Comparing the Structure of the Light Harvesting Complex II across Species of Purple Bacteria

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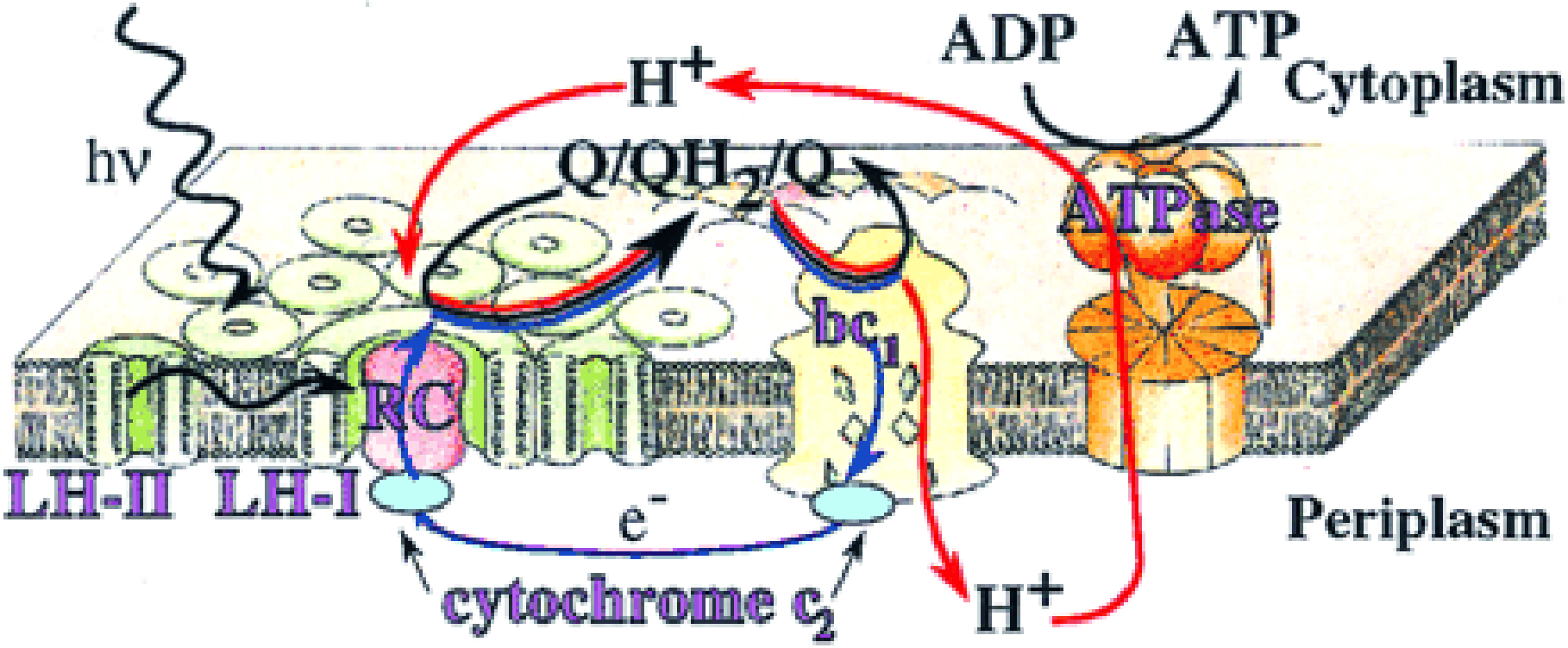
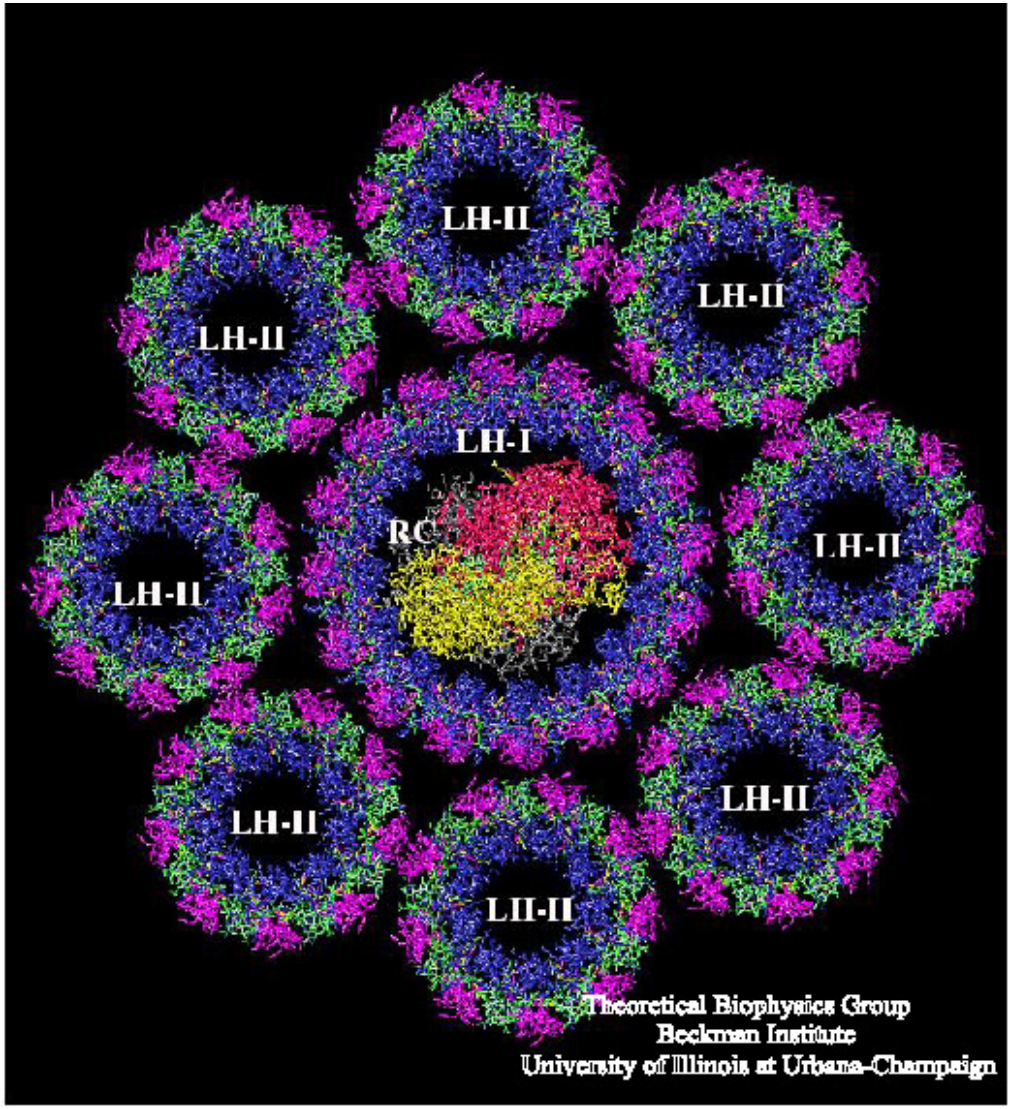
Outline

- Biological Setting: Photosynthetic Unit of Purple Bacteria
- Structural Overview of LH-II
- Sequence Alignment
- Principles Governing our Experiment
- IMIMOL view of the LH-II structure
- Model Building Procedure
- Evaluation of the structure
- Acknowledgments
- References

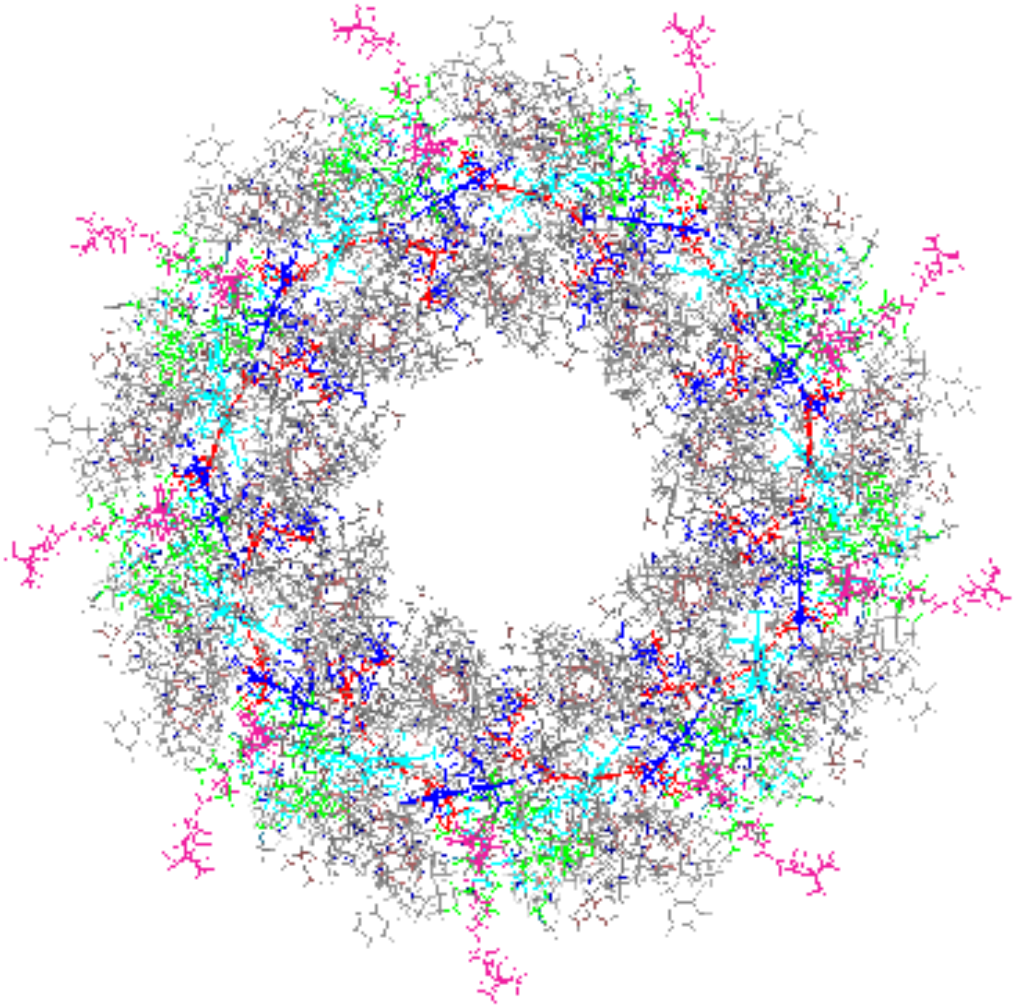
Biological Setting: PSU of Purple Bacteria



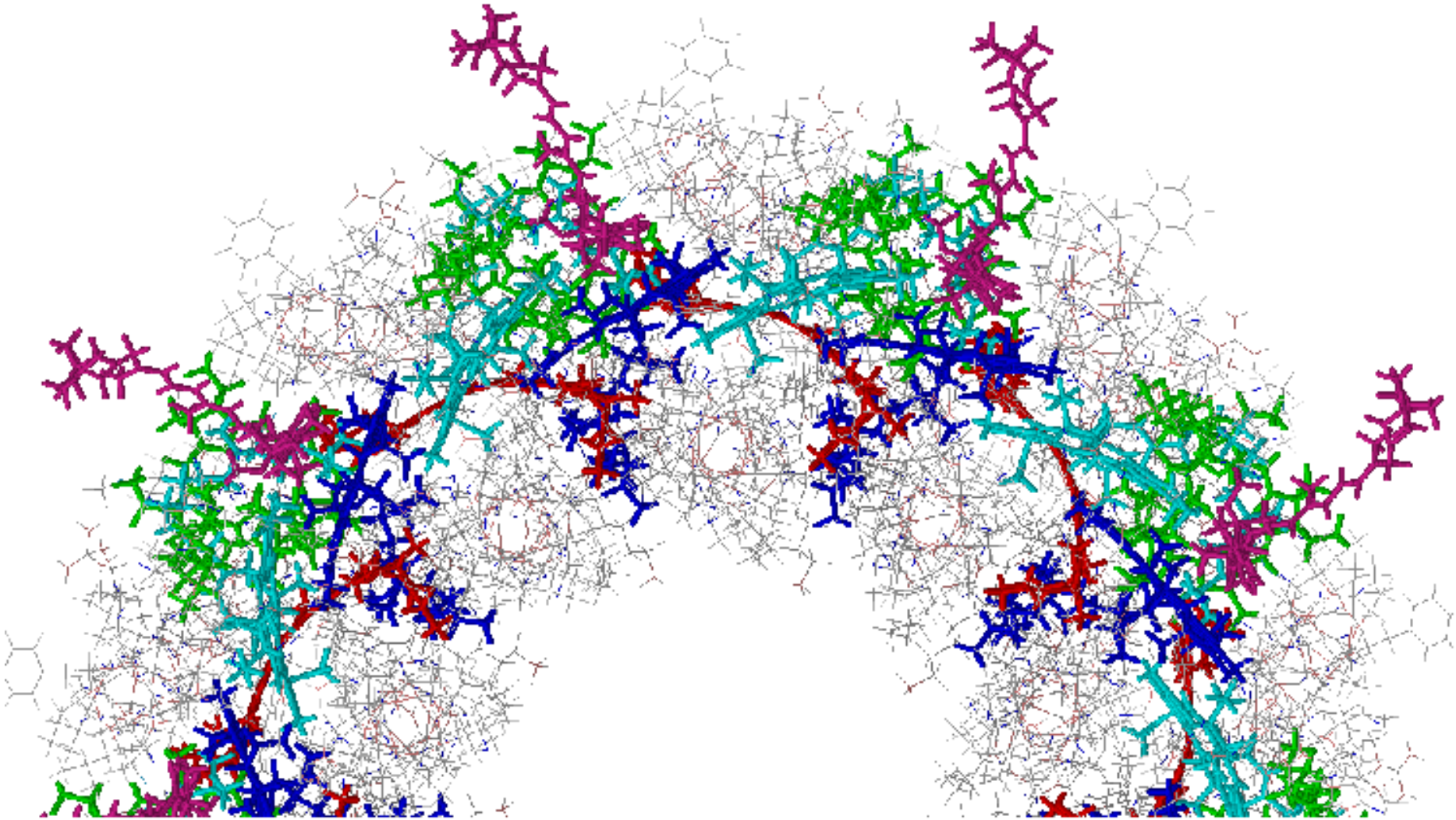
Light Harvesting System



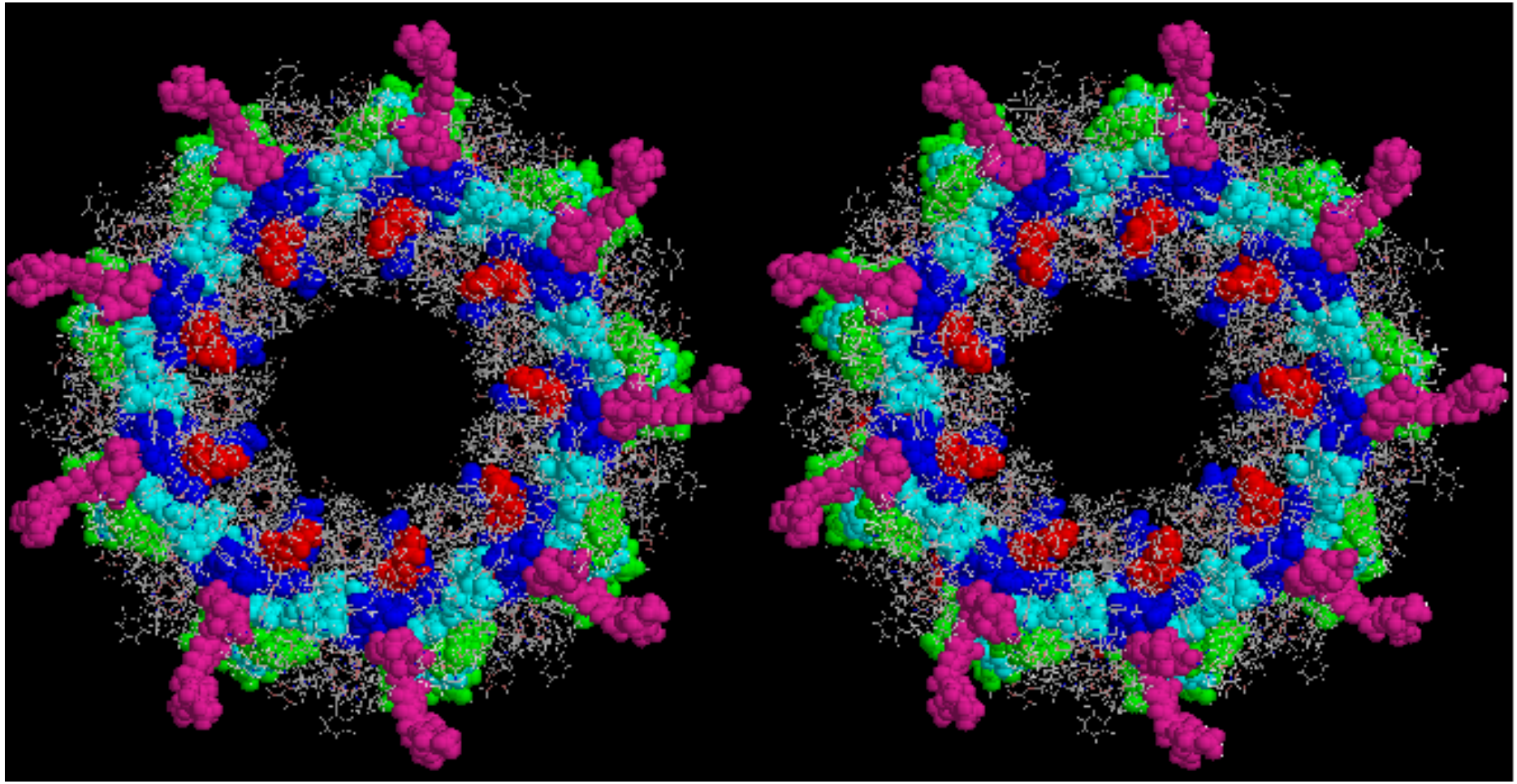
LH-II



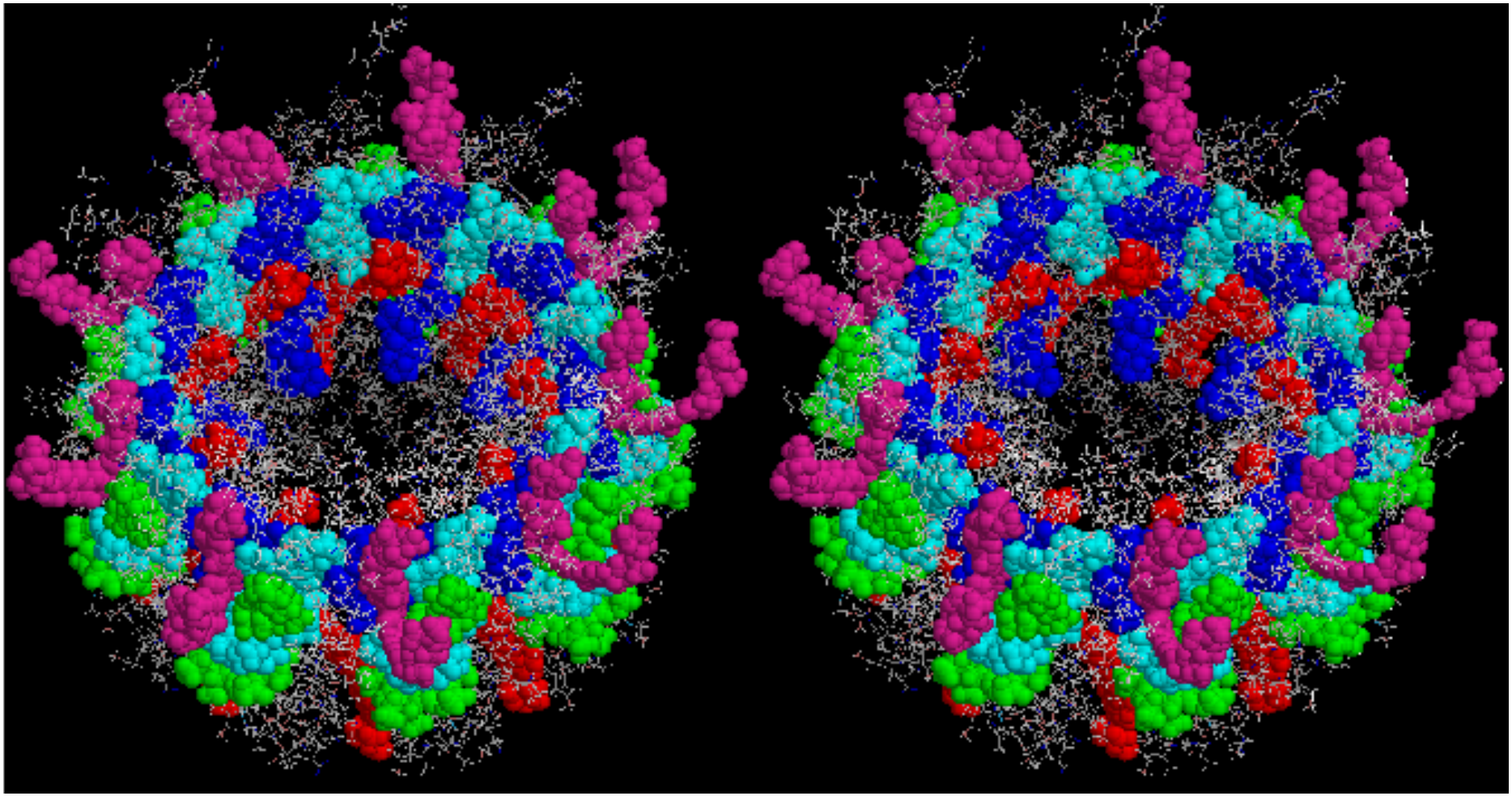
LH-II: closeup



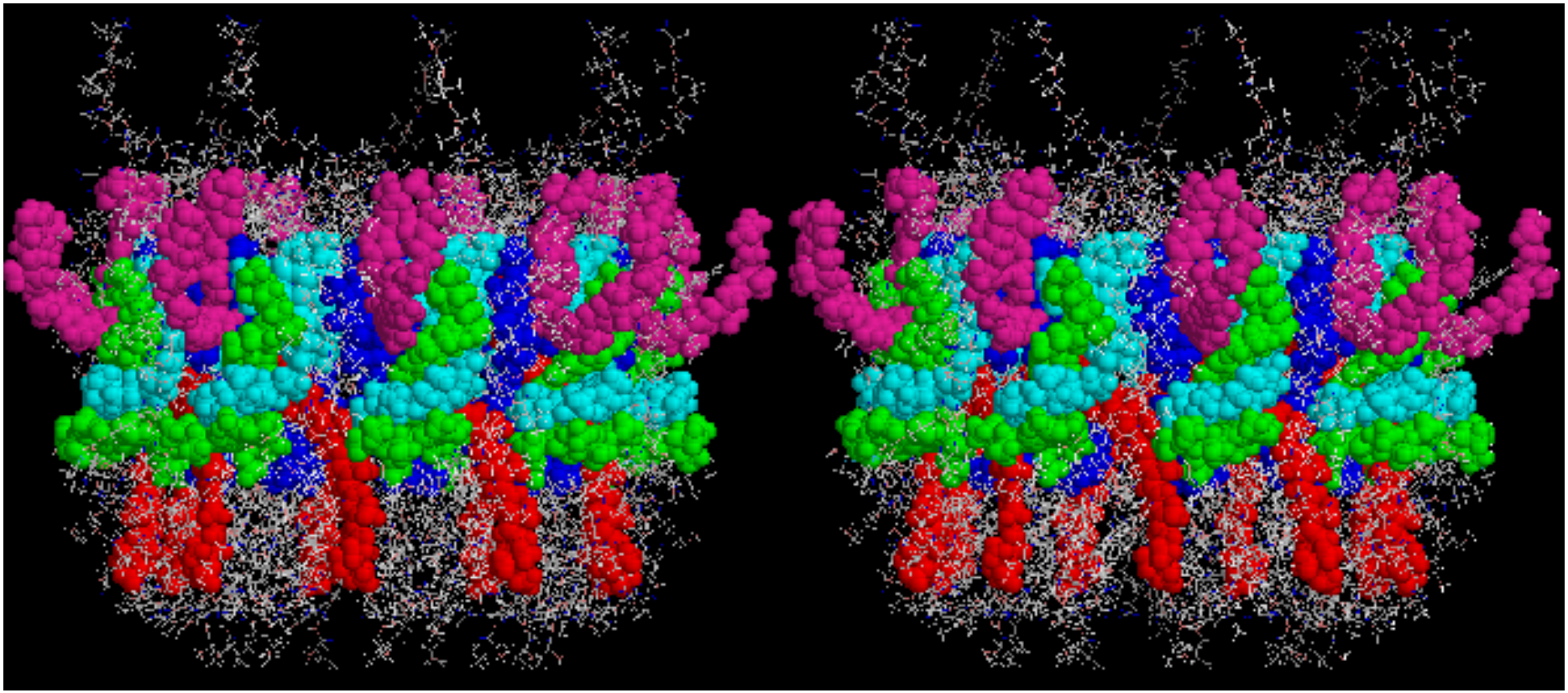
LH-II: stereo top (periplasm) view



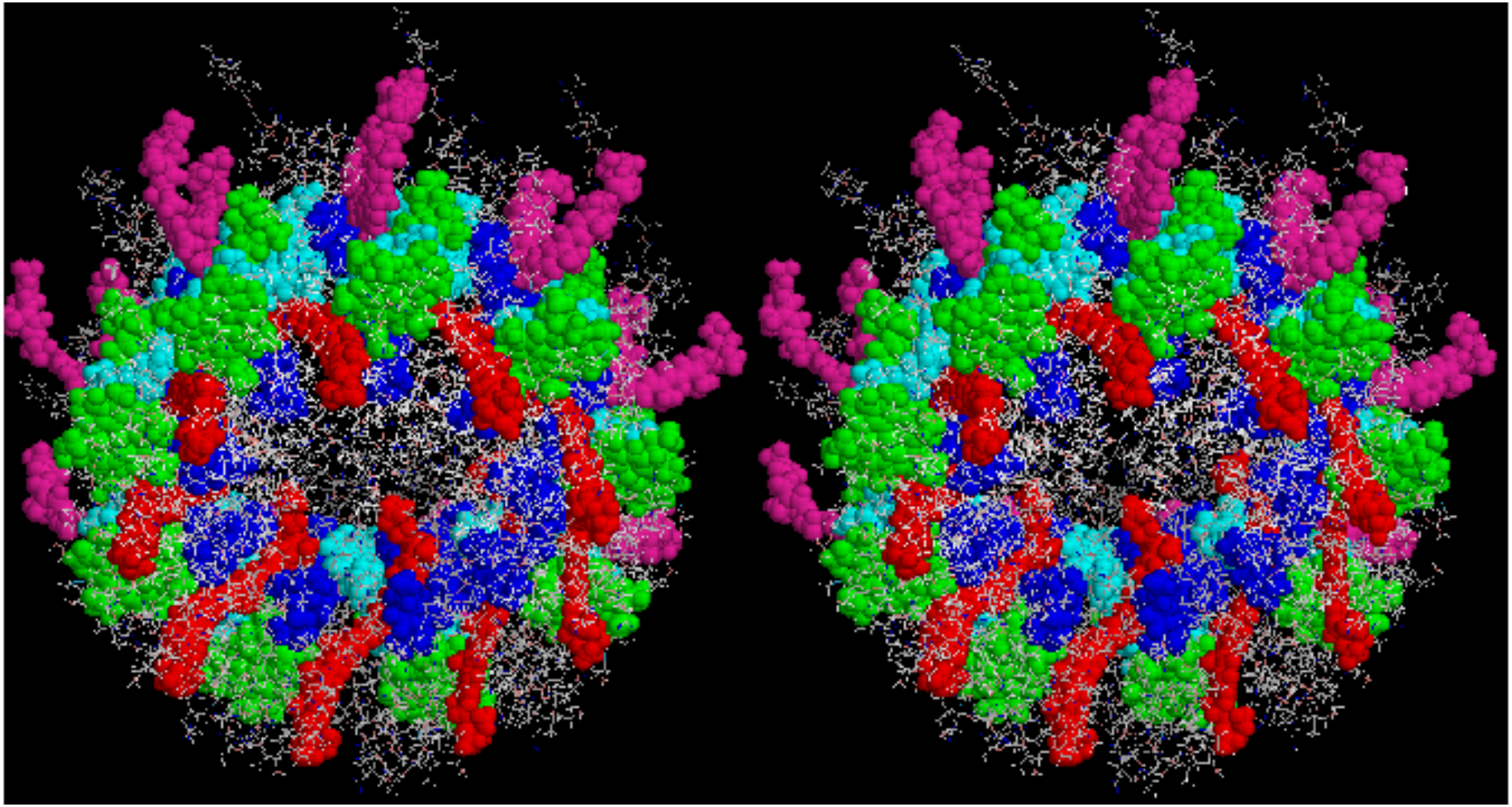
LH-II: stereo upper slant view



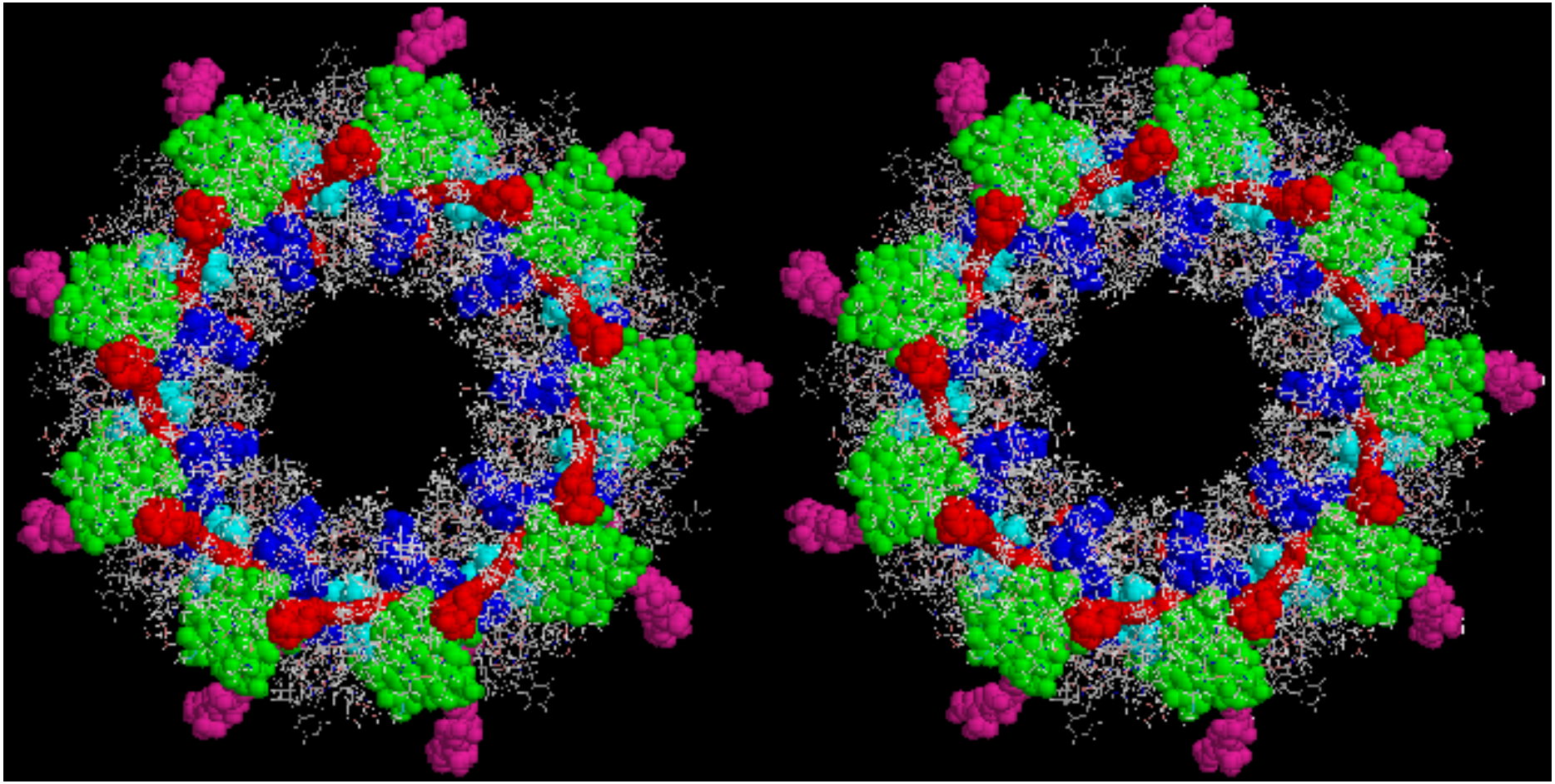
LH-II: stereo side view



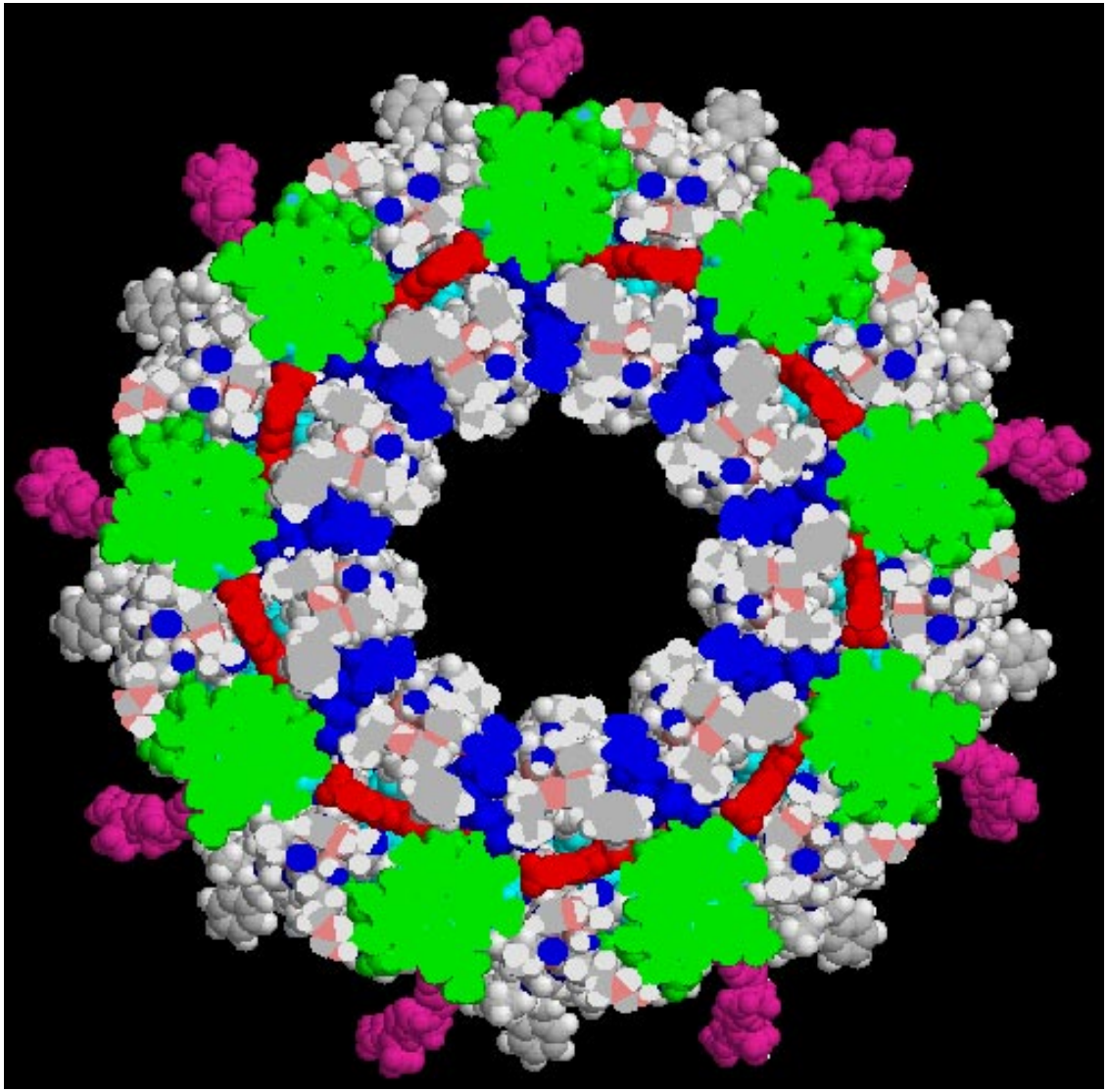
LH-II: stereo lower slant view



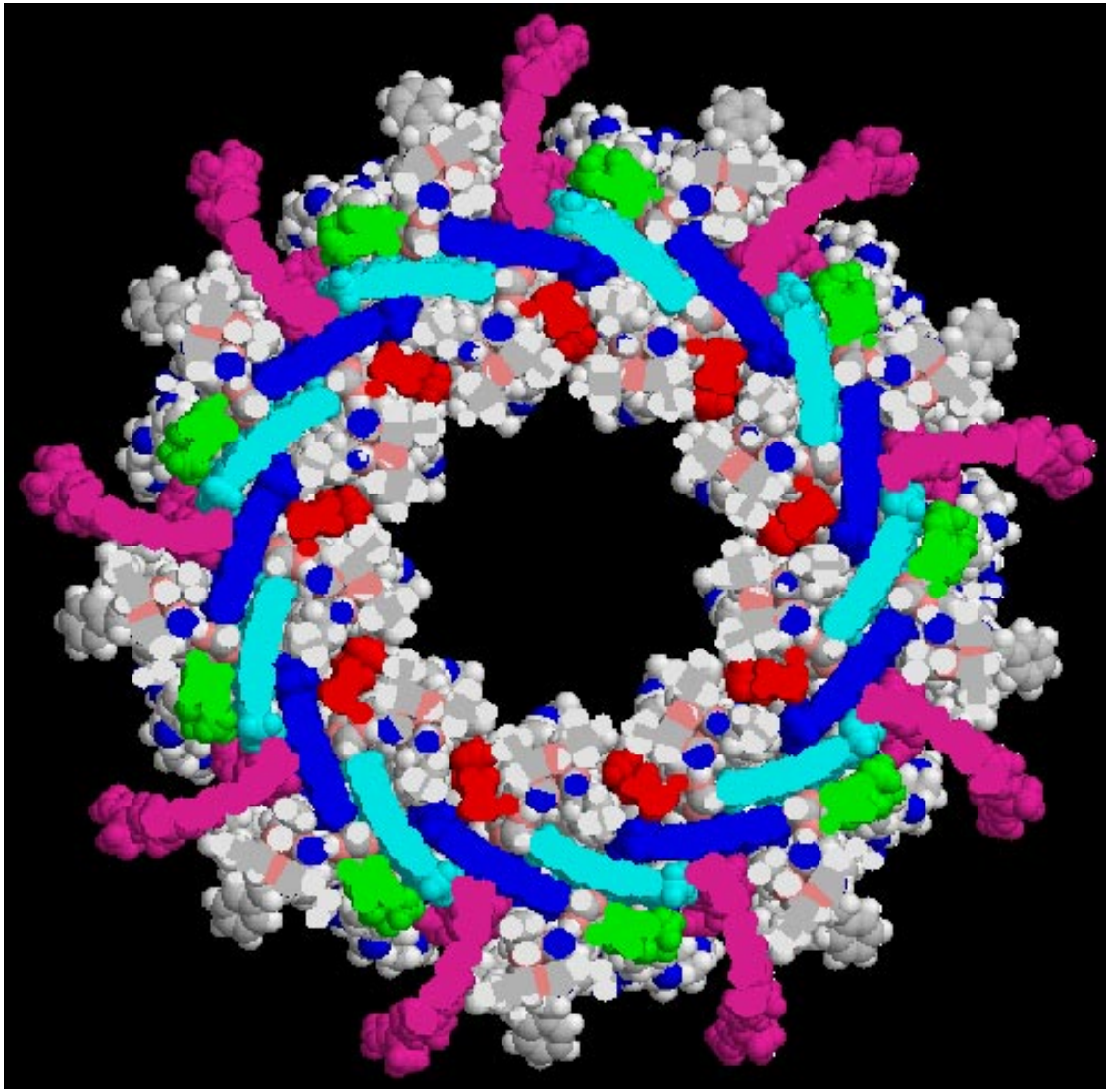
LH-II: stereo bottom (cytoplasm) view



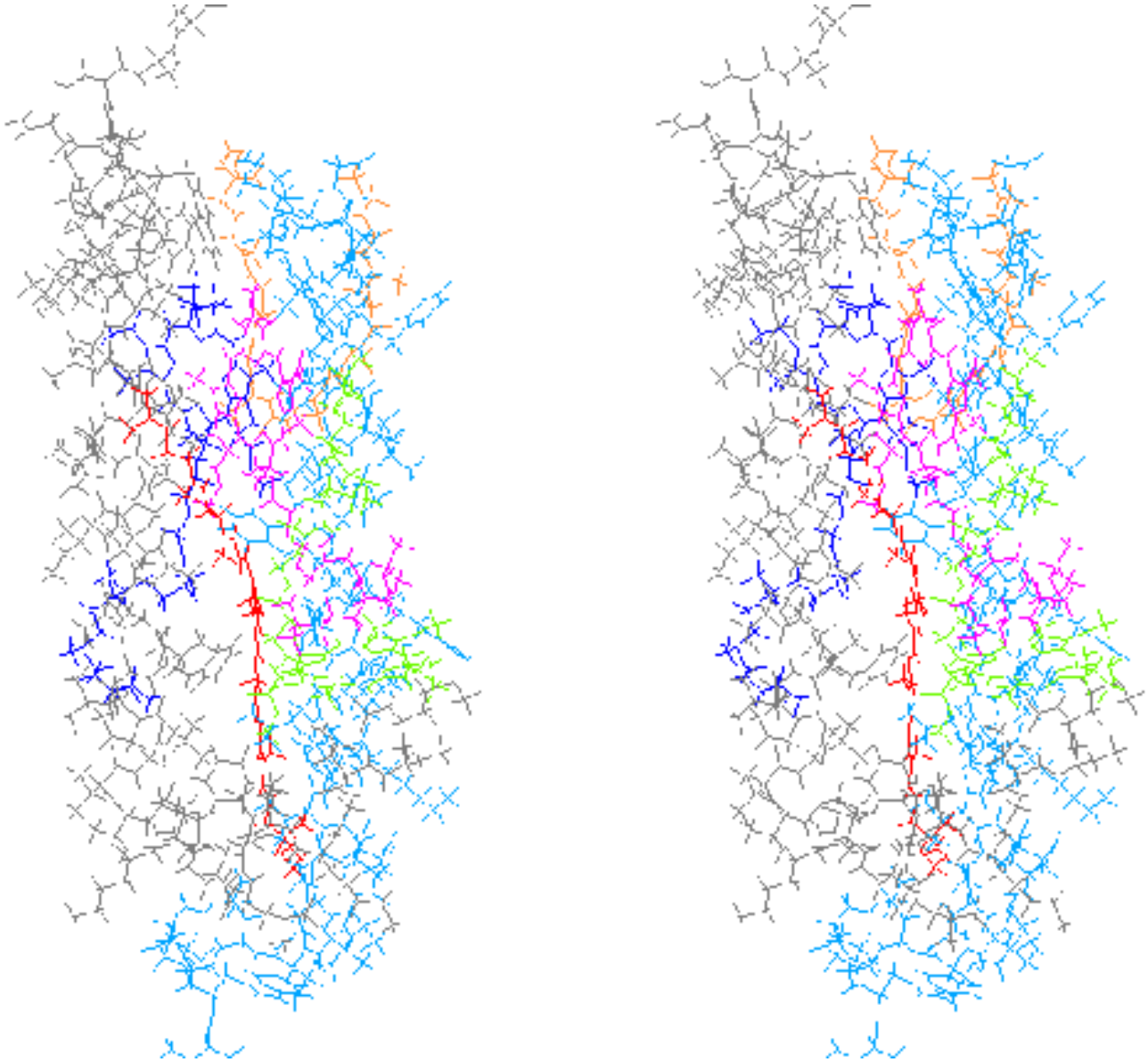
B800 cross section toward periplasm



B850 cross section toward periplasm



Protomer Complex (PC)



Species of Purple Bacteria

Template Species for LH-II

- *Rhodopseudomonas acidophila*. Abbreviated as: *acid.*.
  X-ray crystal structure at 2.0 angstroms known.
- *Rhodospirillum molischianum*. Abbreviated as: *moli.*.
  X-ray crystal structure at 2.4 angstroms known.

Target Species

Rhodobactor sphaeroides. Abbreviated as: *sph.*.

No X-ray structure known.

A homolgy modelling structure based on a 2.4 angstrom X-ray structure of *acid.* was done by Hu, *et. al.*.

Sequence Alignment: α-apoprotein

	10	20	30
sph.	XTNGKIWLVV	KPTVGVPLFL	SAAVIASVII
acid.	XNQGKIWTVV	NPAIGIPALL	GSVTVIAILV
	40	50	
sph.	HAAVLTTTTW	LPAYYQGSAA	VAAE
acid.	HLAILSHTTW	FPAYWQGGVK	KAA-

24 identical, 19 same group, 53 total residues.

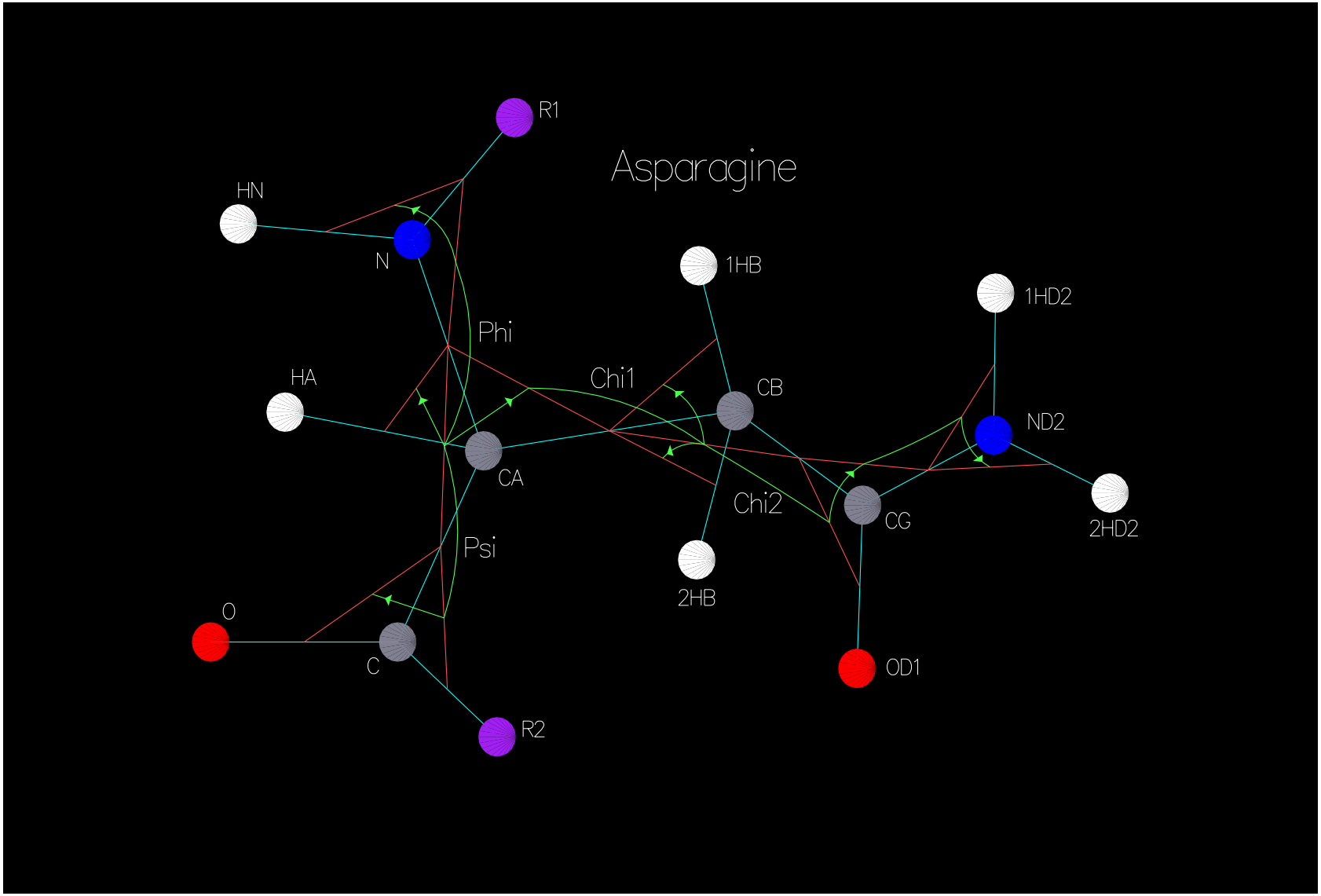
Sequence Alignment: β-apoprotein

	6	16	26
moli.	---AERSLS	GLTEEEAIAV	HDQFKTTFSA
	10	20	30
sph.	TDDLNKVWPS	GLTVAEAEEV	HKQLILGTRV
	1	11	21
acid.	------A	TLTAEQSEEL	HKYVIDGTRV
	36	46	
moli.	FIILAAVAHV	LVWVWKPWF-	*sph.* 7-17
	40	50	
sph.	FGGMALIAHF	LAAAATPWLG	(29,8,44)
	31	41	
acid.	FLGLALVAHF	LAFSATPWLH	*sph.* 18-50

Principles Governing Our Experiment

- **Invariant Core.** Attempt to keep the protein backbones, the pigment conformations, and the relative placements of the components within a PC and the relative placements of the PCs within the LH-II complex invariant.
- **Symmetry.** Maintain perfect nine-fold rotational symmetry about the central axis of LH-II. Hence all the PCs have identical conformations, which must be averaged over the different PC conformations present in the crystal structures.
- **All Atoms.** The known structures do not include the positions of any hydrogen atoms. We assign these positions using the program MolProbity, and include all the atoms in our model.

Z-systems


Asparagine
R1
HN
N
1HB
1HD2
Phi
HA
Chi1
CB
ND2
CA
Chi2
CG
2HD2
Psi
2HB
O
C
OD1
R2

Rotamers

Rotamers are statistically likely shapes of amino acid side chains as found in known biological protein structures.

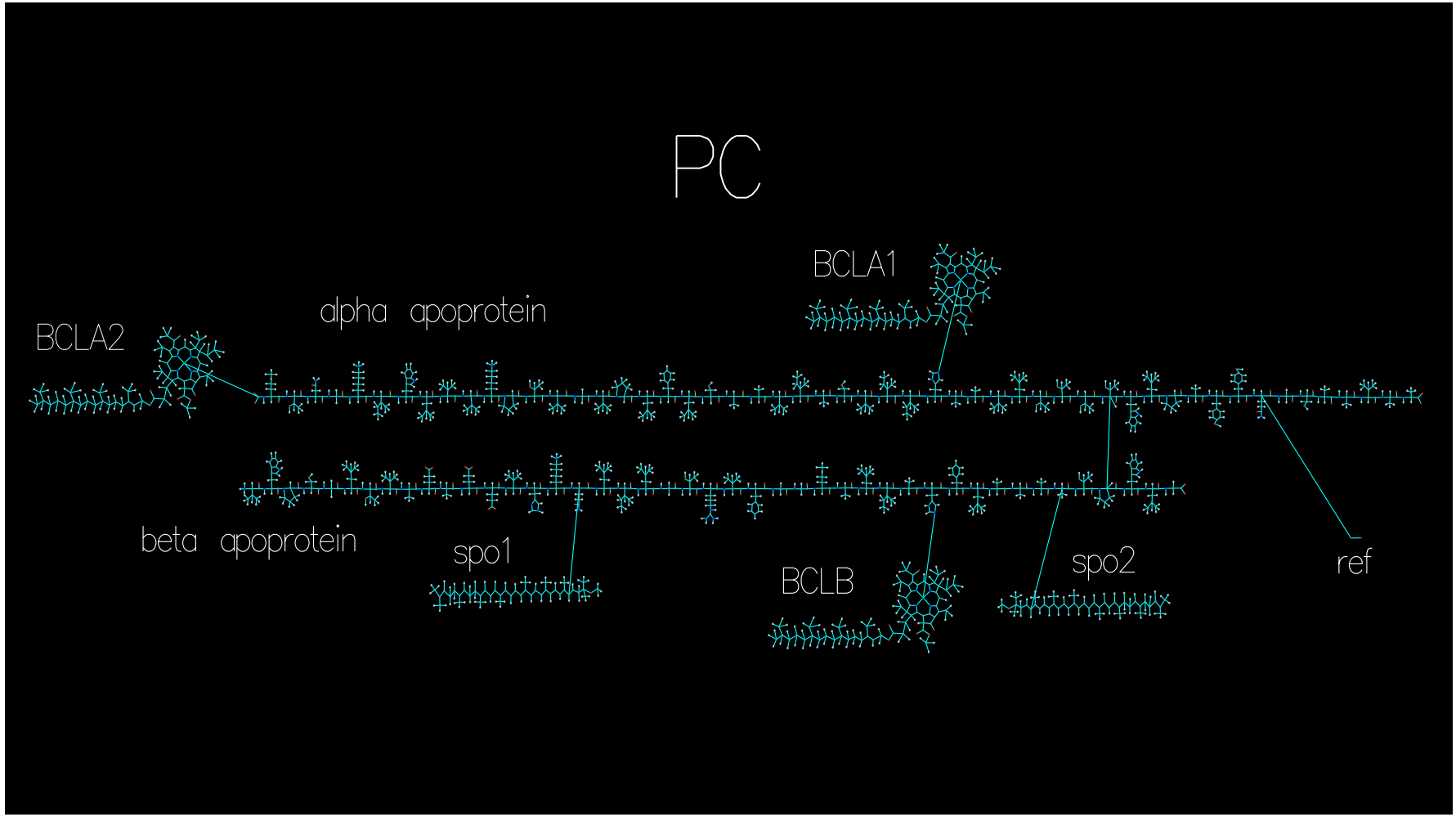
Example: Rotamers of Asparagine. The shape of the side chain of asparagine depends primarily on the values of two torsion angles: χ_1 and χ_2.

name	p-10	p+30	t-20	t+30	m-20	m-80	m+120
freq.	7%	9%	12%	15%	39%	8%	4%
χ_1	62	62	-174	-174	-65	-65	-65
χ_2	-10	30	-20	30	-20	-75	120

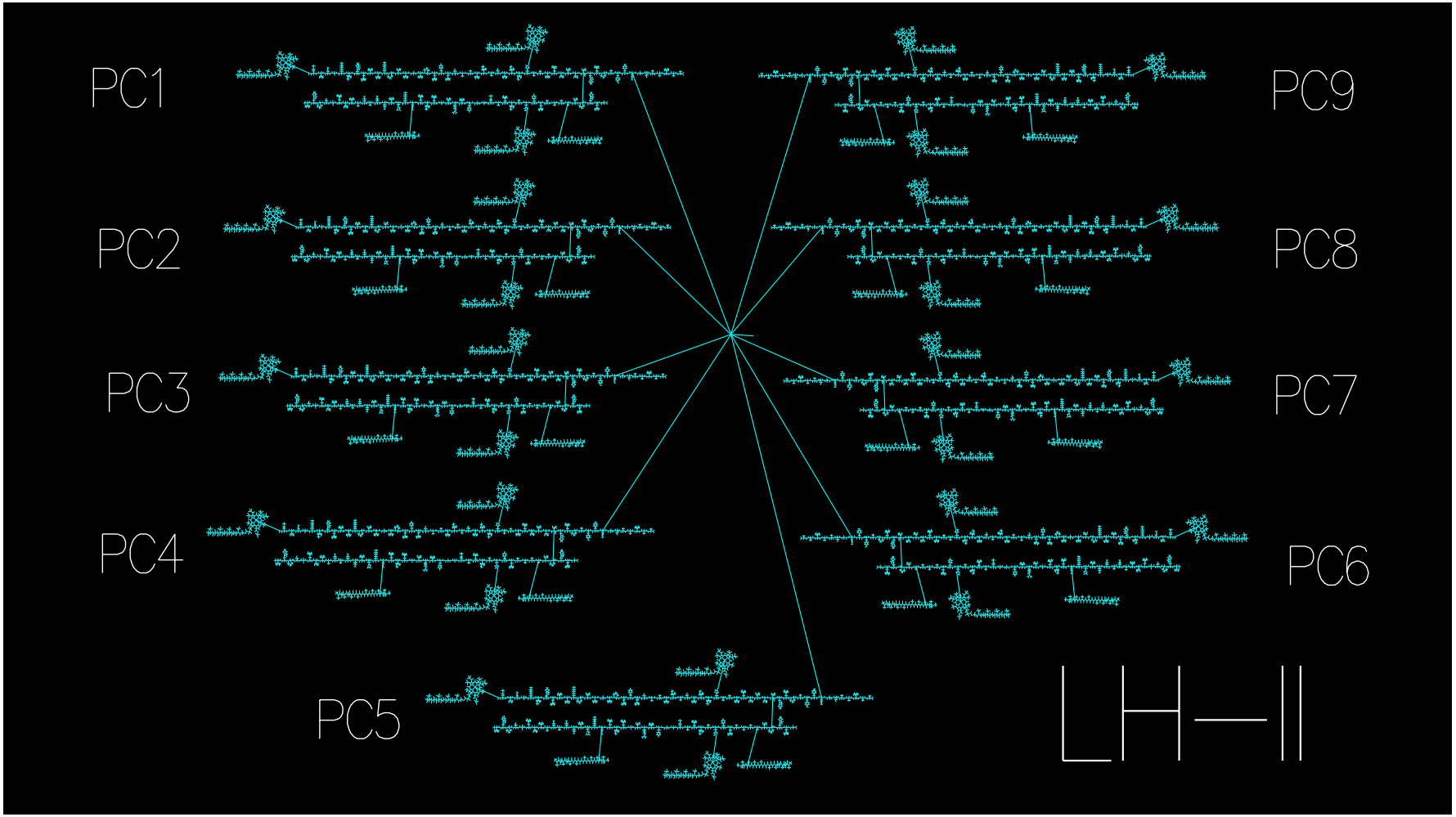
More Principles Governing Our Experiment

- **Internal Coordinates.** Create the structure entirely in Z-system internal coordinates, to facilitate averaging and adjustability.
- **Rotamers.** Attempt to place all conserved residue sidechains in rotameric conformations closest to the average conformation. Attempt to choose rotameric conformations for all the nonconserved residues as well.
- **Steric Consistency.** Choose conformations of all residues so that no two nonbonded atoms are too close to each other in space.
- **Simple Adjustments.** Attempt to achieve this by adjusting a small number of internal coordinates one-by-one by hand so as to pack everything in space consistently.

Z-System of the Protomer Complex



Z-System of LH-II



Model Building Procedure

- Compute averaged PC Z-systems in each of the two template species.
- Delete nonconserved sidechains from the α apoprotein of *acid.* and replace with the corresponding residues from *sph.*.
- Glue residues $\beta 3$–$\beta 13$ of *moli.* to residues $\beta 9$–$\beta 41$ of *acid.* using the average ω wedge angle to obtain residues $\beta 7$–$\beta 50$ of *sph.*.
- Delete all the nonconserved residues from the β apoprotein and replace them with their *sph.* values.
- Assign nearest rotamers to the conserved residues unless this causes a steric clash or the residue is a tethering site for a BCL.

Procedure (continued)

Working from conserved regions toward nonconserved regions assign rotamers to nonconserved residues, inspecting visually for clashes. Do in the following order:

- Individual α and β apoproteins.
- Docked α–β apoproteins, i.e. the heterodimer.
- Heterodimer plus BCLs.
- Heterodimer plus BCLs and carotenoids, i.e. a PC.
- A pair of docked PCs.

If a rotamer choice causes a clash, backtrack and rechoose the previous rotamer and try again. If there is no rotamer that works default to the average conformation. Choose the average over a rotamer to preserve an H-bond.

Summary of Lessons Learned

Rotamerizability

chain	cons.	flex.	rotamer	noncons.	flex.	rotamer
α	$24/53$	13	9	$29/53$	23	18
β	$29/44$	20	10	$15/44$	9	7

Complex Adjustments. We changed one backbone torsion ($\psi 9 \beta$) by 10° to relax crowding. A few deviations from rotamers or average were needed.

Crowded Areas. The crystal structures contain some clashes, but a couple of new clashes remain after our efforts. This is a surprising (to us) degree of success.

Acknowledgements

- IMIMOL, by Scott Johnson; support: IMI at USC.
- VMD, by Theoretical Biophysics Group UIUC; support: NSF, NIH.
- VMD-IMI, by Matthew Heilsberg and Matt Elder; support: IMI at USC.
- MolProbity, by Ian Davis; support: Richardson lab at Duke.
- Convert, by Jason Rogers at USC.
- Average, by Dan Dix at USC.
- RASMOL, by Roger Sayle; support: Glaxo Wellcome Research and Development.

References

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2. Structure . . . of the B800-850 LH2 Complex from *Rps. acidophila* at 2.0 A resolution and 100 K . . . , M.Z. Papiz, S.M. Prince, T. Howard, R.J. Cogdell, N.W. Isaacs, J. Mol. Biol., **326**, 1523–1538, 2003.

3. The Crystal Structure of the Light Harvesting Complex II (B800-850) from *Rhodospirillum molischianum*, J. Koepke, X. Hu, C. Muenke, K. Schulten, H. Miche, Structure, **4**, 581–597, 1996.

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4. Architecture and mechanism of the light-harvesting apparatus of purple bacteria, X. Hu, A. Damjanovic, T. Ritz, K. Schulten, Proc. Natl. Acad. Sci. USA, **95**, 5935–5941, 1998.