Supplemental Figures:

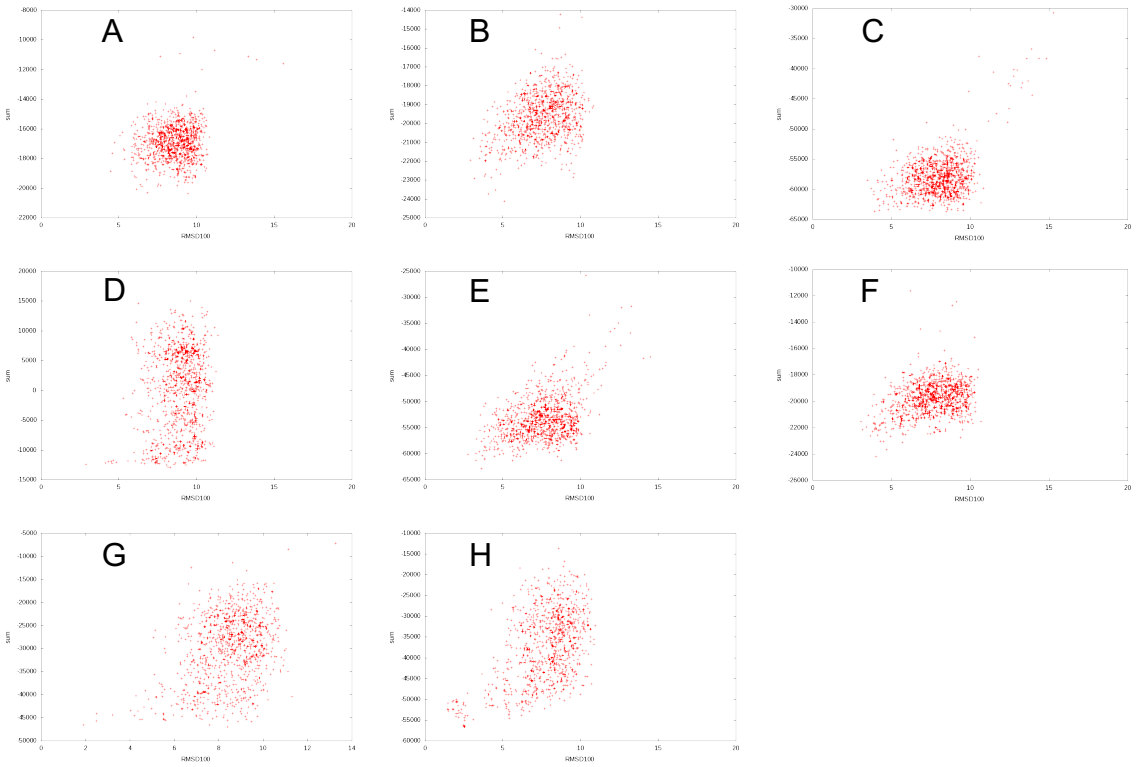


Figure S1. Related to Figure 1. Score versus RMSD100 plot for BCL::MP-Fold assembly of rhodopsin fold. (A) de novo; (B) NMR; (C) EPR; (D) EM; (E) EM_NMR; (F) NMR_EPR; (G) EM_EPR; (H) EM_NMR_EPR.

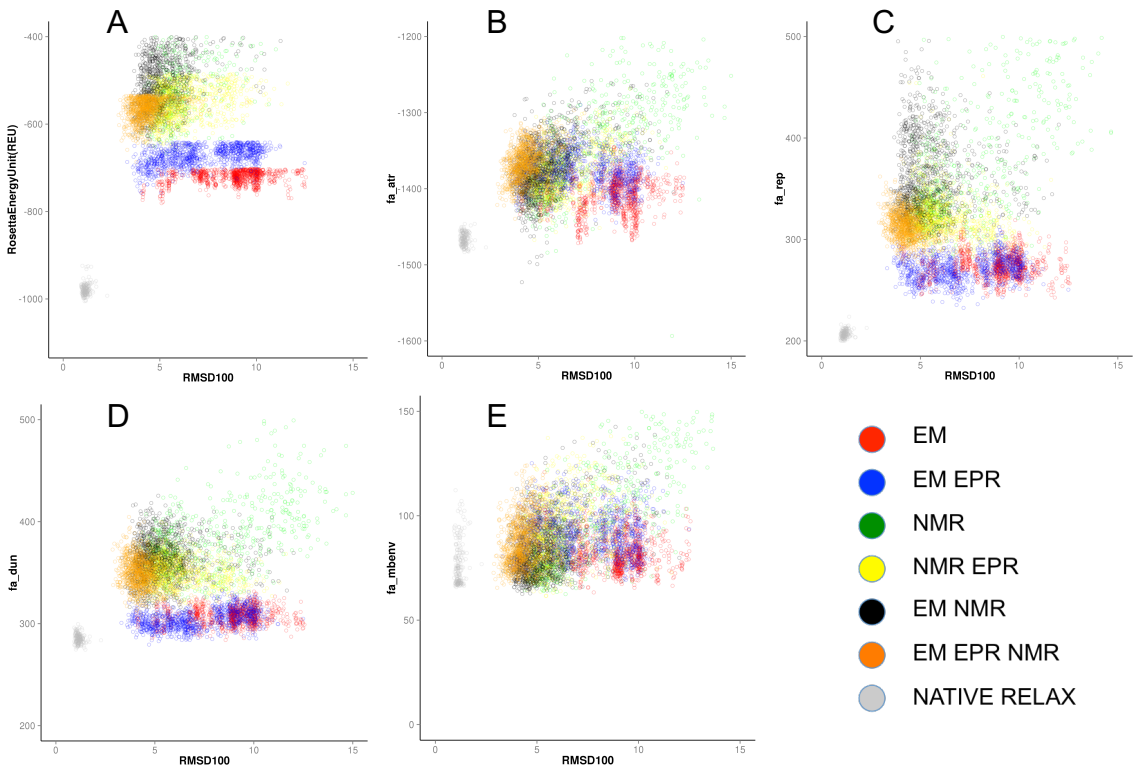


Figure S2. Related to Figure 4 and Discussion. Score versus RMSD100 in TMH for models rescored with original Rosetta membrane scores and individual score terms. fa_atr is the Lennard-Jones attractive energy between atoms in different residues; fa_rep is the Lennard-Jones repulsive energy between atoms in different residues; fa_dun is the internal energy of rotational tautomer of the sidechain, derived from Dunbrack;s statistics of protein sidechains observed in pdb; fa_mbenv is the solvation energy for residues in membrane environment based on amino acids' hydrophobicity.

| Restraint type | Atom 1 | Residue 1 | Atom 2 | Residue 2 | Evaluation Function | lb | ub | sd | Tag /rswitch |
|---|---|---|---|---|---|---|---|---|---|
| AtomPair | H | 75 | 1HG1 | 130 | BOUNDED | 0 | 5.94786 | 1 | NOE |
| AtomPair | 3HD1 | 59 | 3HD2 | 77 | BOUNDED | 0 | 5.33137 | 1 | NOE |
| AtomPair | 2HD1 | 131 | 1HG1 | 254 | BOUNDED | 0 | 4.62996 | 1 | NOE |
| AtomPair | 3HD1 | 76 | 1HD1 | 131 | BOUNDED | 0 | 4.93543 | 1 | NOE |
| AtomPair | 3HG2 | 63 | 3HD2 | 77 | BOUNDED | 0 | 5.92617 | 1 | NOE |
| AtomPair | 2HD1 | 133 | 1HG1 | 218 | BOUNDED | 0 | 4.05534 | 1 | NOE |
| AtomPair | 1HD2 | 125 | 3HD2 | 262 | BOUNDED | 0 | 5.8083 | 1 | NOE |
| AtomPair | 3HG1 | 139 | 3HG2 | 230 | BOUNDED | 0 | 4.66986 | 1 | NOE |
| AtomPair | 2HG2 | 129 | H | 219 | BOUNDED | 0 | 3.95145 | 1 | NOE |
| AtomPair | 1HG1 | 130 | H | 156 | BOUNDED | 0 | 5.00824 | 1 | NOE |
| AtomPair | 3HG1 | 209 | 3HD1 | 214 | BOUNDED | 0 | 5.63787 | 1 | NOE |
| AtomPair | H | 260 | 1HD1 | 305 | BOUNDED | 0 | 4.45914 | 1 | NOE |
| AtomPair | 1HG2 | 129 | H | 219 | BOUNDED | 0 | 5.48106 | 1 | NOE |
| AtomPair | 1HD1 | 128 | 3HD1 | 219 | BOUNDED | 0 | 4.94971 | 1 | NOE |
| AtomPair | 1HD2 | 72 | 3HG2 | 250 | BOUNDED | 0 | 5.42105 | 1 | NOE |
| AtomPair | 2HD2 | 131 | 3HG2 | 254 | BOUNDED | 0 | 4.32513 | 1 | NOE |
| AtomPair | 3HD1 | 131 | H | 254 | BOUNDED | 0 | 5.35469 | 1 | NOE |
| AtomPair | 2HG1 | 139 | H | 230 | BOUNDED | 0 | 4.91498 | 1 | NOE |
| AtomPair | 2HD1 | 75 | 2HG2 | 130 | BOUNDED | 0 | 5.69671 | 1 | NOE |
| AtomPair | 1HD2 | 72 | 1HG1 | 250 | BOUNDED | 0 | 4.5216 | 1 | NOE |
| AtomPair | H | 51 | 1HG2 | 87 | BOUNDED | 0 | 4.4161 | 1 | NOE |
| AtomPair | 2HD2 | 50 | 1HG2 | 304 | BOUNDED | 0 | 4.84477 | 1 | NOE |
| AtomPair | H | 47 | 1HG2 | 300 | BOUNDED | 0 | 5.80309 | 1 | NOE |
| AtomPair | 3HD1 | 219 | 2HG2 | 258 | BOUNDED | 0 | 3.0854 | 1 | NOE |

Table S1. Sample NMR restraints used in Rhodopsin fold determination. Related to STAR Methods section, “Integral membrane protein structure refinement using combined experimental restraints and Rosetta”. NMR restraints were specified in a line-based file. AtomPair specifies the type of restraint to be used, followed by atom name and residue number of the first and second atom. BOUNDED term is used to set the restraint evaluation for calculating a bounded penalty. The lb an ub define the lower and upper bound of the NOE distances, while sd defines the standard deviation of distances. The tag is optional input to specify a rsswitch term, when tag is not numeric, the rswitch is set to default of 0.5.

| Restraint type | Atom 1 | Residue 1 | Atom 2 | Residue 2 | Evaluation Function | EPR descript | Distance value | Weight | Bin size |
|---|---|---|---|---|---|---|---|---|---|
| AtomPair | CB | 5 | CB | 215 | SPLINE | EPR_DISTANCE | 31.6286 | 1 | 0.5 |
| AtomPair | CB | 13 | CB | 210 | SPLINE | EPR_DISTANCE | 32.5877 | 1 | 0.5 |
| AtomPair | CB | 35 | CB | 241 | SPLINE | EPR_DISTANCE | 56.7064 | 1 | 0.5 |
| AtomPair | CB | 39 | CB | 293 | SPLINE | EPR_DISTANCE | 9.27139 | 1 | 0.5 |
| AtomPair | CB | 41 | CB | 159 | SPLINE | EPR_DISTANCE | 35.8508 | 1 | 0.5 |
| AtomPair | CB | 42 | CB | 136 | SPLINE | EPR_DISTANCE | 41.8808 | 1 | 0.5 |
| AtomPair | CB | 57 | CB | 295 | SPLINE | EPR_DISTANCE | 22.5476 | 1 | 0.5 |
| AtomPair | CB | 58 | CB | 223 | SPLINE | EPR_DISTANCE | 25.2647 | 1 | 0.5 |
| AtomPair | CB | 70 | CB | 221 | SPLINE | EPR_DISTANCE | 22.281 | 1 | 0.5 |
| AtomPair | CB | 72 | CB | 128 | SPLINE | EPR_DISTANCE | 11.9059 | 1 | 0.5 |
| AtomPair | CB | 78 | CB | 299 | SPLINE | EPR_DISTANCE | 13.5557 | 1 | 0.5 |
| AtomPair | CB | 81 | CB | 263 | SPLINE | EPR_DISTANCE | 22.6959 | 1 | 0.5 |
| AtomPair | CB | 91 | CB | 165 | SPLINE | EPR_DISTANCE | 19.359 | 1 | 0.5 |
| AtomPair | CB | 97 | CB | 285 | SPLINE | EPR_DISTANCE | 13.7844 | 1 | 0.5 |
| AtomPair | CB | 115 | CB | 291 | SPLINE | EPR_DISTANCE | 18.7978 | 1 | 0.5 |
| AtomPair | CB | 116 | CB | 205 | SPLINE | EPR_DISTANCE | 23.0765 | 1 | 0.5 |
| AtomPair | CB | 131 | CB | 261 | SPLINE | EPR_DISTANCE | 11.0256 | 1 | 0.5 |
| AtomPair | CB | 131 | CB | 291 | SPLINE | EPR_DISTANCE | 25.1033 | 1 | 0.5 |
| AtomPair | CB | 135 | CB | 167 | SPLINE | EPR_DISTANCE | 23.5482 | 1 | 0.5 |
| AtomPair | CB | 140 | CB | 226 | SPLINE | EPR_DISTANCE | 7.02843 | 1 | 0.5 |
| AtomPair | CB | 158 | CB | 212 | SPLINE | EPR_DISTANCE | 21.0541 | 1 | 0.5 |
| AtomPair | CB | 162 | CB | 249 | SPLINE | EPR_DISTANCE | 29.4457 | 1 | 0.5 |
| AtomPair | CB | 200 | CB | 301 | SPLINE | EPR_DISTANCE | 30.2289 | 1 | 0.5 |
| AtomPair | CB | 213 | CB | 267 | SPLINE | EPR_DISTANCE | 16.8667 | 1 | 0.5 |
| AtomPair | CB | 230 | CB | 290 | SPLINE | EPR_DISTANCE | 37.2075 | 1 | 0.5 |
| AtomPair | CB | 247 | CB | 306 | SPLINE | EPR_DISTANCE | 16.5986 | 1 | 0.5 |
| AtomPair | CB | 274 | CB | 300 | SPLINE | EPR_DISTANCE | 26.0892 | 1 | 0.5 |

Table S2. Sample EPR restraints used in Rhodopsin fold determination. Related to STAR Methods section, “Integral membrane protein structure refinement using combined experimental restraints and Rosetta”. EPR DEER distance restraints were specified in a line-based file, AtomPair specifies the type of restraint to be used, followed by atom name and residue number of the first and second atom. SPLINE and EPR_DISTANCE would specify the program read in a histogram file and create cubic spline for the RosettaEPR knowledge-based potential. Experimental distances are set in the next column. Weight sets the numerical multiplier for the score term when linearly adding it to the total energy evaluation. Bin size set the histogram bins, in this case, distances are evaluated by a 0.5Å bin.

## Method S1, related to STAR Methods

We documented the protocol for structure determination using hybrid experimental restraints using BCL::MP-Fold and Rosetta frame work. command lines used for generating the test restraint sets for structure determination and model production using the two stage BCL::MP-Fold and Rosetta structure prediction suite. The following steps were taken to prepare the simulated restraints files used in each stage of the pipeline and running structural prediction with experimental data in BCL::MP-Fold and Rosetta

| Step | Text | Commands | Comments |
|---|---|---|---|
| 1. Simulate EPR DEER distance restraints | EPR distance restraints were simulated using BCL by first predicting the optimum a.a. pairs, then simulating spin label distances with uncertainty added. | 1.1 bcl.exe restraint:OptimizeDataSetPairwise<br>-fasta 1GZM.fasta<br>-pool secondary_structure.pool<br>-exclude_residue_types GLYCINE<br>-restaint_distance_structures native.ls<br>-read_mutates_start mutate_start.table<br>-read_mutates_optimization mutate_opt.table<br>-read_scores_optimization score_opt_bipolar.table<br>-read_mutates_end mutate_end.table<br>-nmodels 100 -mc_number_iterations 10000<br><br>1.2 bcl.exe restraint:SimulateDistances<br>-pdb 1GZM.pdb<br>-skip_undefined_aas<br>-simulate_distance_restraints<br>-add_distance_uncertainty sl-cb_distances.histograms<br>-output_file 1GZM.epr_cst_bcl<br>-restraint_list restraint.ls | 1.1 The OptimizeDataSetPairwise outputs the set of amino acid pairing in the protein sequence and a score for the set.<br>Input:<br>1GZM.fasta #fasta file<br>secondary_structure.pool #secondary structure pool<br>native.ls #directory to native pdb<br>mutate_start.table #specify number of restraint set<br>Output:<br>bcl.data #table of optimized set of EPR spin labeling a.a. pairs<br><br>1.2 SimulateDistances outputs the EPR distance restraints of the given sets of a.a. pairs.<br>Input:<br>1GZM.pdb #native pdb<br>sl-cb_distances.histograms #spin label to $C_{beta}$ distance histogram used to simulate uncertainty<br>restraint.ls #table of a.a. pairs from step 1.1.<br>Output:<br>1GZM.epr_cst_bcl #EPR distance file |
| 2. Simulate NMR restraints | Sparse NMR restraints were simulated as NOEs as 1 restraint per a.a. residue using BCL. When NMR restraints were used in folding, secondary structure information predicted from backbone chemical shift simulated by TALOS+ was also incorporated. | 2.1 bcl.exe restraint:SimulateDistances<br>-pdb 1GZM.pdb<br>-simulate_nmr_distance_restraints<br>-num_restraint_fraction 1<br>-output_file 1GZM.noe_star<br>-aaclass AAComplete<br>-add_distance_uncertainty<br>noe_knowledge_based.histogram<br><br>2.2.1 chemical shift simulation were done using SPARTA+ server<br><br>2.2.2 bcl.exe protein:CreatSSEPool<br>-prefix 1GZM<br>-pool_min_sse_length 9 5 999<br>-ssmethod TALOS<br>-factory SSPredThreshold<br>-join_separate | 2.1 SimulateDistances outputs the NOE distance restraints by randomly picking 1 restraint per residue.<br>Input:<br>1GZM.pdb #native pdb (protonated)<br>noe_knowledge_based.histogram # histogram used to add NOE distance uncertainty.<br>Output:<br>1GZM.noe_star #restraint in NMR-STAR 3.1 file formate<br>2.2.1 Input:1GZM.pdb 1GZM.fasta<br>Output: 1GZMSS.tab<br>2.2.2 Input:1GZM.fasta 1GZMSS.tab from step 2.2.1<br>Output: 1GZM.TALOS.pool #SSE pool for BCL folding |
| 3. Prepare input files for BCL fold | Other input files such as TM and secondary structure prediction pool were prepared using octopus and JUFO9D. Stage file were used to guide prediction with different experimental data in each BCL phases of assembly and refinement. Score weights files were adjusted to | 3.1.1 Perform SSE prediction using Octopus and JUFO9D<br><br>3.1.2 bcl.exe protein:CreatSSEPool<br>-prefix 1GZM<br>-pool_min_sse_length 9 5 999<br>-ssmethod SSE_prediction_method<br>-factory SSPredThreshold<br><br>3.2 Generate Stage file and corresponding scoring function weight set file for each stage specified by stage file | 3.1.1<br>Input: 1GZM.fasta<br>Output: SSE prediction file such as *.jufo9d<br>And *.octo_topo<br>2.1.2.<br>Input: SSE prediction files with the same prefix '1GZM'<br>Output: *.pool #SSE pool<br>3.2 See sample file format below. |

| | | | |
|---|---|---|---|
| | account for different restraint's presence. | | |
| 4. Running BCL::MP-fold with hybrid experimental restraints | Running BCL:MP-Fold using the membrane environment and experimental restraints. The command line utilizes the files prepared in previous steps. Sections in '-restraint_types' and '-body_restraint' points to the BCL modules that could be mixed and matched to use different types of restraints. | bcl.exe protein:Fold<br>-stages_read stages.txt<br>-mc_temperature_fraction 0.25 0.05<br>-native 1GZM.pdb<br>-quality RMSD GDT_TS -superimpose RMSD<br>-pool_separate 1<br>-pool_min_sse_lengths 5 999<br>-sspred JUFO9D OCTOPUS TALOS<br>-sequence_data /directory_to_SSE_prediction_data/ 1GZM<br>-pool_prefix 1GZM -pool 1GZM.SSPredHighest_TALOS.pool<br>-membrane<br>-tm_helices 1GZM.SSPredHighest_OCTOPUS.pool<br><br>-restraint_types NOE DistanceEPR<br>-restraint_prefix 1GZM<br><br>-body_restraint 1GZM_body.pdb 2.5 2.5 5.0 5.0 -1.0<br>-print_body_assignment<br>-score_density_connectivity 1GZM.mrc<br><br>-nmodels *<br>-prefix prefix_for_output_pdbs<br>-protein_storage /directory_to_save_models/<br>-random_seed | Input:<br>stage.txt #Stage file<br>1GZM.pdb #native pdb<br>1GZM.SSPredHighest_OCTOPUS.pool #TM helices to guide membrane positioning<br>1GZM_body.pdb #body restraint pdb to guide EM fold movers<br>1GZM.mrc #EM density file<br><br>Output:<br>prefix_for_output_pdbs.pdb |
| 5. Running Rosetta loop modeling with hybrid experimental restraints | Rosetta takes the coarse-grained models produced in previous BCL stage and models their loops and atomic details.<br>Several preparations steps needs to be taken to generate fragment files and restraints | 5.1.1 fragment_picker.default.linuxgccrelease<br>-database /rosetta/main/database/<br>-in::file::vall /rosetta/tools/fragment_tools/vall.jul19.2011.gz<br>-frags::n_frags 200<br>-frags::frag_sizes 3 9<br>-frags::sigmoid_cs_A 2<br>-frags::sigmoid_cs_B 4<br>-out::file::frag_prefix.score<br>-frags::describe_fragments 1GZM.fsc.score<br>-frags::scoring::config scores.score.cfg<br>-in:file:fasta 1GZM.fasta<br>-in:file:talos_cs 1GZM.talos<br>-frags::ss_pred predSS.tab talos<br>-in::file::talos_phi_psi pred.tab<br><br>5.1.2 Prepare loop definition files<br><br>5.1.3 Prepare TM definition files<br>/rosetta/tools/membrane_tools/octopus2span.pl 1GZM. octo_topo<br><br>5.1.4 Prepare Rosetta Format restraint files<br>bcl.exe restraint:NmrFileConvert<br>-pdb_file 1GZM.pdb<br>-input_file 1GZM.noe_star star noe<br>-output_file 1GZM_nmr.cst ROSETTA<br><br>5.2 loopmodel.linuxgccrelease<br>-database /rosetta/main/database/<br>-in:file:s 1GZM_bcl.pdb<br>-loops:loop_file 1GZM.loops<br>-in:file:native 1GZM.pdb<br>-evaluation:rmsd NATIVE _FULL FULL<br>-evaluation:gdtmm<br><br>-loops::frag_sizes 9 3 1 | 5.1.1<br>Input: vall database installed in rosetta<br>1GZM.fasta<br>1GZM.talos #chemical shift predicted from Sparta+<br>Output:<br>aa1GZM09_05.200_v1_3 #3mer fragments<br>aa1GZM09_05.200_v1_9 #9mer fragments<br>5.1.2<br>example loop file format:<br>LOOP 1 22 0 0.0 0<br>#1st and 2nd column indicates start and end of loop residues to be modeled<br>5.1.3<br>Input: 1GZM.octo_topo #from step 3.1.1<br>Output: 1GZM.span<br>5.1.4<br>Input: 1GZM.noe_star #step 2.1<br>Output: 1GZM_nmr.cst # restraints in Rosetta format<br>5.2<br>Input:<br>1GZM_bcl.pdb #bcl models that will be further refined by rosetta<br>1GZM.loops #step 5.1.2<br>1GZM.pdb #native pdb<br>aa1GZM09_05.200_v1_3 #step 5.1.1<br>aa1GZM09_05.200_v1_9 #step 5.1.1<br>1GZM_centroid_restraint.cst #step 5.1.4<br>1GZM_full_atom.cst #step 5.1.4<br>1GZM.mrc #EM density file |

| | | | |
|---|---|---|---|
| | | -loops::frag_files aa1GZM09_05.200_v1_3 aa1GZM03_05.200_v1_3 none<br>-loops::remodel quick_ccd<br>-loops::intermedrelax no<br>-loops::refine refine_ccd<br>-loops::relax fastrelax<br>-ex1<br>-ex2<br><br>-constraints:cst_file 1GZM_centroid_restraint.cst<br>-constraints:cst_weight 5.0<br>-constraints:cst_fa_file 1GZM_full_atom.cst<br>-constraints:cst_fa_weight 5<br>-constraints:epr_distance<br>-constraints:viol<br>-constraints:viol_level 101<br><br>-edensity::mapfile 1GZM.mrc<br>-edensity::sliding_window 9<br>-edensity::mapreso 5.5<br>-edensity::grid_spacing 4.0<br>-whole_structure_allatom_wt 0.1<br><br>-score:weights membrane_highres_Menv_smooth.wts<br>-membrane:no_interpolate_Mpair<br>-membrane:Menv_penalties<br>-in:file:spanfile 1GZM.span<br><br>-out:pdb<br>-out:output<br>-out:file:scorefile score_file.sc<br>-out:nstruct *<br>-out:prefix /directory_to_save_models/prefix | 1GZM.span #step 5.1.3<br>Output:<br>score_file.sc #score file<br>/directory_to_save_models/prefix.pdb #models produced by loopmodeling |
| 6. Running Rosetta refinement with hybrid experimental restraints | A final refinement step was used to relax the predicted model to their energy minimum using the Rosetta relax application. Top scoring models from loop modeling were taken | 6 relax.linuxgccrelease<br>-database /rosetta/main/database/<br>-in:file:s 1GZM_loopmodeled.pdb<br>-in:file:fullatom<br>-in:file:native 1GZM.pdb<br>-evaluation:rmsd NATIVE _FULL FULL<br>-evaluation:gdtmm<br>-relax:fast<br>-relax:membrane<br>-ex1<br>-ex2<br><br>-constraints:cst_fa_file 1GZM_full_atom.cst<br>-constraints:cst_fa_weight 5<br>-constraints:epr_distance<br>-constraints:viol<br>-constraints:viol_level 101<br><br>-edensity::mapfile 1GZM.mrc<br>-edensity::sliding_window 9<br>-edensity::mapreso 5.5<br>-edensity::grid_spacing 4.0<br>-whole_structure_allatom_wt 0.1<br><br>-score:weights membrane_highres_Menv_smooth.wts<br>-membrane:no_interpolate_Mpair<br>-membrane:Menv_penalties<br>-in:file:spanfile 1GZM.span<br><br>-out:pdb<br>-out:output<br>-out:file:scorefile score_file.sc<br>-out:nstruct *<br>-out:prefix /directory_to_save_models/prefix | 6<br>Input:<br>1GZM_loopmodeled.pdb #best scoring models after loop modeling<br>1GZM.pdb #native pdb<br>aa1GZM09_05.200_v1_3 #step 5.1.1<br>aa1GZM09_05.200_v1_9 #step 5.1.1<br>1GZM_full_atom.cst #step 5.1.4<br>1GZM.mrc #EM density file<br>1GZM.span #step 5.1.3<br><br>Output:<br>score_file.sc #score file<br>/directory_to_save_models/prefix.pdb #models produced by relax |

*Example BCL Stage file format:*

The BCL stage files sets the parameters for BCL::MP-Fold for the specific restraints used in structure prediction. In the example file, SCORE_PROTOCOLS specifies the membrane environment and the used of distance restraint and EM density; MUTATE_PROTOCOLS specifies the particular mutate moves in the program that are tailored to efficiently sample protein conformations for the given environment.

```
NUMBER_CYCLES 1
STAGE Stage_assembly_1
        SCORE_PROTOCOLS Default Membrane Restraint EM
        SCORE_WEIGHTSET_FILE assembly_1.scoreweights
        MUTATE_PROTOCOLS Default Assembly Membrane Restraint EM
        NUMBER_ITERATIONS 2000 400
STAGE_END
STAGE Stage_assembly_2
        SCORE_PROTOCOLS Default Membrane Restraint EM
        SCORE_WEIGHTSET_FILE assembly_2.scoreweights
        MUTATE_PROTOCOLS Default Assembly Membrane Restraint EM
        NUMBER_ITERATIONS 2000 400
STAGE_END
STAGE Stage_assembly_3
        SCORE_PROTOCOLS Default Membrane Restraint EM
        SCORE_WEIGHTSET_FILE assembly_3.scoreweights
        MUTATE_PROTOCOLS Default Assembly Membrane Restraint EM
        NUMBER_ITERATIONS 2000 400
STAGE_END
STAGE Stage_assembly_4
        SCORE_PROTOCOLS Default Membrane Restraint EM
        SCORE_WEIGHTSET_FILE assembly_4.scoreweights
        MUTATE_PROTOCOLS Default Assembly Membrane Restraint EM
        NUMBER_ITERATIONS 2000 400
STAGE_END
STAGE Stage_refinement_1
        SCORE_PROTOCOLS Default Membrane Restraint EM
        SCORE_WEIGHTSET_FILE refinement_1.scoreweights
        MUTATE_PROTOCOLS Default Refinement Membrane Restraint EM
        NUMBER_ITERATIONS 2000 400
        PRINT_END_MODEL true
STAGE_END
```

*Example BCL weightset file format:*

A sample weightset file used in BCL stage is presented below. The first line corresponds to the various scoring terms used in the BCL scoring during each Monte-Carlo Metropolis minimization step. The second line corresponds to the weight for in each scoring term. Specifically, the body_agreement and connectivity score terms are EM specific; the noe_restraint, noe_penalty, ss_TALOS, ss_TALOS_ent score terms are NMR specific; the epr_distance, epr_lower_penalty, epr_upper_penalty are EPR specific. The scoreweight used in the current manuscript makes an equal contribution to the scores. It is possible for users to tweak the weightset based on the confidence of experimental data.

```
bcl::storage::Table<double> aaclash aadist aaneigh aaneigh_ent loop loop_closure_gradient rgyr sseclash ssepack_fr strand_fr co_score ss_JUFO9D ss_JUFO9D_ent ss_OCTOPUS ss_OCTOPUS_ent ssealign mp_helix_topology ss_OCTOPUS_env ss_JUFO9D_env body_agreement connectivity noe_restraint noe_penalty ss_TALOS ss_TALOS_ent epr_distance epr_lower_penalty epr_upper_penalty
weights 375 0.35 50 50 10 50000 5 375
8 20 0.5 1 1 1 1 8 500
20 5 300 450 5 5 10 10
20.0 24 24
```