 and name HA   )(segid b and resid 270 and name HN  ) 0.0 0.0 6.0
assign (segid b and resid 267 and name HB#  )(segid b and resid 269 and name HN  ) 0.0 1.5 6.5
assign (segid b and resid 267 and name HN   )(segid b and resid 269 and name HN  ) 0.0 0.0 6.0
assign (segid b and resid 267 and name HN   )(segid b and resid 270 and name HN  ) 0.0 0.0 5.0
assign (segid b and resid 268 and name HA   )(segid b and resid 270 and name HN  ) 0.0 0.0 3.5
assign (segid b and resid 268 and name HA   )(segid b and resid 271 and name HB#  ) 0.0 1.0 4.5
assign (segid b and resid 268 and name HA   )(segid b and resid 271 and name HN  ) 0.0 0.0 3.5
assign (segid b and resid 268 and name HG#  )(segid b and resid 272 and name HG#  ) 0.0 2.0 7.0
assign (segid b and resid 269 and name HA   )(segid b and resid 272 and name HB#  ) 0.0 1.0 4.5
assign (segid b and resid 269 and name HA   )(segid b and resid 272 and name HN  ) 0.0 0.0 5.0
assign (segid b and resid 269 and name HB#  )(segid b and resid 271 and name HN  ) 0.0 1.0 7.0
assign (segid b and resid 269 and name HB#  )(segid b and resid 272 and name HN  ) 0.0 1.0 7.0
assign (segid b and resid 269 and name HN   )(segid b and resid 271 and name HN  ) 0.0 0.0 5.0
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Table A.4. *(continued)*

```
assign (segid b and resid 270 and name HA   )(segid b and resid 273 and name HB#  ) 0.0 1.0 7.0
assign (segid b and resid 270 and name HA   )(segid b and resid 273 and name HN  ) 0.0 0.0 5.0
assign (segid b and resid 270 and name HG2# )(segid b and resid 272 and name HN  ) 0.0 1.5 6.5
assign (segid b and resid 270 and name HG2# )(segid b and resid 274 and name HG1# ) 0.0 2.5 6.0
assign (segid b and resid 270 and name HN   )(segid b and resid 272 and name HN  ) 0.0 0.0 6.0
assign (segid b and resid 271 and name HA   )(segid b and resid 274 and name HB  ) 0.0 0.0 3.5
assign (segid b and resid 271 and name HA   )(segid b and resid 274 and name HN  ) 0.0 0.0 3.5
assign (segid b and resid 271 and name HA   )(segid b and resid 275 and name HN  ) 0.0 0.0 6.0
assign (segid b and resid 271 and name HN   )(segid b and resid 273 and name HN  ) 0.0 0.0 6.0
assign (segid b and resid 271 and name HN   )(segid b and resid 274 and name HB  ) 0.0 0.0 5.0
assign (segid b and resid 271 and name HN   )(segid b and resid 274 and name HD1# ) 0.0 1.5 6.5
assign (segid b and resid 271 and name HN   )(segid b and resid 274 and name HN  ) 0.0 0.0 6.0
assign (segid b and resid 272 and name HA   )(segid b and resid 274 and name HN  ) 0.0 0.0 5.0
assign (segid b and resid 272 and name HA   )(segid b and resid 275 and name HN  ) 0.0 0.0 2.9
assign (segid b and resid 272 and name HB#  )(segid b and resid 274 and name HN  ) 0.0 1.0 6.0
assign (segid b and resid 272 and name HN   )(segid b and resid 274 and name HB  ) 0.0 0.0 5.0
assign (segid b and resid 272 and name HN   )(segid b and resid 274 and name HN  ) 0.0 0.0 6.0
assign (segid b and resid 272 and name HN   )(segid b and resid 275 and name HN  ) 0.0 0.0 5.0
assign (segid b and resid 273 and name HA   )(segid b and resid 275 and name HN  ) 0.0 0.0 6.0
assign (segid b and resid 273 and name HA   )(segid b and resid 276 and name HB#  ) 0.0 1.0 6.0
assign (segid b and resid 273 and name HA   )(segid b and resid 276 and name HN  ) 0.0 0.0 5.0
assign (segid b and resid 273 and name HA   )(segid b and resid 277 and name HN  ) 0.0 0.0 5.0
assign (segid b and resid 273 and name HB#  )(segid b and resid 275 and name HN  ) 0.0 1.0 6.0
assign (segid b and resid 273 and name HB#  )(segid b and resid 276 and name HN  ) 0.0 1.0 6.0
assign (segid b and resid 273 and name HN   )(segid b and resid 275 and name HN  ) 0.0 0.0 5.0
assign (segid b and resid 274 and name HA   )(segid b and resid 277 and name HB#  ) 0.0 1.0 6.0
assign (segid b and resid 274 and name HA   )(segid b and resid 277 and name HN  ) 0.0 0.0 5.0
assign (segid b and resid 274 and name HA   )(segid b and resid 278 and name HN  ) 0.0 0.0 5.0
assign (segid b and resid 274 and name HD1# )(segid b and resid 277 and name HN  ) 0.0 1.5 6.5
assign (segid b and resid 274 and name HN   )(segid b and resid 276 and name HN  ) 0.0 0.0 5.0
assign (segid b and resid 275 and name HA   )(segid b and resid 278 and name HB#  ) 0.0 1.0 3.9
assign (segid b and resid 275 and name HA   )(segid b and resid 278 and name HN  ) 0.0 0.0 3.5
assign (segid b and resid 276 and name HA   )(segid b and resid 278 and name HN  ) 0.0 0.0 6.0
assign (segid b and resid 276 and name HA   )(segid b and resid 279 and name HB#  ) 0.0 1.5 4.4
assign (segid b and resid 276 and name HB#  )(segid b and resid 278 and name HN  ) 0.0 1.0 7.0
assign (segid b and resid 276 and name HG#  )(segid b and resid 278 and name HN  ) 0.0 1.0 6.0
assign (segid b and resid 276 and name HG#  )(segid b and resid 280 and name HD1# ) 0.0 2.5 7.5
assign (segid b and resid 276 and name HN   )(segid b and resid 278 and name HN  ) 0.0 0.0 5.0
assign (segid b and resid 276 and name HN   )(segid b and resid 279 and name HB#  ) 0.0 1.5 6.5
assign (segid b and resid 276 and name HN   )(segid b and resid 279 and name HN  ) 0.0 0.0 5.0
assign (segid b and resid 276 and name HN   )(segid b and resid 280 and name HG1# ) 0.0 1.0 6.0
assign (segid b and resid 277 and name HA   )(segid b and resid 279 and name HN  ) 0.0 0.0 5.0
assign (segid b and resid 277 and name HA   )(segid b and resid 280 and name HB  ) 0.0 0.0 5.0
assign (segid b and resid 277 and name HA   )(segid b and resid 280 and name HD1# ) 0.0 1.5 6.5
assign (segid b and resid 277 and name HA   )(segid b and resid 280 and name HN  ) 0.0 0.0 5.0
assign (segid b and resid 277 and name HN   )(segid b and resid 281 and name HG1# ) 0.0 1.0 6.0
assign (segid b and resid 278 and name HA   )(segid b and resid 280 and name HD1# ) 0.0 1.5 5.0
assign (segid b and resid 278 and name HA   )(segid b and resid 281 and name HB  ) 0.0 0.0 6.0
assign (segid b and resid 278 and name HA   )(segid b and resid 281 and name HN  ) 0.0 0.0 5.0
assign (segid b and resid 278 and name HA   )(segid b and resid 282 and name HN  ) 0.0 0.0 5.0
assign (segid b and resid 278 and name HN   )(segid b and resid 280 and name HD1# ) 0.0 1.5 6.5
assign (segid b and resid 278 and name HN   )(segid b and resid 280 and name HN  ) 0.0 0.0 6.0
assign (segid b and resid 278 and name HN   )(segid b and resid 281 and name HG1# ) 0.0 1.0 6.0
assign (segid b and resid 279 and name HA   )(segid b and resid 282 and name HB#  ) 0.0 1.0 3.9
assign (segid b and resid 279 and name HA   )(segid b and resid 282 and name HN  ) 0.0 0.0 5.0
assign (segid b and resid 279 and name HB#  )(segid b and resid 281 and name HN  ) 0.0 1.5 6.5
assign (segid b and resid 279 and name HB#  )(segid b and resid 282 and name HN  ) 0.0 1.5 6.5
assign (segid b and resid 279 and name HB#  )(segid b and resid 283 and name HN  ) 0.0 1.5 6.5
assign (segid b and resid 279 and name HN   )(segid b and resid 281 and name HN  ) 0.0 0.0 5.0
assign (segid b and resid 280 and name HA   )(segid b and resid 283 and name HB#  ) 0.0 1.0 7.0
assign (segid b and resid 280 and name HA   )(segid b and resid 283 and name HG#  ) 0.0 1.0 7.0
assign (segid b and resid 280 and name HA   )(segid b and resid 283 and name HN  ) 0.0 0.0 5.0
assign (segid b and resid 280 and name HN   )(segid b and resid 282 and name HN  ) 0.0 0.0 6.0
assign (segid b and resid 280 and name HN   )(segid b and resid 283 and name HG#  ) 0.0 1.0 7.0
assign (segid b and resid 280 and name HN   )(segid b and resid 283 and name HN  ) 0.0 0.0 5.0
assign (segid b and resid 281 and name HA   )(segid b and resid 283 and name HN  ) 0.0 0.0 6.0
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Table A.4. *(continued)*

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assign (segid b and resid 281 and name HA  )(segid b and resid 284 and name HB#  ) 0.0 1.0 6.0
assign (segid b and resid 281 and name HA  )(segid b and resid 284 and name HN   ) 0.0 0.0 5.0
assign (segid b and resid 281 and name HA  )(segid b and resid 285 and name HN   ) 0.0 0.0 5.0
assign (segid b and resid 281 and name HB  )(segid b and resid 283 and name HN   ) 0.0 0.0 6.0
assign (segid b and resid 281 and name HD1# )(segid b and resid 284 and name HN   ) 0.0 1.5 6.5
assign (segid b and resid 282 and name HA  )(segid b and resid 284 and name HN   ) 0.0 0.0 6.0
assign (segid b and resid 282 and name HA  )(segid b and resid 285 and name HB   ) 0.0 0.0 3.5
assign (segid b and resid 282 and name HA  )(segid b and resid 285 and name HN   ) 0.0 0.0 5.0
assign (segid b and resid 282 and name HN  )(segid b and resid 284 and name HN   ) 0.0 0.0 5.0
assign (segid b and resid 282 and name HN  )(segid b and resid 285 and name HN   ) 0.0 0.0 5.0
assign (segid b and resid 283 and name HA  )(segid b and resid 285 and name HN   ) 0.0 0.0 6.0
assign (segid b and resid 283 and name HA  )(segid b and resid 286 and name HB#  ) 0.0 1.0 4.5
assign (segid b and resid 283 and name HA  )(segid b and resid 286 and name HN   ) 0.0 0.0 6.0
assign (segid b and resid 283 and name HA  )(segid b and resid 287 and name HN   ) 0.0 0.0 6.0
assign (segid b and resid 283 and name HN  )(segid b and resid 285 and name HN   ) 0.0 0.0 6.0
assign (segid b and resid 283 and name HN  )(segid b and resid 286 and name HB#  ) 0.0 1.0 7.0
assign (segid b and resid 284 and name HA  )(segid b and resid 286 and name HN   ) 0.0 0.0 5.0
assign (segid b and resid 284 and name HA  )(segid b and resid 287 and name HB#  ) 0.0 1.0 7.0
assign (segid b and resid 284 and name HA  )(segid b and resid 287 and name HN   ) 0.0 0.0 5.0
assign (segid b and resid 284 and name HB#  )(segid b and resid 287 and name HN   ) 0.0 1.0 7.0
assign (segid b and resid 285 and name HA  )(segid b and resid 287 and name HN   ) 0.0 0.0 6.0
assign (segid b and resid 285 and name HA  )(segid b and resid 288 and name HD1# ) 0.0 1.5 6.5
assign (segid b and resid 285 and name HA  )(segid b and resid 288 and name HN   ) 0.0 0.0 5.0
assign (segid b and resid 285 and name HB  )(segid b and resid 287 and name HN   ) 0.0 0.0 6.0
assign (segid b and resid 285 and name HB  )(segid b and resid 288 and name HN   ) 0.0 0.0 6.0
assign (segid b and resid 285 and name HD1# )(segid b and resid 287 and name HN   ) 0.0 1.5 6.5
assign (segid b and resid 285 and name HD1# )(segid b and resid 288 and name HD#  ) 0.0 3.9 6.8
assign (segid b and resid 285 and name HG2# )(segid b and resid 288 and name HD#  ) 0.0 3.9 6.8
assign (segid b and resid 285 and name HG2# )(segid b and resid 288 and name HN   ) 0.0 1.5 6.5
assign (segid b and resid 286 and name HA  )(segid b and resid 288 and name HN   ) 0.0 0.0 6.0
assign (segid b and resid 286 and name HA  )(segid b and resid 289 and name HB#  ) 0.0 1.0 6.0
assign (segid b and resid 286 and name HA  )(segid b and resid 289 and name HD#  ) 0.0 1.0 4.5
assign (segid b and resid 286 and name HA  )(segid b and resid 289 and name HG#  ) 0.0 1.0 4.5
assign (segid b and resid 286 and name HA  )(segid b and resid 289 and name HN   ) 0.0 0.0 6.0
assign (segid b and resid 286 and name HB#  )(segid b and resid 288 and name HN   ) 0.0 1.0 6.0
assign (segid b and resid 286 and name HB#  )(segid b and resid 289 and name HN   ) 0.0 1.0 7.0
assign (segid b and resid 286 and name HN  )(segid b and resid 288 and name HN   ) 0.0 0.0 5.0
assign (segid b and resid 287 and name HA  )(segid b and resid 289 and name HN   ) 0.0 0.0 5.0
assign (segid b and resid 287 and name HB#  )(segid b and resid 289 and name HN   ) 0.0 1.0 6.0
assign (segid b and resid 287 and name HN  )(segid b and resid 289 and name HN   ) 0.0 0.0 6.0
assign (segid a and resid 237 and name HG  )(segid a and resid 288 and name HD1# ) 0.0 1.5 6.5
assign (segid a and resid 237 and name HG  )(segid a and resid 288 and name HD2# ) 0.0 1.5 5.0
assign (segid a and resid 241 and name HG#  )(segid a and resid 281 and name HD1# ) 0.0 3.9 6.8
assign (segid a and resid 241 and name HG#  )(segid a and resid 281 and name HG2# ) 0.0 3.9 6.8
assign (segid a and resid 249 and name HB#  )(segid a and resid 271 and name HN   ) 0.0 1.0 6.0
assign (segid a and resid 252 and name HB  )(segid a and resid 270 and name HD1# ) 0.0 1.5 5.0
assign (segid a and resid 252 and name HD#  )(segid a and resid 257 and name HN   ) 0.0 1.5 6.5
assign (segid a and resid 252 and name HG2# )(segid a and resid 257 and name HN   ) 0.0 1.5 6.5
assign (segid a and resid 252 and name HG2# )(segid a and resid 274 and name HG1# ) 0.0 2.5 8.5
assign (segid a and resid 256 and name HA  )(segid a and resid 267 and name HA   ) 0.0 0.0 6.0
assign (segid a and resid 256 and name HB  )(segid a and resid 267 and name HA   ) 0.0 0.0 5.0
assign (segid a and resid 256 and name HG2# )(segid a and resid 267 and name HA   ) 0.0 1.5 5.0
assign (segid a and resid 256 and name HG2# )(segid a and resid 267 and name HB#  ) 0.0 3.0 5.9
assign (segid a and resid 256 and name HG2# )(segid a and resid 270 and name HB   ) 0.0 1.5 5.0
assign (segid a and resid 256 and name HG2# )(segid a and resid 270 and name HD1# ) 0.0 3.0 5.9
assign (segid a and resid 256 and name HG2# )(segid a and resid 270 and name HG2# ) 0.0 3.0 5.9
assign (segid a and resid 256 and name HG2# )(segid a and resid 271 and name HD2# ) 0.0 2.5 7.5
assign (segid a and resid 256 and name HG2# )(segid a and resid 271 and name HN   ) 0.0 1.5 6.5
assign (segid a and resid 256 and name HN  )(segid a and resid 270 and name HD1# ) 0.0 1.5 6.5
assign (segid a and resid 258 and name HB#  )(segid a and resid 266 and name HD#  ) 0.0 3.4 8.4
assign (segid a and resid 258 and name HG#  )(segid a and resid 266 and name HD#  ) 0.0 3.4 8.4
assign (segid a and resid 259 and name HB#  )(segid a and resid 264 and name HN   ) 0.0 1.0 7.0
assign (segid a and resid 259 and name HN  )(segid a and resid 266 and name HD1# ) 0.0 0.0 5.0
assign (segid b and resid 237 and name HG  )(segid b and resid 288 and name HD1# ) 0.0 1.5 6.5
assign (segid b and resid 237 and name HG  )(segid b and resid 288 and name HD2# ) 0.0 1.5 5.0
assign (segid b and resid 241 and name HG#  )(segid b and resid 281 and name HD1# ) 0.0 3.9 6.8
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Table A.4. *(continued)*

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assign (segid b and resid 241 and name HG#  )(segid b and resid 281 and name HG2# ) 0.0 3.9 6.8
assign (segid b and resid 249 and name HB#  )(segid b and resid 271 and name HN   ) 0.0 1.0 6.0
assign (segid b and resid 252 and name HB  )(segid b and resid 270 and name HD1# ) 0.0 1.5 5.0
assign (segid b and resid 252 and name HD#  )(segid b and resid 257 and name HN   ) 0.0 1.5 6.5
assign (segid b and resid 252 and name HG2# )(segid b and resid 257 and name HN   ) 0.0 1.5 6.5
assign (segid b and resid 252 and name HG2# )(segid b and resid 274 and name HG1# ) 0.0 2.5 8.5
assign (segid b and resid 256 and name HA  )(segid b and resid 267 and name HA   ) 0.0 0.0 6.0
assign (segid b and resid 256 and name HB  )(segid b and resid 267 and name HA   ) 0.0 0.0 5.0
assign (segid b and resid 256 and name HG2# )(segid b and resid 267 and name HA   ) 0.0 1.5 5.0
assign (segid b and resid 256 and name HG2# )(segid b and resid 267 and name HB#  ) 0.0 3.0 5.9
assign (segid b and resid 256 and name HG2# )(segid b and resid 270 and name HB   ) 0.0 1.5 5.0
assign (segid b and resid 256 and name HG2# )(segid b and resid 270 and name HD1# ) 0.0 3.0 5.9
assign (segid b and resid 256 and name HG2# )(segid b and resid 270 and name HG2# ) 0.0 3.0 5.9
assign (segid b and resid 256 and name HG2# )(segid b and resid 271 and name HD2# ) 0.0 2.5 7.5
assign (segid b and resid 256 and name HG2# )(segid b and resid 271 and name HN   ) 0.0 1.5 6.5
assign (segid b and resid 256 and name HN  )(segid b and resid 270 and name HD1# ) 0.0 1.5 6.5
assign (segid b and resid 258 and name HB#  )(segid b and resid 266 and name HD#  ) 0.0 3.4 8.4
assign (segid b and resid 258 and name HG#  )(segid b and resid 266 and name HD#  ) 0.0 3.4 8.4
assign (segid b and resid 259 and name HB#  )(segid b and resid 264 and name HN   ) 0.0 1.0 7.0
assign (segid b and resid 259 and name HN  )(segid b and resid 266 and name HD1# ) 0.0 0.0 5.0
! Intersubuint NOEs
assign (segid a and resid 266 and name HD#  )(segid b and resid 255 and name HA   ) 0.0 2.4 5.3
assign (segid a and resid 255 and name HA  )(segid b and resid 266 and name HD#  ) 0.0 2.4 5.3
assign (segid a and resid 241 and name HG1 )(segid b and resid 280 and name HG2# ) 0.0 3.0 5.9
assign (segid a and resid 280 and name HG2# )(segid b and resid 241 and name HG1# ) 0.0 3.0 5.9
assign (segid a and resid 255 and name HB#  )(segid b and resid 270 and name HD1# ) 0.0 3.0 5.9
assign (segid a and resid 270 and name HD1# )(segid b and resid 255 and name HB#  ) 0.0 3.0 5.9
assign (segid a and resid 252 and name HD1# )(segid b and resid 270 and name HG2# ) 0.0 3.0 5.9
assign (segid a and resid 270 and name HG2# )(segid b and resid 252 and name HD1# ) 0.0 3.0 5.9
assign (segid a and resid 256 and name HG2# )(segid b and resid 270 and name HD1# ) 0.0 3.0 5.9
assign (segid a and resid 270 and name HD1# )(segid b and resid 256 and name HG2# ) 0.0 3.0 5.9
assign (segid a and resid 245 and name HD#  )(segid b and resid 277 and name HA   ) 0.0 2.4 5.3
assign (segid a and resid 277 and name HA  )(segid b and resid 245 and name HD#  ) 0.0 2.4 5.3
assign (segid a and resid 236 and name HD2# )(segid b and resid 287 and name HB#  ) 0.0 3.5 8.5
assign (segid a and resid 287 and name HE#  )(segid b and resid 236 and name HD2# ) 0.0 3.5 8.5
assign (segid a and resid 236 and name HD1# )(segid b and resid 284 and name HD#  ) 0.0 3.5 8.5
assign (segid a and resid 284 and name HD#  )(segid b and resid 236 and name HD1# ) 0.0 3.5 8.5
assign (segid a and resid 241 and name HG2# )(segid b and resid 284 and name HD#  ) 0.0 3.5 8.5
assign (segid a and resid 284 and name HD#  )(segid b and resid 241 and name HG2# ) 0.0 3.5 8.5
assign (segid a and resid 241 and name HG1# )(segid b and resid 287 and name HE#  ) 0.0 3.5 8.5
assign (segid a and resid 287 and name HE#  )(segid b and resid 241 and name HG1# ) 0.0 3.5 8.5
assign (segid a and resid 229 and name HG#  )(segid b and resid 229 and name HG#  ) 0.0 2.0 4.9
assign (segid a and resid 262 and name HG#  )(segid b and resid 262 and name HG#  ) 0.0 2.0 4.9
assign (segid a and resid 241 and name HG#  )(segid b and resid 241 and name HG#  ) 0.0 4.8 7.7
assign (segid a and resid 252 and name HG2# )(segid b and resid 252 and name HG2# ) 0.0 3.0 5.9
assign (segid a and resid 288 and name HD#  )(segid b and resid 288 and name HD#  ) 0.0 2.4 5.3
assign (segid a and resid 256 and name HG1 )(segid b and resid 256 and name HG2# ) 0.0 2.4 5.3
assign (segid a and resid 256 and name HG2# )(segid b and resid 256 and name HG1 ) 0.0 2.4 5.3
! Hydrogen bond
assign (segid a and resid 248 and name O   )(segid a and resid 252 and name N   ) 0.0 0.0 3.3
assign (segid a and resid 248 and name O   )(segid a and resid 252 and name HN  ) 0.0 0.0 2.3
assign (segid a and resid 249 and name O   )(segid a and resid 253 and name N   ) 0.0 0.0 3.3
assign (segid a and resid 249 and name O   )(segid a and resid 253 and name HN  ) 0.0 0.0 2.3
assign (segid a and resid 250 and name O   )(segid a and resid 254 and name N   ) 0.0 0.0 3.3
assign (segid a and resid 250 and name O   )(segid a and resid 254 and name HN  ) 0.0 0.0 2.3
assign (segid a and resid 251 and name O   )(segid a and resid 255 and name N   ) 0.0 0.0 3.3
assign (segid a and resid 251 and name O   )(segid a and resid 255 and name HN  ) 0.0 0.0 2.3
assign (segid a and resid 252 and name O   )(segid a and resid 256 and name N   ) 0.0 0.0 3.3
assign (segid a and resid 252 and name O   )(segid a and resid 256 and name HN  ) 0.0 0.0 2.3
assign (segid a and resid 253 and name O   )(segid a and resid 257 and name N   ) 0.0 0.0 3.3
assign (segid a and resid 253 and name O   )(segid a and resid 257 and name HN  ) 0.0 0.0 2.3
assign (segid a and resid 254 and name O   )(segid a and resid 258 and name N   ) 0.0 0.0 3.3
assign (segid a and resid 254 and name O   )(segid a and resid 258 and name HN  ) 0.0 0.0 2.3
assign (segid a and resid 265 and name O   )(segid a and resid 269 and name N   ) 0.0 0.0 3.3
assign (segid a and resid 265 and name O   )(segid a and resid 269 and name HN  ) 0.0 0.0 2.3
assign (segid a and resid 266 and name O   )(segid a and resid 270 and name N   ) 0.0 0.0 3.3
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Table A.4. *(continued)*

assign	(segid a and resid	266	and	name O	)	(segid a and resid	270	and	name HN	)	0.0	0.0	2.3
assign	(segid a and resid	267	and	name O	)	(segid a and resid	271	and	name N	)	0.0	0.0	3.3
assign	(segid a and resid	267	and	name O	)	(segid a and resid	271	and	name HN	)	0.0	0.0	2.3
assign	(segid a and resid	268	and	name O	)	(segid a and resid	272	and	name N	)	0.0	0.0	3.3
assign	(segid a and resid	268	and	name O	)	(segid a and resid	272	and	name HN	)	0.0	0.0	2.3
assign	(segid a and resid	269	and	name O	)	(segid a and resid	273	and	name N	)	0.0	0.0	3.3
assign	(segid a and resid	269	and	name O	)	(segid a and resid	273	and	name HN	)	0.0	0.0	2.3
assign	(segid a and resid	270	and	name O	)	(segid a and resid	274	and	name N	)	0.0	0.0	3.3
assign	(segid a and resid	270	and	name O	)	(segid a and resid	274	and	name HN	)	0.0	0.0	2.3
assign	(segid a and resid	271	and	name O	)	(segid a and resid	275	and	name N	)	0.0	0.0	3.3
assign	(segid a and resid	271	and	name O	)	(segid a and resid	275	and	name HN	)	0.0	0.0	2.3
assign	(segid a and resid	272	and	name O	)	(segid a and resid	276	and	name N	)	0.0	0.0	3.3
assign	(segid a and resid	272	and	name O	)	(segid a and resid	276	and	name HN	)	0.0	0.0	2.3
assign	(segid a and resid	273	and	name O	)	(segid a and resid	277	and	name N	)	0.0	0.0	3.3
assign	(segid a and resid	273	and	name O	)	(segid a and resid	277	and	name HN	)	0.0	0.0	2.3
assign	(segid a and resid	274	and	name O	)	(segid a and resid	278	and	name N	)	0.0	0.0	3.3
assign	(segid a and resid	274	and	name O	)	(segid a and resid	278	and	name HN	)	0.0	0.0	2.3
assign	(segid a and resid	275	and	name O	)	(segid a and resid	279	and	name N	)	0.0	0.0	3.3
assign	(segid a and resid	275	and	name O	)	(segid a and resid	279	and	name HN	)	0.0	0.0	2.3
assign	(segid a and resid	276	and	name O	)	(segid a and resid	280	and	name N	)	0.0	0.0	3.3
assign	(segid a and resid	276	and	name O	)	(segid a and resid	280	and	name HN	)	0.0	0.0	2.3
assign	(segid a and resid	277	and	name O	)	(segid a and resid	281	and	name N	)	0.0	0.0	3.3
assign	(segid a and resid	277	and	name O	)	(segid a and resid	281	and	name HN	)	0.0	0.0	2.3
assign	(segid a and resid	278	and	name O	)	(segid a and resid	282	and	name N	)	0.0	0.0	3.3
assign	(segid a and resid	278	and	name O	)	(segid a and resid	282	and	name HN	)	0.0	0.0	2.3
assign	(segid a and resid	279	and	name O	)	(segid a and resid	283	and	name N	)	0.0	0.0	3.3
assign	(segid a and resid	279	and	name O	)	(segid a and resid	283	and	name HN	)	0.0	0.0	2.3
assign	(segid a and resid	280	and	name O	)	(segid a and resid	284	and	name N	)	0.0	0.0	3.3
assign	(segid a and resid	280	and	name O	)	(segid a and resid	284	and	name HN	)	0.0	0.0	2.3
assign	(segid a and resid	281	and	name O	)	(segid a and resid	285	and	name N	)	0.0	0.0	3.3
assign	(segid a and resid	281	and	name O	)	(segid a and resid	285	and	name HN	)	0.0	0.0	2.3
assign	(segid a and resid	282	and	name O	)	(segid a and resid	286	and	name N	)	0.0	0.0	3.3
assign	(segid a and resid	282	and	name O	)	(segid a and resid	286	and	name HN	)	0.0	0.0	2.3
assign	(segid b and resid	248	and	name O	)	(segid b and resid	252	and	name N	)	0.0	0.0	3.3
assign	(segid b and resid	248	and	name O	)	(segid b and resid	252	and	name HN	)	0.0	0.0	2.3
assign	(segid b and resid	249	and	name O	)	(segid b and resid	253	and	name N	)	0.0	0.0	3.3
assign	(segid b and resid	249	and	name O	)	(segid b and resid	253	and	name HN	)	0.0	0.0	2.3
assign	(segid b and resid	250	and	name O	)	(segid b and resid	254	and	name N	)	0.0	0.0	3.3
assign	(segid b and resid	250	and	name O	)	(segid b and resid	254	and	name HN	)	0.0	0.0	2.3
assign	(segid b and resid	251	and	name O	)	(segid b and resid	255	and	name N	)	0.0	0.0	3.3
assign	(segid b and resid	251	and	name O	)	(segid b and resid	255	and	name HN	)	0.0	0.0	2.3
assign	(segid b and resid	252	and	name O	)	(segid b and resid	256	and	name N	)	0.0	0.0	3.3
assign	(segid b and resid	252	and	name O	)	(segid b and resid	256	and	name HN	)	0.0	0.0	2.3
assign	(segid b and resid	253	and	name O	)	(segid b and resid	257	and	name N	)	0.0	0.0	3.3
assign	(segid b and resid	253	and	name O	)	(segid b and resid	257	and	name HN	)	0.0	0.0	2.3
assign	(segid b and resid	254	and	name O	)	(segid b and resid	258	and	name N	)	0.0	0.0	3.3
assign	(segid b and resid	254	and	name O	)	(segid b and resid	258	and	name HN	)	0.0	0.0	2.3
assign	(segid b and resid	265	and	name O	)	(segid b and resid	269	and	name N	)	0.0	0.0	3.3
assign	(segid b and resid	265	and	name O	)	(segid b and resid	269	and	name HN	)	0.0	0.0	2.3
assign	(segid b and resid	266	and	name O	)	(segid b and resid	270	and	name N	)	0.0	0.0	3.3
assign	(segid b and resid	266	and	name O	)	(segid b and resid	270	and	name HN	)	0.0	0.0	2.3
assign	(segid b and resid	267	and	name O	)	(segid b and resid	271	and	name N	)	0.0	0.0	3.3
assign	(segid b and resid	267	and	name O	)	(segid b and resid	271	and	name HN	)	0.0	0.0	2.3
assign	(segid b and resid	268	and	name O	)	(segid b and resid	272	and	name N	)	0.0	0.0	3.3
assign	(segid b and resid	268	and	name O	)	(segid b and resid	272	and	name HN	)	0.0	0.0	2.3
assign	(segid b and resid	269	and	name O	)	(segid b and resid	273	and	name N	)	0.0	0.0	3.3
assign	(segid b and resid	269	and	name O	)	(segid b and resid	273	and	name HN	)	0.0	0.0	2.3
assign	(segid b and resid	270	and	name O	)	(segid b and resid	274	and	name N	)	0.0	0.0	3.3
assign	(segid b and resid	270	and	name O	)	(segid b and resid	274	and	name HN	)	0.0	0.0	2.3
assign	(segid b and resid	271	and	name O	)	(segid b and resid	275	and	name N	)	0.0	0.0	3.3
assign	(segid b and resid	271	and	name O	)	(segid b and resid	275	and	name HN	)	0.0	0.0	2.3
assign	(segid b and resid	272	and	name O	)	(segid b and resid	276	and	name N	)	0.0	0.0	3.3
assign	(segid b and resid	272	and	name O	)	(segid b and resid	276	and	name HN	)	0.0	0.0	2.3
assign	(segid b and resid	273	and	name O	)	(segid b and resid	277	and	name N	)	0.0	0.0	3.3
assign	(segid b and resid	273	and	name O	)	(segid b and resid	277	and	name HN	)	0.0	0.0	2.3
assign	(segid b and resid	274	and	name O	)	(segid b and resid	278	and	name N	)	0.0	0.0	3.3

Table A.4. *(continued)*

assign	(segid b and resid	274	and	name O	)	(segid b and resid	278	and	name HN	)	0.0	0.0	2.3
assign	(segid b and resid	275	and	name O	)	(segid b and resid	279	and	name N	)	0.0	0.0	3.3
assign	(segid b and resid	275	and	name O	)	(segid b and resid	279	and	name HN	)	0.0	0.0	2.3
assign	(segid b and resid	276	and	name O	)	(segid b and resid	280	and	name N	)	0.0	0.0	3.3
assign	(segid b and resid	276	and	name O	)	(segid b and resid	280	and	name HN	)	0.0	0.0	2.3
assign	(segid b and resid	277	and	name O	)	(segid b and resid	281	and	name N	)	0.0	0.0	3.3
assign	(segid b and resid	277	and	name O	)	(segid b and resid	281	and	name HN	)	0.0	0.0	2.3
assign	(segid b and resid	278	and	name O	)	(segid b and resid	282	and	name N	)	0.0	0.0	3.3
assign	(segid b and resid	278	and	name O	)	(segid b and resid	282	and	name HN	)	0.0	0.0	2.3
assign	(segid b and resid	279	and	name O	)	(segid b and resid	283	and	name N	)	0.0	0.0	3.3
assign	(segid b and resid	279	and	name O	)	(segid b and resid	283	and	name HN	)	0.0	0.0	2.3
assign	(segid b and resid	280	and	name O	)	(segid b and resid	284	and	name N	)	0.0	0.0	3.3
assign	(segid b and resid	280	and	name O	)	(segid b and resid	284	and	name HN	)	0.0	0.0	2.3
assign	(segid b and resid	281	and	name O	)	(segid b and resid	285	and	name N	)	0.0	0.0	3.3
assign	(segid b and resid	281	and	name O	)	(segid b and resid	285	and	name HN	)	0.0	0.0	2.3
assign	(segid b and resid	282	and	name O	)	(segid b and resid	286	and	name N	)	0.0	0.0	3.3
assign	(segid b and resid	282	and	name O	)	(segid b and resid	286	and	name HN	)	0.0	0.0	2.3

Table A.5. *Dihedral Angle Constraints Used for Structure Calculation of Domain A*

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! phi dihedral angle constraints from chemical shift index & J
assign (segid a and resid  233 and name c) (segid a and resid  234 and name n)
(segid a and resid  234 and name ca)(segid a and resid  234 and name c) 1 -60.0   30.0  2
assign (segid a and resid  234 and name c) (segid a and resid  235 and name n)
(segid a and resid  235 and name ca)(segid a and resid  235 and name c) 1 -60.0   30.0  2
assign (segid a and resid  236 and name c) (segid a and resid  237 and name n)
(segid a and resid  237 and name ca)(segid a and resid  237 and name c) 1 -60.0   30.0  2
assign (segid a and resid  237 and name c) (segid a and resid  238 and name n)
(segid a and resid  238 and name ca)(segid a and resid  238 and name c) 1 -60.0   30.0  2
assign (segid a and resid  238 and name c) (segid a and resid  239 and name n)
(segid a and resid  239 and name ca)(segid a and resid  239 and name c) 1 -60.0   30.0  2
assign (segid a and resid  240 and name c) (segid a and resid  241 and name n)
(segid a and resid  241 and name ca)(segid a and resid  241 and name c) 1 -60.0   30.0  2
assign (segid a and resid  241 and name c) (segid a and resid  242 and name n)
(segid a and resid  242 and name ca)(segid a and resid  242 and name c) 1 -60.0   30.0  2
assign (segid a and resid  242 and name c) (segid a and resid  243 and name n)
(segid a and resid  243 and name ca)(segid a and resid  243 and name c) 1 -60.0   30.0  2
assign (segid a and resid  243 and name c) (segid a and resid  244 and name n)
(segid a and resid  244 and name ca)(segid a and resid  244 and name c) 1 -60.0   30.0  2
assign (segid a and resid  244 and name c) (segid a and resid  245 and name n)
(segid a and resid  245 and name ca)(segid a and resid  245 and name c) 1 -60.0   30.0  2
assign (segid a and resid  245 and name c) (segid a and resid  246 and name n)
(segid a and resid  246 and name ca)(segid a and resid  246 and name c) 1 -60.0   30.0  2
assign (segid a and resid  246 and name c) (segid a and resid  247 and name n)
(segid a and resid  247 and name ca)(segid a and resid  247 and name c) 1 -60.0   30.0  2
assign (segid a and resid  247 and name c) (segid a and resid  248 and name n)
(segid a and resid  248 and name ca)(segid a and resid  248 and name c) 1 -60.0   30.0  2
assign (segid a and resid  248 and name c) (segid a and resid  249 and name n)
(segid a and resid  249 and name ca)(segid a and resid  249 and name c) 1 -60.0   30.0  2
assign (segid a and resid  250 and name c) (segid a and resid  251 and name n)
(segid a and resid  251 and name ca)(segid a and resid  251 and name c) 1 -60.0   30.0  2
assign (segid a and resid  252 and name c) (segid a and resid  253 and name n)
(segid a and resid  253 and name ca)(segid a and resid  253 and name c) 1 -60.0   30.0  2
assign (segid a and resid  253 and name c) (segid a and resid  254 and name n)
(segid a and resid  254 and name ca)(segid a and resid  254 and name c) 1 -60.0   30.0  2
assign (segid a and resid  254 and name c) (segid a and resid  255 and name n)
(segid a and resid  255 and name ca)(segid a and resid  255 and name c) 1 -60.0   30.0  2
assign (segid a and resid  255 and name c) (segid a and resid  256 and name n)
(segid a and resid  256 and name ca)(segid a and resid  256 and name c) 1 -60.0   30.0  2
assign (segid a and resid  263 and name c) (segid a and resid  264 and name n)
(segid a and resid  264 and name ca)(segid a and resid  264 and name c) 1 -60.0   30.0  2
assign (segid a and resid  264 and name c) (segid a and resid  265 and name n)
(segid a and resid  265 and name ca)(segid a and resid  265 and name c) 1 -60.0   30.0  2
assign (segid a and resid  265 and name c) (segid a and resid  266 and name n)
(segid a and resid  266 and name ca)(segid a and resid  266 and name c) 1 -60.0   30.0  2
assign (segid a and resid  268 and name c) (segid a and resid  269 and name n)
(segid a and resid  269 and name ca)(segid a and resid  269 and name c) 1 -60.0   30.0  2
assign (segid a and resid  269 and name c) (segid a and resid  270 and name n)
(segid a and resid  270 and name ca)(segid a and resid  270 and name c) 1 -60.0   30.0  2
assign (segid a and resid  270 and name c) (segid a and resid  271 and name n)
(segid a and resid  271 and name ca)(segid a and resid  271 and name c) 1 -60.0   30.0  2
assign (segid a and resid  271 and name c) (segid a and resid  272 and name n)
(segid a and resid  272 and name ca)(segid a and resid  272 and name c) 1 -60.0   30.0  2
assign (segid a and resid  272 and name c) (segid a and resid  273 and name n)
(segid a and resid  273 and name ca)(segid a and resid  273 and name c) 1 -60.0   30.0  2
assign (segid a and resid  274 and name c) (segid a and resid  275 and name n)
(segid a and resid  275 and name ca)(segid a and resid  275 and name c) 1 -60.0   30.0  2
assign (segid a and resid  275 and name c) (segid a and resid  276 and name n)
(segid a and resid  276 and name ca)(segid a and resid  276 and name c) 1 -60.0   30.0  2
assign (segid a and resid  276 and name c) (segid a and resid  277 and name n)
(segid a and resid  277 and name ca)(segid a and resid  277 and name c) 1 -60.0   30.0  2
assign (segid a and resid  277 and name c) (segid a and resid  278 and name n)
(segid a and resid  278 and name ca)(segid a and resid  278 and name c) 1 -60.0   30.0  2
assign (segid a and resid  278 and name c) (segid a and resid  279 and name n)
(segid a and resid  279 and name ca)(segid a and resid  279 and name c) 1 -60.0   30.0  2
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Table A.5. *(continued)*

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assign (segid a and resid  280 and name c) (segid a and resid  281 and name n)
(segid a and resid  281 and name ca)(segid a and resid  281 and name c) 1 -60.0   30.0  2
assign (segid a and resid  281 and name c) (segid a and resid  282 and name n)
(segid a and resid  282 and name ca)(segid a and resid  282 and name c) 1 -60.0   30.0  2
assign (segid a and resid  284 and name c) (segid a and resid  285 and name n)
(segid a and resid  285 and name ca)(segid a and resid  285 and name c) 1 -60.0   30.0  2
assign (segid b and resid  233 and name c) (segid b and resid  234 and name n)
(segid b and resid  234 and name ca)(segid b and resid  234 and name c) 1 -60.0   30.0  2
assign (segid b and resid  234 and name c) (segid b and resid  235 and name n)
(segid b and resid  235 and name ca)(segid b and resid  235 and name c) 1 -60.0   30.0  2
assign (segid b and resid  236 and name c) (segid b and resid  237 and name n)
(segid b and resid  237 and name ca)(segid b and resid  237 and name c) 1 -60.0   30.0  2
assign (segid b and resid  237 and name c) (segid b and resid  238 and name n)
(segid b and resid  238 and name ca)(segid b and resid  238 and name c) 1 -60.0   30.0  2
assign (segid b and resid  238 and name c) (segid b and resid  239 and name n)
(segid b and resid  239 and name ca)(segid b and resid  239 and name c) 1 -60.0   30.0  2
assign (segid b and resid  240 and name c) (segid b and resid  241 and name n)
(segid b and resid  241 and name ca)(segid b and resid  241 and name c) 1 -60.0   30.0  2
assign (segid b and resid  241 and name c) (segid b and resid  242 and name n)
(segid b and resid  242 and name ca)(segid b and resid  242 and name c) 1 -60.0   30.0  2
assign (segid b and resid  242 and name c) (segid b and resid  243 and name n)
(segid b and resid  243 and name ca)(segid b and resid  243 and name c) 1 -60.0   30.0  2
assign (segid b and resid  243 and name c) (segid b and resid  244 and name n)
(segid b and resid  244 and name ca)(segid b and resid  244 and name c) 1 -60.0   30.0  2
assign (segid b and resid  244 and name c) (segid b and resid  245 and name n)
(segid b and resid  245 and name ca)(segid b and resid  245 and name c) 1 -60.0   30.0  2
assign (segid b and resid  245 and name c) (segid b and resid  246 and name n)
(segid b and resid  246 and name ca)(segid b and resid  246 and name c) 1 -60.0   30.0  2
assign (segid b and resid  246 and name c) (segid b and resid  247 and name n)
(segid b and resid  247 and name ca)(segid b and resid  247 and name c) 1 -60.0   30.0  2
assign (segid b and resid  247 and name c) (segid b and resid  248 and name n)
(segid b and resid  248 and name ca)(segid b and resid  248 and name c) 1 -60.0   30.0  2
assign (segid b and resid  248 and name c) (segid b and resid  249 and name n)
(segid b and resid  249 and name ca)(segid b and resid  249 and name c) 1 -60.0   30.0  2
assign (segid b and resid  250 and name c) (segid b and resid  251 and name n)
(segid b and resid  251 and name ca)(segid b and resid  251 and name c) 1 -60.0   30.0  2
assign (segid b and resid  252 and name c) (segid b and resid  253 and name n)
(segid b and resid  253 and name ca)(segid b and resid  253 and name c) 1 -60.0   30.0  2
assign (segid b and resid  253 and name c) (segid b and resid  254 and name n)
(segid b and resid  254 and name ca)(segid b and resid  254 and name c) 1 -60.0   30.0  2
assign (segid b and resid  254 and name c) (segid b and resid  255 and name n)
(segid b and resid  255 and name ca)(segid b and resid  255 and name c) 1 -60.0   30.0  2
assign (segid b and resid  255 and name c) (segid b and resid  256 and name n)
(segid b and resid  256 and name ca)(segid b and resid  256 and name c) 1 -60.0   30.0  2
assign (segid b and resid  263 and name c) (segid b and resid  264 and name n)
(segid b and resid  264 and name ca)(segid b and resid  264 and name c) 1 -60.0   30.0  2
assign (segid b and resid  264 and name c) (segid b and resid  265 and name n)
(segid b and resid  265 and name ca)(segid b and resid  265 and name c) 1 -60.0   30.0  2
assign (segid b and resid  265 and name c) (segid b and resid  266 and name n)
(segid b and resid  266 and name ca)(segid b and resid  266 and name c) 1 -60.0   30.0  2
assign (segid b and resid  268 and name c) (segid b and resid  269 and name n)
(segid b and resid  269 and name ca)(segid b and resid  269 and name c) 1 -60.0   30.0  2
assign (segid b and resid  269 and name c) (segid b and resid  270 and name n)
(segid b and resid  270 and name ca)(segid b and resid  270 and name c) 1 -60.0   30.0  2
assign (segid b and resid  270 and name c) (segid b and resid  271 and name n)
(segid b and resid  271 and name ca)(segid b and resid  271 and name c) 1 -60.0   30.0  2
assign (segid b and resid  271 and name c) (segid b and resid  272 and name n)
(segid b and resid  272 and name ca)(segid b and resid  272 and name c) 1 -60.0   30.0  2
assign (segid b and resid  272 and name c) (segid b and resid  273 and name n)
(segid b and resid  273 and name ca)(segid b and resid  273 and name c) 1 -60.0   30.0  2
assign (segid b and resid  273 and name c) (segid b and resid  274 and name n)
(segid b and resid  274 and name ca)(segid b and resid  274 and name c) 1 -60.0   50.0  2
assign (segid b and resid  274 and name c) (segid b and resid  275 and name n)
(segid b and resid  275 and name ca)(segid b and resid  275 and name c) 1 -60.0   30.0  2
assign (segid b and resid  275 and name c) (segid b and resid  276 and name n)
(segid b and resid  276 and name ca)(segid b and resid  276 and name c) 1 -60.0   30.0  2
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Table A.5. *(continued)*

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assign (segid b and resid 276 and name c) (segid b and resid 277 and name n)
(segid b and resid 277 and name ca)(segid b and resid 277 and name c) 1 -60.0  30.0  2
assign (segid b and resid 277 and name c) (segid b and resid 278 and name n)
(segid b and resid 278 and name ca)(segid b and resid 278 and name c) 1 -60.0  30.0  2
assign (segid b and resid 278 and name c) (segid b and resid 279 and name n)
(segid b and resid 279 and name ca)(segid b and resid 279 and name c) 1 -60.0  30.0  2
assign (segid b and resid 280 and name c) (segid b and resid 281 and name n)
(segid b and resid 281 and name ca)(segid b and resid 281 and name c) 1 -60.0  30.0  2
assign (segid b and resid 281 and name c) (segid b and resid 282 and name n)
(segid b and resid 282 and name ca)(segid b and resid 282 and name c) 1 -60.0  30.0  2
assign (segid b and resid 284 and name c) (segid b and resid 285 and name n)
(segid b and resid 285 and name ca)(segid b and resid 285 and name c) 1 -60.0  30.0  2
assign (segid a and resid 234 and name n) (segid a and resid 234 and name ca)
! psi dihedral angle constraints from chemical shift index
(segid a and resid 234 and name c)(segid a and resid 235 and name n) 1 -50.0  30.0  2
assign (segid a and resid 235 and name n) (segid a and resid 235 and name ca)
(segid a and resid 235 and name c)(segid a and resid 236 and name n) 1 -50.0  30.0  2
assign (segid a and resid 236 and name n) (segid a and resid 236 and name ca)
(segid a and resid 236 and name c)(segid a and resid 237 and name n) 1 -50.0  30.0  2
assign (segid a and resid 237 and name n) (segid a and resid 237 and name ca)
(segid a and resid 237 and name c)(segid a and resid 238 and name n) 1 -50.0  30.0  2
assign (segid a and resid 238 and name n) (segid a and resid 238 and name ca)
(segid a and resid 238 and name c)(segid a and resid 239 and name n) 1 -50.0  30.0  2
assign (segid a and resid 239 and name n) (segid a and resid 239 and name ca)
(segid a and resid 239 and name c)(segid a and resid 240 and name n) 1 -50.0  30.0  2
assign (segid a and resid 240 and name n) (segid a and resid 240 and name ca)
(segid a and resid 240 and name c)(segid a and resid 241 and name n) 1 -50.0  30.0  2
assign (segid a and resid 241 and name n) (segid a and resid 241 and name ca)
(segid a and resid 241 and name c)(segid a and resid 242 and name n) 1 -50.0  30.0  2
assign (segid a and resid 242 and name n) (segid a and resid 242 and name ca)
(segid a and resid 242 and name c)(segid a and resid 243 and name n) 1 -50.0  30.0  2
assign (segid a and resid 243 and name n) (segid a and resid 243 and name ca)
(segid a and resid 243 and name c)(segid a and resid 244 and name n) 1 -50.0  30.0  2
assign (segid a and resid 244 and name n) (segid a and resid 244 and name ca)
(segid a and resid 244 and name c)(segid a and resid 245 and name n) 1 -50.0  30.0  2
assign (segid a and resid 246 and name n) (segid a and resid 246 and name ca)
(segid a and resid 246 and name c)(segid a and resid 247 and name n) 1 -50.0  30.0  2
assign (segid a and resid 247 and name n) (segid a and resid 247 and name ca)
(segid a and resid 247 and name c)(segid a and resid 248 and name n) 1 -50.0  30.0  2
assign (segid a and resid 248 and name n) (segid a and resid 248 and name ca)
(segid a and resid 248 and name c)(segid a and resid 249 and name n) 1 -50.0  30.0  2
assign (segid a and resid 249 and name n) (segid a and resid 249 and name ca)
(segid a and resid 249 and name c)(segid a and resid 250 and name n) 1 -50.0  30.0  2
assign (segid a and resid 250 and name n) (segid a and resid 250 and name ca)
(segid a and resid 250 and name c)(segid a and resid 251 and name n) 1 -50.0  30.0  2
assign (segid a and resid 251 and name n) (segid a and resid 251 and name ca)
(segid a and resid 251 and name c)(segid a and resid 252 and name n) 1 -50.0  30.0  2
assign (segid a and resid 253 and name n) (segid a and resid 253 and name ca)
(segid a and resid 253 and name c)(segid a and resid 254 and name n) 1 -50.0  30.0  2
assign (segid a and resid 254 and name n) (segid a and resid 254 and name ca)
(segid a and resid 254 and name c)(segid a and resid 255 and name n) 1 -50.0  30.0  2
assign (segid a and resid 255 and name n) (segid a and resid 255 and name ca)
(segid a and resid 255 and name c)(segid a and resid 256 and name n) 1 -50.0  30.0  2
assign (segid a and resid 256 and name n) (segid a and resid 256 and name ca)
(segid a and resid 256 and name c)(segid a and resid 257 and name n) 1 -50.0  30.0  2
assign (segid a and resid 257 and name n) (segid a and resid 257 and name ca)
(segid a and resid 257 and name c)(segid a and resid 258 and name n) 1 -50.0  30.0  2
assign (segid a and resid 264 and name n) (segid a and resid 264 and name ca)
(segid a and resid 264 and name c)(segid a and resid 265 and name n) 1 -50.0  30.0  2
assign (segid a and resid 265 and name n) (segid a and resid 265 and name ca)
(segid a and resid 265 and name c)(segid a and resid 266 and name n) 1 -50.0  30.0  2
assign (segid a and resid 266 and name n) (segid a and resid 266 and name ca)
(segid a and resid 266 and name c)(segid a and resid 267 and name n) 1 -50.0  30.0  2
assign (segid a and resid 267 and name n) (segid a and resid 267 and name ca)
(segid a and resid 267 and name c)(segid a and resid 268 and name n) 1 -50.0  30.0  2
```


Table A.5. *(continued)*

```
assign (segid a and resid 268 and name n) (segid a and resid 268 and name ca)
(segid a and resid 268 and name c)(segid a and resid 269 and name n) 1 -50.0  30.0  2
assign (segid a and resid 269 and name n) (segid a and resid 269 and name ca)
(segid a and resid 269 and name c)(segid a and resid 270 and name n) 1 -50.0  30.0  2
assign (segid a and resid 270 and name n) (segid a and resid 270 and name ca)
(segid a and resid 270 and name c)(segid a and resid 271 and name n) 1 -50.0  30.0  2
assign (segid a and resid 271 and name n) (segid a and resid 271 and name ca)
(segid a and resid 271 and name c)(segid a and resid 272 and name n) 1 -50.0  30.0  2
assign (segid a and resid 272 and name n) (segid a and resid 272 and name ca)
(segid a and resid 272 and name c)(segid a and resid 273 and name n) 1 -50.0  30.0  2
assign (segid a and resid 273 and name n) (segid a and resid 273 and name ca)
(segid a and resid 273 and name c)(segid a and resid 274 and name n) 1 -50.0  30.0  2
assign (segid a and resid 274 and name n) (segid a and resid 274 and name ca)
(segid a and resid 274 and name c)(segid a and resid 275 and name n) 1 -50.0  30.0  2
assign (segid a and resid 275 and name n) (segid a and resid 275 and name ca)
(segid a and resid 275 and name c)(segid a and resid 276 and name n) 1 -50.0  50.0  2
assign (segid a and resid 276 and name n) (segid a and resid 276 and name ca)
(segid a and resid 276 and name c)(segid a and resid 277 and name n) 1 -50.0  30.0  2
assign (segid a and resid 277 and name n) (segid a and resid 277 and name ca)
(segid a and resid 277 and name c)(segid a and resid 278 and name n) 1 -50.0  30.0  2
assign (segid a and resid 278 and name n) (segid a and resid 278 and name ca)
(segid a and resid 278 and name c)(segid a and resid 279 and name n) 1 -50.0  30.0  2
assign (segid a and resid 279 and name n) (segid a and resid 279 and name ca)
(segid a and resid 279 and name c)(segid a and resid 280 and name n) 1 -50.0  30.0  2
assign (segid a and resid 280 and name n) (segid a and resid 280 and name ca)
(segid a and resid 280 and name c)(segid a and resid 281 and name n) 1 -50.0  30.0  2
assign (segid a and resid 281 and name n) (segid a and resid 281 and name ca)
(segid a and resid 281 and name c)(segid a and resid 282 and name n) 1 -50.0  30.0  2
assign (segid a and resid 282 and name n) (segid a and resid 282 and name ca)
(segid a and resid 282 and name c)(segid a and resid 283 and name n) 1 -50.0  30.0  2
assign (segid a and resid 283 and name n) (segid a and resid 283 and name ca)
(segid a and resid 283 and name c)(segid a and resid 284 and name n) 1 -50.0  30.0  2
assign (segid a and resid 284 and name n) (segid a and resid 284 and name ca)
(segid a and resid 284 and name c)(segid a and resid 285 and name n) 1 -50.0  50.0  2
assign (segid a and resid 285 and name n) (segid a and resid 285 and name ca)
(segid a and resid 285 and name c)(segid a and resid 286 and name n) 1 -50.0  30.0  2
assign (segid a and resid 286 and name n) (segid a and resid 286 and name ca)
(segid a and resid 286 and name c)(segid a and resid 287 and name n) 1 -50.0  30.0  2
assign (segid b and resid 234 and name n) (segid b and resid 234 and name ca)
(segid b and resid 234 and name c)(segid b and resid 235 and name n) 1 -50.0  30.0  2
assign (segid b and resid 235 and name n) (segid b and resid 235 and name ca)
(segid b and resid 235 and name c)(segid b and resid 236 and name n) 1 -50.0  30.0  2
assign (segid b and resid 236 and name n) (segid b and resid 236 and name ca)
(segid b and resid 236 and name c)(segid b and resid 237 and name n) 1 -50.0  30.0  2
assign (segid b and resid 237 and name n) (segid b and resid 237 and name ca)
(segid b and resid 237 and name c)(segid b and resid 238 and name n) 1 -50.0  30.0  2
assign (segid b and resid 238 and name n) (segid b and resid 238 and name ca)
(segid b and resid 238 and name c)(segid b and resid 239 and name n) 1 -50.0  30.0  2
assign (segid b and resid 239 and name n) (segid b and resid 239 and name ca)
(segid b and resid 239 and name c)(segid b and resid 240 and name n) 1 -50.0  30.0  2
assign (segid b and resid 240 and name n) (segid b and resid 240 and name ca)
(segid b and resid 240 and name c)(segid b and resid 241 and name n) 1 -50.0  30.0  2
assign (segid b and resid 241 and name n) (segid b and resid 241 and name ca)
(segid b and resid 241 and name c)(segid b and resid 242 and name n) 1 -50.0  30.0  2
assign (segid b and resid 242 and name n) (segid b and resid 242 and name ca)
(segid b and resid 242 and name c)(segid b and resid 243 and name n) 1 -50.0  30.0  2
assign (segid b and resid 243 and name n) (segid b and resid 243 and name ca)
(segid b and resid 243 and name c)(segid b and resid 244 and name n) 1 -50.0  30.0  2
assign (segid b and resid 244 and name n) (segid b and resid 244 and name ca)
(segid b and resid 244 and name c)(segid b and resid 245 and name n) 1 -50.0  30.0  2
assign (segid b and resid 246 and name n) (segid b and resid 246 and name ca)
(segid b and resid 246 and name c)(segid b and resid 247 and name n) 1 -50.0  30.0  2
assign (segid b and resid 247 and name n) (segid b and resid 247 and name ca)
(segid b and resid 247 and name c)(segid b and resid 248 and name n) 1 -50.0  30.0  2
assign (segid b and resid 248 and name n) (segid b and resid 248 and name ca)
(segid b and resid 248 and name c)(segid b and resid 249 and name n) 1 -50.0  30.0  2
```

Table A.5. *(continued)*

```
assign (segid b and resid  249 and name n) (segid b and resid  249 and name ca)
(segid b and resid  249 and name c)(segid b and resid  250 and name n) 1 -50.0   30.0  2
assign (segid b and resid  250 and name n) (segid b and resid  250 and name ca)
(segid b and resid  250 and name c)(segid b and resid  251 and name n) 1 -50.0   30.0  2
assign (segid b and resid  251 and name n) (segid b and resid  251 and name ca)
(segid b and resid  251 and name c)(segid b and resid  252 and name n) 1 -50.0   30.0  2
assign (segid b and resid  253 and name n) (segid b and resid  253 and name ca)
(segid b and resid  253 and name c)(segid b and resid  254 and name n) 1 -50.0   30.0  2
assign (segid b and resid  254 and name n) (segid b and resid  254 and name ca)
(segid b and resid  254 and name c)(segid b and resid  255 and name n) 1 -50.0   30.0  2
assign (segid b and resid  255 and name n) (segid b and resid  255 and name ca)
(segid b and resid  255 and name c)(segid b and resid  256 and name n) 1 -50.0   30.0  2
assign (segid b and resid  256 and name n) (segid b and resid  256 and name ca)
(segid b and resid  256 and name c)(segid b and resid  257 and name n) 1 -50.0   30.0  2
assign (segid b and resid  257 and name n) (segid b and resid  257 and name ca)
(segid b and resid  257 and name c)(segid b and resid  258 and name n) 1 -50.0   30.0  2
assign (segid b and resid  264 and name n) (segid b and resid  264 and name ca)
(segid b and resid  264 and name c)(segid b and resid  265 and name n) 1 -50.0   30.0  2
assign (segid b and resid  265 and name n) (segid b and resid  265 and name ca)
(segid b and resid  265 and name c)(segid b and resid  266 and name n) 1 -50.0   30.0  2
assign (segid b and resid  266 and name n) (segid b and resid  266 and name ca)
(segid b and resid  266 and name c)(segid b and resid  267 and name n) 1 -50.0   30.0  2
assign (segid b and resid  267 and name n) (segid b and resid  267 and name ca)
(segid b and resid  267 and name c)(segid b and resid  268 and name n) 1 -50.0   30.0  2
assign (segid b and resid  268 and name n) (segid b and resid  268 and name ca)
(segid b and resid  268 and name c)(segid b and resid  269 and name n) 1 -50.0   30.0  2
assign (segid b and resid  269 and name n) (segid b and resid  269 and name ca)
(segid b and resid  269 and name c)(segid b and resid  270 and name n) 1 -50.0   30.0  2
assign (segid b and resid  270 and name n) (segid b and resid  270 and name ca)
(segid b and resid  270 and name c)(segid b and resid  271 and name n) 1 -50.0   30.0  2
assign (segid b and resid  271 and name n) (segid b and resid  271 and name ca)
(segid b and resid  271 and name c)(segid b and resid  272 and name n) 1 -50.0   30.0  2
assign (segid b and resid  272 and name n) (segid b and resid  272 and name ca)
(segid b and resid  272 and name c)(segid b and resid  273 and name n) 1 -50.0   30.0  2
assign (segid b and resid  273 and name n) (segid b and resid  273 and name ca)
(segid b and resid  273 and name c)(segid b and resid  274 and name n) 1 -50.0   30.0  2
assign (segid b and resid  274 and name n) (segid b and resid  274 and name ca)
(segid b and resid  274 and name c)(segid b and resid  275 and name n) 1 -50.0   30.0  2
assign (segid b and resid  275 and name n) (segid b and resid  275 and name ca)
(segid b and resid  275 and name c)(segid b and resid  276 and name n) 1 -50.0   50.0  2
assign (segid b and resid  276 and name n) (segid b and resid  276 and name ca)
(segid b and resid  276 and name c)(segid b and resid  277 and name n) 1 -50.0   30.0  2
assign (segid b and resid  277 and name n) (segid b and resid  277 and name ca)
(segid b and resid  277 and name c)(segid b and resid  278 and name n) 1 -50.0   30.0  2
assign (segid b and resid  278 and name n) (segid b and resid  278 and name ca)
(segid b and resid  278 and name c)(segid b and resid  279 and name n) 1 -50.0   30.0  2
assign (segid b and resid  279 and name n) (segid b and resid  279 and name ca)
(segid b and resid  279 and name c)(segid b and resid  280 and name n) 1 -50.0   30.0  2
assign (segid b and resid  280 and name n) (segid b and resid  280 and name ca)
(segid b and resid  280 and name c)(segid b and resid  281 and name n) 1 -50.0   30.0  2
assign (segid b and resid  281 and name n) (segid b and resid  281 and name ca)
(segid b and resid  281 and name c)(segid b and resid  282 and name n) 1 -50.0   30.0  2
assign (segid b and resid  282 and name n) (segid b and resid  282 and name ca)
(segid b and resid  282 and name c)(segid b and resid  283 and name n) 1 -50.0   30.0  2
assign (segid b and resid  283 and name n) (segid b and resid  283 and name ca)
(segid b and resid  283 and name c)(segid b and resid  284 and name n) 1 -50.0   30.0  2
assign (segid b and resid  284 and name n) (segid b and resid  284 and name ca)
(segid b and resid  284 and name c)(segid b and resid  285 and name n) 1 -50.0   50.0  2
assign (segid b and resid  285 and name n) (segid b and resid  285 and name ca)
(segid b and resid  285 and name c)(segid b and resid  286 and name n) 1 -50.0   30.0  2
assign (segid b and resid  286 and name n) (segid b and resid  286 and name ca)
(segid b and resid  286 and name c)(segid b and resid  287 and name n) 1 -50.0   30.0  2
```


Program B.1. Program for Calculating CSI

```
/* csi_SV_calc2.c  from csi_SV_calc2.c 990122 */
/* Biochemistry 1994, 33, 3287-3295  Y.K.Chaeet.al;
J.Mol.Biol. 1996, 264,1101-1116  R.A. Venters et.al.;
J.A.C.S. 1991, 113, 5490-5492  S.Spera & A.Bax*/

#include<stdio.h>
#include<math.h>
#define fname0 "csi_table"
#define fname1 "csi_std_tbl"

main()
{
int no, no1, i, j, HN2D_id[3000], HN2D_no[3000], CSI_no[3000], csi_ha[3000],
csi_co[3000], csi_ca[3000];
float NOESY_ca[3000], NOESY_cb[3000], HN2D_hn[3000], tocsy_ha[3000], HN2D_co[3000],
delta_ca[3000], delta_cb[3000], delta_co[3000], delta_ha[3000], csi_ave[3000],
delta_cacb[3000];
float std_ca[3000], std_cb[3000], std_co[3000], std_ha[3000];
char HN2D_type[300][3];
char CSI_type[3000][3];
FILE *fi;

if ((fi = fopen(fname0, "r")) == NULL)

   {
    printf("Cannot open file");
   }
i = 0;
while (fscanf(fi, "%d %s %d  %f %f %f %f %f",
          &HN2D_id[i], HN2D_type[i], &HN2D_no[i], &NOESY_ca[i], &NOESY_cb[i],
&HN2D_co[i], &tocsy_ha[i], &HN2D_hn[i]) !=EOF)
i++;
no = i;
fclose(fi);

if ((fi = fopen(fname1, "r")) == NULL)
   {
   printf("Cannot open file");
   }
i = 0;
while (fscanf(fi, "%d %s %f %f %f %f",
          &CSI_no[i], CSI_type[i], &std_ca[i], &std_cb[i], &std_co[i],
&std_ha[i])!=EOF)
i++;
no1 = i;
fclose(fi);


/* CSI  */
printf ("CSI = 0.25*(1*dCaCb[i-1]+2*dCaCb[i]+1*dCaCb[i+1]\n");
printf ("hsqc   ID        dCa      dCb      dCaCb     csi\n\n");
for (i = 0; i <= no-1; i++)
    {
    for (j = 0; j <= no-1; j++)
    if(strcmp(HN2D_type[i], CSI_type[j])==0)
    {
    delta_ca[i] = NOESY_ca[i] - std_ca[j];
    delta_cb[i] = NOESY_cb[i] - std_cb[j];
    delta_cacb[i] = delta_ca[i] - delta_cb[i];
    csi_ave[i] = 0.25*(1*delta_cacb[i-1] + 2*delta_cacb[i] + 1*delta_cacb[i+1]);
```

Program B.1. *(continued)*

```
    printf ("%4d %3s %4d  %6.2f  %6.2f  %6.2f  %6.2f\n", HN2D_id[i], HN2D_type[i],
HN2D_no[i], delta_ca[i], delta_cb[i], delta_cacb[i], csi_ave[i]);
    }
  }
}
```


Program B.2. Program for Sorting Out Candidates from Assignment Table

```
/* listUP.c  revised from listup.c for envZ1_ASG2.tbl
   sorting out peaks from the assignment table*/

#include<stdio.h>
#include<math.h>
#include<string.h>
#include<stdlib.h>
#define fname0 "envZ1_ASG2.tbl"
#define err_h 0.08
#define err_c 0.50
#define err_n 1.00
#define N_area 100.00

main(argc,argv)
    int   argc;
    float *argv[];
{
 int no, i;
 float cn_shift[1000], h_shift[1000];
 float shift_x, diff_h, diff_cn, cn_comp;
 char res_id[500][5], atom_id[500][5];
 FILE *fi;

 shift_x = atof(argv[1]);

 if ((fi = fopen(fname0, "r")) == NULL)
    {
     printf("Cannot open file");
    }
 i = 1;
 while (fscanf(fi, "%s %s %f %f",
        res_id[i], atom_id[i], &cn_shift[i], &h_shift[i])
        !=EOF)
 i++;
 no = i ;
 fclose(fi);

     for (i = 1; i <= no ; i++)
         {
         diff_h = fabs(shift_x - h_shift[i]);
      if (diff_h <= err_h )
           {
          printf ("%5s %-5s  %6.2f  %4.2f | dH %6.2f\n",
                res_id[i], atom_id[i], cn_shift[i], h_shift[i], diff_h); }
       diff_cn = fabs(shift_x - cn_shift[i]);
       cn_comp = N_area - shift_x;
        {
       if (cn_comp > 0 && diff_cn <= err_c)
         {
        printf ("%5s %-5s  %6.2f  %4.2f | dC %6.2f\n",
        res_id[i], atom_id[i], cn_shift[i], h_shift[i], diff_cn); }
       if (cn_comp <= 0 && diff_cn <= err_n )
       {
       printf ("%5s %-5s  %6.2f  %4.2f | dN %6.2f\n",
         res_id[i], atom_id[i], cn_shift[i], h_shift[i], diff_cn); }
       }
     }
}
```

Program B.3. *Program for Searching Slices*

```
/* slice_search_temp.c      980109*/
/* this program will show the slice number of peaks for each experiment */

#include<stdio.h>
#include<math.h>
#include<string.h>
#include<stdlib.h>
#define fname0 "slice_C13n.TBL"
#define fname1 "slice_NOESYc.TBL"
#define fname2 "slice_NOESYc2.TBL"
#define fname3 "slice_CN.TBL"
#define fname4 "slice_15NNOE.TBL"
#define fname5 "slice_HCCH.TBL"
#define err_c 0.18       /*err_XXX == Z_diff*/
#define err_nc 0.15
#define err_nc2 0.19
#define err_cnC 0.16
#define err_cnN 0.39
#define err_15N 0.23
#define err_HCCH 0.20

main(argc,argv)
int   argc;
float *argv[];
{
 int no, no1, no2, i, slice_no[500], slice_no2[500], slice_no3[500];
 int no3, slice_no4[500], no4, slice_no5[500], no5, slice_no6[500];
 float Cshift_1[300], Cshift_2[300], Cshift_3[300], Cshift_4[300];
 float Cshift_5[300], shift_x, diff_c1, diff_c2, diff_c3, diff_c4;
 float  diff_c5, diff_c6, diff_c7, diff_c8, diff_c9, diff_c10;
 float Cshift_6[300], Cshift_7[300], Cshift_8[300], Cshift_9[300];
 float Cshift_10[300], Cshift_11[300], Cshift_12[300], Cshift_13[300];
 float Cshift_14[300], Cshift_15[300];
 float diff_c11, diff_c12, diff_c13, diff_c14, diff_c15;
 float Cshift_16[300], Cshift_17[300], Cshift_18[300], Cshift_19[300];
 float Cshift_20[300], Nshift_1[300];
 float Nshift_2[300], Nshift_3[300], Nshift_4[300], Nshift_5[300];
 float diff_c16, diff_c17, diff_c18, diff_c19, diff_c20, diff_n1;
 float Nshift_6[300], Cshift_21[300], Cshift_22[300],Cshift_23[300];
 float diff_n2, diff_n3, diff_n4, diff_n5, diff_n6;
 float diff_c21, diff_c22, diff_c23;
 FILE *fi;


shift_x = atof(argv[1]);

  printf ("GO & SEE  \n");
  printf ("----------------------------------\n");

   if ((fi = fopen(fname0, "r")) == NULL)
     {
      printf("Cannot open file");
     }
   i = 0;
   while (fscanf(fi, "%d %f %f %f %f %f",
            &slice_no[i], &Cshift_1[i], &Cshift_2[i], &Cshift_3[i], &Cshift_4[i],
&Cshift_5[i])
      !=EOF)
   i++;
   no = i ;
```

Program B.3. *(continued)*

```
   fclose(fi);

   if ((fi = fopen(fname1, "r")) == NULL)
    {
    printf("Cannot open file");
    }
    i = 0;
    while (fscanf(fi, "%d %f %f %f %f %f",
            &slice_no2[i], &Cshift_6[i], &Cshift_7[i], &Cshift_8[i], &Cshift_9[i],
&Cshift_10[i]) !=EOF)
    i++;
    no1 = i;
    fclose(fi);

    if ((fi = fopen(fname2, "r")) == NULL)
    {
    printf("Cannot open file");
    }
    i = 0;
    while (fscanf(fi, "%d %f %f %f %f %f",
            &slice_no3[i], &Cshift_11[i], &Cshift_12[i], &Cshift_13[i],
&Cshift_14[i], &Cshift_15[i]) !=EOF)
    i++;
    no2 = i;
    fclose(fi);

    if ((fi = fopen(fname3, "r")) == NULL)
    {
    printf("Cannot open file");
    }
    i = 0;
    while (fscanf(fi, "%d %f %f %f %f %f %f",
            &slice_no4[i], &Cshift_16[i], &Cshift_17[i], &Cshift_18[i],
&Cshift_19[i], &Cshift_20[i], &Nshift_1[i]) !=EOF)
    i++;
    no3 = i;
    fclose(fi);

    if ((fi = fopen(fname4, "r")) == NULL)
    {
    printf("Cannot open file");
    }
    i = 0;
    while (fscanf(fi, "%d %f %f %f %f %f",
            &slice_no5[i], &Nshift_2[i], &Nshift_3[i], &Nshift_4[i], &Nshift_5[i],
&Nshift_6[i]) !=EOF)
    i++;
    no4 = i;
    fclose(fi);

    if ((fi = fopen(fname5, "r")) == NULL)
    {
    printf("Cannot open file");
    }
    i = 0;
    while (fscanf(fi, "%d %f %f %f",
         &slice_no6[i], &Cshift_21[i], &Cshift_22[i], &Cshift_23[i]) !=EOF)
     i++;
     no5 = i;
     fclose(fi);
```

```
for (i = 0; i <= no ; i++)
   {

   diff_c1 = fabs(shift_x - Cshift_1[i]);
   if (diff_c1 <= err_c )
   {
   printf ("slice %4d of C13noesy (-) \n", slice_no[i]); }

   diff_c2 = fabs(shift_x - Cshift_2[i]);
   if (diff_c2 <= err_c )
   {
   printf ("slice %4d of C13noesy (+) \n", slice_no[i]);}

   diff_c3 = fabs(shift_x - Cshift_3[i]);
   if (diff_c3 <= err_c )
   {
   printf ("slice %4d of C13noesy (-) \n", slice_no[i]);}

   diff_c4 = fabs(shift_x - Cshift_4[i]);
   if (diff_c4 <= err_c )
   {
   printf ("slice %4d of C13noesy (+) \n", slice_no[i]);}

   diff_c5 = fabs(shift_x - Cshift_5[i]);
   if (diff_c5 <= err_c )
   {
   printf ("slice %4d of C13noesy (-) \n", slice_no[i]);}


   diff_c6 = fabs(shift_x - Cshift_6[i]);
   if (diff_c6 <= err_nc)
   {
   printf ("slice %4d of noesy_cpurge(h2o) (-)\n", slice_no2[i]);}

   diff_c7 = fabs(shift_x - Cshift_7[i]);
   if (diff_c7 <= err_nc)
   {
   printf ("slice %4d of noesy_cpurge(h2o) (+) \n", slice_no2[i]);}

   diff_c8 = fabs(shift_x - Cshift_8[i]);
   if (diff_c8 <= err_nc)
   {
   printf ("slice %4d of noesy_cpurge(h2o) (-)\n", slice_no2[i]);}

   diff_c9 = fabs(shift_x - Cshift_9[i]);
   if (diff_c9 <= err_nc)
   {
   printf ("slice %4d of noesy_cpurge(h2o) (+)\n", slice_no2[i]);}

   diff_c10 = fabs(shift_x - Cshift_10[i]);
   if (diff_c10 <= err_nc)
   {
   printf ("slice %4d of noesy_cpurge(h2o) (-)\n", slice_no2[i]);}

   diff_c11 = fabs(shift_x - Cshift_11[i]);
   if (diff_c11 <= err_nc2)
   {
   printf ("slice %4d of noesy_cpurge(d20) (-)\n", slice_no3[i]);}

   diff_c12 = fabs(shift_x - Cshift_12[i]);
```



```
   if (diff_c12 <= err_nc2)
   {
   printf ("slice %4d of noesy_cpurge(d20) (+)\n", slice_no3[i]);}

   diff_c13 = fabs(shift_x - Cshift_13[i]);
   if (diff_c13 <= err_nc2)
   {
   printf ("slice %4d of noesy_cpurge(d20) (-)\n", slice_no3[i]);}

   diff_c14 = fabs(shift_x - Cshift_14[i]);
   if (diff_c14 <= err_nc2)
   {
   printf ("slice %4d of noesy_cpurge(d20) (+)\n", slice_no3[i]);}

   diff_c15 = fabs(shift_x - Cshift_15[i]);
   if (diff_c15 <= err_nc2)
   {
   printf ("slice %4d of noesy_cpurge(d20) (-)\n", slice_no3[i]);}

   diff_c16 = fabs(shift_x - Cshift_16[i]);
   if (diff_c16 <= err_cnC)
   {
   printf ("slice %4d of CN_noesy (-)\n", slice_no4[i]);}

   diff_c17 = fabs(shift_x - Cshift_17[i]);
   if (diff_c17 <= err_cnC)
   {
   printf ("slice %4d of CN_noesy (+) \n", slice_no4[i]);}

   diff_c18 = fabs(shift_x - Cshift_18[i]);
   if (diff_c18 <= err_cnC)
   {
   printf ("slice %4d of CN_noesy (-)\n", slice_no4[i]);}

   diff_c19 = fabs(shift_x - Cshift_19[i]);
   if (diff_c19 <= err_cnC)
   {
   printf ("slice %4d of CN_noesy (+)\n", slice_no4[i]);}

   diff_c20 = fabs(shift_x - Cshift_20[i]);
   if (diff_c20 <= err_cnC)
   {
   printf ("slice %4d of CN_noesy (-)\n", slice_no4[i]);}

   diff_n1 = fabs(shift_x - Nshift_1[i]);
   if (diff_n1 <= err_cnN)
   {
   printf ("slice %4d of CN_noesy (N)\n", slice_no4[i]);}

   diff_n2 = fabs(shift_x - Nshift_2[i]);
   if (diff_n2 <= err_15N)
   {
   printf ("slice %4d of 15Nnoesy (-)\n", slice_no5[i]);}

   diff_n3 = fabs(shift_x - Nshift_3[i]);
   if (diff_n3 <= err_15N)
   {
   printf ("slice %4d of 15Nnoesy (+)\n", slice_no5[i]);}

   diff_n4 = fabs(shift_x - Nshift_4[i]);
```

Program B.3. *(continued)*

```
        if (diff_n4 <= err_15N)
        {
        printf ("slice %4d of 15Nnoesy (-)\n", slice_no5[i]);}

        diff_n5 = fabs(shift_x - Nshift_5[i]);
        if (diff_n5 <= err_15N)
        {
        printf ("slice %4d of 15Nnoesy (+)\n", slice_no5[i]);}

        diff_n6 = fabs(shift_x - Nshift_6[i]);
        if (diff_n6 <= err_15N)
        {
        printf ("slice %4d of 15Nnoesy (-)\n", slice_no5[i]);}

        diff_c21 = fabs(shift_x - Cshift_21[i]);
        if (diff_c21 <= err_HCCH)
        {
        printf ("slice %4d of HCCH-TOCSY (-)\n", slice_no6[i]);}

        diff_c22 = fabs(shift_x - Cshift_22[i]);
        if (diff_c22 <= err_HCCH)
        {
        printf ("slice %4d of HCCH-TOCSY (+)\n", slice_no6[i]);}

        diff_c23 = fabs(shift_x - Cshift_23[i]);
        if (diff_c23 <= err_HCCH)
        {
        printf ("slice %4d of HCCH-TOCSY (-)\n", slice_no6[i]);}
    }
}
```


Program B.4. Program for Finding Mirror Image

```
/* find_mirror_image2.c
   sorting out the diagonal peaks from the output of capp*/

#include<stdio.h>
#include<math.h>
#include<string.h>
#define fname0 "envZ_HCCH.PCK"
#define tor_x 0.05
#define tor_y 0.05
#define Z_range 23.94    /* sweep width/spectrometer freq.*/

main(argc,argv)
    int argc;
    char *argv[];
{
 int no, i, j, Peak_id[9000];
 float Peak_x[9000], Peak_y[9000], Peak_z[9000], Peak_int[9000];
 float x_a, y_a, z_a, z_plus, z_minus, int_a, diff_xy, diff_yx;
 float z_plus1, z_minus1;
 int id_a, slice_a, Slice_no[9000];
 FILE *fi;

 if(argc != 2)
   {
   printf("argument 1:  id number to be searched\n");
   exit(1);
   }

 id_a = atoi(argv[1]);

 if ((fi = fopen(fname0, "r")) == NULL)
    {
     printf("Cannot open file");
    }
 i = 1;
 while (fscanf(fi, "%d %d %f %f %f %e",
        &Peak_id[i], &Slice_no[i], &Peak_x[i], &Peak_y[i], &Peak_z[i],
        &Peak_int[i] )
        !=EOF)
 i++;
 no = i ;
 fclose(fi);

   for (j = 1; j <= no ; j++)
     {
     if(Peak_id[j] == id_a)
       {
        x_a = Peak_x[j];
        y_a = Peak_y[j];
        z_a = Peak_z[j];
      z_plus = z_a + Z_range;
      z_minus = z_a - Z_range;
        slice_a = Slice_no[j];
        int_a = Peak_int[j];
        }
     }
     printf ("%4d  %3d  %6.2f  %6.2f  %7.2f (%6.2f/%6.2f) %8.3e \n",
                  id_a, slice_a, x_a, y_a, z_a, z_plus, z_minus, int_a);
     printf ("-------------------------------------------------------------\n");
```

Program B.4. *(continued)*

```
    for (i = 1; i <= no ; i++)
      {
        diff_xy = fabs(x_a - Peak_y[i]);
        diff_yx = fabs(y_a - Peak_x[i]);

      if (diff_xy <= tor_x && diff_yx <= tor_y)
            {
            z_plus1 = Peak_z[i] + Z_range;
            z_minus1 = Peak_z[i] - Z_range;
          {
          printf ("%4d  %3d  %6.2f  %6.2f  %7.2f (%6.2f/%6.2f) %8.3e\n",
                  Peak_id[i], Slice_no[i], Peak_x[i], Peak_y[i], Peak_z[i],z_plus1,
z_minus1, Peak_int[i]);
            }
          }
  }
}
```


Program B.5. Program for Analyzing Hydrogen Exchanging Data

```
/* H_exchange.c   971125 for H-bond data by hsqc with/without h2o
presat. */

#include<stdio.h>
#define fname0 "hsqc_with_h2o.TBL"
#define fname1 "hsqc_no_h2o.TBL"
#define error_hn  0.0301
#define error_n15 0.101
#define offset_wh_hn  0.000       /* hsqc_hn + offset_hn */
#define offset_wh_n15 0.000     /* hsqc_hx + offset_hx   */
#define BigT 0.001375

main()
{
int no, no1, i, j;
int  hsqc_id[200], hsqc2_id[200], hsqc_slicenum[200];
int  hsqc2_slicenum[200];
float hsqc_hn_tmp, hsqc_n15_tmp;
float delta_hn, delta_n15, intn_ratio, ex_rate;
float hsqc_hn[200], hsqc2_HN[200], hsqc_n15[200], hsqc2_N15[200], hsqc_intn[200],
hsqc2_intn[200];
FILE *fi;


if ((fi = fopen(fname0, "r")) == NULL)
   {
    printf("Cannot open file");
   }
i = 0;
while (fscanf(fi, "%d %f %f %f",
              &hsqc_id[i], &hsqc_hn[i], &hsqc_n15[i], &hsqc_intn[i]) !=EOF)
i++;
no = i;
fclose(fi);

if ((fi = fopen(fname1, "r")) == NULL)
    {
    printf("cannot open file");
    }
i = 0;
while (fscanf(fi, "%d %f %f %f",
         &hsqc2_id[i], &hsqc2_HN[i], &hsqc2_N15[i], &hsqc2_intn[i]) !=EOF)
i++;
no1 = i;
fclose(fi);


/* hsqc  */

printf ("hsqc(+h) vs. hsqc(-h) \n\n");
printf ("OFFSET FOR HN (+h2o presat.): %5.4f \n", offset_wh_hn );
printf ("OFFSET FOR N  (+h2o presat.): %5.4f \n", offset_wh_n15);
printf ("BigT : %7.6f \n", BigT);
printf ("\n\n");

for (i = 0; i <= no-1; i++)
    {
    hsqc_hn_tmp = hsqc_hn[i] + offset_wh_hn;
    hsqc_n15_tmp = hsqc_n15[i] + offset_wh_n15;
```

Program B.5. *(continued)*

```
    for (j = 0; j <= no1-1; j++)
        {
         delta_hn = hsqc2_HN[j] - hsqc_hn_tmp;
         if (delta_hn <= 0) delta_hn = -1*delta_hn;

         delta_n15 = hsqc2_N15[j] - hsqc_n15_tmp;
         if (delta_n15  <= 0) delta_n15  = -1*delta_n15;

         if(delta_hn <= error_hn && delta_n15  <= error_n15 )
        {
      intn_ratio = hsqc_intn[i]/hsqc2_intn[j];
      ex_rate =(1/intn_ratio - 1)/(BigT*100);

      printf ("%4d    %6.2f  %6.2f  %+6.2e\n", hsqc_id[i], hsqc_hn_tmp,
hsqc_n15_tmp, hsqc_intn[i]);
      printf ("%4d    %6.2f  %6.2f  %+6.2e    %6.3f  %6.3f\n\n", hsqc2_id[j],
hsqc2_HN[j], hsqc2_N15[j], hsqc2_intn[j], intn_ratio, ex_rate);
        }
       }
     }
}
```


Program B.6. Program for Analyzing HNHA Data

```
/* hnha_special2.c   970030  */

#include<stdio.h>
#include<math.h>
#define fname0 "envZ_HNHA.PCK"
#define fname1 "ASG_tbl"
#define error_hn 0.0301
#define error_hx 0.0301
#define error_n15 0.301
#define error_dhn  0.0501
#define error_dn15 0.501
#define offset_hn  0.000      /* HNHA_hn + offset_hn */
#define offset_hx 0.000    /* HNHA_hx + offset_hx  */
#define offset_n15 0.000    /* HNHA_n15 + offset_n15  */
#define water_shift 4.77
#define pai 3.14159
#define param 0.0268      /* 2*(1/4Jxh)+2*BigT   */
#define n15_range  16.44  /* Z_range obtained from Z_SW/Z_SF */

main()
{
int no, no1, i, j, k, HNHA_id[3000], HNHA_slicenum[3000], hsqc_id[1000],
res_id[1000];
float HNHA_hn_tmp, HNHA_n15_tmp, delta_hn, delta_n15, delta_hx, delta_nx,
HNHA_hx_tmp;
float HNHA_hn[3000], HNHA_hx[3000], HNHA_n15[3000], HNHA_intn[3000];
float HNHA_hn_tmp2, HNHA_hx_tmp2, HNHA_n15_tmp2, delta_hx2, delta_nx2, HNHA_dev_tmp;
float asg_n15[300], asg_hn[300], asg_co[300], asg_ca[300], asg_ha[300], asg_cb[300],
asg_hb[300] ;
float diff_n15, diff_n15_add, diff_n15_sub, diff_hn;
char aa_type[300][3];
double j_hnha;


FILE *fi;

if ((fi = fopen(fname0, "r")) == NULL)

   {
    printf("Cannot open file");
   }
i = 0;
while (fscanf(fi, "%d %d %f %f %f %f",
                &HNHA_id[i], &HNHA_slicenum[i], &HNHA_hn[i],  &HNHA_hx[i],
&HNHA_n15[i], &HNHA_intn[i]) !=EOF)
i++;
no = i;
fclose(fi);


if ((fi = fopen(fname1, "r")) == NULL)
   {
   printf("Cannot open file");
   }
i = 0;
while (fscanf(fi, "%d %s %d %f %f %f %f %f %f %f ",
                              &hsqc_id[i], aa_type[i], &res_id[i], &asg_n15[i],
&asg_hn[i], &asg_co[i], &asg_ca[i], &asg_ha[i], &asg_cb[i], &asg_hb[i] ) !=EOF)
i++;
no1 = i;
```

```
fclose(fi);

/* HNHA  */

printf ("HNHA list");
printf ("\n\n");
printf (" pk#    sl#    hn      hx    n15      intn    - Iha/Ihn");
printf ("\n");
for (i = 0; i <= no-1; i++)
    {
    HNHA_hn_tmp = HNHA_hn[i] + offset_hn;
    HNHA_hx_tmp = HNHA_hx[i] + offset_hx;
    delta_nx = HNHA_hn_tmp - HNHA_hx_tmp;
    if (delta_nx <= 0) delta_nx = -1*delta_nx;
     delta_hx = HNHA_hx[i] - water_shift;
     if (delta_hx <= 0) delta_hx = -1*delta_hx;
     if (delta_hx >= error_hx && delta_nx <= error_hn)
     {
       for (j = 0; j <= no-1; j++)
      {
      if(j != i)
        {
        HNHA_hn_tmp2 = HNHA_hn[j] + offset_hn;
        delta_hn = HNHA_hn_tmp2 - HNHA_hn_tmp;
        if (delta_hn <= 0) delta_hn = -1*delta_hn;
        HNHA_hx_tmp2 = HNHA_hx[j] + offset_hx;
      delta_nx2 = HNHA_hn_tmp2 - HNHA_hx_tmp2;
        HNHA_n15_tmp = HNHA_n15[i] + offset_n15;
      HNHA_n15_tmp2 = HNHA_n15[j] + offset_n15;
        delta_n15 = HNHA_n15_tmp2 - HNHA_n15_tmp;
        if (delta_n15 <= 0) delta_n15 = -1*delta_n15;
      delta_hx2 = HNHA_hx[j] - water_shift;
      if (delta_hx2 <= 0) delta_hx2 = -1*delta_hx2;

        if(delta_hn <= error_hn && delta_n15 <= error_n15 && delta_hx2 >= error_hx &&
delta_nx2 >= error_hn)
          {
          HNHA_dev_tmp = -1*(HNHA_intn[j]/HNHA_intn[i]);
        if(HNHA_dev_tmp >= 0)
        {
        j_hnha = (atan(sqrt(HNHA_dev_tmp)))/(pai*param);
          printf ("%4d  %4d  %6.2f  %6.2f  %6.2f  %+6.2e \n", HNHA_id[i],
HNHA_slicenum[i], HNHA_hn_tmp, HNHA_hx_tmp, HNHA_n15_tmp, HNHA_intn[i]);
          printf ("%4d  %4d  %6.2f  %6.2f  %6.2f  %+6.2e  %6.3f %6.2f\n", HNHA_id[j],
HNHA_slicenum[j], HNHA_hn_tmp2, HNHA_hx_tmp2, HNHA_n15_tmp2, HNHA_intn[j],
HNHA_dev_tmp, j_hnha);
          }
         for (k=0; k <= no1-1; k++)
         {
         diff_n15 = asg_n15[k] - HNHA_n15_tmp2;
         if (diff_n15 < 0) diff_n15 = -1*diff_n15;

         diff_n15_add = asg_n15[k] - (HNHA_n15_tmp2 + n15_range);
         if (diff_n15_add < 0) diff_n15_add = -1*diff_n15_add;

         diff_n15_sub = asg_n15[k] - (HNHA_n15_tmp2 - n15_range);
         if (diff_n15_sub < 0) diff_n15_sub = -1*diff_n15_sub;

         diff_hn = asg_hn[k] - HNHA_hn_tmp2;
         if (diff_hn < 0) diff_hn = -1*diff_hn;
```



```
         if (diff_n15 <= error_dn15 && diff_hn <= error_dhn)
         {
         printf ( "                                                          %4d %2s
%6.2f \n", res_id[k], aa_type[k], asg_ha[k]);
         }

           if (diff_n15_add <= error_dn15 && diff_hn <= error_dhn)
         {
         printf ( "                                                          %4d %2s
%6.2f \n", res_id[k], aa_type[k], asg_ha[k]);
         }

           if (diff_n15_sub <= error_dn15 && diff_hn <= error_dhn)
         {
         printf ( "                                                          %4d %2s
%6.2f \n", res_id[k], aa_type[k], asg_ha[k]);
         }
        }
        printf ("\n");
       }
      }
     }
    }
   }
  }
```

Program B.7. Program for Analyzing HNHB Data

```
/* search_hnhb3.c     971208    */

#include<stdio.h>
#define fname1 "envZ_HNHB.PCK"
#define error_hn  0.0301
#define error_n15 0.0501
#define error_hnhx 0.0301
#define offset_hn  0.000       /* HNHB_hn + offset_hn */
#define offset_n15 0.000     /* HNHB_n15 + offset_n15  */

main()
{
int  no1, i, j, HNHB_id[1000], HNHB_slicenum[500];
float delta_hn, delta_hnhx;
float delta_n15, ratio_hnhx;
float HNHB_hn[1000], HNHB_hx[1000], HNHB_n15[1000], HNHB_intn[1000];

FILE *fi;

if ((fi = fopen(fname1, "r")) == NULL)
   {
    printf("Cannot open file");
   }
i = 0;
while (fscanf(fi, "%d %d %f %f %f %f",
              &HNHB_id[i], &HNHB_slicenum[i], &HNHB_hn[i], &HNHB_hx[i],
&HNHB_n15[i], &HNHB_intn[i]) !=EOF)
i++;
no1 = i;
fclose(fi);


/* HNHB  */

printf ("HNHB  \n\n");
printf ("ERROR FOR HN  : %5.4f \n", error_hn);
printf ("ERROR FOR N15 : %5.4f \n", error_n15);
printf ("OFFSET FOR HN : %5.4f \n", offset_hn );
printf ("OFFSET FOR N15: %5.4f \n", offset_n15);
printf ("\n\n");
printf ("  pk#  sl#      HN      HX     n15      intn     Ic/Id");


for (i = 0; i <= no1-1; i++)
    {
    delta_hnhx = HNHB_hn[i] - HNHB_hx[i];
    if (delta_hnhx <= 0) delta_hnhx = -1*delta_hnhx;
    if (delta_hnhx <= error_hnhx)
    {
    printf ("\n");
    printf ("*%4d %4d   %6.2f  %6.2f  %6.2f  %+6.2e\n", HNHB_id[i],
 HNHB_slicenum[i], HNHB_hn[i], HNHB_hx[i], HNHB_n15[i], HNHB_intn[i]);
    for (j = 0; j <= no1-1; j++)
    {
    if (j != i)
    {
    delta_n15 = HNHB_n15[i] - HNHB_n15[j];
    if (delta_n15 <= 0) delta_n15 = -1*delta_n15;

    delta_hn = HNHB_hn[i] - HNHB_hn[j];
```


Program B.7. *(continued)*

```
    if (delta_hn <= 0) delta_hn = -1*delta_hn;

    if (delta_n15 <= error_n15 && delta_hn <= error_hn )
    {
     ratio_hnhx = (HNHB_intn[j]/HNHB_intn[i]);
     printf (" %4d %4d   %6.2f  %6.2f  %6.2f  %+6.2e  %6.2f\n", HNHB_id[j],
HNHB_slicenum[j], HNHB_hn[j], HNHB_hx[j], HNHB_n15[j], HNHB_intn[j], ratio_hnhx);
      }
     }
    }
   }
  }
 }
```