

core.init: Checking for fconfig files in pwd and ./rosetta/flags
core.init.score_function_corrections: [**WARNING**] Flag -restore_talaris_behavior is set but -weights are also specified. Not changing input weights file!
core.init: Rosetta version: rosetta.binary.mac.release-247 r247 2020.08+release.cb1cabafd74
cb1cabafd7463ab703f6abf5efa33d2707b85924 <https://www.rosettacommons.org> 2020-02-22T06:57:31.821199
core.init: command:
/Users/andreserobian/rosetta_workshop/rosetta/main/source/build/src/release/macos/10.14/64/x86/clang/10.0/default/pepspec_anchor_dock.default.macosclangrelease -database
/Users/andreserobian/Documents/PyRosetta4/setup/pyrosetta/database @dock.args -corrections::restore_talaris_behavior
basic.random.init_random_generator: 'RNG device' seed mode, using '/dev/urandom', seed=-1745446643 seed_offset=0
real_seed=-1745446643
basic.random.init_random_generator: RandomGenerator:init: Normal mode, seed=-1745446643 RG_type=mt19937
core.chemical.GlobalResidueTypeSet: Finished initializing fa_standard residue type set. Created 544 residue types
core.chemical.GlobalResidueTypeSet: Total time to initialize 0.385531 seconds.
core.import_pose.import_pose: File 'aln_2n2a_AB.pdb' automatically determined to be of type PDB
core.io.pose_from_sfr.PoseFromSFRBuilder: [**WARNING**] discarding 4 atoms at position 1 in file aln_2n2a_AB.pdb. Best match rsd_type: ALA:NtermProteinFull
core.io.pose_from_sfr.PoseFromSFRBuilder: [**WARNING**] discarding 4 atoms at position 2 in file aln_2n2a_AB.pdb. Best match rsd_type: GLU
core.io.pose_from_sfr.PoseFromSFRBuilder: [**WARNING**] discarding 6 atoms at position 3 in file aln_2n2a_AB.pdb. Best match rsd_type: GLN
core.io.pose_from_sfr.PoseFromSFRBuilder: [**WARNING**] discarding 10 atoms at position 4 in file aln_2n2a_AB.pdb. Best match rsd_type: ARG
core.io.pose_from_sfr.PoseFromSFRBuilder: [**WARNING**] discarding 3 atoms at position 5 in file aln_2n2a_AB.pdb. Best match rsd_type: ALA
core.io.pose_from_sfr.PoseFromSFRBuilder: [**WARNING**] discarding 2 atoms at position 6 in file aln_2n2a_AB.pdb. Best match rsd_type: SER
core.io.pose_from_sfr.PoseFromSFRBuilder: [**WARNING**] discarding 6 atoms at position 7 in file aln_2n2a_AB.pdb. Best match rsd_type: PRO
core.io.pose_from_sfr.PoseFromSFRBuilder: [**WARNING**] discarding 8 atoms at position 8 in file aln_2n2a_AB.pdb. Best match rsd_type: LEU
core.io.pose_from_sfr.PoseFromSFRBuilder: [**WARNING**] discarding 3 atoms at position 9 in file aln_2n2a_AB.pdb. Best match rsd_type: THR
core.io.pose_from_sfr.PoseFromSFRBuilder: [**WARNING**] discarding 2 atoms at position 10 in file aln_2n2a_AB.pdb. Best match rsd_type: SER
core.io.pose_from_sfr.PoseFromSFRBuilder: [**WARNING**] discarding 8 atoms at position 11 in file aln_2n2a_AB.pdb. Best match rsd_type: ILE
core.io.pose_from_sfr.PoseFromSFRBuilder: [**WARNING**] discarding 8 atoms at position 12 in file aln_2n2a_AB.pdb. Best match rsd_type: ILE
core.io.pose_from_sfr.PoseFromSFRBuilder: [**WARNING**] discarding 2 atoms at position 13 in file aln_2n2a_AB.pdb. Best match rsd_type: SER
core.io.pose_from_sfr.PoseFromSFRBuilder: [**WARNING**] discarding 3 atoms at position 14 in file aln_2n2a_AB.pdb. Best match rsd_type: ALA
core.io.pose_from_sfr.PoseFromSFRBuilder: [**WARNING**] discarding 6 atoms at position 15 in file aln_2n2a_AB.pdb. Best match rsd_type: VAL
core.io.pose_from_sfr.PoseFromSFRBuilder: [**WARNING**] discarding 6 atoms at position 16 in file aln_2n2a_AB.pdb. Best match rsd_type: VAL
core.io.pose_from_sfr.PoseFromSFRBuilder: [**WARNING**] discarding 2 atoms at position 17 in file aln_2n2a_AB.pdb. Best match rsd_type: GLY
core.io.pose_from_sfr.PoseFromSFRBuilder: [**WARNING**] discarding 8 atoms at position 18 in file aln_2n2a_AB.pdb. Best match rsd_type: ILE
core.io.pose_from_sfr.PoseFromSFRBuilder: [**WARNING**] discarding 8 atoms at position 19 in file aln_2n2a_AB.pdb. Best match rsd_type: LEU
core.io.pose_from_sfr.PoseFromSFRBuilder: [**WARNING**] discarding 8 atoms at position 20 in file aln_2n2a_AB.pdb. Best match rsd_type: LEU
core.io.pose_from_sfr.PoseFromSFRBuilder: [**WARNING**] discarding 6 atoms at position 21 in file aln_2n2a_AB.pdb. Best match rsd_type: VAL

core.io.pose_from_sfr.PoseFromSFRBuilder: [**WARNING**] discarding 4 atoms at position 50 in file aln_2n2a_AB.pdb. Best match rsd_type: GLU

core.io.pose_from_sfr.PoseFromSFRBuilder: [**WARNING**] discarding 3 atoms at position 51 in file aln_2n2a_AB.pdb. Best match rsd_type: THR

core.io.pose_from_sfr.PoseFromSFRBuilder: [**WARNING**] discarding 4 atoms at position 52 in file aln_2n2a_AB.pdb. Best match rsd_type: GLU

core.io.pose_from_sfr.PoseFromSFRBuilder: [**WARNING**] discarding 8 atoms at position 53 in file aln_2n2a_AB.pdb. Best match rsd_type: LEU

core.io.pose_from_sfr.PoseFromSFRBuilder: [**WARNING**] discarding 6 atoms at position 54 in file aln_2n2a_AB.pdb. Best match rsd_type: VAL

core.io.pose_from_sfr.PoseFromSFRBuilder: [**WARNING**] discarding 4 atoms at position 55 in file aln_2n2a_AB.pdb. Best match rsd_type: GLU

core.io.pose_from_sfr.PoseFromSFRBuilder: [**WARNING**] discarding 6 atoms at position 56 in file aln_2n2a_AB.pdb. Best match rsd_type: PRO

core.io.pose_from_sfr.PoseFromSFRBuilder: [**WARNING**] discarding 8 atoms at position 57 in file aln_2n2a_AB.pdb. Best match rsd_type: LEU

core.io.pose_from_sfr.PoseFromSFRBuilder: [**WARNING**] discarding 2 atoms at position 58 in file aln_2n2a_AB.pdb. Best match rsd_type: GLY:CtermProteinFull

core.io.pose_from_sfr.PoseFromSFRBuilder: [**WARNING**] discarding 4 atoms at position 59 in file aln_2n2a_AB.pdb. Best match rsd_type: ALA:NtermProteinFull

core.io.pose_from_sfr.PoseFromSFRBuilder: [**WARNING**] discarding 4 atoms at position 60 in file aln_2n2a_AB.pdb. Best match rsd_type: GLU

core.io.pose_from_sfr.PoseFromSFRBuilder: [**WARNING**] discarding 6 atoms at position 61 in file aln_2n2a_AB.pdb. Best match rsd_type: GLN

core.io.pose_from_sfr.PoseFromSFRBuilder: [**WARNING**] discarding 10 atoms at position 62 in file aln_2n2a_AB.pdb. Best match rsd_type: ARG

core.io.pose_from_sfr.PoseFromSFRBuilder: [**WARNING**] discarding 3 atoms at position 63 in file aln_2n2a_AB.pdb. Best match rsd_type: ALA

core.io.pose_from_sfr.PoseFromSFRBuilder: [**WARNING**] discarding 2 atoms at position 64 in file aln_2n2a_AB.pdb. Best match rsd_type: SER

core.io.pose_from_sfr.PoseFromSFRBuilder: [**WARNING**] discarding 6 atoms at position 65 in file aln_2n2a_AB.pdb. Best match rsd_type: PRO

core.io.pose_from_sfr.PoseFromSFRBuilder: [**WARNING**] discarding 8 atoms at position 66 in file aln_2n2a_AB.pdb. Best match rsd_type: LEU

core.io.pose_from_sfr.PoseFromSFRBuilder: [**WARNING**] discarding 3 atoms at position 67 in file aln_2n2a_AB.pdb. Best match rsd_type: THR

core.io.pose_from_sfr.PoseFromSFRBuilder: [**WARNING**] discarding 2 atoms at position 68 in file aln_2n2a_AB.pdb. Best match rsd_type: SER

core.io.pose_from_sfr.PoseFromSFRBuilder: [**WARNING**] discarding 8 atoms at position 69 in file aln_2n2a_AB.pdb. Best match rsd_type: ILE

core.io.pose_from_sfr.PoseFromSFRBuilder: [**WARNING**] discarding 8 atoms at position 70 in file aln_2n2a_AB.pdb. Best match rsd_type: ILE

core.io.pose_from_sfr.PoseFromSFRBuilder: [**WARNING**] discarding 2 atoms at position 71 in file aln_2n2a_AB.pdb. Best match rsd_type: SER

core.io.pose_from_sfr.PoseFromSFRBuilder: [**WARNING**] discarding 3 atoms at position 72 in file aln_2n2a_AB.pdb. Best match rsd_type: ALA

core.io.pose_from_sfr.PoseFromSFRBuilder: [**WARNING**] discarding 6 atoms at position 73 in file aln_2n2a_AB.pdb. Best match rsd_type: VAL

core.io.pose_from_sfr.PoseFromSFRBuilder: [**WARNING**] discarding 6 atoms at position 74 in file aln_2n2a_AB.pdb. Best match rsd_type: VAL

core.io.pose_from_sfr.PoseFromSFRBuilder: [**WARNING**] discarding 2 atoms at position 75 in file aln_2n2a_AB.pdb. Best match rsd_type: GLY

core.io.pose_from_sfr.PoseFromSFRBuilder: [**WARNING**] discarding 8 atoms at position 76 in file aln_2n2a_AB.pdb. Best match rsd_type: ILE

core.io.pose_from_sfr.PoseFromSFRBuilder: [**WARNING**] discarding 8 atoms at position 77 in file aln_2n2a_AB.pdb. Best match rsd_type: LEU

core.io.pose_from_sfr.PoseFromSFRBuilder: [**WARNING**] discarding 8 atoms at position 106 in file aln_2n2a_AB.pdb.
Best match rsd_type: LEU

core.io.pose_from_sfr.PoseFromSFRBuilder: [**WARNING**] discarding 6 atoms at position 107 in file aln_2n2a_AB.pdb.
Best match rsd_type: GLN

core.io.pose_from_sfr.PoseFromSFRBuilder: [**WARNING**] discarding 4 atoms at position 108 in file aln_2n2a_AB.pdb.
Best match rsd_type: GLU

core.io.pose_from_sfr.PoseFromSFRBuilder: [**WARNING**] discarding 3 atoms at position 109 in file aln_2n2a_AB.pdb.
Best match rsd_type: THR

core.io.pose_from_sfr.PoseFromSFRBuilder: [**WARNING**] discarding 4 atoms at position 110 in file aln_2n2a_AB.pdb.
Best match rsd_type: GLU

core.io.pose_from_sfr.PoseFromSFRBuilder: [**WARNING**] discarding 8 atoms at position 111 in file aln_2n2a_AB.pdb.
Best match rsd_type: LEU

core.io.pose_from_sfr.PoseFromSFRBuilder: [**WARNING**] discarding 6 atoms at position 112 in file aln_2n2a_AB.pdb.
Best match rsd_type: VAL

core.io.pose_from_sfr.PoseFromSFRBuilder: [**WARNING**] discarding 4 atoms at position 113 in file aln_2n2a_AB.pdb.
Best match rsd_type: GLU

core.io.pose_from_sfr.PoseFromSFRBuilder: [**WARNING**] discarding 6 atoms at position 114 in file aln_2n2a_AB.pdb.
Best match rsd_type: PRO

core.io.pose_from_sfr.PoseFromSFRBuilder: [**WARNING**] discarding 8 atoms at position 115 in file aln_2n2a_AB.pdb.
Best match rsd_type: LEU

core.io.pose_from_sfr.PoseFromSFRBuilder: [**WARNING**] discarding 2 atoms at position 116 in file aln_2n2a_AB.pdb.
Best match rsd_type: GLY:CtermProteinFull

core.conformation.Conformation: [**WARNING**] missing heavyatom: OXT on residue GLY:CtermProteinFull 58

core.conformation.Conformation: [**WARNING**] missing heavyatom: OXT on residue GLY:CtermProteinFull 116

core.scoring.ScoreFunctionFactory: SCOREFUNCTION: [talaris2013.wts](#)

core.scoring.etable: Starting energy table calculation

core.scoring.etable: smooth_etable: changing atr/rep split to bottom of energy well

core.scoring.etable: smooth_etable: spline smoothing lj etables (maxdis = 6)

core.scoring.etable: smooth_etable: spline smoothing solvation etables (max_dis = 6)

core.scoring.etable: Finished calculating energy tables.

basic.io.database: Database file opened: scoring/score_functions/hbonds/sp2_elec_params/HBPoly1D.csv

basic.io.database: Database file opened: scoring/score_functions/hbonds/sp2_elec_params/HBFadeIntervals.csv

basic.io.database: Database file opened: scoring/score_functions/hbonds/sp2_elec_params/HBEval.csv

basic.io.database: Database file opened: scoring/score_functions/rama/Rama_smooth_dyn.dat_ss_6.4

basic.io.database: Database file opened: scoring/score_functions/P_AA_pp/P_AA

basic.io.database: Database file opened: scoring/score_functions/P_AA_pp/P_AA_n

basic.io.database: Database file opened: scoring/score_functions/P_AA_pp/P_AA_pp

core.scoring.etable: Using alternate parameters: LJ_RADIUS_SOFT in Etable construction.

core.scoring.etable: Starting energy table calculation

core.scoring.etable: smooth_etable: changing atr/rep split to bottom of energy well

core.scoring.etable: smooth_etable: spline smoothing lj etables (maxdis = 6)

core.scoring.etable: smooth_etable: spline smoothing solvation etables (max_dis = 6)

core.scoring.etable: Finished calculating energy tables.

basic.io.database: Database file opened: scoring/score_functions/PairEPotential/pdb_pair_stats_fine

apps.pilot.chrisk/pep_prep: Initializing prep_1.pdb with aln_2n2a_AB.pdb

core.import_pose.import_pose: File 'aln_2n2a_AB.pdb' automatically determined to be of type PDB

core.io.pose_from_sfr.PoseFromSFRBuilder: [**WARNING**] discarding 4 atoms at position 1 in file aln_2n2a_AB.pdb. Best match rsd_type: ALA:NtermProteinFull

core.io.pose_from_sfr.PoseFromSFRBuilder: [**WARNING**] discarding 4 atoms at position 2 in file aln_2n2a_AB.pdb. Best match rsd_type: GLU

core.io.pose_from_sfr.PoseFromSFRBuilder: [**WARNING**] discarding 6 atoms at position 3 in file aln_2n2a_AB.pdb. Best match rsd_type: GLN

core.io.pose_from_sfr.PoseFromSFRBuilder: [**WARNING**] discarding 10 atoms at position 4 in file aln_2n2a_AB.pdb. Best match rsd_type: ARG

core.io.pose_from_sfr.PoseFromSFRBuilder: [**WARNING**] discarding 3 atoms at position 5 in file aln_2n2a_AB.pdb. Best match rsd_type: ALA

core.io.pose_from_sfr.PoseFromSFRBuilder: [**WARNING**] discarding 10 atoms at position 34 in file aln_2n2a_AB.pdb.
Best match rsd_type: ARG

core.io.pose_from_sfr.PoseFromSFRBuilder: [**WARNING**] discarding 10 atoms at position 35 in file aln_2n2a_AB.pdb.
Best match rsd_type: ARG

core.io.pose_from_sfr.PoseFromSFRBuilder: [**WARNING**] discarding 6 atoms at position 36 in file aln_2n2a_AB.pdb. Best
match rsd_type: GLN

core.io.pose_from_sfr.PoseFromSFRBuilder: [**WARNING**] discarding 6 atoms at position 37 in file aln_2n2a_AB.pdb. Best
match rsd_type: GLN

core.io.pose_from_sfr.PoseFromSFRBuilder: [**WARNING**] discarding 11 atoms at position 38 in file aln_2n2a_AB.pdb.
Best match rsd_type: LYS

core.io.pose_from_sfr.PoseFromSFRBuilder: [**WARNING**] discarding 8 atoms at position 39 in file aln_2n2a_AB.pdb. Best
match rsd_type: ILE

core.io.pose_from_sfr.PoseFromSFRBuilder: [**WARNING**] discarding 10 atoms at position 40 in file aln_2n2a_AB.pdb.
Best match rsd_type: ARG

core.io.pose_from_sfr.PoseFromSFRBuilder: [**WARNING**] discarding 11 atoms at position 41 in file aln_2n2a_AB.pdb.
Best match rsd_type: LYS

core.io.pose_from_sfr.PoseFromSFRBuilder: [**WARNING**] discarding 2 atoms at position 42 in file aln_2n2a_AB.pdb. Best
match rsd_type: TYR

core.io.pose_from_sfr.PoseFromSFRBuilder: [**WARNING**] discarding 3 atoms at position 43 in file aln_2n2a_AB.pdb. Best
match rsd_type: THR

core.io.pose_from_sfr.PoseFromSFRBuilder: [**WARNING**] discarding 7 atoms at position 44 in file aln_2n2a_AB.pdb. Best
match rsd_type: MET

core.io.pose_from_sfr.PoseFromSFRBuilder: [**WARNING**] discarding 10 atoms at position 45 in file aln_2n2a_AB.pdb.
Best match rsd_type: ARG

core.io.pose_from_sfr.PoseFromSFRBuilder: [**WARNING**] discarding 10 atoms at position 46 in file aln_2n2a_AB.pdb.
Best match rsd_type: ARG

core.io.pose_from_sfr.PoseFromSFRBuilder: [**WARNING**] discarding 8 atoms at position 47 in file aln_2n2a_AB.pdb. Best
match rsd_type: LEU

core.io.pose_from_sfr.PoseFromSFRBuilder: [**WARNING**] discarding 8 atoms at position 48 in file aln_2n2a_AB.pdb. Best
match rsd_type: LEU

core.io.pose_from_sfr.PoseFromSFRBuilder: [**WARNING**] discarding 6 atoms at position 49 in file aln_2n2a_AB.pdb. Best
match rsd_type: GLN

core.io.pose_from_sfr.PoseFromSFRBuilder: [**WARNING**] discarding 4 atoms at position 50 in file aln_2n2a_AB.pdb. Best
match rsd_type: GLU

core.io.pose_from_sfr.PoseFromSFRBuilder: [**WARNING**] discarding 3 atoms at position 51 in file aln_2n2a_AB.pdb. Best
match rsd_type: THR

core.io.pose_from_sfr.PoseFromSFRBuilder: [**WARNING**] discarding 4 atoms at position 52 in file aln_2n2a_AB.pdb. Best
match rsd_type: GLU

core.io.pose_from_sfr.PoseFromSFRBuilder: [**WARNING**] discarding 8 atoms at position 53 in file aln_2n2a_AB.pdb. Best
match rsd_type: LEU

core.io.pose_from_sfr.PoseFromSFRBuilder: [**WARNING**] discarding 6 atoms at position 54 in file aln_2n2a_AB.pdb. Best
match rsd_type: VAL

core.io.pose_from_sfr.PoseFromSFRBuilder: [**WARNING**] discarding 4 atoms at position 55 in file aln_2n2a_AB.pdb. Best
match rsd_type: GLU

core.io.pose_from_sfr.PoseFromSFRBuilder: [**WARNING**] discarding 6 atoms at position 56 in file aln_2n2a_AB.pdb. Best
match rsd_type: PRO

core.io.pose_from_sfr.PoseFromSFRBuilder: [**WARNING**] discarding 8 atoms at position 57 in file aln_2n2a_AB.pdb. Best
match rsd_type: LEU

core.io.pose_from_sfr.PoseFromSFRBuilder: [**WARNING**] discarding 2 atoms at position 58 in file aln_2n2a_AB.pdb. Best
match rsd_type: GLY:CtermProteinFull

core.io.pose_from_sfr.PoseFromSFRBuilder: [**WARNING**] discarding 4 atoms at position 59 in file aln_2n2a_AB.pdb. Best
match rsd_type: ALA:NtermProteinFull

core.io.pose_from_sfr.PoseFromSFRBuilder: [**WARNING**] discarding 4 atoms at position 60 in file aln_2n2a_AB.pdb. Best
match rsd_type: GLU

core.io.pose_from_sfr.PoseFromSFRBuilder: [**WARNING**] discarding 6 atoms at position 61 in file aln_2n2a_AB.pdb. Best
match rsd_type: GLN

core.io.pose_from_sfr.PoseFromSFRBuilder: [**WARNING**] discarding 8 atoms at position 90 in file aln_2n2a_AB.pdb. Best match rsd_type: ILE
core.io.pose_from_sfr.PoseFromSFRBuilder: [**WARNING**] discarding 11 atoms at position 91 in file aln_2n2a_AB.pdb. Best match rsd_type: LYS
core.io.pose_from_sfr.PoseFromSFRBuilder: [**WARNING**] discarding 10 atoms at position 92 in file aln_2n2a_AB.pdb. Best match rsd_type: ARG
core.io.pose_from_sfr.PoseFromSFRBuilder: [**WARNING**] discarding 10 atoms at position 93 in file aln_2n2a_AB.pdb. Best match rsd_type: ARG
core.io.pose_from_sfr.PoseFromSFRBuilder: [**WARNING**] discarding 6 atoms at position 94 in file aln_2n2a_AB.pdb. Best match rsd_type: GLN
core.io.pose_from_sfr.PoseFromSFRBuilder: [**WARNING**] discarding 6 atoms at position 95 in file aln_2n2a_AB.pdb. Best match rsd_type: GLN
core.io.pose_from_sfr.PoseFromSFRBuilder: [**WARNING**] discarding 11 atoms at position 96 in file aln_2n2a_AB.pdb. Best match rsd_type: LYS
core.io.pose_from_sfr.PoseFromSFRBuilder: [**WARNING**] discarding 8 atoms at position 97 in file aln_2n2a_AB.pdb. Best match rsd_type: ILE
core.io.pose_from_sfr.PoseFromSFRBuilder: [**WARNING**] discarding 10 atoms at position 98 in file aln_2n2a_AB.pdb. Best match rsd_type: ARG
core.io.pose_from_sfr.PoseFromSFRBuilder: [**WARNING**] discarding 11 atoms at position 99 in file aln_2n2a_AB.pdb. Best match rsd_type: LYS
core.io.pose_from_sfr.PoseFromSFRBuilder: [**WARNING**] discarding 2 atoms at position 100 in file aln_2n2a_AB.pdb. Best match rsd_type: TYR
core.io.pose_from_sfr.PoseFromSFRBuilder: [**WARNING**] discarding 3 atoms at position 101 in file aln_2n2a_AB.pdb. Best match rsd_type: THR
core.io.pose_from_sfr.PoseFromSFRBuilder: [**WARNING**] discarding 7 atoms at position 102 in file aln_2n2a_AB.pdb. Best match rsd_type: MET
core.io.pose_from_sfr.PoseFromSFRBuilder: [**WARNING**] discarding 10 atoms at position 103 in file aln_2n2a_AB.pdb. Best match rsd_type: ARG
core.io.pose_from_sfr.PoseFromSFRBuilder: [**WARNING**] discarding 10 atoms at position 104 in file aln_2n2a_AB.pdb. Best match rsd_type: ARG
core.io.pose_from_sfr.PoseFromSFRBuilder: [**WARNING**] discarding 8 atoms at position 105 in file aln_2n2a_AB.pdb. Best match rsd_type: LEU
core.io.pose_from_sfr.PoseFromSFRBuilder: [**WARNING**] discarding 8 atoms at position 106 in file aln_2n2a_AB.pdb. Best match rsd_type: LEU
core.io.pose_from_sfr.PoseFromSFRBuilder: [**WARNING**] discarding 6 atoms at position 107 in file aln_2n2a_AB.pdb. Best match rsd_type: GLN
core.io.pose_from_sfr.PoseFromSFRBuilder: [**WARNING**] discarding 4 atoms at position 108 in file aln_2n2a_AB.pdb. Best match rsd_type: GLU
core.io.pose_from_sfr.PoseFromSFRBuilder: [**WARNING**] discarding 3 atoms at position 109 in file aln_2n2a_AB.pdb. Best match rsd_type: THR
core.io.pose_from_sfr.PoseFromSFRBuilder: [**WARNING**] discarding 4 atoms at position 110 in file aln_2n2a_AB.pdb. Best match rsd_type: GLU
core.io.pose_from_sfr.PoseFromSFRBuilder: [**WARNING**] discarding 8 atoms at position 111 in file aln_2n2a_AB.pdb. Best match rsd_type: LEU
core.io.pose_from_sfr.PoseFromSFRBuilder: [**WARNING**] discarding 6 atoms at position 112 in file aln_2n2a_AB.pdb. Best match rsd_type: VAL
core.io.pose_from_sfr.PoseFromSFRBuilder: [**WARNING**] discarding 4 atoms at position 113 in file aln_2n2a_AB.pdb. Best match rsd_type: GLU
core.io.pose_from_sfr.PoseFromSFRBuilder: [**WARNING**] discarding 6 atoms at position 114 in file aln_2n2a_AB.pdb. Best match rsd_type: PRO
core.io.pose_from_sfr.PoseFromSFRBuilder: [**WARNING**] discarding 8 atoms at position 115 in file aln_2n2a_AB.pdb. Best match rsd_type: LEU
core.io.pose_from_sfr.PoseFromSFRBuilder: [**WARNING**] discarding 2 atoms at position 116 in file aln_2n2a_AB.pdb. Best match rsd_type: GLY:CtermProteinFull
core.conformation.Conformation: [**WARNING**] missing heavyatom: OXT on residue GLY:CtermProteinFull 58
core.conformation.Conformation: [**WARNING**] missing heavyatom: OXT on residue GLY:CtermProteinFull 116

core.pack.dunbrack.RotamerLibrary: Using Dunbrack library binary file
'/Users/andreserobian/Documents/PyRosetta4/setup/pyrosetta/database/rotamer/ExtendedOpt1-5/Dunbrack10.lib.bin'.
core.pack.dunbrack.RotamerLibrary: Dunbrack 2010 library took 0.151104 seconds to load from binary
apps.pilot.chrisk/pep_prep: Loading TOMs3m.pdb: pep anchor @ chain B seqpos 71
core.import_pose.import_pose: File 'TOMs3m.pdb' automatically determined to be of type PDB
core.io.pose_from_sfr.PoseFromSFRBuilder: [**WARNING**] PDB reader is ignoring atom 3HA in residue 10 C. Pass flag
-ignore_zero_occupancy false to change this behavior
core.io.pose_from_sfr.PoseFromSFRBuilder: [**WARNING**] PDB reader is ignoring atom 3HA in residue 18 C. Pass flag
-ignore_zero_occupancy false to change this behavior
core.io.pose_from_sfr.PoseFromSFRBuilder: [**WARNING**] PDB reader is ignoring atom 3HA in residue 22 C. Pass flag
-ignore_zero_occupancy false to change this behavior
core.io.pose_from_sfr.PoseFromSFRBuilder: [**WARNING**] discarding 1 atoms at position 117 in file TOMs3m.pdb. Best
match rsd_type: LEU:NtermProteinFull
core.io.pose_from_sfr.PoseFromSFRBuilder: [**WARNING**] discarding 1 atoms at position 118 in file TOMs3m.pdb. Best
match rsd_type: THR
core.io.pose_from_sfr.PoseFromSFRBuilder: [**WARNING**] discarding 1 atoms at position 119 in file TOMs3m.pdb. Best
match rsd_type: SER
core.io.pose_from_sfr.PoseFromSFRBuilder: [**WARNING**] discarding 1 atoms at position 120 in file TOMs3m.pdb. Best
match rsd_type: ILE
core.io.pose_from_sfr.PoseFromSFRBuilder: [**WARNING**] discarding 1 atoms at position 121 in file TOMs3m.pdb. Best
match rsd_type: ILE
core.io.pose_from_sfr.PoseFromSFRBuilder: [**WARNING**] discarding 1 atoms at position 122 in file TOMs3m.pdb. Best
match rsd_type: SER
core.io.pose_from_sfr.PoseFromSFRBuilder: [**WARNING**] discarding 1 atoms at position 126 in file TOMs3m.pdb. Best
match rsd_type: GLY
core.io.pose_from_sfr.PoseFromSFRBuilder: [**WARNING**] discarding 1 atoms at position 127 in file TOMs3m.pdb. Best
match rsd_type: ILE
core.io.pose_from_sfr.PoseFromSFRBuilder: [**WARNING**] discarding 1 atoms at position 128 in file TOMs3m.pdb. Best
match rsd_type: LEU
core.io.pose_from_sfr.PoseFromSFRBuilder: [**WARNING**] discarding 1 atoms at position 129 in file TOMs3m.pdb. Best
match rsd_type: LEU
core.io.pose_from_sfr.PoseFromSFRBuilder: [**WARNING**] discarding 1 atoms at position 133 in file TOMs3m.pdb. Best
match rsd_type: LEU
core.io.pose_from_sfr.PoseFromSFRBuilder: [**WARNING**] discarding 1 atoms at position 134 in file TOMs3m.pdb. Best
match rsd_type: GLY
core.io.pose_from_sfr.PoseFromSFRBuilder: [**WARNING**] discarding 5 atoms at position 137 in file TOMs3m.pdb. Best
match rsd_type: PHE
core.io.pose_from_sfr.PoseFromSFRBuilder: [**WARNING**] discarding 1 atoms at position 138 in file TOMs3m.pdb. Best
match rsd_type: GLY
core.io.pose_from_sfr.PoseFromSFRBuilder: [**WARNING**] discarding 1 atoms at position 139 in file TOMs3m.pdb. Best
match rsd_type: ILE
core.io.pose_from_sfr.PoseFromSFRBuilder: [**WARNING**] discarding 1 atoms at position 140 in file TOMs3m.pdb. Best
match rsd_type: LEU
core.io.pose_from_sfr.PoseFromSFRBuilder: [**WARNING**] discarding 1 atoms at position 141 in file TOMs3m.pdb. Best
match rsd_type: ILE:CtermProteinFull
core.conformation.Conformation: [**WARNING**] missing heavyatom: OXT on residue ILE:CtermProteinFull 141
core.io.pose_from_sfr.PoseFromSFRBuilder: [**WARNING**] can't find pose atom for file-residue 117 atom 3HB (trying to
store temperature in PDBInfo)
core.io.pose_from_sfr.PoseFromSFRBuilder: [**WARNING**] can't find pose atom for file-residue 118 atom 1HG (trying to
store temperature in PDBInfo)
core.io.pose_from_sfr.PoseFromSFRBuilder: [**WARNING**] can't find pose atom for file-residue 119 atom 3HB (trying to
store temperature in PDBInfo)
core.io.pose_from_sfr.PoseFromSFRBuilder: [**WARNING**] can't find pose atom for file-residue 120 atom 3HG1 (trying to
store temperature in PDBInfo)
core.io.pose_from_sfr.PoseFromSFRBuilder: [**WARNING**] can't find pose atom for file-residue 121 atom 3HG1 (trying to
store temperature in PDBInfo)

core.io.pose_from_sfr.PoseFromSFRBuilder: [**WARNING**] can't find pose atom for file-residue 122 atom 3HB (trying to store temperature in PDBInfo)

core.io.pose_from_sfr.PoseFromSFRBuilder: [**WARNING**] can't find pose atom for file-residue 127 atom 3HG1 (trying to store temperature in PDBInfo)

core.io.pose_from_sfr.PoseFromSFRBuilder: [**WARNING**] can't find pose atom for file-residue 128 atom 3HB (trying to store temperature in PDBInfo)

core.io.pose_from_sfr.PoseFromSFRBuilder: [**WARNING**] can't find pose atom for file-residue 129 atom 3HB (trying to store temperature in PDBInfo)

core.io.pose_from_sfr.PoseFromSFRBuilder: [**WARNING**] can't find pose atom for file-residue 133 atom 3HB (trying to store temperature in PDBInfo)

core.io.pose_from_sfr.PoseFromSFRBuilder: [**WARNING**] can't find pose atom for file-residue 137 atom 1HD (trying to store temperature in PDBInfo)

core.io.pose_from_sfr.PoseFromSFRBuilder: [**WARNING**] can't find pose atom for file-residue 137 atom 1HE (trying to store temperature in PDBInfo)

core.io.pose_from_sfr.PoseFromSFRBuilder: [**WARNING**] can't find pose atom for file-residue 137 atom 2HD (trying to store temperature in PDBInfo)

core.io.pose_from_sfr.PoseFromSFRBuilder: [**WARNING**] can't find pose atom for file-residue 137 atom 2HE (trying to store temperature in PDBInfo)

core.io.pose_from_sfr.PoseFromSFRBuilder: [**WARNING**] can't find pose atom for file-residue 137 atom 3HB (trying to store temperature in PDBInfo)

core.io.pose_from_sfr.PoseFromSFRBuilder: [**WARNING**] can't find pose atom for file-residue 139 atom 3HG1 (trying to store temperature in PDBInfo)

core.io.pose_from_sfr.PoseFromSFRBuilder: [**WARNING**] can't find pose atom for file-residue 140 atom 3HB (trying to store temperature in PDBInfo)

core.io.pose_from_sfr.PoseFromSFRBuilder: [**WARNING**] can't find pose atom for file-residue 141 atom 3HG1 (trying to store temperature in PDBInfo)

apps.pilot.chrisk/pep_prep: RB translation: x, y, z: -18.9369, 8.25101, 18.9872

apps.pilot.chrisk/pep_prep: RB rotation: bond, tor1, tor2: 70.1161, -32.3851, 153.285

apps.pilot.chrisk/pep_prep: peptide stub atoms: CB CA N

RB translation avg: x, y, z: -18.9369, 8.25101, 18.9872

apps.pilot.chrisk/pep_prep: Max RB translation deviation: x, y, z: 0, 0, 0

apps.pilot.chrisk/pep_prep: RB rotation avg: jump_bond_angle, jump_tor1, jump_tor2: 70.1161, -32.3851, 153.285

apps.pilot.chrisk/pep_prep: Max RB rotation deviation: jump_bond_angle, jump_tor1, jump_tor2: 0, 0, 0

core.pack.task: Packer task: initialize from command line()

core.pack.pack_rotamers: built 430 rotamers at 33 positions.

core.pack.interaction_graph.interaction_graph_factory: Instantiating DensePDInteractionGraph

core.pack.task: Packer task: initialize from command line()

core.pack.pack_rotamers: built 430 rotamers at 33 positions.

core.pack.interaction_graph.interaction_graph_factory: Instantiating DensePDInteractionGraph

core.pack.task: Packer task: initialize from command line()

core.pack.pack_rotamers: built 430 rotamers at 33 positions.

core.pack.interaction_graph.interaction_graph_factory: Instantiating DensePDInteractionGraph

core.pack.task: Packer task: initialize from command line()

core.pack.pack_rotamers: built 430 rotamers at 33 positions.

core.pack.interaction_graph.interaction_graph_factory: Instantiating DensePDInteractionGraph

core.pack.task: Packer task: initialize from command line()

core.pack.pack_rotamers: built 430 rotamers at 33 positions.

core.pack.interaction_graph.interaction_graph_factory: Instantiating DensePDInteractionGraph

core.pack.task: Packer task: initialize from command line()

core.pack.pack_rotamers: built 430 rotamers at 33 positions.

core.pack.interaction_graph.interaction_graph_factory: Instantiating DensePDInteractionGraph

core.pack.task: Packer task: initialize from command line()

core.pack.pack_rotamers: built 432 rotamers at 34 positions.

core.pack.interaction_graph.interaction_graph_factory: Instantiating DensePDInteractionGraph

core.pack.task: Packer task: initialize from command line()
core.pack.pack_rotamers: built 430 rotamers at 33 positions.
core.pack.interaction_graph.interaction_graph_factory: Instantiating DensePDInteractionGraph
core.pack.task: Packer task: initialize from command line()
core.pack.pack_rotamers: built 430 rotamers at 33 positions.
core.pack.interaction_graph.interaction_graph_factory: Instantiating DensePDInteractionGraph
apps.pilot.chrisk/pep_prep: Ignoring clash residues: 9, 11, 12, 15, 16, 18, 19, 22, 43, 44, 67, 69, 70, 71, 73, 74, 76, 77, 80, 81, 84, 85, 88, 101, 102,
fa_rep: 1418.250082789848 at S71-P117
apps.pilot.chrisk/pep_prep: Failed to resolve clash in iter 1
Initializing prep_1.pdb with aln_2n2a_AB.pdb
core.import_pose.import_pose: File 'aln_2n2a_AB.pdb' automatically determined to be of type PDB
core.io.pose_from_sfr.PoseFromSFRBuilder: [**WARNING**] discarding 4 atoms at position 1 in file aln_2n2a_AB.pdb. Best match rsd_type: ALA:NtermProteinFull
core.io.pose_from_sfr.PoseFromSFRBuilder: [**WARNING**] discarding 4 atoms at position 2 in file aln_2n2a_AB.pdb. Best match rsd_type: GLU
core.io.pose_from_sfr.PoseFromSFRBuilder: [**WARNING**] discarding 6 atoms at position 3 in file aln_2n2a_AB.pdb. Best match rsd_type: GLN
core.io.pose_from_sfr.PoseFromSFRBuilder: [**WARNING**] discarding 10 atoms at position 4 in file aln_2n2a_AB.pdb. Best match rsd_type: ARG
core.io.pose_from_sfr.PoseFromSFRBuilder: [**WARNING**] discarding 3 atoms at position 5 in file aln_2n2a_AB.pdb. Best match rsd_type: ALA
core.io.pose_from_sfr.PoseFromSFRBuilder: [**WARNING**] discarding 2 atoms at position 6 in file aln_2n2a_AB.pdb. Best match rsd_type: SER
core.io.pose_from_sfr.PoseFromSFRBuilder: [**WARNING**] discarding 6 atoms at position 7 in file aln_2n2a_AB.pdb. Best match rsd_type: PRO
core.io.pose_from_sfr.PoseFromSFRBuilder: [**WARNING**] discarding 8 atoms at position 8 in file aln_2n2a_AB.pdb. Best match rsd_type: LEU
core.io.pose_from_sfr.PoseFromSFRBuilder: [**WARNING**] discarding 3 atoms at position 9 in file aln_2n2a_AB.pdb. Best match rsd_type: THR
core.io.pose_from_sfr.PoseFromSFRBuilder: [**WARNING**] discarding 2 atoms at position 10 in file aln_2n2a_AB.pdb. Best match rsd_type: SER
core.io.pose_from_sfr.PoseFromSFRBuilder: [**WARNING**] discarding 8 atoms at position 11 in file aln_2n2a_AB.pdb. Best match rsd_type: ILE
core.io.pose_from_sfr.PoseFromSFRBuilder: [**WARNING**] discarding 8 atoms at position 12 in file aln_2n2a_AB.pdb. Best match rsd_type: ILE
core.io.pose_from_sfr.PoseFromSFRBuilder: [**WARNING**] discarding 2 atoms at position 13 in file aln_2n2a_AB.pdb. Best match rsd_type: SER
core.io.pose_from_sfr.PoseFromSFRBuilder: [**WARNING**] discarding 3 atoms at position 14 in file aln_2n2a_AB.pdb. Best match rsd_type: ALA
core.io.pose_from_sfr.PoseFromSFRBuilder: [**WARNING**] discarding 6 atoms at position 15 in file aln_2n2a_AB.pdb. Best match rsd_type: VAL
core.io.pose_from_sfr.PoseFromSFRBuilder: [**WARNING**] discarding 6 atoms at position 16 in file aln_2n2a_AB.pdb. Best match rsd_type: VAL
core.io.pose_from_sfr.PoseFromSFRBuilder: [**WARNING**] discarding 2 atoms at position 17 in file aln_2n2a_AB.pdb. Best match rsd_type: GLY
core.io.pose_from_sfr.PoseFromSFRBuilder: [**WARNING**] discarding 8 atoms at position 18 in file aln_2n2a_AB.pdb. Best match rsd_type: ILE
core.io.pose_from_sfr.PoseFromSFRBuilder: [**WARNING**] discarding 8 atoms at position 19 in file aln_2n2a_AB.pdb. Best match rsd_type: LEU
core.io.pose_from_sfr.PoseFromSFRBuilder: [**WARNING**] discarding 8 atoms at position 20 in file aln_2n2a_AB.pdb. Best match rsd_type: LEU
core.io.pose_from_sfr.PoseFromSFRBuilder: [**WARNING**] discarding 6 atoms at position 21 in file aln_2n2a_AB.pdb. Best match rsd_type: VAL
core.io.pose_from_sfr.PoseFromSFRBuilder: [**WARNING**] discarding 6 atoms at position 22 in file aln_2n2a_AB.pdb. Best match rsd_type: VAL

core.io.pose_from_sfr.PoseFromSFRBuilder: [**WARNING**] discarding 3 atoms at position 51 in file aln_2n2a_AB.pdb. Best match rsd_type: THR

core.io.pose_from_sfr.PoseFromSFRBuilder: [**WARNING**] discarding 4 atoms at position 52 in file aln_2n2a_AB.pdb. Best match rsd_type: GLU

core.io.pose_from_sfr.PoseFromSFRBuilder: [**WARNING**] discarding 8 atoms at position 53 in file aln_2n2a_AB.pdb. Best match rsd_type: LEU

core.io.pose_from_sfr.PoseFromSFRBuilder: [**WARNING**] discarding 6 atoms at position 54 in file aln_2n2a_AB.pdb. Best match rsd_type: VAL

core.io.pose_from_sfr.PoseFromSFRBuilder: [**WARNING**] discarding 4 atoms at position 55 in file aln_2n2a_AB.pdb. Best match rsd_type: GLU

core.io.pose_from_sfr.PoseFromSFRBuilder: [**WARNING**] discarding 6 atoms at position 56 in file aln_2n2a_AB.pdb. Best match rsd_type: PRO

core.io.pose_from_sfr.PoseFromSFRBuilder: [**WARNING**] discarding 8 atoms at position 57 in file aln_2n2a_AB.pdb. Best match rsd_type: LEU

core.io.pose_from_sfr.PoseFromSFRBuilder: [**WARNING**] discarding 2 atoms at position 58 in file aln_2n2a_AB.pdb. Best match rsd_type: GLY:CtermProteinFull

core.io.pose_from_sfr.PoseFromSFRBuilder: [**WARNING**] discarding 4 atoms at position 59 in file aln_2n2a_AB.pdb. Best match rsd_type: ALA:NtermProteinFull

core.io.pose_from_sfr.PoseFromSFRBuilder: [**WARNING**] discarding 4 atoms at position 60 in file aln_2n2a_AB.pdb. Best match rsd_type: GLU

core.io.pose_from_sfr.PoseFromSFRBuilder: [**WARNING**] discarding 6 atoms at position 61 in file aln_2n2a_AB.pdb. Best match rsd_type: GLN

core.io.pose_from_sfr.PoseFromSFRBuilder: [**WARNING**] discarding 10 atoms at position 62 in file aln_2n2a_AB.pdb. Best match rsd_type: ARG

core.io.pose_from_sfr.PoseFromSFRBuilder: [**WARNING**] discarding 3 atoms at position 63 in file aln_2n2a_AB.pdb. Best match rsd_type: ALA

core.io.pose_from_sfr.PoseFromSFRBuilder: [**WARNING**] discarding 2 atoms at position 64 in file aln_2n2a_AB.pdb. Best match rsd_type: SER

core.io.pose_from_sfr.PoseFromSFRBuilder: [**WARNING**] discarding 6 atoms at position 65 in file aln_2n2a_AB.pdb. Best match rsd_type: PRO

core.io.pose_from_sfr.PoseFromSFRBuilder: [**WARNING**] discarding 8 atoms at position 66 in file aln_2n2a_AB.pdb. Best match rsd_type: LEU

core.io.pose_from_sfr.PoseFromSFRBuilder: [**WARNING**] discarding 3 atoms at position 67 in file aln_2n2a_AB.pdb. Best match rsd_type: THR

core.io.pose_from_sfr.PoseFromSFRBuilder: [**WARNING**] discarding 2 atoms at position 68 in file aln_2n2a_AB.pdb. Best match rsd_type: SER

core.io.pose_from_sfr.PoseFromSFRBuilder: [**WARNING**] discarding 8 atoms at position 69 in file aln_2n2a_AB.pdb. Best match rsd_type: ILE

core.io.pose_from_sfr.PoseFromSFRBuilder: [**WARNING**] discarding 8 atoms at position 70 in file aln_2n2a_AB.pdb. Best match rsd_type: ILE

core.io.pose_from_sfr.PoseFromSFRBuilder: [**WARNING**] discarding 2 atoms at position 71 in file aln_2n2a_AB.pdb. Best match rsd_type: SER

core.io.pose_from_sfr.PoseFromSFRBuilder: [**WARNING**] discarding 3 atoms at position 72 in file aln_2n2a_AB.pdb. Best match rsd_type: ALA

core.io.pose_from_sfr.PoseFromSFRBuilder: [**WARNING**] discarding 6 atoms at position 73 in file aln_2n2a_AB.pdb. Best match rsd_type: VAL

core.io.pose_from_sfr.PoseFromSFRBuilder: [**WARNING**] discarding 6 atoms at position 74 in file aln_2n2a_AB.pdb. Best match rsd_type: VAL

core.io.pose_from_sfr.PoseFromSFRBuilder: [**WARNING**] discarding 2 atoms at position 75 in file aln_2n2a_AB.pdb. Best match rsd_type: GLY

core.io.pose_from_sfr.PoseFromSFRBuilder: [**WARNING**] discarding 8 atoms at position 76 in file aln_2n2a_AB.pdb. Best match rsd_type: ILE

core.io.pose_from_sfr.PoseFromSFRBuilder: [**WARNING**] discarding 8 atoms at position 77 in file aln_2n2a_AB.pdb. Best match rsd_type: LEU

core.io.pose_from_sfr.PoseFromSFRBuilder: [**WARNING**] discarding 8 atoms at position 78 in file aln_2n2a_AB.pdb. Best match rsd_type: LEU

core.io.pose_from_sfr.PoseFromSFRBuilder: [**WARNING**] discarding 6 atoms at position 107 in file aln_2n2a_AB.pdb.
Best match rsd_type: GLN

core.io.pose_from_sfr.PoseFromSFRBuilder: [**WARNING**] discarding 4 atoms at position 108 in file aln_2n2a_AB.pdb.
Best match rsd_type: GLU

core.io.pose_from_sfr.PoseFromSFRBuilder: [**WARNING**] discarding 3 atoms at position 109 in file aln_2n2a_AB.pdb.
Best match rsd_type: THR

core.io.pose_from_sfr.PoseFromSFRBuilder: [**WARNING**] discarding 4 atoms at position 110 in file aln_2n2a_AB.pdb.
Best match rsd_type: GLU

core.io.pose_from_sfr.PoseFromSFRBuilder: [**WARNING**] discarding 8 atoms at position 111 in file aln_2n2a_AB.pdb.
Best match rsd_type: LEU

core.io.pose_from_sfr.PoseFromSFRBuilder: [**WARNING**] discarding 6 atoms at position 112 in file aln_2n2a_AB.pdb.
Best match rsd_type: VAL

core.io.pose_from_sfr.PoseFromSFRBuilder: [**WARNING**] discarding 4 atoms at position 113 in file aln_2n2a_AB.pdb.
Best match rsd_type: GLU

core.io.pose_from_sfr.PoseFromSFRBuilder: [**WARNING**] discarding 6 atoms at position 114 in file aln_2n2a_AB.pdb.
Best match rsd_type: PRO

core.io.pose_from_sfr.PoseFromSFRBuilder: [**WARNING**] discarding 8 atoms at position 115 in file aln_2n2a_AB.pdb.
Best match rsd_type: LEU

core.io.pose_from_sfr.PoseFromSFRBuilder: [**WARNING**] discarding 2 atoms at position 116 in file aln_2n2a_AB.pdb.
Best match rsd_type: GLY:CtermProteinFull

core.conformation.Conformation: [**WARNING**] missing heavyatom: OXT on residue GLY:CtermProteinFull 58

core.conformation.Conformation: [**WARNING**] missing heavyatom: OXT on residue GLY:CtermProteinFull 116

apps.pilot.chrisk/pep_prep: Loading TOMs3m.pdb: pep anchor @ chain B seqpos 71

core.import_pose.import_pose: File 'TOMs3m.pdb' automatically determined to be of type PDB

core.io.pose_from_sfr.PoseFromSFRBuilder: [**WARNING**] PDB reader is ignoring atom 3HA in residue 10 C. Pass flag
-ignore_zero_occupancy false to change this behavior

core.io.pose_from_sfr.PoseFromSFRBuilder: [**WARNING**] PDB reader is ignoring atom 3HA in residue 18 C. Pass flag
-ignore_zero_occupancy false to change this behavior

core.io.pose_from_sfr.PoseFromSFRBuilder: [**WARNING**] PDB reader is ignoring atom 3HA in residue 22 C. Pass flag
-ignore_zero_occupancy false to change this behavior

core.io.pose_from_sfr.PoseFromSFRBuilder: [**WARNING**] discarding 1 atoms at position 117 in file TOMs3m.pdb. Best
match rsd_type: LEU:NtermProteinFull

core.io.pose_from_sfr.PoseFromSFRBuilder: [**WARNING**] discarding 1 atoms at position 118 in file TOMs3m.pdb. Best
match rsd_type: THR

core.io.pose_from_sfr.PoseFromSFRBuilder: [**WARNING**] discarding 1 atoms at position 119 in file TOMs3m.pdb. Best
match rsd_type: SER

core.io.pose_from_sfr.PoseFromSFRBuilder: [**WARNING**] discarding 1 atoms at position 120 in file TOMs3m.pdb. Best
match rsd_type: ILE

core.io.pose_from_sfr.PoseFromSFRBuilder: [**WARNING**] discarding 1 atoms at position 121 in file TOMs3m.pdb. Best
match rsd_type: ILE

core.io.pose_from_sfr.PoseFromSFRBuilder: [**WARNING**] discarding 1 atoms at position 122 in file TOMs3m.pdb. Best
match rsd_type: SER

core.io.pose_from_sfr.PoseFromSFRBuilder: [**WARNING**] discarding 1 atoms at position 126 in file TOMs3m.pdb. Best
match rsd_type: GLY

core.io.pose_from_sfr.PoseFromSFRBuilder: [**WARNING**] discarding 1 atoms at position 127 in file TOMs3m.pdb. Best
match rsd_type: ILE

core.io.pose_from_sfr.PoseFromSFRBuilder: [**WARNING**] discarding 1 atoms at position 128 in file TOMs3m.pdb. Best
match rsd_type: LEU

core.io.pose_from_sfr.PoseFromSFRBuilder: [**WARNING**] discarding 1 atoms at position 129 in file TOMs3m.pdb. Best
match rsd_type: LEU

core.io.pose_from_sfr.PoseFromSFRBuilder: [**WARNING**] discarding 1 atoms at position 133 in file TOMs3m.pdb. Best
match rsd_type: LEU

core.io.pose_from_sfr.PoseFromSFRBuilder: [**WARNING**] discarding 1 atoms at position 134 in file TOMs3m.pdb. Best
match rsd_type: GLY

core.io.pose_from_sfr.PoseFromSFRBuilder: [**WARNING**] discarding 5 atoms at position 137 in file TOMs3m.pdb. Best
match rsd_type: PHE

core.io.pose_from_sfr.PoseFromSFRBuilder: [**WARNING**] discarding 1 atoms at position 138 in file TOMs3m.pdb. Best match rsd_type: GLY

core.io.pose_from_sfr.PoseFromSFRBuilder: [**WARNING**] discarding 1 atoms at position 139 in file TOMs3m.pdb. Best match rsd_type: ILE

core.io.pose_from_sfr.PoseFromSFRBuilder: [**WARNING**] discarding 1 atoms at position 140 in file TOMs3m.pdb. Best match rsd_type: LEU

core.io.pose_from_sfr.PoseFromSFRBuilder: [**WARNING**] discarding 1 atoms at position 141 in file TOMs3m.pdb. Best match rsd_type: ILE:CtermProteinFull

core.conformation.Conformation: [**WARNING**] missing heavyatom: OXT on residue ILE:CtermProteinFull 141

core.io.pose_from_sfr.PoseFromSFRBuilder: [**WARNING**] can't find pose atom for file-residue 117 atom 3HB (trying to store temperature in PDBInfo)

core.io.pose_from_sfr.PoseFromSFRBuilder: [**WARNING**] can't find pose atom for file-residue 118 atom 1HG (trying to store temperature in PDBInfo)

core.io.pose_from_sfr.PoseFromSFRBuilder: [**WARNING**] can't find pose atom for file-residue 119 atom 3HB (trying to store temperature in PDBInfo)

core.io.pose_from_sfr.PoseFromSFRBuilder: [**WARNING**] can't find pose atom for file-residue 120 atom 3HG1 (trying to store temperature in PDBInfo)

core.io.pose_from_sfr.PoseFromSFRBuilder: [**WARNING**] can't find pose atom for file-residue 121 atom 3HG1 (trying to store temperature in PDBInfo)

core.io.pose_from_sfr.PoseFromSFRBuilder: [**WARNING**] can't find pose atom for file-residue 122 atom 3HB (trying to store temperature in PDBInfo)

core.io.pose_from_sfr.PoseFromSFRBuilder: [**WARNING**] can't find pose atom for file-residue 127 atom 3HG1 (trying to store temperature in PDBInfo)

core.io.pose_from_sfr.PoseFromSFRBuilder: [**WARNING**] can't find pose atom for file-residue 128 atom 3HB (trying to store temperature in PDBInfo)

core.io.pose_from_sfr.PoseFromSFRBuilder: [**WARNING**] can't find pose atom for file-residue 129 atom 3HB (trying to store temperature in PDBInfo)

core.io.pose_from_sfr.PoseFromSFRBuilder: [**WARNING**] can't find pose atom for file-residue 133 atom 3HB (trying to store temperature in PDBInfo)

core.io.pose_from_sfr.PoseFromSFRBuilder: [**WARNING**] can't find pose atom for file-residue 137 atom 1HD (trying to store temperature in PDBInfo)

core.io.pose_from_sfr.PoseFromSFRBuilder: [**WARNING**] can't find pose atom for file-residue 137 atom 1HE (trying to store temperature in PDBInfo)

core.io.pose_from_sfr.PoseFromSFRBuilder: [**WARNING**] can't find pose atom for file-residue 137 atom 2HD (trying to store temperature in PDBInfo)

core.io.pose_from_sfr.PoseFromSFRBuilder: [**WARNING**] can't find pose atom for file-residue 137 atom 2HE (trying to store temperature in PDBInfo)

core.io.pose_from_sfr.PoseFromSFRBuilder: [**WARNING**] can't find pose atom for file-residue 137 atom 3HB (trying to store temperature in PDBInfo)

core.io.pose_from_sfr.PoseFromSFRBuilder: [**WARNING**] can't find pose atom for file-residue 139 atom 3HG1 (trying to store temperature in PDBInfo)

core.io.pose_from_sfr.PoseFromSFRBuilder: [**WARNING**] can't find pose atom for file-residue 140 atom 3HB (trying to store temperature in PDBInfo)

core.io.pose_from_sfr.PoseFromSFRBuilder: [**WARNING**] can't find pose atom for file-residue 141 atom 3HG1 (trying to store temperature in PDBInfo)

apps.pilot.chrisk/pep_prep: RB translation: x, y, z: -18.9369, 8.25101, 18.9872

apps.pilot.chrisk/pep_prep: RB rotation: bond, tor1, tor2: 70.1161, -32.3851, 153.285

apps.pilot.chrisk/pep_prep: peptide stub atoms: CB CA N

RB translation avg: x, y, z: -18.9369, 8.25101, 18.9872

apps.pilot.chrisk/pep_prep: Max RB translation deviation: x, y, z: 0, 0, 0

apps.pilot.chrisk/pep_prep: RB rotation avg: jump_bond_angle, jump_tor1, jump_tor2: 70.1161, -32.3851, 153.285

apps.pilot.chrisk/pep_prep: Max RB rotation deviation: jump_bond_angle, jump_tor1, jump_tor2: 0, 0, 0

core.pack.task: Packer task: initialize from command line()

core.pack.pack_rotamers: built 430 rotamers at 33 positions.

core.pack.interaction_graph.interaction_graph_factory: Instantiating DensePDInteractionGraph

core.pack.task: Packer task: initialize from command line()

core.pack.pack_rotamers: built 428 rotamers at 32 positions.

core.pack.interaction_graph.interaction_graph_factory: Instantiating DensePDInteractionGraph
core.pack.task: Packer task: initialize from command line()
core.pack.pack_rotamers: built 428 rotamers at 32 positions.
core.pack.interaction_graph.interaction_graph_factory: Instantiating DensePDInteractionGraph
core.pack.task: Packer task: initialize from command line()
core.pack.pack_rotamers: built 428 rotamers at 32 positions.
core.pack.interaction_graph.interaction_graph_factory: Instantiating DensePDInteractionGraph
core.pack.task: Packer task: initialize from command line()
core.pack.pack_rotamers: built 428 rotamers at 32 positions.
core.pack.interaction_graph.interaction_graph_factory: Instantiating DensePDInteractionGraph
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core.pack.task: Packer task: initialize from command line()
core.pack.pack_rotamers: built 430 rotamers at 33 positions.
apps.pilot.chrisk/pep_prep: Ignoring clash residues: 9, 11, 12, 15, 16, 18, 19, 22, 43, 44, 67, 69, 70, 71, 73, 74, 76, 77, 80, 81, 84, 85, 88, 101, 102,
fa_rep: 419.8969709986635 at S71-P117
apps.pilot.chrisk/pep_prep: Failed to resolve clash in iter 1
Initializing prep_1.pdb with aln_2n2a_AB.pdb
core.import_pose.import_pose: File 'aln_2n2a_AB.pdb' automatically determined to be of type PDB
core.io.pose_from_sfr.PoseFromSFRBuilder: [**WARNING**] discarding 4 atoms at position 1 in file aln_2n2a_AB.pdb. Best match rsd_type: ALA:NtermProteinFull
core.io.pose_from_sfr.PoseFromSFRBuilder: [**WARNING**] discarding 4 atoms at position 2 in file aln_2n2a_AB.pdb. Best match rsd_type: GLU
core.io.pose_from_sfr.PoseFromSFRBuilder: [**WARNING**] discarding 6 atoms at position 3 in file aln_2n2a_AB.pdb. Best match rsd_type: GLN
core.io.pose_from_sfr.PoseFromSFRBuilder: [**WARNING**] discarding 10 atoms at position 4 in file aln_2n2a_AB.pdb. Best match rsd_type: ARG
core.io.pose_from_sfr.PoseFromSFRBuilder: [**WARNING**] discarding 3 atoms at position 5 in file aln_2n2a_AB.pdb. Best match rsd_type: ALA
core.io.pose_from_sfr.PoseFromSFRBuilder: [**WARNING**] discarding 2 atoms at position 6 in file aln_2n2a_AB.pdb. Best match rsd_type: SER
core.io.pose_from_sfr.PoseFromSFRBuilder: [**WARNING**] discarding 6 atoms at position 7 in file aln_2n2a_AB.pdb. Best match rsd_type: PRO
core.io.pose_from_sfr.PoseFromSFRBuilder: [**WARNING**] discarding 8 atoms at position 8 in file aln_2n2a_AB.pdb. Best match rsd_type: LEU
core.io.pose_from_sfr.PoseFromSFRBuilder: [**WARNING**] discarding 3 atoms at position 9 in file aln_2n2a_AB.pdb. Best match rsd_type: THR
core.io.pose_from_sfr.PoseFromSFRBuilder: [**WARNING**] discarding 2 atoms at position 10 in file aln_2n2a_AB.pdb. Best match rsd_type: SER
core.io.pose_from_sfr.PoseFromSFRBuilder: [**WARNING**] discarding 8 atoms at position 11 in file aln_2n2a_AB.pdb. Best match rsd_type: ILE
core.io.pose_from_sfr.PoseFromSFRBuilder: [**WARNING**] discarding 8 atoms at position 12 in file aln_2n2a_AB.pdb. Best match rsd_type: ILE
core.io.pose_from_sfr.PoseFromSFRBuilder: [**WARNING**] discarding 2 atoms at position 13 in file aln_2n2a_AB.pdb. Best match rsd_type: SER

core.io.pose_from_sfr.PoseFromSFRBuilder: [**WARNING**] discarding 3 atoms at position 14 in file aln_2n2a_AB.pdb. Best match rsd_type: ALA

core.io.pose_from_sfr.PoseFromSFRBuilder: [**WARNING**] discarding 6 atoms at position 15 in file aln_2n2a_AB.pdb. Best match rsd_type: VAL

core.io.pose_from_sfr.PoseFromSFRBuilder: [**WARNING**] discarding 6 atoms at position 16 in file aln_2n2a_AB.pdb. Best match rsd_type: VAL

core.io.pose_from_sfr.PoseFromSFRBuilder: [**WARNING**] discarding 2 atoms at position 17 in file aln_2n2a_AB.pdb. Best match rsd_type: GLY

core.io.pose_from_sfr.PoseFromSFRBuilder: [**WARNING**] discarding 8 atoms at position 18 in file aln_2n2a_AB.pdb. Best match rsd_type: ILE

core.io.pose_from_sfr.PoseFromSFRBuilder: [**WARNING**] discarding 8 atoms at position 19 in file aln_2n2a_AB.pdb. Best match rsd_type: LEU

core.io.pose_from_sfr.PoseFromSFRBuilder: [**WARNING**] discarding 8 atoms at position 20 in file aln_2n2a_AB.pdb. Best match rsd_type: LEU

core.io.pose_from_sfr.PoseFromSFRBuilder: [**WARNING**] discarding 6 atoms at position 21 in file aln_2n2a_AB.pdb. Best match rsd_type: VAL

core.io.pose_from_sfr.PoseFromSFRBuilder: [**WARNING**] discarding 6 atoms at position 22 in file aln_2n2a_AB.pdb. Best match rsd_type: VAL

core.io.pose_from_sfr.PoseFromSFRBuilder: [**WARNING**] discarding 6 atoms at position 23 in file aln_2n2a_AB.pdb. Best match rsd_type: VAL

core.io.pose_from_sfr.PoseFromSFRBuilder: [**WARNING**] discarding 8 atoms at position 24 in file aln_2n2a_AB.pdb. Best match rsd_type: LEU

core.io.pose_from_sfr.PoseFromSFRBuilder: [**WARNING**] discarding 2 atoms at position 25 in file aln_2n2a_AB.pdb. Best match rsd_type: GLY

core.io.pose_from_sfr.PoseFromSFRBuilder: [**WARNING**] discarding 6 atoms at position 26 in file aln_2n2a_AB.pdb. Best match rsd_type: VAL

core.io.pose_from_sfr.PoseFromSFRBuilder: [**WARNING**] discarding 6 atoms at position 27 in file aln_2n2a_AB.pdb. Best match rsd_type: VAL

core.io.pose_from_sfr.PoseFromSFRBuilder: [**WARNING**] discarding 2 atoms at position 28 in file aln_2n2a_AB.pdb. Best match rsd_type: PHE