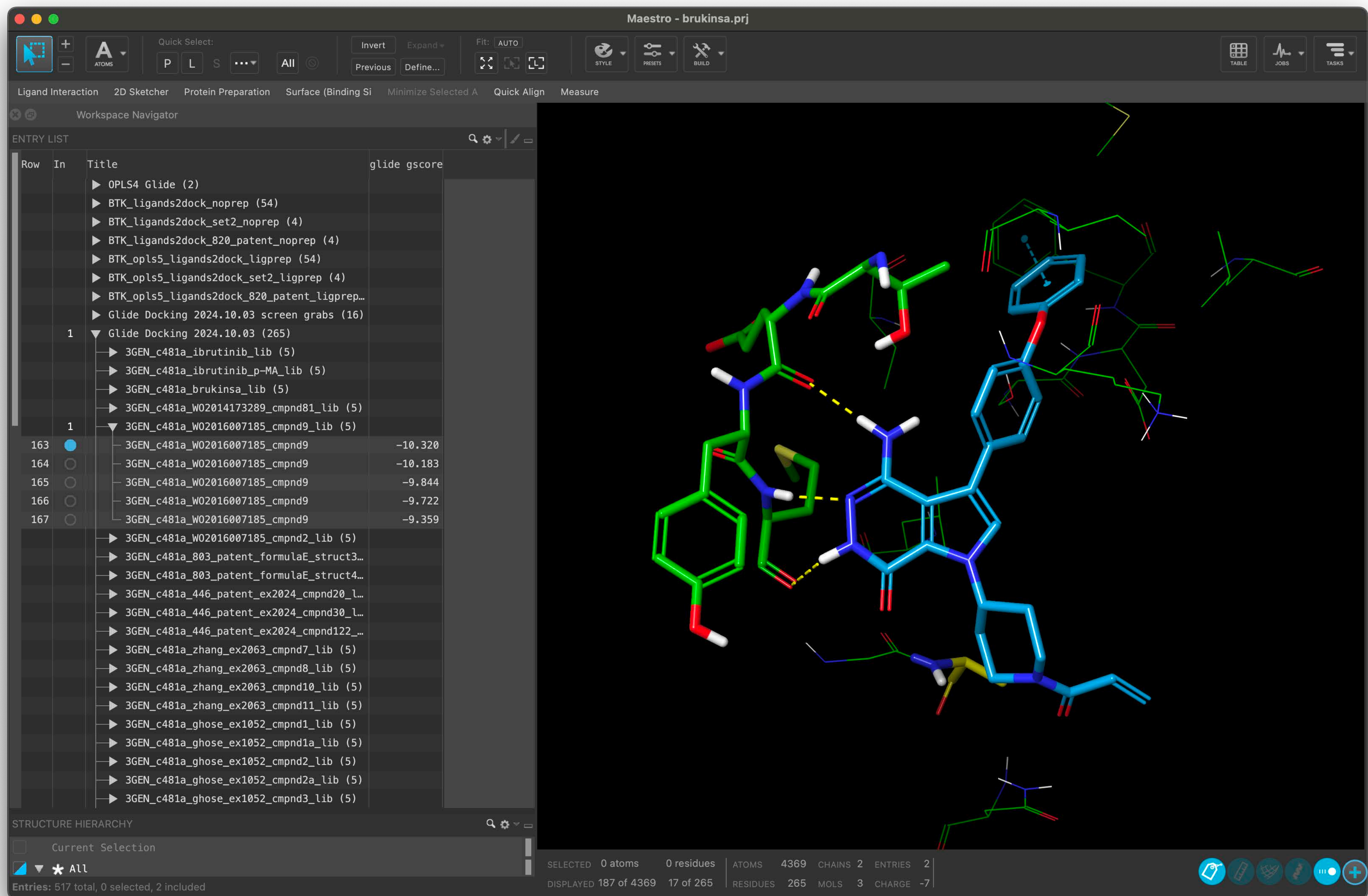
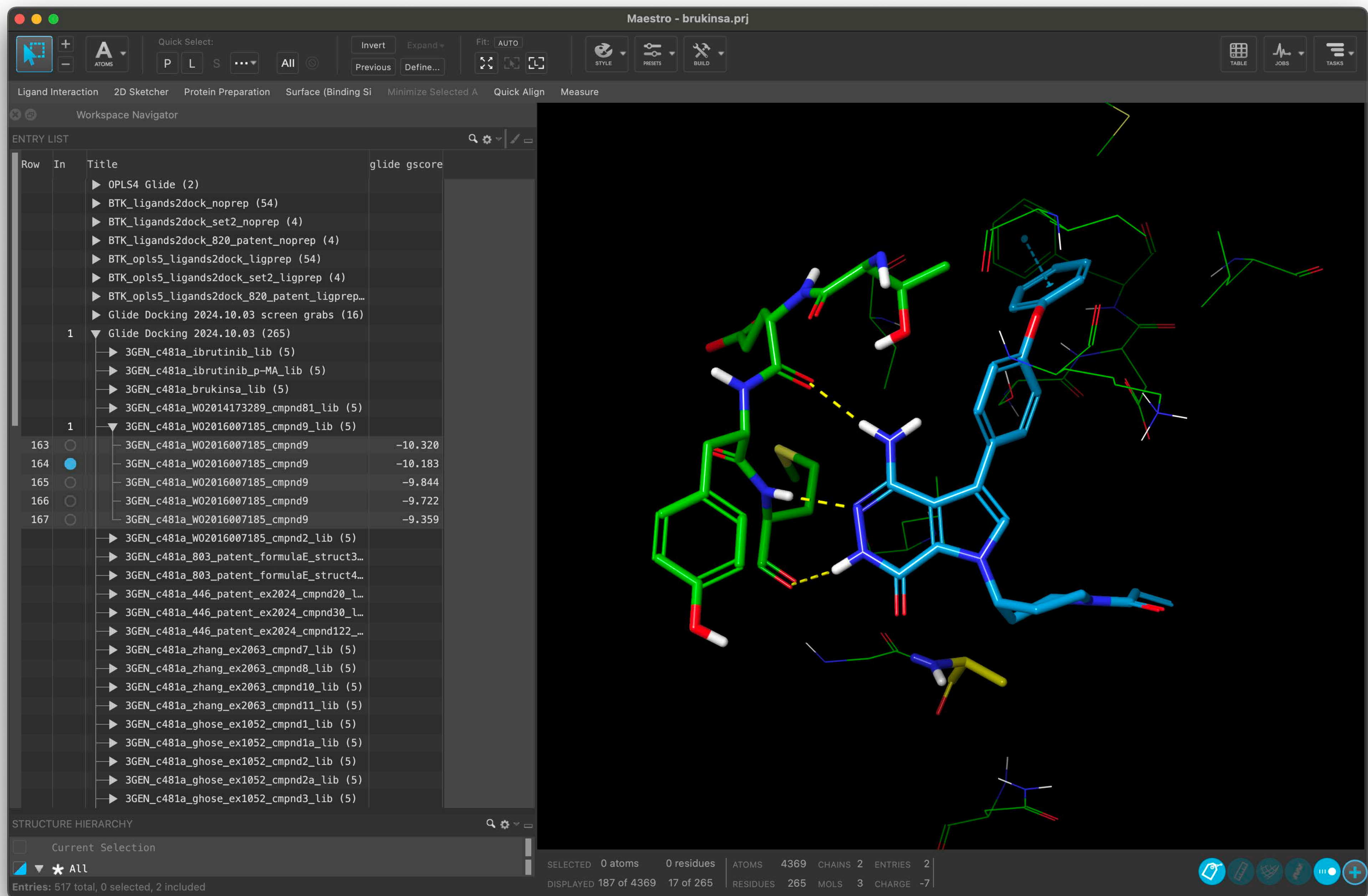
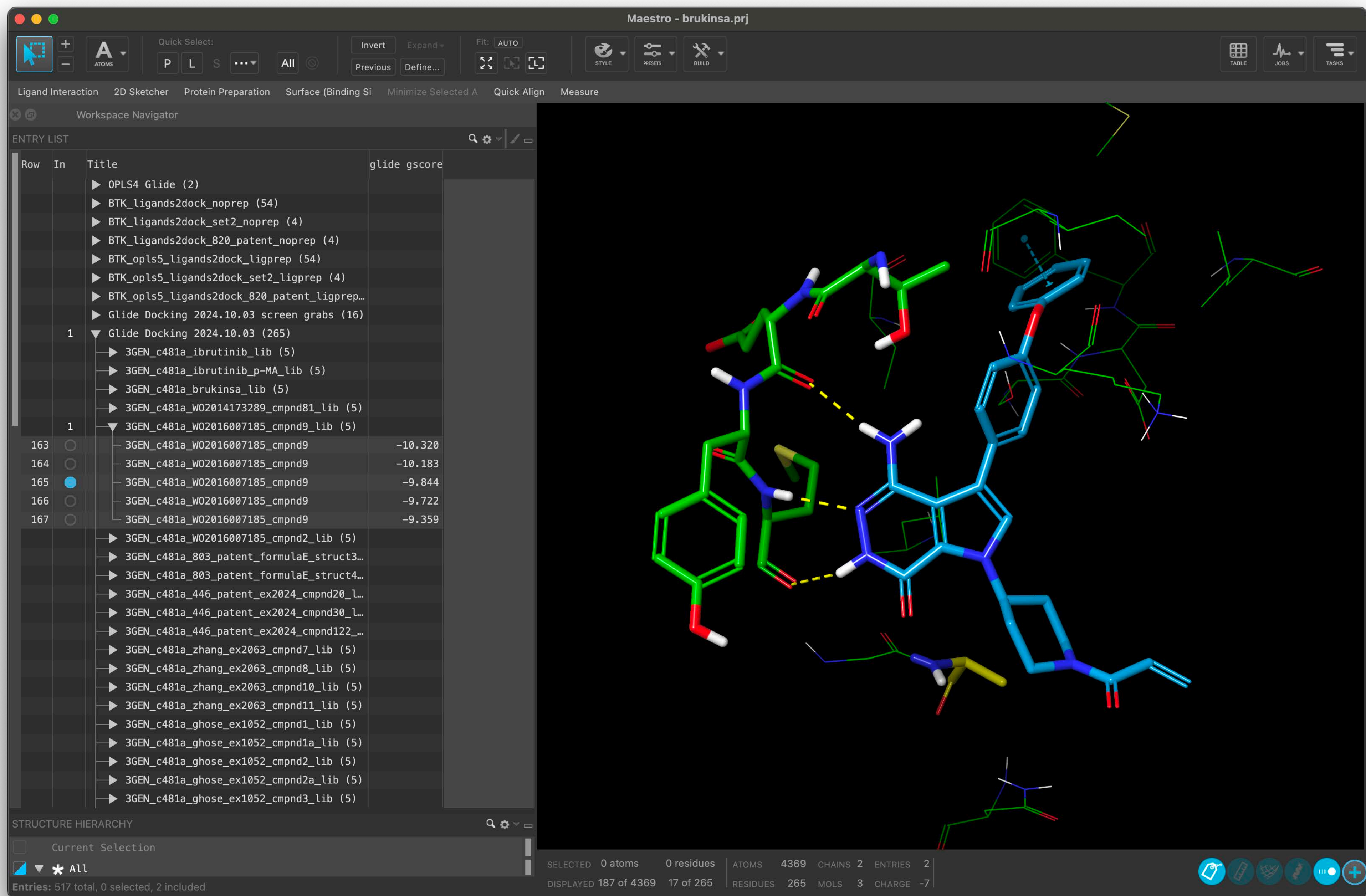
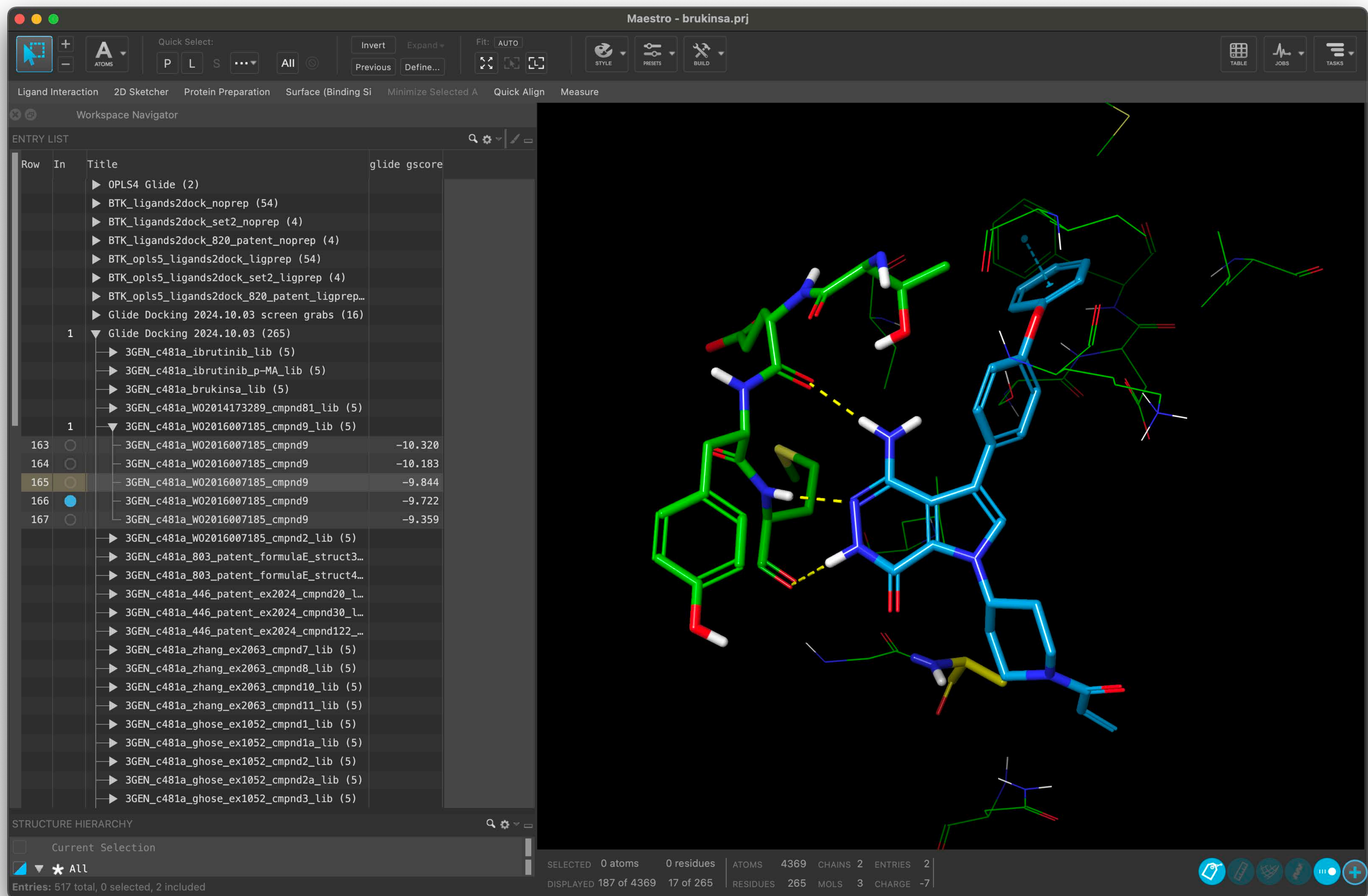










Maestro - brukinsa.prj

Quick Select: P L S ... All Invert Expand Fit: AUTO STYLE PRESETS BUILD TABLE JOBS TASKS

Ligand Interaction 2D Sketcher Protein Preparation Surface (Binding Si) Minimize Selected A Quick Align Measure

Workspace Navigator

ENTRY LIST

Row	In	Title	glide gscore
		▶ OPLS4 Glide (2)	
		▶ BTK_ligands2dock_noprep (54)	
		▶ BTK_ligands2dock_set2_noprep (4)	
		▶ BTK_ligands2dock_820_patent_noprep (4)	
		▶ BTK_opls5_ligands2dock_ligprep (54)	
		▶ BTK_opls5_ligands2dock_set2_ligprep (4)	
		▶ BTK_opls5_ligands2dock_820_patent_ligprep...	
		▶ Glide Docking 2024.10.03 screen grabs (16)	
	1	▼ Glide Docking 2024.10.03 (265)	
		▶ 3GEN_c481a_ibrutinib_lib (5)	
		▶ 3GEN_c481a_ibrutinib_p-MA_lib (5)	
		▶ 3GEN_c481a_brukinsa_lib (5)	
		▶ 3GEN_c481a_W02014173289_cmpnd81_lib (5)	
	1	▼ 3GEN_c481a_W02016007185_cmpnd9_lib (5)	
163	☐	3GEN_c481a_W02016007185_cmpnd9	-10.320
164	☐	3GEN_c481a_W02016007185_cmpnd9	-10.183
165	☐	3GEN_c481a_W02016007185_cmpnd9	-9.844
166	☐	3GEN_c481a_W02016007185_cmpnd9	-9.722
167	☒	3GEN_c481a_W02016007185_cmpnd9	-9.359
		▶ 3GEN_c481a_W02016007185_cmpnd2_lib (5)	
		▶ 3GEN_c481a_803_patent_formulaE_struct3...	
		▶ 3GEN_c481a_803_patent_formulaE_struct4...	
		▶ 3GEN_c481a_446_patent_ex2024_cmpnd20_l...	
		▶ 3GEN_c481a_446_patent_ex2024_cmpnd30_l...	
		▶ 3GEN_c481a_446_patent_ex2024_cmpnd122...	
		▶ 3GEN_c481a_zhang_ex2063_cmpnd7_lib (5)	
		▶ 3GEN_c481a_zhang_ex2063_cmpnd8_lib (5)	
		▶ 3GEN_c481a_zhang_ex2063_cmpnd10_lib (5)	
		▶ 3GEN_c481a_zhang_ex2063_cmpnd11_lib (5)	
		▶ 3GEN_c481a_ghose_ex1052_cmpnd1_lib (5)	
		▶ 3GEN_c481a_ghose_ex1052_cmpnd1a_lib (5)	
		▶ 3GEN_c481a_ghose_ex1052_cmpnd2_lib (5)	
		▶ 3GEN_c481a_ghose_ex1052_cmpnd2a_lib (5)	
		▶ 3GEN_c481a_ghose_ex1052_cmpnd3_lib (5)	

STRUCTURE HIERARCHY

☐ Current Selection

☒ ☐ ☒ All

Entries: 517 total, 0 selected, 2 included

SELECTED 0 atoms 0 residues | ATOMS 4369 CHAINS 2 ENTRIES 2
DISPLAYED 187 of 4369 17 of 265 | RESIDUES 265 MOLS 3 CHARGE -7