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Conformational control of cofactors in nature – Functional tetrapyrrole conformations in the photosynthetic reaction centers of purple bacteria

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Chemically identical tetrapyrrole cofactors such as hemes and chlorophylls participate in functionally diverse biological roles. An analysis of the available protein structural data for the bacteriochlorophylls in the photosynthetic reaction center gives statistically reliable evidence of the hypothesis that the protein induced cofactor conformation is a modulator of the bio-molecular function of each reaction center. The results serve as a general model to illustrate conformational control of tetrapyrrole cofactors in other proteins.

Tetrapyrrole containing proteins are one of the most fundamental classes of enzymes found in nature and it is an open question to give a chemical rationale for the multitude of biological reactions that can be catalyzed by these pigment-protein complexes.[1] A critical factor for all biological functions is the close structural interplay between bound cofactors and the respective apoprotein in addition to factors such as hydrogen bonding or electronic effects. In individual tetrapyrrolic systems there is considerable evidence[2] that nonplanarity is the key geometric factor affecting their physicochemical properties. Thus, the biological diversity of chemically identical tetrapyrroles has been linked with distinct, conserved conformations.[2a,2c,3] However, except for studies based on individual structures, no convincing general proof has been given for this concept of conformational control thus far.

Using the cofactors of the photosynthetic reaction center in purple bacteria we present the first statistically reliable analysis of such systems for this hypothesis and show that the various chromophores of the reaction center have different conformations which can be correlated with their chemical role. This shows that the protein scaffold exerts functional conformational control on the porphyrin macrocycle and that modulation of the macrocycle conformation is an effective and general means to fine-tune the cofactor properties *in vivo* and to utilize the same cofactor for different chemical reactions. The results serve as a general model for the structural factors involved in cofactor regulation in nature.

The initial steps of photosynthesis take place in the reaction center (RC); the processes of light-harvesting, charge-separation and photoprotection all involve and indeed depend upon numerous tetrapyrrole cofactors.[4] In fact, the RC is itself a true testament to the versatility of these cofactors where chemically identical species perform one or more of these highly specialized functions within the same protein. The focus here is on the six tetrapyrrole cofactors of the electron transfer chain (ETC) from the RCs of the purple photosynthetic bacteria (Fig. 1). The cofactors of the ETC are anchored to one of two reaction center proteins (L or M), via numerous interactions and are arranged in pairs of approximate C_2 symmetry.[5] An interesting enigma, addressed further in this article, is the preferential electron transfer along the L-branch.[6]

In the past conformational aspects of porphyrin structures have been described using typical core structural data, such as bond lengths, tilt angles, skeletal deviation plots or out-of-plane displacements which gave rise to the identification of some general types of macrocycle conformations (e.g. ruffled, doomed, saddle).[2a,8] However, these data do not lend itself to a quantitative analysis of chemically very distinct species and so here we use the method of normal-coordinate structural decomposition (NSD)[3b,9] which overcomes this issue. This technique was developed by Shelnutt and affords clear separation of the contributing distortions (normal-modes) to the macrocycle conformation in a quantitative fashion allowing a comparative analysis of conformational effects in porphyrins and is valid for use with the porphyrinoid cofactors in protein structures.[3b,9b]

Our approach involved the determination of the NSD for every ETC cofactor [bacteriochlorophyll (BChl) and bacteriopheophytin (BPhe)] of photosynthetic bacteria from relevant crystal structures obtained from the Protein Data Bank (PDB; structure overview Table 1). Via a methodical statistical route, including investigation of the nature and reliability of each crystal structure, we refined the dataset and extracted the best estimate of the actual conformations present in the crystal.

Table 1. Summary of RC crystal structures (details in Section 6, S.I.)

Species	Crystal structures[a]	Resolution(s)[b]
B. viridis	15 (14)	1.86-3.21 (2.36)
R. sphaeroides	77 (27)	1.80-4.60 (2.66)

[a] Independent RC crystal structures assessed (retained for best estimate in parenthesis) [b] Resolution range (mean) of all structures.

Agglomerative hierarchical clustering of the cofactor conformations revealed that their major determinant was indeed their functional position in the ETC. However, closer inspection indicated secondary features that were related to entire crystal structures and we sought to assess the experimental correlations that were present and so performed further analyses where the conformations of each cofactor reflected each structure's observable variables.

In the *R. sphaeroides* data, the inter-crystal structure Euclidean dissimilarities highlighted that a number of structures did not exhibit *any* degree of experimental variation (Fig. 2) and were therefore removed them further consideration; it is likely that they originate from the practice of rigid-body refinement. Next, a two-factor analysis revealed that structures exhibited either: planar cofactors, functionally distinct nonplanar cofactors or functionally distinct nonplanar cofactors with unusual in-plane contractions (Fig. 2). Based on a comparison to high-resolution chlorin analogues from the Cambridge Structural Database[10] and others reasons we concluded that the first nonplanar set mentioned above presents the most reliable cofactor conformations. The NSD results of these structures' cofactors (Fig. 3) show clearly the distinct conformations present at each position of the ETC. Notably, the absolute nature of this

conformational superstructure varies with species but retains some general features and in some cases almost conserved conformations.

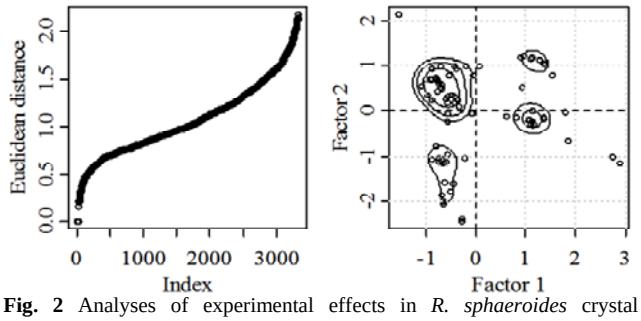

Fig. 2 Analyses of experimental effects in *R. sphaeroides* crystal structures. [Left] Euclidean dissimilarities between each structures' BChl conformations; cluster near zero indicates structures that exhibit no experimental variation. [Right] Plot of PDB structure scores on the Varimax rotated factors, computed by the regression method with kernel density contours overlaid. F1 (22.6% total variance) correlates with increasing planarity and F2 (21.5%) negatively with in-plane contraction.

In general, the deformation of the special pair cofactors is always the greatest (of at least the bacteriochlorophylls (BChls)) with a degree of asymmetry existing between the two, specifically that the B-branch cofactor exhibits greater distortion than that of the A-branch. With respect to the accessory pigments, the BChls are usually the least distorted of all the cofactors and the bacteriopheophytins are considerably distorted. An important deviation from this pattern exists for the B-branch accessory BChl of *R. sphaeroides* in that this cofactor displays a far greater distortion than its A-branch counterpart such that its relative distortion is comparable to that of the B-branch special pair cofactor. In both species, the conformations of the accessory BPhes are dominated by a 0.3-0.5Å B_{1u} distortion, with noticeable contributions from other modes. In terms of the cause of the distortions, that the special-pairs of both species are generally the most distorted cofactors indicates that their mutual interaction is a crucial factor, whereas the differences within each accessory pair must be mediated by the apoprotein alone. The fact that we may attribute at least the increased distortion of the special-pair cofactors to their dimerization points to a new paradigm for its original formation (in addition to their excitonic coupling), since this feature may be crucial to the overall ET process. Note that we have previously described such effects in small molecule bischlorin crystal structures.[11]

In light of the fact that increasing nonplanarity of tetrapyrroles has been linked with easier oxidation and more difficult reduction[12] of the molecule, a point which has recently been exploited for heme redox modification via protein induced distortion *in vitro*,[13] and that photosynthetic electron transfer is subject to the Marcus theory, the relative conformations of the BChl cofactors (above; in particular that the special-pairs are always the most distorted and BA is always relatively planar) would seem to assist in charge-separation on the whole. The conformations may also contribute to the preference for L-branch electron transfer in both species. Mechanistically, the ET asymmetry is dominated by the initial charge transfer asymmetry of the special-pair in *B. viridis*, which is echoed by the asymmetry in the extent of the nonplanar distortion exhibited by each half of the special-pair dimer in this species (Fig.'s. 3 and 4).

In *R. sphaeroides* the asymmetry of ET may begin with the conformational differences in the special-pair but could also be enhanced by stabilization of the $SP^{+}BA^{-}$ intermediate[14] compared to the alternative $SP^{+}BB^{-}$ intermediate, recalling the distortion of BB and that this will affect its hindered reduction. Note, that the rate of electron transfer is greater in *B. viridis* than in *R. sphaeroides*,[15] which again correlates with the greater distortion of the SP of the former (Fig. 4). The idea of the conformationally induced initial charge-transfer asymmetry (i.e. electron hole asymmetry at the special-pair) is supported by a recent study by Daviso *et al*. who concluded that the preferential localization of electron spin density to DL of the special-pair radical cation is intrinsic to the dimer and "… [is] predominantly attributable to local conformational conservation…".[16] Thus, our hypothesis is consistent with, and aids in the understanding of, the observed properties of the ETC and provides a rationale for these properties that would be observed as intrinsic in keeping with these recent computational findings. However, to this end, the idea of the easier oxidation of the more nonplanar macrocycle would in fact imply that it should be DM that exhibits the greater hole density.

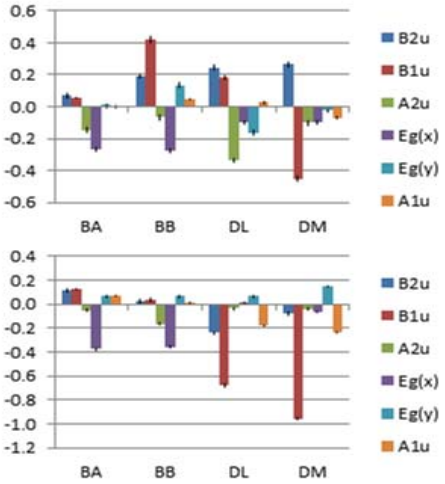

Fig. 3 Mean out-of-plane minimum basis NSDs of each ETC bacteriochlorin cofactor in *R. sphaeroides* (top) and *B. viridis* (bottom). Y-axes in Å; error bars indicate two standard errors. *B. viridis*, n = 14 for each cofactor; *R. sphaeroides*, n = 32 for each cofactor

On the other hand, not only is the understanding of ET aided by conformational considerations but also that of photoprotection since it has recently been shown that increasing macrocycle distortion affects lower yields of singlet oxygen generation from the triplet state.[17] This implies that the distortion of all but the advantageously planar cofactors (i.e. BA; see above) may be beneficial to the RC in reducing the risk of oxidative damage. In addition, the apparently apoprotein modulated distortion of BB in *R. sphaeroides* may be a specific enhancement of its photoprotective role whilst the planar BB in *B. viridis* can account for the lack of efficient triplet quenching in this species.[18] This argument is also valid in terms of the triplet transfer to the carotenoid since the distortion induced red-shift may be what allows BB in *R. sphaeroides* to absorb the low energy triplet state of the SP in the first place.

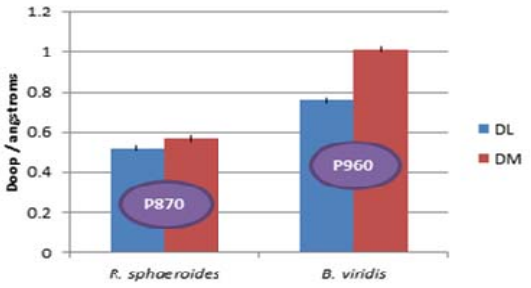

Fig. 4 Comparison of the total out-of-plane distortion (D_{oop}) of the special-pairs from each species. *R. sphaeroides*, n = 32 (right) and B. viridis, n = 14 (left) for each cofactor.

Further experimental observations and reaction center properties can also be explained with reference to the uncovered conformations. Resonance Raman (RR) studies of RCs yield conformational information on the tetrapyrroles in solution. One such study of *R. sphaeroides*[19] indicated that of the four ETC BChls, one is conformationally unique and suggested that it is DL that is different. Our analysis shows that this cofactor is unique in that its conformation is dominated by a relatively large A_{2u} distortion. Also, RR spectral studies indicate a more symmetric binding environment for the cofactors of P960 (the special-pair of *B. viridis*), yet electron paramagnetic resonance and electron nuclear double resonance studies show that CT is more asymmetric in P960 than in P865.[15] However, we can now see that the difference in overall nonplanarity is greater in the *B. viridis* special-pair. With this in mind the optical and near-infrared absorption spectra of the bacteriochlorin cofactors in RCs of *B. viridis* and *R. sphaeroides*[20] may also be conformationally modulated since the considerable red shift of the Qy band of P960[20a] compared to P865[15,20b] (95 nm shift) can only in part be attributed to the different C8 substituents since the isolated compounds absorb at only 770 and 795 nm, respectively, in solution[21] (25 nm shift). However, the NSDs show P960 to be far more distorted than P870; this type of red-shift is another known effect of porphyrin nonplanarity and more specifically, the large $B_{1u(2)}$ distortion exhibited by P960 has been directly liked to such spectral shifts.[2b]

We suggest that these statistics represent the actual conformations found in the crystal and we provide coordinates for these cofactors. The conformations, together with the current understanding of the effects of nonplanarity, tie in with the observed physical properties of electron transfer in photosynthetic systems such as the species variant extent of the bathochromic shift of the special-pair, the preference for L-branch ET or the photoprotective action of BB in *R. sphaeroides* amongst others and therefore provide a new chemical rationale for understanding these processes. It is thus valid to suppose that the conformation contributes to some of these observables, possibly in a deliberate rather than coincidental way; that nature has not only selected the primary structure of proteins to affect the desired protein conformations and cofactor spatial arrangements but also to induce particular cofactor conformations. The concept of conformational control of tetrapyrrole cofactors can clearly be used to address questions of functional significance in the bacterial photosynthetic reaction center in a statistically reliable manner. This indicates the general validity this concept and indicates that it can be extended to hemes and other systems and serve as a model for structural cofactor modulation in general.

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Notes and references

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† Electronic Supplementary Information (ESI) available: Explicit descriptions of the R packages and functions used and data configurations, detailed descriptions of the analytic process, all relevant conformational data for all subsets and NSD bases (including coordinates), details of each PDB structure assessed and classified, and all individual cofactor NSDs. See DOI: 10.1039/b000000x/

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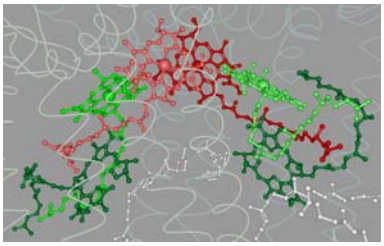
GRAPHICAL ABSTRACT:



Each of the chemically identical cofactors of the electron transfer chain of purple bacteria adopts distinct conformations induced by the apoprotein. In describing how these conformational modifications contribute to ETC function, a chemical rationale for their biofunctional utility is proposed in which the protein exerts conformational influence upon the cofactor to affect desired properties. This serves as a general model for the control of tetrapyrrole function in nature.

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Supplementary Information

Conformational control of cofactors in nature – Conservation of tetrapyrrole conformations in the photosynthetic reaction centers of purple bacteria

Stuart A. MacGowan and Mathias O. Senge

Contents

1 Note on content

Other than to provide the appropriate data and detailed experimental methods used by and produced from our analyses there are three major purposes of this supplement. The first is to show how we proved that almost the entire set of published reaction centre (RC) crystal structures was in agreement of with the idea of distinct conformations for each of the cofactor functionalities of the electron transfer chain (ETC). The second point is to provide explicit justification and to describe the process for/by which we have partitioned the reaction centre crystal structures, in particular the *R. sphaeroides* set, based on the resolved conformations of their ETC cofactors (Section 4). Finally, the third purpose is to illustrate the local nonplanar distortions of the cofactors (*i.e.* in terms of their individual atomic z-axis displacements; Section 5) and consequently, to demonstrate the specific adequacies of the NSD reduced basis sets that are cited in our work as a suitable vantage point from which to compare their conformations.

In brief, Section 2 contains the detailed experimental methodology that would be required to reproduce our work. A brief account of the analysis that confirmed that the crystal structure data were consistent with, and would yield, distinct cofactor conformations for each of the functionalities is relayed in Section 3 followed by the logic, rationale and analysis behind the crystal structure partitioning in Section 4, including our argument for the selection of the best candidate crystal structure set to derive the mean cofactor conformations. Section 5 provides the full, quantitative conformational description of the conformations of each cofactor from each of the crystal structure subsets as well as the appropriate descriptive statistics. This includes the NSD data of the reduced basis deemed adequate for describing each particular conformation in both chart and tabular form; skeletal deviation plots of the cofactors from the most relevant subsets and the cofactor coordinates that we have derived. We have also provided brief descriptive conformational overviews of the cofactors we consider to be the most important from the set of crystal structures we determined to be most reliable, to place the data in context, and in addition we include a brief discussion of the magnitude of the potential physicochemical impact of the distortions. Finally, the PDB structures that were included in the study are presented in Section 6, references in Section 1 and the individual NSDs for each of the cofactors are given in Section 8.

2 Experimental Methodology

2.1 Data-acquisition, processing and NSD

The raw data, *i.e.* the cofactor atomic coordinates, were downloaded in batches by PDB ligand I.D. from the PDB Ligand Expo site (www.ligand-expo.rcsb.org; last accessed: 30th April 2011), which is part of the RCSB PDB[1] (www.pdb.org) project. Specifically, every BCL (BChl a), BCB (BChl b), BPH (BPhe a) and BPB (BPhe b) found in the directory as of 18/10/2010 was downloaded in .ipdb format on that day; the BH1 cofactors (BPhe a of structures 2BNP, 2BNS and 2BOZ) were downloaded subsequently on 28/03/2011. Additionally, any cofactor structure that included alternate conformations was recompiled as two separate structures and the NSD of both were obtained. The PDB structures included are identified in Section 6.

The macrocycle of each cofactor was decomposed into deformations along its normal deformations by the procedure of normal-coordinate structural decomposition[2] (NSD). The NSD computations were carried out using the online NSD Web Program[3] with each cofactor oriented consistently, as described in the program's online documentation; the program automatically performs the NSD computation on any tetrapyrrole structure in PDB format. In order to speed up the tedious process of loading the coordinates, running the decomposition, re-orienting the structure to obtain consistent signs (phases) for the normal-coordinates and storing the results, a short macro that automated much of the process (excepting operator verification of the cofactor orientation) was written and implemented in the AutoHotkey scripting language.

2.2 Statistical analyses

The preliminary analysis that is described in Section 3 involved the agglomerative hierarchical clustering (AHC) of each of the cofactors' minimum basis NSD results in order to discover whether or not the crystal structure data were consistent with the idea of distinct cofactor conformations for each of the functionalities. Thus, the AHC was performed on data matrices containing observations of the NSD minimum basis for each of the cofactors of a given species' with the XL Stat plugin for Microsoft Excel using the Euclidean distance measure to build the dissimilarity matrix and Ward's method for the agglomeration.

The collected NSD data were then treated so that each X-ray structure (PDB entry) was considered as an individual observation and the minimum basis NSD deformations of its cofactors the observables. In detail, the data was formed into an *m* x *n* matrix where *m* is the number of crystal structures included and *n*, the number of variables, equals the number of cofactors included (*i.e.* four bacteriochlorophylls or two bacteriopheophytins) times the number of basis parameters used (*i.e.* B2u_m_BA* is a distinct *variable* from B2u_m_BB and there is no categorical variable for cofactor function); in the analyses of the experimental effects that follow, the 12 normal-coordinates of the minimum basis were used for each cofactor. The result of this approach was the potential to isolate so-called batch effects that are present from particular (sets of) structure determinations *via* variable-axis rotations from methods such as principal component and factor analysis (PCA and FA). The analyses presented in Section 4 were all performed on data matrices in this configuration.

* *i.e.* minimum basis B2u displacement of cofactor BA

The kernel density estimations, Euclidean dissimilarities, FAs and the PCAs used were calculated in the R programing environment[4] using the *kde*, *daisy*, *factanal* and *prcomp* functions in the ks, cluster and base libraries, respectively. The bandwidth parameters, h, of the KDEs were chosen using the plug-in selector, executed with the hpi (or Hpi for bivariate KDEs) function also in the ks library. The decision as to the number of factors extracted in the factor analyses was made based on our initial exploratory analyses (Section 4). The data matrices were untransformed; Varimax rotation was performed in the FAs and the crystal structure scores were computed using the regression method.

Once the crystal structure set partitioning was complete, the mean (arithmetic) normal-coordinates were calculated to yield the average conformation of each of the cofactors in each subset of crystal structures (Section 5). Both the sample standard deviation (SD) and standard error of the mean (SE) are given where appropriate as measures of the sample variation; the SD represents the observed single experiment precision of each of the measured parameters whereas the SE should provide appropriate confidence intervals for the precision of the sample[*].

2.3 Re-centred NSD

Included also in Section 5 are tabular listings of NSD data that we have termed as the 're-centred NSD' (Section 5.7). These data were obtained by performing the NSD computation on coordinates that were obtained from the statistical mean complete basis NSD for each cofactor of each subset (coordinates which are approximately equivalent to averaged atomic coordinates). For example, the re-centred NSD of cofactor DL from subset RBC4 was obtained by converting the corresponding statistical average NSD deformations of the complete basis to Cartesian coordinates and then performing the NSD computation on this structure. The reason for doing this was twofold; to obtain the Doop and δoop parameters for the mean conformation and also to ensure that the mean NSD deformations were representative of the NSD of the mean conformation. This latter point was considered a prudent check since the extended and complete basis sets are not completely orthogonal[2b], although we did not expect any substantial deviation owing to the relatively small dot products of the normal-deformation vectors[2b] and our own analysis of the numerical stability of NSD based on the condition numbers of the basis matrices. Whilst the complete basis re-centred molecular conformations are precisely the same as those given by the mean results the NSD description of this conformation may have been different due to the nonorthogonality of the complete basis.

3 Preliminary analysis: Confirming experimental consistency with distinct cofactor conformations

Preliminary analysis of the collected data was performed using agglomerative hierarchical clustering (for AHC details see Section 2.2) to identify structures bearing similar conformations, in terms of the in– and out-of-plane distortions of the minimum basis.

The *Blastochloris viridis* AHC (Figure 1) shows that there were six clusters of cofactors bearing similar conformations (including one cluster of a single structure, indicating its relative uniqueness) each of which contained predominantly only structures of one particular ETC functionality. Specifically, the cluster pattern demonstrates that the DM and DL cofactors (*i.e.* each half of the special-pair) are conformationally distinct from the accessory monomers and also from each other (although they are related relative to the rest as seen by the position of their cluster union in the dendrogram; top right, Figure 1). It is also seen that the first accessory cofactors (BA and BB) form a distinct group but are on the whole not distinguishable from each other whilst the second accessories (ΦA and ΦB) form two groups, each predominantly composed of one of either ΦA or ΦB, but not exclusively, and that these clusters are also closely related. The cluster that consists of a single observation was identified as a DM cofactor from a 'hetero-dimer' mutant structure where the DM bacteriochlorophyll had been replaced with a bacteriopheophytin; but note its proximity to the main DM cluster. The OOP mean conformations of each of the cofactors that were correctly classified are also displayed with these results (bottom left, Figure 1).

Similar to the above, the *R. sphaeroides* AHC proved that there were distinct conformations for each of the functionalities in this species too (Figure 2), the main difference being the presence of a cluster that predominantly contained the BB cofactors and the closeness of the DL group to that of the BA's (implying their conformational similarity). In addition, whilst there were two groups for the accessory bacteriopheophytins, the cluster membership for each group was split equally between ΦAs and ΦBs. Also note that the BA group not only contained the vast majority of the BA cofactors, but also a significant number of the other bacteriochlorin functionalities (*i.e.* BB, DM, and DL; bottom right, Figure 2).

[*] Whilst we do not assert that the samples themselves are normally distributed we do invoke the Central Limit Theorem to state that the sample mean should be so and hence the SE provides approximate 95% confidence intervals for the means. The SDs may provide a useful test to see whether we have accounted for all of the systematic variation of the data by comparing them to the theoretical precision of a single experiment. However, we have not attempted this here as this calculation, to our knowledge, is not trivial. To do so, one would need to know the approximate experimental error in each NSD at a given resolution and would need to take into account: the theoretical mean atomic positional error, a reduced dimensionality component owing to separation of the in- and out-of-plane coordinates (already performed by Jentzen *et al*), the error in the calculation of the mean plane, the effect of restraints on these errors and possibly, owing to the random distribution of positional error, its probabilistic propagation into each mode given the nodal (phase change) patterns of the different normal-deformations. In addition to this later point, should probabilistic concerns be minor, at the very least one would need to know entrywise condition numbers for the NSD calculations.

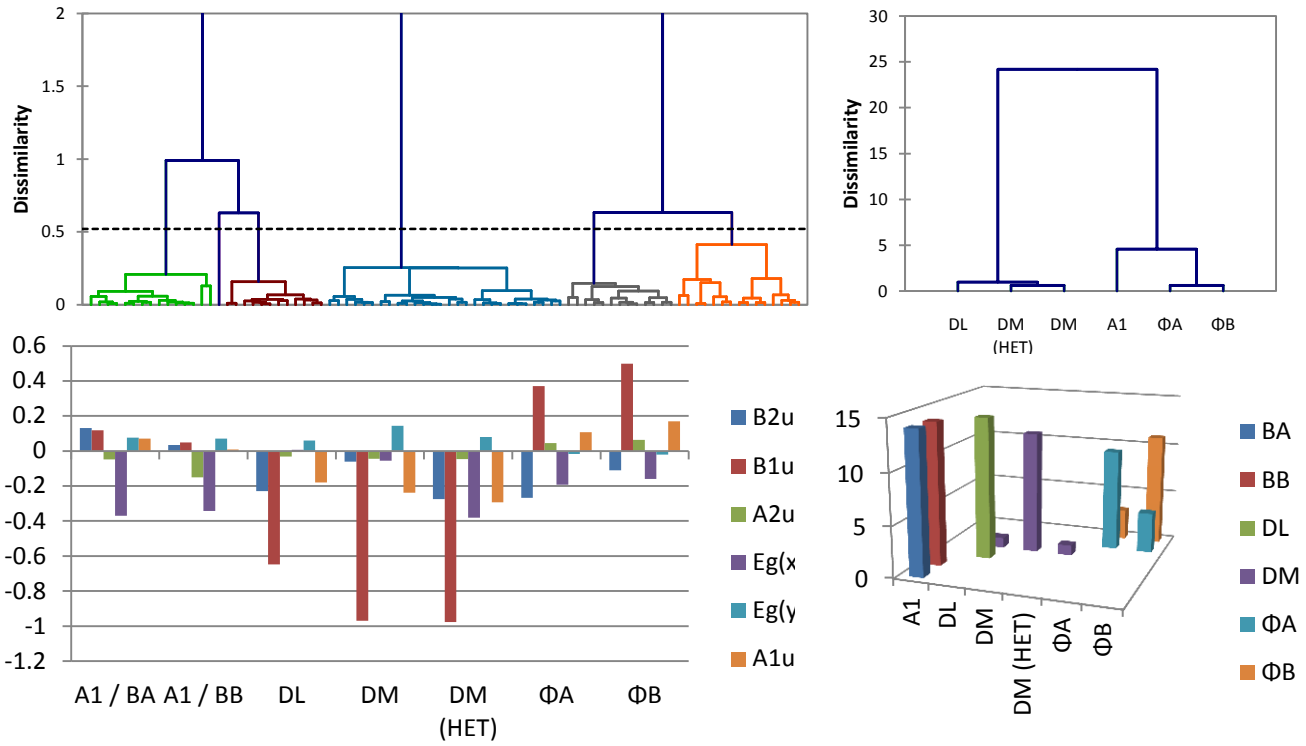

Figure 1: Initial AHC of *B. viridis* data. Cluster dendrograms (top) showing the clusters that predominantly contain DL (green), DM (brown), A1 (blue), ΦA (grey) and ΦB (orange) cofactors and their relationship; dissimilarity is given by Wards' criterion. Cluster assignment by function (bottom right); the axis labels indicate the cluster as seen in the dendrogram and the coloured bars enumerate how many cofactors of that functionality were present in the cluster. Mean minimum basis distortions of the correctly classified cofactors (bottom left; *i.e.* of cofactors that were present in the cluster pertaining to their functionality). n= 84, within class variance = 0.053 (12.59%), between class variance = 0.371 (87.41%).

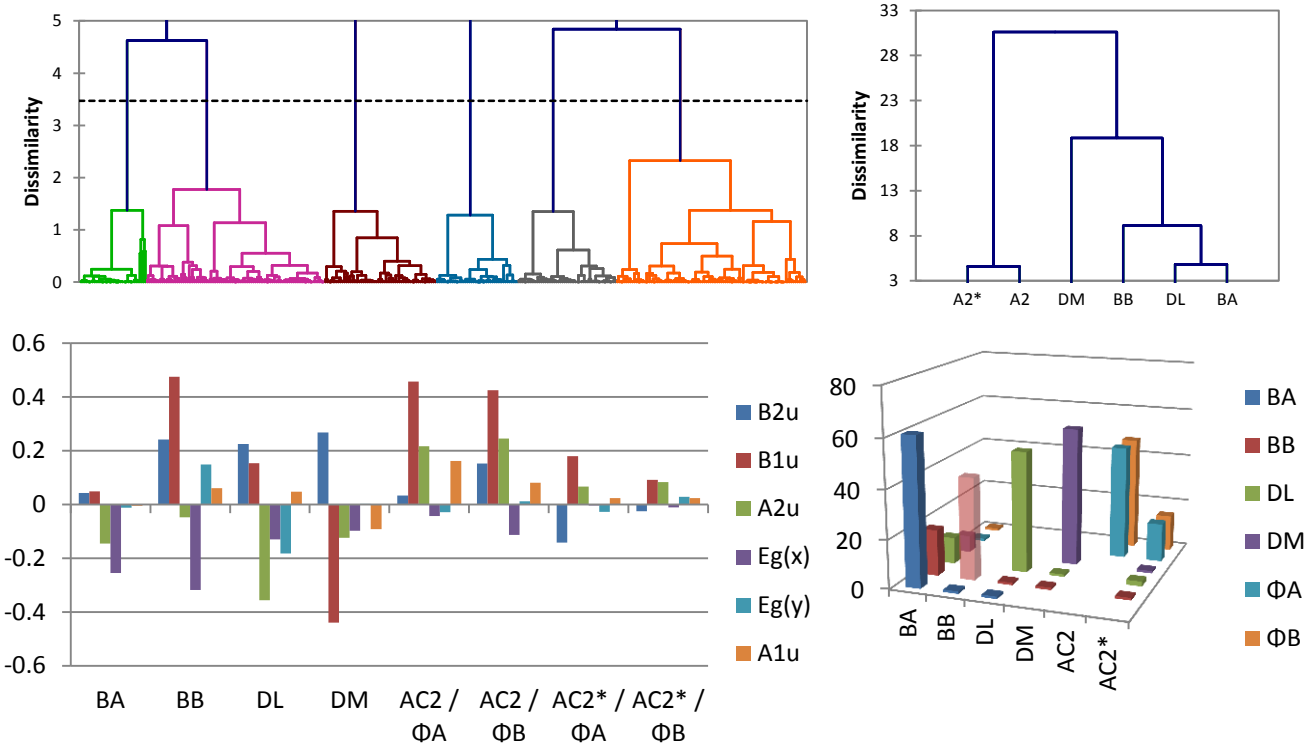

Figure 2: Initial AHC of *R. sphaeroides* data. Cluster dendrograms (top) showing the clusters that predominantly contain DL (grey), DM (brown), BA (orange), BB (blue), and the two clusters containing the bacteriopheophytin, AC2 (pink) and AC2* (green) cofactors and their relationship; dissimilarity is given by Wards' criterion. Cluster assignment by function (bottom right); the axis labels indicate the cluster as seen in the dendrogram and the coloured bars enumerate how many cofactors of that functionality were present in the cluster. Mean minimum basis distortions of the correctly classified cofactors (bottom left; *i.e.* of cofactors that were present in the cluster pertaining to their functionality). n = 383, within class variance = 0.104 (37.04%) and between class variance = 0.177 (62.96%).

The explanation of these features rest in the conformations of the functionalities, as captured by the mean deformations (bottom left, Figures 1 and 2). Thus, in *B. viridis* the BAs and BBs are similar in their relative absences of the B1u (ruffle) deformation and the DLs and DMs differ mostly in the extent, rather than make-up, of their distortions (DM being the most distorted cofactor). In contrast, the *R. sphaeroides* BB cofactor exhibits a predominant and considerable B1u distortion and its DL is very different from DM owing to a phase change of the B1u mode and the predominance of a large A2u (dome) distortion. Furthermore, owing to the relative planarity of the BA type in *R. sphaeroides* (which appears to be a conserved feature between the species) it should be clear that the 'misclassified' (*i.e.* non BA cofactors in this group) display similar, near planar conformations and it should also be noted the AC2* set contains relatively planar ΦAs and ΦBs. Finally, whilst in both species the bacteriopheophytins are quite distinct from the bacteriochlorin cofactors (particularly in *R. sphaeroides*), neither species contains completely differentiable second accessories (in terms of A- / B- branch differentiation).

The interpretation of these results goes as far as to say that our initial hypothesis was somewhat validated; in that the protein scaffold imposes a rigid conformation on each of the cofactors, illustrated by the overall correct grouping of the cofactors' conformations by functionality. However, a critique of these observations would in fact point out that the only conclusion that can be definitively drawn is that the *majority* of the data is consistent with this hypothesis. In fact, on closer inspection we find that, for example, the PDB structures that contain planar DMs (a significantly nonplanar cofactor in most of the structures) report planar conformations for all the cofactors. Thus, a minority of structures are actually consistent with all of the cofactors having planar conformations. Of course, one could say simply that these are anomalous given their lesser numbers, but this would not be proper scientific process.

Fortunately, these types of results were anticipated at the outset of the investigation owing to the fact that the process of crystal structure determination is not always just a measurement of molecular dimensions; it often uses chemical knowledge to fill in the gaps that are present from lower resolution studies such as these. With this in mind, the extent of any aromatic planarity restraints, or in the extreme case, the presence of any such constraints may affect the observations of the planar macrocycles. Alternatively, it may be simply that the crystallographer felt that owing to the low resolution of his study, he could not comment accurately on the detailed conformation of the cofactors, and solved this part of the structure using rigid-body refinement of planar macrocycles.

There was one other such systematic variation between some of the structures in the *R. sphaeroides* data that became apparent during the initial AHCs. Notice in the dendrogram (top left, Figure 2) that there is a systematic pattern within each of the clusters, which indicates that there is more order to the data than simply the distinct conformations of the functionalities. Since the complete description of this variation *via* the more detailed AHCs that were carried out is laborious and difficult to follow, it suffices to say that following a similar method we discovered a subset of structures that differed in the extent of their nonplanarity and exhibited an unusual in-plane conformation and then to move on to the mode of analysis which uncovered the patterns of experimental origin.

4 Analysis of Measurement Effects

4.1 Justification of the Partitioning of the Crystal Structure Datasets

The significance of the following classification of the X-ray crystal structures of the bacterial electron transfer chains under study, based on the observed conformations of their tetrapyrrole cofactors rests on only one simple hypothesis:

> ***That for the most part, there is no physical reason that the conformations of the cofactors should be coupled, beyond that of the possibility of conformational change in charge separated states, perturbations to cofactor geometry induced by point mutations of the apoprotein or steric and electronic interaction of the special-pair, so that any such observed conformational coupling results predominantly from experimental origins.***

That is to say that the cofactors are sufficiently removed from one another that the observed systematic differences between all of the cofactors of a given structure and another's geometries arise because of systematic differences between the measurements and not because of systematic differences between their conformations. As an example, consider two hypothetical crystal structures A and B. If the four bacteriochlorophyll cofactors of A exhibit consistently and quantitatively precise increased nonplanarity over those of B, such that the relative difference between the conformations of the cofactors within each structure is maintained then we may draw two conclusions:

1) The relative differences of this conformational parameter between the specific cofactor functionalities has been measured precisely by both experiments
2) In the absence of any chemical or physical explanation of this difference the effect must arise from a systematic difference between the measurements of the two samples.

This is an ideal example (with obvious conclusions); in reality due to the random distribution of experimental error it is highly unlikely that such differences would obtain quantitative precision. However, this does not present a problem since our dataset (particularly of structures of *R. sphaeroides*) is moderately large and our applications of principal component analysis (PCA) and, in particular, factor analysis (FA) are able to resolve such features over this noise.

With reference to the possible exceptions stated in this hypothesis, it was assumed that the experimentally correlated systematic differences would overwhelm such features. For instance, it is reasonable to suppose that in the charge-separated state a change of the conformations of the P^{+} and ΦA^{-} cofactors, relative to their ground-state neutral counterparts would occur, however subtle. This would manifest itself as a systematic difference between structures in these two states and may be recoverable as a factor in the FA. We have not, however, found such a factor and though its definitive exclusion would require an even deeper statistical analysis, it is likely that the combination of the slightness of the change and the relatively low resolutions of the structures would make a feature such as this presently unobservable. Also, point mutations close to any of the cofactors may sometimes affect a change in their conformation, as has recently been demonstrated experimentally and were these perturbations larger than the experimental error one would expect systematic differences to be observed between structures of different mutations. However, again we have not been able to detect such features but if they are present there is no reason for them to have an effect on our results stated in this work.

However, on the other hand, it cannot be asserted with absolute authority that the inter-crystal structure set differences to be described do not represent real conformational differences; we consider this is quite unlikely (see also Section 4.6). In any case, the structure subsets should not be treated together since in such a situation that there was a chemical or physical reason for the coupling of the conformations so that the differences were actual (that we have not picked up on), these differences are so large compared to those within each set that they would have to be taken as an indication that the cofactors adopted multiple discrete conformations and so they would need to be treated separately anyway. It is for this reason that we have provided details of all the crystal structure subsets in this supplement.

4.2 *Rhodobacter sphaeroides* bacteriochlorophylls

Our exploratory analyses indicated that there were systematic differences between sets of structures as well as the inter-cofactor conformational data structure that was our target. These structure solution based differences are 'batch effects' of the crystal structure determinations and knowledge of their precise identity, character, elemental composition and origin were required to ensure a sound analysis. We identified four distinct sets in the *R. sphaeroides* bacteriochlorophyll dataset:

1. Structures that did not exhibit reasonable experimental variation (**RBC1**; n = 9)
2. Structures that resolved the cofactors as planar or near planar (**RBC2**; n = 18)
3. Structures with unusual in-plane conformations (**RBC3**; n = 16)
4. Structures that appear most reliable (**RBC4**; n = 32)

The purpose of this supplementary section is to provide the necessary information and derivation required to partition the data (*R. sphaeroides* bacteriochlorophyll set) into these clusters and also the (publically available) material required for their explanation.

4.2.1 *Tied* structures

The inter-structure Euclidean distance plot (Figure 3) shows a distinct group of outliers with near zero dissimilarity; it is clear that they originate from a different statistical distribution since they are present only after a distinct discontinuity of the empirical cumulative distribution of this parameter. Close inspection of the source of these outliers shows that they are closely related in terms of their experimental circumstance (*i.e.* they were measured at the same time by the same group (see Section 6, Table 41) and share a common starting model. We therefore interpret this subset as erroneous due to lack of appropriate experimental variability as they are replicas and do not represent independent measurements. The structures identified as such are labelled RBC1 (Section 6.1, Table 41) whilst the mean conformations exhibited by each cofactor may be found in Section 5.4.1, Figure 12.

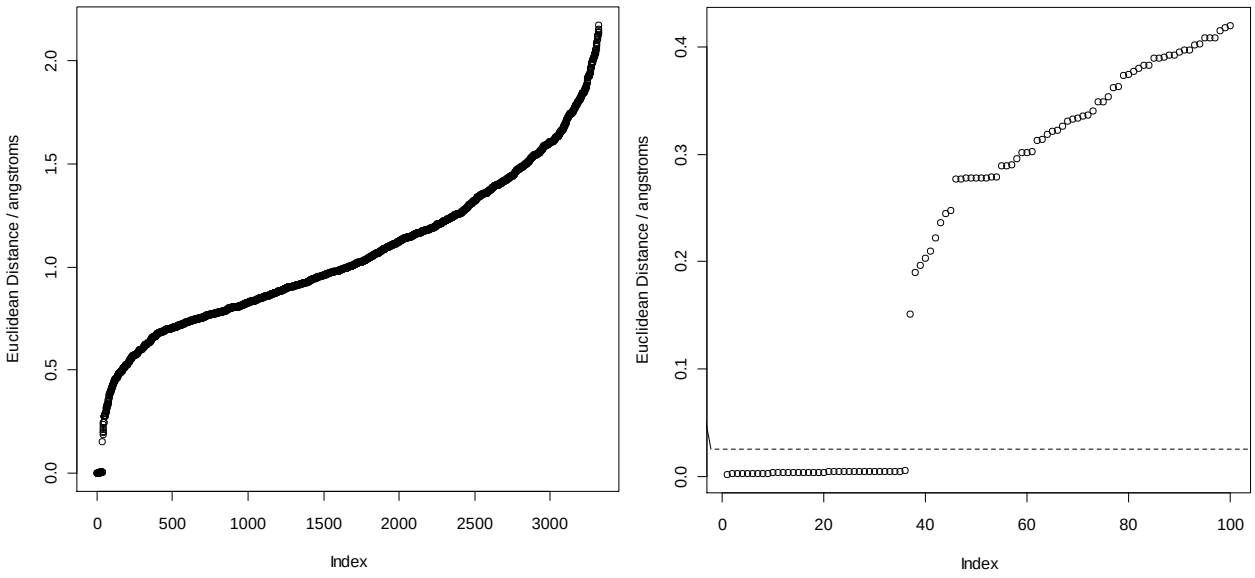

Figure 3: Plot of inter-structure Euclidean distances of minimum basis from all *R. sphaeroides* bacteriochlorophyll cofactors.

4.2.2 Factor analysis: Identification of Crystal Structure Experimental Variations

Subsets **RBC2** (planar / near planar bacteriochlorophylls) and **RBC3** (contracted bacteriochlorophylls) were identified in our original analyses through a combination of graphical and numerical exploratory measures. However, we found that we could express these findings most concisely in the form of an exploratory factor analysis (EFA). The optimal EFA was found to consist of two Varimax rotated factors, accounting for 44.1% of the total variance (22.6 and 21.5% each, respectively), extracted from the structure bacteriochlorophyll minimum basis data matrix. The factor loadings (Table 1) demonstrate that Factor 1 (F1) is mostly related to the nonplanarity exhibited by the cofactors in the structure determination whilst Factor 2 (F2) accounts for the observed structures with unusual in-plane conformations. With these loadings in mind, the apparent clusters observable in the plot of the structure scores (Figure 4) are readily identified, *i.e.* structures with a large negative score on F2 (mostly bottom left in Figure 4) exhibit unusually contracted macrocycles together with enhanced nonplanarity, particularly along the higher energy normal-modes (illustrated by *δoop* loading) whilst those crystal structures with a positive F1 value have resolved near planar cofactors. We therefore identify the bottom left cluster as **RBC3** and the top and middle right clusters, which exhibit near planar and minimally nonplanar conformations (respectively) as corresponding to **RBC2** (with descriptive statistics given separately as RBC2a and -2b, respectively, in Section 5.4.1) The remaining cluster (top left), which contains the highest proportion of structures of a single cluster, is identified as **RBC4** which contains structures that exhibit significant nonplanarity with in-plane deformations akin to those of isolated related compounds. Also, note that we have treated structures that fall significantly outwith the level 25 regions of the KDE contours as outliers (OLs; see Section 6.1 for affected structures).

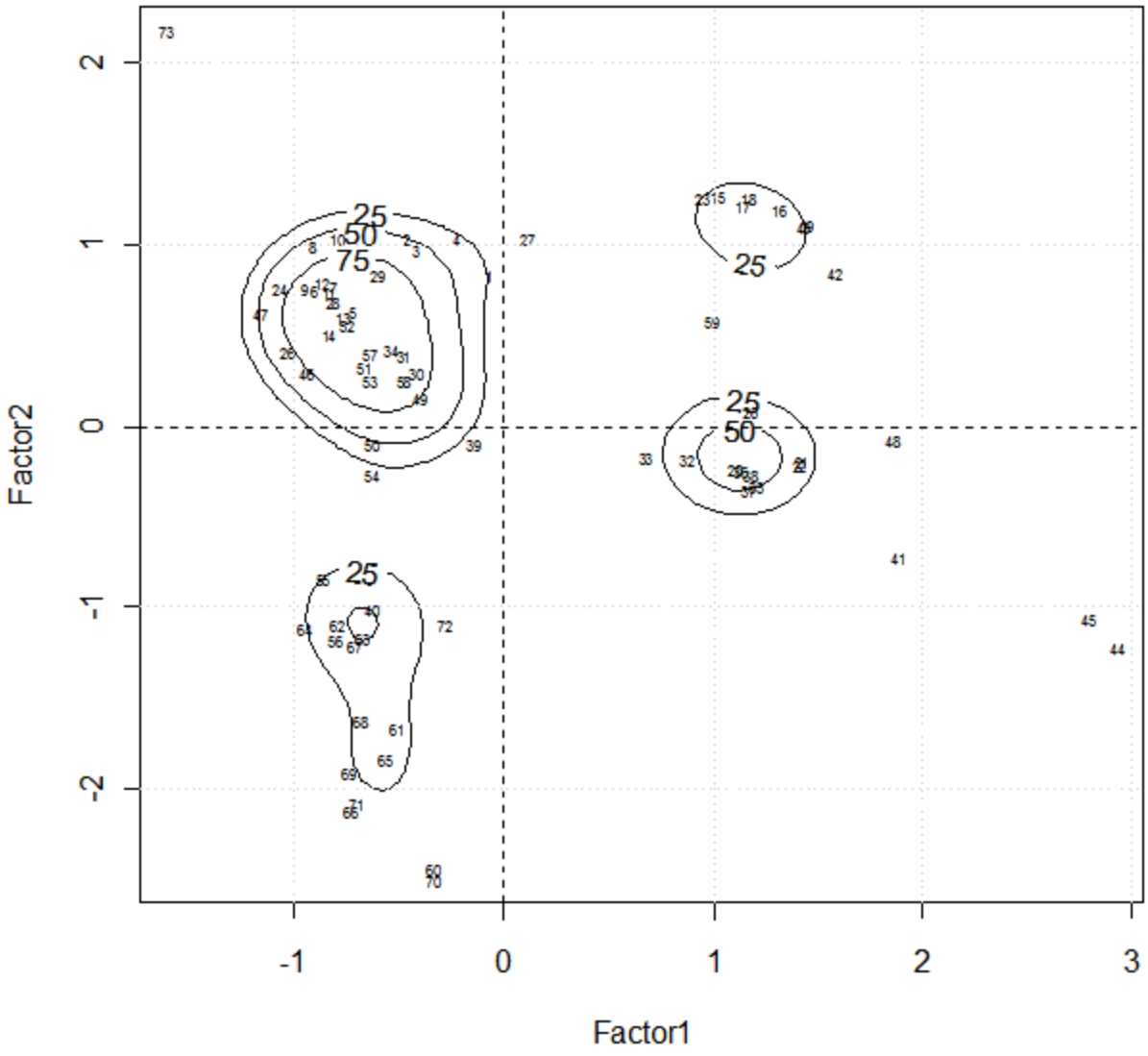

Figure 4: Plot of the structure scores, on the Varimax rotated factors, computed by the regression method with kernel density contours overlaid (bandwidth matrix computed using the plug-in selector). Structure key in Section 6.1.

Table 1: Loadings of the original variables onto the Varimax rotated factors. Loadings in highest 25% for each factor are marked in bold italic.

	DM	DL	BB	BA	DM	DL	BB	BA
		Doop				***Dip***		
F1	***-0.857***	***-0.844***	***-0.823***	***-0.767***	0.301	0.082	-0.067	-0.011
F2	-0.406	-0.428	-0.411	-0.457	0.290	0.522	0.264	0.263
		δoop				***δip***		
F1	-0.435	-0.543	-0.419	-0.512	***0.851***	***0.798***	***0.687***	***0.731***
F2	***-0.743***	***-0.752***	***-0.707***	***-0.733***	-0.210	-0.246	-0.013	-0.072
		B2u				***B2g***		
F1	***-0.697***	-0.526	***-0.712***	-0.421	0.496	0.243	0.084	-0.115
F2	-0.319	-0.128	-0.273	0.066	-0.297	-0.410	***-0.586***	-0.382
		B1u				***B1g***		
F1	***0.837***	***-0.618***	***-0.797***	-0.295	0.196	0.194	0.359	0.372
F2	0.341	0.225	-0.357	0.178	0.230	0.262	0.299	0.378
		A2u				***Eu(x)***		
F1	0.389	***0.784***	-0.100	0.240	-0.382	-0.191	-0.338	-0.273
F2	0.341	0.419	-0.105	0.207	-0.100	-0.209	-0.286	-0.048
		Eg(x)				***Eu(y)***		
F1	0.467	0.343	***0.745***	***0.735***	0.443	0.167	0.551	-0.014
F2	0.286	***0.645***	0.496	***0.563***	0.010	0.338	0.228	-0.172
		Eg(y)				***A1g***		
F1	0.272	0.597	-0.397	0.243	0.028	0.136	0.071	0.063
F2	-0.224	0.479	-0.244	0.390	***0.807***	***0.824***	***0.904***	***0.797***
		A1u				***A2g***		
F1	0.472	-0.477	-0.335	-0.164	0.087	-0.083	0.048	0.022
F2	0.550	***-0.584***	-0.432	0.098	***0.863***	***0.771***	***0.875***	***0.838***

4.3 *Rhodobacter sphaeroides* bacteriopheophytins

Given the nature of subsets identified within the *R. sphaeroides* bacteriochlorophyll data, it was expected that similar groups should arise within that of the bacteriopheophytins, in particular, subsets **RBC1** and **RBC2**. Thus, the same analytical methodology (inter-structure Euclidean distance plots and two-factor EFA) was applied here and confirmed the presence and identity of the analogous subsets:

1. Structures that did not exhibit reasonable experimental variation (**RBP1**; n = 10)
2. Structures that resolved the cofactors as planar or near planar (**RBP2**; n = 16)
3. A set consisting mostly of the structures found in **RBC3** (**RBP3**; n = 17)
4. A set consisting mostly of the structures found in **RBC4** (**RBP4**; n = 16)

In addition, in this case, the EFA defined another subset (**RBP5**; n = 10) that had no explicit counterpart in the *R. sphaeroides* bacteriochlorophyll dataset (but does appear to be fairly related to **RBC4**).

4.3.1 *Tied* Structures

The inter-structure Euclidean distance plot based on the *Rhodobacter* bacteriopheophytin data (Figure 5) shows the presence of a subset of structures that exhibit effectively no experimental variation. As would be expected, included in this set are the structures from its counterpart in the bacteriochlorophyll data, **RBC1** (see Section 6.1). However, in this case there is one extra structure exhibiting the lack of any experimental variance, namely PDB ID: 1QOV.

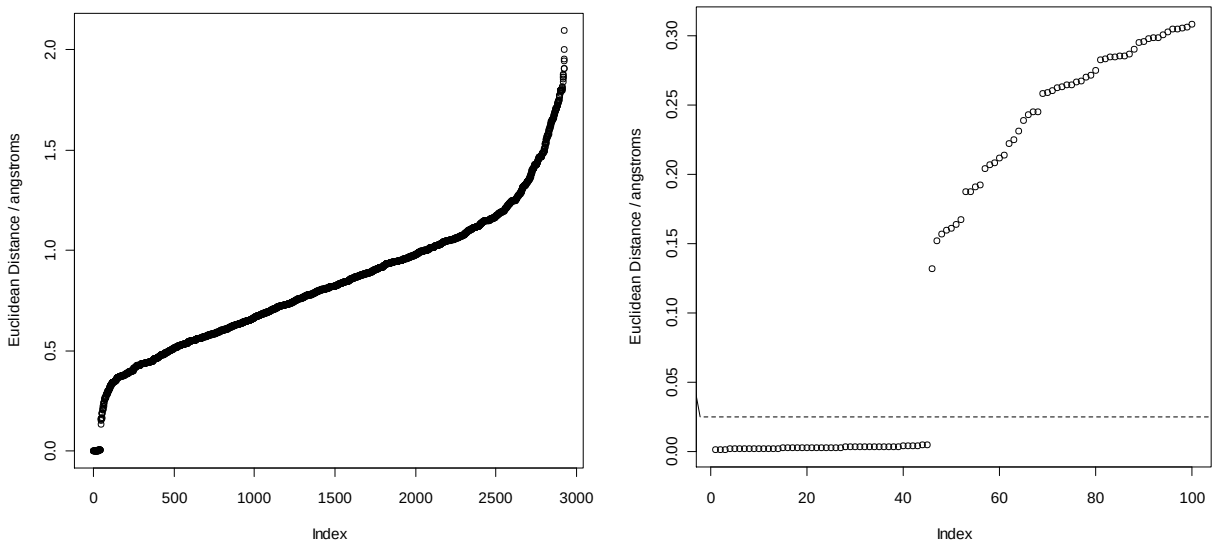

Figure 5: Plot of inter-structure Euclidean distances of minimum basis from all Rhodobacter bacteriopheophytin cofactors.

4.3.2 Factor Analysis

Factor 1 (26.2% total variance; F1) of the *Rhodobacter* bacteriopheophytin EFA (Figure 6 and Table 2) is seen to correlate principally with the observed nonplanarity of the bacteriopheophytins and serves to differentiate, in order of increasing nonplanarity, subsets **RBP2**, **-3** and **-4**. The nature of **RBP2** is a somewhat trivial matter; it is the bacteriopheophytin counterpart of **RBC2** in both composition (PDB structures; see Section 6.1) and conformational structure (planar cofactors). The differentiation of **RBP3** and **-4**, however, is more interesting since these sets are composed of the same structures that are found in **RBC3** and **-4** (Section 6.1) and whilst in this case they are not separated on account of an in-plane A1g contraction, they are separated by numerous in- and out-of-plane parameters (Table 2), such that the difference between **RBP3** and **-4** is quite similar, qualitatively (compare NSDs in Section 5.4.3), as that of **RBC3** and **-4**. This is particularly apparent from the large positive Doop and δoop on F1, but is more readily apparent from the relevant mean δoop values as well as the reduced basis/actual conformation comparisons in Sections 5.4 and 5.5.1. Note also that factor 2 accounts for 14.1% of the total variance and that the total variance accounted for by the two factors is 40.3%, which is very similar to the variance accounted for by the two factors in the corresponding bacteriochlorophyll analysis (44.1%) which confirms their relationship further. That F2 in this analysis accounts for less variance than its counterpart in the bacteriochlorophyll set is readily acceptable since by comparison of the two analyses (below, Figure 6 and Section 4.2.2, Figure 4) shows that in this analysis RBP3 is differentiated from RBP4 by a combination of F2 and F1, as opposed to the differentiation of the related bacteriochlorophyll crystal structure sets (RBC3 and RBC4) by F2 alone.

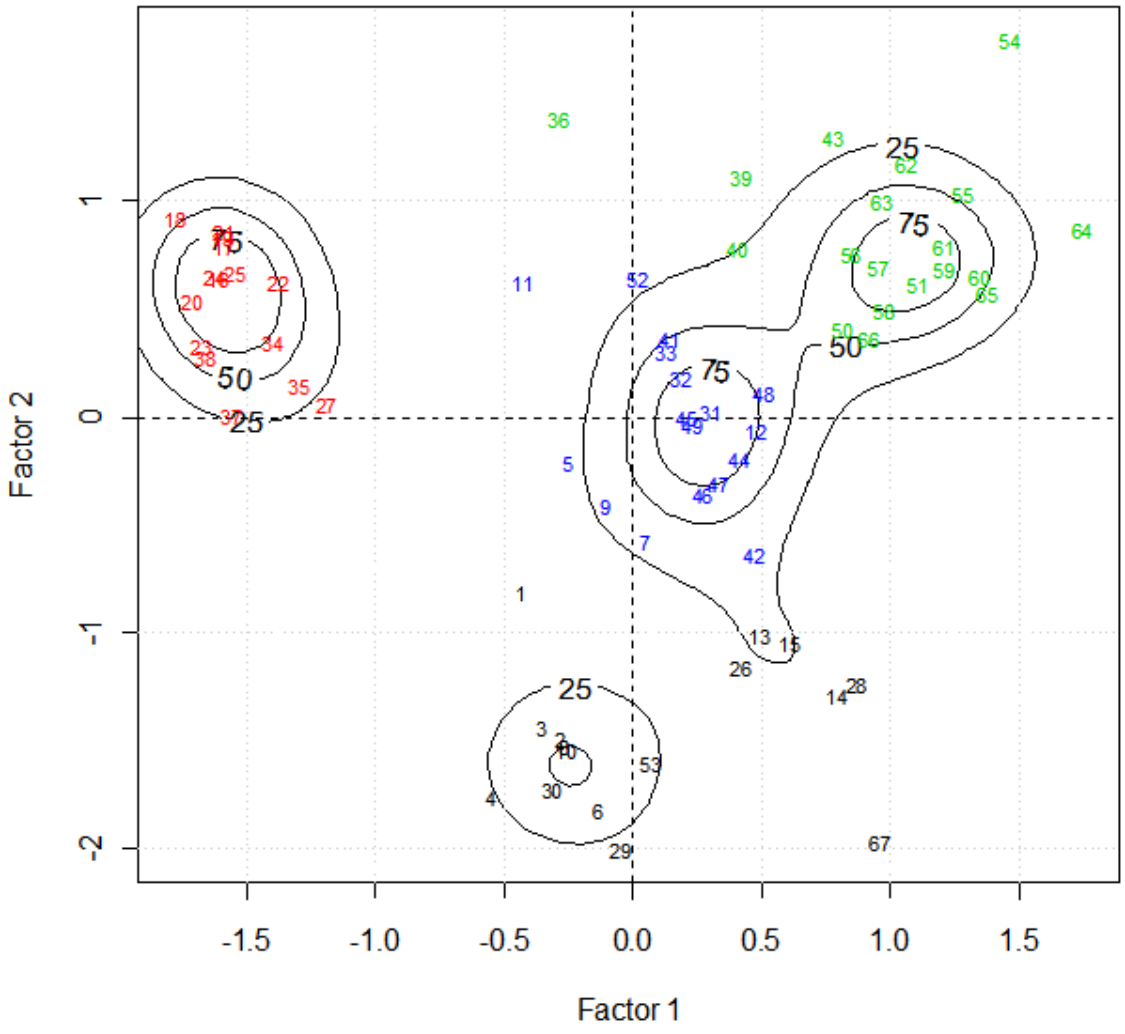

Figure 6: Plot of the structure scores, on the Varimax rotated factors, computed by the regression method with kernel density contours overlaid (bandwidth matrix computed using the plug-in selector). Structure key in Section 6.1; colouring for illustrative purposes only.

Table 2: Loadings of the original variables onto the Varimax rotated factors. Loadings in highest 25% for each factor are marked in bold italic.

	Factor 1		*Factor 2*			*Factor 1*		*Factor 2*	
	ΦA	***ΦB***	***ΦA***	***ΦB***		***ΦA***	***ΦB***	***ΦA***	***ΦB***
Doop	***0.842***	***0.921***	-0.037	-0.087	***Dip***	0.291	0.187	***0.583***	***0.869***
δoop	***0.870***	***0.830***	0.213	0.285	***δip***	0.008	0.044	***0.459***	***0.670***
B2u	0.220	0.596	0.032	0.155	***B2g***	0.213	0.302	***0.681***	***0.579***
B1u	***0.741***	0.663	-0.205	-0.279	***B1g***	-0.277	-0.105	-0.392	***-0.732***
A2u	***0.758***	***0.797***	0.030	-0.040	***Eu(x)***	-0.389	0.019	-0.142	-0.093
Eg(x)	-0.287	-0.438	-0.200	-0.241	***Eu(y)***	-0.047	-0.176	-0.374	-0.315
Eg(y)	-0.155	0.056	0.122	-0.234	***A1g***	-0.018	-0.036	0.117	***0.562***
A1u	0.730	0.431	0.407	0.096	***A2g***	***-0.841***	-0.038	-0.171	-0.038

4.4 *Blastochloris viridis* bacteriochlorophylls

The dataset comprising the conformations of the *B. viridis* bacteriochlorophyll cofactors was neither as large nor subject to as many experimental variations as that of *R. sphaeroides* described previously. However, we found in our exploratory analysis a single structure that appeared to resolve less cofactor nonplanarity than the rest of the experiments (analogous to RBC2, albeit not as extreme). The principal component analysis* of the data was found to best illustrate the deviation of this structure, namely 1PRC, and the overall consistency of the

* Note that the preference of FA over PCA in the preceding section owed itself to the the rotation of the factors allowing their ease of interpretation; FA could not be used here since this data forms an underdetermined matrix.

rest. The first PC of the *B. viridis* bacteriochlorophyll cofactors notably correlates with a number of the nonplanarity parameters (Table 3) such that the negative score of the outlying structure (1PRC; Figure 7) indicates that its cofactors are consistently less nonplanar than the rest of the data. Note also that this PC accounts for 36.72% of the total variance in the data and that the scree plot is consistent with there being the only one significant principle component.

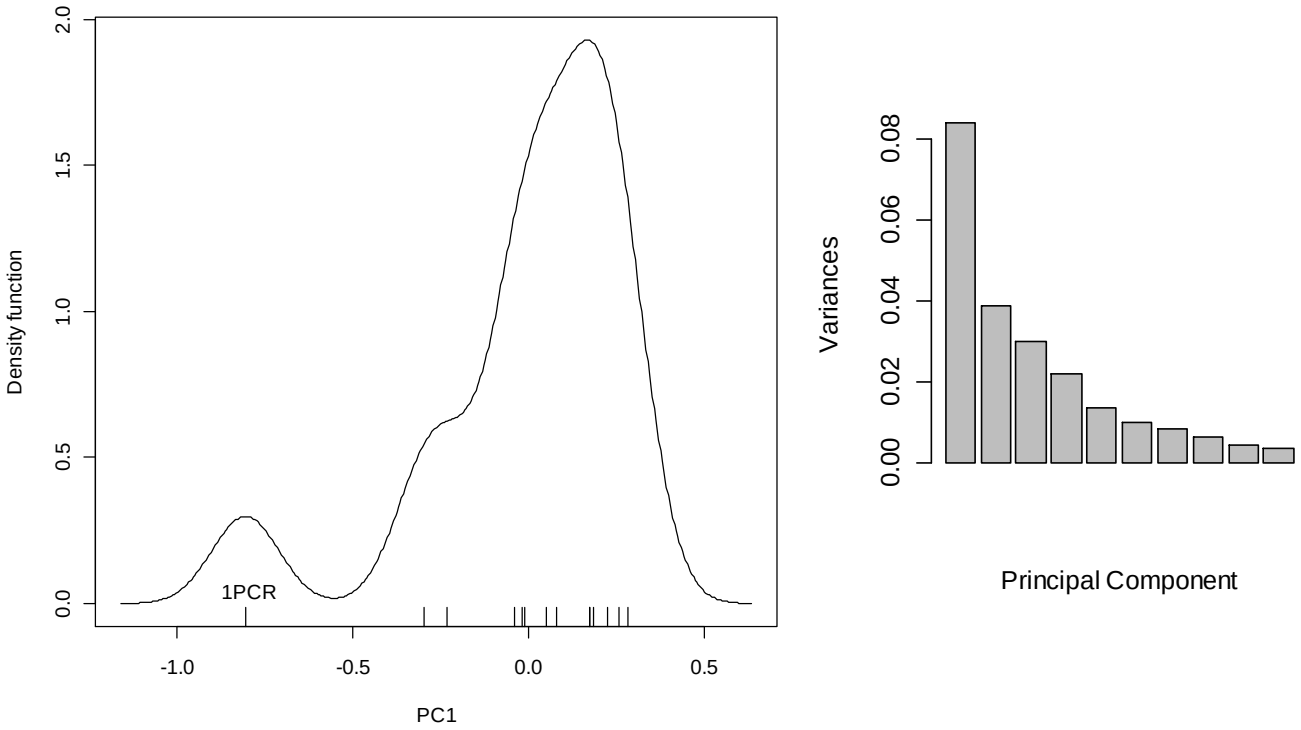

Figure 7: PCA of *B. viridis* bacteriochlorophyll dataset. Kernel density estimate of the distribution of the structure scores on the first principle component (right; bandwidth determined by the plug-in selector, h = 0.0957) and the PCA scree plot (left).

Table 3: Loadings of the original variables onto the first principal component. Loadings in highest 20% are marked in bold italic.

	DM	DL	BB	BA		DM	DL	BB	BA
Doop	***0.281***	***0.363***	***0.270***	***0.205***	***Dip***	0.097	0.032	0.115	0.143
δoop	-0.015	0.001	-0.001	0.002	***δip***	-0.015	-0.014	-0.011	-0.008
B2u	***-0.254***	***-0.159***	-0.157	0.004	***B2g***	-0.092	-0.016	-0.020	-0.033
B1u	***-0.278***	***-0.344***	-0.048	0.039	***B1g***	-0.147	0.019	-0.137	***-0.168***
A2u	-0.039	-0.064	***-0.182***	***0.158***	***Eu(x)***	-0.088	-0.048	-0.039	-0.118
Eg(x)	-0.107	0.060	***-0.255***	***-0.196***	***Eu(y)***	0.107	0.012	0.010	0.031
Eg(y)	0.059	-0.046	-0.005	0.003	***A1g***	0.144	0.076	0.042	0.063
A1u	0.019	-0.032	0.016	0.010	***A2g***	-0.040	0.003	-0.020	-0.11

4.5 *Blastochloris viridis* bacteriopheophytins

Whilst we found no systematic variation in the *B. viridis* bacteriopheophytin conformations that correlated with the crystal structure determinations during our exploratory analyses, we felt it was appropriate to demonstrate this formally (particularly since this result is in contrast to what was found in the *R. sphaeroides* set, where experimental correlations in the bacteriochlorophyll data were echoed in their bacteriopheophytins). As confirmation, the PCA of this dataset (Figure 8) did not exhibit any significant structure in either the scree plot (meaning there are no significant PCs) or the distribution of the structure scores (*i.e.* no readily interpretable features).

However, whilst there is no definite structure to the PCA, the two observations to the right of the plot (Figure 8) flag as potential outliers in the KDE and were therefore assessed separately; it was found that these structures exhibited in-plane conformations that were quite elongated compared to the rest (Section 5.4.4).

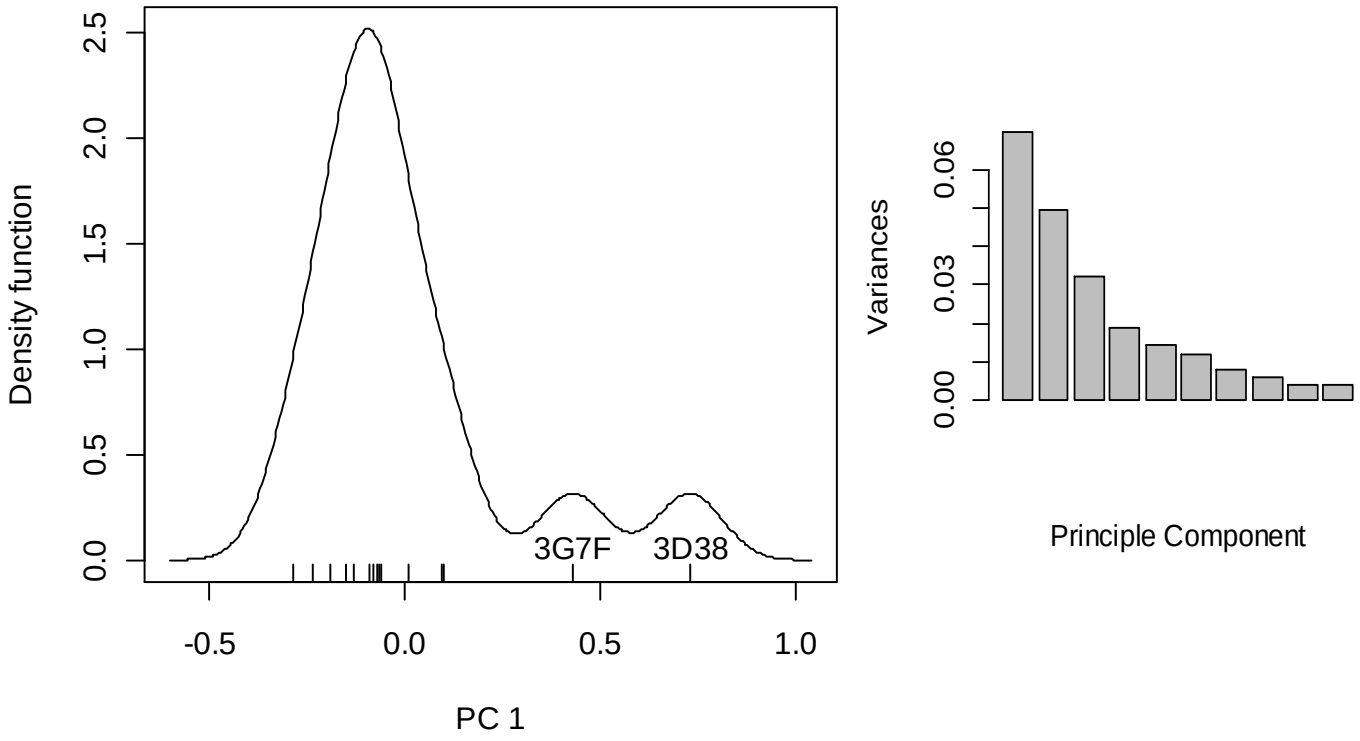

Figure 8: PCA of *B. viridis* bacteriopheophytin dataset. Kernel density estimate of the distribution of the structure scores on the first principle component (right; bandwidth determined by the plug-in selector, h = 0.08419132) and PCA scree plot (left).

Table 4: Loadings of the original variables onto the first principal component. Loadings in highest 20% are marked in bold italic.

	ΦA	***ΦB***		***ΦA***	***ΦB***
Doop	0.017	0.020	***Dip***	***0.310***	***0.350***
δoop	0.027	0.024	***δip***	0.042	0.040
B2u	0.083	***0.296***	***B2g***	0.111	0.223
B1u	-0.072	-0.073	***B1g***	***-0.428***	***-0.309***
A2u	-0.219	0.236	***Eu(x)***	-0.036	-0.117
Eg(x)	0.114	-0.063	***Eu(y)***	-0.042	0.002
Eg(y)	***-0.364***	0.170	***A1g***	0.044	-0.014
A1u	-0.020	0.085	***A2g***	-0.101	-0.108

4.6 Assessment of the Quality of the Conformations

As argued in the justification for the data driven partitioning of the crystal structure determinations (Section 4.1) we believe that the major experimental correlations uncovered in the reaction centre data do not represent any actual differences between cofactor conformations. The need therefore arises for us to assess each of the candidate sets for their potential to deliver reliable structures since it is our view that only one should be correct.

4.6.1 *R. sphaeroides* Crystal Structure Sets

The fact that the experimental types elucidated by each of the *R. sphaeroides* FAs are on the whole correspondent by crystal structure (Table 5, below and Table 41, Section 6), confirms the experimental dependance between the resolved conformations of the BChls and the BPhes. In the case of the *R. sphaeroides* candidates, both the tied structure set (RBC1 and RBP1) as well as the planar structure set (RBC2 and RBP2) of experiments should be rejected and not used for derivation of the mean cofactor geometries. The reasons for this are: the tied structures do not represent independent measurements of the cofactor's geometries and would therefore unduly weight their singular contribution[*] to an average conformation whereas the planar sets are deemed as erroneous since high-resolution crystal structures of isolated and related molecules (*e.g.* Mg-chlorins) exhibit significant nonplanarity and also because of the relatively small number of structures exhibiting this

[*] These cofactor structures were most probably obtained via rigid-body refinement based on the cofactor coordinates from the oldest structure in the set; for this reason it would have been acceptable to allow a single structure from RBC1 to contribute to the average conformation but since our final dataset is still quite large it was unnecessary to do so.

feature (n = 18). In addition to these arguments, a cursory look at the resolutions of the experiments involved shows that these sets contain structure determinations that are generally on the lower resolution side of the crystal structures (Table 6).

We must then decide between sets RBC3 and RBC4 (and of course, the corresponding bacteriopheophytin sets); sets both exhibiting cofactors that are substantially nonplanar. The key to this decision in our opinion rests in their conformational comparison to related small molecule crystal structures. Recalling that the most obvious feature of the RBC3 crystal structures is that the cofactors all exhibit a striking absence of the A1g distortion (which represents the degree of in-plane macrocycle expansion/contraction) when compared to each of the other subsets; we have found in our investigations of isolated chlorin crystal structures that this deformation is, without exception, almost entirely dependent on the central ion that is present in the macrocycle. Thus, the A1g deformation exhibited by the cofactors in RBC3 is in fact that of a metalated Cu macrocycle whilst that exhibited by RBC4 (and indeed the other subsets as well as the *B. viridis* bacteriochlorophylls) is consistent with Mg coordinated in the central cavity (specifically, we have compared them to Mg-chlorophyllides). In addition, the excessive higher energy distortions exhibited by the RBC3 cofactors (this feature is also shared with RBP3) are quite unprecedented in porphyrinoid cofactor conformations that are induced by protein interaction alone, since the energies required for their induction are significantly greater than that required by a combination of only lowest-energy normal-deformations. Finally, if the previous arguments are not sufficient, then it should be noted that the vast majority of the cofactors in this set (RBC3) were part of the same study (see Section 6.1); most of them were made at the same time by the same group and all of them were diffracted in the same place. Thus we suppose that at some point during their measurement or refinement a systematic error has been introduced (which we cannot specifically identify at this time) that has gone unnoticed since the goal of their study was quite different from determination and analysis of accurate conformations of the bacteriochlorophyll cofactors. It is for these reasons, and the appearance of the set's independence of measurement, that we believe the RBC4 (n = 32) structures to be the best candidates to provide accurate and reliable cofactor conformations.

Table 5: Contingency table of PDB structure count in RBC group (columns) and RBP group (rows). OL = outlier; NA = not included in factor analysis and 4, 5 (RBP group) = structures containing two RCs in asymmetric unit with one classed as RBP4 and the other as RBP5.

	1	2	3	4	OL	NA
1	**9**			1		
2		**13**				1
3			**14**		3	
4				**13**		
OL			1	*5*	2	1
NA		2	1	*3*		
5				*2*	2	1
4, 5				*3*		

Table 6: Summary of crystal structures present in each set. [a] mean in parenthesis, [b] relates to structures with two RCs in asymmetric unit where each RC was classified differently as RBP4 or RBP5.

	Crystal structures	Resolution(s)[a]
Total in PDB	77	1.80-4.60 (2.66)
	R. sphaeroides bacteriochlorophyll factor analysis	
RBC1	9	2.70-3.20 (3.02)
RBC2	15 (18 RCs)	2.10-4.60 (2.95)
RBC3	16	1.87-2.88 (2.36)
RBC4	27 (32 RCs)	1.80-3.00 (2.53)
OL	7	2.20-3.10 (2.76)
NA	3	2.50-3.00 (2.77)
	R. sphaeroides bacteriopheophytin factor analysis	
RBP1	10	2.10-3.20 (2.93)
RBP2	14 (16 RCs)	2.35-4.60 (2.99)
RBP3	17	1.87-2.88 (2.36)
RBP4	13 (+3, 16 RCs)[b]	2.30-3.00 (2.61)
RBP5	5 (+3, 10 RCs)[b]	2.20-3.10 (2.68)
OL	9	2.55-2.90 (2.70)
NA	6	1.80-2.80 (2.32)

4.6.2 *B. viridis* Crystal Structure Sets

For the *B. viridis* bacteriochlorophyll cofactors, the arguments stated above for the exclusion of the planar cofactor set, apply also to our decision in proceeding with their analysis using the BBC2 set of structures and not with structure 1PRC, even though the bacteriopheophytin cofactors of 1PRC do not reflect this feature. This lack of corroboration can be explained though since it is possible that different restraints have been applied to the bacteriopheophytins in this structure and so, since the conformations of the BChl cofactors of 1PRC are all consistently and significantly less distorted than the rest, we feel it to remain reasonable to assume that this aspect is an experimental artefact.

As for the apparent outliers in the *B. viridis* bacteriopheophytin PCA, assessment of their individual conformations showed that the reason for this was that on the whole, the structures exhibited greater in-plane distortion as well as changes to the out-of-plane distortion pattern (Section 5.4.4).

5 Macrocycle Conformations

5.1 Illustrations of the Lowest Energy Normal-deformations

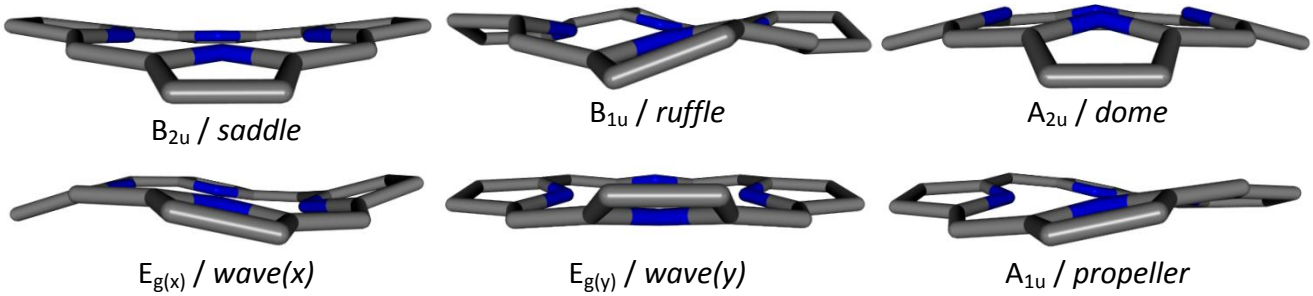

Figure 9: Illustrations of the six lowest-energy out-of-plane normal-deformations.

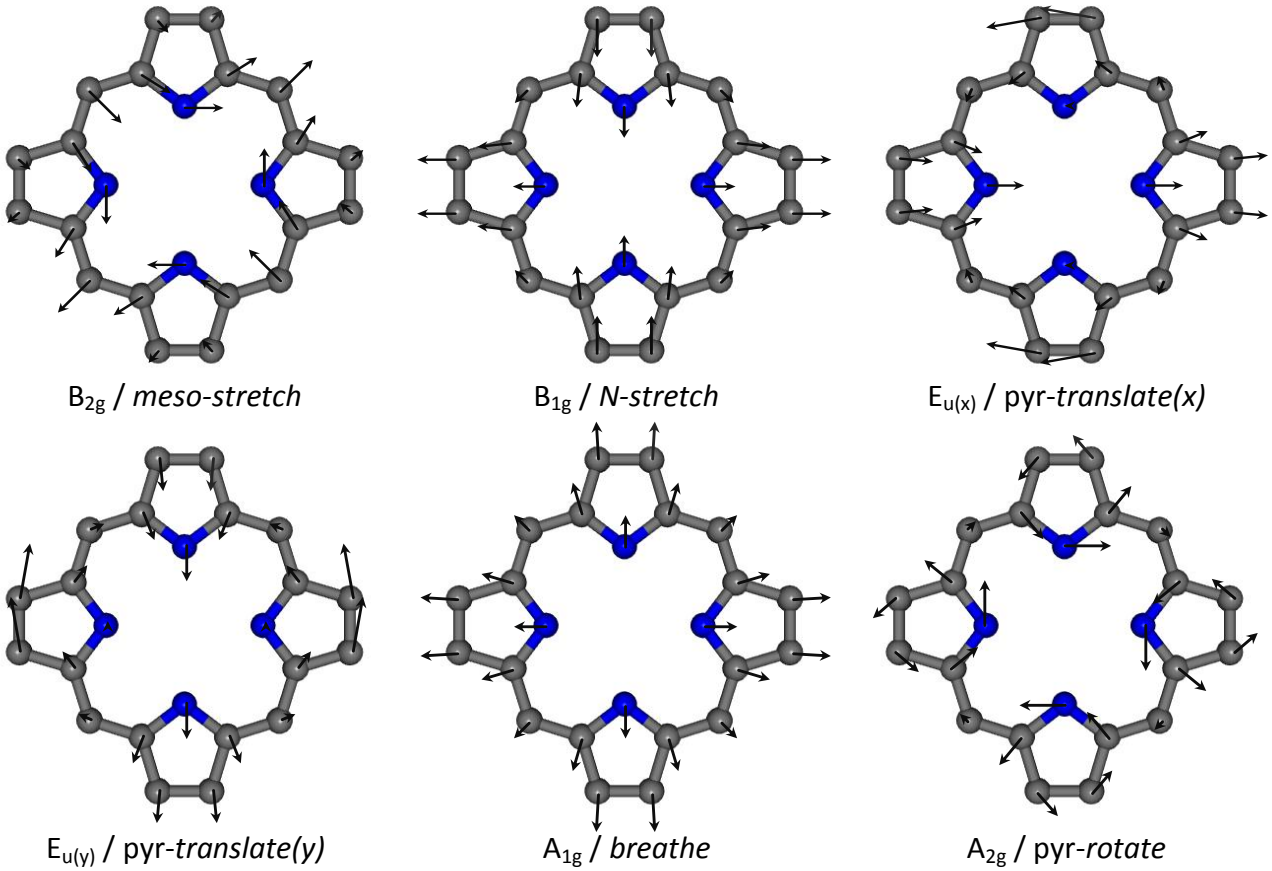

Figure 10: Illustrations of the six lowest-energy in-plane normal-deformations.

5.2 Nomenclature of Cofactor Nuclei and Ring Subunits

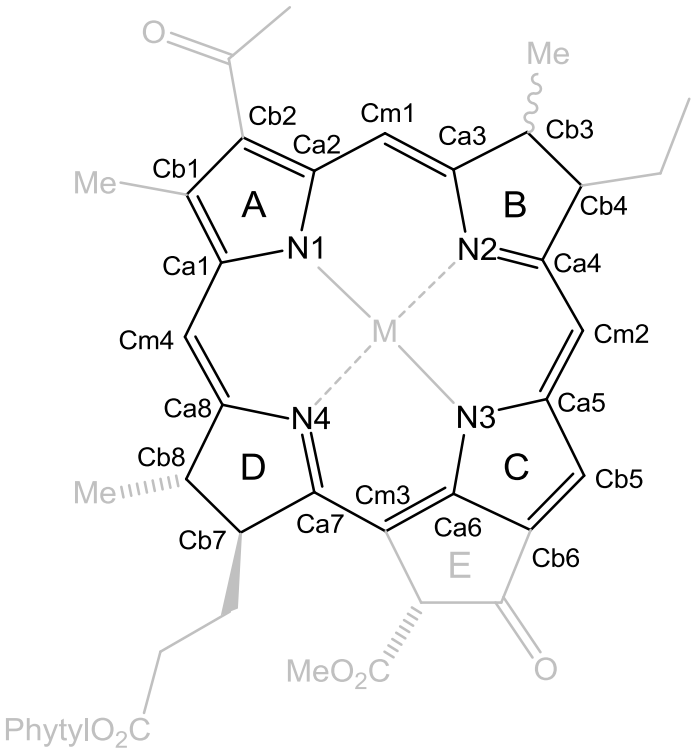

Figure 11: Nomenclature of cofactor nuclei and ring subunits used throughout.

5.3 Overviews of Most Relevant Cofactor Conformations

5.3.1 *R. sphaeroides* RBC4 cofactors

The minimum basis was deemed to be acceptable since the mean deviation between the simulated and actual conformations, δoop values (Section 5.6.3 for descriptives of RBC4 dataset and Section 5.7.1 for δoop of mean conformation), were either within or close to Jentzen *et al's* criterion[2b] (i.e. close to 0.03). From the NSDs (Section 5.4.1), it is immediately apparent that the cofactors assume statistically significant, unique nonplanar geometries and share a much more common IP conformation, showing that the IP conformation is mostly effected by the chemical structure and that the OOP deformation is controlled by the protein/cofactor environment. The key features of the NSDs of the cofactors are that BA is the most planar; BB is the most nonplanar, exhibiting a large B1u distortion; DL is quite nonplanar and exhibits a dominant A2u distortion with contributions from B2u and B1u, and DM is considerably nonplanar showing significant B2u distortion and a large, negative B1u deformation (see Doop values in Section 5.6.3 and 5.7.1). In terms of skeletal displacements (Section 0), DL stands apart in that rings A, B and C (for nomenclature see Section 5.2) exhibit a 'tilt' in one direction along their Cα-Cα axes, which originates from the A2u mode, although the OOP orientation of ring A may be somewhat conserved among the four. It should also be readily observed that the only real failing of the minimum basis is that the SP^3-hybridisation of the β-carbons of the reduced rings (B and D) that leads to their displacement above and below the plane is not entirely encapsulated (red/blue comparison, Section 0). This validates the use of the minimum basis for the conformational comparisons of these structures in our paper since these must be the distortions that are induced by the protein/cofactor- and, in the case of the special-pair, the cofactor/cofactor interactions.

In addition, it is also noteworthy to draw attention to the differences of the Doop and δoop parameters between the descriptive statistics of the RBC4 dataset and their re-centred NSDs (i.e. the values of these parameters for the mean conformation). In particular, the reduction in the δoop value of the minimum basis of the mean conformations (the re-centred value) compared to the mean value for the cofactors, indicates that the minimum basis provides a better description of the mean conformation than it does for most of the individual observations. It is possible to interpret this fact as showing that the averaging process has resulted in the removal of spurious higher-energy distortions. Considering this together with the knowledge that the remaining higher-energy distortions are required only to describe the SP^3-hybridisation of the β-carbons of the reduced rings (as noted above) we may conclude that the force exerted by the protein upon the cofactor is only energetically capable of inducing these lower energy distortions.*

5.3.2 *B. viridis* BBC1 cofactors

Here it was found that the extended basis was required to obtain sufficient agreement between the simulated conformations and the observed mean conformation (to ensure that δ_{oop} was close to 0.03; Section 5.4.2) mostly due to, as the next-to-lowest energy deformations

* Of course, this conclusion is dependent upon our being correct about the erroneous nature of the RBC3 structures.

show (Figure 18, Section 5.4.2), a strong B1u(2)* and A1u(2) distortion in each of the special-pair cofactors and also a strong Eg(x)(2) deformation in the accessory bacteriochlorophyll monomers (in particular of BB). In contrast to *R. sphaeroides*, the A/B-branch asymmetry of the special-pair originates from the extent rather than the make-up of the conformation (thus DL exhibits a large negative B1u distortion, although to a lesser extent than DM and does not show the A2u mode that contributed to DLs uniqueness in *R. sphaeroides*;) and the accessory bacteriochlorophyll monomers do not exhibit A/B-branch asymmetry of the order that was found in *R. sphaeroides* (although note the considerably larger Eg(x)(2) distortion of BB). Similar to the case for *R. sphaeroides* and the adequacy of the minimum basis in that case, here the extended basis captures the majority of the cofactors' conformations (Section 5.5.2) excepting the localised perturbation of the SP^3-hybridisation of the β-carbons on rings B and D.

5.4 Magnitude of the Physicochemical Effects of the Cofactor Distortions

One way to assess the physicochemical impact of the observed macrocyclic distortion in the RC in the context of their relative importance compared to the other forms of functional modulation that the protein scaffold is known to exert, it is necessary to approximate the distortions' perturbation energy (deformation energy) and to then compare these energies with those that have been determined for the other factors. These deformation energies can be obtained directly from the NSD analysis[2b] since it has been shown that the total macrocycle distortion energy (E_d) is obtained from the linear sum of the contributions of each of the normal-deformations (δE_i), in turn given by the square of the normal-coordinate displacement (d_i^2) multiplied by the respective force constant of the mode (K_i), as shown below:-

$$E_d = \sum_{i=1}^{n} \delta E_i = \sum_{i=1}^{n} K_i \, d_i^2$$

The energies then give an idea of the potential magnitude of the effect that can be induced by macrocyclic distortion on an energetically determined quantity (e.g., reduction potential or absorption maximum). The force constants used were calculated by Jentzen *et al*[2b] and are expected to give reasonable estimates of the distortion energies for this purpose.

Table 7: Total macrocycle distortion energies derived from minimum basis NSD of each cofactors mean conformation.

	R. sphaeroides				B. viridis			
	BA	BB	DL	DM	BA	BB	DL	DM
E_d/ kJ mol^{-1}	5.8941	10.2961	8.2253	6.2451	11.4459	10.1356	16.4346	30.5355
E_d / meV molecule^{-1}	61	107	85	65	119	105	170	317

Table 8: Influences of both H-bonding to- and the introduction of polarised residues near P870 (data from Allen and Williams[5]).

	H-bonding	Polarised residues
Qy-band	-8 to -22nm shift (blue-shift) of Qy upon removal of DL acetyl-HIS H-bond	Unavailable
$P/P^{\bullet+}$ Midpoint potential	420 to 765mV (+60-125mV / H-bond; 100meV Hückel model stabilisation)	(Δ) -60 to +50mV (-ve charge / +ve charge 10Å from donor; exponential dependence on distance and dielectric constant)

Comparison of the estimated conformational distortion energies and experimental values of physicochemical changes brought about by other protein interactions derived from RC mutagenesis studies[5] (Table 7Table 8) reveals that the nonplanar distortions represent energetic perturbations on a par with those brought about by H-bonding and electrostatic influences. For example, the estimated 100meV stabilisation induced by each additional H-bond to an acetyl-oxygen of a BChl constituent of the special-pair is certainly matched by the range of distortion energies exhibited by the cofactors (Table 7). This approach is valid on the basis of simple MO theory considering that the distortion of the macrocycle from its preferred geometry raises the energy of the MOs, including the HOMO, which affects decreased ionisation energy and consequently a decreased midpoint potential. Furthermore, this facile analysis may be improved somewhat by an assumption, employed by Zucchelli *et al,*[6] that a distortion of a given symmetry modifies the energy-level of an orbital with the same symmetry; this then allows specific estimation of the effect of the cofactor conformations on the Gouterman frontier orbitals[7] of the BChls enabling a more balanced approach and a direct assessment of the conformationally induced spectral shift of the Qy-band.

Briefly, the four-orbital model describes the electronic structure of porphyrins by a configuration interaction between the HOMO, HOMO-1, LUMO and LUMO-1 of the conjugated π-system which gives rise to the high energy Soret and low energy Q-bands observed in their UV/Vis absorption spectra.[7] The symmetries of these orbitals, when the model is applied to the D2h symmetric BChl macrocycle are Au, B1u, B2g and B3g, respectively.[8] Furthermore, after considering how the NSD basis-modes transform in the D2h point-group, the normal-modes corresponding to these symmetries are the *ruf*, *dom*, *wav(x)* and *wav(y)* distortions (details not shown). The individual contributions to the

* The parenthetic "2" following the symmetry of the distortion denotes that it is the second lowest, or "next-to-lowest", energy distortion of that symmetry that is referred to.

total deformation energies (δE_i) for each of the NSD minimum basis modes of these symmetries for each cofactor are presented (Table 9) as well as this models consequent effect on the four-orbital transitions (Table 10).

Table 9: Normal-deformation energies of the modes of the minimum basis associated with the two highest and lowest energy molecular orbitals of the BChl cofactors by symmetry.

Orbital	D2h orbital symmetry[8]	Matching (D2h) normal-mode(s)	Perturbation / meV							
			R. sphaeroides				*B. viridis*			
			BA	BB	DL	DM	BA	BB	DL	DM
LUMO+1	B3g	saddle / wave (y) [reduced axis]	0	16	24	7	5	3	8	16
LUMO	B2g	wave (x)	51	53	6	7	98	90	0	3
HOMO	Au	ruffle	1	31	6	35	3	0	79	157
HOMO-1	B1u	dome	9	2	48	4	1	12	1	1

Table 10: Distortion induced shift of the LUMO←HOMO and LUMO+1←HOMO-1 transitions predicted by like-symmetry assumptions of Zucchelli *et al*[6].

	R. sphaeroides				*B. viridis*			
	BA	BB	DL	DM	BA	BB	DL	DM
$\Delta E_{B2g\leftarrow Au}$ / meV	50	22	0	-28	95	90	-79	-154
$\Delta E_{B3g\leftarrow B1u}$ / meV	-9	14	-24	3	4	-9	7	15

Since it has been shown that the B2g←Au transition contributes greater than 90% of the Qy-band transition,[8] the first row of entries in Table 10 provides a good estimate of the spectral shift due to conformational distortion (relative to a planar macrocycle). Thus, a blue-shift is predicted for all of the BChl accessory monomers, a slight red-shit for DM of *R. sphaeroides* and a considerable red-shift of the components of the *B. viridis* special-pair (P960). Thus, taking the solution Qy-absorption maximum of 795nm for BChl b as reference[9] (in this model, assumed to be planar), $\Delta E_{B2g\leftarrow Au}$ for DL predicts a shift to 837nm whilst in DM the estimated maximum would be shifted to 882nm. Within the limits of the preceding approximations then, the red-shift of P960 relative to P870 may be assisted as much by conformational control as it is by the greater excitonic coupling of the former special-pair.

Another approach to the question of the magnitude of the physicochemical changes associated with the varying degrees of distortion of the cofactors is to draw on experimental results from conformationally designed synthetic porphyrins. The relevant results from two such studies concerning the effect of a gradual sterically induced, ruffle distortion of nickel porphyrins on redox and absorption properties,[10] and that of a graded saddle distortion of free-base and zinc porphyrins on their photophysical behaviours[11] have been extracted and are illustrated below (Figure 12 Figure 13). These studies also demonstrate that the potential physicochemical effects of macrocycle distortion of the extent observed in the RC are significant in the context of the other protein modulated influences.

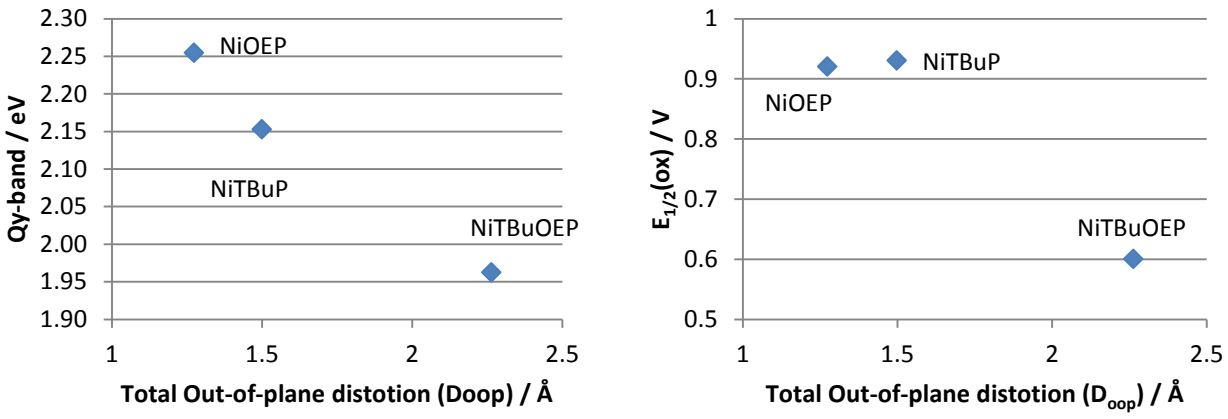

Figure 12: Illustration of the relation between the total out-of-plane distortion (Doop) and the energy of the Qy-band (left) and the first half-wave oxidation potential (right) a a series of conformationally designed, sterically crowded ruffle Ni-porphyrins; data from Senge *et al*[10].

For example, the approximate one angstrom shift in the total distortion of (5,10,15,20-tetrabutyl-2,3,7,8,12,13,17,18-octaethylporphyrinato)nickel(II) (NiTBuOEP) relative to (2,3,7,8,12,13,17,18-octaethylporphyrinato)nickel(II) (NiOEP) leads to a 0.3V reduction in the first half-wave oxidation potential a 0.29eV reduction in the Qy-band of the former relative to the latter[10] (Figure 12); this level of

distortion is similar to that exhibited by the special-pair cofactors of *B. viridis*. Concerning redox properties again, in a recent study by Olea *et al*[12] mutations to the haem binding pocket of H-NOX, decreasing the total degree of distortion from 2.180Å in the wild-type to 0.870Å in the mutant affected a decrease of the haem midpoint potential by 171mV. Note that this reversal in the trend between macrocycle distortion and redox potential is of course due the fact that the haem oxidation is a metal centred process. The relevance of this result to the BChl redox processes (macrocycle centred) is only apparent when one considers that reduction potentials are related to electron density; applying a pseudo-conservation principle coupled with the knowledge that the distortion of the wild-type H-NOX cofactor was confirmed to affect a measured decrease in electron density at the iron-centre,[12] renders the proposal acceptable that potentials of macrocycle and metal-centred redox process, when affected predominantly by conformational effects, are inversely proportional. As another example, the decreasing singlet oxygen yields affected by a gradually increasing saddle distortion[11] (Figure 13) as a consequence of the distortions' effects on numerous photo-physical parameters[11] lends weight to the idea of a photo-protective role of the distortion of the BB cofactor in *R. sphaeroides*.

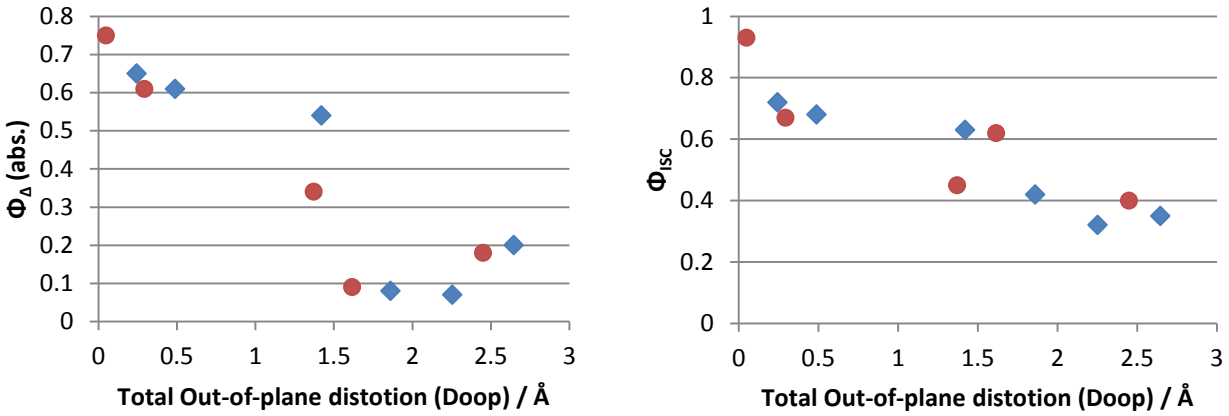

Figure 13: Illustrations of the association between the total out-of-plane distortion (Doop) and the singlet-oxygen (left) and the intersystem crossing quantum yields of a series of conformationally designed free-base- (blue diamonds) and Zn (red circles) saddled porphyrins; data from Roder *et al*[11].

5.5 NSD Descriptive Statistics

5.5.1 *Rhodobacter sphaeroides* bacteriochlorophylls

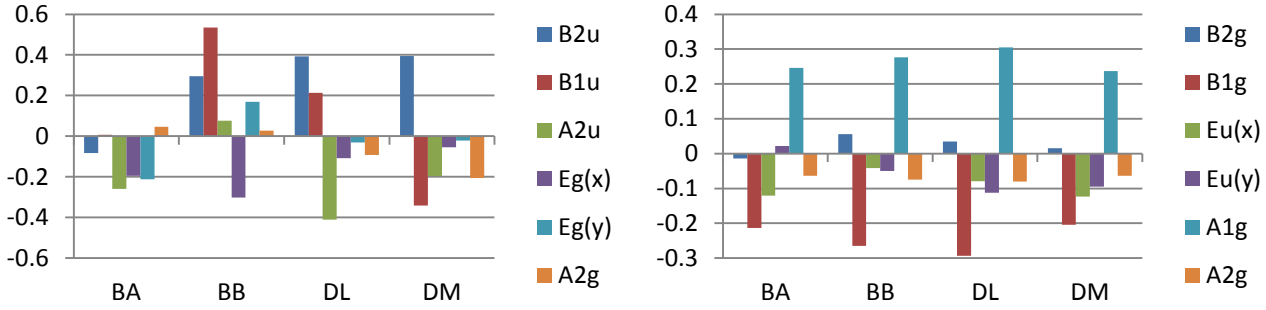

Figure 14: Mean minimum basis normal-coordinate displacements of each ETC cofactor in RBC1 ('no error set'). Out-of-plane (left) and in-plane (right). Y-axes in angstroms; error bars indicate two standard errors (not visible since all are less than 0.00023Å). n = 9.

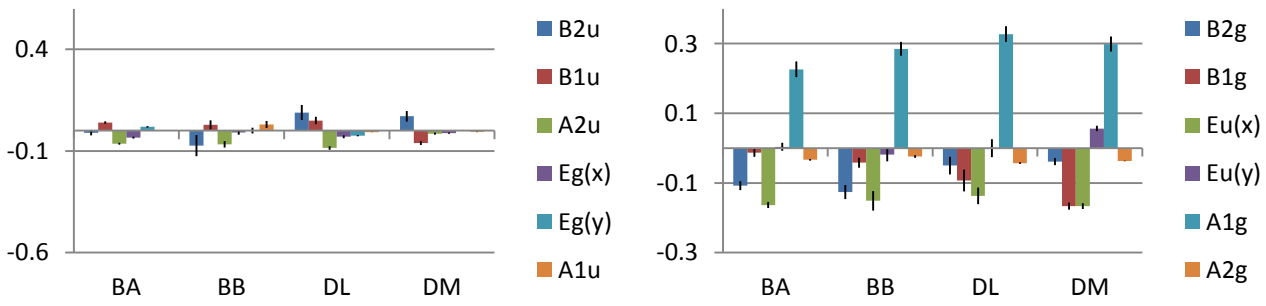

Figure 15: Mean minimum basis normal-coordinate displacements of each ETC cofactor in RBC2a ('planar set'). Out-of-plane (left) and in-plane (right). Y-axes in angstroms; error bars indicate two standard errors. n = 8.

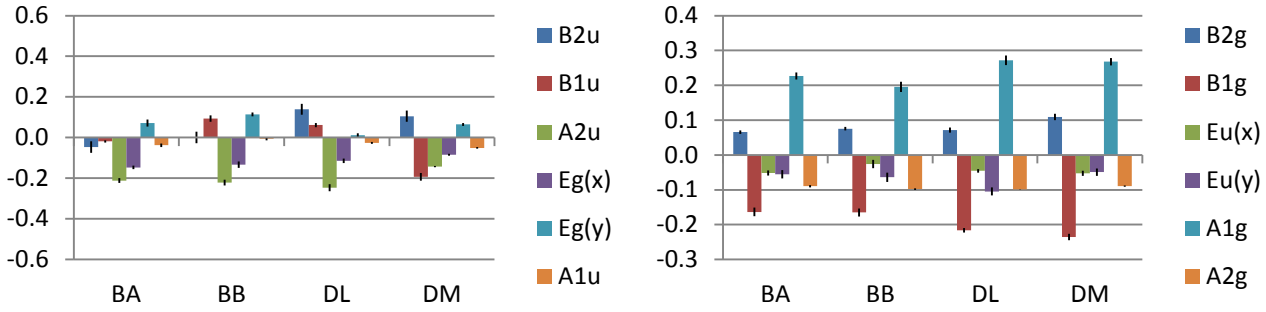

Figure 16: Mean minimum basis normal-coordinate displacements of each ETC cofactor in RBC2b ('planar set'). Out-of-plane (left) and in-plane (right). Y-axes in angstroms; error bars indicate two standard errors. n = 10.

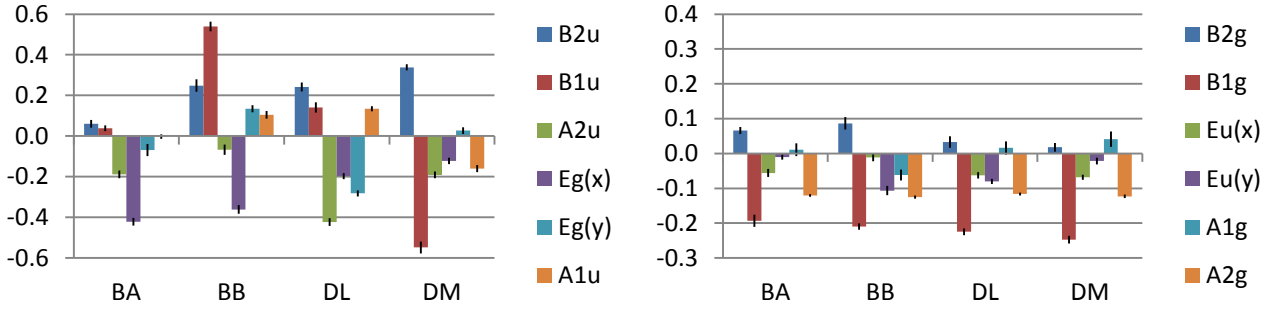

Figure 17: Mean minimum basis normal-coordinate displacements of each ETC cofactor in RBC3 ('unusual IP conformation set'). Out-of-plane (left) and in-plane (right). Y-axes in angstroms; error bars indicate two standard errors. n = 16.

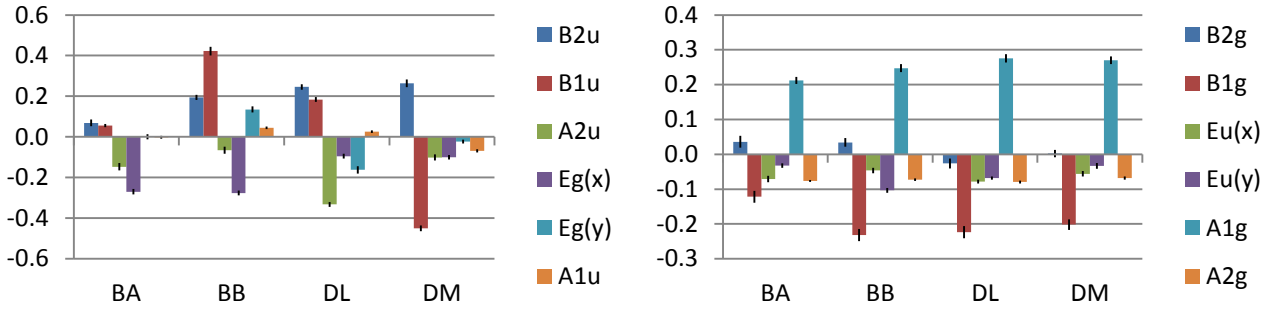

Figure 18: Mean minimum basis normal-coordinate displacements of each ETC cofactor in RBC4 ('deemed as most reliable set'). Out-of-plane (left) and in-plane (right). Y-axes in angstroms; error bars indicate two standard errors. n = 32.

5.5.2 *Blastochloris viridis* bacteriochlorophylls

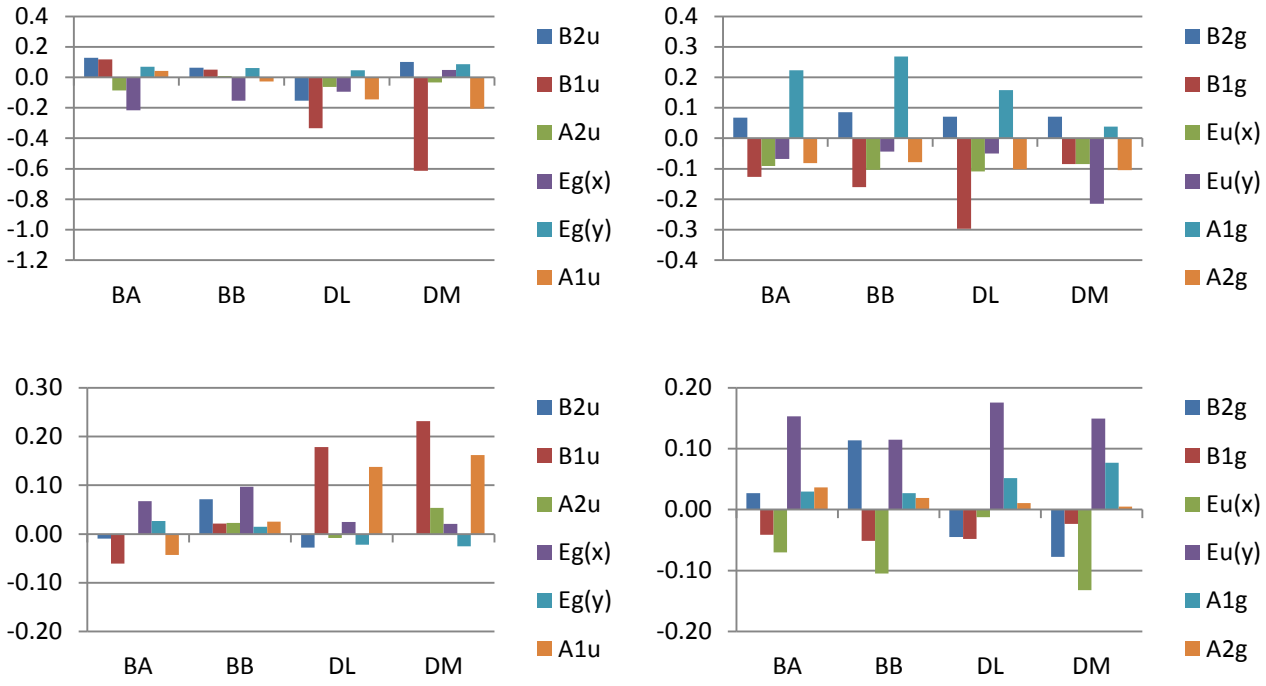

Figure 19: Extended basis normal-coordinate displacements of each ETC cofactor in 1PRC. Out-of-plane (left), in-plane (right), lowest energy (top) and next-to-lowest energy (bottom). Y-axes in angstroms.

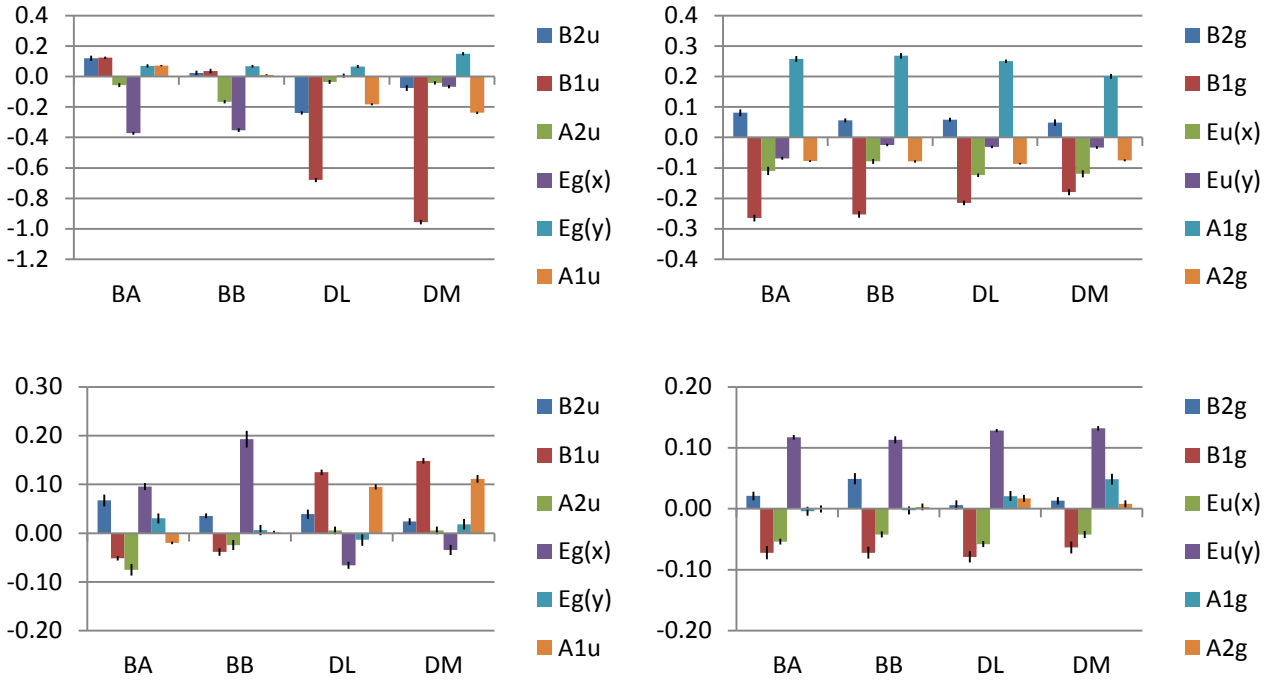

Figure 20: Mean extended basis normal-coordinate displacements of each ETC cofactor in BBC1. Out-of-plane (left), in-plane (right), lowest energy (top) and next-to-lowest energy (bottom). Y-axes in angstroms; error bars indicate two standard errors; n = 13.

5.5.3 *Rhodobacter sphaeroides* bacteriopheophytins

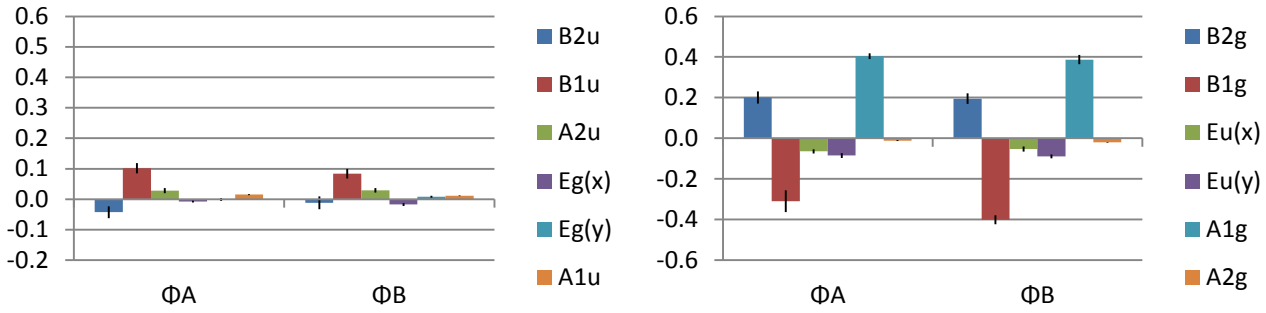

Figure 21: Mean minimum basis normal-coordinate displacements of each ETC cofactor in RBP2. Out-of-plane (left) and in-plane (right). Y-axes in angstroms; error bars indicate two standard errors and n = 16.

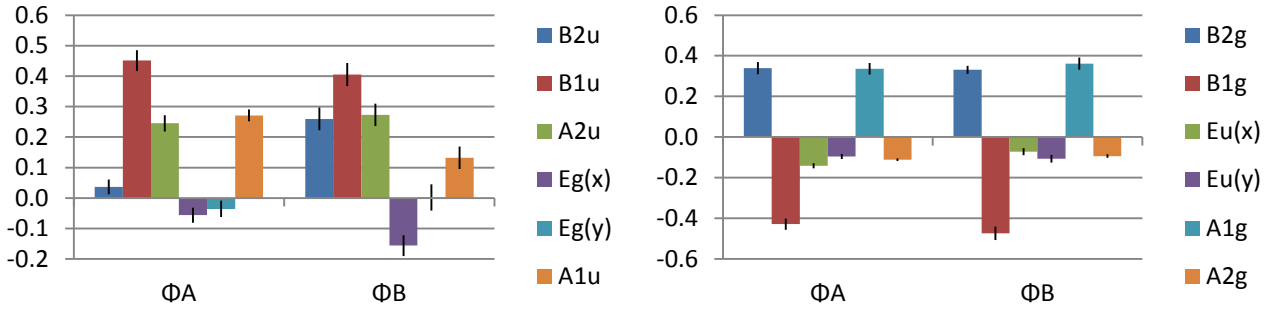

Figure 22: Mean minimum basis normal-coordinate displacements of each ETC cofactor in RBP3. Out-of-plane (left) and in-plane (right). Y-axes in angstroms; error bars indicate two standard errors and n = 17.

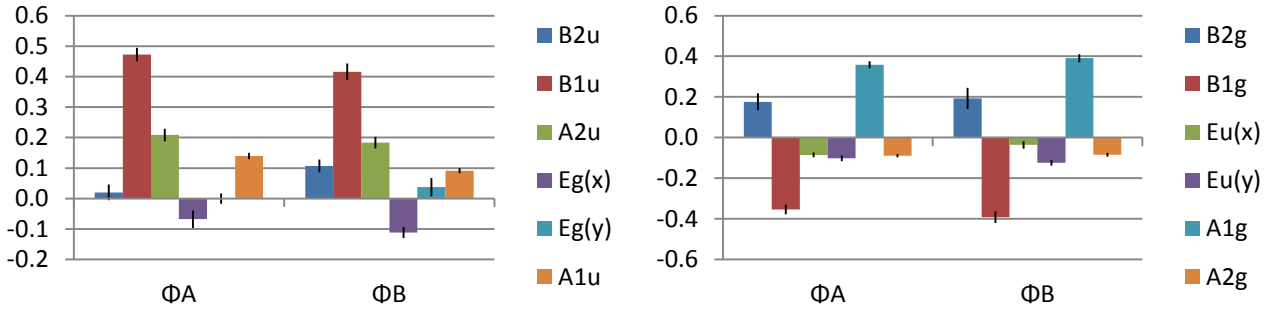

Figure 23: Mean minimum basis normal-coordinate displacements of each ETC cofactor in RBP4. Out-of-plane (left) and in-plane (right). Y-axes in angstroms; error bars indicate two standard errors and n = 16.

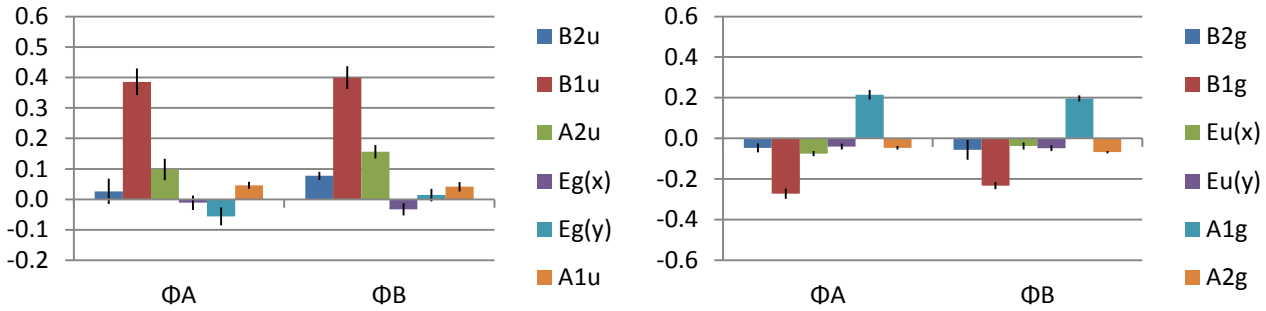

Figure 24: Mean minimum basis normal-coordinate displacements of each ETC cofactor in RBP5. Out-of-plane (left) and in-plane (right). Y-axes in angstroms; error bars indicate two standard errors and n = 10.

5.5.4 Blastochloris viridis bacteriopheophytins

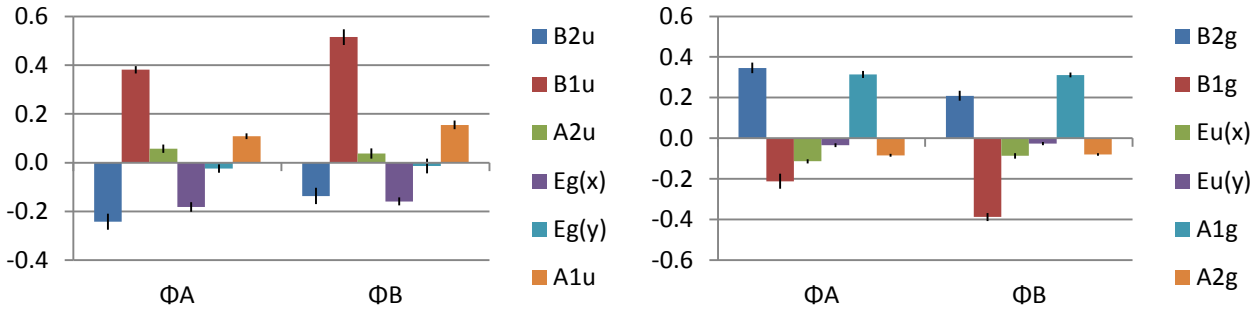

Figure 25: Mean minimum basis normal-coordinate displacements of each ETC cofactor in BBP1. Out-of-plane (left) and in-plane (right). Y-axes in angstroms; error bars indicate two standard errors and n = 13.

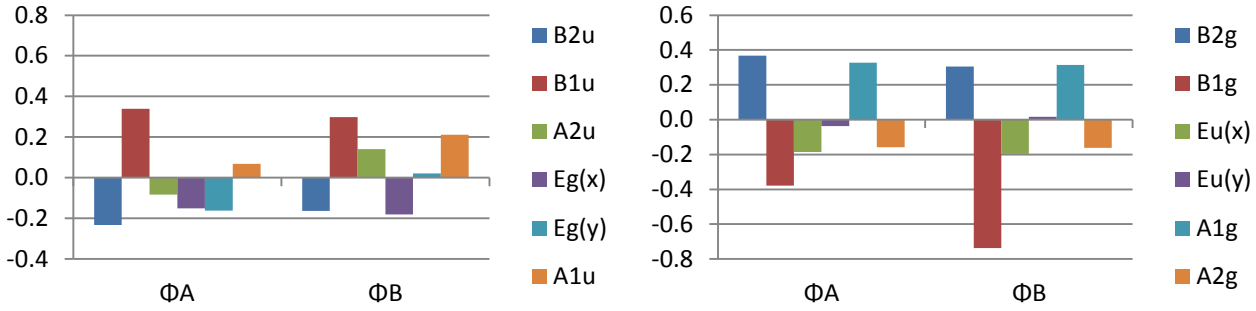

Figure 26: Minimum basis normal-coordinate displacements of each ETC cofactor in 3D38. Out-of-plane (left) and in-plane (right). Y-axes in angstroms.

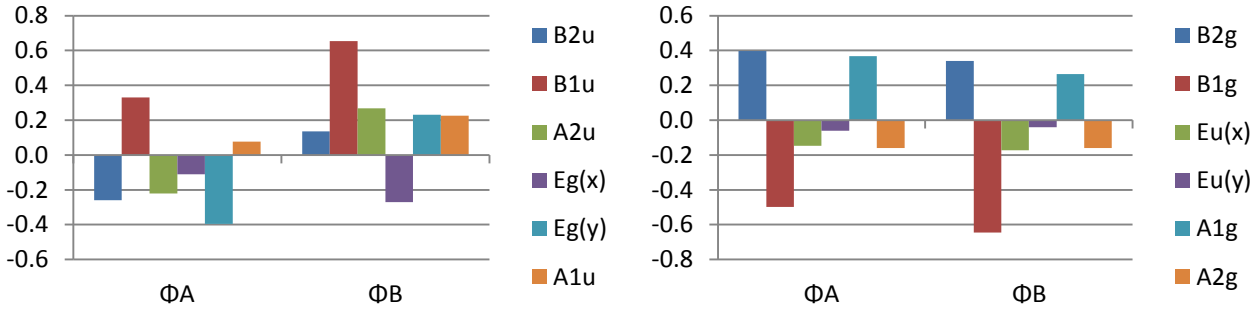

Figure 27: Minimum basis normal-coordinate displacements of each ETC cofactor in 3G7F. Out-of-plane (left) and in-plane (right). Y-axes in angstroms.

5.6 Skeletal Deviation Plots: Local Nonplanarity

5.6.1 *Rhodobacter sphaeroides* bacteriochlorophylls

Skeletal Deviation Plots of Averaged Conformations (RBC3)

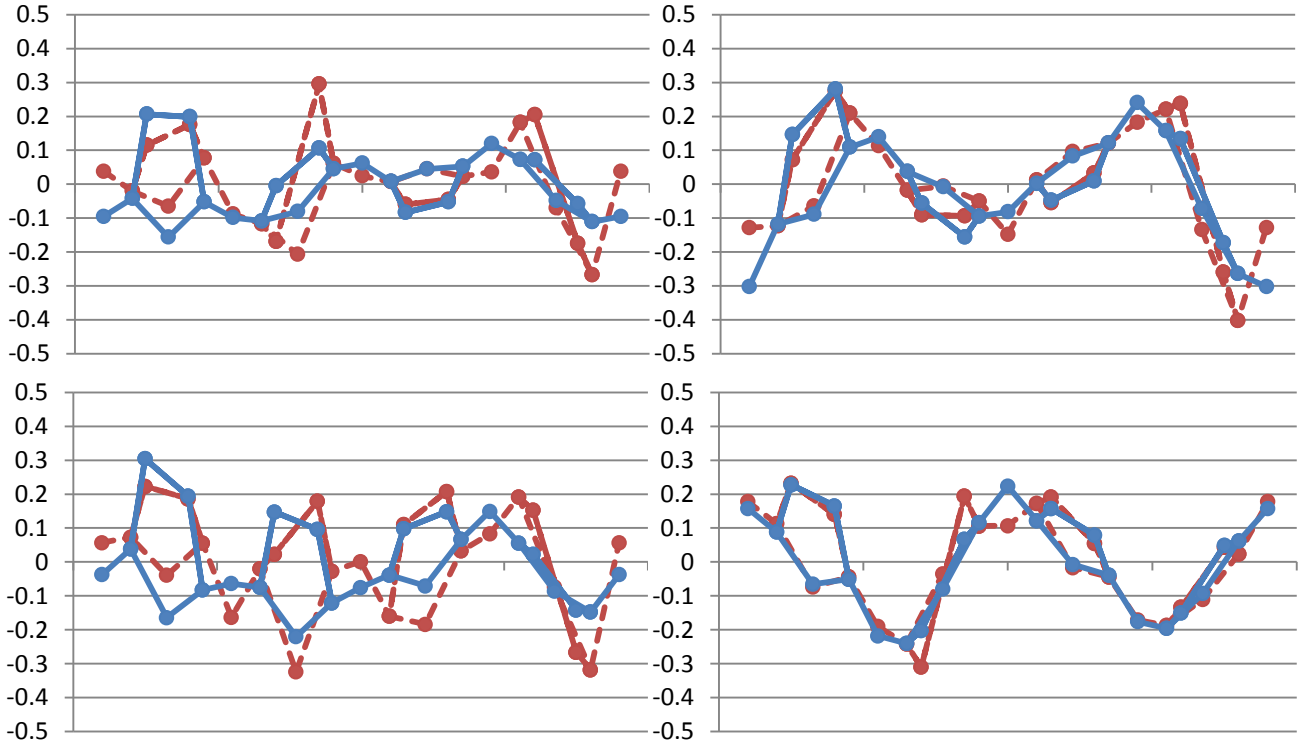

Figure 28: Skeletal plots of z-axis displacements from the NSD minimum (blue) and extended basis (red) simulation of re-centred RBC3. BA (top left), BB (top right), DL (bottom left) and DM (bottom right). Y-axes in angstroms.

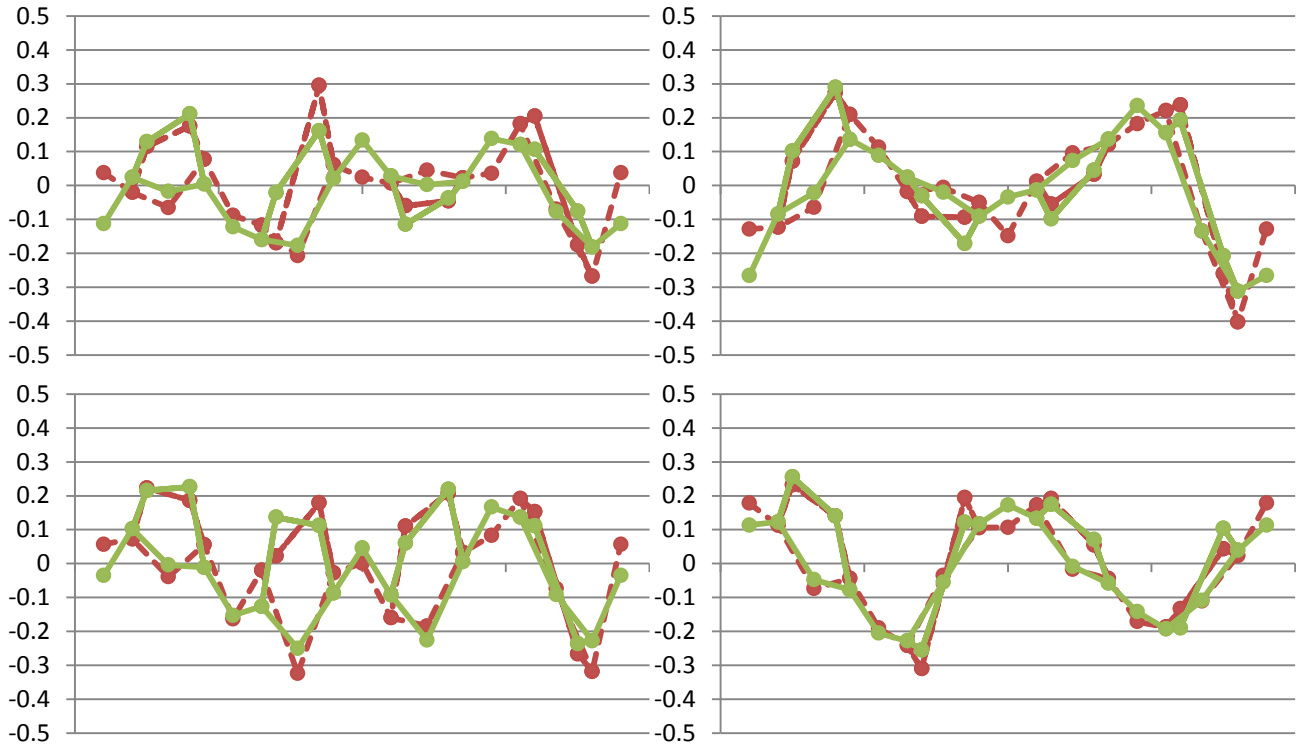

Figure 29: Skeletal plots of z-axis displacements from the NSD extended basis simulation (green) and complete basis, *i.e.* the observed structure, (red) of re-centred RBC3. BA (top left), BB (top right), DL (bottom left) and DM (bottom right). Y-axes in angstroms.

Skeletal Deviation Plots of Averaged Conformations (RBC4)

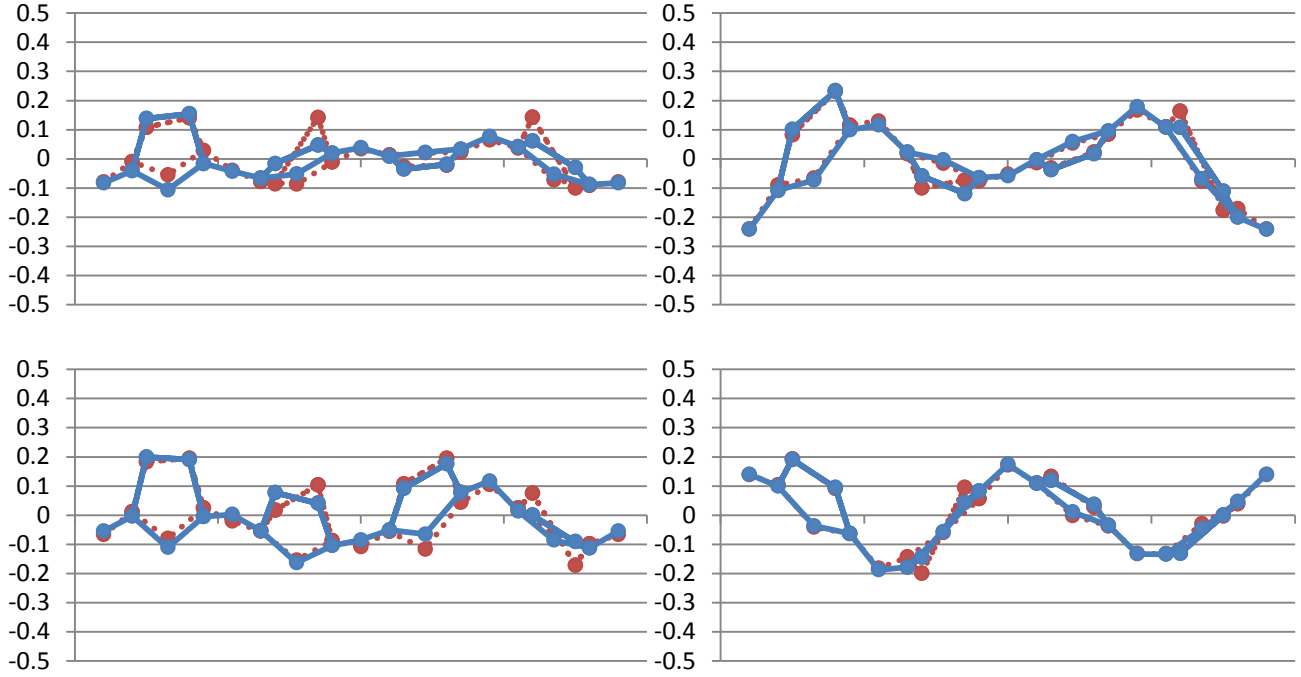

Figure 30: Comparison of minimum basis simulated (blue), with the observed (red), Z-axis displacements of: BA (top left), BB (top right), DL (bottom left) and DM (bottom right); axes in angstroms.

5.6.2 *Blastochloris viridis* bacteriochlorophylls

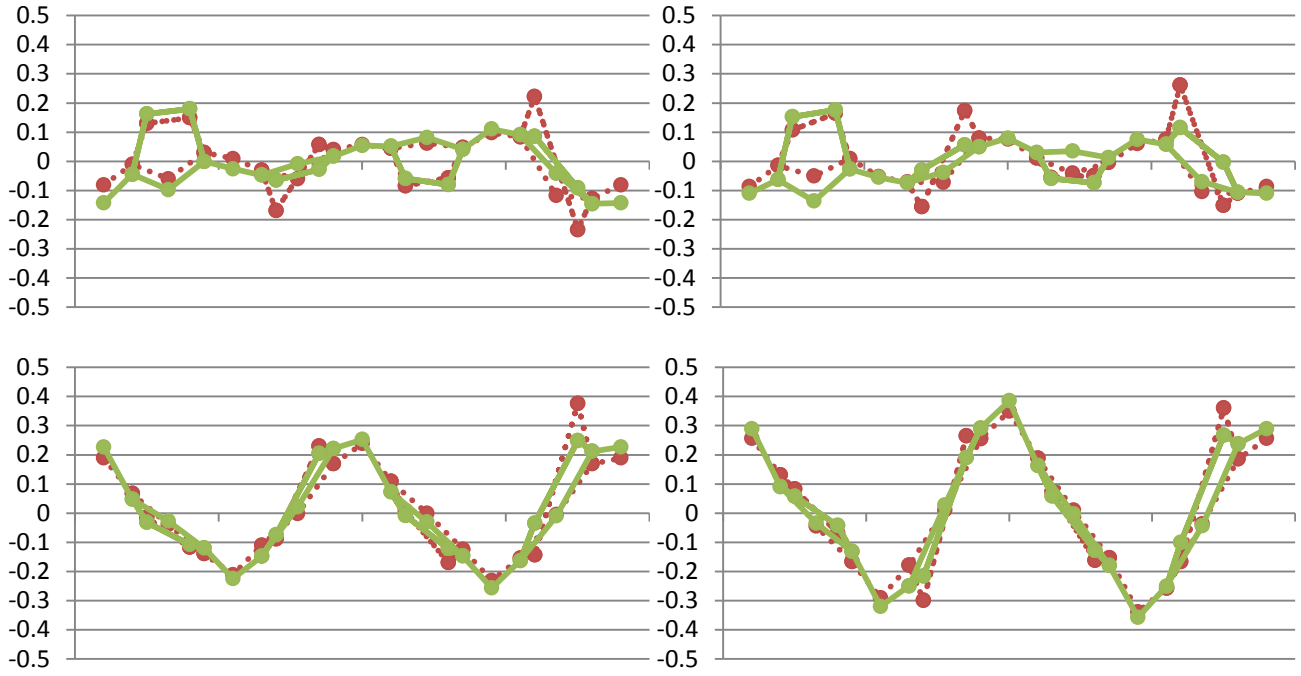

Figure 31: Comparison of the extended basis simulated (green) Z-axis distortions with those that are observed (red) for: BA (top left), BB (top right), DL (bottom left) and DM (bottom right). Y-Axes / angstroms

5.6.3 *Rhodobacter sphaeroides* bacteriopheophytins

Skeletal deviation plots (RBP4)

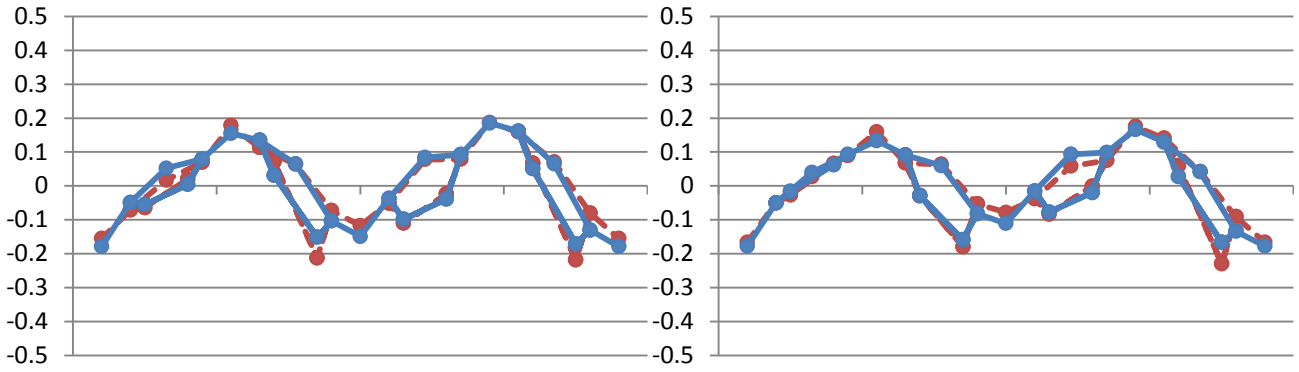

Figure 32: Comparison of the minimum basis simulated (blue) Z-axis distortions with those that are observed (red) for: ΦA (left) and ΦB (right). Y-Axes / angstroms.

Skeletal deviation plots (RBP5)

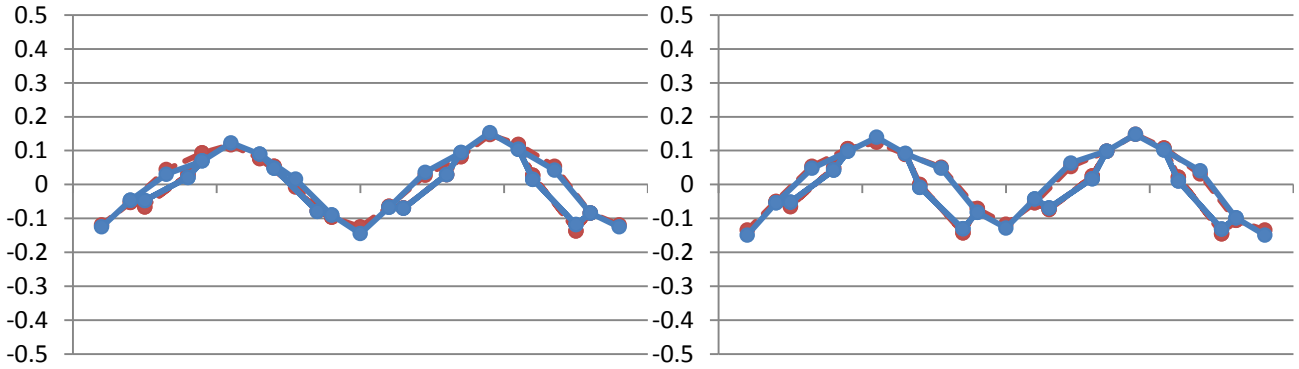

Figure 33: Comparison of the minimum basis simulated (blue) Z-axis distortions with those that are observed (red) for: ΦA (left) and ΦB (right). Y-Axes / angstroms.

5.6.4 *Blastochloris viridis* bacteriopheophytins

Skeletal plots (BBP1)

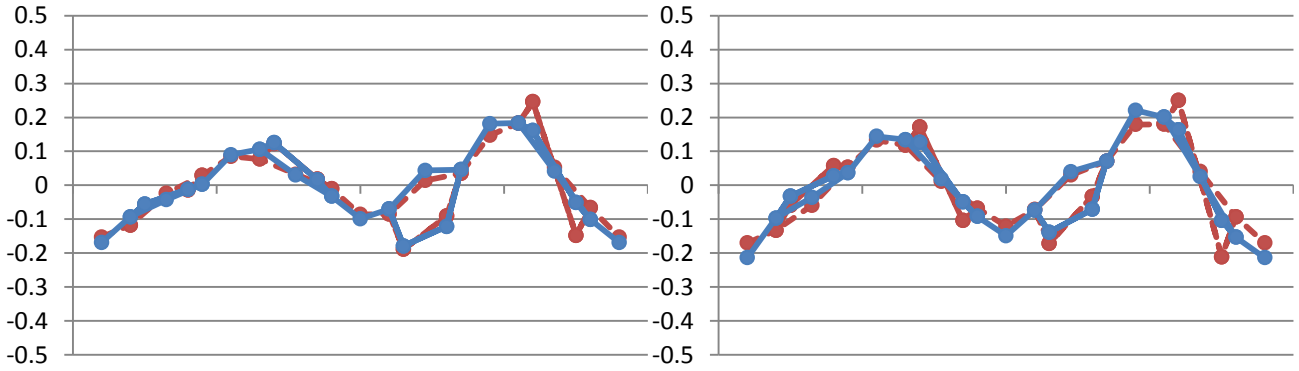

Figure 34: Comparison of the minimum basis simulated (blue) Z-axis distortions with those that are observed (red) for: ΦA (left) and ΦB (right). Y-Axes / angstroms.

5.7 Tabular NSD descriptive statistics

5.7.1 *Rhodobacter sphaeroides* bacteriochlorophylls – RBC2

Table 11: Descriptive statistics of minimum basis out-of-plane parameters and normal-coordinate displacements for each ETC cofactor in all RBC2a experiments. n = 8.

	BA	BB	DL	DM	BA	BB	DL	DM
			Doop				***Dip***	
MEAN	0.0948	0.1851	0.1766	0.1122	0.3096	0.3686	0.4009	0.3937
SSD	0.0156	0.0869	0.0372	0.0481	0.0511	0.0453	0.0478	0.0391
SE	0.0055	0.0307	0.0132	0.0170	0.0181	0.0160	0.0169	0.0138
			δoop				***δip***	
MEAN	0.0061	0.0110	0.0045	0.0032	0.0588	0.0683	0.0621	0.0643
SSD	0.0011	0.0111	0.0010	0.0006	0.0018	0.0157	0.0020	0.0027
SE	0.0004	0.0039	0.0004	0.0002	0.0006	0.0056	0.0007	0.0009
			B2u				***B2g***	
MEAN	-0.0102	-0.0737	0.0895	0.0707	-0.1075	-0.1260	-0.0501	-0.0392
SSD	0.0376	0.1481	0.1064	0.0721	0.0367	0.0564	0.0718	0.0288
SE	0.0133	0.0524	0.0376	0.0255	0.0130	0.0199	0.0254	0.0102
			B1u				***B1g***	
MEAN	0.0393	0.0285	0.0501	-0.0613	-0.0127	-0.0419	-0.0933	-0.1664
SSD	0.0181	0.0655	0.0498	0.0267	0.0350	0.0410	0.0888	0.0291
SE	0.0064	0.0232	0.0176	0.0094	0.0124	0.0145	0.0314	0.0103
			A2u				***Eu(x)***	
MEAN	-0.0640	-0.0679	-0.0851	-0.0146	-0.1636	-0.1513	-0.1373	-0.1664
SSD	0.0124	0.0447	0.0256	0.0139	0.0253	0.0789	0.0678	0.0232
SE	0.0044	0.0158	0.0091	0.0049	0.0089	0.0279	0.0240	0.0082
			Eg(x)				***Eu(y)***	
MEAN	-0.0343	-0.0088	-0.0297	-0.0126	0.0039	-0.0189	-0.0005	0.0561
SSD	0.0140	0.0294	0.0206	0.0083	0.0335	0.0533	0.0729	0.0221
SE	0.0049	0.0104	0.0073	0.0029	0.0118	0.0189	0.0258	0.0078
			Eg(y)				***A1g***	
MEAN	0.0187	0.0000	-0.0248	0.0020	0.2261	0.2850	0.3273	0.2989
SSD	0.0109	0.0406	0.0078	0.0048	0.0641	0.0553	0.0637	0.0608
SE	0.0039	0.0144	0.0027	0.0017	0.0227	0.0196	0.0225	0.0215
			A1u				***A2g***	
MEAN	0.0003	0.0303	-0.0069	-0.0058	-0.0337	-0.0242	-0.0432	-0.0370
SSD	0.0031	0.0492	0.0031	0.0052	0.0068	0.0112	0.0059	0.0027
SE	0.0011	0.0174	0.0011	0.0018	0.0024	0.0040	0.0021	0.0010

Table 12: Descriptive statistics of minimum basis out-of-plane parameters and normal-coordinate displacements for each ETC cofactor in all RBC2b experiments. n = 10.

	BA	BB	DL	DM	BA	BB	DL	DM
			Doop				***Dip***	
MEAN	0.2903	0.3159	0.3275	0.2980	0.3143	0.3003	0.3888	0.3947
SSD	0.0629	0.0604	0.0586	0.0712	0.0449	0.0432	0.0367	0.0239
SE	0.0199	0.0191	0.0185	0.0225	0.0142	0.0137	0.0116	0.0076
			δoop				***δip***	
MEAN	0.0238	0.0228	0.0188	0.0142	0.0687	0.0684	0.0661	0.0701
SSD	0.0070	0.0062	0.0053	0.0026	0.0046	0.0021	0.0016	0.0012

	BA	BB	DL	DM	BA	BB	DL	DM
SE	0.0022	0.0020	0.0017	0.0008	0.0014	0.0007	0.0005	0.0004
			B2u				***B2g***	
MEAN	-0.0468	0.0006	0.1391	0.1049	0.0655	0.0753	0.0719	0.1090
SSD	0.0878	0.0884	0.0841	0.0865	0.0163	0.0163	0.0232	0.0281
SE	0.0278	0.0280	0.0266	0.0273	0.0051	0.0052	0.0073	0.0089
			B1u				***B1g***	
MEAN	-0.0192	0.0937	0.0614	-0.1933	-0.1634	-0.1652	-0.2160	-0.2355
SSD	0.0175	0.0501	0.0328	0.0594	0.0396	0.0372	0.0199	0.0286
SE	0.0055	0.0159	0.0104	0.0188	0.0125	0.0117	0.0063	0.0090
			A2u				***Eu(x)***	
MEAN	-0.2114	-0.2212	-0.2472	-0.1426	-0.0519	-0.0261	-0.0456	-0.0526
SSD	0.0367	0.0443	0.0558	0.0099	0.0236	0.0382	0.0165	0.0240
SE	0.0116	0.0140	0.0176	0.0031	0.0075	0.0121	0.0052	0.0076
			Eg(x)				***Eu(y)***	
MEAN	-0.1473	-0.1332	-0.1148	-0.0847	-0.0552	-0.0641	-0.1046	-0.0493
SSD	0.0270	0.0504	0.0339	0.0135	0.0385	0.0413	0.0370	0.0339
SE	0.0085	0.0159	0.0107	0.0043	0.0122	0.0131	0.0117	0.0107
			Eg(y)				***A1g***	
MEAN	0.0713	0.1134	0.0121	0.0646	0.2266	0.1956	0.2717	0.2678
SSD	0.0547	0.0296	0.0288	0.0218	0.0317	0.0455	0.0431	0.0333
SE	0.0173	0.0094	0.0091	0.0069	0.0100	0.0144	0.0136	0.0105
			A1u				***A2g***	
MEAN	-0.0378	-0.0055	-0.0260	-0.0511	-0.0897	-0.0980	-0.0989	-0.0896
SSD	0.0264	0.0251	0.0165	0.0130	0.0110	0.0073	0.0018	0.0062
SE	0.0084	0.0079	0.0052	0.0041	0.0035	0.0023	0.0006	0.0020

5.7.2 *Rhodobacter sphaeroides* bacteriochlorophylls – RBC3

Table 13: Descriptive statistics of minimum basis out-of-plane parameters and normal-coordinate displacements for each ETC cofactor in all RBC3 experiments. n = 16.

	BA	BB	DL	DM	BA	BB	DL	DM
			Doop				***Dip***	
MEAN	0.4995	0.7487	0.6498	0.7200	0.2698	0.3092	0.2952	0.3108
SSD	0.0900	0.0756	0.0578	0.0890	0.0322	0.0387	0.0393	0.0285
SE	0.0225	0.0189	0.0145	0.0223	0.0080	0.0097	0.0098	0.0071
			δoop				***δip***	
MEAN	0.0946	0.0737	0.0979	0.0666	0.0506	0.0528	0.0539	0.0556
SSD	0.0237	0.0233	0.0168	0.0249	0.0059	0.0053	0.0057	0.0050
SE	0.0059	0.0058	0.0042	0.0062	0.0015	0.0013	0.0014	0.0012
			B2u				***B2g***	
MEAN	0.0604	0.2486	0.2418	0.3382	0.0661	0.0866	0.0326	0.0180
SSD	0.0760	0.1230	0.0874	0.0596	0.0403	0.0729	0.0669	0.0493
SE	0.0190	0.0307	0.0218	0.0149	0.0101	0.0182	0.0167	0.0123
			B1u				***B1g***	
MEAN	0.0387	0.5398	0.1404	-0.5483	-0.1934	-0.2099	-0.2247	-0.2478
SSD	0.0579	0.0946	0.1019	0.1179	0.0698	0.0370	0.0386	0.0441
SE	0.0145	0.0237	0.0255	0.0295	0.0174	0.0093	0.0097	0.0110
			A2u				***Eu(x)***	
MEAN	-0.1881	-0.0672	-0.4238	-0.1913	-0.0562	-0.0115	-0.0627	-0.0681

	BA	BB	DL	DM	BA	BB	DL	DM
SSD	0.0747	0.0983	0.0746	0.0675	0.0460	0.0424	0.0358	0.0288
SE	0.0187	0.0246	0.0186	0.0169	0.0115	0.0106	0.0089	0.0072
			Eg(x)				***Eu(y)***	
MEAN	-0.4214	-0.3613	-0.1966	-0.1219	-0.0101	-0.1067	-0.0800	-0.0217
SSD	0.0761	0.0859	0.0596	0.0622	0.0298	0.0528	0.0296	0.0381
SE	0.0190	0.0215	0.0149	0.0156	0.0074	0.0132	0.0074	0.0095
			Eg(y)				***A1g***	
MEAN	-0.0684	0.1348	-0.2822	0.0270	0.0109	-0.0621	0.0159	0.0411
SSD	0.1190	0.0696	0.0614	0.0655	0.0727	0.0618	0.0736	0.0870
SE	0.0297	0.0174	0.0154	0.0164	0.0182	0.0154	0.0184	0.0217
			A1u				***A2g***	
MEAN	-0.0023	0.1053	0.1342	-0.1601	-0.1205	-0.1252	-0.1163	-0.1230
SSD	0.0435	0.0758	0.0495	0.0708	0.0161	0.0175	0.0160	0.0211
SE	0.0109	0.0190	0.0124	0.0177	0.0040	0.0044	0.0040	0.0053

5.7.3 *Rhodobacter sphaeroides* bacteriochlorophylls – RBC4

Table 14: Descriptive statistics of minimum basis out-of-plane parameters and normal-coordinate displacements for each ETC cofactor in all RBC4 experiments. n = 32.

	BA	BB	DL	DM	BA	BB	DL	DM
			Doop				***Dip***	
MEAN	0.3611	0.5848	0.5168	0.5694	0.3052	0.3894	0.4031	0.3704
SSD	0.0688	0.1244	0.0677	0.0824	0.0740	0.0692	0.0609	0.0735
SE	0.0122	0.0220	0.0120	0.0146	0.0131	0.0122	0.0108	0.0130
			δoop				***δip***	
MEAN	0.0340	0.0255	0.0349	0.0205	0.0498	0.0519	0.0499	0.0546
SSD	0.0153	0.0144	0.0155	0.0116	0.0050	0.0053	0.0046	0.0044
SE	0.0027	0.0025	0.0027	0.0020	0.0009	0.0009	0.0008	0.0008
			B2u				***B2g***	
MEAN	0.0691	0.1940	0.2457	0.2630	0.0358	0.0341	-0.0261	0.0021
SSD	0.0961	0.0702	0.0757	0.1078	0.0973	0.0693	0.0799	0.0609
SE	0.0170	0.0124	0.0134	0.0191	0.0172	0.0122	0.0141	0.0108
			B1u				***B1g***	
MEAN	0.0551	0.4220	0.1835	-0.4504	-0.1219	-0.2318	-0.2237	-0.2019
SSD	0.0451	0.1220	0.0678	0.0808	0.0956	0.1012	0.0992	0.0874
SE	0.0080	0.0216	0.0120	0.0143	0.0169	0.0179	0.0175	0.0154
			A2u				***Eu(x)***	
MEAN	-0.1472	-0.0656	-0.3326	-0.1012	-0.0713	-0.0463	-0.0785	-0.0559
SSD	0.1008	0.0953	0.0673	0.0858	0.0520	0.0436	0.0318	0.0450
SE	0.0178	0.0169	0.0119	0.0152	0.0092	0.0077	0.0056	0.0079
			Eg(x)				***Eu(y)***	
MEAN	-0.2699	-0.2761	-0.0951	-0.1004	-0.0323	-0.1035	-0.0684	-0.0335
SSD	0.0739	0.0682	0.0672	0.0620	0.0370	0.0377	0.0253	0.0483
SE	0.0131	0.0121	0.0119	0.0110	0.0065	0.0067	0.0045	0.0085
			Eg(y)				***A1g***	
MEAN	0.0001	0.1349	-0.1625	-0.0228	0.2122	0.2472	0.2754	0.2702
SSD	0.0729	0.0842	0.1054	0.0522	0.0558	0.0642	0.0686	0.0632
SE	0.0129	0.0149	0.0186	0.0092	0.0099	0.0113	0.0121	0.0112

	BA	BB	DL	DM	BA	BB	DL	DM
			A1u				***A2g***	
MEAN	-0.0022	0.0451	0.0253	-0.0689	-0.0766	-0.0729	-0.0796	-0.0685
SSD	0.0383	0.0342	0.0348	0.0463	0.0164	0.0185	0.0224	0.0262
SE	0.0068	0.0060	0.0061	0.0082	0.0029	0.0033	0.0040	0.0046

5.7.4 Blastochloris viridis bacteriochlorophylls – 1PRC

Minimum Basis

Table 15: Minimum basis out-of-plane parameters and normal-coordinate displacements for each ETC cofactor in 1PRC.

BA	BB	DL	DM	BA	BB	DL	DM
		Doop				***Dip***	
0.3019	0.1875	0.4142	0.663	0.2998	0.3533	0.3796	0.2809
		δoop				***δip***	
0.0394	0.0458	0.0401	0.0518	0.0472	0.0492	0.0515	0.0521
		B2u				***B2g***	
0.1285	0.0619	-0.154	0.1016	0.0674	0.0859	0.0714	0.0714
		B1u				***B1g***	
0.1168	0.0503	-0.3335	-0.6127	-0.1271	-0.1604	-0.2989	-0.0871
		A2u				***Eu(x)***	
-0.0856	0.0065	-0.0628	-0.0368	-0.0911	-0.1037	-0.1082	-0.0834
		Eg(x)				***Eu(y)***	
-0.2169	-0.1562	-0.0963	0.0465	-0.0692	-0.0454	-0.0525	-0.2157
		Eg(y)				***A1g***	
0.0698	0.06	0.0452	0.0876	0.2218	0.2691	0.1565	0.0381
		A1u				***A2g***	
0.0412	-0.0272	-0.146	-0.2064	-0.083	-0.0804	-0.1035	-0.1063

Extended Basis

Table 16: Extended basis parameters and normal-coordinate displacements for each ETC cofactor in 1PRC.

	BA	BB	DL	DM	BA	BB	DL	DM
			Doop				***Dip***	
N/A	0.3201	0.2294	0.4737	0.7232	0.3503	0.4072	0.4272	0.3634
			δoop				***δip***	
N/A	0.0401	0.0443	0.0176	0.0145	0.0360	0.0332	0.0345	0.0314
			B2u				***B2g***	
1st	0.1280	0.0627	-0.1544	0.1016	0.0673	0.0853	0.0711	0.0703
2nd	-0.0093	0.0711	-0.0282	-0.0004	0.0271	0.1138	-0.0451	-0.0778
			B1u				***B1g***	
1st	0.1168	0.0503	-0.3335	-0.6127	-0.1266	-0.1601	-0.2967	-0.0844
2nd	-0.0607	0.0215	0.1784	0.2313	-0.0411	-0.0514	-0.0484	-0.0237
			A2u				***Eu(x)***	
1st	-0.0857	0.0078	-0.0636	-0.0341	-0.0910	-0.1040	-0.1094	-0.0847
2nd	-0.0011	0.0228	-0.0085	0.0537	-0.0701	-0.1047	-0.0125	-0.1323
			Eg(x)				***Eu(y)***	
1st	-0.2160	-0.1544	-0.0956	0.0480	-0.0681	-0.0442	-0.0499	-0.2148
2nd	0.0673	0.0967	0.0244	0.0206	0.1532	0.1146	0.1754	0.1494

	BA	BB	DL	DM	BA	BB	DL	DM
			Eg(y)				***A1g***	
1st	0.0700	0.0599	0.0454	0.0855	0.2228	0.2681	0.1576	0.0379
2nd	0.0264	0.0150	-0.0219	-0.0252	0.0294	0.0271	0.0515	0.0771
			A1u				***A2g***	
1st	0.0412	-0.0272	-0.1460	-0.2064	-0.0811	-0.0789	-0.1017	-0.1052
2nd	-0.0431	0.0254	0.1378	0.1618	0.0363	0.0192	0.0107	0.0050

5.7.5 Blastochloris viridis bacteriochlorophylls – BBC1

Minimum Basis

Table 17: Descriptive statistics of minimum basis out-of-plane parameters and normal-coordinate displacements for each ETC cofactor in all BBC1 experiments; n = 13.

	BA	BB	DL	DM	BA	BB	DL	DM
			Doop				***Dip***	
MEAN	0.4466	0.4269	0.7582	1.0145	0.4245	0.3956	0.3739	0.3259
SSD	0.0619	0.0590	0.0794	0.0765	0.0337	0.0664	0.0399	0.0465
SE	0.0109	0.0104	0.0140	0.0135	0.0060	0.0117	0.0071	0.0082
			δoop				***δip***	
MEAN	0.0493	0.0528	0.0383	0.0415	0.0450	0.0453	0.0459	0.0437
SSD	0.0084	0.0071	0.0067	0.0104	0.0059	0.0067	0.0072	0.0078
SE	0.0015	0.0012	0.0012	0.0018	0.0010	0.0012	0.0013	0.0014
			B2u				***B2g***	
MEAN	0.1173	0.0225	-0.2394	-0.0766	0.0803	0.0551	0.0568	0.0482
SSD	0.0956	0.0802	0.0608	0.1066	0.0597	0.0379	0.0359	0.0609
SE	0.0169	0.0142	0.0107	0.0188	0.0105	0.0067	0.0063	0.0108
			B1u				***B1g***	
MEAN	0.1230	0.0359	-0.6792	-0.9567	-0.2644	-0.2521	-0.2148	-0.1793
SSD	0.0408	0.0865	0.0748	0.0837	0.0600	0.0594	0.0431	0.0549
SE	0.0072	0.0153	0.0132	0.0148	0.0106	0.0105	0.0076	0.0097
			A2u				***Eu(x)***	
MEAN	-0.0514	-0.1636	-0.0365	-0.0416	-0.1096	-0.0781	-0.1234	-0.1188
SSD	0.0685	0.0606	0.0693	0.0619	0.0759	0.0431	0.0331	0.0664
SE	0.0121	0.0107	0.0122	0.0109	0.0134	0.0076	0.0059	0.0117
			Eg(x)				***Eu(y)***	
MEAN	-0.3750	-0.3589	0.0070	-0.0661	-0.0703	-0.0260	-0.0328	-0.0347
SSD	0.0563	0.0672	0.0746	0.0589	0.0292	0.0230	0.0243	0.0250
SE	0.0099	0.0119	0.0132	0.0104	0.0052	0.0041	0.0043	0.0044
			Eg(y)				***A1g***	
MEAN	0.0677	0.0670	0.0655	0.1498	0.2568	0.2671	0.2493	0.1993
SSD	0.0601	0.0517	0.0622	0.0554	0.0554	0.0514	0.0351	0.0432
SE	0.0106	0.0091	0.0110	0.0098	0.0098	0.0091	0.0062	0.0076
			A1u				***A2g***	
MEAN	0.0706	0.0113	-0.1827	-0.2380	-0.0782	-0.0792	-0.0877	-0.0762
SSD	0.0244	0.0229	0.0348	0.0435	0.0161	0.0186	0.0141	0.0180
SE	0.0043	0.0041	0.0061	0.0077	0.0028	0.0033	0.0025	0.0032

Extended Basis

Table 18: Descriptive statistics of extended basis out-of-plane parameters and lowest energy normal-coordinate displacements for each ETC cofactor in all BBC1 experiments; n = 13.

	BA	BB	DL	DM	BA	BB	DL	DM
			Doop				***Dip***	
MEAN	0.4852	0.4897	0.7864	1.0385	0.4590	0.4333	0.4180	0.3760
SSD	0.0749	0.0661	0.0787	0.0771	0.0378	0.0656	0.0396	0.0380
SE	0.0132	0.0117	0.0139	0.0136	0.0067	0.0116	0.0070	0.0067
			δoop				***δip***	
MEAN	0.0375	0.0367	0.0220	0.0205	0.0283	0.0290	0.0275	0.0254
SSD	0.0105	0.0099	0.0073	0.0084	0.0088	0.0091	0.0088	0.0084
SE	0.0019	0.0017	0.0013	0.0015	0.0016	0.0016	0.0016	0.0015
			B2u				***B2g***	
MEAN	0.1191	0.0234	-0.2389	-0.0765	0.0808	0.0560	0.0578	0.0489
SSD	0.0967	0.0802	0.0611	0.1067	0.0597	0.0375	0.0360	0.0608
SE	0.0171	0.0142	0.0108	0.0189	0.0106	0.0066	0.0064	0.0108
			B1u				***B1g***	
MEAN	0.1230	0.0359	-0.6792	-0.9567	-0.2646	-0.2525	-0.2150	-0.1797
SSD	0.0408	0.0865	0.0748	0.0837	0.0610	0.0600	0.0434	0.0551
SE	0.0072	0.0153	0.0132	0.0148	0.0108	0.0106	0.0077	0.0097
			A2u				***Eu(x)***	
MEAN	-0.0567	-0.1664	-0.0365	-0.0421	-0.1101	-0.0787	-0.1239	-0.1193
SSD	0.0682	0.0617	0.0698	0.0632	0.0761	0.0431	0.0331	0.0663
SE	0.0121	0.0109	0.0123	0.0112	0.0134	0.0076	0.0059	0.0117
			Eg(x)				***Eu(y)***	
MEAN	-0.3728	-0.3527	0.0054	-0.0670	-0.0686	-0.0245	-0.0312	-0.0331
SSD	0.0561	0.0658	0.0751	0.0586	0.0286	0.0229	0.0240	0.0253
SE	0.0099	0.0116	0.0133	0.0104	0.0051	0.0041	0.0043	0.0045
			Eg(y)				***A1g***	
MEAN	0.0686	0.0671	0.0645	0.1488	0.2576	0.2679	0.2499	0.2006
SSD	0.0602	0.0515	0.0620	0.0557	0.0558	0.0518	0.0352	0.0434
SE	0.0106	0.0091	0.0110	0.0098	0.0099	0.0092	0.0062	0.0077
			A1u				***A2g***	
MEAN	0.0706	0.0113	-0.1827	-0.2380	-0.0777	-0.0788	-0.0866	-0.0752
SSD	0.0244	0.0229	0.0348	0.0435	0.0160	0.0187	0.0143	0.0180
SE	0.0043	0.0041	0.0061	0.0077	0.0028	0.0033	0.0025	0.0032

Table 19: Descriptive statistics of extended basis out-of-plane next-to-lowest energy normal-coordinate displacements for each ETC cofactor in all BBC1 experiments; n = 13.

	BA	BB	DL	DM	BA	BB	DL	DM
			B2u				***B2g***	
MEAN	0.0670	0.0354	0.0390	0.0236	0.0210	0.0493	0.0062	0.0131
SSD	0.0705	0.0287	0.0539	0.0393	0.0400	0.0507	0.0423	0.0332
SE	0.0125	0.0051	0.0095	0.0069	0.0071	0.0090	0.0075	0.0059
			B1u				***B1g***	
MEAN	-0.0514	-0.0386	0.1249	0.1483	-0.0720	-0.0721	-0.0789	-0.0634
SSD	0.0266	0.0426	0.0324	0.0302	0.0608	0.0543	0.0515	0.0549
SE	0.0047	0.0075	0.0057	0.0053	0.0108	0.0096	0.0091	0.0097

	BA	BB	DL	DM	BA	BB	DL	DM
			A2u				***Eu(x)***	
MEAN	-0.0752	-0.0243	0.0056	0.0056	-0.0541	-0.0424	-0.0580	-0.0425
SSD	0.0657	0.0563	0.0435	0.0442	0.0265	0.0282	0.0280	0.0327
SE	0.0116	0.0100	0.0077	0.0078	0.0047	0.0050	0.0050	0.0058
			Eg(x)				***Eu(y)***	
MEAN	0.0955	0.1926	-0.0660	-0.0347	0.1171	0.1132	0.1282	0.1320
SSD	0.0424	0.0964	0.0425	0.0593	0.0208	0.0320	0.0141	0.0203
SE	0.0075	0.0170	0.0075	0.0105	0.0037	0.0057	0.0025	0.0036
			Eg(y)				***A1g***	
MEAN	0.0303	0.0062	-0.0135	0.0184	-0.0038	-0.0027	0.0208	0.0485
SSD	0.0581	0.0603	0.0705	0.0615	0.0415	0.0378	0.0465	0.0519
SE	0.0103	0.0107	0.0125	0.0109	0.0073	0.0067	0.0082	0.0092
			A1u				***A2g***	
MEAN	-0.0201	0.0018	0.0948	0.1111	-0.0003	0.0029	0.0170	0.0080
SSD	0.0159	0.0187	0.0309	0.0449	0.0323	0.0317	0.0335	0.0326
SE	0.0028	0.0033	0.0055	0.0079	0.0057	0.0056	0.0059	0.0058

5.7.6 *Rhodobacter sphaeroides* bacteriopheophytins – RBP2

Table 20: Descriptive statistics of minimum basis in- and out-of-plane parameters and normal-coordinate displacements for each ETC cofactor in all RBP2 experiments; n = 16.

	ΦA	ΦB	ΦA	ΦB
	Doop		***Dip***	
MEAN	0.1482	0.1301	0.6048	0.6185
SSD	0.0442	0.0545	0.0630	0.0642
SE	0.0114	0.0141	0.0163	0.0166
	δoop		***δip***	
MEAN	0.0039	0.0037	0.0596	0.0613
SSD	0.0010	0.0010	0.0035	0.0049
SE	0.0003	0.0002	0.0009	0.0013
	B2u		***B2g***	
MEAN	-0.0426	-0.0119	0.2010	0.1948
SSD	0.0741	0.0825	0.1171	0.1008
SE	0.0191	0.0213	0.0302	0.0260
	B1u		***B1g***	
MEAN	0.1017	0.0839	-0.3097	-0.4009
SSD	0.0650	0.0618	0.2054	0.0861
SE	0.0168	0.0159	0.0530	0.0222
	A2u		***Eu(x)***	
MEAN	0.0279	0.0295	-0.0645	-0.0524
SSD	0.0329	0.0284	0.0401	0.0494
SE	0.0085	0.0073	0.0104	0.0128
	Eg(x)		***Eu(y)***	
MEAN	-0.0077	-0.0175	-0.0852	-0.0891
SSD	0.0128	0.0198	0.0437	0.0354
SE	0.0033	0.0051	0.0113	0.0091
	Eg(y)		***A1g***	
MEAN	-0.0006	0.0077	0.4041	0.3869
SSD	0.0180	0.0123	0.0550	0.0873

	ΦA	ΦB	ΦA	ΦB
SE	0.0046	0.0032	0.0142	0.0225
	A1u		***A2g***	
MEAN	0.0151	0.0110	-0.0115	-0.0200
SSD	0.0065	0.0040	0.0108	0.0044
SE	0.0017	0.0010	0.0028	0.0011

5.7.7 *Rhodobacter sphaeroides* bacteriopheophytins – RBP3

Table 21: Descriptive statistics of minimum basis in- and out-of-plane parameters and normal-coordinate displacements for each ETC cofactor in all RBP3 experiments; n = 17.

	ΦA	ΦB	ΦA	ΦB
	Doop		***Dip***	
MEAN	0.6118	0.6362	0.6870	0.7161
SSD	0.0638	0.1280	0.0670	0.0488
SE	0.0213	0.0427	0.0223	0.0163
	δoop		***δip***	
MEAN	0.0648	0.0768	0.0605	0.0653
SSD	0.0178	0.0254	0.0049	0.0073
SE	0.0059	0.0085	0.0016	0.0024
	B2u		***B2g***	
MEAN	0.0365	0.2596	0.3392	0.3309
SSD	0.0722	0.1128	0.0883	0.0581
SE	0.0241	0.0376	0.0294	0.0194
	B1u		***B1g***	
MEAN	0.4511	0.4048	-0.4287	-0.4732
SSD	0.1022	0.1135	0.0809	0.0986
SE	0.0341	0.0378	0.0270	0.0329
	A2u		***Eu(x)***	
MEAN	0.2451	0.2729	-0.1415	-0.0723
SSD	0.0802	0.1109	0.0387	0.0509
SE	0.0267	0.0370	0.0129	0.0170
	Eg(x)		***Eu(y)***	
MEAN	-0.0564	-0.1562	-0.0955	-0.1070
SSD	0.0742	0.1017	0.0358	0.0571
SE	0.0247	0.0339	0.0119	0.0190
	Eg(y)		***A1g***	
MEAN	-0.0355	0.0019	0.3354	0.3609
SSD	0.0798	0.1304	0.0850	0.0895
SE	0.0266	0.0435	0.0283	0.0298
	A1u		***A2g***	
MEAN	0.2711	0.1321	-0.1118	-0.0934
SSD	0.0590	0.1090	0.0191	0.0250
SE	0.0197	0.0363	0.0064	0.0083

5.7.8 *Rhodobacter sphaeroides* bacteriopheophytins – RBP4

Table 22: Descriptive statistics of minimum basis in- and out-of-plane parameters and normal-coordinate displacements for each ETC cofactor in all RBP4 experiments; n = 16.

	ΦA	ΦB	ΦA	ΦB
	Doop		***Dip***	
MEAN	0.5585	0.5080	0.5779	0.6320
SSD	0.0514	0.0779	0.0498	0.0818
SE	0.0171	0.0260	0.0166	0.0273
	δoop		***δip***	
MEAN	0.0260	0.0232	0.0553	0.0561
SSD	0.0074	0.0060	0.0068	0.0046
SE	0.0025	0.0020	0.0023	0.0015
	B2u		***B2g***	
MEAN	0.0200	0.1073	0.1757	0.1929
SSD	0.0766	0.0633	0.1255	0.1563
SE	0.0255	0.0211	0.0418	0.0521
	B1u		***B1g***	
MEAN	0.4724	0.4156	-0.3540	-0.3919
SSD	0.0659	0.0821	0.0731	0.0851
SE	0.0220	0.0274	0.0244	0.0284
	A2u		***Eu(x)***	
MEAN	0.2084	0.1835	-0.0855	-0.0360
SSD	0.0609	0.0567	0.0348	0.0535
SE	0.0203	0.0189	0.0116	0.0178
	Eg(x)		***Eu(y)***	
MEAN	-0.0677	-0.1116	-0.1022	-0.1241
SSD	0.0862	0.0525	0.0433	0.0438
SE	0.0287	0.0175	0.0144	0.0146
	Eg(y)		***A1g***	
MEAN	-0.0004	0.0373	0.3586	0.3909
SSD	0.0511	0.0894	0.0520	0.0601
SE	0.0170	0.0298		
	A1u		***A2g***	
MEAN	0.1394	0.0912	-0.0898	-0.0839
SSD	0.0301	0.0241	0.0230	0.0286
SE	0.0100	0.0080	0.0077	0.0095

5.7.9 *Rhodobacter sphaeroides* bacteriopheophytins – RBP5

Table 23: Descriptive statistics of minimum basis in- and out-of-plane parameters and normal-coordinate displacements for each ETC cofactor in all RBP5 experiments; n = 9.

	ΦA	ΦB	ΦA	ΦB
	Doop		***Dip***	
MEAN	0.4511	0.4571	0.3801	0.3615
SSD	0.1181	0.0972	0.0681	0.0323
SE	0.0394	0.0324	0.0227	0.0108
	δoop		***δip***	
MEAN	0.0169	0.0159	0.0549	0.0541
SSD	0.0069	0.0076	0.0041	0.0016
SE	0.0023	0.0025	0.0014	0.0005

	ΦA	ΦB	ΦA	ΦB
	B2u		***B2g***	
MEAN	0.0265	0.0769	-0.0469	-0.0557
SSD	0.1259	0.0397	0.0657	0.1468
SE	0.0420	0.0132	0.0219	0.0489
	B1u		***B1g***	
MEAN	0.3857	0.3992	-0.2718	-0.2325
SSD	0.1314	0.1119	0.0769	0.0526
SE	0.0438	0.0373	0.0256	0.0175
	A2u		***Eu(x)***	
MEAN	0.0981	0.1564	-0.0748	-0.0376
SSD	0.1047	0.0655	0.0391	0.0521
SE	0.0349	0.0218	0.0130	0.0174
	Eg(x)		***Eu(y)***	
MEAN	-0.0111	-0.0329	-0.0409	-0.0483
SSD	0.0706	0.0592	0.0425	0.0417
SE	0.0235	0.0197	0.0142	0.0139
	Eg(y)		***A1g***	
MEAN	-0.0560	0.0141	0.2143	0.1965
SSD	0.0877	0.0607	0.0711	0.0432
SE	0.0292	0.0202	0.0237	0.0144
	A1u		***A2g***	
MEAN	0.0460	0.0415	-0.0462	-0.0679
SSD	0.0333	0.0460	0.0266	0.0160
SE	0.0111	0.0153	0.0089	0.0053

5.7.10 *Blastochloris viridis* bacteriopheophytins – BBP1

Table 24: Descriptive statistics of minimum basis in- and out-of-plane parameters and normal-coordinate displacements for each ETC cofactor in all BBP1 experiments; n = 13.

	ΦA	ΦB	ΦA	ΦB
	Doop		***Dip***	
MEAN	0.5271	0.6099	0.5529	0.5665
SSD	0.0650	0.1122	0.0984	0.0417
SE	0.0180	0.0311	0.0273	0.0116
	δoop		***δip***	
MEAN	0.0301	0.0378	0.0493	0.0485
SSD	0.0066	0.0093	0.0081	0.0101
SE	0.0018	0.0026	0.0022	0.0028
	B2u		***B2g***	
MEAN	-0.2420	-0.1369	0.3464	0.2090
SSD	0.1193	0.1210	0.0923	0.0882
SE	0.0331	0.0336	0.0256	0.0245
	B1u		***B1g***	
MEAN	0.3812	0.5148	-0.2115	-0.3877
SSD	0.0540	0.1144	0.1323	0.0713
SE	0.0150	0.0317	0.0367	0.0198
	A2u		***Eu(x)***	
MEAN	0.0571	0.0380	-0.1132	-0.0869
SSD	0.0617	0.0756	0.0374	0.0479

	ΦA	ΦB	ΦA	ΦB
SE	0.0171	0.0210	0.0104	0.0133
	Eg(x)		***Eu(y)***	
MEAN	-0.1818	-0.1591	-0.0338	-0.0265
SSD	0.0709	0.0603	0.0340	0.0268
SE	0.0197	0.0167	0.0094	0.0074
	Eg(y)		***A1g***	
MEAN	-0.0243	-0.0140	0.3136	0.3117
SSD	0.0616	0.1088	0.0627	0.0421
SE	0.0171	0.0302	0.0174	0.0117
	A1u		***A2g***	
MEAN	0.1082	0.1547	-0.0838	-0.0801
SSD	0.0435	0.0648	0.0264	0.0217
SE	0.0121	0.0180	0.0073	0.0060

5.8 Tabular re-centred NSD deformations and parameters

5.8.1 *Rhodobacter sphaeroides* bacteriochlorophylls – RBC4

Table 25: Minimum basis parameters and normal-coordinate displacements of each ETC cofactor in RBC4 (average coordinates).

BA	BB	DL	DM	BA	BB	DL	DM
	Doop				***Dip***		
0.3198	0.5623	0.4905	0.5447	0.2704	0.3662	0.3792	0.3501
	δoop				***δip***		
0.0268	0.0170	0.0267	0.0110	0.0445	0.0463	0.0445	0.0488
	B2u				***B2g***		
0.0688	0.1937	0.2455	0.2625	0.0361	0.0340	-0.0261	0.0022
	B1u				***B1g***		
0.0557	0.4215	0.1834	-0.4498	-0.1221	-0.2316	-0.2238	-0.2020
	A2u				***Eu(x)***		
-0.1467	-0.0658	-0.3326	-0.1008	-0.0718	-0.0465	-0.0786	-0.0558
	Eg(x)				***Eu(y)***		
-0.2700	-0.2763	-0.0953	-0.1004	-0.0323	-0.1038	-0.0680	-0.0337
	Eg(y)				***A1g***		
0.0004	0.1352	-0.1623	-0.0229	0.2120	0.2471	0.2753	0.2700
	A1u				***A2g***		
-0.0025	0.0452	0.0256	-0.0688	-0.0762	-0.0728	-0.0799	-0.0677

5.8.2 *Blastochloris viridis* bacteriochlorophylls – BBC1

Minimum Basis

Table 26: Minimum basis parameters and normal-coordinate displacements of each ETC cofactor in BBC1 (from averaged coordinates).

BA	BB	DL	DM	BA	BB	DL	DM
	Doop				***Dip***		
0.4262	0.4024	0.7467	1.0031	0.4066	0.3884	0.3682	0.3088
	δoop				***δip***		
0.0424	0.0443	0.0319	0.0365	0.0377	0.0367	0.0389	0.0347
	B2u				***B2g***		
0.1174	0.0226	-0.2390	-0.0769	0.0802	0.0549	0.0568	0.0481

		B1u				***B1g***	
0.123	0.0363	-0.6791	-0.9567	-0.2642	-0.2519	-0.2148	-0.1792
		A2u				***Eu(x)***	
-0.0517	-0.1638	-0.0366	-0.0417	-0.1098	-0.0784	-0.1237	-0.1189
		Eg(x)				***Eu(y)***	
-0.3750	-0.3588	0.0071	-0.0662	-0.0701	-0.0262	-0.0323	-0.0351
		Eg(y)				***A1g***	
0.0671	0.0670	0.0654	0.1497	0.2569	0.2670	0.2495	0.1992
		A1u				***A2g***	
0.0704	0.0110	-0.1833	-0.2377	-0.0783	-0.0789	-0.0875	-0.0767

Extended Basis

Table 27: Extended basis parameters and normal-coordinate displacements of each ETC cofactor in BBC1 (from averaged coordinates).

	BA	BB	DL	DM	BA	BB	DL	DM
			Doop				***Dip***	
N/A	0.4525	0.4505	0.7672	1.0212	0.4331	0.4158	0.4029	0.3481
			δoop				***δip***	
N/A	0.0341	0.034	0.0192	0.0158	0.0223	0.0229	0.0213	0.0179
			B2u				***B2g***	
1st	0.1192	0.0235	-0.2386	-0.0767	0.0807	0.0558	0.0578	0.0488
2nd	0.0672	0.0352	0.0391	0.0236	0.0208	0.0495	0.0057	0.0133
			B1u				***B1g***	
1st	0.1230	0.0363	-0.6791	-0.9567	-0.2645	-0.2522	-0.215	-0.1796
2nd	-0.0510	-0.0382	0.1247	0.1481	-0.0722	-0.0720	-0.0787	-0.0630
			A2u				***Eu(x)***	
1st	-0.057	-0.1666	-0.0366	-0.0421	-0.1103	-0.0790	-0.1243	-0.1194
2nd	-0.0752	-0.0242	0.0055	0.006	-0.0541	-0.0426	-0.0576	-0.0429
			Eg(x)				***Eu(y)***	
1st	-0.3728	-0.3526	0.0054	-0.0671	-0.0684	-0.0247	-0.0307	-0.0335
2nd	0.0951	0.1926	-0.0663	-0.0351	0.1173	0.1130	0.1288	0.1323
			Eg(y)				***A1g***	
1st	0.0681	0.067	0.0643	0.1488	0.2577	0.2679	0.25	0.2005
2nd	0.0306	0.0064	-0.0134	0.0187	-0.0042	-0.0024	0.0204	0.0479
			A1u				***A2g***	
1st	0.0704	0.011	-0.1833	-0.2377	-0.0778	-0.0785	-0.0865	-0.0757
2nd	-0.0200	0.0022	0.0949	0.1107	-0.0005	0.0029	0.0169	0.0081

5.8.3 *Rhodobacter sphaeroides* bacteriopheophytins – RBP4

Table 28: Minimum basis in- and out-of-plane parameters and normal-coordinate displacements for each ETC cofactor in all RBP4 experiments.

ΦA	ΦB	ΦA	ΦB
	Doop		***Dip***
0.5394	0.4902	0.5573	0.6061
	δoop		***δip***
0.0211	0.0184	0.0494	0.0518
	B2u		***B2g***
0.0204	0.1073	0.1755	0.1923

B1u		***B1g***	
0.4724	0.4156	-0.3539	-0.3921
A2u		***Eu(x)***	
0.2083	0.1838	-0.0851	-0.0358
Eg(x)		***Eu(y)***	
-0.0673	-0.1114	-0.1020	-0.1245
Eg(y)		***A1g***	
-0.0004	0.0372	0.3590	0.3909
A1u		***A2g***	
0.1395	0.0916	-0.0897	-0.0836

5.8.4 *Rhodobacter sphaeroides* bacteriopheophytins – RBP5

Table 29: Minimum basis in- and out-of-plane parameters and normal-coordinate displacements for each ETC cofactor in all RBP5 experiments.

ΦA	ΦB	ΦA	ΦB
Doop		***Dip***	
0.4057	0.4391	0.3632	0.3226
δoop		***δip***	
0.0101	0.0085	0.0527	0.0513
B2u		***B2g***	
0.0263	0.0774	-0.0475	-0.0556
B1u		***B1g***	
0.386	0.3993	-0.2727	-0.2323
A2u		***Eu(x)***	
0.0978	0.1564	-0.075	-0.0382
Eg(x)		***Eu(y)***	
-0.0113	-0.0326	-0.0406	-0.0479
Eg(y)		***A1g***	
-0.056	0.0141	0.2143	0.1967
A1u		***A2g***	
0.0458	0.0409	-0.0459	-0.0679

5.8.5 *Blastochloris viridis* bacteriopheophytins – BBP1

Table 30: Minimum basis in- and out-of-plane parameters and normal-coordinate displacements for each ETC cofactor in all BBP1 experiments.

ΦA	ΦB	ΦA	ΦB
Doop		***Dip***	
0.5021	0.5783	0.5329	0.5529
δoop		***δip***	
0.0218	0.0325	0.0425	0.0415
B2u		***B2g***	
-0.2419	-0.1368	0.3464	0.2088
B1u		***B1g***	
0.381	0.5147	-0.2112	-0.388
A2u		***Eu(x)***	
0.0571	0.0381	-0.1131	-0.0867

Eg(x)		***Eu(y)***	
-0.1815	-0.159	-0.0343	-0.0263
Eg(y)		***A1g***	
-0.0245	-0.0137	0.3137	0.3114
A1u		***A2g***	
0.1077	0.1546	-0.0838	-0.08

5.9 Cofactor Coordinates

5.9.1 Rhodobacter sphaeroides bacteriochlorophylls – RBC4

Table 31: Atomic coordinates of the best estimate (RBC4) of the conformation of the *R. sphaeroides* BA macrocycle (angstroms). n = 32.

	Minimum			Extended			Complete		
Atom	x	y	z	x	y	z	x	y	z
N1	-2.0330	-0.0311	-0.1061	-2.0343	0.0010	-0.0364	-2.0640	0.0060	-0.0550
N2	-0.0114	2.0712	-0.0518	0.0173	2.0694	-0.0922	0.0210	2.0591	-0.0870
N3	2.0005	0.0297	0.0226	1.9808	0.0648	0.0100	2.0010	0.0630	0.0209
N4	0.0145	-2.0566	-0.0520	0.0389	-2.0811	-0.0675	0.0311	-2.0689	-0.0721
Cm1	-2.4203	2.4363	-0.0426	-2.4322	2.4073	-0.0540	-2.4150	2.4080	-0.0390
Cm2	2.4323	2.4467	0.0382	2.4712	2.4492	0.0570	2.4500	2.4411	0.0339
Cm3	2.4201	-2.4268	0.0774	2.4181	-2.3973	0.0866	2.4431	-2.3819	0.0650
Cm4	-2.4220	-2.4607	-0.0821	-2.3987	-2.4028	-0.1020	-2.4069	-2.4080	-0.0790
Ca1	-2.8697	-1.1304	-0.0406	-2.8580	-1.0843	-0.0143	-2.8569	-1.1040	-0.0100
Ca2	-2.8410	1.0898	-0.0160	-2.8698	1.0820	0.0158	-2.8770	1.1050	0.0290
Ca3	-1.0982	2.9136	-0.0658	-1.1022	2.8813	-0.0976	-1.0910	2.8481	-0.0780
Ca4	1.1050	2.8852	0.0204	1.1346	2.8982	0.0165	1.1410	2.8662	-0.0111
Ca5	2.8500	1.1140	0.0092	2.8683	1.1134	0.0127	2.8810	1.1152	0.0129
Ca6	2.8112	-1.0866	0.0334	2.7735	-1.0541	0.0228	2.7661	-1.0438	0.0229
Ca7	1.1085	-2.8912	0.0423	1.1269	-2.9201	0.0529	1.1471	-2.8930	0.0379
Ca8	-1.0859	-2.8853	-0.0879	-1.0744	-2.8832	-0.1144	-1.0869	-2.8500	-0.0910
Cb1	-4.2498	-0.6850	0.1380	-4.2539	-0.6820	0.1170	-4.2269	-0.6970	0.1080
Cb2	-4.2267	0.6769	0.1548	-4.2597	0.6713	0.1471	-4.2470	0.6790	0.1410
Cb3	-0.6441	4.3007	-0.0160	-0.6724	4.2724	-0.0208	-0.7361	4.3121	-0.0850
Cb4	0.7168	4.2755	0.0470	0.6958	4.2812	0.0737	0.7429	4.3021	0.1420
Cb5	4.2241	0.6599	-0.0353	4.2357	0.6287	-0.0362	4.2180	0.6352	-0.0271
Cb6	4.1931	-0.6963	-0.0187	4.1627	-0.7184	-0.0232	4.1471	-0.7388	-0.0221
Cb7	0.6923	-4.2786	0.0614	0.6989	-4.3134	0.0809	0.7542	-4.3459	0.1429
Cb8	-0.6661	-4.2709	-0.0299	-0.6672	-4.2836	-0.0345	-0.7358	-4.3089	-0.1000

Table 32: Atomic coordinates of the best estimate (RBC4) of the conformation of the *R. sphaeroides* BB macrocycle (angstroms). n = 32.

	Minimum			Extended			Complete		
Atom	x	y	z	x	y	z	x	y	z
N1	-2.0131	-0.0312	-0.0726	-2.0167	0.0037	-0.0515	-2.0511	0.0151	-0.0651
N2	-0.0115	2.1156	-0.0030	0.0191	2.1124	-0.0180	0.0171	2.0960	-0.0150
N3	1.9921	0.0267	0.0591	1.9732	0.0622	0.0416	1.9960	0.0629	0.0540
N4	0.0135	-2.0685	-0.0675	0.0395	-2.0930	-0.0657	0.0349	-2.0819	-0.0771
Cm1	-2.4221	2.4442	0.1166	-2.4265	2.4145	0.1126	-2.4060	2.4141	0.1299
Cm2	2.4318	2.4575	-0.0584	2.4681	2.4566	-0.0397	2.4501	2.4449	-0.0530
Cm3	2.4084	-2.4438	0.1793	2.3987	-2.4141	0.1834	2.4229	-2.3981	0.1669

	Minimum			Extended			Complete		
Atom	x	y	z	x	y	z	x	y	z
Cm4	-2.4116	-2.4724	-0.2415	-2.3824	-2.4077	-0.2434	-2.3921	-2.4109	-0.2401
Ca1	-2.8430	-1.1398	-0.1080	-2.8328	-1.0910	-0.1046	-2.8411	-1.1139	-0.0901
Ca2	-2.8271	1.0862	0.0997	-2.8566	1.0788	0.1158	-2.8610	1.1072	0.1159
Ca3	-1.1051	2.9532	0.0229	-1.1035	2.9224	0.0087	-1.0949	2.8901	0.0180
Ca4	1.1069	2.9295	-0.0640	1.1350	2.9399	-0.0599	1.1401	2.9070	-0.0760
Ca5	2.8431	1.1122	-0.0030	2.8639	1.1113	-0.0082	2.8760	1.1120	-0.0130
Ca6	2.7949	-1.1011	0.0962	2.7544	-1.0680	0.0902	2.7519	-1.0541	0.0850
Ca7	1.1004	-2.9102	0.1088	1.1145	-2.9441	0.1168	1.1348	-2.9130	0.1100
Ca8	-1.0832	-2.9010	-0.1996	-1.0678	-2.8951	-0.2044	-1.0812	-2.8639	-0.1711
Cb1	-4.2218	-0.7098	0.1015	-4.2298	-0.7133	0.0917	-4.2000	-0.7288	0.0829
Cb2	-4.2087	0.6519	0.2338	-4.2442	0.6402	0.2339	-4.2230	0.6422	0.2319
Cb3	-0.6554	4.3478	-0.0581	-0.6839	4.3225	-0.0573	-0.7559	4.3541	-0.1000
Cb4	0.7096	4.3263	-0.1191	0.6873	4.3309	-0.1174	0.7452	4.3650	-0.0730
Cb5	4.2152	0.6364	-0.0373	4.2306	0.6107	-0.0363	4.2090	0.6179	-0.0320
Cb6	4.1768	-0.7215	0.0178	4.1455	-0.7386	0.0171	4.1279	-0.7621	0.0230
Cb7	0.6833	-4.2992	0.1076	0.6888	-4.3406	0.1196	0.7368	-4.3770	0.1639
Cb8	-0.6734	-4.2891	-0.1111	-0.6747	-4.3007	-0.1249	-0.7362	-4.3250	-0.1761

Table 33: Atomic coordinates of the best estimate (RBC4) of the conformation of the *R. sphaeroides* DL macrocycle (angstroms). n = 32.

	Minimum			Extended			Complete		
Atom	x	y	z	x	y	z	x	y	z
N1	-2.0275	-0.0179	-0.1108	-2.0302	0.0160	-0.0650	-2.0610	0.0169	-0.0801
N2	-0.0274	2.1116	-0.1629	0.0013	2.1080	-0.1517	0.0010	2.0979	-0.1541
N3	1.9919	0.0150	-0.0654	1.9740	0.0499	-0.1208	2.0030	0.0509	-0.1171
N4	0.0307	-2.0808	-0.0856	0.0545	-2.1041	-0.0603	0.0430	-2.0900	-0.0661
Cm1	-2.4338	2.4619	0.0024	-2.4429	2.4381	-0.0303	-2.4301	2.4399	-0.0201
Cm2	2.4209	2.4464	-0.0849	2.4600	2.4499	-0.0733	2.4399	2.4339	-0.1081
Cm3	2.4282	-2.4537	0.1170	2.4221	-2.4285	0.1153	2.4430	-2.4221	0.1040
Cm4	-2.4042	-2.4641	-0.0550	-2.3806	-2.4066	-0.0847	-2.3821	-2.4071	-0.0672
Ca1	-2.8527	-1.1299	-0.0035	-2.8421	-1.0852	0.0059	-2.8461	-1.1040	0.0108
Ca2	-2.8426	1.1034	-0.0047	-2.8708	1.0990	0.0138	-2.8780	1.1209	0.0239
Ca3	-1.1130	2.9615	-0.0537	-1.1144	2.9319	-0.0720	-1.1061	2.8969	-0.0551
Ca4	1.0977	2.9167	-0.1044	1.1265	2.9260	-0.0827	1.1330	2.8989	-0.0880
Ca5	2.8362	1.1052	-0.0511	2.8571	1.1068	-0.0762	2.8760	1.1079	-0.0561
Ca6	2.8050	-1.1066	0.0778	2.7657	-1.0766	0.0508	2.7600	-1.0641	0.0440
Ca7	1.1198	-2.9259	0.0144	1.1348	-2.9574	0.0411	1.1530	-2.9311	0.0240
Ca8	-1.0723	-2.9055	-0.1128	-1.0601	-2.9006	-0.1251	-1.0711	-2.8721	-0.0981
Cb1	-4.2356	-0.6938	0.1990	-4.2406	-0.6971	0.1939	-4.2110	-0.7121	0.1829
Cb2	-4.2250	0.6699	0.1904	-4.2568	0.6591	0.1961	-4.2410	0.6689	0.1948
Cb3	-0.6470	4.3525	0.0772	-0.6747	4.3263	0.0667	-0.7471	4.3569	0.0169
Cb4	0.7174	4.3163	0.0405	0.6958	4.3183	0.0539	0.7579	4.3469	0.1039
Cb5	4.2114	0.6439	0.0914	4.2254	0.6182	0.1057	4.2019	0.6290	0.1070
Cb6	4.1842	-0.7136	0.1755	4.1523	-0.7313	0.1911	4.1290	-0.7490	0.1950
Cb7	0.6984	-4.3148	0.0002	0.7045	-4.3521	0.0215	0.7650	-4.3841	0.0750
Cb8	-0.6606	-4.2977	-0.0909	-0.6612	-4.3079	-0.1134	-0.7320	-4.3301	-0.1721

Table 34: Atomic coordinates of the best estimate (RBC4) of the conformation of the *R. sphaeroides* DM macrocycle (angstroms). n = 32.

	Minimum			Extended			Complete		
Atom	x	y	z	x	y	z	x	y	z
N1	-2.0255	-0.0205	-0.0368	-2.0277	0.0208	-0.0370	-2.0599	0.0190	-0.0410
N2	-0.0175	2.0985	-0.0570	0.0095	2.0927	-0.0571	0.0111	2.0860	-0.0599
N3	2.0002	0.0191	0.0111	1.9823	0.0644	-0.0007	2.0051	0.0650	-0.0019
N4	0.0199	-2.0833	-0.0460	0.0438	-2.1112	-0.0361	0.0361	-2.0960	-0.0290
Cm1	-2.4267	2.4539	-0.1880	-2.4396	2.4252	-0.1768	-2.4209	2.4310	-0.1820
Cm2	2.4247	2.4524	0.1747	2.4615	2.4561	0.1689	2.4370	2.4460	0.1711
Cm3	2.4251	-2.4471	-0.1331	2.4121	-2.4079	-0.1212	2.4381	-2.3960	-0.1310
Cm4	-2.4153	-2.4639	0.1402	-2.3800	-2.3996	0.1270	-2.3889	-2.3990	0.1390
Ca1	-2.8562	-1.1274	0.0999	-2.8363	-1.0757	0.1096	-2.8409	-1.0950	0.1030
Ca2	-2.8383	1.1011	-0.0629	-2.8754	1.0964	-0.0728	-2.8849	1.1240	-0.0640
Ca3	-1.1064	2.9430	-0.1785	-1.1097	2.9075	-0.1726	-1.0980	2.8760	-0.1440
Ca4	1.1000	2.9122	0.0828	1.1268	2.9222	0.0780	1.1301	2.8920	0.0561
Ca5	2.8422	1.1129	0.1092	2.8671	1.1164	0.1179	2.8811	1.1140	0.1101
Ca6	2.8139	-1.1004	-0.0353	2.7712	-1.0605	-0.0535	2.7651	-1.0470	-0.0370
Ca7	1.1132	-2.9227	-0.1340	1.1259	-2.9532	-0.1197	1.1471	-2.9230	-0.1329
Ca8	-1.0840	-2.9093	0.0467	-1.0669	-2.9123	0.0414	-1.0809	-2.8750	0.0390
Cb1	-4.2373	-0.6848	0.1903	-4.2369	-0.6850	0.1903	-4.2049	-0.7030	0.1920
Cb2	-4.2218	0.6779	0.0942	-4.2629	0.6693	0.0952	-4.2449	0.6740	0.0909
Cb3	-0.6538	4.3338	-0.1451	-0.6789	4.3024	-0.1677	-0.7349	4.3280	-0.2000
Cb4	0.7090	4.3080	0.0433	0.6902	4.3112	0.0636	0.7330	4.3390	0.0941
Cb5	4.2183	0.6594	0.1192	4.2371	0.6232	0.1242	4.2211	0.6290	0.1321
Cb6	4.1946	-0.6989	0.0363	4.1633	-0.7263	0.0358	4.1431	-0.7460	0.0271
Cb7	0.6908	-4.3130	-0.1311	0.6954	-4.3536	-0.1515	0.7671	-4.3880	-0.1290
Cb8	-0.6693	-4.3008	-0.0001	-0.6717	-4.3223	0.0148	-0.7559	-4.3550	-0.0030

5.9.2 *Blastochloris viridis* bacteriochlorophylls – BBC1

Table 35: Atomic coordinates of the best estimate of the conformation of the *B.viridis* BA macrocycle (angstroms); n = 13.

	Minimum			Extended			Complete		
Atom	x	y	z	x	y	z	x	y	z
N1	-2.0231	-0.0432	-0.0973	-2.0189	-0.0088	-0.0423	-2.0310	-0.0041	-0.0600
N2	-0.0005	2.1162	-0.0092	0.0168	2.1130	-0.0383	0.0270	2.1050	-0.0599
N3	1.9734	0.0402	0.0815	1.9564	0.0763	0.0449	1.9719	0.0800	0.0621
N4	0.0052	-2.0844	-0.0411	0.0203	-2.1090	-0.0999	0.0210	-2.1121	-0.1170
Cm1	-2.4065	2.4444	-0.0258	-2.4374	2.4342	-0.0312	-2.4191	2.4480	0.0091
Cm2	2.4387	2.4665	0.0541	2.4855	2.4760	0.1111	2.4599	2.4660	0.0571
Cm3	2.4028	-2.4314	0.1112	2.4086	-2.4075	0.1494	2.4450	-2.4021	0.0980
Cm4	-2.4195	-2.4894	-0.1426	-2.4118	-2.4485	-0.1082	-2.4120	-2.4551	-0.0800
Ca1	-2.8578	-1.1511	-0.0445	-2.8385	-1.1133	-0.0149	-2.8360	-1.1221	-0.0110
Ca2	-2.8242	1.0862	-0.0008	-2.8519	1.0866	0.0332	-2.8481	1.1009	0.0301
Ca3	-1.0885	2.9567	-0.0472	-1.1045	2.9324	-0.0723	-1.0911	2.9100	-0.0309
Ca4	1.1185	2.9319	0.0174	1.1501	2.9352	0.0331	1.1400	2.9370	0.0391
Ca5	2.8310	1.1217	0.0513	2.8511	1.1272	0.0331	2.8559	1.1220	0.0441
Ca6	2.7755	-1.0855	0.0412	2.7415	-1.0555	0.0503	2.7229	-1.0470	0.0480
Ca7	1.1014	-2.9154	0.0908	1.1204	-2.9387	0.0901	1.1380	-2.9040	0.0839

	Minimum			Extended			Complete		
Atom	x	y	z	x	y	z	x	y	z
Ca8	-1.0864	-2.9249	-0.1452	-1.0872	-2.9290	-0.1775	-1.1110	-2.9031	-0.1280
Cb1	-4.2356	-0.7017	0.1627	-4.2255	-0.7054	0.1351	-4.2200	-0.7241	0.1300
Cb2	-4.2101	0.6626	0.1800	-4.2341	0.6509	0.1617	-4.2330	0.6539	0.1491
Cb3	-0.6296	4.3521	-0.0644	-0.6472	4.3240	-0.0629	-0.6991	4.3489	-0.1689
Cb4	0.7344	4.3281	-0.0274	0.7250	4.3208	-0.0336	0.7669	4.3160	0.0582
Cb5	4.1988	0.6491	-0.0590	4.2088	0.6235	-0.0836	4.2130	0.6300	-0.0839
Cb6	4.1562	-0.7065	-0.0800	4.1261	-0.7236	-0.0756	4.1100	-0.7409	-0.0569
Cb7	0.7024	-4.3097	0.0857	0.7067	-4.3358	0.1225	0.7320	-4.3501	0.2219
Cb8	-0.6561	-4.3125	-0.0914	-0.6605	-4.3249	-0.1243	-0.7030	-4.3530	-0.2341

Table 36: Atomic coordinates of the best estimate of the conformation of the *B.viridis* BB macrocycle (angstroms); n = 13.

	Minimum			Extended			Complete		
Atom	x	y	z	x	y	z	x	y	z
N1	-2.0204	-0.0363	-0.1362	-2.0149	-0.0044	-0.0351	-2.0309	0.0039	-0.0510
N2	-0.0075	2.1059	-0.0380	0.0079	2.1033	-0.0548	0.0191	2.0989	-0.0720
N3	1.9849	0.0352	0.0349	1.9693	0.0712	-0.0503	1.9821	0.0839	-0.0411
N4	0.0108	-2.0940	-0.0699	0.0211	-2.1181	-0.0928	0.0210	-2.1190	-0.1040
Cm1	-2.4111	2.4485	-0.0546	-2.4410	2.4388	-0.0899	-2.4160	2.4479	-0.0521
Cm2	2.4308	2.4656	0.0794	2.4761	2.4724	0.1323	2.4501	2.4590	0.0748
Cm3	2.4123	-2.4375	0.0752	2.4154	-2.4114	0.1085	2.4581	-2.4120	0.0610
Cm4	-2.4210	-2.4802	-0.1101	-2.4163	-2.4418	-0.1211	-2.4189	-2.4480	-0.0870
Ca1	-2.8576	-1.1403	-0.0627	-2.8413	-1.1024	-0.0194	-2.8399	-1.1091	-0.0140
Ca2	-2.8227	1.0934	-0.0261	-2.8451	1.0947	0.0178	-2.8440	1.1099	0.0090
Ca3	-1.0943	2.9491	-0.0733	-1.1122	2.9257	-0.1116	-1.0979	2.9060	-0.0711
Ca4	1.1085	2.9232	0.0500	1.1370	2.9265	0.0789	1.1260	2.9250	0.0799
Ca5	2.8347	1.1242	0.0300	2.8583	1.1269	-0.0030	2.8591	1.1230	0.0119
Ca6	2.7917	-1.0880	0.0129	2.7565	-1.0589	-0.0145	2.7391	-1.0500	-0.0041
Ca7	1.1067	-2.9279	0.0582	1.1246	-2.9461	0.0900	1.1441	-2.9110	0.0741
Ca8	-1.0888	-2.9264	-0.1061	-1.0906	-2.9347	-0.1522	-1.1139	-2.9100	-0.1100
Cb1	-4.2353	-0.6845	0.1527	-4.2271	-0.6789	0.1222	-4.2199	-0.6960	0.1071
Cb2	-4.2080	0.6789	0.1763	-4.2271	0.6764	0.1664	-4.2229	0.6749	0.1650
Cb3	-0.6412	4.3425	-0.0301	-0.6674	4.3155	-0.0494	-0.7130	4.3430	-0.1551
Cb4	0.7214	4.3185	0.0567	0.7033	4.3119	0.0790	0.7351	4.3030	0.1738
Cb5	4.2061	0.6633	-0.0586	4.2203	0.6296	-0.0642	4.2261	0.6420	-0.0561
Cb6	4.1724	-0.6938	-0.0733	4.1423	-0.7192	-0.0540	4.1271	-0.7451	-0.0491
Cb7	0.6941	-4.3221	0.1154	0.7100	-4.3442	0.1590	0.7371	-4.3530	0.2611
Cb8	-0.6664	-4.3172	-0.0027	-0.6591	-4.3327	-0.0419	-0.7069	-4.3671	-0.1510

Table 37: Atomic coordinates of the best estimate of the conformation of the *B.viridis* DL macrocycle (angstroms); n = 13.

	Minimum			Extended			Complete		
Atom	x	y	z	x	y	z	x	y	z
N1	-2.0343	-0.0394	-0.0276	-2.0301	0.0000	-0.0430	-2.0419	0.0050	-0.0399
N2	-0.0085	2.0966	0.0215	0.0104	2.0936	0.0006	0.0251	2.0861	-0.0020
N3	1.9783	0.0380	-0.0310	1.9605	0.0760	0.0175	1.9750	0.0831	0.0000
N4	0.0138	-2.0820	-0.0097	0.0295	-2.1093	-0.0173	0.0220	-2.1050	-0.0051

	Minimum			Extended			Complete		
Atom	x	y	z	x	y	z	x	y	z
Cm1	-2.4113	2.4466	-0.2244	-2.4359	2.4314	-0.1772	-2.4210	2.4420	-0.2118
Cm2	2.4341	2.4579	0.2524	2.4801	2.4580	0.2049	2.4570	2.4430	0.2380
Cm3	2.4146	-2.4286	-0.2567	2.4112	-2.3979	-0.2368	2.4510	-2.3899	-0.2311
Cm4	-2.4201	-2.4804	0.2265	-2.4067	-2.4258	0.1977	-2.4090	-2.4380	0.1890
Ca1	-2.8709	-1.1436	0.0474	-2.8511	-1.0980	0.0703	-2.8450	-1.1080	0.0670
Ca2	-2.8337	1.0924	-0.1195	-2.8628	1.0898	-0.1541	-2.8640	1.1030	-0.1389
Ca3	-1.0907	2.9437	-0.1486	-1.1026	2.9220	-0.1285	-1.0900	2.8980	-0.1098
Ca4	1.1125	2.9083	0.2210	1.1450	2.9074	0.1814	1.1340	2.9090	0.1691
Ca5	2.8333	1.1201	0.0723	2.8572	1.1217	0.1253	2.8580	1.1180	0.1080
Ca6	2.7861	-1.0821	-0.1471	2.7478	-1.0459	-0.1611	2.7311	-1.0379	-0.1241
Ca7	1.1116	-2.9133	-0.1635	1.1263	-2.9430	-0.1632	1.1421	-2.9090	-0.1551
Ca8	-1.0828	-2.9165	0.2119	-1.0819	-2.9173	0.2026	-1.1029	-2.8940	0.1689
Cb1	-4.2504	-0.6864	-0.0315	-4.2437	-0.6996	-0.0211	-4.2339	-0.7120	-0.0159
Cb2	-4.2211	0.6784	-0.1074	-4.2491	0.6559	-0.1172	-4.2500	0.6600	-0.1169
Cb3	-0.6242	4.3347	-0.0748	-0.6411	4.3114	-0.1159	-0.6870	4.3421	-0.0889
Cb4	0.7380	4.3030	0.2048	0.7295	4.2939	0.2595	0.7650	4.2870	0.2301
Cb5	4.2032	0.6592	-0.0083	4.2193	0.6402	-0.0028	4.2241	0.6431	0.0079
Cb6	4.1660	-0.6957	-0.1215	4.1352	-0.7051	-0.1445	4.1210	-0.7189	-0.1702
Cb7	0.7081	-4.3063	-0.0349	0.7109	-4.3417	-0.0998	0.7231	-4.3740	-0.1442
Cb8	-0.6515	-4.3047	0.2489	-0.6578	-4.3178	0.3227	-0.6839	-4.3329	0.3759

Table 38: Atomic coordinates of the best estimate of the conformation of the *B.viridis* DM macrocycle (angstroms); n = 13.

	Minimum			Extended			Complete		
Atom	x	y	z	x	y	z	x	y	z
N1	-2.0301	-0.0342	-0.0348	-2.0272	0.0055	-0.0413	-2.0420	0.0100	-0.0450
N2	-0.0076	2.0803	0.0280	0.0067	2.0755	0.0286	0.0160	2.0760	0.0102
N3	1.9762	0.0327	-0.0032	1.9632	0.0725	0.0241	1.9770	0.0749	0.0102
N4	0.0127	-2.0644	-0.0433	0.0242	-2.0907	-0.0602	0.0170	-2.0950	-0.0370
Cm1	-2.4109	2.4409	-0.3202	-2.4275	2.4232	-0.2775	-2.4140	2.4340	-0.2909
Cm2	2.4309	2.4484	0.3855	2.4626	2.4438	0.3308	2.4400	2.4350	0.3493
Cm3	2.4134	-2.4238	-0.3573	2.3968	-2.3847	-0.3198	2.4380	-2.3730	-0.3389
Cm4	-2.4168	-2.4703	0.2894	-2.3919	-2.4151	0.2540	-2.4000	-2.4240	0.2559
Ca1	-2.8646	-1.1368	0.0905	-2.8425	-1.0911	0.1280	-2.8370	-1.0970	0.1309
Ca2	-2.8335	1.0911	-0.1316	-2.8634	1.0890	-0.1746	-2.8630	1.0990	-0.1670
Ca3	-1.0894	2.9258	-0.2499	-1.0971	2.9050	-0.2241	-1.0829	2.8840	-0.1789
Ca4	1.1101	2.8928	0.2914	1.1319	2.8906	0.2638	1.1120	2.9000	0.2543
Ca5	2.8291	1.1133	0.1627	2.8552	1.1143	0.2060	2.8580	1.1060	0.1873
Ca6	2.7871	-1.0820	-0.1795	2.7511	-1.0435	-0.2014	2.7350	-1.0359	-0.1528
Ca7	1.1089	-2.8952	-0.2508	1.1144	-2.9201	-0.2452	1.1250	-2.8910	-0.2580
Ca8	-1.0809	-2.8992	0.2374	-1.0736	-2.9058	0.2161	-1.0950	-2.8800	0.1859
Cb1	-4.2438	-0.6874	0.0578	-4.2375	-0.6973	0.0762	-4.2260	-0.7100	0.0829
Cb2	-4.2192	0.6760	-0.0431	-4.2503	0.6580	-0.0611	-4.2490	0.6580	-0.0691
Cb3	-0.6271	4.3139	-0.2154	-0.6416	4.2942	-0.2757	-0.6450	4.3080	-0.2988
Cb4	0.7337	4.2846	0.1899	0.7253	4.2783	0.2564	0.7280	4.2740	0.2653
Cb5	4.1989	0.6584	0.0580	4.2211	0.6353	0.0652	4.2310	0.6370	0.0733
Cb6	4.1657	-0.6954	-0.1284	4.1415	-0.7102	-0.1446	4.1250	-0.7240	-0.1627

	Minimum			Extended			Complete		
Atom	x	y	z	x	y	z	x	y	z
Cb7	0.7075	-4.2849	-0.1003	0.7117	-4.3203	-0.1704	0.7280	-4.3510	-0.1661
Cb8	-0.6505	-4.2846	0.2672	-0.6531	-4.3062	0.3467	-0.6761	-4.3151	0.3599

5.9.3 *Rhodobacter sphaeroides* bacteriopheophytins – RBP4

Table 39: Atomic coordinates of the best estimate of the conformation of the ΦA macrocycle (RBP4, angstroms); n = 16.

	Minimum			Extended			Complete		
Atom	x	y	z	x	y	z	x	y	z
N1	-2.0206	-0.0702	0.0520	-2.0312	-0.0431	0.0126	-2.0640	-0.0411	0.0170
N2	0.0188	2.1611	0.0649	0.0639	2.1581	0.0640	0.0530	2.1450	0.0640
N3	1.9820	0.0659	0.0840	1.9612	0.0971	0.0680	1.9970	0.0960	0.0779
N4	-0.0152	-2.1149	0.0651	0.0204	-2.1351	0.0809	0.0131	-2.1430	0.0710
Cm1	-2.3942	2.4382	0.1551	-2.3825	2.4025	0.1625	-2.3620	2.3979	0.1779
Cm2	2.4618	2.5038	-0.1489	2.4985	2.5104	-0.1121	2.4750	2.5010	-0.1170
Cm3	2.3834	-2.4314	0.1852	2.3755	-2.4149	0.1784	2.3962	-2.4060	0.1871
Cm4	-2.4391	-2.5249	-0.1786	-2.4064	-2.4593	-0.1400	-2.4179	-2.4541	-0.1550
Ca1	-2.8652	-1.1795	-0.0489	-2.8702	-1.1324	-0.0822	-2.8719	-1.1461	-0.0710
Ca2	-2.8109	1.0705	0.0795	-2.8343	1.0632	0.0898	-2.8400	1.0919	0.0699
Ca3	-1.0814	2.9898	0.1347	-1.0696	2.9495	0.1336	-1.0611	2.9039	0.1129
Ca4	1.1376	2.9870	-0.1033	1.1659	3.0106	-0.0907	1.1699	2.9800	-0.0730
Ca5	2.8518	1.1470	-0.0367	2.8710	1.1465	-0.0540	2.8920	1.1501	-0.0510
Ca6	2.7657	-1.0797	0.0920	2.7198	-1.0578	0.1048	2.7071	-1.0590	0.0791
Ca7	1.0848	-2.9415	0.1618	1.1037	-2.9793	0.1584	1.1261	-2.9470	0.1590
Ca8	-1.1062	-2.9651	-0.1302	-1.0810	-2.9511	-0.1021	-1.0879	-2.9261	-0.0800
Cb1	-4.2397	-0.7181	-0.0551	-4.2632	-0.7059	-0.0603	-4.2369	-0.7162	-0.0641
Cb2	-4.2009	0.6479	0.0044	-4.2345	0.6539	0.0134	-4.2170	0.6508	0.0199
Cb3	-0.6329	4.3969	0.0315	-0.6838	4.3665	0.0581	-0.7611	4.4009	0.0719
Cb4	0.7355	4.3867	-0.1513	0.6889	4.4030	-0.1978	0.7629	4.4430	-0.2121
Cb5	4.2169	0.6445	-0.0984	4.2291	0.6083	-0.1014	4.2090	0.6232	-0.1099
Cb6	4.1532	-0.7147	-0.0387	4.1142	-0.7440	-0.0391	4.0841	-0.7639	-0.0239
Cb7	0.6874	-4.3444	0.0505	0.7049	-4.3874	0.0672	0.7632	-4.4050	0.0671
Cb8	-0.6728	-4.3549	-0.1708	-0.6602	-4.3594	-0.2119	-0.7288	-4.3761	-0.2179

Table 40: Atomic coordinates of the best estimate of the conformation of the ΦB macrocycle (RBP4, angstroms); n = 16.

	Minimum			Extended			Complete		
Atom	x	y	z	x	y	z	x	y	z
N1	-2.0084	-0.0730	0.0400	-2.0203	-0.0430	0.0286	-2.0559	-0.0349	0.0270
N2	0.0236	2.1799	0.0596	0.0721	2.1752	0.0616	0.0671	2.1760	0.0640
N3	1.9922	0.0677	0.0931	1.9715	0.1037	0.0468	2.0081	0.1010	0.0581
N4	-0.0220	-2.1235	0.0419	0.0128	-2.1448	0.0546	0.0080	-2.1550	0.0421
Cm1	-2.3941	2.4363	0.1332	-2.3812	2.4030	0.1371	-2.3699	2.3931	0.1599
Cm2	2.4656	2.5161	-0.1110	2.5066	2.5261	-0.0707	2.4821	2.5170	-0.0780
Cm3	2.3762	-2.4392	0.1662	2.3638	-2.4231	0.1786	2.3730	-2.4140	0.1751
Cm4	-2.4427	-2.5307	-0.1771	-2.4085	-2.4635	-0.1537	-2.4160	-2.4639	-0.1660
Ca1	-2.8541	-1.1834	-0.0504	-2.8614	-1.1331	-0.0651	-2.8609	-1.1539	-0.0499
Ca2	-2.8015	1.0654	0.0928	-2.8239	1.0627	0.1072	-2.8309	1.0901	0.0900
Ca3	-1.0850	3.0011	0.0915	-1.0732	2.9567	0.0839	-1.0639	2.9141	0.0678

	Minimum			Extended			Complete		
Atom	x	y	z	x	y	z	x	y	z
Ca4	1.1390	3.0118	-0.0818	1.1674	3.0373	-0.0600	1.1731	3.0080	-0.0531
Ca5	2.8612	1.1530	-0.0150	2.8874	1.1539	-0.0391	2.9061	1.1560	-0.0380
Ca6	2.7698	-1.0859	0.0984	2.7163	-1.0652	0.0944	2.7051	-1.0630	0.0751
Ca7	1.0753	-2.9527	0.1293	1.0939	-2.9909	0.1398	1.1140	-2.9610	0.1402
Ca8	-1.1146	-2.9745	-0.1333	-1.0864	-2.9629	-0.1210	-1.0950	-2.9329	-0.0908
Cb1	-4.2268	-0.7271	-0.0165	-4.2530	-0.7072	-0.0229	-4.2279	-0.7159	-0.0270
Cb2	-4.1900	0.6377	0.0625	-4.2227	0.6519	0.0641	-4.1998	0.6551	0.0660
Cb3	-0.6505	4.4130	-0.0285	-0.7150	4.3786	-0.0239	-0.7928	4.4071	-0.0291
Cb4	0.7198	4.4129	-0.1586	0.6592	4.4297	-0.1848	0.7342	4.4590	-0.1791
Cb5	4.2272	0.6400	-0.0774	4.2448	0.5925	-0.0751	4.2231	0.6050	-0.0829
Cb6	4.1601	-0.7220	-0.0197	4.1145	-0.7631	-0.0171	4.0901	-0.7790	-0.0009
Cb7	0.6701	-4.3571	0.0272	0.7002	-4.4014	0.0424	0.7590	-4.4230	0.0592
Cb8	-0.6902	-4.3658	-0.1665	-0.6647	-4.3732	-0.2058	-0.7300	-4.3850	-0.2298

5.9.4 *Rhodobacter sphaeroides* bacteriopheophytins – RBP5

Table 41: Atomic coordinates of the best estimate of the conformation of the ΦA macrocycle (RBP5, angstroms); n = 10.

	Minimum			Extended			Complete		
Atom	x	y	z	x	y	z	x	y	z
N1	-2.0051	-0.0024	0.0305	-2.0048	0.0173	0.0458	-2.0270	0.0239	0.0440
N2	-0.0230	2.1026	0.0159	0.0140	2.1128	-0.0095	0.0169	2.0900	-0.0080
N3	1.9711	0.0007	0.0359	1.9423	0.0239	0.0251	1.9470	0.0351	0.0270
N4	0.0262	-2.0842	0.0426	0.0611	-2.1114	0.0558	0.0591	-2.0950	0.0540
Cm1	-2.4247	2.4665	0.1230	-2.4231	2.4013	0.1203	-2.4051	2.4029	0.1171
Cm2	2.4063	2.4397	-0.1449	2.4371	2.4188	-0.1213	2.4270	2.4111	-0.1250
Cm3	2.4233	-2.4571	0.1529	2.4300	-2.4128	0.1457	2.4402	-2.4079	0.1470
Cm4	-2.3944	-2.4548	-0.1250	-2.3682	-2.3739	-0.1244	-2.3759	-2.3781	-0.1190
Ca1	-2.8240	-1.1159	-0.0466	-2.8214	-1.0585	-0.0494	-2.8450	-1.0670	-0.0531
Ca2	-2.8259	1.1121	0.0693	-2.8509	1.0783	0.0867	-2.8720	1.0969	0.0930
Ca3	-1.1060	2.9516	0.0892	-1.1049	2.9178	0.0755	-1.1031	2.8880	0.0760
Ca4	1.0916	2.9137	-0.0894	1.1252	2.9393	-0.0944	1.1289	2.9010	-0.0961
Ca5	2.8045	1.0973	-0.0669	2.8079	1.0766	-0.0651	2.8260	1.0801	-0.0640
Ca6	2.7938	-1.1102	0.0939	2.7631	-1.0679	0.0859	2.7780	-1.0459	0.0821
Ca7	1.1158	-2.9259	0.1041	1.1438	-2.9584	0.1157	1.1511	-2.9390	0.1180
Ca8	-1.0707	-2.9114	-0.0836	-1.0581	-2.9003	-0.0834	-1.0699	-2.8650	-0.0840
Cb1	-4.2043	-0.6862	-0.0468	-4.2231	-0.6767	-0.0650	-4.1890	-0.7061	-0.0660
Cb2	-4.2031	0.6755	0.0207	-4.2421	0.6708	0.0304	-4.2090	0.6859	0.0300
Cb3	-0.6524	4.3407	0.0480	-0.6811	4.3204	0.0561	-0.7571	4.3570	0.0540
Cb4	0.7093	4.3115	-0.0791	0.6919	4.3360	-0.0809	0.7559	4.3710	-0.0771
Cb5	4.1782	0.6553	-0.0701	4.1820	0.6277	-0.0715	4.1380	0.6411	-0.0690
Cb6	4.1672	-0.7005	0.0295	4.1457	-0.7131	0.0300	4.1520	-0.7509	0.0290
Cb7	0.7024	-4.3148	0.0152	0.7019	-4.3549	0.0264	0.7651	-4.3920	0.0270
Cb8	-0.6560	-4.3039	-0.1183	-0.6682	-4.3130	-0.1344	-0.7318	-4.3370	-0.1370

Table 42: Atomic coordinates of the best estimate of the conformation of the ΦB macrocycle (RBP5, angstroms); n = 10.

	Minimum			Extended			Complete		
Atom	x	y	z	x	y	z	x	y	z

	Minimum			Extended			Complete		
Atom	x	y	z	x	y	z	x	y	z
N1	-2.0011	-0.0069	0.0479	-1.9969	0.0068	0.0559	-2.0150	0.0139	0.0540
N2	-0.0320	2.0930	0.0476	0.0001	2.1068	0.0519	0.0070	2.0789	0.0511
N3	1.9837	0.0048	0.0634	1.9553	0.0231	0.0511	1.9621	0.0290	0.0531
N4	0.0336	-2.0713	0.0409	0.0630	-2.0977	0.0331	0.0640	-2.0771	0.0311
Cm1	-2.4308	2.4590	0.1394	-2.4320	2.3912	0.1269	-2.4180	2.3969	0.1241
Cm2	2.4043	2.4371	-0.1283	2.4325	2.4094	-0.1130	2.4260	2.4069	-0.1170
Cm3	2.4256	-2.4561	0.1477	2.4367	-2.4085	0.1467	2.4461	-2.3931	0.1480
Cm4	-2.3938	-2.4467	-0.1491	-2.3761	-2.3698	-0.1368	-2.3849	-2.3751	-0.1340
Ca1	-2.8248	-1.1137	-0.0541	-2.8243	-1.0578	-0.0514	-2.8470	-1.0681	-0.0500
Ca2	-2.8224	1.1053	0.0978	-2.8410	1.0675	0.1034	-2.8620	1.0839	0.1060
Ca3	-1.1147	2.9427	0.0911	-1.1186	2.9130	0.0899	-1.1121	2.8859	0.0890
Ca4	1.0837	2.9014	-0.0822	1.1156	2.9269	-0.0758	1.1209	2.8900	-0.0709
Ca5	2.8191	1.0987	-0.0425	2.8203	1.0717	-0.0525	2.8350	1.0729	-0.0539
Ca6	2.8018	-1.1099	0.0981	2.7764	-1.0675	0.1002	2.7950	-1.0441	0.0980
Ca7	1.1160	-2.9203	0.1015	1.1457	-2.9457	0.1036	1.1541	-2.9241	0.1080
Ca8	-1.0694	-2.8908	-0.0978	-1.0628	-2.8833	-0.1042	-1.0720	-2.8491	-0.1060
Cb1	-4.2043	-0.6846	-0.0518	-4.2229	-0.6678	-0.0606	-4.1940	-0.6991	-0.0650
Cb2	-4.1989	0.6753	0.0420	-4.2316	0.6764	0.0461	-4.1990	0.6928	0.0490
Cb3	-0.6627	4.3300	-0.0084	-0.6926	4.3137	-0.0020	-0.7661	4.3599	0.0000
Cb4	0.6987	4.2978	-0.1306	0.6814	4.3237	-0.1410	0.7360	4.3490	-0.1429
Cb5	4.1943	0.6501	-0.0687	4.1975	0.6200	-0.0785	4.1490	0.6310	-0.0739
Cb6	4.1773	-0.7067	0.0170	4.1609	-0.7206	0.0280	4.1670	-0.7610	0.0251
Cb7	0.6871	-4.3055	0.0100	0.6919	-4.3384	0.0250	0.7540	-4.3801	0.0220
Cb8	-0.6705	-4.2827	-0.1308	-0.6786	-4.2929	-0.1462	-0.7460	-4.3201	-0.1450

5.9.5 *Blastochloris viridis* bacteriopheophytins - BBP1

Table 43: Atomic coordinates of the best estimate of the conformation of the *B.viridis* ΦA macrocycle (BBP1, angstroms); n = 13.

	Minimum			Extended			Complete		
Atom	x	y	z	x	y	z	x	y	z
N1	-2.0454	-0.1085	-0.0429	-2.0421	-0.0745	-0.0225	-2.0437	-0.0767	-0.0240
N2	0.0625	2.1091	0.0302	0.0886	2.1087	0.0301	0.1007	2.1146	0.0315
N3	1.9941	0.1070	0.0438	1.9722	0.1450	0.0087	1.9903	0.1623	0.0143
N4	-0.0576	-2.0938	0.0418	-0.0354	-2.1216	0.0609	-0.0427	-2.1263	0.0534
Cm1	-2.3597	2.3935	0.0897	-2.3848	2.3689	0.0582	-2.3590	2.3821	0.0852
Cm2	2.4986	2.5226	-0.0988	2.5481	2.5282	-0.0644	2.5203	2.5132	-0.0856
Cm3	2.3621	-2.3773	0.1815	2.3684	-2.3475	0.1627	2.4042	-2.3595	0.1469
Cm4	-2.4851	-2.5435	-0.1689	-2.4720	-2.4890	-0.1611	-2.4711	-2.4944	-0.1530
Ca1	-2.9148	-1.1986	-0.0935	-2.8990	-1.1521	-0.1124	-2.8969	-1.1563	-0.1180
Ca2	-2.8126	1.0433	0.0026	-2.8414	1.0363	0.0356	-2.8387	1.0537	0.0289
Ca3	-1.0428	2.9211	0.1061	-1.0557	2.8901	0.0820	-1.0576	2.8620	0.0772
Ca4	1.1683	2.9551	-0.0327	1.2042	2.9663	-0.0087	1.1893	2.9647	-0.0102
Ca5	2.8811	1.1762	-0.0699	2.9006	1.1769	-0.1031	2.9056	1.1697	-0.0851
Ca6	2.7683	-1.0347	0.0457	2.7291	-0.9998	0.0491	2.7172	-0.9917	0.0352
Ca7	1.0613	-2.8919	0.1835	1.0851	-2.9203	0.1885	1.0941	-2.8890	0.1834
Ca8	-1.1405	-2.9611	-0.1011	-1.1370	-2.9621	-0.0911	-1.1543	-2.9326	-0.0664
Cb1	-4.2845	-0.7062	-0.0555	-4.2817	-0.7038	-0.0654	-4.2768	-0.7227	-0.0588

	Minimum			Extended			Complete		
Atom	x	y	z	x	y	z	x	y	z
Cb2	-4.2141	0.6600	-0.0122	-4.2433	0.6522	-0.0038	-4.2508	0.6580	-0.0140
Cb3	-0.6110	4.3268	0.1252	-0.6382	4.2961	0.1550	-0.7033	4.3089	0.1232
Cb4	0.7530	4.3398	0.0162	0.7354	4.3409	-0.0150	0.8011	4.3412	0.0176
Cb5	4.2418	0.6784	-0.1792	4.2520	0.6459	-0.1745	4.2569	0.6574	-0.1890
Cb6	4.1631	-0.6787	-0.1219	4.1294	-0.7007	-0.1121	4.1067	-0.7162	-0.0911
Cb7	0.6876	-4.2990	0.1614	0.6946	-4.3315	0.2071	0.7284	-4.3440	0.2462
Cb8	-0.6737	-4.3396	-0.0513	-0.6770	-4.3526	-0.1037	-0.7198	-4.3785	-0.1477

Table 44: Atomic coordinates of the best estimate of the conformation of the *B.viridis* ΦB macrocycle (BBP1, angstroms); n = 13.

	Minimum			Extended			Complete		
Atom	x	y	z	x	y	z	x	y	z
N1	-2.0050	-0.0740	-0.0359	-2.0019	-0.0388	-0.0574	-2.0019	-0.0265	-0.0588
N2	0.0297	2.1411	0.0189	0.0561	2.1398	0.0136	0.0640	2.1552	0.0107
N3	1.9656	0.0728	0.0400	1.9436	0.1131	0.0289	1.9511	0.1295	0.0303
N4	-0.0260	-2.1291	0.0255	-0.0039	-2.1572	0.0479	-0.0130	-2.1668	0.0412
Cm1	-2.3736	2.4329	0.1440	-2.4017	2.4105	0.1140	-2.3722	2.4168	0.1330
Cm2	2.4557	2.5107	-0.1490	2.5069	2.5208	-0.0954	2.4760	2.5135	-0.1212
Cm3	2.3753	-2.4205	0.2210	2.3828	-2.3914	0.1776	2.4206	-2.4024	0.1793
Cm4	-2.4453	-2.5268	-0.2136	-2.4318	-2.4752	-0.1663	-2.4307	-2.4838	-0.1703
Ca1	-2.8573	-1.1747	-0.0969	-2.8400	-1.1287	-0.1396	-2.8423	-1.1321	-0.1331
Ca2	-2.7868	1.0716	0.0362	-2.8169	1.0672	0.0642	-2.8124	1.0826	0.0525
Ca3	-1.0651	2.9693	0.1344	-1.0796	2.9356	0.1236	-1.0808	2.9058	0.1177
Ca4	1.1365	2.9771	-0.0919	1.1725	2.9900	-0.0802	1.1544	2.9923	-0.0676
Ca5	2.8316	1.1574	-0.0733	2.8518	1.1604	-0.1011	2.8571	1.1576	-0.0721
Ca6	2.7527	-1.0652	0.0710	2.7122	-1.0310	0.0923	2.7034	-1.0261	0.0707
Ca7	1.0792	-2.9467	0.2008	1.1041	-2.9736	0.1970	1.1131	-2.9424	0.1797
Ca8	-1.1151	-2.9815	-0.1531	-1.1108	-2.9853	-0.1265	-1.1315	-2.9561	-0.0935
Cb1	-4.2267	-0.6948	-0.0323	-4.2217	-0.6882	-0.0564	-4.2233	-0.6999	-0.0592
Cb2	-4.1765	0.6699	0.0273	-4.2060	0.6667	0.0572	-4.2074	0.6608	0.0578
Cb3	-0.6292	4.3746	0.1267	-0.6587	4.3403	0.1883	-0.7068	4.3497	0.1720
Cb4	0.7349	4.3718	-0.0495	0.7149	4.3732	-0.1186	0.7684	4.3651	-0.1035
Cb5	4.1940	0.6731	-0.1385	4.2036	0.6349	-0.1550	4.2115	0.6393	-0.1716
Cb6	4.1373	-0.6847	-0.0709	4.1019	-0.7126	-0.0519	4.0859	-0.7272	-0.0330
Cb7	0.6880	-4.3531	0.1631	0.6974	-4.3838	0.2174	0.7255	-4.3982	0.2501
Cb8	-0.6740	-4.3714	-0.1039	-0.6747	-4.3865	-0.1737	-0.7089	-4.4068	-0.2113

6 PDB Structures

The raw data, i.e. the cofactor atomic coordinates, were downloaded in batches by PDB ligand I.D. from the PDB Ligand Expo site. Specifically, every BCL (BChl a), BCB (BChl b), BPH (BPheo a) and BPB (BPheo b) found in the directory as of 18/10/2010 was downloaded in .ipdb format on that day and the BH1 (BPheo a), in structures 2BNP, 2BNS and 2BOZ, cofactors were downloaded on 28/03/2011. Additionally, any cofactor structure that included alternate conformations was recompiled as two separate structures and both were included in the final analysis.

6.1 *Rhodobacter sphaeroides* RC crystal structures

Table 45: Information relating to the PDB structures of the *R. sphaeroides* reaction center that were included in the analysis. [a] OL denotes outlier in relevant factor analysis; [b] structures containing two RCs in asymmetric unit and therefore two measurements of each cofactor; [c] not included in factor analysis because of erroneous, missing or chemically different cofactor (see comments) and [d] not included in relevant factor analysis since structures do not exhibit any reasonable experimental variation.

PDB ID	Space	R	Res.	T / K	Comments	Key 1	Key 2	RBC[a]	RBP[a]	Ref.
1AIG[b]	P 43 21 2	0.215	2.6	77	Light	1, 2	1, 2	4	5	[13]
1AIJ[b]	P 43 21 2	0.216	2.2	77	Dark	3, 4	3, 4	4	5	[13]
1DS8[b]	P 43 21 2	0.227	2.5	90	Dark; Cd^{2+} PT inhibitor	5, 6	5, 6	4	4, 5	[14]
1DV3[b]	P 43 21 2	0.226	2.5	90	Light; Cd^{2+} PT inhibitor	7, 8	7, 8	4	4, 5	[14]
1DV6[b]	P 43 21 2	0.238	2.5	90	Dark; Zn^{2+} PT inhibitor	9, 10	9, 10	4	4, 5	[14]
1E14	P 31 2 1	0.226	2.7	100	FM197R/GM203D [BA]	11	11	4	OL	[15]
1E6D	P 31 2 1	0.174	2.3	298	WM115F/ FM197R [BA / P]	12	12	4	4	[16]
1F6N	P 31 2 1	0.221	2.8	277	Error in BCL L304 (BA)	NA[c]	13	-	OL	[17]
1FNP	P 31 2 1	0.216	2.6	277	PL209Y	13	14	4	OL	[17]
1FNQ	P 31 2 1	0.217	2.6	277	PL209E	14	15	4	OL	[17]
1JGW	P 31 2 1	0.211	2.8	298	TM21L	15	16	2A	2	[18]
1JGX	P 31 2 1	0.211	3.01	298	TM21D	16	17	2A	2	[18]
1JGY	P 31 2 1	0.218	2.7	298	YM76F	17	18	2A	2	[18]
1JGZ	P 31 2 1	0.215	2.7	298	YM76K	18	19	2A	2	[18]
1JH0	P 31 2 1	0.225	3.5	298	EL205L	19	20	2A	2	[18]
1K6L	P 31 2 1	0.193	3.1	293		NA[d]	NA[d]	1	1	[19]
1K6N	P 31 2 1	0.203	3.1	293	EL212A/DL213A	NA[d]	NA[d]	1	1	[19]
1KBY	P 31 2 1	0.195	2.5	298	HM202L [DM → BPheo]	NA[c]	21	-	2	[20]
1L9B	P 1 21 1	0.22	2.4	100	Cytochrome C_2 bound	20	22	2B	2	[21]
1L9J[b]	P 1 21 1	0.248	3.25	100	Cytochrome C_2 bound	21, 22	23, 24	2B	2	[21]
1M3X	P 31 2 1	0.185	2.55	298	Surface lipids [BA / ΦB]	23	25	2A	2	[22]
1MPS	P 31 2 1	0.194	2.55	298	YM177F/FM197R [P]	24	26	4	OL	[22]
1OGV	P 42 21 2	0.214	2.35	100		25	27	2B	2	[23]
1PCR	P 31 2 1	0.186	2.65	NA		26	28	4	OL	[24]
1PSS	P 21 21 21	0.223	3.0	NA	See ref.	27	29	OL	5	[25]
1PST	P 21 21 21	0.218	3.0	NA	See ref. [DM → BPheo]	NA[c]	30	-	5	[25]
1QOV	P 31 2 1	0.169	2.1	298	AM260W	28	NA[d]	4	1	[26]
1RG5	P 31 2 1	0.155	2.5	298	R-26.1	29	31	4	4	[27]
1RGN	P 31 2 1	0.189	2.8	100	R-26.1 reconstituted spheroidene	30	32	4	4	[27]
1RQK	P 31 2 1	0.162	2.7	298	R-26.1 reconstituted with 3,4-dihydrospheroidene	31	33	4	4	[27]
1RVJ	P 31 2 1	0.218	2.75	100	DL213N/RH177H; [ΦA is BPheo b]	32	NA[c]	2B	-	[28]
1RY5	P 31 2 1	0.211	2.1	292	DL213N; [ΦA is BPheo b]	33	NA[c]	2B	-	[28]
1RZH	P 31 2 1	0.221	1.8	100	DL213N/RM233C; [ΦA is BPheo b]	34	NA[c]	4	-	[28]

PDB ID	Space	R	Res.	T / K	Comments	Key 1	Key 2	RBC[a]	RBP[a]	Ref.
1RZZ[b]	P 43 21 2	0.216	2.4	100	DL213N/RM233C; [ΦA is BPheo b]	35, 36	NA[c], 34	2B	2	[28]
1S00[b]	P 43 21 2	0.226	2.6	100	DL213N/RM233C; [ΦA is BPheo b]	37, 38	NA[c], 35	2B	2	[28]
1UMX	P 31 2 1	0.224	2.8	298	RM267L; [ΦA/B is BPheo b]	39	NA[c]	4	-	[29]
1YF6	P 31 2 1	0.197	2.25	100	Quintuple mutant [Q(A) deficient; ΦA → BChl]	40	NA[c]	3	-	[30]
1YST	P 21 21 21	0.234	3.0	NA	Rhodobacter sphaeroides Y	41	36	OL	OL	[31]
1Z9J	P 42 2 2	0.299	4.5	298	Redox active metal centre	42	37	2A	2	[32]
1Z9K	P 42 2 2	0.33	4.6	298	As above	43	38	2A	2	[32]
2BNP	P 42 21 2	0.21	2.7	100	Dark	44	39	OL	3	[33]
2BNS	P 42 21 2	0.209	2.5	100	Light	45	40	OL	3	[33]
2BOZ	P 31 2 1	0.174	2.4	100	GM203L [BA]	46	41	4	4	[34]
2GMR	P 21 21 21	0.215	2.5	100	DL210N	47	42	4	4	[35]
2GNU	P 42 21 2	0.2	2.2	100		48	43	OL	3	[36]
2HG3	P 31 2 1	0.164	2.7	100	R-26.1	49	44	4	4	[37]
2HG9	P 31 2 1	0.179	2.45	100	R-26.1	50	45	4	4	[37]
2HH1	P 31 2 1	0.178	2.55	100	R-26.1	51	46	4	4	[37]
2HHK	P 31 2 1	0.172	2.5	100	R-26.1	52	47	4	4	[37]
2HIT	P 31 2 1	0.182	2.75	NA	R-26.1	53	48	4	4	[37]
2HJ6	P 31 2 1	0.174	3.0	100	R-26.1	54	49	4	4	[37]
2J8C	P 31 2 1	0.178	1.87	100	Dark, pH8	55	50	3	3	[38]
2J8D	P 31 2 1	0.197	2.07	100	Light, pH8	56	51	3	3	[38]
2JIY	P 31 2 1	0.181	2.2	100	AM149W [ΦB exclusion]	57	NA[c]	4	-	[39]
2JJ0	P 31 2 1	0.203	2.8	100	AM248W [QA exclusion]	58	52	4	4	[39]
2RCR	P 21 21 21		3.1	NA		59	53	OL	5	[40]
2UWS	P 31 2 1	0.202	2.9	100	Light, pH6.5	60	54	3	OL	[38]
2UWT	P 31 2 1	0.196	2.5	100	As above	61	55	3	3	[38]
2UWU	P 31 2 1	0.208	2.04	100	Dark, pH6.5	62	56	3	3	[38]
2UWV	P 31 2 1	0.225	2.13	100	Light pH6.5	63	57	3	3	[38]
2UWW	P 31 2 1	0.205	2.05	100	Dark, pH6.5	64	58	3	3	[38]
2UX3	P 31 2 1	0.185	2.5	100	Dark, pH9	65	59	3	3	[38]
2UX4	P 31 2 1	0.19	2.51	100	Light, pH9	66	60	3	3	[38]
2UX5	P 31 2 1	0.202	2.21	100	As above	67	61	3	3	[38]
2UXJ	P 43 21 2	0.194	2.25	100	Dark, pH10	68	62	3	3	[38]
2UXK	P 43 21 2	0.19	2.31	100	Light, pH10	69	63	3	3	[38]
2UXL	P 31 2 1	0.176	2.88	100	Dark, pH10	70	64	3	3	[38]
2UXM	P 31 2 1	0.186	2.7	100	Light, pH10	71	65	3	3	[38]
2WX5	P 31 2 1	0.237	2.63	100	FL181R [BB hexacoordinated]	72	66	3	3	[41]
3DSY	P 31 2 1	0.191	3.0	293	EL212Q	NA[d]	NA[d]	1	1	[42]
3DTA	P 31 2 1	0.199	3.2	293	EL212Q, NM44D	NA[d]	NA[d]	1	1	[42]
3DTR	P 31 2 1	0.195	3.1	293	EL212Q, LL227F	NA[d]	NA[d]	1	1	[42]
3DTS	P 31 2 1	0.209	3.1	293	EL212Q, DL213A, RM233L	NA[d]	NA[d]	1	1	[42]
3DU2	P 31 2 1	0.192	3.1	293	EL212A	NA[d]	NA[d]	1	1	[42]
3DU3	P 31 2 1	0.191	2.8	273	EL212Q, DL213A, AM249Y	NA[d]	NA[d]	1	1	[43]
3DUQ	P 31 2 1	0.209	2.7	273	EL212Q, DL213A, NM5D	NA[d]	NA[d]	1	1	[43]
4RCR	P 21 21 21	0.227	2.8	NA	R-26	73	67	OL	OL	[44]

6.2 *Blastochloris viridis* RC crystal structures

Table 46: Information relating to the PDB structures of the *B. viridis* reaction center that were included in the analysis.

PDB ID	Space Group	R	Res.	T / K	Comments	BBC	BBP	Ref.
1DXR	P 43 21 2	0.194	2.00	263	HL168F [DL lost H-bond; ↑↑P interaction]	2	1	[45]
1PRC	P 43 21 2	0.193	2.30	NA		1	1	[46]
1R2C	P 43 21 2	0.202	2.86	293		2	1	[47]
1VRN	P 43 21 2	0.191	2.20	100		2	1	[48]
2I5N	P 43 21 2	0.173	1.96	NA		2	1	[49]
2JBL	P 43 21 2	0.190	2.40	263	Stigmatellin inhibited	2	1	[50]
2PRC	P 43 21 2	0.182	2.45	263	Ubiquinone-2 complex [QB]	2	1	[51]
2WJM	P 21 21 2	0.174	1.95	100	Lipidic sponge phase	2	1	[52]
2WJN	P 21 21 2	0.172	1.86	100	As above	2	1	[52]
3D38	P 31 2 1	0.194	3.21	100	Crystallised with methyl-beta-cyclodextrin	2	OL	[53]
3G7F	P 43 21 2	0.177	2.50	100	HM200L, [heterodimer (DM)]	NA	OL	[54]
3PRC	P 43 21 2	0.178	2.40	263	QB depleted	2	1	[51]
5PRC	P 43 21 2	0.190	2.35	263	Atrazine complex	2	1	[55]
6PRC	P 43 21 2	0.184	2.30	263	Triazine complex	2	1	[55]
7PRC	P 43 21 2	0.184	2.65	263	As above	2	1	[55]

7 References

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8 Cofactor NSDs

8.1 *Rhodobacter sphaeroides* bacteriochlorin cofactor NSDs

Table 47: Minimum basis normal-mode displacements and conformational parameters of all BA cofactors from crystal structures of *Rhodobacter sphaeroides*.

Cofactor ID	Dip	δip	B2g	B1g	Eu(x)	Eu(y)	A1g	A2g	Doop	δoop	B2u	B1u	A2u	Eg(x)	Eg(y)	A1u
1AIG - BCL L283	0.2438	0.0511	-0.1464	-0.0317	-0.0548	-0.0913	0.1495	-0.0577	0.2084	0.0182	0.0474	0.0271	-0.1257	-0.1475	0.0532	0.0088
1AIG - BCL N284	0.1836	0.0538	-0.0930	0.0513	-0.0102	0.0041	0.1292	-0.0748	0.3500	0.0215	0.2086	-0.0296	-0.2045	-0.1762	0.0700	0.0173
1AIJ - BCL L283	0.2276	0.0504	-0.0266	-0.0253	-0.0311	-0.0748	0.1991	-0.0655	0.2906	0.0186	0.0390	0.1024	-0.2276	-0.1321	0.0527	0.0197
1AIJ - BCL R283	0.2667	0.0536	-0.0683	-0.0228	-0.0225	-0.0626	0.2415	-0.0567	0.2422	0.0159	0.0789	0.0780	-0.1436	-0.1560	0.0362	0.0096
1DS8 - BCL L1004	0.2114	0.0550	-0.0806	-0.0721	-0.0340	-0.0665	0.1508	-0.0682	0.4044	0.0335	0.0275	0.1393	-0.2324	-0.2970	0.0321	0.0122
1DS8 - BCL R2004	0.1991	0.0518	0.0422	-0.0038	0.0046	0.0128	0.1763	-0.0812	0.4173	0.0329	-0.0959	0.0701	-0.2796	-0.2853	0.0100	0.0199
1DV3 - BCL M1004	0.2020	0.0567	-0.0810	0.0064	-0.0059	-0.1032	0.1372	-0.0687	0.3817	0.0302	-0.0004	0.1161	-0.2133	-0.2937	0.0105	0.0177
1DV3 - BCL R2004	0.2018	0.0511	0.0263	-0.0353	-0.0029	-0.0264	0.1820	-0.0703	0.4227	0.0327	-0.0529	0.0768	-0.3067	-0.2718	0.0201	0.0410
1DV6 - BCL M1004	0.2269	0.0537	-0.1174	-0.0307	-0.0176	0.0134	0.1714	-0.0831	0.4116	0.0333	0.0020	0.0957	-0.2645	-0.2996	0.0221	0.0084
1DV6 - BCL R2004	0.2308	0.0527	-0.0341	-0.0441	0.0012	-0.0968	0.1905	-0.0670	0.3700	0.0319	-0.0262	0.0496	-0.2664	-0.2442	0.0322	0.0458
1E14 - BCL C304	0.3628	0.0531	0.0594	-0.1872	-0.1495	0.0128	0.2617	-0.0456	0.4230	0.0312	0.2734	-0.0584	-0.2793	-0.1494	-0.0167	0.0134
1E6D - BCL C304	0.3886	0.0490	0.1456	-0.2406	-0.0653	-0.0073	0.2497	-0.0724	0.3354	0.0265	0.0545	0.0299	-0.1113	-0.3072	0.0393	-0.0178
1EYS - BCL L604	0.3555	0.0473	-0.0100	-0.2209	-0.1714	-0.0821	0.1766	-0.1009	0.3242	0.0841	-0.0252	0.0741	-0.0668	-0.2226	0.2103	0.0274
1F6N - BCL L304	0.5775	0.1251	-0.4794	-0.2220	0.0024	-0.0609	0.2165	-0.0616	0.4998	0.1051	0.0812	0.0541	-0.3487	-0.2869	0.1597	-0.1047
1FNP - BCL L304	0.2985	0.0446	0.0817	-0.1718	-0.0717	-0.0167	0.2088	-0.0627	0.4363	0.0737	0.1052	0.0090	-0.2267	-0.3252	0.0708	-0.1306
1FNQ - BCL L304	0.3266	0.0431	0.0660	-0.1919	-0.1009	-0.0499	0.2194	-0.0684	0.3786	0.0713	0.1821	0.0156	-0.1782	-0.2610	-0.0040	-0.1002
1JGW - BCL M853	0.3162	0.0567	-0.1092	0.0099	-0.1693	-0.0036	0.2412	-0.0337	0.1149	0.0066	0.0245	0.0494	-0.0864	-0.0508	0.0108	-0.0010
1JGX - BCL L853	0.3372	0.0579	-0.0818	-0.0074	-0.1347	-0.0234	0.2949	-0.0361	0.0948	0.0070	-0.0090	0.0341	-0.0697	-0.0426	0.0322	0.0044
1JGY - BCL M853	0.3054	0.0587	-0.1010	0.0147	-0.1770	-0.0082	0.2246	-0.0322	0.0821	0.0056	-0.0551	0.0178	-0.0490	-0.0270	0.0153	0.0047
1JGZ - BCL M853	0.3463	0.0578	-0.1271	-0.0252	-0.1818	0.0208	0.2610	-0.0394	0.0965	0.0059	-0.0161	0.0643	-0.0588	-0.0378	0.0061	-0.0017
1JH0 - BCL L853	0.3901	0.0589	-0.1727	0.0132	-0.1988	0.0081	0.2844	-0.0418	0.0881	0.0053	-0.0016	0.0441	-0.0700	-0.0238	0.0187	0.0008
1K6L - BCL L304	0.3538	0.0509	-0.0142	-0.2130	-0.1207	0.0217	0.2460	-0.0640	0.3996	0.0676	-0.0823	0.0064	-0.2593	-0.1959	-0.2126	0.0455
1K6N - BCL L304	0.3543	0.0509	-0.0141	-0.2133	-0.1204	0.0218	0.2466	-0.0636	0.3994	0.0677	-0.0827	0.0073	-0.2590	-0.1954	-0.2128	0.0458
1KBY - BCL L853	0.3604	0.0572	-0.0543	-0.0105	-0.1948	0.0154	0.2960	-0.0322	0.1179	0.0063	0.0210	0.0583	-0.0858	-0.0470	0.0219	-0.0025
1L9B - BCL L1004	0.3172	0.0672	0.0626	-0.1595	-0.0413	-0.0886	0.2328	-0.0865	0.2477	0.0204	-0.0052	-0.0017	-0.1939	-0.1394	0.0526	-0.0394
1L9J - BCL L1004	0.3274	0.0690	0.0649	-0.1897	-0.0656	-0.0925	0.2169	-0.0842	0.2517	0.0182	-0.0150	-0.0442	-0.1971	-0.1184	0.0831	-0.0375
1L9J - BCL R2004	0.3469	0.0676	0.0520	-0.1871	-0.0900	-0.0982	0.2376	-0.0919	0.2316	0.0145	-0.0193	-0.0126	-0.1918	-0.1127	0.0489	-0.0356
1M3X - BCL L853	0.2869	0.0576	-0.0562	0.0214	-0.1317	-0.0388	0.2423	-0.0333	0.1197	0.0077	0.0468	0.0607	-0.0703	-0.0523	0.0276	-0.0015
1MPS - BCL L304	0.4180	0.0378	0.0595	-0.1927	-0.0773	-0.0651	0.3446	-0.0717	0.3985	0.0665	-0.0181	0.1227	-0.2287	-0.2995	-0.0368	0.0101
1OGV - BCL L1283	0.3790	0.0672	0.0648	-0.2053	-0.0621	-0.0836	0.2779	-0.0959	0.2626	0.0244	-0.0293	0.0023	-0.1911	-0.1383	0.1111	-0.0092
1PCR - BCL L304	0.3538	0.0509	-0.0162	-0.2140	-0.1206	0.0215	0.2450	-0.0644	0.3995	0.0676	-0.0819	0.0051	-0.2585	-0.1962	-0.2132	0.0455
1PSS - BCL M4	0.2549	0.0511	0.0183	-0.0403	-0.0639	-0.1118	0.2045	-0.0679	0.2358	0.0137	0.1027	0.1654	-0.1037	-0.0763	-0.0096	0.0326
1PST - BCL L4	0.2235	0.0512	-0.0102	-0.0236	-0.0722	-0.0653	0.1886	-0.0650	0.3788	0.0195	0.1329	0.2703	-0.2148	-0.0663	0.0224	0.0416
1PYH - BCL B304	0.3416	0.0498	0.0603	-0.2854	-0.1234	-0.0362	0.0902	-0.0830	0.3696	0.0339	-0.0124	0.0563	-0.0969	-0.3498	-0.0113	-0.0373

Cofactor ID	Dip	δip	B2g	B1g	Eu(x)	Eu(y)	A1g	A2g	Doop	δoop	B2u	B1u	A2u	Eg(x)	Eg(y)	A1u
1QOV - BCL L1304	0.3753	0.0492	0.0943	-0.2763	-0.0331	-0.0127	0.2255	-0.0589	0.3965	0.0388	0.0303	0.0440	-0.1016	-0.3686	-0.0667	-0.0610
1RG5 - BCL L304	0.4007	0.0444	0.0127	-0.1858	-0.1069	-0.0433	0.3246	-0.0849	0.3473	0.0316	-0.0238	0.1166	-0.0986	-0.3078	0.0433	-0.0093
1RGN - BCL L304	0.3384	0.0560	0.0914	-0.1629	-0.2087	-0.0656	0.1651	-0.0674	0.2506	0.0234	0.1011	0.0193	-0.0885	-0.1900	-0.0909	0.0018
1RQK - BCL L304	0.2783	0.0448	0.0292	-0.1355	-0.0876	-0.0103	0.2073	-0.0862	0.2790	0.0245	0.1465	0.0899	0.0222	-0.2029	0.0808	0.0107
1RVJ - BCL M854	0.2508	0.0814	0.0905	-0.0787	-0.0171	-0.0168	0.2102	-0.0615	0.3183	0.0349	-0.0046	-0.0235	-0.2223	-0.2087	-0.0319	-0.0820
1RY5 - BCL L854	0.3785	0.0672	0.0647	-0.2050	-0.0625	-0.0835	0.2774	-0.0960	0.2623	0.0243	-0.0287	0.0018	-0.1907	-0.1384	0.1114	-0.0095
1RZH - BCL L854	0.3753	0.0492	0.0944	-0.2767	-0.0329	-0.0126	0.2251	-0.0589	0.3962	0.0387	0.0303	0.0441	-0.1011	-0.3684	-0.0662	-0.0614
1RZZ - BCL L1004	0.2621	0.0685	0.0300	-0.1193	-0.0563	-0.0504	0.1993	-0.0903	0.2664	0.0185	-0.0627	-0.0291	-0.1953	-0.1483	0.0401	-0.0666
1S00 - BCL L1004	0.2741	0.0667	0.0758	-0.1518	-0.0726	-0.0287	0.1778	-0.0929	0.2591	0.0189	0.0871	-0.0464	-0.1766	-0.1457	0.0227	-0.0668
1S00 - BCL S2004	0.3035	0.0664	0.0720	-0.1734	-0.0240	0.0025	0.2156	-0.0991	0.4091	0.0314	-0.2209	-0.0213	-0.2745	-0.1534	0.1380	-0.0117
1UMX - BCL L1283	0.4510	0.0608	0.3753	0.0933	-0.1439	0.0032	0.1415	-0.1144	0.2370	0.0229	0.0877	0.0451	-0.0632	-0.1948	0.0599	-0.0299
1YF6 - BCL L854	0.2429	0.0477	0.0907	-0.0873	-0.0168	0.0422	0.1724	-0.1066	0.4600	0.0557	0.1055	0.1351	-0.2827	-0.3023	-0.0338	-0.0986
1YST - BCL L275	0.3032	0.0598	-0.0709	-0.2094	0.0159	-0.1061	0.1446	-0.1032	0.1613	0.0113	-0.0475	0.0577	-0.1209	-0.0532	0.0547	-0.0029
1Z9J - BCL B853	0.2730	0.0605	-0.1327	-0.0625	-0.1771	0.0033	0.1460	-0.0191	0.0738	0.0067	-0.0041	0.0219	-0.0556	-0.0280	0.0324	-0.0043
1Z9K - BCL B853	0.2215	0.0621	-0.0789	-0.0656	-0.1380	0.0729	0.1142	-0.0338	0.0888	0.0043	-0.0673	0.0221	-0.0518	-0.0122	0.0062	0.0012
2BNP - BCL A1283	0.3664	0.0733	0.2269	0.2039	-0.1132	-0.0207	0.1006	-0.1334	0.0443	0.0145	0.0070	-0.0141	-0.0139	-0.0389	0.0014	0.0017
2BNS - BCL A1283	0.1855	0.0685	-0.0256	0.0106	-0.1096	0.0284	0.0304	-0.1411	0.0498	0.0179	-0.0048	0.0093	-0.0275	-0.0361	-0.0176	-0.0004
2BOZ - BCL L1283	0.3445	0.0497	-0.0006	-0.2228	-0.1121	-0.0469	0.2118	-0.0968	0.4451	0.0302	0.0695	0.0825	-0.1701	-0.3503	-0.1867	0.0007
2GMR - BCL L304	0.4409	0.0434	0.0313	-0.2069	-0.0985	-0.0468	0.3663	-0.0671	0.5235	0.0498	0.0259	-0.0024	-0.2649	-0.4496	-0.0020	0.0329
2GNU - BCL L1283	0.3649	0.0630	0.1906	-0.0942	-0.0630	-0.0287	0.2645	-0.1149	0.1103	0.0257	0.0217	0.0152	-0.0728	-0.0638	-0.0370	0.0270
2HG3 - BCL L314	0.3021	0.0505	0.0699	-0.1492	-0.0535	0.0040	0.2301	-0.0911	0.3375	0.0281	0.1466	0.0139	-0.0489	-0.2932	-0.0621	-0.0003
2HG9 - BCL L314	0.2843	0.0503	0.1064	-0.1050	-0.1017	-0.0339	0.2032	-0.0753	0.3336	0.0346	0.0778	0.0586	-0.0571	-0.3125	-0.0287	-0.0056
2HH1 - BCL L314	0.3409	0.0453	0.1364	-0.1345	-0.0821	-0.0589	0.2506	-0.0809	0.3182	0.0304	0.1501	0.0972	0.0143	-0.2583	-0.0483	0.0003
2HHK - BCL L314	0.3012	0.0457	0.1046	-0.0783	-0.0939	-0.0594	0.2223	-0.1089	0.3388	0.0287	0.1129	0.0532	-0.0446	-0.3115	-0.0114	0.0055
2HIT - BCL L314	0.3049	0.0448	0.1006	-0.1184	-0.1377	0.0244	0.1947	-0.1066	0.4170	0.0246	0.2950	0.0534	0.0450	-0.2746	0.0810	0.0018
2HJ6 - BCL L314	0.2975	0.0565	0.0110	-0.2110	-0.0239	-0.0024	0.1878	-0.0893	0.3737	0.0260	0.1626	0.0516	-0.0228	-0.3122	0.1116	-0.0079
2J8C - BCL L1282	0.2781	0.0472	0.0057	-0.2001	-0.1100	-0.0272	0.0939	-0.1252	0.5174	0.0638	-0.0443	0.0442	-0.2034	-0.4673	-0.0636	-0.0043
2J8D - BCL L1283	0.3066	0.0468	-0.0370	-0.2552	-0.0249	-0.0207	0.0925	-0.1338	0.4486	0.1009	0.0359	0.0470	-0.1009	-0.4066	-0.1489	-0.0058
2JIY - BCL L1284	0.3125	0.0432	0.0620	-0.1740	-0.1168	-0.0059	0.2049	-0.0886	0.3683	0.0275	-0.0679	0.0744	-0.1382	-0.3224	-0.0488	0.0116
2JJ0 - BCL L1284	0.2755	0.0529	0.0108	-0.1519	-0.0913	-0.0693	0.1738	-0.0969	0.3215	0.0228	0.1223	0.0721	-0.0461	-0.2774	0.0614	0.0192
2RCR - BCL L450	0.2986	0.0501	0.1434	-0.1608	0.0869	-0.0868	0.1394	-0.0907	0.3557	0.0155	-0.0686	0.1306	-0.2415	-0.0096	0.2131	0.0302
2UWS - BCL L1282	0.2596	0.0574	0.1174	-0.1750	-0.0776	-0.0175	-0.0779	-0.1030	0.4339	0.1203	0.1436	0.1193	-0.1374	-0.3195	0.1728	0.0510
2UWT - BCL L1283	0.2612	0.0511	0.0631	-0.1935	-0.1051	-0.0387	0.0276	-0.1163	0.4506	0.1023	0.1138	0.0048	-0.1507	-0.4020	0.0560	0.0511
2UWU - BCL L1282	0.3008	0.0420	0.0717	-0.2639	-0.0464	-0.0380	0.0232	-0.1075	0.4686	0.0901	0.0857	0.0067	-0.1050	-0.4480	-0.0202	-0.0086
2UWV - BCL L1282	0.2996	0.0420	0.0688	-0.2545	-0.0594	-0.0126	0.0427	-0.1212	0.4425	0.0743	0.1728	0.0182	-0.1089	-0.3905	0.0249	-0.0265
2UWW - BCL L1282	0.2780	0.0433	0.0984	-0.2315	-0.0373	-0.0237	0.0211	-0.1079	0.4934	0.0919	0.1125	-0.0020	-0.1076	-0.4664	-0.0379	-0.0161
2UX3 - BCL L1282	0.2680	0.0547	0.0786	-0.2030	-0.0553	-0.0467	-0.0267	-0.1360	0.5292	0.1024	0.0545	0.0414	-0.1873	-0.4513	-0.1805	0.0635
2UX4 - BCL L1282	0.2308	0.0595	0.0483	-0.1832	-0.0331	-0.0155	-0.0298	-0.1232	0.6637	0.1103	0.0071	-0.0260	-0.3127	-0.5468	-0.2060	0.0247
2UX5 - BCL L1282	0.3327	0.0453	0.0675	-0.2903	-0.0219	-0.0191	0.0884	-0.1149	0.5147	0.0791	0.0511	0.0356	-0.2114	-0.4474	-0.1122	-0.0599
2UXJ - BCL L1282	0.2783	0.0513	0.1216	-0.2115	-0.0241	0.0363	-0.0485	-0.1169	0.4981	0.1074	0.1029	0.1190	-0.2495	-0.3920	0.0846	-0.0160
2UXK - BCL L1282	0.2100	0.0536	0.0491	-0.1414	-0.0448	-0.0352	-0.0453	-0.1280	0.5448	0.1118	0.0591	0.0377	-0.1975	-0.4694	-0.1781	0.0291
2UXL - BCL L1282	0.2278	0.0534	0.0598	-0.1391	-0.0168	-0.0147	-0.0468	-0.1620	0.6437	0.1273	-0.1455	0.1012	-0.2687	-0.5087	-0.2248	0.0376
2UXM - BCL L1283	0.2853	0.0594	0.0489	-0.2426	-0.0351	0.0339	-0.0236	-0.1312	0.5963	0.1244	0.0640	-0.0853	-0.2845	-0.4641	-0.2173	-0.0247

Cofactor ID	Dip	δip	B2g	B1g	Eu(x)	Eu(y)	A1g	A2g	Doop	δoop	B2u	B1u	A2u	Eg(x)	Eg(y)	A1u
2WX5 - BCL M1304	0.2572	0.0554	0.1051	-0.0220	-0.1907	0.0361	-0.0890	-0.0948	0.2858	0.0522	0.0477	0.0215	-0.1012	-0.2599	-0.0098	-0.0327
3DSY - BCL L501	0.3536	0.0509	-0.0139	-0.2129	-0.1210	0.0218	0.2456	-0.0639	0.3998	0.0676	-0.0826	0.0070	-0.2593	-0.1960	-0.2126	0.0456
3DTA - BCL L501	0.3540	0.0509	-0.0142	-0.2129	-0.1210	0.0222	0.2461	-0.0642	0.3996	0.0677	-0.0824	0.0063	-0.2595	-0.1956	-0.2124	0.0458
3DTR - BCL L501	0.3541	0.0509	-0.0142	-0.2130	-0.1210	0.0219	0.2460	-0.0645	0.3993	0.0676	-0.0822	0.0068	-0.2590	-0.1963	-0.2121	0.0450
3DTS - BCL L501	0.3546	0.0509	-0.0144	-0.2135	-0.1200	0.0219	0.2471	-0.0631	0.3996	0.0677	-0.0828	0.0068	-0.2593	-0.1953	-0.2128	0.0458
3DU2 - BCL L501	0.3537	0.0510	-0.0142	-0.2130	-0.1206	0.0216	0.2458	-0.0638	0.4000	0.0677	-0.0827	0.0059	-0.2595	-0.1958	-0.2129	0.0463
3DU3 - BCL L501	0.3548	0.0510	-0.0150	-0.2135	-0.1204	0.0212	0.2471	-0.0636	0.3995	0.0679	-0.0821	0.0064	-0.2592	-0.1953	-0.2131	0.0460
3DUQ - BCL L501	0.3549	0.0509	-0.0148	-0.2134	-0.1209	0.0219	0.2470	-0.0637	0.3992	0.0676	-0.0822	0.0075	-0.2590	-0.1950	-0.2130	0.0460
4RCR - BCL M311	0.5346	0.0592	0.0850	-0.0551	0.2437	-0.0723	0.4591	0.0112	0.5349	0.0596	0.4237	0.0466	-0.0377	-0.1265	0.2615	0.1366

Table 48 : Minimum basis normal-mode displacements and conformational parameters of all BB cofactors from crystal structures of *Rhodobacter sphaeroides*.

Cofactor ID	Dip	δip	B2g	B1g	Eu(x)	Eu(y)	A1g	A2g	Doop	δoop	B2u	B1u	A2u	Eg(x)	Eg(y)	A1u
1AIG - BCL M309	0.2535	0.0528	-0.1265	-0.0414	-0.0650	-0.1063	0.1652	-0.0609	0.2137	0.0103	0.0670	0.1026	-0.0893	-0.1461	-0.0360	0.0071
1AIG - BCL N282	0.3205	0.0522	-0.0282	-0.0834	-0.0728	-0.0747	0.2881	-0.0328	0.3919	0.0155	0.0863	0.3518	-0.1160	-0.0765	0.0445	0.0325
1AIJ - BCL M309	0.2613	0.0528	-0.0120	-0.0886	-0.0324	-0.0684	0.2272	-0.0541	0.4255	0.0148	0.2147	0.2992	-0.1330	-0.1522	0.0626	0.0257
1AIJ - BCL S309	0.2824	0.0527	-0.0075	-0.0826	-0.0302	-0.0870	0.2488	-0.0499	0.3895	0.0107	0.1001	0.2955	-0.1664	-0.1538	0.0412	0.0363
1DS8 - BCL L1001	0.2808	0.0562	-0.1079	-0.0859	-0.0718	-0.0520	0.2107	-0.0872	0.5191	0.0261	0.1839	0.3608	-0.1362	-0.2837	0.0488	0.0642
1DS8 - BCL R2001	0.3153	0.0561	0.0273	-0.0928	0.0397	-0.1206	0.2656	-0.0582	0.6416	0.0195	0.2234	0.5110	-0.1836	-0.2347	0.0376	0.1017
1DV3 - BCL L1001	0.2850	0.0571	-0.0097	-0.0975	-0.0383	-0.0929	0.2334	-0.0838	0.5403	0.0234	0.2381	0.3578	-0.1330	-0.2632	0.1364	0.0393
1DV3 - BCL S2001	0.3816	0.0598	0.0394	-0.1468	0.0274	-0.0826	0.3362	-0.0437	0.6704	0.0198	0.1106	0.5845	-0.1899	-0.2139	0.0660	0.0974
1DV6 - BCL M1001	0.3066	0.0554	-0.0667	-0.1097	-0.0134	-0.0646	0.2580	-0.0813	0.5867	0.0253	0.2313	0.4361	-0.1217	-0.2677	0.1032	0.0590
1DV6 - BCL S2001	0.3454	0.0599	-0.0360	-0.1250	0.0345	-0.0662	0.3065	-0.0534	0.6357	0.0161	0.0842	0.5298	-0.2329	-0.2397	0.0188	0.0652
1E14 - BCL C301	0.4279	0.0575	0.1211	-0.2730	-0.0862	-0.1041	0.2669	-0.0664	0.7275	0.0240	0.1794	0.5817	0.0245	-0.3362	0.2069	0.0474
1E6D - BCL C301	0.3809	0.0549	0.1028	-0.2285	-0.0795	-0.0735	0.2610	-0.0500	0.7048	0.0183	0.2315	0.5498	-0.0038	-0.3019	0.2206	0.0325
1EYS - BCL M601	0.3635	0.0469	-0.0262	-0.1883	-0.1691	-0.1448	0.1887	-0.1043	0.4407	0.0796	-0.1807	0.2928	0.0383	-0.1586	0.2088	0.0751
1F6N - BCL L301	0.4289	0.0398	0.0912	-0.2319	-0.0378	-0.0720	0.3328	-0.0673	0.6966	0.0678	0.2936	0.4649	-0.3115	-0.2838	0.0727	-0.0023
1FNP - BCL M801	0.4687	0.0426	0.0939	-0.2842	-0.0560	-0.0861	0.3409	-0.0580	0.6014	0.0562	0.2617	0.4019	-0.2005	-0.2423	0.1810	-0.0080
1FNQ - BCL M801	0.4188	0.0393	0.0736	-0.2464	-0.0320	-0.0993	0.3062	-0.0677	0.6395	0.0669	0.3098	0.3877	-0.1787	-0.3498	0.0724	-0.0563
1JGW - BCL L850	0.3482	0.0594	-0.0687	-0.0741	-0.1192	-0.0521	0.3051	-0.0313	0.1296	0.0056	0.0333	0.0908	-0.0743	-0.0350	0.0262	0.0029
1JGX - BCL L850	0.3107	0.0917	-0.1649	0.0025	-0.0529	0.0279	0.2562	-0.0118	0.3260	0.0286	-0.2679	-0.0567	-0.1195	0.0213	-0.0612	0.1133
1JGY - BCL L850	0.3850	0.0574	-0.0802	-0.0728	-0.1733	-0.0626	0.3182	-0.0359	0.1066	0.0048	0.0465	0.0469	-0.0759	-0.0238	0.0258	0.0029
1JGZ - BCL L850	0.4048	0.0604	-0.1196	-0.0294	-0.0814	-0.0703	0.3693	-0.0267	0.1237	0.0046	0.0713	0.0603	-0.0760	-0.0249	0.0134	0.0015
1JH0 - BCL M850	0.3492	0.0953	-0.1982	0.0261	-0.1148	0.0850	0.2480	-0.0056	0.3177	0.0293	-0.2561	-0.0753	-0.1120	0.0361	-0.0686	0.1054
1K6L - BCL M501	0.3999	0.0510	0.0561	-0.2651	-0.0414	-0.0496	0.2767	-0.0754	0.7070	0.0167	0.2957	0.5347	0.0763	-0.3020	0.1696	0.0277
1K6N - BCL M501	0.3996	0.0509	0.0563	-0.2649	-0.0417	-0.0503	0.2766	-0.0745	0.7071	0.0167	0.2956	0.5347	0.0757	-0.3022	0.1696	0.0274
1KBY - BCL L850	0.3286	0.0925	-0.1424	0.0106	-0.0620	0.0708	0.2806	-0.0056	0.3002	0.0275	-0.2372	-0.0477	-0.1223	0.0351	-0.0659	0.1052
1L9B - BCL M1001	0.3114	0.0694	0.0718	-0.1698	-0.0565	0.0134	0.2217	-0.1023	0.2383	0.0143	0.0696	0.0403	-0.1768	-0.0898	0.1049	-0.0021
1L9J - BCL M1001	0.3050	0.0684	0.0555	-0.1579	-0.0417	-0.0914	0.2133	-0.0971	0.2716	0.0220	0.0612	0.0485	-0.1965	-0.0938	0.1415	0.0154
1L9J - BCL S2001	0.3264	0.0636	0.0857	-0.2270	-0.0392	-0.1140	0.1453	-0.1095	0.2835	0.0209	-0.1015	0.0250	-0.2133	-0.1180	0.0936	-0.0354
1M3X - BCL L850	0.3535	0.0588	-0.0751	-0.0505	-0.1391	-0.0487	0.3065	-0.0332	0.1489	0.0052	0.0797	0.0869	-0.0797	-0.0380	0.0216	-0.0031
1MPS - BCL M801	0.4539	0.0435	0.0685	-0.2337	-0.0614	-0.1079	0.3571	-0.0613	0.4879	0.0453	0.1566	0.2909	-0.1276	-0.3097	0.1263	0.0282

Cofactor ID	Dip	δip	B2g	B1g	Eu(x)	Eu(y)	A1g	A2g	Doop	δoop	B2u	B1u	A2u	Eg(x)	Eg(y)	A1u
1OGV - BCL M1302	0.3841	0.0657	0.0604	-0.2366	-0.0764	-0.0613	0.2641	-0.0926	0.2882	0.0182	-0.1606	0.0884	-0.1861	-0.0831	0.0883	0.0117
1PCR - BCL L301	0.4079	0.0427	0.0831	-0.3037	-0.0868	-0.1492	0.1850	-0.0567	0.6496	0.0666	0.2258	0.5127	-0.1166	-0.2878	0.1072	-0.0151
1PSS - BCL M1	0.3011	0.0498	-0.0452	-0.1467	-0.0491	-0.1044	0.2265	-0.0497	0.2196	0.0053	-0.0060	0.2016	-0.0825	-0.0158	-0.0071	0.0206
1PST - BCL M1	0.2866	0.0510	-0.0482	-0.0650	-0.0095	-0.1400	0.2313	-0.0488	0.3476	0.0124	0.1133	0.2480	-0.1944	-0.0810	0.0388	0.0249
1PYH - BCL A301	0.3851	0.0495	0.0445	-0.3138	-0.0295	-0.1179	0.1610	-0.0850	0.6579	0.0217	0.2545	0.5034	0.0455	-0.2947	0.1489	0.0597
1QOV - BCL M1301	0.3990	0.0509	0.0560	-0.2647	-0.0402	-0.0503	0.2760	-0.0752	0.7064	0.0166	0.2950	0.5341	0.0772	-0.3021	0.1694	0.0278
1RG5 - BCL M501	0.5280	0.0546	-0.0171	-0.3444	-0.0438	-0.1158	0.3699	-0.0878	0.4964	0.0179	0.2581	0.2676	-0.0089	-0.2889	0.1438	0.0634
1RGN - BCL M908	0.4439	0.0574	0.0959	-0.2912	-0.0658	-0.1830	0.2438	-0.0761	0.7149	0.0270	0.1433	0.5595	-0.0290	-0.2404	0.3355	0.0799
1RQK - BCL M501	0.4305	0.0576	-0.1019	-0.3233	0.0479	-0.1258	0.2160	-0.0753	0.6429	0.0192	0.3049	0.3734	-0.0288	-0.3181	0.2759	0.0535
1RVJ - BCL L851	0.2970	0.0696	0.0794	-0.1334	-0.0307	-0.0608	0.2241	-0.0959	0.3694	0.0266	0.0322	0.1921	-0.2119	-0.1798	0.1452	0.0127
1RY5 - BCL L851	0.3118	0.0702	0.0846	-0.1528	0.0684	-0.0996	0.2130	-0.0822	0.4116	0.0347	-0.0918	0.0967	-0.2908	-0.2446	0.0627	-0.0575
1RZH - BCL M851	0.3985	0.0508	0.0557	-0.2646	-0.0401	-0.0503	0.2756	-0.0750	0.7059	0.0167	0.2942	0.5342	0.0772	-0.3019	0.1688	0.0281
1RZZ - BCL L1001	0.2524	0.0691	0.1004	-0.1348	-0.0276	-0.0228	0.1522	-0.1048	0.3487	0.0252	0.0264	0.1112	-0.2655	-0.1474	0.1275	-0.0105
1RZZ - BCL S2001	0.3075	0.0686	0.0728	-0.1552	-0.0205	-0.0814	0.2195	-0.0997	0.3211	0.0218	0.1048	0.1125	-0.2132	-0.1122	0.1441	0.0254
1RZZ - BCL S2004	0.3033	0.0659	0.0779	-0.1642	-0.0276	-0.0119	0.2200	-0.0983	0.3946	0.0326	-0.1689	-0.0169	-0.2809	-0.1698	0.1372	-0.0192
1S00 - BCL L1001	0.2212	0.0683	0.0921	-0.1325	-0.0097	-0.0239	0.1129	-0.0975	0.3834	0.0283	-0.0016	0.1428	-0.2870	-0.1584	0.1381	-0.0070
1S00 - BCL S2001	0.2858	0.0706	0.0501	-0.1520	-0.0273	-0.0988	0.1897	-0.0980	0.2427	0.0156	0.0671	0.0793	-0.1713	-0.1048	0.0877	-0.0076
1UMX - BCL M1303	0.4439	0.0499	0.0752	-0.3831	-0.0014	-0.1558	0.1051	-0.0966	0.6360	0.0193	0.2411	0.4211	-0.0617	-0.2715	0.3014	0.0271
1YF6 - BCL M851	0.2939	0.0574	0.0200	-0.2547	-0.0667	0.0226	0.0592	-0.1122	0.7856	0.0500	0.4103	0.5667	-0.0063	-0.3300	0.0767	0.1133
1YST - BCL M307	0.4590	0.0825	0.2431	-0.3530	0.1105	-0.0305	0.0719	-0.0930	0.1919	0.0194	-0.1126	0.1104	-0.0344	-0.0912	-0.0201	0.0454
1Z9J - BCL A850	0.3415	0.0596	-0.0945	-0.0961	-0.2532	-0.0022	0.1845	-0.0171	0.1739	0.0055	-0.1710	-0.0025	0.0145	0.0198	0.0111	0.0164
1Z9K - BCL A850	0.4561	0.0635	-0.2067	-0.0408	-0.2765	-0.0285	0.2922	-0.0316	0.1545	0.0044	-0.1255	0.0777	-0.0201	-0.0258	0.0315	0.0029
2BNP - BCL B1302	0.4237	0.0648	0.3391	-0.1075	-0.1815	0.0120	0.0629	-0.1261	0.0588	0.0126	-0.0114	0.0450	-0.0153	-0.0246	0.0116	0.0179
2BNS - BCL B1302	0.3922	0.0636	0.2442	-0.2180	-0.1424	0.0404	0.0968	-0.1241	0.0463	0.0136	-0.0187	0.0262	-0.0217	-0.0131	0.0029	0.0213
2BOZ - BCL M1303	0.3776	0.0503	0.0667	-0.2654	-0.0702	-0.1660	0.1582	-0.1007	0.7540	0.0196	0.1165	0.6149	0.0010	-0.3593	0.2145	0.0404
2GMR - BCL L301	0.4544	0.0438	0.1092	-0.2831	-0.0551	-0.1281	0.2995	-0.0721	0.7773	0.0448	0.2214	0.6166	-0.1716	-0.3228	0.1622	0.1222
2GNU - BCL M1302	0.3649	0.0630	0.1906	-0.0942	-0.0630	-0.0287	0.2645	-0.1149	0.1103	0.0257	0.0217	0.0152	-0.0728	-0.0638	-0.0370	0.0270
2HG3 - BCL M311	0.4036	0.0540	0.1315	-0.2693	-0.0438	-0.1211	0.2267	-0.0714	0.4403	0.0204	0.0892	0.2861	0.0907	-0.2943	0.0672	0.0686
2HG9 - BCL M311	0.3912	0.0534	0.0238	-0.3093	-0.0059	-0.1077	0.1780	-0.1161	0.5694	0.0210	0.1874	0.3904	0.0488	-0.3236	0.1592	0.0653
2HH1 - BCL M311	0.4494	0.0532	0.0720	-0.3404	-0.0673	-0.0900	0.2469	-0.0854	0.5193	0.0203	0.1546	0.3240	0.0351	-0.3423	0.1388	0.0565
2HHK - BCL M311	0.4506	0.0481	0.0570	-0.3124	-0.0779	-0.0528	0.2932	-0.0859	0.4986	0.0216	0.2002	0.2789	0.0829	-0.3291	0.1154	0.0474
2HIT - BCL M311	0.3859	0.0458	0.1079	-0.2379	-0.1309	-0.0937	0.2152	-0.0921	0.5316	0.0217	0.2172	0.3790	0.0374	-0.2604	0.1390	0.0577
2HJ6 - BCL M311	0.4560	0.0492	0.0999	-0.3601	-0.1317	-0.1672	0.1154	-0.0981	0.5971	0.0216	0.1591	0.4633	-0.0424	-0.3137	0.1134	0.0590
2J8C - BCL M1303	0.2969	0.0474	-0.0200	-0.2141	-0.0504	-0.1305	0.0854	-0.1228	0.7657	0.0584	0.2673	0.5909	-0.0086	-0.3939	0.0691	0.0755
2J8D - BCL M1308	0.3057	0.0487	0.1381	-0.2227	-0.0429	-0.0697	-0.0467	-0.1262	0.7106	0.0648	0.3075	0.5430	-0.0154	-0.3092	0.1364	0.0320
2JIY - BCL L1282	0.4434	0.0524	-0.0007	-0.3531	-0.0431	-0.0950	0.2343	-0.0783	0.6573	0.0234	0.2707	0.4388	-0.0699	-0.3739	0.1417	0.0384
2JJ0 - BCL L1282	0.4152	0.0539	0.0446	-0.2935	-0.0889	-0.1727	0.2000	-0.0809	0.6402	0.0256	0.1504	0.4684	-0.0309	-0.3327	0.2319	0.0496
2RCR - BCL M601	0.4219	0.0490	0.1877	-0.2922	0.0016	-0.0743	0.2153	-0.0745	0.4668	0.0122	0.0730	-0.3431	-0.2001	0.0942	0.2142	0.0083
2UWS - BCL M1303	0.3906	0.0600	0.1873	-0.2200	-0.0180	-0.1891	-0.1053	-0.1481	0.8644	0.1258	0.2499	0.5925	-0.2174	-0.4535	0.0331	0.2822
2UWT - BCL M1303	0.3370	0.0514	0.1077	-0.2356	0.0213	-0.1263	-0.0902	-0.1481	0.6665	0.0831	0.2573	0.5176	-0.0420	-0.2500	0.1619	0.1402
2UWU - BCL M1303	0.2621	0.0515	0.0063	-0.2045	0.0117	-0.1073	-0.0296	-0.1196	0.6749	0.0613	0.2918	0.4875	-0.0290	-0.3242	0.1623	0.0196
2UWV - BCL M1303	0.3006	0.0463	0.0614	-0.2132	0.0371	-0.1351	-0.0927	-0.1136	0.6852	0.0520	0.2719	0.4911	-0.0183	-0.3548	0.1670	0.0176
2UWW - BCL M1304	0.2847	0.0534	0.0271	-0.2405	0.0095	-0.0962	-0.0145	-0.1136	0.7212	0.0617	0.3027	0.5324	-0.0363	-0.3406	0.1489	0.0738

Cofactor ID	Dip	δip	B2g	B1g	Eu(x)	Eu(y)	A1g	A2g	Doop	δoop	B2u	B1u	A2u	Eg(x)	Eg(y)	A1u
2UX3 - BCL M1303	0.3460	0.0579	0.1588	-0.2301	0.0587	-0.1042	-0.0865	-0.1406	0.7221	0.0924	0.3256	0.4942	-0.0176	-0.3762	0.0888	0.1465
2UX4 - BCL M1303	0.2855	0.0539	0.0605	-0.1882	0.0130	-0.1451	-0.0786	-0.1225	0.7575	0.0916	0.2903	0.5850	-0.0347	-0.3129	0.2054	0.0776
2UX5 - BCL M1304	0.2849	0.0480	0.0952	-0.1696	0.0290	-0.0836	-0.1515	-0.1120	0.6859	0.0576	0.2777	0.4723	-0.0301	-0.3674	0.1848	0.0144
2UXJ - BCL M1303	0.3096	0.0464	0.0674	-0.2379	-0.0573	-0.0497	-0.0753	-0.1525	0.8292	0.0655	0.2615	0.6530	-0.0934	-0.4142	0.0790	0.0787
2UXK - BCL M1303	0.3165	0.0557	0.1401	-0.1888	-0.0463	-0.1577	-0.0644	-0.1173	0.9027	0.0846	0.2629	0.7494	-0.0236	-0.3620	0.1399	0.1818
2UXL - BCL M1303	0.3512	0.0578	0.1555	-0.2449	-0.0832	-0.0435	-0.0932	-0.1472	0.7851	0.1044	-0.1329	0.3059	-0.3823	-0.5951	0.0153	0.0666
2UXM - BCL M1303	0.3495	0.0626	0.2045	-0.1905	-0.0233	-0.1364	-0.1063	-0.1167	0.7930	0.0892	0.2749	0.5599	-0.0521	-0.3850	0.2199	0.2012
2WX5 - BCL L1282	0.2332	0.0465	-0.0241	-0.1037	0.0237	-0.1547	-0.1026	-0.0897	0.6298	0.0364	0.0581	0.4958	-0.0684	-0.2113	0.2675	0.1631
3DSY - BCL M501	0.3998	0.0509	0.0562	-0.2653	-0.0412	-0.0501	0.2765	-0.0752	0.7070	0.0167	0.2953	0.5349	0.0764	-0.3017	0.1697	0.0276
3DTA - BCL M501	0.3998	0.0509	0.0560	-0.2648	-0.0414	-0.0496	0.2770	-0.0753	0.7072	0.0167	0.2959	0.5347	0.0764	-0.3018	0.1701	0.0276
3DTR - BCL M501	0.3999	0.0509	0.0562	-0.2654	-0.0410	-0.0493	0.2767	-0.0752	0.7070	0.0167	0.2954	0.5347	0.0767	-0.3019	0.1697	0.0280
3DTS - BCL M501	0.3993	0.0510	0.0560	-0.2652	-0.0417	-0.0504	0.2761	-0.0740	0.7069	0.0168	0.2954	0.5346	0.0758	-0.3025	0.1696	0.0275
3DU2 - BCL M501	0.3998	0.0509	0.0563	-0.2653	-0.0413	-0.0499	0.2764	-0.0754	0.7069	0.0167	0.2954	0.5345	0.0760	-0.3024	0.1697	0.0277
3DU3 - BCL M501	0.4002	0.0509	0.0563	-0.2652	-0.0419	-0.0505	0.2770	-0.0752	0.7077	0.0167	0.2965	0.5348	0.0759	-0.3020	0.1706	0.0280
3DUQ - BCL M501	0.3993	0.0511	0.0568	-0.2651	-0.0410	-0.0501	0.2761	-0.0743	0.7063	0.0167	0.2951	0.5341	0.0755	-0.3023	0.1695	0.0278
4RCR - BCL L282	0.4363	0.0352	-0.0276	-0.0790	-0.0280	-0.0289	0.4261	0.0124	0.5507	0.0679	0.0452	0.1944	-0.4909	-0.1241	-0.0534	0.0645

Table 49: Minimum basis normal-mode displacements and conformational parameters of all DL cofactors from crystal structures of *Rhodobacter sphaeroides*.

Cofactor ID	Dip	δip	B2g	B1g	Eu(x)	Eu(y)	A1g	A2g	Doop	δoop	B2u	B1u	A2u	Eg(x)	Eg(y)	A1u
1AIG - BCL L282	0.3228	0.0501	-0.1203	-0.1097	-0.0909	-0.0711	0.2463	-0.0611	0.3885	0.0137	0.1476	0.2466	-0.2148	-0.1123	-0.0895	0.0398
1AIG - BCL N283	0.3080	0.0473	-0.1176	-0.0447	-0.0518	-0.0563	0.2646	-0.0565	0.5026	0.0142	0.2475	0.3314	-0.2642	-0.0376	-0.0943	0.0374
1AIJ - BCL L282	0.3189	0.0514	-0.1060	-0.0897	-0.0671	-0.0765	0.2615	-0.0607	0.5339	0.0178	0.2361	0.3183	-0.3421	-0.0713	-0.0669	0.0379
1AIJ - BCL R282	0.3119	0.0524	-0.0853	-0.0715	-0.0553	-0.0694	0.2706	-0.0615	0.4597	0.0138	0.1835	0.2907	-0.2933	-0.0633	-0.0498	0.0261
1DS8 - BCL L1002	0.3526	0.0500	-0.0885	-0.1272	-0.0370	-0.0812	0.2972	-0.0634	0.5818	0.0236	0.2350	0.2720	-0.4176	-0.1203	-0.1254	0.0690
1DS8 - BCL R2002	0.3831	0.0524	-0.1432	-0.0295	-0.0248	-0.0475	0.3419	-0.0747	0.5400	0.0270	0.2527	0.1746	-0.4259	-0.1029	-0.0544	0.0475
1DV3 - BCL L1002	0.4262	0.0498	-0.1481	-0.1424	-0.0915	-0.0570	0.3520	-0.0624	0.5381	0.0223	0.2591	0.2146	-0.3968	-0.1155	-0.0493	0.0556
1DV3 - BCL R2002	0.4262	0.0543	-0.1693	-0.1426	-0.0495	-0.0606	0.3515	-0.0543	0.5753	0.0239	0.3118	0.2079	-0.4185	-0.0931	-0.0682	0.0458
1DV6 - BCL L1002	0.3918	0.0488	-0.1278	-0.1336	-0.0627	-0.0908	0.3218	-0.0597	0.6248	0.0320	0.3377	0.2801	-0.4267	-0.0908	-0.0663	0.0560
1DV6 - BCL R2002	0.4355	0.0542	-0.1988	-0.1528	-0.0550	-0.0638	0.3384	-0.0719	0.5839	0.0159	0.2564	0.1774	-0.4777	-0.0623	-0.0895	0.0601
1E14 - BCL C302	0.3921	0.0490	-0.0332	-0.2689	-0.0892	-0.0020	0.2630	-0.0566	0.5775	0.0367	0.3764	0.0944	-0.3565	-0.1681	-0.1525	0.0653
1E6D - BCL C302	0.3782	0.0533	0.0583	-0.1952	-0.0740	-0.0380	0.3032	-0.0520	0.4879	0.0368	0.2350	0.2113	-0.3415	0.0491	-0.1227	0.0642
1EYS - BCL L602	0.3696	0.0483	0.0333	-0.2302	-0.1334	-0.1109	0.2063	-0.0991	0.3721	0.0770	0.0960	0.2987	-0.0824	-0.0220	0.1380	0.1172
1F6N - BCL L302	0.4508	0.0444	0.0507	-0.2407	-0.0848	-0.0471	0.3588	-0.0673	0.4775	0.0714	0.1672	0.2189	-0.3465	-0.0978	-0.1483	-0.0224
1FNP - BCL L302	0.4599	0.0449	0.0555	-0.2386	-0.0535	-0.0806	0.3718	-0.0619	0.3882	0.0651	0.1333	0.1403	-0.2517	-0.1793	-0.1264	-0.0423
1FNQ - BCL L302	0.4275	0.0460	0.0664	-0.2221	-0.0677	-0.0688	0.3395	-0.0672	0.4338	0.0653	0.1472	0.1807	-0.2785	-0.2026	-0.1129	-0.0496
1JGW - BCL L851	0.4276	0.0611	-0.0748	-0.1215	-0.1391	0.0202	0.3752	-0.0441	0.2104	0.0052	0.1548	0.0789	-0.1092	-0.0413	-0.0210	-0.0037
1JGX - BCL L851	0.4276	0.0611	-0.0726	-0.1092	-0.1744	0.0338	0.3639	-0.0409	0.1543	0.0041	0.1060	0.0692	-0.0769	-0.0344	-0.0255	-0.0026
1JGY - BCL L851	0.4186	0.0624	-0.0596	-0.1116	-0.2007	0.0072	0.3424	-0.0401	0.1888	0.0051	0.1216	0.0739	-0.1136	-0.0412	-0.0275	-0.0076
1JGZ - BCL L851	0.4694	0.0637	0.1225	0.1217	0.0227	-0.1585	0.4040	-0.0413	0.2034	0.0048	-0.1639	-0.0672	-0.0898	0.0195	-0.0385	-0.0077
1JH0 - BCL L851	0.3830	0.0601	-0.0804	-0.1076	-0.1475	0.0013	0.3230	-0.0504	0.1301	0.0040	0.0809	0.0437	-0.0811	-0.0333	-0.0275	-0.0064
1K6L - BCL L302	0.4536	0.0425	0.0343	-0.2938	-0.0789	-0.1124	0.3049	-0.0801	0.6247	0.0683	0.3929	0.2137	-0.4111	-0.1081	-0.0313	-0.0919

Cofactor ID	Dip	δip	B2g	B1g	Eu(x)	Eu(y)	A1g	A2g	Doop	δoop	B2u	B1u	A2u	Eg(x)	Eg(y)	A1u
1K6N - BCL L302	0.4541	0.0425	0.0341	-0.2939	-0.0790	-0.1123	0.3056	-0.0804	0.6250	0.0684	0.3934	0.2138	-0.4112	-0.1079	-0.0309	-0.0921
1KBY - BCL L851	0.4042	0.0614	-0.0891	-0.1238	-0.1738	-0.0001	0.3293	-0.0384	0.1935	0.0047	0.1442	0.0797	-0.0922	-0.0383	-0.0182	-0.0034
1L9B - BCL L1002	0.3123	0.0665	0.1276	-0.1925	-0.0510	-0.0429	0.1747	-0.0960	0.4147	0.0166	0.3190	0.1024	-0.2242	-0.0855	0.0008	-0.0464
1L9J - BCL L1002	0.3656	0.0672	0.0848	-0.2345	-0.0516	-0.0738	0.2314	-0.0991	0.2491	0.0123	0.1748	0.0053	-0.1512	-0.0747	-0.0200	-0.0512
1L9J - BCL R2002	0.4015	0.0675	0.0755	-0.2436	-0.0713	-0.0636	0.2783	-0.0978	0.3087	0.0124	0.2249	0.0436	-0.1846	-0.0772	-0.0285	-0.0445
1M3X - BCL L851	0.3815	0.0616	-0.0694	-0.1138	-0.1395	-0.0123	0.3261	-0.0428	0.2320	0.0061	0.1756	0.0901	-0.1098	-0.0452	-0.0267	-0.0073
1MPS - BCL L302	0.3868	0.0398	0.0265	-0.1674	-0.0756	-0.0508	0.3280	-0.0713	0.4811	0.0713	0.1227	0.1287	-0.3999	-0.1818	-0.0812	0.0156
1OGV - BCL L1282	0.4347	0.0669	0.0607	-0.2246	-0.0240	-0.1555	0.3169	-0.0983	0.2680	0.0154	0.0878	0.0767	-0.2204	-0.0965	0.0016	-0.0196
1PCR - BCL L302	0.4526	0.0424	0.0346	-0.2927	-0.0782	-0.1119	0.3046	-0.0809	0.6250	0.0682	0.3930	0.2134	-0.4114	-0.1091	-0.0310	-0.0920
1PSS - BCL L2	0.3045	0.0488	-0.0885	-0.1093	-0.0882	-0.0459	0.2420	-0.0672	0.3645	0.0164	0.2000	0.2224	-0.1886	-0.0337	-0.0810	0.0108
1PST - BCL L2	0.2791	0.0511	-0.0644	-0.1023	-0.0367	-0.0897	0.2261	-0.0527	0.3880	0.0173	0.3099	0.1784	-0.1355	-0.0362	-0.0539	0.0080
1PYH - BCL A302	0.3853	0.0566	-0.0220	-0.3352	-0.0776	-0.0818	0.1242	-0.0863	0.5192	0.0368	0.2774	0.2176	-0.2976	-0.0291	-0.2327	0.0412
1QOV - BCL L1302	0.4287	0.0580	-0.0089	-0.2861	-0.0742	-0.0387	0.3056	-0.0385	0.4977	0.0379	0.2693	0.1404	-0.3481	0.0218	-0.1815	0.0293
1RG5 - BCL L302	0.5426	0.0516	0.0267	-0.3597	-0.1361	-0.0609	0.3649	-0.0943	0.4459	0.0307	0.2442	0.1771	-0.2878	0.0014	-0.1575	0.0133
1RGN - BCL L302	0.3755	0.0474	0.0113	-0.2674	-0.0735	-0.0620	0.2111	-0.1248	0.4595	0.0286	0.1219	0.1541	-0.3515	-0.1217	-0.1848	0.0077
1RQK - BCL L302	0.3903	0.0499	0.0116	-0.3144	-0.0629	-0.0613	0.1871	-0.1032	0.4177	0.0325	0.2460	0.1447	-0.2722	-0.0091	-0.1365	0.0134
1RVJ - BCL L852	0.3678	0.0638	0.0487	-0.2034	-0.0555	-0.1045	0.2600	-0.0996	0.3837	0.0250	0.0828	0.0846	-0.3229	-0.1699	-0.0015	-0.0095
1RY5 - BCL L852	0.3659	0.0663	0.0706	-0.2040	-0.0242	-0.1027	0.2579	-0.0982	0.4144	0.0292	0.1486	0.1110	-0.3308	-0.1670	-0.0005	0.0000
1RZH - BCL L852	0.3470	0.0637	0.0250	-0.2004	-0.0060	-0.0838	0.2479	-0.1053	0.4236	0.0285	0.1994	0.1344	-0.3005	-0.1747	-0.0277	-0.0072
1RZZ - BCL L1002	0.4029	0.0670	0.0560	-0.2024	-0.0328	-0.1585	0.2874	-0.0973	0.3022	0.0177	0.1159	0.0369	-0.2506	-0.1102	0.0326	-0.0226
1RZZ - BCL R2002	0.3952	0.0664	0.0473	-0.1945	-0.0566	-0.1089	0.3020	-0.0993	0.2892	0.0187	0.0514	0.0400	-0.2525	-0.1122	0.0507	-0.0222
1S00 - BCL L1002	0.4294	0.0628	0.0778	-0.2457	-0.0589	-0.1151	0.3013	-0.1023	0.3077	0.0209	0.0470	0.0673	-0.2633	-0.1310	0.0296	-0.0238
1S00 - BCL R2002	0.4130	0.0670	0.0698	-0.2145	-0.0299	-0.1205	0.3068	-0.1007	0.3375	0.0195	0.1391	0.0460	-0.2712	-0.1237	0.0566	-0.0206
1UMX - BCL L1282	0.4720	0.0456	0.0079	-0.3432	-0.1154	-0.0191	0.2876	-0.0924	0.5350	0.0344	0.2488	0.1390	-0.2941	-0.0034	-0.3429	0.0305
1YF6 - BCL L852	0.3679	0.0472	0.1712	-0.2688	-0.0504	-0.0787	0.0545	-0.1487	0.5873	0.0820	0.3700	0.1044	-0.3382	-0.1907	-0.1728	0.1286
1YST - BCL L274	0.5150	0.0862	0.0687	-0.4734	0.0044	-0.1493	0.0800	-0.0879	0.2573	0.0269	0.2162	-0.0795	-0.0332	-0.0889	0.0196	-0.0616
1Z9J - BCL A851	0.3070	0.0662	-0.0549	-0.1479	-0.1666	0.0028	0.1972	-0.0520	0.1562	0.0042	0.1258	0.0639	-0.0538	-0.0318	-0.0204	-0.0130
1Z9K - BCL A851	0.3921	0.0609	-0.1119	-0.1561	-0.1531	0.1016	0.2863	-0.0336	0.1373	0.0028	0.1154	0.0482	-0.0462	-0.0300	-0.0113	-0.0067
2BNP - BCL A1282	0.2271	0.0664	0.0492	-0.0506	-0.1029	0.0070	0.0908	-0.1665	0.0378	0.0115	0.0136	0.0063	-0.0293	-0.0161	-0.0006	0.0094
2BNS - BCL A1282	0.2856	0.0760	0.1254	0.0296	-0.1046	-0.0180	0.1861	-0.1382	0.0681	0.0182	0.0060	0.0001	-0.0654	-0.0045	-0.0172	0.0022
2BOZ - BCL L1282	0.5802	0.0494	-0.0414	-0.4030	-0.1413	-0.1119	0.3579	-0.1095	0.6128	0.0381	0.3480	0.2434	-0.2838	-0.0596	-0.3300	0.0465
2GMR - BCL L302	0.4447	0.0443	0.0623	-0.1761	-0.0951	-0.0853	0.3767	-0.0683	0.4996	0.0578	0.1976	0.1618	-0.3514	-0.1910	-0.1443	0.0596
2GNU - BCL L1282	0.6186	0.0704	0.0542	-0.3151	-0.1418	-0.0900	0.4869	-0.1230	0.1138	0.0196	0.0300	0.0045	-0.0919	-0.0074	-0.0567	0.0178
2HG3 - BCL L312	0.4103	0.0463	0.0260	-0.3305	-0.1269	-0.0764	0.1606	-0.1035	0.5951	0.0378	0.3501	0.1936	-0.2296	-0.0781	-0.3663	0.0322
2HG9 - BCL L312	0.4090	0.0522	0.0555	-0.3111	-0.0953	-0.0928	0.1921	-0.1129	0.5719	0.0358	0.3483	0.0908	-0.2982	-0.0986	-0.3134	0.0273
2HH1 - BCL L312	0.4196	0.0519	-0.0323	-0.3292	-0.0449	-0.1259	0.1938	-0.1058	0.5273	0.0342	0.2839	0.1221	-0.3105	-0.1472	-0.2517	0.0334
2HHK - BCL L312	0.4078	0.0514	0.0009	-0.3008	-0.0907	-0.0779	0.2226	-0.1095	0.5212	0.0381	0.2946	0.1081	-0.3342	-0.1000	-0.2267	0.0068
2HIT - BCL L312	0.4057	0.0457	0.0384	-0.3173	-0.0785	-0.0631	0.2090	-0.0927	0.5515	0.0344	0.2026	0.0972	-0.3036	-0.1369	-0.3772	0.0213
2HJ6 - BCL L312	0.3099	0.0548	0.0983	-0.2172	-0.1121	-0.0536	0.1284	-0.0851	0.5819	0.0348	0.1437	0.0655	-0.4250	-0.2079	-0.2995	0.0142
2J8C - BCL L1288	0.3189	0.0493	-0.0452	-0.2470	-0.1027	-0.0512	0.1097	-0.1160	0.5932	0.0842	0.2641	0.1077	-0.4043	-0.1731	-0.2715	0.0586
2J8D - BCL L1282	0.3394	0.0482	-0.0651	-0.2733	-0.0691	-0.0766	0.0857	-0.1350	0.7244	0.0879	0.3731	0.2989	-0.3848	-0.1845	-0.3288	0.0783
2JIY - BCL L1283	0.3828	0.0494	-0.0273	-0.2894	-0.1104	-0.0614	0.1986	-0.0814	0.5225	0.0351	0.2990	0.1969	-0.2846	-0.0307	-0.2496	0.0242
2JJ0 - BCL L1283	0.3997	0.0477	0.0065	-0.2824	-0.1244	-0.0889	0.2131	-0.1054	0.4516	0.0303	0.1887	0.2214	-0.2521	-0.0478	-0.2302	0.0222

Cofactor ID	Dip	δip	B2g	B1g	Eu(x)	Eu(y)	A1g	A2g	Doop	δoop	B2u	B1u	A2u	Eg(x)	Eg(y)	A1u
2RCR - BCL L350	0.5712	0.0533	0.3052	-0.3630	-0.0339	-0.0535	0.3058	-0.0620	0.2543	0.0117	-0.0699	0.2246	-0.0303	0.0654	-0.0618	0.0170
2UWS - BCL L1286	0.3297	0.0609	0.1197	-0.2363	-0.0333	-0.1303	-0.0704	-0.1243	0.7939	0.1242	0.1688	0.1538	-0.5220	-0.3638	-0.3458	0.2317
2UWT - BCL L1282	0.2880	0.0519	0.0172	-0.2389	-0.0694	-0.0614	0.0442	-0.1226	0.6692	0.0918	0.2558	0.1370	-0.4400	-0.2265	-0.3210	0.1252
2UWU - BCL L1288	0.2650	0.0507	-0.0139	-0.2107	-0.0657	-0.0357	0.0613	-0.1278	0.6218	0.0931	0.2580	0.2014	-0.4327	-0.1263	-0.2586	0.0969
2UWV - BCL L1286	0.3120	0.0503	0.0341	-0.2667	-0.0434	-0.1008	0.0334	-0.1091	0.5929	0.0892	0.2394	0.2032	-0.3914	-0.1543	-0.2581	0.0965
2UWW - BCL L1290	0.2718	0.0499	-0.0226	-0.2264	-0.0532	-0.0671	0.0518	-0.1100	0.6568	0.0937	0.2399	0.2401	-0.4570	-0.1526	-0.2568	0.1344
2UX3 - BCL L1286	0.2430	0.0593	0.0066	-0.1882	-0.0921	-0.0412	0.0202	-0.1139	0.6003	0.1043	0.1036	0.0652	-0.4600	-0.2274	-0.2776	0.0714
2UX4 - BCL L1288	0.2177	0.0582	0.0338	-0.1194	-0.0726	-0.1127	-0.0174	-0.1172	0.6632	0.1146	0.1410	0.1036	-0.4504	-0.2549	-0.3370	0.1670
2UX5 - BCL L1287	0.2739	0.0486	0.0612	-0.2350	-0.0505	-0.0834	0.0142	-0.0797	0.6225	0.0844	0.2999	0.1177	-0.3742	-0.1818	-0.3103	0.1201
2UXJ - BCL L1287	0.3006	0.0547	0.1447	-0.1990	-0.0485	-0.1108	0.0102	-0.1228	0.6532	0.0976	0.2640	0.1794	-0.4325	-0.1175	-0.3333	0.1134
2UXK - BCL L1289	0.2723	0.0585	-0.0054	-0.2134	-0.0211	-0.1241	0.0328	-0.1080	0.6286	0.1221	0.2530	0.0589	-0.4329	-0.2196	-0.2513	0.1698
2UXL - BCL L1285	0.3013	0.0667	0.0252	-0.2602	0.0124	-0.0779	0.0170	-0.1263	0.7357	0.1193	0.1719	-0.1359	-0.5748	-0.1948	-0.2856	0.2081
2UXM - BCL L1282	0.2787	0.0582	0.0730	-0.2080	-0.1096	-0.0852	0.0203	-0.0972	0.6244	0.1133	0.0984	0.2760	-0.4460	-0.2309	-0.1397	0.1798
2WX5 - BCL L1283	0.3434	0.0495	-0.0126	-0.2040	-0.1345	-0.0433	-0.2138	-0.1023	0.6288	0.0651	0.3679	0.1344	-0.2390	-0.1474	-0.3676	0.1673
3DSY - BCL L502	0.4535	0.0426	0.0343	-0.2938	-0.0788	-0.1123	0.3049	-0.0800	0.6248	0.0684	0.3929	0.2142	-0.4110	-0.1083	-0.0312	-0.0921
3DTA - BCL L502	0.4537	0.0425	0.0352	-0.2939	-0.0785	-0.1119	0.3051	-0.0804	0.6246	0.0683	0.3931	0.2136	-0.4108	-0.1078	-0.0314	-0.0921
3DTR - BCL L502	0.4534	0.0425	0.0343	-0.2939	-0.0792	-0.1118	0.3049	-0.0795	0.6249	0.0682	0.3932	0.2136	-0.4111	-0.1081	-0.0315	-0.0924
3DTS - BCL L502	0.4540	0.0426	0.0338	-0.2936	-0.0785	-0.1119	0.3060	-0.0801	0.6247	0.0684	0.3930	0.2142	-0.4108	-0.1082	-0.0308	-0.0922
3DU2 - BCL L502	0.4535	0.0424	0.0340	-0.2936	-0.0794	-0.1121	0.3050	-0.0802	0.6246	0.0683	0.3927	0.2136	-0.4114	-0.1081	-0.0312	-0.0918
3DU3 - BCL L502	0.4536	0.0425	0.0346	-0.2932	-0.0783	-0.1124	0.3054	-0.0809	0.6246	0.0683	0.3930	0.2135	-0.4111	-0.1084	-0.0304	-0.0917
3DUQ - BCL L502	0.4543	0.0426	0.0343	-0.2938	-0.0792	-0.1125	0.3059	-0.0801	0.6252	0.0684	0.3933	0.2142	-0.4112	-0.1084	-0.0311	-0.0921
4RCR - BCL L283	0.4704	0.0321	0.0093	-0.0412	0.0165	-0.0264	0.4674	0.0045	0.4383	0.0545	-0.1066	0.2263	-0.3132	0.0843	-0.1161	0.1043

Table 50: Minimum basis normal-mode displacements and conformational parameters of all DM cofactors from crystal structures of *Rhodobacter sphaeroides*.

Cofactor ID	Dip	δip	B2g	B1g	Eu(x)	Eu(y)	A1g	A2g	Doop	δoop	B2u	B1u	A2u	Eg(x)	Eg(y)	A1u
1AIG - BCL M310	0.2195	0.0529	-0.0848	-0.0591	-0.0386	0.0306	0.1798	-0.0524	0.5709	0.0109	0.1763	-0.5362	-0.0251	-0.0350	0.0213	-0.0710
1AIG - BCL O309	0.2874	0.0505	-0.0225	-0.1271	-0.0538	-0.0953	0.2242	-0.0607	0.5059	0.0081	0.1904	-0.4236	-0.1558	-0.1159	0.0142	-0.0486
1AIJ - BCL M310	0.2868	0.0538	-0.0813	-0.0924	-0.0306	-0.0394	0.2508	-0.0417	0.4576	0.0063	0.1534	-0.3713	-0.2000	-0.0753	0.0081	-0.0471
1AIJ - BCL S310	0.2896	0.0547	-0.0323	-0.0865	-0.0526	-0.0630	0.2587	-0.0407	0.4303	0.0089	0.0643	-0.3731	-0.1898	-0.0556	0.0083	-0.0514
1DS8 - BCL M1003	0.3197	0.0529	-0.0089	-0.1479	0.0161	0.0236	0.2761	-0.0563	0.5475	0.0098	0.1740	-0.4810	-0.1555	-0.0951	0.0247	-0.0655
1DS8 - BCL S2003	0.3344	0.0548	0.0284	-0.1371	-0.0049	-0.0967	0.2842	-0.0452	0.6457	0.0149	0.2696	-0.5346	-0.1710	-0.1530	-0.0588	-0.0477
1DV3 - BCL M1003	0.3580	0.0561	-0.0498	-0.1486	0.0378	-0.0606	0.3111	-0.0418	0.6492	0.0149	0.2195	-0.5329	-0.2547	-0.1413	0.0159	-0.0643
1DV3 - BCL S2003	0.3471	0.0567	0.0028	-0.1184	0.0026	-0.0478	0.3211	-0.0323	0.5507	0.0151	0.2526	-0.4100	-0.2272	-0.1164	-0.0679	-0.0401
1DV6 - BCL M1003	0.3464	0.0541	0.0411	-0.1661	-0.0338	-0.0412	0.2938	-0.0401	0.6063	0.0140	0.2009	-0.5076	-0.2071	-0.1556	-0.0103	-0.0485
1DV6 - BCL S2003	0.3549	0.0537	-0.0604	-0.0725	-0.0493	-0.0639	0.3315	-0.0243	0.4480	0.0135	0.1393	-0.3606	-0.2075	-0.0765	-0.0064	-0.0484
1E14 - BCL C303	0.4081	0.0483	0.0002	-0.2448	-0.0655	-0.0078	0.3084	-0.0845	0.5337	0.0161	-0.0863	-0.4248	-0.2290	0.1013	-0.1813	-0.0372
1E6D - BCL C303	0.4427	0.0540	0.0134	-0.2579	-0.0973	-0.0380	0.3355	-0.0759	0.6207	0.0130	0.3210	-0.5271	-0.0293	-0.0504	-0.0240	-0.0200
1EYS - BCL M603	0.4142	0.0543	0.0437	-0.2423	-0.2294	-0.0932	0.1971	-0.1038	0.5242	0.0713	0.0825	-0.3768	-0.0241	-0.0353	0.3514	-0.0255
1F6N - BCL M801	0.4203	0.0501	0.0777	-0.2415	-0.0980	-0.1045	0.2969	-0.0602	0.4833	0.0483	0.3129	-0.3119	-0.0596	0.0593	0.0575	-0.1674
1FNP - BCL M802	0.4430	0.0482	0.0484	-0.2599	-0.0971	-0.1028	0.3202	-0.0619	0.5034	0.0435	0.2854	-0.3504	-0.1402	-0.0412	0.0107	-0.1667
1FNQ - BCL M802	0.3968	0.0480	0.0759	-0.2357	-0.1248	-0.0860	0.2649	-0.0549	0.5459	0.0452	0.3037	-0.4068	-0.0583	-0.0504	0.0149	-0.1848

Cofactor ID	Dip	δip	B2g	B1g	Eu(x)	Eu(y)	A1g	A2g	Doop	δoop	B2u	B1u	A2u	Eg(x)	Eg(y)	A1u
1JGW - BCL M852	0.4422	0.0617	-0.0155	-0.1576	-0.2056	0.0857	0.3456	-0.0380	0.1489	0.0040	0.1224	-0.0750	-0.0309	-0.0196	0.0061	-0.0134
1JGX - BCL M852	0.4199	0.0649	-0.0372	-0.1552	-0.1621	0.0445	0.3485	-0.0336	0.0922	0.0026	0.0648	-0.0628	-0.0177	-0.0048	0.0019	-0.0030
1JGY - BCL M852	0.3718	0.0654	-0.0274	-0.1417	-0.1340	0.0234	0.3120	-0.0398	0.1485	0.0029	0.1247	-0.0761	-0.0182	-0.0177	-0.0031	-0.0069
1JGZ - BCL M852	0.4067	0.0627	-0.0276	-0.1563	-0.1808	0.0594	0.3204	-0.0370	0.1231	0.0038	0.0976	-0.0726	-0.0028	-0.0157	0.0025	-0.0102
1JH0 - BCL M852	0.3866	0.0656	-0.0365	-0.1566	-0.1793	0.0887	0.2870	-0.0344	0.1031	0.0029	0.0846	-0.0569	-0.0101	-0.0057	-0.0072	-0.0062
1K6L - BCL M502	0.3551	0.0476	0.0157	-0.2045	-0.1230	-0.0944	0.2365	-0.0637	0.5968	0.0532	0.3942	-0.3404	-0.1970	-0.0538	-0.0215	-0.2068
1K6N - BCL M502	0.3557	0.0475	0.0157	-0.2045	-0.1240	-0.0949	0.2366	-0.0642	0.5966	0.0533	0.3938	-0.3407	-0.1970	-0.0541	-0.0206	-0.2064
1L9B - BCL M1003	0.3513	0.0701	0.1327	-0.2434	-0.0419	-0.0422	0.1855	-0.0929	0.3479	0.0172	0.2036	-0.2002	-0.1420	-0.1106	0.0374	-0.0757
1L9J - BCL M1003	0.4260	0.0692	0.1320	-0.2810	-0.0930	-0.0047	0.2593	-0.0958	0.2271	0.0115	0.1061	-0.1051	-0.1403	-0.0766	0.0403	-0.0459
1L9J - BCL S2003	0.4298	0.0692	0.1134	-0.2624	-0.0935	-0.0376	0.2889	-0.0971	0.2012	0.0094	-0.0271	-0.1163	-0.1279	-0.0734	0.0575	-0.0343
1M3X - BCL M852	0.4304	0.0623	-0.0078	-0.1526	-0.1676	0.0504	0.3607	-0.0338	0.1758	0.0039	0.1407	-0.0969	-0.0355	-0.0198	0.0045	-0.0079
1MPS - BCL M802	0.4673	0.0459	0.0394	-0.2609	-0.1164	-0.0605	0.3553	-0.0726	0.5981	0.0475	0.2760	-0.5092	-0.0972	-0.0231	-0.0612	-0.0926
1OGV - BCL M1303	0.3817	0.0713	0.0959	-0.2072	-0.0581	-0.0685	0.2786	-0.0889	0.3016	0.0145	0.1632	-0.1735	-0.1388	-0.0844	0.0730	-0.0502
1PCR - BCL M801	0.3554	0.0476	0.0163	-0.2040	-0.1227	-0.0941	0.2376	-0.0633	0.5950	0.0531	0.3929	-0.3392	-0.1963	-0.0534	-0.0196	-0.2068
1PSS - BCL M3	0.2186	0.0518	-0.0652	-0.0537	-0.0539	-0.0404	0.1856	-0.0411	0.4652	0.0100	0.0920	-0.4111	-0.1896	-0.0212	-0.0260	-0.0432
1PYH - BCL B303	0.3838	0.0538	0.0139	-0.3229	-0.0643	-0.0409	0.1682	-0.0937	0.5453	0.0172	0.3057	-0.4235	-0.0837	-0.1039	-0.0382	-0.0728
1QOV - BCL L1303	0.4501	0.0552	0.0592	-0.3198	-0.0362	-0.0439	0.3007	-0.0560	0.5190	0.0184	0.3066	-0.3792	-0.0795	-0.1177	-0.0699	-0.0804
1RG5 - BCL M502	0.4867	0.0561	-0.0130	-0.3086	-0.0827	-0.0350	0.3560	-0.0818	0.5276	0.0129	0.3037	-0.4141	-0.0611	-0.0979	0.0102	-0.0343
1RGN - BCL M909	0.3324	0.0602	-0.0322	-0.1967	-0.0923	-0.0096	0.2306	-0.0949	0.5593	0.0155	0.2779	-0.4318	-0.0328	-0.1967	-0.0891	-0.0373
1RQK - BCL M502	0.3218	0.0551	0.0321	-0.2795	-0.0621	0.0202	0.1118	-0.0877	0.5896	0.0171	0.2808	-0.4721	-0.0544	-0.2034	-0.0159	-0.0355
1RVJ - BCL M853	0.3732	0.0703	0.0405	-0.1799	-0.0566	-0.0146	0.3104	-0.0744	0.3154	0.0129	0.1042	-0.2402	-0.1425	-0.0830	0.0347	-0.0501
1RY5 - BCL M853	0.4050	0.0686	0.0954	-0.2551	-0.0301	-0.0275	0.2835	-0.0888	0.4563	0.0182	0.2521	-0.3102	-0.1667	-0.1073	0.0627	-0.0725
1RZH - BCL M853	0.4498	0.0553	0.0589	-0.3195	-0.0362	-0.0433	0.3007	-0.0560	0.5195	0.0183	0.3063	-0.3802	-0.0798	-0.1179	-0.0696	-0.0802
1RZZ - BCL M1003	0.3865	0.0688	0.1296	-0.2375	-0.0520	-0.0259	0.2545	-0.0898	0.3136	0.0156	0.1278	-0.2121	-0.1433	-0.0809	0.0887	-0.0459
1RZZ - BCL S2003	0.4062	0.0726	0.1106	-0.2385	-0.0292	-0.0945	0.2804	-0.0867	0.2699	0.0139	0.0592	-0.1905	-0.1358	-0.0809	0.0776	-0.0454
1S00 - BCL M1003	0.4009	0.0705	0.1319	-0.2250	-0.0422	-0.0751	0.2773	-0.0916	0.2977	0.0155	0.0544	-0.2185	-0.1414	-0.0791	0.0965	-0.0487
1S00 - BCL S2003	0.3864	0.0700	0.1079	-0.2248	-0.0291	-0.1028	0.2599	-0.0902	0.2491	0.0135	0.0054	-0.1661	-0.1471	-0.0707	0.0777	-0.0419
1UMX - BCL M1304	0.4539	0.0582	0.1215	-0.3426	-0.0987	-0.0980	0.2010	-0.1189	0.4517	0.0168	0.3171	-0.3053	0.0551	-0.0740	-0.0027	-0.0418
1YF6 - BCL M853	0.3439	0.0585	-0.0479	-0.2872	-0.0964	0.0002	0.0994	-0.1197	0.7078	0.0646	0.2993	-0.5617	-0.1744	-0.1773	-0.0070	-0.1847
1YST - BCL M308	0.5612	0.0721	0.1643	-0.5218	-0.0954	0.0339	-0.0459	-0.0579	0.2931	0.0143	0.2239	-0.1653	-0.0684	0.0428	0.0235	-0.0376
1Z9J - BCL B852	0.3693	0.0697	-0.0972	-0.2344	-0.1382	0.0558	0.2195	-0.0401	0.0833	0.0028	-0.0714	-0.0417	-0.0074	0.0013	0.0070	-0.0016
1Z9K - BCL B852	0.3228	0.0622	-0.0640	-0.1764	-0.1638	0.0407	0.1974	-0.0390	0.0225	0.0028	0.0018	-0.0086	0.0060	-0.0191	0.0043	0.0032
2BNP - BCL B1303	0.4239	0.0896	0.3688	0.1399	-0.0685	0.0900	0.0203	-0.1044	0.0604	0.0076	0.0071	-0.0363	-0.0062	-0.0386	0.0218	-0.0165
2BNS - BCL B1303	0.4077	0.0845	0.2825	0.1281	-0.1186	0.1138	0.1798	-0.1034	0.0569	0.0119	0.0062	-0.0338	-0.0333	-0.0268	0.0069	-0.0134
2BOZ - BCL M1304	0.5506	0.0573	-0.0576	-0.3871	-0.1053	-0.0131	0.3574	-0.1046	0.6155	0.0194	0.3873	-0.4427	-0.0810	-0.1473	-0.0481	-0.0477
2GMR - BCL M309	0.4207	0.0465	0.0665	-0.2113	-0.1130	-0.0540	0.3281	-0.0672	0.4781	0.0300	0.1483	-0.3588	-0.1676	-0.1544	0.0204	-0.1598
2GNU - BCL M1303	0.5770	0.0754	0.1890	-0.2752	-0.0964	0.0756	0.4478	-0.0769	0.1342	0.0161	0.0190	-0.0920	-0.0540	-0.0614	0.0280	-0.0416
2HG3 - BCL M313	0.3861	0.0617	0.0872	-0.2472	-0.0098	0.0927	0.2484	-0.1000	0.5754	0.0187	0.2738	-0.4926	-0.0122	-0.0601	-0.0263	-0.0949
2HG9 - BCL M313	0.3138	0.0620	-0.0983	-0.1982	0.0004	0.0810	0.1868	-0.0895	0.7413	0.0238	0.3897	-0.6149	-0.0479	-0.0944	-0.0773	-0.0492
2HH1 - BCL M313	0.2779	0.0629	-0.0582	-0.1151	-0.0338	-0.0084	0.2328	-0.0720	0.7147	0.0224	0.3884	-0.5782	-0.1007	-0.0976	-0.0518	-0.0576
2HHK - BCL M313	0.3865	0.0556	-0.1288	-0.2424	-0.0554	-0.0037	0.2656	-0.0190	0.6524	0.0215	0.4019	-0.4962	-0.0245	-0.1006	-0.0748	-0.0397
2HIT - BCL M313	0.4032	0.0568	0.1075	-0.0632	-0.0439	-0.0679	0.3595	-0.1061	0.6521	0.0231	0.3892	-0.5082	0.0462	-0.1015	-0.0355	-0.0428
2HJ6 - BCL M313	0.2734	0.0587	-0.0167	-0.1330	-0.1341	-0.0291	0.1628	-0.1071	0.7505	0.0247	0.3908	-0.6047	-0.0058	-0.1988	0.0263	-0.0684

Cofactor ID	Dip	δip	B2g	B1g	Eu(x)	Eu(y)	A1g	A2g	Doop	δoop	B2u	B1u	A2u	Eg(x)	Eg(y)	A1u
2J8C - BCL M1304	0.3378	0.0539	0.0021	-0.2277	-0.1203	-0.0444	0.1879	-0.1026	0.6806	0.0392	0.4009	-0.4873	-0.1965	-0.0925	0.0427	-0.1269
2J8D - BCL M1309	0.3616	0.0497	0.0863	-0.2800	-0.0866	-0.0177	0.1545	-0.1149	0.6529	0.0548	0.3685	-0.4490	-0.1806	-0.1801	0.0557	-0.1441
2JIY - BCL M1303	0.3647	0.0545	0.0134	-0.2264	-0.0465	-0.0021	0.2691	-0.0840	0.4891	0.0195	0.2359	-0.3865	-0.0387	-0.1203	0.1200	-0.0620
2JIY - BCL M1303	0.4142	0.0567	0.0211	-0.3401	-0.0144	0.0351	0.2127	-0.0936	0.8693	0.0238	0.3532	-0.6541	-0.1044	-0.3614	-0.2439	-0.0453
2JJ0 - BCL M1304	0.3250	0.0586	-0.0009	-0.2501	-0.0078	-0.0143	0.1818	-0.0985	0.5755	0.0187	0.2866	-0.4581	-0.0109	-0.1921	-0.0346	-0.0322
2RCR - BCL M400	0.4293	0.0564	0.0548	-0.2590	-0.0970	-0.0098	0.3132	-0.0816	0.3314	0.0160	-0.2153	-0.1327	-0.0749	0.0592	0.1899	0.0254
2UWS - BCL M1304	0.3208	0.0596	-0.0217	-0.2609	-0.0866	0.0238	-0.0990	-0.1284	0.5590	0.1203	0.3233	-0.3066	-0.1494	0.0221	0.0932	-0.2871
2UWT - BCL M1304	0.2852	0.0565	0.0674	-0.2230	-0.0756	-0.0406	0.0143	-0.1396	0.7054	0.0614	0.3371	-0.5653	-0.1378	-0.1071	-0.0188	-0.1833
2UWU - BCL M1304	0.3065	0.0533	0.0654	-0.2579	-0.0488	0.0004	0.1002	-0.1036	0.7158	0.0456	0.3914	-0.5487	-0.1606	-0.1540	-0.0131	-0.0917
2UWV - BCL M1304	0.3080	0.0560	0.0187	-0.2790	-0.0526	0.0271	0.0359	-0.1090	0.7130	0.0463	0.4304	-0.5182	-0.1119	-0.1480	0.0006	-0.1421
2UWW - BCL M1305	0.3049	0.0513	0.0651	-0.2503	-0.0541	-0.0153	0.0954	-0.1174	0.7234	0.0468	0.3648	-0.5470	-0.2192	-0.1242	-0.0843	-0.1432
2UX3 - BCL M1304	0.2917	0.0597	0.0223	-0.2397	-0.0776	-0.0287	0.0594	-0.1295	0.8342	0.0502	0.3188	-0.7137	-0.2142	-0.1535	0.0085	-0.1241
2UX4 - BCL M1304	0.2558	0.0582	-0.0274	-0.1638	-0.0673	-0.0283	-0.0292	-0.1780	0.8600	0.0808	0.2779	-0.7625	-0.1979	-0.1211	0.1028	-0.1285
2UX5 - BCL M1305	0.3436	0.0579	0.0744	-0.3069	-0.0478	-0.0052	0.0909	-0.0883	0.7179	0.0503	0.3887	-0.5573	-0.1309	-0.1239	0.0863	-0.1174
2UXJ - BCL M1304	0.3275	0.0510	0.0174	-0.2903	-0.0490	-0.0050	0.0658	-0.1264	0.6800	0.0684	0.3786	-0.4812	-0.1909	-0.1137	0.0192	-0.1943
2UXK - BCL M1304	0.3010	0.0546	0.0359	-0.2546	-0.0295	-0.0079	0.0564	-0.1427	0.7310	0.0903	0.3517	-0.5209	-0.2764	-0.1071	-0.0801	-0.2124
2UXL - BCL M1304	0.3066	0.0614	0.0355	-0.2621	-0.0242	-0.0718	-0.0267	-0.1327	0.7250	0.1098	0.2030	-0.5218	-0.3889	-0.2436	0.0385	0.0086
2UXM - BCL M1304	0.3137	0.0640	-0.0901	-0.2406	-0.1213	-0.0043	-0.0065	-0.1328	0.9139	0.0917	0.3276	-0.7688	-0.2065	-0.1131	0.1673	-0.2312
2WX5 - BCL M1303	0.2648	0.0441	-0.0148	-0.1401	-0.0519	-0.1301	-0.1417	-0.1030	0.5996	0.0450	0.2492	-0.4629	-0.1245	-0.0129	0.0198	-0.2589
3DSY - BCL M502	0.3552	0.0476	0.0155	-0.2045	-0.1226	-0.0944	0.2368	-0.0638	0.5969	0.0532	0.3945	-0.3405	-0.1971	-0.0537	-0.0210	-0.2064
3DTA - BCL M502	0.3556	0.0476	0.0156	-0.2046	-0.1234	-0.0946	0.2368	-0.0642	0.5975	0.0533	0.3946	-0.3410	-0.1972	-0.0535	-0.0215	-0.2069
3DTR - BCL M502	0.3550	0.0475	0.0158	-0.2042	-0.1228	-0.0940	0.2368	-0.0636	0.5969	0.0533	0.3946	-0.3403	-0.1972	-0.0530	-0.0210	-0.2066
3DTS - BCL M502	0.3557	0.0476	0.0157	-0.2043	-0.1238	-0.0951	0.2367	-0.0644	0.5968	0.0532	0.3940	-0.3413	-0.1960	-0.0539	-0.0203	-0.2066
3DU2 - BCL M502	0.3549	0.0475	0.0148	-0.2041	-0.1224	-0.0948	0.2368	-0.0635	0.5970	0.0532	0.3942	-0.3403	-0.1975	-0.0543	-0.0210	-0.2069
3DU3 - BCL M502	0.3559	0.0476	0.0157	-0.2040	-0.1244	-0.0951	0.2370	-0.0641	0.5969	0.0532	0.3943	-0.3410	-0.1967	-0.0536	-0.0211	-0.2061
3DUQ - BCL M502	0.3556	0.0477	0.0157	-0.2048	-0.1236	-0.0951	0.2365	-0.0631	0.5965	0.0533	0.3940	-0.3403	-0.1971	-0.0548	-0.0205	-0.2063
4RCR - BCL M310	0.4911	0.0361	-0.0187	-0.0729	0.0347	-0.0235	0.4833	-0.0118	0.6497	0.0499	0.3028	-0.4903	-0.2372	-0.1071	0.1246	-0.0824

8.2 *Blastochloris Viridis* bacteriochlorin cofactor NSDs

8.2.1 Minimum Basis

Table 51: Minimum basis normal-mode displacements and conformational parameters of all BA cofactors from crystal structures of *Blastochloris viridis*.

Cofactor ID	Dip	δip	B2g	B1g	Eu(x)	Eu(y)	A1g	A2g	Doop	δoop	B2u	B1u	A2u	Eg(x)	Eg(y)	A1u
1DXR - BCB L401	0.4577	0.0405	0.0365	-0.3396	-0.1465	-0.0943	0.2405	-0.0680	0.4287	0.0380	0.0403	0.0633	0.0065	-0.4170	0.0168	0.0634
1PRC - BCB L604	0.2998	0.0472	0.0674	-0.1271	-0.0911	-0.0692	0.2218	-0.0830	0.3019	0.0394	0.1285	0.1168	-0.0856	-0.2169	0.0698	0.0412
1R2C - BCB L304	0.4282	0.0425	0.0700	-0.2552	-0.1371	-0.0632	0.2925	-0.0705	0.4264	0.0443	0.0515	0.1304	-0.1755	-0.3065	0.1698	0.0927
1VRN - BCB L404	0.4577	0.0430	0.0569	-0.2671	-0.1183	-0.0633	0.3337	-0.0744	0.4822	0.0439	0.1453	0.1305	-0.0666	-0.4179	0.0954	0.0788
2I5N - BCB L401	0.4610	0.0511	0.1045	-0.2378	-0.1177	-0.0694	0.3407	-0.1015	0.4916	0.0542	0.0374	0.1917	0.0053	-0.4484	-0.0128	0.0472
2JBL - BCB L1275	0.4483	0.0434	0.0658	-0.2574	-0.1038	-0.0598	0.3336	-0.0687	0.5172	0.0421	0.0969	0.1673	-0.1616	-0.4348	0.0962	0.0754
2PRC - BCB L304	0.4361	0.0398	0.0317	-0.2727	-0.1688	-0.0320	0.2803	-0.0816	0.4685	0.0445	0.0795	0.1079	-0.0944	-0.4156	0.1242	0.0670
2WJM - BCB L1275	0.3556	0.0555	0.1857	-0.0921	-0.0021	-0.1073	0.2624	-0.0558	0.3394	0.0526	0.1035	0.1158	-0.0536	-0.2730	0.0410	0.1094

Cofactor ID	Dip	δip	B2g	B1g	Eu(x)	Eu(y)	A1g	A2g	Doop	δoop	B2u	B1u	A2u	Eg(x)	Eg(y)	A1u
2WJN - BCB L1275	0.3934	0.0567	0.1247	-0.2501	0.1131	-0.1165	0.2159	-0.0605	0.4083	0.0650	0.1385	0.1465	-0.0301	-0.3368	0.0862	0.0656
3D38 - BCB L401	0.4476	0.0485	0.1597	-0.2732	-0.1179	-0.1144	0.2494	-0.1050	0.3813	0.0358	-0.0657	0.1787	-0.1202	-0.3012	-0.0432	0.0457
3G7F - BCB L401	0.4295	0.0481	0.1701	-0.2407	-0.1289	-0.0383	0.2609	-0.1072	0.3820	0.0513	0.1441	0.0823	-0.0562	-0.3388	0.0116	0.0178
3PRC - BCB L304	0.4128	0.0402	0.0391	-0.2884	-0.1395	-0.0634	0.2370	-0.0779	0.4827	0.0557	0.2220	0.0686	0.0236	-0.4073	0.0985	0.0536
5PRC - BCB L304	0.3615	0.0418	-0.0100	-0.2666	-0.1498	-0.0415	0.1726	-0.0744	0.4154	0.0512	0.1569	0.0936	-0.0579	-0.3447	0.1002	0.0836
6PRC - BCB L304	0.4188	0.0393	0.0261	-0.3139	-0.1499	-0.0855	0.1990	-0.0824	0.4530	0.0510	0.1489	0.0927	0.0146	-0.4045	0.0382	0.0957
7PRC - BCB L304	0.4344	0.0402	0.0629	-0.3462	-0.1668	-0.0352	0.1770	-0.0668	0.5752	0.0610	0.3437	0.1532	0.0467	-0.4035	0.1250	0.0930

Table 52: Minimum basis normal-mode displacements and conformational parameters of all BB cofactors from crystal structures of *Blastochloris viridis*.

Cofactor ID	Dip	δip	B2g	B1g	Eu(x)	Eu(y)	A1g	A2g	Doop	δoop	B2u	B1u	A2u	Eg(x)	Eg(y)	A1u
1DXR - BCB M400	0.4516	0.0419	0.0220	-0.2919	-0.0906	0.0084	0.3220	-0.0790	0.4471	0.0451	0.0847	0.0114	-0.0372	-0.4345	0.0464	0.0143
1PRC - BCB M601	0.3533	0.0492	0.0859	-0.1604	-0.1037	-0.0454	0.2691	-0.0804	0.1875	0.0458	0.0619	0.0503	0.0065	-0.1562	0.0600	-0.0272
1R2C - BCB M1301	0.4663	0.0397	0.0566	-0.2977	-0.1141	-0.0242	0.3266	-0.0726	0.3731	0.0614	0.1120	0.0027	-0.1717	-0.2659	0.1622	0.0119
1VRN - BCB M401	0.4273	0.0417	0.0730	-0.2373	-0.1001	-0.0349	0.3232	-0.0724	0.3815	0.0497	-0.0084	0.0157	-0.1532	-0.3453	0.0465	0.0194
2I5N - BCB M400	0.4203	0.0491	0.0427	-0.2724	-0.0769	-0.0616	0.2849	-0.0986	0.4511	0.0463	-0.1011	0.1467	-0.1801	-0.3721	0.0268	-0.0141
2JBL - BCB L1278	0.4259	0.042	0.0643	-0.2291	-0.1067	-0.0099	0.3281	-0.0750	0.5413	0.0496	-0.0419	0.0166	-0.3232	-0.4023	0.1514	0.0422
2PRC - BCB M805	0.4284	0.04	0.0902	-0.3069	-0.0657	-0.0161	0.2654	-0.0786	0.4866	0.0497	0.0484	0.0640	-0.1548	-0.4455	0.0849	0.0275
2WJM - BCB M1324	0.2845	0.0569	0.0467	-0.1321	0.0519	-0.0173	0.2343	-0.0586	0.3269	0.0478	0.1233	0.1253	-0.1395	-0.2250	0.0640	0.0425
2WJN - BCB M1324	0.2334	0.057	0.0432	-0.1278	-0.0405	-0.0631	0.1702	-0.0410	0.3525	0.0613	0.1550	0.0028	-0.1650	-0.2639	0.0461	0.0348
3D38 - BCB M400	0.4047	0.0511	-0.0379	-0.2981	-0.0773	-0.0055	0.2310	-0.1188	0.4574	0.0417	-0.0971	-0.1217	-0.1815	-0.3899	-0.0041	-0.0016
3G7F - BCB M400	0.4373	0.0534	0.1277	-0.3233	-0.1110	-0.0015	0.2182	-0.1025	0.4771	0.0536	0.0181	0.2400	-0.1861	-0.3627	0.0557	-0.0191
3PRC - BCB M805	0.449	0.0408	0.0901	-0.2733	-0.1142	-0.0311	0.3139	-0.0790	0.4253	0.0503	0.0371	0.0165	-0.1808	-0.3712	0.0914	0.0205
5PRC - BCB M805	0.3589	0.04	0.0587	-0.2606	-0.0646	-0.0211	0.2156	-0.0797	0.3919	0.0624	-0.0508	-0.0008	-0.1009	-0.3679	0.0685	-0.0287
6PRC - BCB M805	0.3815	0.0403	0.0349	-0.2313	-0.0871	-0.0225	0.2767	-0.0783	0.3973	0.0629	0.0561	0.0083	-0.1559	-0.3413	0.1162	0.0196
7PRC - BCB M805	0.3691	0.0397	0.0585	-0.2480	-0.0961	-0.0638	0.2290	-0.0742	0.4673	0.0575	-0.0206	-0.0246	-0.1600	-0.4373	-0.0176	-0.0115

Table 53: Minimum basis normal-mode displacements and conformational parameters of all DL cofactors from crystal structures of *Blastochloris viridis*.

Cofactor ID	Dip	δip	B2g	B1g	Eu(x)	Eu(y)	A1g	A2g	Doop	δoop	B2u	B1u	A2u	Eg(x)	Eg(y)	A1u
1DXR - BCB L400	0.3642	0.0432	0.0761	-0.1851	-0.1309	-0.0213	0.2594	-0.0877	0.6675	0.0369	-0.1356	-0.6097	-0.0545	0.0164	0.0788	-0.2142
1PRC - BCB L602	0.3796	0.0515	0.0714	-0.2989	-0.1082	-0.0525	0.1565	-0.1035	0.4142	0.0401	-0.1540	-0.3335	-0.0628	-0.0963	0.0452	-0.1460
1R2C - BCB L302	0.3952	0.0431	0.0736	-0.2640	-0.1524	-0.0099	0.2274	-0.0775	0.6191	0.0339	-0.2842	-0.5396	0.0273	0.0025	0.0048	-0.1026
1VRN - BCB L402	0.4232	0.0401	0.0549	-0.2417	-0.1364	-0.0311	0.3055	-0.0687	0.7993	0.0395	-0.2273	-0.7262	0.0554	0.0256	0.0251	-0.2354
2I5N - BCB L400	0.3712	0.0471	0.0433	-0.1956	-0.0853	-0.0246	0.2801	-0.1067	0.8137	0.0527	-0.2829	-0.6912	-0.0597	-0.1813	0.1546	-0.2099
2JBL - BCB L1274	0.4053	0.0402	0.0522	-0.2438	-0.1313	-0.0361	0.2789	-0.0762	0.8316	0.0302	-0.2768	-0.7508	-0.0485	0.0314	-0.0439	-0.2142
2PRC - BCB L302	0.3387	0.0461	0.0588	-0.1843	-0.1140	0.0011	0.2357	-0.0933	0.7697	0.0434	-0.3183	-0.6704	-0.0628	0.0918	0.0242	-0.1691
2WJM - BCB L1274	0.3344	0.0600	0.0958	-0.1111	-0.0502	-0.0534	0.2801	-0.0807	0.7138	0.0372	-0.1294	-0.6433	0.0907	0.0178	0.1678	-0.2052
2WJN - BCB L1274	0.3556	0.0629	0.0536	-0.2123	-0.0755	-0.0178	0.2610	-0.0665	0.7064	0.0420	-0.1611	-0.6453	0.0398	0.0298	0.1125	-0.2038
3D38 - BCB L400	0.4314	0.0507	0.1269	-0.2275	-0.1473	-0.0827	0.2810	-0.1036	0.8735	0.0500	-0.3069	-0.7682	-0.1401	-0.0955	0.1295	-0.1823
3G7F - BCB L400	0.4065	0.0427	0.0733	-0.2609	-0.1680	-0.0439	0.2198	-0.1156	0.8106	0.0360	-0.2221	-0.7575	-0.0100	-0.0477	0.0891	-0.1536

Cofactor ID	Dip	δip	B2g	B1g	Eu(x)	Eu(y)	A1g	A2g	Doop	δoop	B2u	B1u	A2u	Eg(x)	Eg(y)	A1u
3PRC - BCB L302	0.4032	0.0433	0.0230	-0.2658	-0.1418	-0.0245	0.2530	-0.0819	0.7212	0.0357	-0.2206	-0.6532	-0.0345	0.0889	0.0164	-0.1880
5PRC - BCB L302	0.2949	0.0406	0.0075	-0.1809	-0.1143	-0.0034	0.1811	-0.0913	0.7247	0.0332	-0.2736	-0.6334	-0.1208	-0.0160	0.0946	-0.1591
6PRC - BCB L302	0.3283	0.0416	-0.0162	-0.1929	-0.1255	-0.0718	0.2046	-0.0866	0.6822	0.0312	-0.2425	-0.6105	-0.0836	0.0633	0.0201	-0.1501
7PRC - BCB L302	0.3831	0.0408	0.0724	-0.2407	-0.1544	-0.0396	0.2231	-0.0920	0.8808	0.0338	-0.2702	-0.8092	-0.1099	0.0712	0.0437	-0.1698

Table 54: Minimum basis normal-mode displacements and conformational parameters of all DM cofactors from crystal structures of *Blastochloris viridis*.

Cofactor ID	Dip	δip	B2g	B1g	Eu(x)	Eu(y)	A1g	A2g	Doop	δoop	B2u	B1u	A2u	Eg(x)	Eg(y)	A1u
1DXR - BCB M401	0.3393	0.0405	0.0407	-0.1697	-0.1475	-0.0320	0.2391	-0.0688	0.8485	0.0343	-0.1055	-0.7896	0.0154	-0.1413	0.1457	-0.2097
1PRC - BCB M603	0.2809	0.0521	0.0714	-0.0871	-0.0834	-0.2157	0.0381	-0.1063	0.6630	0.0518	0.1016	-0.6127	-0.0368	0.0465	0.0876	-0.2064
1R2C - BCB M1303	0.3299	0.0362	0.0960	-0.1696	-0.2055	-0.0276	0.1493	-0.0744	1.0678	0.0392	-0.2000	-1.0022	0.0344	-0.1134	0.1458	-0.2462
1VRN - BCB M403	0.3625	0.0391	0.0489	-0.2320	-0.1281	-0.0248	0.2300	-0.0722	1.1001	0.0363	-0.0507	-1.0594	0.0506	-0.0177	0.0999	-0.2692
2I5N - BCB M401	0.3278	0.0500	-0.0401	-0.2469	-0.0651	-0.0429	0.1691	-0.1011	1.1229	0.0576	-0.0776	-1.0376	-0.1059	-0.1277	0.2509	-0.2962
2JBL - BCB M1324	0.3689	0.0395	0.0389	-0.1859	-0.2027	-0.0187	0.2312	-0.0717	1.0042	0.0269	-0.1067	-0.9563	-0.0135	-0.0724	0.1875	-0.2046
2PRC - BCB M806	0.2626	0.0373	-0.0289	-0.1333	-0.1417	-0.0981	0.1183	-0.0817	1.0783	0.0311	-0.1390	-1.0334	-0.1197	-0.0009	0.1803	-0.1695
2WJM - BCB M1325	0.2634	0.0610	0.1694	-0.0586	0.0055	0.0077	0.1861	-0.0501	1.0496	0.0559	0.1314	-0.9883	0.0021	-0.0162	0.1559	-0.2883
2WJN - BCB M1325	0.2371	0.0575	0.1009	-0.1309	-0.0261	-0.0302	0.1592	-0.0443	1.0096	0.0532	0.0926	-0.9426	-0.0525	-0.0102	0.1628	-0.3046
3D38 - BCB M401	0.3846	0.0430	0.1239	-0.2622	-0.0469	-0.0577	0.2131	-0.1134	0.9181	0.0541	-0.2597	-0.7987	-0.0166	-0.1838	0.2161	-0.2382
3PRC - BCB M806	0.3314	0.0379	0.0460	-0.1440	-0.1327	-0.0312	0.2481	-0.0826	0.9802	0.0372	-0.1396	-0.9353	-0.0174	-0.0157	0.0849	-0.2426
5PRC - BCB M806	0.3374	0.0400	0.0239	-0.1881	-0.1807	-0.0262	0.1983	-0.0720	0.9599	0.0325	-0.0442	-0.9183	-0.0737	-0.0609	0.1690	-0.1966
6PRC - BCB M806	0.3119	0.0404	-0.0144	-0.1992	-0.1294	-0.0179	0.1848	-0.0785	1.0536	0.0371	-0.0860	-1.0110	-0.1147	-0.0691	0.0508	-0.2449
7PRC - BCB M806	0.3803	0.0454	0.0220	-0.2106	-0.1436	-0.0517	0.2647	-0.0801	0.9954	0.0436	-0.0113	-0.9643	-0.1297	-0.0297	0.0976	-0.1835

8.2.2 Extended Basis (Lowest Energy)

Table 55: Extended conformational parameters and lowest energy basis normal-mode displacements of all BA cofactors from crystal structures of *Blastochloris viridis*.

Cofactor ID	Dip_e	δip_e	B2g_e	B1g_e	Eu(x)_e	Eu(y)_e	A1g_e	A2g_e	Doop_e	δoop_e	B2u_e	B1u_e	A2u_e	Eg(x)_e	Eg(y)_e	A1u_e
1DXR - BCB L401	0.4845	0.0240	0.0373	-0.3408	-0.1471	-0.0933	0.2413	-0.0672	0.4501	0.0312	0.0417	0.0633	0.0032	-0.4159	0.0193	0.0634
1PRC - BCB L604	0.3503	0.0360	0.0673	-0.1266	-0.0910	-0.0681	0.2228	-0.0811	0.3201	0.0401	0.1280	0.1168	-0.0857	-0.2160	0.0700	0.0412
1R2C - BCB L304	0.4606	0.0253	0.0700	-0.2562	-0.1379	-0.0618	0.2939	-0.0704	0.4918	0.0255	0.0511	0.1304	-0.1809	-0.2993	0.1729	0.0928
1VRN - BCB L404	0.4886	0.0252	0.0574	-0.2683	-0.1192	-0.0619	0.3347	-0.0740	0.5250	0.0274	0.1480	0.1305	-0.0702	-0.4136	0.0972	0.0788
2I5N - BCB L401	0.5162	0.0247	0.1052	-0.2371	-0.1179	-0.0670	0.3428	-0.1013	0.5026	0.0526	0.0388	0.1917	-0.0011	-0.4473	-0.0112	0.0472
2JBL - BCB L1275	0.4800	0.0263	0.0660	-0.2582	-0.1049	-0.0585	0.3351	-0.0681	0.5474	0.0284	0.0984	0.1673	-0.1691	-0.4317	0.0949	0.0754
2PRC - BCB L304	0.4625	0.0247	0.0323	-0.2741	-0.1694	-0.0310	0.2810	-0.0810	0.5037	0.0320	0.0811	0.1079	-0.1001	-0.4129	0.1266	0.0670
2WJM - BCB L1275	0.3827	0.0487	0.1859	-0.0899	-0.0030	-0.1039	0.2605	-0.0561	0.3714	0.0492	0.1046	0.1158	-0.0557	-0.2730	0.0419	0.1094
2WJN - BCB L1275	0.4247	0.0490	0.1246	-0.2473	0.1136	-0.1130	0.2140	-0.0599	0.4450	0.0575	0.1406	0.1465	-0.0280	-0.3370	0.0877	0.0656
3D38 - BCB L401	0.4982	0.0256	0.1610	-0.2726	-0.1176	-0.1124	0.2509	-0.1046	0.3883	0.0362	-0.0648	0.1787	-0.1236	-0.3011	-0.0432	0.0457
3G7F - BCB L401	0.4802	0.0263	0.1711	-0.2399	-0.1294	-0.0368	0.2625	-0.1065	0.3924	0.0511	0.1450	0.0823	-0.0610	-0.3380	0.0111	0.0178
3PRC - BCB L304	0.4421	0.0241	0.0395	-0.2896	-0.1400	-0.0622	0.2379	-0.0773	0.5445	0.0340	0.2252	0.0686	0.0169	-0.4026	0.1006	0.0536
5PRC - BCB L304	0.3963	0.0250	-0.0095	-0.2680	-0.1505	-0.0401	0.1733	-0.0738	0.4749	0.0326	0.1575	0.0936	-0.0673	-0.3411	0.1028	0.0836
6PRC - BCB L304	0.4477	0.0221	0.0264	-0.3151	-0.1508	-0.0842	0.2000	-0.0818	0.5003	0.0362	0.1511	0.0927	0.0057	-0.4041	0.0394	0.0957

Cofactor ID	Dip_e	δip_e	B2g_e	B1g_e	Eu(x)_e	Eu(y)_e	A1g_e	A2g_e	Doop_e	δoop_e	B2u_e	B1u_e	A2u_e	Eg(x)_e	Eg(y)_e	A1u_e
7PRC - BCB L304	0.4618	0.0245	0.0634	-0.3478	-0.1673	-0.0341	0.1782	-0.0659	0.6558	0.0313	0.3488	0.1532	0.0377	-0.4018	0.1204	0.0930

Table 56: Extended conformational parameters and lowest energy basis normal-mode displacements of all BB cofactors from crystal structures of *Blastochloris viridis*.

Cofactor ID	Dip_e	δip_e	B2g_e	B1g_e	Eu(x)_e	Eu(y)_e	A1g_e	A2g_e	Doop_e	δoop_e	B2u_e	B1u_e	A2u_e	Eg(x)_e	Eg(y)_e	A1u_e
1DXR - BCB M400	0.4817	0.0250	0.0225	-0.2933	-0.0917	0.0099	0.3225	-0.0786	0.4935	0.0324	0.0867	0.0114	-0.0384	-0.4291	0.0495	0.0143
1PRC - BCB M601	0.4072	0.0332	0.0853	-0.1601	-0.1040	-0.0442	0.2681	-0.0789	0.2294	0.0443	0.0627	0.0503	0.0078	-0.1544	0.0599	-0.0272
1R2C - BCB M1301	0.4886	0.0270	0.0572	-0.2990	-0.1145	-0.0234	0.3281	-0.0721	0.4917	0.0308	0.1136	0.0027	-0.1806	-0.2569	0.1593	0.0119
1VRN - BCB M401	0.4585	0.0247	0.0733	-0.2384	-0.1009	-0.0335	0.3242	-0.0720	0.4597	0.0276	-0.0070	0.0157	-0.1531	-0.3371	0.0500	0.0194
2I5N - BCB M400	0.4727	0.0262	0.0439	-0.2722	-0.0770	-0.0605	0.2865	-0.0981	0.4631	0.0440	-0.0996	0.1466	-0.1835	-0.3708	0.0274	-0.0141
2JBL - BCB L1278	0.4551	0.0277	0.0645	-0.2302	-0.1074	-0.0083	0.3300	-0.0747	0.6043	0.0269	-0.0415	0.0166	-0.3276	-0.3928	0.1532	0.0422
2PRC - BCB M805	0.4559	0.0249	0.0906	-0.3080	-0.0668	-0.0148	0.2660	-0.0783	0.5455	0.0296	0.0495	0.0640	-0.1584	-0.4372	0.0847	0.0275
2WJM - BCB M1324	0.3237	0.0516	0.0494	-0.1296	0.0515	-0.0138	0.2327	-0.0593	0.3490	0.0469	0.1236	0.1253	-0.1411	-0.2241	0.0652	0.0425
2WJN - BCB M1324	0.2781	0.0489	0.0450	-0.1267	-0.0423	-0.0602	0.1690	-0.0401	0.3881	0.0586	0.1562	0.0028	-0.1669	-0.2641	0.0475	0.0348
3D38 - BCB M400	0.4685	0.0260	-0.0358	-0.2975	-0.0777	-0.0050	0.2334	-0.1184	0.4620	0.0411	-0.0959	-0.1217	-0.1843	-0.3900	-0.0039	-0.0016
3G7F - BCB M400	0.5039	0.0240	0.1283	-0.3224	-0.1111	0.0004	0.2196	-0.1027	0.4952	0.0513	0.0190	0.2400	-0.1900	-0.3612	0.0562	-0.0191
3PRC - BCB M805	0.4753	0.0259	0.0908	-0.2742	-0.1148	-0.0302	0.3148	-0.0784	0.4897	0.0312	0.0376	0.0165	-0.1861	-0.3644	0.0869	0.0205
5PRC - BCB M805	0.3939	0.0233	0.0593	-0.2617	-0.0653	-0.0199	0.2163	-0.0794	0.5268	0.0312	-0.0505	-0.0008	-0.0998	-0.3549	0.0688	-0.0287
6PRC - BCB M805	0.4136	0.0248	0.0356	-0.2326	-0.0873	-0.0213	0.2776	-0.0781	0.5252	0.0311	0.0562	0.0083	-0.1594	-0.3290	0.1155	0.0196
7PRC - BCB M805	0.3966	0.0265	0.0599	-0.2490	-0.0967	-0.0629	0.2300	-0.0733	0.5626	0.0314	-0.0198	-0.0246	-0.1606	-0.4262	-0.0215	-0.0115

Table 57: Extended conformational parameters and lowest energy basis normal-mode displacements of all DL cofactors from crystal structures of *Blastochloris viridis*.

Cofactor ID	Dip_e	δip_e	B2g_e	B1g_e	Eu(x)_e	Eu(y)_e	A1g_e	A2g_e	Doop_e	δoop_e	B2u_e	B1u_e	A2u_e	Eg(x)_e	Eg(y)_e	A1u_e
1DXR - BCB L400	0.4080	0.0231	0.0770	-0.1862	-0.1315	-0.0201	0.2601	-0.0865	0.6993	0.0151	-0.1345	-0.6097	-0.0560	0.0137	0.0775	-0.2142
1PRC - BCB L602	0.4272	0.0345	0.0711	-0.2967	-0.1094	-0.0499	0.1576	-0.1017	0.4737	0.0176	-0.1544	-0.3335	-0.0636	-0.0956	0.0454	-0.1460
1R2C - BCB L302	0.4301	0.0264	0.0737	-0.2648	-0.1531	-0.0087	0.2282	-0.0761	0.6480	0.0136	-0.2833	-0.5396	0.0326	0.0022	0.0103	-0.1026
1VRN - BCB L402	0.4539	0.0225	0.0554	-0.2427	-0.1372	-0.0299	0.3066	-0.0676	0.8283	0.0215	-0.2264	-0.7262	0.0546	0.0229	0.0240	-0.2354
2I5N - BCB L400	0.4275	0.0247	0.0448	-0.1950	-0.0856	-0.0232	0.2822	-0.1055	0.8586	0.0359	-0.2808	-0.6912	-0.0591	-0.1841	0.1538	-0.2099
2JBL - BCB L1274	0.4365	0.0231	0.0530	-0.2445	-0.1321	-0.0348	0.2801	-0.0753	0.8462	0.0198	-0.2772	-0.7508	-0.0493	0.0327	-0.0457	-0.2142
2PRC - BCB L302	0.3868	0.0271	0.0597	-0.1849	-0.1150	0.0021	0.2361	-0.0926	0.8059	0.0184	-0.3198	-0.6704	-0.0683	0.0906	0.0178	-0.1691
2WJM - BCB L1274	0.3804	0.0501	0.0981	-0.1097	-0.0506	-0.0492	0.2778	-0.0807	0.7402	0.0229	-0.1289	-0.6433	0.0909	0.0161	0.1651	-0.2052
2WJN - BCB L1274	0.4247	0.0459	0.0556	-0.2107	-0.0759	-0.0144	0.2585	-0.0636	0.7458	0.0214	-0.1596	-0.6453	0.0422	0.0266	0.1108	-0.2038
3D38 - BCB L400	0.4952	0.0225	0.1284	-0.2273	-0.1474	-0.0808	0.2836	-0.1022	0.9069	0.0384	-0.3050	-0.7682	-0.1367	-0.0991	0.1286	-0.1823
3G7F - BCB L400	0.4434	0.0251	0.0738	-0.2606	-0.1678	-0.0429	0.2211	-0.1146	0.8309	0.0271	-0.2207	-0.7575	-0.0088	-0.0507	0.0891	-0.1536
3PRC - BCB L302	0.4402	0.0242	0.0237	-0.2666	-0.1427	-0.0234	0.2539	-0.0806	0.7510	0.0148	-0.2201	-0.6532	-0.0370	0.0843	0.0149	-0.1880
5PRC - BCB L302	0.3365	0.0247	0.0084	-0.1819	-0.1148	-0.0023	0.1817	-0.0901	0.7450	0.0198	-0.2742	-0.6334	-0.1203	-0.0148	0.0955	-0.1591
6PRC - BCB L302	0.3705	0.0223	-0.0154	-0.1938	-0.1264	-0.0705	0.2048	-0.0854	0.7041	0.0201	-0.2428	-0.6105	-0.0844	0.0628	0.0198	-0.1501
7PRC - BCB L302	0.4188	0.0238	0.0733	-0.2412	-0.1549	-0.0387	0.2236	-0.0916	0.8994	0.0189	-0.2717	-0.8092	-0.1115	0.0721	0.0409	-0.1698

Table 58: Extended conformational parameters and lowest energy basis normal-mode displacements of all DM cofactors from crystal structures of *Blastochloris viridis*.

Cofactor ID	Dip_e	δip_e	B2g_e	B1g_e	Eu(x)_e	Eu(y)_e	A1g_e	A2g_e	Doop_e	δoop_e	B2u_e	B1u_e	A2u_e	Eg(x)_e	Eg(y)_e	A1u_e
1DXR - BCB M401	0.3817	0.0211	0.0405	-0.1704	-0.1481	-0.0307	0.2406	-0.0681	0.8672	0.0163	-0.1052	-0.7896	0.0168	-0.1426	0.1460	-0.2097
1PRC - BCB M603	0.3634	0.0314	0.0703	-0.0844	-0.0847	-0.2148	0.0379	-0.1052	0.7232	0.0145	0.1016	-0.6127	-0.0341	0.0480	0.0855	-0.2064
1R2C - BCB M1303	0.3621	0.0219	0.0957	-0.1702	-0.2056	-0.0266	0.1506	-0.0741	1.0864	0.0205	-0.2011	-1.0022	0.0369	-0.1082	0.1436	-0.2462
1VRN - BCB M403	0.4044	0.0189	0.0491	-0.2328	-0.1288	-0.0234	0.2316	-0.0716	1.1192	0.0109	-0.0507	-1.0594	0.0498	-0.0193	0.1007	-0.2692
2I5N - BCB M401	0.4032	0.0214	-0.0388	-0.2464	-0.0657	-0.0412	0.1716	-0.1001	1.1564	0.0368	-0.0765	-1.0376	-0.1040	-0.1299	0.2493	-0.2962
2JBL - BCB M1324	0.4052	0.0223	0.0390	-0.1869	-0.2029	-0.0174	0.2329	-0.0712	1.0151	0.0108	-0.1071	-0.9563	-0.0127	-0.0724	0.1888	-0.2046
2PRC - BCB M806	0.3070	0.0228	-0.0282	-0.1338	-0.1426	-0.0969	0.1196	-0.0809	1.0896	0.0180	-0.1401	-1.0334	-0.1206	-0.0035	0.1793	-0.1695
2WJM - BCB M1325	0.3402	0.0453	0.1699	-0.0577	0.0048	0.0111	0.1853	-0.0500	1.0914	0.0257	0.1322	-0.9883	0.0000	-0.0200	0.1567	-0.2883
2WJN - BCB M1325	0.3198	0.0423	0.1030	-0.1304	-0.0270	-0.0276	0.1589	-0.0414	1.0480	0.0269	0.0937	-0.9426	-0.0539	-0.0148	0.1633	-0.3046
3D38 - BCB M401	0.4304	0.0223	0.1246	-0.2619	-0.0467	-0.0559	0.2148	-0.1110	0.9604	0.0354	-0.2578	-0.7987	-0.0157	-0.1867	0.2147	-0.2382
3PRC - BCB M806	0.3695	0.0216	0.0461	-0.1449	-0.1334	-0.0299	0.2491	-0.0818	0.9981	0.0157	-0.1393	-0.9353	-0.0165	-0.0176	0.0831	-0.2426
5PRC - BCB M806	0.3808	0.0220	0.0243	-0.1892	-0.1810	-0.0247	0.1996	-0.0711	0.9731	0.0159	-0.0441	-0.9183	-0.0727	-0.0612	0.1674	-0.1966
6PRC - BCB M806	0.3606	0.0207	-0.0133	-0.2003	-0.1301	-0.0166	0.1865	-0.0778	1.0714	0.0169	-0.0863	-1.0110	-0.1173	-0.0695	0.0509	-0.2449
7PRC - BCB M806	0.4232	0.0270	0.0239	-0.2118	-0.1440	-0.0506	0.2667	-0.0791	1.0237	0.0166	-0.0116	-0.9643	-0.1369	-0.0249	0.0908	-0.1835

8.2.3 Extended Basis (Next-to-lowest Energy)

Table 59: Extended conformational parameters and next-to-lowest energy basis normal-mode displacements of all BA cofactors from crystal structures of *Blastochloris viridis*.

Cofactor ID	B2g_2	B1g_2	Eu(x)_2	Eu(y)_2	A1g_2	A2g_2	B2u_2	B1u_2	A2u_2	Eg(x)_2	Eg(y)_2	A1u_2
1DXR - BCB L401	-0.0113	-0.0905	-0.0579	0.1156	0.0009	-0.0163	0.0648	-0.0546	-0.0550	0.0568	0.0697	-0.0200
1PRC - BCB L604	0.0271	-0.0411	-0.0701	0.1532	0.0294	0.0363	-0.0093	-0.0607	-0.0011	0.0673	0.0264	-0.0431
1R2C - BCB L304	0.0308	-0.1028	-0.0569	0.1160	-0.0008	-0.0240	-0.0254	-0.0624	-0.0985	0.1956	0.0802	-0.0354
1VRN - BCB L404	0.0109	-0.1059	-0.0553	0.1203	-0.0069	-0.0189	0.1296	-0.0432	-0.0671	0.1282	0.0522	-0.0307
2I5N - BCB L401	0.0821	-0.0862	-0.0944	0.1668	-0.0513	0.0169	0.0100	-0.0191	-0.0221	0.0929	-0.0140	0.0187
2JBL - BCB L1275	0.0165	-0.1017	-0.0543	0.1251	-0.0003	-0.0165	0.0688	-0.0310	-0.1319	0.0944	-0.0144	-0.0192
2PRC - BCB L304	0.0007	-0.1000	-0.0400	0.1076	-0.0031	-0.0262	0.0659	-0.0814	-0.1003	0.0833	0.0779	-0.0175
2WJM - BCB L1275	-0.0302	0.0667	0.0110	0.0911	0.0631	0.0498	0.0365	-0.0840	-0.0150	0.0885	0.0616	-0.0344
2WJN - BCB L1275	-0.0233	0.0737	-0.0367	0.0791	0.0779	0.0809	0.0678	-0.0365	0.0201	0.1310	0.0697	-0.0211
3D38 - BCB L401	0.0935	-0.1027	-0.0489	0.1405	-0.0757	0.0197	0.0062	-0.0307	0.0177	0.0451	-0.0356	-0.0158
3G7F - BCB L401	0.0894	-0.0942	-0.0919	0.1280	-0.0635	0.0085	0.0003	-0.0002	-0.0080	0.0767	-0.0360	0.0081
3PRC - BCB L304	-0.0004	-0.0994	-0.0496	0.1104	0.0011	-0.0223	0.1516	-0.0427	-0.1187	0.1368	0.0735	-0.0297
5PRC - BCB L304	0.0080	-0.1023	-0.0336	0.1187	-0.0006	-0.0263	0.0221	-0.0694	-0.1630	0.1110	0.0877	-0.0342
6PRC - BCB L304	0.0054	-0.0793	-0.0703	0.1164	-0.0044	-0.0175	0.1005	-0.0761	-0.1558	0.0451	0.0492	-0.0304
7PRC - BCB L304	0.0223	-0.0840	-0.0782	0.1043	0.0101	-0.0121	0.2388	-0.0876	-0.1552	0.0513	-0.0976	-0.0193

Table 60: Extended conformational parameters and next-to-lowest energy basis normal-mode displacements of all BB cofactors from crystal structures of *Blastochloris viridis*.

Cofactor ID	B2g_2	B1g_2	Eu(x)_2	Eu(y)_2	A1g_2	A2g_2	B2u_2	B1u_2	A2u_2	Eg(x)_2	Eg(y)_2	A1u_2
1DXR - BCB M400	0.0299	-0.0981	-0.0522	0.1210	-0.0055	-0.0218	0.0890	-0.0384	-0.0210	0.1669	0.0748	-0.0145

Cofactor ID	B2g_2	B1g_2	Eu(x)_2	Eu(y)_2	A1g_2	A2g_2	B2u_2	B1u_2	A2u_2	Eg(x)_2	Eg(y)_2	A1u_2
1PRC - BCB M601	0.1138	-0.0514	-0.1047	0.1146	0.0271	0.0192	0.0711	0.0215	0.0228	0.0967	0.0150	0.0254
1R2C - BCB M1301	0.0303	-0.1009	-0.0227	0.0972	0.0017	-0.0166	0.0834	-0.1071	-0.1521	0.2407	-0.0615	0.0086
1VRN - BCB M401	0.0198	-0.1024	-0.0488	0.1191	-0.0044	-0.0185	0.0663	-0.0495	-0.0007	0.2279	0.0832	-0.0073
2I5N - BCB M400	0.0968	-0.0904	-0.0631	0.1504	-0.0482	0.0171	0.0340	0.0307	0.0383	0.0781	0.0028	0.0280
2JBL - BCB L1278	0.0153	-0.1062	-0.0386	0.1110	0.0003	-0.0247	0.0187	-0.0855	-0.0800	0.2381	0.0468	-0.0022
2PRC - BCB M805	0.0134	-0.0912	-0.0428	0.1170	-0.0011	-0.0241	0.0478	-0.0527	-0.0634	0.2272	-0.0046	-0.0079
2WJM - BCB M1324	0.0450	0.0818	-0.0128	0.0617	0.0895	0.0600	0.0057	-0.0427	0.0033	0.0948	0.0528	-0.0077
2WJN - BCB M1324	0.0426	0.0201	-0.1015	0.0492	0.0512	0.0751	0.0436	-0.0456	0.0029	0.1183	0.0752	-0.0142
3D38 - BCB M400	0.1700	-0.0814	-0.0806	0.0974	-0.0583	0.0266	0.0213	-0.0187	0.0338	0.0433	0.0043	-0.0003
3G7F - BCB M400	0.1420	-0.0707	-0.0638	0.1769	-0.0470	0.0115	-0.0069	0.0629	0.0308	0.0939	0.0072	0.0520
3PRC - BCB M805	0.0008	-0.0885	-0.0282	0.1255	-0.0067	-0.0081	0.0237	-0.0473	-0.0887	0.1990	-0.0936	-0.0041
5PRC - BCB M805	0.0369	-0.0947	-0.0241	0.1239	-0.0013	-0.0127	0.0143	-0.0364	0.0233	0.3487	0.0177	-0.0005
6PRC - BCB M805	0.0301	-0.0910	-0.0102	0.1274	-0.0030	-0.0162	0.0120	-0.0461	-0.0585	0.3345	-0.0102	-0.0163
7PRC - BCB M805	0.0168	-0.0961	-0.0035	0.1071	-0.0044	-0.0065	0.0429	-0.0640	-0.0081	0.2846	-0.1077	0.0116

Table 61: Extended conformational parameters and next-to-lowest energy basis normal-mode displacements of all DL cofactors from crystal structures of *Blastochloris viridis*.

Cofactor ID	B2g_2	B1g_2	Eu(x)_2	Eu(y)_2	A1g_2	A2g_2	B2u_2	B1u_2	A2u_2	Eg(x)_2	Eg(y)_2	A1u_2
1DXR - BCB L400	-0.0544	-0.1020	-0.0404	0.1367	0.0015	-0.0101	0.0734	0.1405	-0.0167	-0.0929	-0.0251	0.0918
1PRC - BCB L602	-0.0451	-0.0484	-0.0125	0.1754	0.0515	0.0107	-0.0282	0.1784	-0.0085	0.0244	-0.0219	0.1378
1R2C - BCB L302	-0.0362	-0.1000	-0.0543	0.1165	0.0312	-0.0013	0.0613	0.0747	0.0986	-0.0217	0.1238	0.0470
1VRN - BCB L402	0.0041	-0.0942	-0.0547	0.1215	0.0180	0.0015	0.0632	0.1381	-0.0070	-0.1026	-0.0410	0.1055
2I5N - BCB L400	0.0652	-0.0922	-0.1105	0.1363	-0.0285	0.0193	0.1094	0.1414	0.0296	-0.0930	0.0457	0.1751
2JBL - BCB L1274	0.0012	-0.0910	-0.0478	0.1230	0.0256	0.0005	0.0006	0.1179	-0.0068	-0.0079	-0.0613	0.0814
2PRC - BCB L302	-0.0211	-0.1098	-0.0402	0.1429	0.0208	0.0026	-0.0465	0.1065	-0.0860	-0.0532	-0.1665	0.0787
2WJM - BCB L1274	-0.0128	0.0484	-0.0440	0.1062	0.1196	0.0573	0.0197	0.1451	0.0102	-0.0803	-0.0349	0.0951
2WJN - BCB L1274	-0.0172	0.0336	-0.0634	0.1488	0.1142	0.1161	0.0647	0.1687	0.0355	-0.0815	-0.0306	0.1266
3D38 - BCB L400	0.1055	-0.0831	-0.1230	0.1478	-0.0534	0.0313	0.1257	0.0825	0.0565	-0.1222	0.0559	0.1172
3G7F - BCB L400	0.0285	-0.1014	-0.0691	0.1216	-0.0052	0.0205	0.0876	0.0599	0.0128	-0.0935	0.0493	0.0990
3PRC - BCB L302	-0.0261	-0.1064	-0.0482	0.1292	0.0115	-0.0016	0.0400	0.1337	-0.0346	-0.1206	-0.0457	0.0805
5PRC - BCB L302	0.0069	-0.1149	-0.0477	0.1027	0.0112	-0.0005	-0.0132	0.1465	0.0145	-0.0097	0.0257	0.0847
6PRC - BCB L302	0.0018	-0.0985	-0.0549	0.1299	0.0039	0.0035	0.0046	0.1561	-0.0059	-0.0432	-0.0114	0.0610
7PRC - BCB L302	0.0412	-0.0936	-0.0143	0.1323	0.0213	-0.0006	-0.0443	0.1371	-0.0217	-0.0012	-0.0726	0.0839

Table 62: Extended conformational parameters and next-to-lowest energy basis normal-mode displacements of all DM cofactors from crystal structures of *Blastochloris viridis*.

Cofactor ID	B2g_2	B1g_2	Eu(x)_2	Eu(y)_2	A1g_2	A2g_2	B2u_2	B1u_2	A2u_2	Eg(x)_2	Eg(y)_2	A1u_2
1DXR - BCB M401	-0.0100	-0.0850	-0.0538	0.1410	0.0125	-0.0135	0.0396	0.1353	0.0384	-0.0359	0.0339	0.0894
1PRC - BCB M603	-0.0778	-0.0237	-0.1323	0.1494	0.0771	0.0050	-0.0004	0.2313	0.0537	0.0206	-0.0252	0.1618
1R2C - BCB M1303	0.0185	-0.0817	-0.0230	0.1081	0.0563	-0.0076	-0.0311	0.1381	0.0542	0.0667	-0.0381	0.1098
1VRN - BCB M403	0.0090	-0.0760	-0.0628	0.1398	0.0515	-0.0138	0.0068	0.1453	-0.0020	-0.0703	0.0295	0.1227

Cofactor ID	B2g_2	B1g_2	Eu(x)_2	Eu(y)_2	A1g_2	A2g_2	B2u_2	B1u_2	A2u_2	Eg(x)_2	Eg(y)_2	A1u_2
2I5N - BCB M401	0.0778	-0.0699	-0.1226	0.1690	-0.0017	0.0188	0.0826	0.1676	0.0345	-0.0664	0.0817	0.1653
2JBL - BCB M1324	0.0236	-0.0907	-0.0284	0.1254	0.0520	-0.0094	-0.0042	0.0933	0.0254	-0.0280	0.0555	0.0921
2PRC - BCB M806	-0.0004	-0.0945	-0.0261	0.1107	0.0556	-0.0074	-0.0329	0.1316	-0.0030	-0.0541	-0.0028	0.0585
2WJM - BCB M1325	-0.0236	0.0704	-0.0251	0.1222	0.1487	0.0584	0.0259	0.2096	-0.0185	-0.1056	0.0872	0.1577
2WJN - BCB M1325	-0.0250	0.0462	-0.0626	0.0983	0.1461	0.0922	0.0164	0.1889	0.0196	-0.0985	0.0684	0.1682
3D38 - BCB M401	0.0693	-0.0839	-0.0769	0.1307	-0.0420	0.0205	0.1074	0.1495	0.0140	-0.0861	0.0521	0.1852
3PRC - BCB M806	0.0046	-0.0978	-0.0282	0.1231	0.0338	-0.0034	0.0357	0.1582	0.0325	-0.0413	-0.0157	0.0768
5PRC - BCB M806	0.0412	-0.0907	0.0035	0.1418	0.0287	-0.0136	0.0342	0.1361	0.0278	-0.0100	-0.0022	0.0684
6PRC - BCB M806	0.0082	-0.0759	-0.0180	0.1576	0.0422	-0.0074	0.0117	0.1606	-0.0326	-0.0148	0.0318	0.0975
7PRC - BCB M806	-0.0230	-0.0951	-0.0285	0.1487	0.0466	-0.0102	0.0152	0.1137	-0.1172	0.0936	-0.1424	0.0524

8.3 *Rhodobacter sphaeroides* bacteriopheophytin cofactor NSDs

Table 63: Minimum basis normal-mode displacements and conformational parameters of all ΦA cofactors from crystal structures of *Rhodobacter sphaeroides*.

Cofactor ID	Dip	δip	B2g	B1g	Eu(x)	Eu(y)	A1g	A2g	Doop	δoop	B2u	B1u	A2u	Eg(x)	Eg(y)	A1u
1AIG - BPH L285	0.4884	0.0528	-0.1092	-0.2954	-0.1178	-0.0998	0.3392	-0.0208	0.3981	0.0239	0.0879	0.2889	0.1891	0.0419	-0.1721	0.0151
1AIG - BPH N285	0.4382	0.0540	-0.0240	-0.3856	-0.1054	0.0097	0.1754	-0.0273	0.3523	0.0212	-0.0020	0.2709	0.1849	-0.0190	-0.1270	0.0068
1AIJ - BPH L285	0.3360	0.0564	0.0283	-0.2012	-0.0527	-0.1369	0.2213	-0.0339	0.5337	0.0159	-0.0208	0.4973	0.1379	0.0169	0.1095	0.0763
1AIJ - BPH R284	0.2221	0.0573	0.0066	-0.1490	-0.0355	-0.0667	0.1394	-0.0442	0.4808	0.0098	-0.0538	0.4696	-0.0552	-0.0213	0.0459	0.0463
1DS8 - BPH L1006	0.5479	0.0536	0.1067	-0.3558	-0.1224	-0.0541	0.3772	-0.0441	0.4603	0.0257	-0.1218	0.4170	0.0668	-0.0154	-0.0367	0.1308
1DS8 - BPH R2006	0.3976	0.0580	0.0174	-0.2860	-0.0812	-0.0121	0.2610	-0.0346	0.3726	0.0171	-0.1286	0.3208	-0.0241	-0.1033	-0.0532	0.0731
1DV3 - BPH L1006	0.6311	0.0516	0.1952	-0.3608	-0.0854	-0.0882	0.4579	-0.0722	0.5521	0.0193	-0.0304	0.5098	0.1507	-0.0073	0.0032	0.1456
1DV3 - BPH R2006	0.4072	0.0612	-0.0131	-0.2271	-0.1329	-0.0261	0.3078	-0.0303	0.3342	0.0161	-0.0595	0.2927	0.0689	-0.0889	-0.0720	0.0681
1DV6 - BPH L1006	0.5299	0.0530	0.2150	-0.2609	-0.0218	-0.1688	0.3650	-0.0659	0.5638	0.0152	-0.0520	0.4873	0.2364	0.0441	-0.0057	0.1409
1DV6 - BPH R2006	0.4297	0.0564	-0.0797	-0.2765	-0.1025	-0.0174	0.2992	-0.0394	0.3698	0.0118	-0.0138	0.3553	0.0433	0.0048	-0.0448	0.0800
1E14 - BPH C401	0.6322	0.0524	0.3910	-0.4283	-0.0098	-0.0479	0.2383	-0.0650	0.3607	0.0163	-0.1045	0.2664	0.1319	0.0456	-0.1618	0.0510
1E6D - BPH C402	0.6319	0.0496	0.3728	-0.3596	-0.0631	-0.0801	0.3409	-0.0657	0.6228	0.0158	-0.0346	0.5801	0.2072	-0.0393	0.0168	0.0741
1EYS - BPH L606	0.3180	0.0465	-0.0287	-0.1243	-0.1064	-0.1313	0.2282	-0.0645	0.5690	0.0368	-0.1249	0.4716	0.1020	-0.1726	-0.0768	0.1992
1F6N - BPH L402	0.5206	0.0471	0.0973	-0.3361	-0.0531	-0.0686	0.3683	-0.0735	0.5027	0.0483	-0.0875	0.4274	0.2325	-0.0732	-0.0319	0.0439
1FNP - BPH L402	0.5116	0.0475	0.0788	-0.3343	-0.0642	-0.0913	0.3554	-0.0709	0.5875	0.0489	-0.1941	0.4834	0.2659	-0.0315	-0.0240	0.0397
1FNQ - BPH L402	0.5491	0.0447	0.1409	-0.3360	-0.0442	-0.1126	0.3868	-0.0677	0.5648	0.0468	-0.0640	0.4998	0.2456	-0.0349	-0.0042	0.0590
1JGW - BPH L855	0.5334	0.0601	0.1595	-0.3232	-0.0773	-0.1054	0.3708	-0.0033	0.1376	0.0039	-0.0926	0.0986	-0.0044	-0.0129	-0.0126	0.0172
1JGX - BPH L855	0.6901	0.0615	0.2718	-0.4386	-0.0883	-0.1250	0.4320	0.0056	0.1322	0.0041	-0.0615	0.1104	0.0296	-0.0019	0.0037	0.0246
1JGY - BPH L855	0.5503	0.0639	0.1226	-0.3298	-0.0780	-0.1087	0.4014	0.0076	0.1137	0.0031	-0.0983	0.0277	0.0451	0.0089	0.0023	0.0196
1JGZ - BPH L855	0.6407	0.0640	0.2405	-0.4085	-0.0967	-0.1277	0.4000	-0.0124	0.1313	0.0041	-0.0745	0.0991	0.0317	0.0075	0.0112	0.0261
1JH0 - BPH L855	0.4852	0.0613	0.1679	-0.3072	-0.0736	-0.1096	0.3087	-0.0123	0.0714	0.0045	-0.0253	0.0572	-0.0087	-0.0227	-0.0216	0.0115
1K6L - BPH L402	0.6155	0.0511	0.3574	-0.3546	-0.0652	-0.0714	0.3344	-0.0647	0.5802	0.0246	0.0494	0.5182	0.2346	0.0294	-0.0110	0.0982
1K6N - BPH L402	0.6153	0.0511	0.3574	-0.3542	-0.0651	-0.0717	0.3344	-0.0650	0.5800	0.0245	0.0498	0.5178	0.2346	0.0305	-0.0114	0.0982
1KBY - BPH L855	0.5784	0.0632	0.2232	-0.3161	-0.0475	-0.1113	0.4125	-0.0030	0.1673	0.0051	-0.0997	0.1284	-0.0141	-0.0172	-0.0263	0.0196
1L9B - BPH M1006	0.6199	0.0567	0.2271	-0.3097	-0.0508	-0.0500	0.4807	-0.0249	0.1966	0.0038	-0.1458	0.1250	0.0368	-0.0168	-0.0039	0.0101
1L9J - BPH M1006	0.5620	0.0560	0.1771	-0.3143	-0.0640	-0.0450	0.4230	-0.0266	0.1074	0.0026	-0.0660	0.0834	-0.0017	-0.0094	0.0045	0.0107

1L9J - BPH S2006	0.6332	0.0560	0.1443	-0.3892	-0.0581	-0.0551	0.4707	-0.0267	0.1484	0.0023	-0.0694	0.1288	0.0012	-0.0232	-0.0031	0.0073
1M3X - BPH L855	0.5807	0.0613	0.2665	-0.3141	-0.0731	-0.0751	0.3956	-0.0083	0.1642	0.0047	-0.1042	0.1242	0.0031	-0.0127	-0.0131	0.0182
1MPS - BPH L402	0.5143	0.0466	0.1175	-0.3502	-0.0253	-0.0827	0.3404	-0.0686	0.4977	0.0359	-0.0899	0.4663	0.1259	-0.0032	0.0423	0.0675
1OGV - BPH L1284	0.6081	0.0533	0.3247	-0.3004	-0.0968	-0.0486	0.4028	-0.0121	0.2269	0.0051	-0.0165	0.2030	0.0967	-0.0197	-0.0100	0.0126
1PCR - BPH L402	0.5072	0.0446	-0.0766	-0.3733	-0.0447	-0.0899	0.3117	-0.0695	0.6375	0.0622	-0.0288	0.5427	0.2831	0.0568	-0.1444	0.0822
1PSS - BPH L271	0.3879	0.0492	-0.0767	-0.3617	-0.0128	-0.0509	0.0931	-0.0484	0.7109	0.0318	0.1138	0.6605	0.1477	0.1151	-0.1404	0.0355
1PST - BPH L271	0.4356	0.0529	-0.1588	-0.3238	-0.0503	-0.0440	0.2311	-0.0425	0.4625	0.0195	0.1139	0.3345	0.2822	0.0611	-0.0607	0.0443
1PYH - BPH B402	0.4077	0.0538	0.1947	-0.2791	-0.0825	-0.0674	0.1655	-0.1083	0.5344	0.0275	0.0122	0.4690	0.1952	0.0172	-0.0204	0.1634
1QOV - BPH M1402	0.6158	0.0509	0.3575	-0.3552	-0.0644	-0.0715	0.3342	-0.0654	0.5808	0.0246	0.0488	0.5191	0.2339	0.0292	-0.0109	0.0987
1RG5 - BPH L402	0.6140	0.0584	0.1220	-0.4189	-0.0796	-0.0520	0.4060	-0.1132	0.5603	0.0242	-0.0677	0.5084	0.1651	-0.0563	-0.0141	0.1424
1RGN - BPH L402	0.6515	0.0721	0.2400	-0.4500	-0.0972	-0.1061	0.3642	-0.1052	0.6317	0.0292	0.1323	0.5175	0.2671	-0.1324	0.0717	0.1406
1RQK - BPH L402	0.5809	0.0610	0.2082	-0.3866	-0.0714	-0.0341	0.3605	-0.0914	0.5046	0.0226	-0.0124	0.4393	0.1971	-0.0597	-0.0056	0.1380
1RZZ - BPH R2006	0.6731	0.0584	0.3016	-0.3238	-0.0792	-0.0699	0.4960	-0.0109	0.1836	0.0050	-0.0021	0.1620	0.0737	-0.0121	0.0400	0.0161
1S00 - BPH R2006	0.6650	0.0564	0.3539	-0.3800	-0.0659	-0.0298	0.4089	-0.0153	0.2018	0.0049	0.0119	0.1879	0.0636	-0.0078	0.0276	0.0201
1YST - BPH L276	0.4536	0.0707	0.0966	-0.3500	-0.1722	-0.1621	0.0794	-0.1081	0.9179	0.0235	-0.8485	0.2982	0.1157	-0.0938	-0.0968	0.0461
1Z9J - BPH A855	0.7012	0.0574	0.1766	-0.5748	-0.0886	-0.0327	0.3472	-0.0236	0.1599	0.0020	0.1436	-0.0524	0.0448	0.0048	0.0096	0.0098
1Z9K - BPH A855	0.5509	0.0638	-0.1422	0.3846	0.0698	-0.1844	0.3105	-0.0067	0.0808	0.0035	0.0608	0.0415	0.0204	0.0196	-0.0173	0.0029
2BNP - BH1 A1284	0.8103	0.0637	0.5344	-0.5624	-0.1597	-0.0498	0.1318	-0.0962	0.6204	0.0427	-0.1010	0.5215	0.1244	0.0375	-0.0807	0.2815
2BNS - BH1 A1284	0.6335	0.0608	0.2431	-0.5288	-0.1446	-0.0832	0.1540	-0.1052	0.6253	0.0433	-0.0526	0.5379	0.1048	-0.0381	-0.0741	0.2844
2BOZ - BH1 L1284	0.5774	0.0583	0.3171	-0.3097	-0.1560	-0.0767	0.3032	-0.1214	0.5300	0.0218	0.0101	0.4588	0.2327	-0.0088	-0.0305	0.1233
2GMR - BPH L305	0.4917	0.0429	0.1690	-0.2697	-0.1193	-0.0501	0.3417	-0.0836	0.5610	0.0460	0.0491	0.4600	0.2088	0.0539	-0.0378	0.2299
2GNU - BPH M1284	0.7457	0.0534	0.5193	-0.4235	-0.1196	-0.0527	0.2527	-0.1615	0.6376	0.0434	-0.0116	0.5357	0.1502	-0.0626	-0.1036	0.2866
2HG3 - BPH L402	0.6095	0.0528	0.1962	-0.4010	-0.0555	-0.1332	0.3746	-0.1051	0.5755	0.0267	0.0914	0.4761	0.2630	-0.0385	-0.0564	0.1495
2HG9 - BPH L402	0.5530	0.0587	0.1865	-0.3979	-0.0985	-0.0894	0.2942	-0.0922	0.5238	0.0266	0.0526	0.4644	0.1763	-0.0825	-0.0198	0.1329
2HH1 - BPH L402	0.5694	0.0490	0.2537	-0.3855	-0.1016	-0.1572	0.2655	-0.0756	0.6199	0.0244	0.0035	0.5685	0.1320	-0.1307	-0.0714	0.1465
2HHK - BPH L402	0.5832	0.0548	0.2444	-0.3391	-0.0726	-0.1109	0.3725	-0.0953	0.5718	0.0295	0.0540	0.4982	0.2153	-0.1102	-0.0473	0.1230
2HIT - BPH L402	0.6377	0.0487	-0.0498	-0.4170	-0.1015	-0.1531	0.4346	-0.0875	0.6360	0.0361	0.1505	0.4570	0.3195	-0.2030	0.0838	0.1507
2HJ6 - BPH L402	0.4891	0.0621	-0.1414	-0.1610	-0.0236	-0.1559	0.3877	-0.1348	0.4928	0.0246	-0.0187	0.2957	0.2459	-0.2727	0.0427	0.1355
2J8C - BPH L1286	0.6192	0.0556	0.3542	-0.3139	-0.1635	-0.1151	0.3309	-0.0998	0.5735	0.0595	-0.0437	0.3648	0.2629	-0.1975	-0.0677	0.2850
2J8D - BPH L1287	0.6544	0.0580	0.3989	-0.3041	-0.1733	-0.1256	0.3359	-0.1344	0.6162	0.0627	0.0534	0.4652	0.2343	-0.1475	-0.1158	0.2654
2JIY - BPH L1285	0.5703	0.0516	0.2941	-0.3051	-0.1449	-0.1025	0.3242	-0.0952	0.5500	0.0266	-0.0112	0.4669	0.2401	-0.0800	-0.0003	0.1427
2JJ0 - BPH L1285	0.5479	0.0589	0.1755	-0.3900	-0.0991	-0.1247	0.2912	-0.0841	0.5288	0.0278	0.1136	0.4209	0.2505	-0.0236	0.1003	0.1269
2RCR - BPH L550	0.3669	0.0488	-0.1225	-0.2357	-0.1000	-0.0239	0.2007	-0.1148	0.4431	0.0091	0.2890	0.2695	0.0973	-0.0655	-0.1617	-0.0165
2UWS - BPH L1284	0.7749	0.0772	0.2606	-0.5799	-0.0725	-0.0724	0.4119	-0.1270	0.6226	0.0925	0.4440	0.3452	0.0993	-0.0597	-0.1899	0.1479
2UWT - BPH L1284	0.8073	0.0622	0.3718	-0.5793	-0.1326	-0.0503	0.3820	-0.1091	0.6540	0.0569	0.1462	0.4787	0.3472	0.0045	0.0332	0.2354
2UWU - BPH L1286	0.6345	0.0592	0.2670	-0.3772	-0.1640	-0.1275	0.3687	-0.0997	0.6783	0.0544	0.1306	0.5125	0.3039	0.0007	-0.0708	0.2881
2UWV - BPH L1284	0.6543	0.0596	0.2867	-0.3964	-0.1378	-0.1137	0.3807	-0.1096	0.6360	0.0582	0.0835	0.5196	0.2417	-0.0286	-0.0815	0.2483
2UWW - BPH L1288	0.6468	0.0558	0.2903	-0.3439	-0.1497	-0.1112	0.4058	-0.1276	0.6604	0.0582	0.1179	0.5151	0.2730	-0.0332	-0.1109	0.2627
2UX3 - BPH L1284	0.6441	0.0652	0.2699	-0.4030	-0.1237	-0.0648	0.3868	-0.1025	0.6268	0.0773	0.0766	0.5421	0.2588	0.0279	-0.1094	0.1158
2UX4 - BPH L1286	0.7019	0.0665	0.2938	-0.4614	-0.1241	-0.0645	0.4017	-0.1116	0.5144	0.0763	0.0042	0.2670	0.3336	-0.0671	0.0411	0.2754
2UX5 - BPH L1285	0.7401	0.0549	0.3620	-0.4835	-0.1689	-0.1273	0.3595	-0.0950	0.7209	0.0570	0.1141	0.6134	0.2379	-0.0661	-0.1394	0.2236
2UXJ - BPH L1285	0.7545	0.0565	0.4055	-0.4360	-0.2077	-0.1403	0.3825	-0.0756	0.5690	0.0866	-0.0275	0.3166	0.1925	0.0070	0.1196	0.4140
2UXK - BPH L1287	0.6651	0.0593	0.3241	-0.3421	-0.1693	-0.1238	0.4047	-0.1122	0.5058	0.0823	0.0598	0.3589	0.2099	-0.0367	0.0041	0.2794
2UXL - BPH L1283	0.6053	0.0633	0.2613	-0.4149	-0.0610	-0.1043	0.3139	-0.1131	0.5534	0.1106	-0.0249	0.3024	0.2197	-0.2168	0.0744	0.3367

2UXM - BPH L1285	0.7443	0.0726	0.3517	-0.4676	-0.0529	-0.1366	0.4195	-0.1190	0.5163	0.0751	0.0644	0.3556	0.2482	-0.1181	0.0667	0.2365
2WX5 - BPH L1288	0.6179	0.0613	0.2321	-0.4500	-0.1528	-0.0322	0.2907	-0.1282	0.6917	0.0579	0.0312	0.4619	0.4238	-0.0239	0.0116	0.2895
3DSY - BPH L503	0.6154	0.0511	0.3574	-0.3543	-0.0654	-0.0710	0.3344	-0.0652	0.5802	0.0246	0.0495	0.5183	0.2344	0.0292	-0.0111	0.0983
3DTA - BPH L503	0.6161	0.0510	0.3581	-0.3546	-0.0653	-0.0710	0.3347	-0.0651	0.5803	0.0246	0.0496	0.5186	0.2343	0.0296	-0.0113	0.0976
3DTR - BPH L503	0.6155	0.0510	0.3576	-0.3546	-0.0649	-0.0715	0.3342	-0.0652	0.5803	0.0246	0.0493	0.5181	0.2348	0.0300	-0.0104	0.0982
3DTS - BPH M503	0.6155	0.0512	0.3574	-0.3545	-0.0651	-0.0717	0.3345	-0.0648	0.5802	0.0245	0.0494	0.5182	0.2346	0.0300	-0.0114	0.0983
3DU2 - BPH L503	0.6156	0.0511	0.3575	-0.3549	-0.0653	-0.0711	0.3342	-0.0645	0.5808	0.0245	0.0490	0.5187	0.2349	0.0295	-0.0112	0.0985
3DU3 - BPH L503	0.6152	0.0512	0.3574	-0.3542	-0.0652	-0.0717	0.3340	-0.0648	0.5800	0.0245	0.0496	0.5177	0.2349	0.0303	-0.0111	0.0986
3DUQ - BPH L503	0.6156	0.0512	0.3582	-0.3541	-0.0662	-0.0717	0.3341	-0.0647	0.5796	0.0245	0.0492	0.5175	0.2345	0.0301	-0.0116	0.0987
4RCR - BPH L284	0.9389	0.0734	-0.0490	0.0605	-0.3647	0.0652	0.8469	-0.1449	0.5748	0.0656	-0.3945	0.3542	0.1690	0.0892	-0.1107	0.0212

Table 64: Minimum basis normal-mode displacements and conformational parameters of all ΦB cofactors from crystal structures of *Rhodobacter sphaeroides*.

Cofactor ID	Dip	δip	B2g	B1g	Eu(x)	Eu(y)	A1g	A2g	Doop	δoop	B2u	B1u	A2u	Eg(x)	Eg(y)	A1u
1AIG - BPH L284	0.5380	0.0523	-0.0690	-0.4624	-0.1405	-0.0401	0.2173	-0.0478	0.3987	0.0140	0.1589	0.3008	0.1983	-0.0307	-0.0034	0.0542
1AIG - BPH O310	0.3845	0.0526	0.0921	-0.3202	0.0242	0.0314	0.1715	-0.0764	0.4820	0.0156	0.0902	0.4525	0.1283	-0.0056	0.0076	0.0539
1AIJ - BPH L284	0.3654	0.0556	-0.0596	-0.3055	0.0078	-0.0822	0.1637	-0.0546	0.3703	0.0080	0.0115	0.3204	0.1733	-0.0299	0.0220	0.0544
1AIJ - BPH S311	0.3484	0.0557	-0.1869	-0.2032	-0.0215	-0.0592	0.1907	-0.0692	0.3831	0.0142	0.0646	0.3739	0.0144	0.0201	-0.0101	0.0451
1DS8 - BPH M1005	0.5662	0.0607	0.1405	-0.4141	-0.0660	-0.0950	0.3375	-0.0467	0.4376	0.0181	0.1610	0.3532	0.1540	-0.0692	-0.0695	0.0863
1DS8 - BPH S2005	0.3448	0.0536	-0.1976	-0.1550	-0.0078	-0.0649	0.2160	-0.0699	0.5905	0.0151	0.0728	0.5285	0.2290	-0.0388	0.0389	0.0934
1DV3 - BPH M1005	0.5338	0.0576	-0.1520	-0.3620	-0.1279	-0.1148	0.3163	-0.0357	0.5405	0.0153	0.1275	0.4946	0.1332	-0.0641	-0.0106	0.0961
1DV3 - BPH S2005	0.3525	0.0532	0.0568	-0.2331	-0.0037	-0.0175	0.2453	-0.0785	0.5335	0.0133	0.0712	0.5057	0.1097	-0.0517	0.0564	0.0775
1DV6 - BPH M1005	0.5502	0.0610	-0.0732	-0.3222	-0.1091	-0.1082	0.4089	-0.0530	0.4441	0.0151	0.0698	0.3895	0.1479	-0.0721	0.0121	0.1160
1DV6 - BPH S2005	0.4118	0.0537	-0.1748	-0.2183	-0.0738	-0.0511	0.2764	-0.0828	0.5122	0.0131	0.1121	0.4637	0.1553	-0.0397	0.0705	0.0641
1E14 - BPH C402	0.7554	0.0500	0.3309	-0.5812	-0.0791	-0.0511	0.3370	-0.0310	0.4218	0.0309	0.0976	0.3438	0.1915	-0.0535	-0.0381	0.0960
1E6D - BPH C401	0.7378	0.0510	0.5331	-0.3359	-0.0493	-0.0820	0.3695	-0.0396	0.7428	0.0270	0.2104	0.6128	0.2559	-0.2022	0.1526	0.0481
1EYS - BPH M605	0.3516	0.0515	0.0469	-0.2230	-0.1139	-0.1044	0.1971	-0.0945	0.4154	0.0384	-0.0204	0.3501	0.1341	0.0124	0.0237	0.1759
1F6N - BPH M401	0.5088	0.0428	0.1135	-0.3729	-0.0406	-0.0673	0.3057	-0.0855	0.6229	0.0489	0.0073	0.5694	0.2204	-0.1218	-0.0063	-0.0170
1FNP - BPH M401	0.4813	0.0443	0.1241	-0.3327	-0.0546	-0.0564	0.3044	-0.0817	0.7131	0.0528	0.0756	0.5844	0.3844	-0.0964	0.0598	-0.0248
1FNQ - BPH M401	0.4984	0.0432	0.1652	-0.3484	-0.0441	-0.0641	0.2956	-0.0795	0.6441	0.0478	0.0545	0.5454	0.3105	-0.1222	0.0458	-0.0319
1JGW - BPH M854	0.6418	0.0656	0.1837	-0.4463	-0.0188	-0.1077	0.4082	-0.0190	0.1237	0.0035	0.0373	0.1125	0.0055	-0.0314	0.0086	0.0129
1JGX - BPH M854	0.6158	0.0662	0.1088	-0.4810	0.0219	-0.1222	0.3465	-0.0243	0.1151	0.0040	0.0211	0.1039	0.0206	-0.0278	0.0235	0.0155
1JGY - BPH M854	0.6821	0.0669	0.1668	-0.4921	-0.0757	-0.1242	0.4171	-0.0090	0.0684	0.0024	-0.0055	0.0629	0.0174	-0.0164	0.0050	0.0102
1JGZ - BPH M854	0.6298	0.0645	0.1679	-0.4568	-0.0825	-0.1518	0.3602	-0.0147	0.0986	0.0030	-0.0115	0.0821	0.0287	-0.0393	0.0194	0.0099
1JH0 - BPH M854	0.6097	0.0659	0.0563	-0.4757	-0.0750	-0.0845	0.3592	-0.0211	0.0905	0.0028	-0.0424	0.0781	-0.0015	-0.0126	0.0067	0.0097
1K6L - BPH M401	0.5899	0.0547	0.3118	-0.3677	-0.0499	-0.0493	0.3320	-0.0215	0.6392	0.0246	0.1635	0.5000	0.3283	-0.1282	0.0314	0.0819
1K6N - BPH M401	0.5898	0.0546	0.3121	-0.3676	-0.0506	-0.0493	0.3316	-0.0213	0.6398	0.0246	0.1633	0.5008	0.3278	-0.1290	0.0321	0.0824
1KBY - BPH L854	0.6727	0.0677	0.2925	-0.3994	-0.0173	-0.1416	0.4321	-0.0206	0.1293	0.0038	0.0520	0.1116	-0.0069	-0.0349	0.0130	0.0114
1L9B - BPH L1005	0.6858	0.0563	0.3573	-0.4019	-0.0081	-0.0577	0.4212	-0.0180	0.1712	0.0051	0.0677	0.1310	0.0700	-0.0471	0.0154	0.0148
1L9J - BPH L1005	0.5871	0.0552	0.2445	-0.3309	-0.0273	-0.0670	0.4120	-0.0205	0.0549	0.0032	-0.0489	-0.0006	0.0055	-0.0054	-0.0224	0.0080
1L9J - BPH R2005	0.6763	0.0559	0.3136	-0.3168	-0.0726	-0.0816	0.4962	-0.0226	0.0741	0.0019	-0.0659	0.0113	0.0282	-0.0116	0.0086	0.0043
1M3X - BPH M854	0.6359	0.0635	0.1857	-0.4455	-0.0104	-0.1001	0.4010	-0.0202	0.1328	0.0039	0.0279	0.1240	0.0012	-0.0344	0.0095	0.0148
1MPS - BPH L401	0.4692	0.0441	0.1733	-0.2707	-0.0852	-0.0460	0.3194	-0.0740	0.6327	0.0433	0.1006	0.4698	0.3158	-0.2157	0.1501	0.0267

1OGV - BPH M1304	0.5610	0.0549	0.2360	-0.3112	-0.0353	-0.0803	0.3921	-0.0271	0.2003	0.0049	0.0615	0.1637	0.0929	-0.0232	0.0163	0.0107
1PCR - BPH M401	0.5480	0.0406	0.1459	-0.4165	-0.0902	-0.0310	0.3003	-0.0792	0.7094	0.0548	-0.0333	0.6579	0.2569	-0.0362	0.0435	-0.0068
1PSS - BPH M5	0.2978	0.0516	-0.0611	-0.2364	-0.0865	-0.0293	0.1371	-0.0438	0.3235	0.0188	0.1485	0.1907	0.2075	0.0156	0.0374	0.0389
1PST - BPH M5	0.3609	0.0540	-0.1806	-0.2330	-0.0404	-0.0452	0.1936	-0.0469	0.3661	0.0106	0.0840	0.2952	0.1954	0.0085	0.0386	0.0096
1PYH - BPH A401	0.4374	0.0630	0.2296	-0.3381	-0.0808	-0.0476	0.1020	-0.0717	0.5845	0.0245	0.0586	0.4901	0.2727	-0.1107	-0.0106	0.1061
1QOV - BPH M1401	0.5905	0.0547	0.3117	-0.3686	-0.0500	-0.0499	0.3319	-0.0215	0.6391	0.0246	0.1633	0.5009	0.3275	-0.1268	0.0304	0.0817
1RG5 - BPH M401	0.6769	0.0560	0.1942	-0.4047	-0.0686	-0.1334	0.4781	-0.0755	0.5593	0.0238	0.0631	0.4887	0.2223	-0.0855	0.0806	0.0821
1RGN - BPH M401	0.6039	0.0549	0.1982	-0.3315	0.0176	-0.2374	0.3850	-0.1030	0.4174	0.0165	0.0870	0.3445	0.0488	-0.1852	0.0854	0.0628
1RQK - BPH M401	0.7398	0.0510	0.2881	-0.6020	-0.0065	-0.0515	0.2918	-0.1183	0.4906	0.0243	0.0902	0.3451	0.1848	-0.0519	0.2697	0.0621
1RVJ - BPH M855	0.6429	0.0551	0.2554	-0.3753	-0.0555	-0.0749	0.4447	-0.0285	0.1366	0.0045	-0.0397	0.1103	0.0580	-0.0267	-0.0086	0.0276
1RY5 - BPH M855	0.6268	0.0553	0.2779	-0.3632	-0.0438	-0.0590	0.4215	-0.0254	0.1566	0.0035	0.0011	0.1410	0.0579	-0.0330	-0.0046	0.0137
1RZH - BPH M855	0.6467	0.0547	0.3163	-0.3685	-0.0429	-0.0722	0.4182	-0.0230	0.1766	0.0041	0.0095	0.1558	0.0767	-0.0268	0.0021	0.0138
1RZZ - BPH M1005	0.5974	0.0558	0.3017	-0.3119	-0.0716	-0.0562	0.3996	-0.0242	0.1997	0.0041	0.0066	0.1795	0.0832	-0.0184	-0.0017	0.0190
1RZZ - BPH S2005	0.5905	0.0550	0.2730	-0.2787	-0.0466	-0.0653	0.4355	-0.0199	0.1439	0.0030	0.0288	0.1307	0.0472	-0.0175	-0.0082	0.0139
1S00 - BPH M1005	0.6231	0.0530	0.2716	-0.4044	-0.0941	-0.0893	0.3651	-0.0287	0.1747	0.0054	-0.0108	0.1480	0.0882	-0.0077	-0.0146	0.0208
1S00 - BPH S2005	0.5427	0.0588	0.2571	-0.2400	-0.0392	-0.0792	0.4033	-0.0183	0.1764	0.0048	0.0439	0.1593	0.0544	0.0066	0.0228	0.0172
1YF6 - BPH L855	0.6177	0.0652	0.0838	-0.4400	-0.0286	-0.1324	0.3958	-0.0768	0.5734	0.0481	0.2192	0.4566	0.1830	-0.0514	-0.1535	0.1121
1YST - BPH M309	1.0367	0.0729	-0.3481	-0.7806	-0.1850	0.1378	0.5319	-0.0897	0.6158	0.0192	-0.5323	-0.2589	0.1182	-0.0875	-0.0659	-0.0538
1Z9J - BPH B854	0.4576	0.0620	0.0623	-0.4127	-0.1548	-0.0249	0.0998	-0.0261	0.1124	0.0038	-0.0918	-0.0522	0.0373	0.0087	-0.0034	0.0028
1Z9K - BPH B854	0.6892	0.0605	0.0158	-0.5247	-0.1450	-0.0481	0.4192	-0.0186	0.2603	0.0048	-0.2525	0.0398	0.0415	0.0243	0.0003	0.0092
2BNP - BH1 B1304	0.7644	0.0621	0.3442	-0.6447	-0.1053	-0.0007	0.1599	-0.1166	0.4476	0.0481	0.1255	0.3483	0.1023	-0.0372	0.1006	0.2032
2BNS - BH1 B1304	0.7404	0.0707	0.2899	-0.6232	-0.1415	-0.0034	0.2079	-0.1117	0.4674	0.0346	0.0597	0.4054	0.1011	-0.0770	0.0538	0.1775
2BOZ - BH1 M1311	0.6823	0.0607	0.2843	-0.3719	-0.0186	-0.1212	0.4737	-0.0836	0.4234	0.0233	0.1558	0.2618	0.2660	-0.0777	-0.0403	0.0895
2GMR - BPH M310	0.5600	0.0464	0.2166	-0.2801	-0.0664	-0.0647	0.4180	-0.0709	0.5242	0.0365	0.1107	0.4456	0.1985	-0.0726	0.0232	0.1372
2GNU - BPH M1304	0.8351	0.0656	0.4146	-0.6099	-0.0330	-0.0531	0.3663	-0.1245	0.5375	0.0372	0.1976	0.3524	0.2408	-0.1601	-0.0172	0.2045
2HG3 - BPH M401	0.6027	0.0515	0.2929	-0.3664	0.0443	-0.1195	0.3383	-0.1122	0.4938	0.0313	0.1189	0.3870	0.2486	-0.0764	0.0098	0.1107
2HG9 - BPH M401	0.6426	0.0562	0.3175	-0.3509	-0.0382	-0.1122	0.4107	-0.0796	0.5306	0.0236	0.0699	0.4711	0.1613	-0.1209	-0.0430	0.1110
2HH1 - BPH M401	0.5507	0.0606	0.1233	-0.3560	0.0226	-0.1568	0.3533	-0.1069	0.5292	0.0209	-0.0164	0.4799	0.1518	-0.1277	0.0459	0.0900
2HHK - BPH M401	0.5356	0.0599	0.1565	-0.3571	-0.0382	-0.1389	0.3258	-0.0889	0.5178	0.0253	0.1094	0.3989	0.2169	-0.1700	-0.0871	0.1162
2HIT - BPH M401	0.6694	0.0621	0.1728	-0.4422	0.0624	-0.1696	0.4260	-0.0928	0.5368	0.0297	0.2362	0.3678	0.2358	-0.1733	0.0310	0.1023
2HJ6 - BPH M401	0.6634	0.0563	0.1344	-0.4063	-0.0837	-0.1381	0.4664	-0.1153	0.5028	0.0228	0.0937	0.4203	0.1697	-0.1745	0.0281	0.0857
2J8C - BPH M1308	0.6741	0.0483	0.3748	-0.3684	-0.1265	-0.1359	0.3649	-0.1027	0.5884	0.0494	0.2864	0.4266	0.1981	-0.1021	-0.1219	0.1328
2J8D - BPH M1317	0.6850	0.0578	0.2968	-0.4257	-0.0793	-0.1188	0.4088	-0.1112	0.5887	0.0749	0.1765	0.3192	0.3995	-0.1697	-0.0568	0.1478
2JJ0 - BPH M1307	0.7963	0.0523	0.2597	-0.5674	-0.0506	-0.1426	0.4551	-0.1210	0.4368	0.0171	0.0295	0.3882	0.1404	-0.0617	0.1082	0.0631
2RCR - BPH M500	0.3875	0.0566	0.2104	-0.1877	-0.1366	-0.1169	0.1746	-0.0887	0.5525	0.0345	0.0376	0.4619	0.1950	-0.1742	-0.1345	-0.0637
2UWS - BPH M1312	0.8828	0.0948	0.4818	-0.6116	-0.0038	-0.1703	0.3730	-0.0701	0.8523	0.1341	0.1989	0.3648	0.7035	0.1201	-0.2097	-0.0203
2UWT - BPH M1312	0.7803	0.0705	0.3520	-0.5302	-0.0398	-0.1740	0.4092	-0.0677	0.7932	0.0802	0.2844	0.5639	0.4109	-0.2402	-0.0605	-0.0055
2UWU - BPH M1312	0.6877	0.0691	0.3003	-0.3696	-0.0450	-0.1059	0.4745	-0.0879	0.4985	0.0823	0.2193	0.1710	0.3037	-0.2473	-0.0484	0.1245
2UWV - BPH M1313	0.7058	0.0700	0.3384	-0.3965	-0.0786	-0.0206	0.4649	-0.0607	0.6215	0.0890	0.3518	0.3553	0.3323	-0.0530	-0.1511	0.0107
2UWW - BPH M1311	0.6725	0.0642	0.3353	-0.3396	-0.0520	-0.1169	0.4516	-0.0653	0.5931	0.0709	0.3621	0.3376	0.2623	-0.1603	-0.0977	0.0509
2UX3 - BPH M1313	0.7602	0.0732	0.4233	-0.4036	-0.0809	-0.1413	0.4473	-0.0956	0.7002	0.0882	0.3255	0.4178	0.4157	-0.1169	0.0249	0.1506
2UX4 - BPH M1311	0.6750	0.0694	0.3271	-0.4305	-0.0707	-0.1210	0.3687	-0.0879	0.8679	0.0936	0.4667	0.6598	0.2380	-0.1131	-0.1621	-0.0662
2UX5 - BPH M1314	0.7420	0.0606	0.4360	-0.4039	-0.0411	-0.1958	0.3889	-0.0781	0.6472	0.1107	0.1656	0.3610	0.2945	-0.3535	0.1368	0.1753
2UXJ - BPH M1313	0.7224	0.0672	0.2062	-0.5610	-0.0833	-0.1338	0.3709	-0.0460	0.7572	0.0802	0.3951	0.5798	0.1771	-0.1182	-0.1876	0.0227

2UXK - BPH M1311	0.6889	0.0748	0.2960	-0.4656	-0.0381	-0.1645	0.3651	-0.0921	0.5881	0.0972	0.1590	0.4292	0.1877	-0.2840	0.0681	0.1258
2UXL - BPH M1309	0.7144	0.0705	0.2812	-0.5855	0.0573	-0.1289	0.2307	-0.1237	0.8223	0.1224	0.4098	0.3948	0.3840	-0.3106	0.2822	0.1698
2UXM - BPH M1314	0.6799	0.0523	0.3198	-0.4548	-0.1638	-0.0883	0.3172	-0.1338	0.7677	0.0970	0.1840	0.4324	0.4370	0.0210	0.1088	0.4065
2WX5 - BPH M1314	0.6462	0.0644	0.2893	-0.4324	-0.1077	-0.1166	0.3388	-0.0830	0.5292	0.0504	0.2450	0.3265	0.1543	-0.1324	0.1600	0.2156
3DSY - BPH M503	0.5895	0.0546	0.3120	-0.3672	-0.0493	-0.0484	0.3319	-0.0214	0.6393	0.0245	0.1634	0.5001	0.3282	-0.1283	0.0312	0.0822
3DTA - BPH M503	0.5901	0.0547	0.3118	-0.3678	-0.0498	-0.0494	0.3320	-0.0222	0.6390	0.0246	0.1638	0.4999	0.3276	-0.1282	0.0312	0.0821
3DTR - BPH M503	0.5896	0.0547	0.3114	-0.3675	-0.0497	-0.0497	0.3321	-0.0215	0.6393	0.0246	0.1635	0.5002	0.3282	-0.1282	0.0318	0.0817
3DTS - BPH M504	0.5895	0.0546	0.3121	-0.3672	-0.0505	-0.0492	0.3313	-0.0219	0.6403	0.0247	0.1631	0.5010	0.3283	-0.1295	0.0329	0.0821
3DU2 - BPH M503	0.5896	0.0548	0.3119	-0.3673	-0.0493	-0.0493	0.3319	-0.0214	0.6393	0.0246	0.1636	0.5000	0.3281	-0.1287	0.0312	0.0818
3DU3 - BPH M503	0.5894	0.0546	0.3113	-0.3675	-0.0499	-0.0498	0.3318	-0.0213	0.6398	0.0247	0.1626	0.5008	0.3282	-0.1288	0.0316	0.0828
3DUQ - BPH M503	0.5897	0.0546	0.3111	-0.3678	-0.0507	-0.0497	0.3320	-0.0216	0.6393	0.0245	0.1631	0.5007	0.3269	-0.1294	0.0325	0.0824
4RCR - BPH M312	0.3044	0.0326	-0.0329	-0.0824	0.0171	0.0362	0.2875	-0.0222	0.7746	0.0616	-0.0862	0.0243	0.5681	0.2713	0.3825	0.2221

8.4 *Blastochloris viridis* bacteriopheophytin cofactor NSDs

Table 65: Minimum basis normal-mode displacements and conformational parameters of all ΦA cofactors from crystal structures of *Blastochloris viridis*.

Cofactor ID	Dip	δip	B2g	B1g	Eu(x)	Eu(y)	A1g	A2g	Doop	δoop	B2u	B1u	A2u	Eg(x)	Eg(y)	A1u
1DXR - BPB L402	0.5550	0.0484	0.4054	-0.1767	-0.0925	-0.0193	0.3123	-0.0775	0.4422	0.0324	-0.1704	0.3278	0.0499	-0.2040	-0.0604	0.1063
1PRC - BPB L606	0.5477	0.0398	0.3293	-0.3321	-0.0897	-0.0962	0.2221	-0.1211	0.6134	0.0363	-0.4735	0.2565	0.0699	-0.2708	0.0634	0.0628
1R2C - BPB L402	0.5673	0.0451	0.3127	-0.3702	-0.1043	-0.0157	0.2663	-0.0709	0.4630	0.0311	-0.0851	0.3559	0.2099	-0.0509	-0.1738	0.0602
1VRN - BPB L406	0.5088	0.0427	0.3084	-0.2362	-0.1420	-0.0686	0.2820	-0.0607	0.4535	0.0276	-0.1886	0.3909	0.0413	-0.0890	-0.0591	0.0646
2I5N - BPB M402	0.7830	0.0708	0.4503	-0.5009	-0.1308	-0.0857	0.3359	-0.1489	0.5253	0.0374	-0.1233	0.4507	0.0667	-0.1348	0.0415	0.1822
2JBL - BPB L1276	0.4210	0.0466	0.2381	-0.1313	-0.1354	-0.0328	0.2815	-0.0679	0.5000	0.0241	-0.2878	0.3875	-0.0277	-0.1074	-0.0111	0.0678
2PRC - BPB L402	0.5959	0.0504	0.4636	-0.0654	-0.1369	-0.0128	0.3349	-0.0698	0.6355	0.0219	-0.3995	0.4354	0.0416	-0.2018	0.0091	0.1102
2WJM - BPB L1276	0.5713	0.0535	0.3012	-0.2175	-0.0120	-0.0411	0.4292	-0.0479	0.5252	0.0408	-0.0998	0.4297	0.1240	-0.1812	0.0332	0.1786
2WJN - BPB L1276	0.6247	0.0578	0.4269	-0.2220	-0.0914	-0.0224	0.3799	-0.0745	0.4559	0.0372	-0.1495	0.3497	0.0463	-0.1659	-0.0656	0.1709
3D38 - BPB L402	0.7689	0.0805	0.3978	-0.4974	-0.1474	-0.0600	0.3669	-0.1599	0.6324	0.0513	-0.2593	0.3295	-0.2208	-0.1107	-0.3965	0.0774
3G7F - BPB L402	0.6681	0.0801	0.3681	-0.3787	-0.1850	-0.0365	0.3274	-0.1573	0.4786	0.0414	-0.2322	0.3386	-0.0838	-0.1502	-0.1619	0.0680
3PRC - BPB L402	0.5293	0.0478	0.4453	-0.0269	-0.1148	-0.0157	0.2440	-0.0903	0.5328	0.0229	-0.2932	0.3869	0.0023	-0.1876	-0.0474	0.1037
5PRC - BPB L402	0.5065	0.0465	0.2843	-0.0699	-0.1593	0.0310	0.3712	-0.0820	0.5783	0.0204	-0.2605	0.4453	0.0072	-0.2433	-0.0218	0.0925
6PRC - BPB L402	0.6010	0.0419	0.3809	-0.2359	-0.1272	-0.0174	0.3702	-0.0832	0.5212	0.0275	-0.2677	0.3580	0.0092	-0.2462	-0.0404	0.0971
7PRC - BPB L402	0.3762	0.0500	0.1562	-0.1645	-0.1356	-0.0428	0.2467	-0.0948	0.6058	0.0321	-0.3472	0.3809	0.1019	-0.2804	0.0159	0.1099

Table 66: Minimum basis normal-mode displacements and conformational parameters of all ΦB cofactors from crystal structures of *Blastochloris viridis*.

Cofactor ID	Dip	δip	B2g	B1g	Eu(x)	Eu(y)	A1g	A2g	Doop	δoop	B2u	B1u	A2u	Eg(x)	Eg(y)	A1u
1DXR - BPB M402	0.5230	0.0433	0.1625	-0.3755	-0.0506	-0.0309	0.3116	-0.0740	0.5691	0.0282	-0.0636	0.5018	0.0706	-0.1905	0.0906	0.1358
1PRC - BPB M605	0.5920	0.0591	0.1832	-0.4341	-0.1320	0.0075	0.3225	-0.0840	0.4007	0.0457	-0.0268	0.3331	-0.0328	-0.0832	-0.0965	0.1777
1R2C - BPB M401	0.5710	0.0434	0.3132	-0.3227	-0.1425	-0.0108	0.3118	-0.0780	0.4208	0.0214	0.0370	0.3787	0.1340	-0.0425	-0.0748	0.0833
1VRN - BPB M405	0.5236	0.0419	0.3217	-0.2688	-0.1032	-0.0602	0.2810	-0.0718	0.5748	0.0292	-0.1484	0.5057	-0.0066	-0.1572	0.0928	0.1390
2I5N - BPB L402	0.6445	0.0764	0.3891	-0.3713	-0.1318	-0.0690	0.2874	-0.1463	0.5267	0.0442	-0.2353	0.3229	-0.0958	-0.2113	-0.2395	0.0815
2JBL - BPB M1325	0.5059	0.0412	0.2175	-0.3309	-0.1331	-0.0240	0.2730	-0.0795	0.5901	0.0266	-0.2301	0.5097	-0.0416	-0.1432	0.0374	0.1091

2PRC - BPB M401	0.5870	0.0467	0.1639	-0.4421	-0.0553	-0.0082	0.3389	-0.0651	0.6715	0.0451	-0.2385	0.5705	0.1238	-0.1405	0.0218	0.1815
2WJM - BPB M1326	0.5635	0.0553	0.2498	-0.3249	0.0175	-0.0130	0.3813	-0.0607	0.6802	0.0519	-0.0695	0.5782	0.1291	-0.0954	0.1537	0.2722
2WJN - BPB M1326	0.5586	0.0498	0.1543	-0.3530	-0.0307	-0.0187	0.3967	-0.0704	0.6782	0.0477	-0.0157	0.5824	0.0822	-0.1556	0.0741	0.2898
3D38 - BPB M402	0.8113	0.0821	0.3403	-0.6448	-0.1734	-0.0398	0.2638	-0.1595	0.8335	0.0590	0.1359	0.6534	0.2675	-0.2715	0.2305	0.2257
3G7F - BPB M402	0.8951	0.0654	0.3056	-0.7375	-0.1970	0.0172	0.3137	-0.1625	0.4615	0.0560	-0.1640	0.2980	0.1402	-0.1804	0.0204	0.2113
3PRC - BPB M401	0.5865	0.0421	0.1601	-0.4654	-0.0634	-0.0652	0.2975	-0.0708	0.6674	0.0332	-0.0180	0.6014	0.1107	-0.2076	0.0206	0.1663
5PRC - BPB M401	0.5389	0.0478	0.0619	-0.4355	-0.0837	-0.0380	0.2888	-0.0710	0.6495	0.0405	-0.3557	0.4869	-0.0217	-0.1976	-0.0672	0.1191
6PRC - BPB M401	0.5384	0.0433	0.1503	-0.3857	-0.1078	-0.0321	0.3169	-0.0734	0.7074	0.0393	-0.2705	0.6055	0.0200	-0.1761	-0.0783	0.1519
7PRC - BPB L401	0.6320	0.0404	0.1898	-0.5306	-0.1128	0.0184	0.2443	-0.0959	0.7928	0.0378	-0.1440	0.7150	0.0217	-0.2679	-0.1161	0.1036