

Supplementary information for:

## Macromolecular modeling and design in Rosetta: new methods and frameworks

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The main documentation page can be found at <https://www.rosettacommons.org/docs/latest/Home>.

Tutorials, demos and protocol captures are documented at <https://www.rosettacommons.org/demos/latest/Home>.

Method	Developers	Lab developed	Paper	Documentation	Protocol capture
<b>Protein prediction structure</b>					
fragment picker	Dominik Gront	(formerly David Baker), Dominik Gront	<sup>1</sup>	<a href="https://www.rosettacommons.org/docs/latest/application_documentation/utilities/app-fragment-picker">https://www.rosettacommons.org/docs/latest/application_documentation/utilities/app-fragment-picker</a>	
RosettaCM	Yifan Song	(formerly David Baker)	<sup>2</sup>	<a href="https://www.rosettacommons.org/docs/latest/application_documentation/structure_prediction/RosettaCM">https://www.rosettacommons.org/docs/latest/application_documentation/structure_prediction/RosettaCM</a>	Supp to <sup>2</sup>
iterative hybridize	Sergey Ovchinnikov, Hahnbeom Park	David Baker, Sergey Ovchinnikov	<sup>3,4</sup>	<a href="https://www.rosettacommons.org/docs/latest/IterativeHybridize">https://www.rosettacommons.org/docs/latest/IterativeHybridize</a>	
RosettaSurface	Michael Pacella	Jeffrey Gray	<sup>5-7</sup>	<a href="https://www.rosettacommons.org/docs/latest/application_documentation/docking/surface-docking">https://www.rosettacommons.org/docs/latest/application_documentation/docking/surface-docking</a>	Supp to <sup>5</sup>
<b>Protein-protein docking</b>					
RosettaDock4.0	Nick Marze, Shourya Roy Burman	Jeffrey Gray	<sup>8</sup>	<a href="https://www.rosettacommons.org/demos/latest/tutorials/Protein-Protein-Docking/Protein-Protein-Docking">https://www.rosettacommons.org/demos/latest/tutorials/Protein-Protein-Docking/Protein-Protein-Docking</a>	
Rosetta SymDock2	Shourya Roy Burman	(formerly Ingemar André), Jeffrey Gray	<sup>9</sup>	<a href="https://www.rosettacommons.org/docs/latest/SymDockProtocol">https://www.rosettacommons.org/docs/latest/SymDockProtocol</a>	
<b>Small molecule ligand docking</b>					
RosettaLigand	Sam DeLuca Darwin Fu, Shannon Smith,	Jens Meiler	<sup>10-12</sup>	<a href="https://www.rosettacommons.org/demos/latest/tutorials/ligand_docking/ligand_docking_tutorial">https://www.rosettacommons.org/demos/latest/tutorials/ligand_docking/ligand_docking_tutorial</a>	

	Rocco Moretti				
RosettaLigandEnsemble	Darwin Fu, Rocco Moretti	Jens Meiler	13	<a href="https://www.rosettacommons.org/docs/latest/scripting_documentation/RosettaScripts/Movers/movers_pages/HighResEnsembleMover">https://www.rosettacommons.org/docs/latest/scripting_documentation/RosettaScripts/Movers/movers_pages/HighResEnsembleMover</a>	
pocket optimization	David Johnson	John Karanicolas	14,15	<a href="https://www.rosettacommons.org/docs/latest/application_documentation/utilities/pocket-relax">https://www.rosettacommons.org/docs/latest/application_documentation/utilities/pocket-relax</a> <a href="https://www.rosettacommons.org/docs/latest/application_documentation/analysis/pocket-measure">https://www.rosettacommons.org/docs/latest/application_documentation/analysis/pocket-measure</a>	Supp to <sup>14,15</sup>
DARC	Ragul Gowthaman, Karen Khar	John Karanicolas	16–18	<a href="https://www.rosettacommons.org/docs/latest/application_documentation/docking/DARC">https://www.rosettacommons.org/docs/latest/application_documentation/docking/DARC</a>	Supp to <sup>16–18</sup>
<b>Protein design</b>					
SEWING	Tim Jacobs, Sharon Guffy, Frank Teets	Brian Kuhlmann	19,20	<a href="https://www.rosettacommons.org/docs/latest/scripting_documentation/RosettaScripts/composite_protocols/sewing/SEWING">https://www.rosettacommons.org/docs/latest/scripting_documentation/RosettaScripts/composite_protocols/sewing/SEWING</a>	
RosettaRemodel	Possu Huang	(formerly David Baker), Possu Huang	21	<a href="https://www.rosettacommons.org/docs/latest/application_documentation/design/rosettaremodel">https://www.rosettacommons.org/docs/latest/application_documentation/design/rosettaremodel</a>	
LooDo	Kristin Blacklock	Sagar Khare	22	<a href="https://www.rosettacommons.org/demos/latest/protocol_capture/loodo/README">https://www.rosettacommons.org/demos/latest/protocol_capture/loodo/README</a>	
RECON	Alex Sevy, Marion Sauer	Jens Meiler	23	<a href="https://www.rosettacommons.org/docs/latest/application_documentation/RECON-multistate-design">https://www.rosettacommons.org/docs/latest/application_documentation/RECON-multistate-design</a>	Supp to <sup>23</sup>
curved $\beta$ -sheet design	Enrique Marcos, Benjamin Basanta	David Baker	24	<a href="https://github.com/basantab/DeNovoCurvedSheetDesign">https://github.com/basantab/DeNovoCurvedSheetDesign</a> <a href="https://www.rosettacommons.org/docs/latest/application_documentation/design/curvedsheetdesign">https://www.rosettacommons.org/docs/latest/application_documentation/design/curvedsheetdesign</a> <a href="https://www.rosettacommons.org/docs/latest/scripting_documentation/RosettaScripts/xsd/filter_StrandCurvatureByLevels_type">https://www.rosettacommons.org/docs/latest/scripting_documentation/RosettaScripts/xsd/filter_StrandCurvatureByLevels_type</a> <a href="https://www.rosettacommons.org/docs/latest/scripting_documentation/RosettaScripts/xsd/filter_HelixBendFilter_type">https://www.rosettacommons.org/docs/latest/scripting_documentation/RosettaScripts/xsd/filter_HelixBendFilter_type</a>	
biased forward folding	Daniel Silva, Enrique Marcos	David Baker	24	<a href="https://www.rosettacommons.org/docs/latest/Biased-forward-folding">https://www.rosettacommons.org/docs/latest/Biased-forward-folding</a> <a href="https://github.com/emarcos/biased_forward_folding/">https://github.com/emarcos/biased_forward_folding/</a>	
fold_from_loops	Bruno Correia	formerly David Baker	25	<a href="https://www.rosettacommons.org/docs/latest/scripting_documentation/RosettaScripts/composite_protocols/fold_from_loops/FunFolDes">https://www.rosettacommons.org/docs/latest/scripting_documentation/RosettaScripts/composite_protocols/fold_from_loops/FunFolDes</a>	

FunFolDes	Jaume Bonet, Andreas Scheck	Bruno Correia	26	<a href="https://www.rosettacommons.org/docs/latest/scripting_documentation/RosettaScripts/composite_protocols/fold_from_loops/FunFolDes">https://www.rosettacommons.org/docs/latest/scripting_documentation/RosettaScripts/composite_protocols/fold_from_loops/FunFolDes</a>	<a href="https://github.com/lpdi-epfl/FunFolDesData">https://github.com/lpdi-epfl/FunFolDesData</a>
<b>Protein interface design</b>					
FlexDDG	Kyle Barlow, Shane O'Connor	Tanja Kortemme	27	<a href="https://www.rosettacommons.org/docs/latest/flex-ddG">https://www.rosettacommons.org/docs/latest/flex-ddG</a>	<a href="https://github.com/Kortemme-Lab/flex_ddG_tutorial">https://github.com/Kortemme-Lab/flex_ddG_tutorial</a>
Coupled Moves	Noah Ollikainen, Rene M. de Jong	Tanja Kortemme & DSM Biotechnology Center	28	<a href="https://www.rosettacommons.org/docs/latest/coupled-moves">https://www.rosettacommons.org/docs/latest/coupled-moves</a>	
Parametric design	Vikram Mulligan	(formerly David Baker) Richard Bonneau	29,30	<a href="https://www.rosettacommons.org/docs/latest/scripting_documentation/RosettaScripts/Movers/movers_pages/MakeBundleMover">https://www.rosettacommons.org/docs/latest/scripting_documentation/RosettaScripts/Movers/movers_pages/MakeBundleMover</a> <a href="https://www.rosettacommons.org/docs/latest/scripting_documentation/RosettaScripts/Movers/movers_pages/BundleGridSamplerMover">https://www.rosettacommons.org/docs/latest/scripting_documentation/RosettaScripts/Movers/movers_pages/BundleGridSamplerMover</a> <a href="https://www.rosettacommons.org/docs/latest/scripting_documentation/RosettaScripts/Movers/movers_pages/PerturbBundleMover">https://www.rosettacommons.org/docs/latest/scripting_documentation/RosettaScripts/Movers/movers_pages/PerturbBundleMover</a> <a href="https://www.rosettacommons.org/docs/latest/scripting_documentation/RosettaScripts/Filters/filter_pages/BundleReporterFilter">https://www.rosettacommons.org/docs/latest/scripting_documentation/RosettaScripts/Filters/filter_pages/BundleReporterFilter</a>	Supp to <sup>29</sup>
<b>Peptides and peptidomimetics</b>					
FlexPepDock	Barak Raveh, Nir London, Lior Zimmerman	Ora Schueler-Furman	31,32	<a href="https://www.rosettacommons.org/docs/latest/application_documentation/docking/flex-pep-dock">https://www.rosettacommons.org/docs/latest/application_documentation/docking/flex-pep-dock</a>	Supp to <sup>32</sup>
PIPER-FlexPepDock	Nawsad Alam, Alisa Khramushin	Ora Schueler-Furman	33	<a href="https://www.rosettacommons.org/docs/latest/application_documentation/docking/flex-pep-dock">https://www.rosettacommons.org/docs/latest/application_documentation/docking/flex-pep-dock</a>	
PeptiDerive	Yuval Sedan, Orly Marcu	Ora Schueler-Furman	34	<a href="https://www.rosettacommons.org/docs/latest/application_documentation/analysis/PeptiDerive">https://www.rosettacommons.org/docs/latest/application_documentation/analysis/PeptiDerive</a>	
simple_cycpep_predict	Vikram Mulligan	(formerly David Baker) Richard Bonneau	29,35,36	<a href="https://www.rosettacommons.org/docs/latest/structure_prediction/simple_cycpep_predict">https://www.rosettacommons.org/docs/latest/structure_prediction/simple_cycpep_predict</a>	Supp to <sup>35,36</sup>
MFPred	Aliza Rubenstein	Sagar Khare	37	<a href="https://www.rosettacommons.org/docs/latest/scripting_documentation/RosettaScripts/Movers/movers_pages/analysis/GenMeanFieldMover">https://www.rosettacommons.org/docs/latest/scripting_documentation/RosettaScripts/Movers/movers_pages/analysis/GenMeanFieldMover</a>	

<b>Loop modeling</b>					
NGK (next-generation KIC)	Amelie Stein	Tanja Kortemme	38	<a href="https://www.rosettacommons.org/docs/latest/application_documentation/structure_prediction/loop_modeling/next-generation-KIC">https://www.rosettacommons.org/docs/latest/application_documentation/structure_prediction/loop_modeling/next-generation-KIC</a> <a href="https://www.rosettacommons.org/docs/latest/application_documentation/structure_prediction/loop_modeling/loopmodel-kinematic(for -vicinity_sampling)">https://www.rosettacommons.org/docs/latest/application_documentation/structure_prediction/loop_modeling/loopmodel-kinematic (for -vicinity_sampling)</a>	
GenKIC (generalized KIC)	Vikram Mulligan	(formerly David Baker) Richard Bonneau	35	<a href="https://www.rosettacommons.org/docs/latest/scripting_documentation/RosettaScripts/composite_protocols/generalized_kic/GeneralizedKIC">https://www.rosettacommons.org/docs/latest/scripting_documentation/RosettaScripts/composite_protocols/generalized_kic/GeneralizedKIC</a> <a href="https://www.rosettacommons.org/docs/latest/scripting_documentation/RosettaScripts/Movers/movers_pages/GeneralizedKICMover">https://www.rosettacommons.org/docs/latest/scripting_documentation/RosettaScripts/Movers/movers_pages/GeneralizedKICMover</a> <a href="https://www.rosettacommons.org/docs/latest/scripting_documentation/RosettaScripts/composite_protocols/generalized_kic/GeneralizedKICperturber">https://www.rosettacommons.org/docs/latest/scripting_documentation/RosettaScripts/composite_protocols/generalized_kic/GeneralizedKICperturber</a> <a href="https://www.rosettacommons.org/docs/latest/scripting_documentation/RosettaScripts/composite_protocols/generalized_kic/GeneralizedKICfilter">https://www.rosettacommons.org/docs/latest/scripting_documentation/RosettaScripts/composite_protocols/generalized_kic/GeneralizedKICfilter</a> <a href="https://www.rosettacommons.org/docs/latest/scripting_documentation/RosettaScripts/composite_protocols/generalized_kic/GeneralizedKICselector">https://www.rosettacommons.org/docs/latest/scripting_documentation/RosettaScripts/composite_protocols/generalized_kic/GeneralizedKICselector</a> <a href="https://www.rosettacommons.org/demos/latest/tutorials/GeneralizedKIC/generalized_kinematic_closure_1">https://www.rosettacommons.org/demos/latest/tutorials/GeneralizedKIC/generalized_kinematic_closure_1</a> <a href="https://www.rosettacommons.org/demos/latest/tutorials/GeneralizedKIC/generalized_kinematic_closure_2">https://www.rosettacommons.org/demos/latest/tutorials/GeneralizedKIC/generalized_kinematic_closure_2</a> <a href="https://www.rosettacommons.org/demos/latest/tutorials/GeneralizedKIC/generalized_kinematic_closure_3">https://www.rosettacommons.org/demos/latest/tutorials/GeneralizedKIC/generalized_kinematic_closure_3</a> <a href="https://www.rosettacommons.org/demos/latest/tutorials/GeneralizedKIC/generalized_kinematic_closure_4">https://www.rosettacommons.org/demos/latest/tutorials/GeneralizedKIC/generalized_kinematic_closure_4</a>	Supp to <sup>29,35</sup>
LoopHashKIC	Xingjie Pan	Tanja Kortemme		<a href="https://www.rosettacommons.org/docs/latest/scripting_documentation/RosettaScripts/Movers/movers_pages/LoopModelerMover">https://www.rosettacommons.org/docs/latest/scripting_documentation/RosettaScripts/Movers/movers_pages/LoopModelerMover</a>	
Consensus_Loop_Design	Enrique Marcos, Tom Linsky	David Baker	24,39	<a href="https://www.rosettacommons.org/docs/latest/scripting_documentation/RosettaScripts/TaskOperations/taskoperations_pages/ConsensusLoopDesignOperation">https://www.rosettacommons.org/docs/latest/scripting_documentation/RosettaScripts/TaskOperations/taskoperations_pages/ConsensusLoopDesignOperation</a>	
<b>Modeling of antibodies and proteins in the immune system</b>					
RosettaAntibody	Jeliazko Jeliazkov, Nick Marze,	Jeffrey Gray	40-43	<a href="https://www.rosettacommons.org/docs/latest/application_documentation/antibody/antibody-protocol">https://www.rosettacommons.org/docs/latest/application_documentation/antibody/antibody-protocol</a>	

	Brian Weitzner, Jared Adolf-Bryfogle Sergey Lyskov, Daisuke Kuroda				
AbPredict	Christoffer Norn, Gideon Lapidoth	Sarel Fleishman	44,45	<a href="https://www.rosettacommons.org/docs/latest/application_documentation/structure_prediction/AbPredict2">https://www.rosettacommons.org/docs/latest/application_documentation/structure_prediction/AbPredict2</a>	
RosettaMHC	Santrupti Nerli	Nik Sgourakis	46	<a href="https://github.com/snerligit/mhc-pep-threader">https://github.com/snerligit/mhc-pep-threader</a>	
TCRModel	Ragul Gowthaman	Brian Pierce	47	<a href="https://www.rosettacommons.org/docs/latest/application_documentation/structure_prediction/TCRmodel">https://www.rosettacommons.org/docs/latest/application_documentation/structure_prediction/TCRmodel</a>	
SnugDock	Jeliazko Jeliazkov, Nick Marze, Brian Weitzner	Jeffrey Gray	48	<a href="https://www.rosettacommons.org/docs/latest/application_documentation/antibody/snugdock">https://www.rosettacommons.org/docs/latest/application_documentation/antibody/snugdock</a>	
RAbD (RosettaAntibodyDesign)	Jared Adolf-Bryfogle, Brian Weitzner	Bill Schief, Roland Dunbrack	49	<a href="https://www.rosettacommons.org/docs/latest/application_documentation/antibody/RosettaAntibodyDesign">https://www.rosettacommons.org/docs/latest/application_documentation/antibody/RosettaAntibodyDesign</a>	
Epitope removal	Indigo King	David Baker, Cyrus Biotechnology	50,51	<a href="https://www.rosettacommons.org/docs/latest/scripting_documentation/RosettaScripts/Movers/movers_pages/GreedyOptMutationMover">https://www.rosettacommons.org/docs/latest/scripting_documentation/RosettaScripts/Movers/movers_pages/GreedyOptMutationMover</a> <a href="https://www.rosettacommons.org/docs/latest/scripting_documentation/RosettaScripts/xsd/filter_NMerSVMEnergy_type">https://www.rosettacommons.org/docs/latest/scripting_documentation/RosettaScripts/xsd/filter_NMerSVMEnergy_type</a>	
AbDesign	Gideon Lapidoth	Sarel Fleishman	52,53	<a href="https://www.rosettacommons.org/docs/latest/scripting_documentation/RosettaScripts/Movers/movers_pages/SpliceMover">https://www.rosettacommons.org/docs/latest/scripting_documentation/RosettaScripts/Movers/movers_pages/SpliceMover</a>	
<b>Modeling experimental data</b>	<b>with</b>				
cryo-EM <i>de novo</i>	Ray Wang	Frank DiMaio, David Baker	54	<a href="https://dimaiolab.ipd.uw.edu/software/">https://dimaiolab.ipd.uw.edu/software/</a>	
cryoEM: RosettaES	Brandon Frenz	Frank DiMaio	55	<a href="https://dimaiolab.ipd.uw.edu/software/">https://dimaiolab.ipd.uw.edu/software/</a>	
cryoEM: iterative refinement	Frank DiMaio, Yifan Song	(formerly David Baker) Frank DiMaio	56,57	<a href="https://dimaiolab.ipd.uw.edu/software/">https://dimaiolab.ipd.uw.edu/software/</a>	
cryoEM: automated refinement	Ray Wang	Frank DiMaio	58	<a href="https://dimaiolab.ipd.uw.edu/software/">https://dimaiolab.ipd.uw.edu/software/</a>	

NMR: CS-Rosetta	(formerly Oliver Lange) Santrupti Nerli	Nik Sgourakis	59	<a href="https://csrosetta.chemistry.ucsc.edu/">https://csrosetta.chemistry.ucsc.edu/</a> <a href="https://github.com/RosettaCommons/csrosetta3">https://github.com/RosettaCommons/csrosetta3</a>	
PCS: PCS-Rosetta, GPS-Rosetta	Christophe Schmitz, Kala Bharath Pilla	Thomas Huber	60,61	<a href="https://www.rosettacommons.org/demos/latest/protocol_capture/gps_rosetta_pcs_nmr_constraints/README">https://www.rosettacommons.org/demos/latest/protocol_capture/gps_rosetta_pcs_nmr_constraints/README</a> <a href="https://github.com/kalabharath/pcs_driven_iterative_resampling">https://github.com/kalabharath/pcs_driven_iterative_resampling</a>	
RosettaNMR framework: using RDC/PRE/PCS/NOE/CS for ab initio, protein-protein docking, ligand docking, symmetric assembly	Georg Kuenze, Julia Koehler Leman	Jens Meiler	62	<a href="https://www.rosettacommons.org/docs/latest/application_documentation/RosettaNMR-with-Paramagnetic-Restraints">https://www.rosettacommons.org/docs/latest/application_documentation/RosettaNMR-with-Paramagnetic-Restraints</a>	Supp to <sup>62</sup>
mass-spec: HRF hydroxyl radical footprinting	Melanie Aprahamian	Steffen Lindert	63,64	<a href="https://www.rosettacommons.org/docs/latest/rosetta_basics/scoring/ms_expdata_score_terms">https://www.rosettacommons.org/docs/latest/rosetta_basics/scoring/ms_expdata_score_terms</a>	Supp to <sup>63</sup>
mass-spec: PyTXMS	Hamed Khakzad	Lars Malmstroem	65	<a href="https://zenodo.org/record/1438111#.XlQUoRNKhBw">https://zenodo.org/record/1438111#.XlQUoRNKhBw</a> <a href="https://www.rosettacommons.org/docs/latest/scripting_documentation/PyRosetta/PyTXMS">https://www.rosettacommons.org/docs/latest/scripting_documentation/PyRosetta/PyTXMS</a>	
<b>DNA and RNA</b>					
RNA applications		Rhiju Das		<a href="https://www.rosettacommons.org/docs/latest/application_documentation/rna/rna-applications">https://www.rosettacommons.org/docs/latest/application_documentation/rna/rna-applications</a>	
SWA (stepwise assembly)	Rhiju Das	Rhiju Das	66,67	<a href="https://www.rosettacommons.org/docs/latest/application_documentation/stepwise/stepwise_assembly/swa-rna-loop">https://www.rosettacommons.org/docs/latest/application_documentation/stepwise/stepwise_assembly/swa-rna-loop</a> <a href="https://www.rosettacommons.org/docs/latest/application_documentation/stepwise/stepwise_assembly/swa-protein-long-loop">https://www.rosettacommons.org/docs/latest/application_documentation/stepwise/stepwise_assembly/swa-protein-long-loop</a> <a href="https://www.rosettacommons.org/docs/latest/application_documentation/stepwise/stepwise_assembly/swa-protein-main">https://www.rosettacommons.org/docs/latest/application_documentation/stepwise/stepwise_assembly/swa-protein-main</a>	
SWM (stepwise Monte-Carlo)	Caleb Geniesse Andrew Watkins	Rhiju Das	68	<a href="https://www.rosettacommons.org/docs/latest/application_documentation/stepwise/stepwise_monte_carlo/stepwise">https://www.rosettacommons.org/docs/latest/application_documentation/stepwise/stepwise_monte_carlo/stepwise</a>	
FARFAR (fragment assembly medium resolution structure prediction)	Andrew Watkins Kalli Kappel	Rhiju Das	69-71	<a href="https://www.rosettacommons.org/docs/latest/application_documentation/rna/rna-denovo">https://www.rosettacommons.org/docs/latest/application_documentation/rna/rna-denovo</a> <a href="https://www.rosettacommons.org/docs/latest/application_documentation/rna/rnp-modeling">https://www.rosettacommons.org/docs/latest/application_documentation/rna/rnp-modeling</a>	
ERRASER (refinement into EM density maps)	Fang-Chieh Chou	Rhiju Das	72,73	<a href="https://www.rosettacommons.org/docs/latest/application_documentation/rna/erraser">https://www.rosettacommons.org/docs/latest/application_documentation/rna/erraser</a>	<a href="https://www.rosettacommons.org/demos/latest/public/erraser/README">https://www.rosettacommons.org/demos/latest/public/erraser/README</a>

CS-Rosetta-RNA (modeling with NMR data)	Parin Sripakdeevong	Rhiju Das	74	<a href="https://www.rosettacommons.org/docs/latest/application_documentation/rna/CS-Rosetta-RNA">https://www.rosettacommons.org/docs/latest/application_documentation/rna/CS-Rosetta-RNA</a>	
RECCES (Reweighting of Energy-function Collection with Conformational Ensemble Sampling)	Fang-Chieh Chou	Rhiju Das			<a href="https://www.rosettacommons.org/demos/latest/public/recces/R_EADME">https://www.rosettacommons.org/demos/latest/public/recces/R_EADME</a>
DRRAFTER ( <i>de novo</i> modeling of protein-RNA complexes into EM densities)	Kalli Kappel	Rhiju Das	75	<a href="https://www.rosettacommons.org/docs/latest/application_documentation/rna/drrafter">https://www.rosettacommons.org/docs/latest/application_documentation/rna/drrafter</a>	<a href="https://www.rosettacommons.org/demos/latest/public/drrafter/R_EADME">https://www.rosettacommons.org/demos/latest/public/drrafter/R_EADME</a>
<b>Membrane proteins</b>					
RosettaMP framework: mp_dock mp_symdock mp_relax mp_ddg	Julia Koehler Leman, Rebecca Alford	Jeffrey Gray	76	<a href="https://www.rosettacommons.org/docs/latest/application_documentation/Application%20Documentation#Membrane-Proteins">https://www.rosettacommons.org/docs/latest/application_documentation/Application%20Documentation#Membrane-Proteins</a>	Supp to <sup>76</sup>
RosettaMP toolkit: mp_score mp_transform mp_mutate_relax helix_from_sequence	Julia Koehler Leman	Jeffrey Gray	77	<a href="https://www.rosettacommons.org/docs/latest/application_documentation/Application%20Documentation#Membrane-Proteins">https://www.rosettacommons.org/docs/latest/application_documentation/Application%20Documentation#Membrane-Proteins</a>	Supp to <sup>77</sup>
mp_lipid_acc	Julia Koehler Leman	Richard Bonneau	78	<a href="https://www.rosettacommons.org/docs/latest/application_documentation/Application%20Documentation#Membrane-Proteins">https://www.rosettacommons.org/docs/latest/application_documentation/Application%20Documentation#Membrane-Proteins</a>	Supp to <sup>78</sup>
mp_domain_assembly	Julia Koehler Leman	Richard Bonneau	79	<a href="https://www.rosettacommons.org/docs/latest/application_documentation/Application%20Documentation#Membrane-Proteins">https://www.rosettacommons.org/docs/latest/application_documentation/Application%20Documentation#Membrane-Proteins</a>	Supp to <sup>79</sup>
RosettaCM for membrane proteins	Brian Bender	Jens Meiler	80	<a href="https://www.rosettacommons.org/docs/latest/application_documentation/Application%20Documentation#Membrane-Proteins">https://www.rosettacommons.org/docs/latest/application_documentation/Application%20Documentation#Membrane-Proteins</a>	Supp to <sup>80</sup>
<b>Carbohydrates</b>					
RosettaCarbohydrate framework	Jason W. Labonte, Jared Adolf-Bryfogle	Jeffrey Gray (Bill Schief)	81,82	<a href="https://www.rosettacommons.org/docs/latest/application_documentation/carbohydrates/WorkingWithGlycans">https://www.rosettacommons.org/docs/latest/application_documentation/carbohydrates/WorkingWithGlycans</a>	
<b>Scorefunction</b>					

REF2015 scorefunction	Hahnbeom Park, Frank DiMaio	Frank DiMaio, David Baker	83,84	<a href="https://www.rosettacommons.org/docs/latest/rosetta_basics/scoring/score-types">https://www.rosettacommons.org/docs/latest/rosetta_basics/scoring/score-types</a>	
cartesian_ddG	Brandon Frenz, Phil Bradley, Yuan Liu	Frank DiMaio, Phil Bradley	83	<a href="https://www.rosettacommons.org/docs/latest/cartesian-ddG">https://www.rosettacommons.org/docs/latest/cartesian-ddG</a>	
HBNet	Scott Boyken, Jack Maguire	David Baker, Brian Kuhlman	85,86	<a href="https://www.rosettacommons.org/docs/latest/scripting_documentation/RosettaScripts/Movers/movers_pages/HBNetMover">https://www.rosettacommons.org/docs/latest/scripting_documentation/RosettaScripts/Movers/movers_pages/HBNetMover</a>	
HBNetEnergy	Vikram Mulligan	(formerly David Baker) Richard Bonneau	85	<a href="https://www.rosettacommons.org/docs/latest/rosetta_basics/scoring/HBNetEnergy">https://www.rosettacommons.org/docs/latest/rosetta_basics/scoring/HBNetEnergy</a>	
AACompositionEnergy	Vikram Mulligan	(formerly David Baker) Richard Bonneau		<a href="https://www.rosettacommons.org/docs/latest/rosetta_basics/scoring/AACompositionEnergy">https://www.rosettacommons.org/docs/latest/rosetta_basics/scoring/AACompositionEnergy</a>	Supp to <sup>36,87</sup>
AARepeatEnergy	Vikram Mulligan	(formerly David Baker) Richard Bonneau		<a href="https://www.rosettacommons.org/docs/latest/rosetta_basics/scoring/Repeat-stretch-energy">https://www.rosettacommons.org/docs/latest/rosetta_basics/scoring/Repeat-stretch-energy</a>	
VoidsPenaltyEnergy	Vikram Mulligan	(formerly David Baker) Richard Bonneau		<a href="https://www.rosettacommons.org/docs/latest/rosetta_basics/scoring/VoidsPenaltyEnergy">https://www.rosettacommons.org/docs/latest/rosetta_basics/scoring/VoidsPenaltyEnergy</a>	
NetChargeEnergy	Vikram Mulligan	(formerly David Baker) Richard Bonneau		<a href="https://www.rosettacommons.org/docs/latest/rosetta_basics/scoring/NetChargeEnergy">https://www.rosettacommons.org/docs/latest/rosetta_basics/scoring/NetChargeEnergy</a>	
BuriedUnsatPenalty	Vikram Mulligan	(formerly David Baker) Richard Bonneau		<a href="https://www.rosettacommons.org/docs/latest/rosetta_basics/scoring/BuriedUnsatPenalty">https://www.rosettacommons.org/docs/latest/rosetta_basics/scoring/BuriedUnsatPenalty</a>	
<b>Interfaces</b>					
PyRosetta	Sergey Lyskov	Jeffrey Gray	88,89	<a href="http://www.pyrosetta.org">http://www.pyrosetta.org</a>	
RosettaScripts	Sarel Fleishman	(formerly David Baker) Sarel Fleishman	80,90	<a href="https://www.rosettacommons.org/docs/latest/scripting_documentation/RosettaScripts/RosettaScripts">https://www.rosettacommons.org/docs/latest/scripting_documentation/RosettaScripts/RosettaScripts</a>	
InteractiveRosetta	Benjamin Walcott	Chris Bystroff	91	<a href="http://www.github.com/BystroffLab/InteractiveROSETTA">www.github.com/BystroffLab/InteractiveROSETTA</a>	
Foldit Standalone	Seth Cooper, Firas Khatib	(formerly David Baker) Seth Cooper, Firas Khatib	92-95	<a href="http://fold.it/standalone">http://fold.it/standalone</a>	
ROSIE server	Sergey Lyskov Rocco Moretti Shane O'Connor	Jeffrey Gray	96,97	<a href="http://rosie.rosettacommons.org/documentation">http://rosie.rosettacommons.org/documentation</a>	
<b>Miscellaneous</b>					

Metalloproteins	Vikram Mulligan	(formerly David Baker) Richard Bonneau	98,99	<a href="https://www.rosettacommons.org/docs/latest/rosetta_basics/non_protein_residues/Metals">https://www.rosettacommons.org/docs/latest/rosetta_basics/non_protein_residues/Metals</a> <a href="https://www.rosettacommons.org/docs/latest/scripting_documentation/RosettaScripts/Movers/movers_pages/SetupMetalsMover">https://www.rosettacommons.org/docs/latest/scripting_documentation/RosettaScripts/Movers/movers_pages/SetupMetalsMover</a> <a href="https://www.rosettacommons.org/docs/latest/scripting_documentation/RosettaScripts/Movers/constraint_generators/MetalContactsConstraintGenerator">https://www.rosettacommons.org/docs/latest/scripting_documentation/RosettaScripts/Movers/constraint_generators/MetalContactsConstraintGenerator</a>	99
Waters	Ryan Pavlovicz	Frank DiMaio	REF?	<a href="https://www.rosettacommons.org/docs/latest/scripting_documentation/RosettaScripts/Movers/WaterBoxMover">https://www.rosettacommons.org/docs/latest/scripting_documentation/RosettaScripts/Movers/WaterBoxMover</a>	
SimpleMetrics	Jared Adolf-Bryfogle	Bill Schief		<a href="https://www.rosettacommons.org/docs/latest/scripting_documentation/RosettaScripts/SimpleMetrics/SimpleMetrics">https://www.rosettacommons.org/docs/latest/scripting_documentation/RosettaScripts/SimpleMetrics/SimpleMetrics</a>	
AmbRose	Kristin Blacklock, Aliza Rubenstein, Michael Szegedy	Sagar Khare		<a href="https://www.rosettacommons.org/docs/latest/AmbRose">https://www.rosettacommons.org/docs/latest/AmbRose</a>	
RosettaRC	Jared Adolf-Bryfogle	William Schief		<a href="https://www.rosettacommons.org/docs/latest/rosetta_basics/running-rosetta-with-options#common-options-and-default-user-configuration">https://www.rosettacommons.org/docs/latest/rosetta_basics/running-rosetta-with-options#common-options-and-default-user-configuration</a>	

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