ATOMIC COORDINATES FOR THE CHLOROPHYLL CORE OF A BACTERIOCHLOROPHYLL a-PROTEIN FROM GREEN PHOTOSYNTHETIC BACTERIA

R. E. Fenna,* L. F. Ten Eyck, and B. W. Matthews

Institute of Molecular Biology and Department of Physics
University of Oregon, Eugene, Oregon 97403, U.S.A.

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Summary: Preliminary atomic coordinates are presented for the seven bacteriochlorophylls constituting the core of one subunit of the trimeric water soluble bacteriochlorophyll a-protein from the green photosynthetic bacterium Prosthecochloris aestuarii, strain 2K, formerly identified as Chlorobium limicola, strain 2K. The coordinates were derived from a 2.8 Å resolution electron density map based on four isomorphous heavy-atom derivatives, and adjusted to have stereochemically acceptable bond lengths and angles.

The three-dimensional structure of a bacteriochlorophyll a-containing protein from a green photosynthetic bacterium has been determined by X-ray crystallography (1). [The bacterium, previously designated Chlorobium limicola, strain 2K, has now been identified as Prosthecochloris aestuarii (Ref. 2 and personal communication from J. M. Olson and N. Pfennig).] The chlorophyll-protein, which mediates in the transfer of excitation energy from the bulk antenna pigment chlorobium chlorophyll to the photochemical reaction centers (3), consists of three identical subunits, each consisting of a core of seven bacteriochlorophylls enclosed within an envelope of protein (Fig. 1).

Recently the quality of the electron density map used for the initial structure determination has been improved by the inclusion of a fourth isomorphous heavy-atom derivative, permitting the structure to be defined with greater certainty (4). In the absence of the amino acid sequence, it is not possible at this time to present coordinates for the whole molecule. However, the electron density map does show the general arrangement of the chlorophyll core quite clearly, and permits us to present preliminary coordinates for this part of the molecule.

*Present address: Molecular Biology Institute, University of California at Los Angeles, Los Angeles, California 90024.

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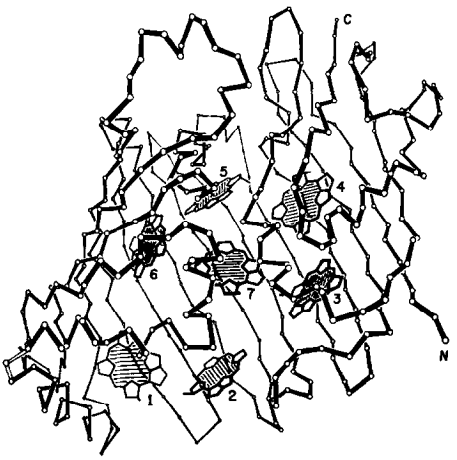

Figure 1. Schematic diagram showing one subunit of the bacteriochlorophyll-protein. For clarity, the magnesium atoms, chlorophyll ring substituents and phytyl chains, except for the first bond, have been omitted. The direction of view is from the three-fold axis, which is horizontal, towards the exterior of the molecule.

The coordinates were obtained by building a skeletal model of the core in a Richards optical comparator (5,6). Because the resolution of the electron density map (2.8 Å) does not permit visualization of individual atoms, the geometry of the model was based, as far as possible, on that of ethyl chlorophyllide a (7). The rigid conjugated portion of each porphyrin ring was first aligned to coincide with the electron density map, and then rotations were made about the various single bonds in order to place the ring substituents and the phytyl chains. Buckling was allowed in Ring II which is saturated in bacteriochlorophyll a (Fig. 2) but not in ethyl chlorophyllide a. Markers were then placed in the electron density map to agree, as well as possible, with both the model and the electron density.

The "raw" coordinates, so obtained, were then checked and idealized by first rotating and translating that part of ethyl chlorophyllide a common to bacteriochlorophyll a so as to minimize the rms deviation between the corresponding atoms, i.e., C1-C6, C9-C22, C27-C30, C32, C33, N1-N4, and O1. (Rms deviations ranged from 0.14 Å to 0.17 Å for the seven chlorophylls.)

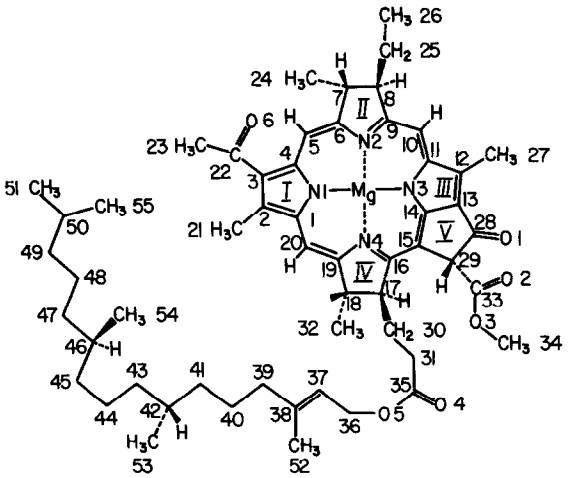

Figure 2. The structure of bacteriochlorophyll a showing the atom numbering used in Table I.

The coordinates of all the remaining atoms were then adjusted by a least squares procedure which enforces bond length and angle constraints, and at the same time requires the idealized model to fit as closely as desired to the raw coordinates (8,9). In this application the bond length and angle constraints were weighted ten times as heavily as adherence to the raw coordinates, except for the conjugated portion of the chlorin ring where weights of a thousand were used to force the atoms to coincide with the rotated ethyl chlorophyllide coordinates described above. The "standard" dimensions of the substituent bond lengths and angles were taken from the Handbook of Chemistry and Physics (10). Each magnesium atom was located equidistant from its four nitrogen ligands, and displaced 0.4 Å from the ring plane toward the apparent fifth ligand.

The idealized coordinates for the seven bacteriochlorophylls are given in Table I, where the numbering scheme, shown in Figure 2, is based on that used for ethyl chlorophyllide a (7). The coordinates are in Angstroms along the orthogonal crystallographic axes a*, b, and c.

Crystals of the chlorophyll protein have space group $P6_3$ with cell

Table I

BCHL	1	MG	75.7	24.6	20.8
	1	N1	75.9	24.7	18.7
	1	N2	73.6	24.4	20.5
	1	N3	75.5	23.7	22.5
	1	N4	77.6	24.3	23.8
	1	O1	77.4	22.4	26.6
	1	O2	79.6	24.9	25.1
	1	O3	80.7	22.9	25.4
	1	O4	78.7	20.1	22.5
	1	O5	78.1	20.4	20.3
	1	O6	73.6	26.0	15.3
	1	C1	77.1	24.7	18.0
	1	C2	76.7	25.0	16.6
	1	C3	75.4	25.1	16.4
	1	C4	74.8	24.9	17.8
	1	C5	73.5	24.9	18.1
	1	C6	72.9	24.7	19.4
	1	C7	71.4	24.6	19.5
	1	C8	71.2	24.3	21.1
	1	C9	72.7	24.1	21.5
	1	C10	73.0	23.8	22.8
	1	C11	74.3	23.6	23.4
	1	C12	74.7	23.2	24.7
	1	C13	76.1	23.1	24.6
	1	C14	76.5	23.4	23.3
	1	C15	77.9	23.4	23.1
	1	C16	78.5	23.7	21.9
	1	C17	80.0	23.6	21.7
	1	C18	80.1	24.3	20.3
	1	C19	78.7	24.3	19.8
	1	C20	78.3	24.6	18.5
	1	C21	77.8	25.1	15.5
	1	C22	76.6	25.3	15.2
	1	C23	75.6	25.3	14.0
	1	C24	70.8	26.3	19.2
	1	C25	70.5	22.9	21.1
	1	C26	70.1	22.5	19.7
	1	C27	73.8	23.0	25.8
	1	C28	77.3	22.7	25.4
	1	C29	78.5	22.9	24.5
	1	C30	80.6	22.2	21.7
	1	C31	80.3	21.3	20.9
	1	C32	80.7	25.7	20.3
	1	C33	79.5	23.7	25.3
	1	C34	81.7	23.7	25.9
	1	C35	78.9	20.5	21.3
	1	C36	76.7	23.5	23.6
	1	C37	75.9	20.6	19.2
	1	C38	74.6	20.7	19.2
	1	C39	73.9	21.2	17.9
	1	C40	74.8	21.1	16.7
	1	C41	74.0	21.4	15.4
	1	C42	74.9	21.2	14.2
	1	C43	73.9	20.9	13.0
	1	C44	73.2	19.6	13.4
	1	C45	71.6	19.7	13.2
	1	C46	71.0	18.3	13.3
	1	C47	71.3	17.7	14.7
	1	C48	70.6	18.4	15.8
	1	C49	70.8	17.5	17.1
	1	C50	70.8	18.4	18.4
	1	C51	72.8	17.9	19.3
	1	C52	73.7	20.7	23.4
	1	C53	75.7	22.5	14.0
	1	C54	69.4	18.5	13.2
	1	C55	69.5	18.2	19.1
BCHL	2	MG	76.7	19.6	32.4
	2	N1	75.5	21.3	31.7
	2	N2	75.3	19.5	34.0
	2	N3	77.2	17.8	32.8
	2	N4	77.5	19.5	30.4
	2	O1	80.0	14.3	31.8
	2	O2	81.9	16.7	31.0
	2	O3	81.3	16.5	28.8
	2	O4	79.4	16.6	25.3
	2	O5	77.4	17.3	24.4
	2	O6	73.2	24.5	33.1
	2	C1	75.7	22.0	30.5
	2	C2	74.8	23.1	30.5
	2	C3	74.1	23.1	31.6
	2	C4	74.5	22.0	32.4
	2	C5	74.0	21.5	33.6
	2	C6	74.4	20.4	34.4
	2	C7	73.7	20.2	35.8
	2	C8	74.4	18.8	36.1
	2	C9	75.3	18.5	35.0
	2	C10	76.2	17.4	34.9
	2	C11	77.1	17.0	33.9
	2	C12	77.9	15.9	33.8
	2	C13	78.5	16.0	32.6
	2	C14	78.1	17.2	32.0
	2	C15	78.7	17.5	30.8
	2	C16	78.4	18.6	30.0
	2	C17	79.0	18.9	28.6
	2	C18	78.6	20.4	28.4
	2	C19	77.5	20.5	29.5
	2	C20	76.6	21.6	29.5
	2	C21	74.7	24.1	29.3
	2	C22	73.0	24.1	32.0
	2	C23	72.0	24.7	31.0
	2	C24	74.3	21.2	36.7
	2	C25	73.3	17.7	36.2
	2	C26	71.9	18.3	36.2
	2	C27	78.0	14.8	34.9
	2	C28	79.4	15.3	31.7
	2	C29	79.6	16.3	30.5
	2	C30	78.6	18.0	27.5
	2	C31	78.5	18.8	26.1
	2	C32	79.7	21.4	28.6
	2	C33	81.0	16.3	30.2
	2	C34	82.5	15.8	28.5
	2	C35	78.4	17.3	25.2
	2	C36	76.1	17.1	24.8
	2	C37	75.2	18.3	24.4
	2	C38	73.9	18.4	24.6
	2	C39	73.1	19.6	24.1
	2	C40	71.7	19.6	24.7
	2	C41	71.6	19.7	23.6
	2	C42	69.2	19.3	24.1
	2	C43	68.3	20.5	24.1
	2	C44	69.3	21.9	24.4
	2	C45	67.9	23.0	24.6
	2	C46	68.3	24.2	23.8
	2	C47	67.4	25.4	24.2
	2	C48	67.1	26.3	22.9
	2	C49	66.1	25.5	22.1
	2	C50	66.0	26.0	20.6
	2	C51	64.7	25.5	20.0
	2	C52	73.0	17.2	24.9
	2	C53	69.4	18.8	25.6
	2	C54	69.8	24.6	24.0
	2	C55	67.2	25.7	19.8
BCHL	3	MG	65.6	14.0	44.9
	3	N1	64.3	15.3	45.8
	3	N2	65.6	12.8	46.6
	3	N3	67.4	13.1	44.5
	3	N4	66.2	15.6	43.5
	3	O1	70.8	12.4	41.3
	3	O2	70.5	15.9	42.1
	3	O3	71.0	15.5	40.1
	3	O4	64.5	17.7	38.0
	3	O5	66.5	17.6	37.0
	3	O6	60.5	16.8	47.8
	3	C1	63.8	16.4	45.2
	3	C2	62.6	16.8	45.9
	3	C3	62.4	15.9	46.9
	3	C4	63.5	14.9	46.8
	3	C5	63.6	13.8	47.6
	3	C6	64.6	12.8	47.5
	3	C7	64.7	11.5	48.4
	3	C8	66.0	10.8	48.0
	3	C9	66.4	11.6	46.8
	3	C10	67.5	11.2	46.1
	3	C11	68.0	11.9	44.9
	3	C12	69.1	11.5	44.1
	3	C13	69.1	12.5	43.1
	3	C14	68.1	13.5	43.4
	3	C15	68.0	14.5	42.5
	3	C16	67.2	15.6	42.5
	3	C17	67.1	16.8	41.6
	3	C18	66.0	17.7	42.3
	3	C19	65.5	16.8	43.4
	3	C20	64.3	17.1	44.1
	3	C21	61.8	18.0	45.6
	3	C22	61.3	15.9	47.9
	3	C23	61.5	15.2	49.2
	3	C24	64.9	11.8	49.9
	3	C25	65.6	9.3	47.7
	3	C26	66.7	8.3	48.1
	3	C27	69.9	10.3	44.3
	3	C28	69.6	12.9	41.9
	3	C29	69.2	19.3	41.5
	3	C30	66.6	16.4	40.2
	3	C31	66.4	17.7	39.4
	3	C32	66.7	18.9	43.0
	3	C33	70.3	15.7	41.2
	3	C34	70.0	16.2	39.3
	3	C35	65.7	17.5	38.0
	3	C36	65.9	17.8	35.7
	3	C37	67.0	17.5	34.6
	3	C38	66.8	17.0	33.4
	3	C39	68.0	16.6	32.6
	3	C40	67.8	16.9	31.1
	3	C41	69.0	16.6	30.2
	3	C42	68.6	15.6	29.0
	3	C43	68.1	16.4	27.8
	3	C44	66.6	16.9	28.1
	3	C45	66.0	17.3	26.8
	3	C46	64.8	18.3	26.9
	3	C47	64.3	18.8	25.5
	3	C48	64.0	20.1	25.3
	3	C49	63.0	20.8	26.4
	3	C50	62.4	21.9	25.9
	3	C51	60.8	21.7	25.8
	3	C52	65.5	17.0	32.6
	3	C53	69.8	14.8	28.6
	3	C54	63.7	17.7	27.8
	3	C55	62.9	22.3	24.6
BCHL	4	MG	54.8	16.8	42.8
	4	N1	55.4	17.7	41.1
	4	N2	56.8	18.1	43.1
	4	N3	54.7	16.5	44.8
	4	N4	53.1	18.1	42.9
	4	O1	52.0	16.7	48.6
	4	O2	53.0	16.0	46.1
	4	O3	49.3	18.2	46.4
	4	O4	52.8	20.3	46.3
	4	O5	54.3	21.7	44.7
	4	O6	58.4	17.4	37.8
	4	C1	54.5	18.9	40.3
	4	C2	55.2	18.7	39.8
	4	C3	56.4	18.1	39.0
	4	C4	56.5	17.4	40.3
	4	C5	57.6	16.7	40.8
	4	C6	57.7	16.1	42.1
	4	C7	58.9	15.1	42.3
	4	C8	58.6	14.6	43.8
	4	C9	57.3	15.4	44.2
	4	C10	56.7	15.3	45.4
	4	C11	55.4	15.8	45.8
	4	C12	54.8	15.7	47.0
	4	C13	53.6	16.4	46.8
	4	C14	53.6	16.9	45.5
	4	C15	52.4	17.7	45.2
	4	C16	52.2	18.2	43.9
	4	C17	51.0	19.0	43.5
	4	C18	51.2	19.2	42.0
	4	C19	52.6	18.7	41.8
	4	C20	53.3	18.9	40.6
	4	C21	54.7	19.5	37.9
	4	C22	57.4	18.1	38.0
	4	C23	57.5	19.5	37.2
	4	C24	58.8	13.7	41.5
	4	C25	59.8	15.0	44.5
	4	C26	60.9	14.1	44.1
	4	C27	55.3	15.0	48.2
	4	C28	52.4	16.9	47.5
	4	C29	51.6	17.7	46.4
	4	C30	50.9	20.4	44.2
	4	C31	51.8	21.4	44.5
	4	C32	50.2	18.3	41.2
	4	C33	50.2	17.2	46.6
	4	C34	47.9	17.8	46.4
	4	C35	53.1	20.9	45.3
	4	C36	55.3	20.9	45.5
	4	C37	56.7	21.0	44.9
	4	C38	57.6	20.0	44.7
	4	C39	58.8	20.3	43.9
	4	C40	60.0	19.3	43.5
	4	C41	61.1	19.8	42.5
	4	C42	61.2	19.0	41.5
	4	C43	62.0	19.7	40.6
	4	C44	63.3	20.4	40.8
	4	C45	63.4	21.8	40.3
	4	C46	64.8	22.1	39.6
	4	C47	65.0	22.1	38.1
	4	C48	66.4	21.7	37.9
	4	C49	66.6	21.4	36.3
	4	C50	68.0	21.6	35.7
	4	C51	67.8	21.7	34.2
	4	C52	57.6	18.7	45.4
	4	C53	61.9	17.6	41.9
	4	C54	65.3	23.4	40.2
	4	C55	68.8	20.4	36.3
BCHL	5	MG	53.3	23.9	31.3
	5	N1	53.1	26.0	31.3
	5	N2	54.7	24.3	29.5
	5	N3	54.3	22.1	31.1
	5	N4	52.6	23.7	33.1
	5	O1	54.5	17.9	33.1
	5	O2	51.8	18.1	34.7
	5	O3	51.2	19.8	33.5
	5	O4	51.8	23.1	39.7
	5	O5	54.0	23.4	39.3
	5	O6	53.9	29.9	29.4
	5	C1	52.4	26.6	32.3
	5	C2	52.3	28.0	32.3
	5	C3	52.9	28.3	30.9
	5	C4	53.5	26.9	30.4
	5	C5	54.2	26.7	29.3
	5	C6	54.8	25.5	28.5
	5	C7	55.7	25.4	27.5
	5	C8	56.2	23.9	27.5
	5	C9	55.4	23.4	28.9
	5	C10	55.6	22.1	29.1
	5	C11	55.1	21.4	30.2
	5	C12	55.3	20.1	30.6
	5	C13	54.6	20.0	31.7
	5	C14	54.3	21.3	32.1
	5	C15	53.2	21.3	33.3
	5	C16	52.6	22.5	33.3
	5	C17	51.8	22.6	35.3
	5	C18	51.1	24.0	34.3
	5	C19	51.9	24.6	33.7
	5	C20	51.8	25.9	33.4
	5	C21	51.5	29.0	32.8
	5	C22	53.1	29.6	30.2
	5	C23	51.7	30.3	30.3
	5	C24	54.8	25.3	26.3
	5	C25	57.7	23.7	27.6
	5	C26	58.3	25.0	26.9
	5	C27	56.0	19.0	29.9
	5	C28	54.2	19.1	32.9
	5	C29	53.3	19.9	33.9
	5	C30	52.6	22.5	36.3
	5	C31	52.1	23.5	37.4
	5	C32	49.6	23.9	34.5
	5	C33	52.2	19.1	34.3
	5	C34	49.9	19.4	33.3
	5	C35	52.6	23.2	38.3
	5	C36	54.3	23.6	40.4
	5	C37	55.9	23.6	40.5
	5	C38	56.7	22.6	40.6
	5	C39	58.2	22.8	40.7
	5	C40	58.8	22.6	39.4
	5	C41	59.2	23.9	38.8
	5	C42	60.6	23.8	38.2
	5	C43	60.5	23.3	36.7
	5	C44	61.9	22.7	36.3
	5	C45	61.8	22.2	34.9
	5	C46	62.1	20.7	34.8
	5	C47	63.5	20.5	34.3
	5	C48	63.8	21.6	33.3
	5	C49	65.5	21.3	31.5
	5	C50	64.6	21.7	30.8
	5	C51	65.4	20.4	30.4
	5	C52	56.3	21.1	40.4
	5	C53	61.3	25.2	38.1
	5	C54	61.9	20.1	36.2
	5	C55	65.5	22.8	31.3
BCHL	6	MG	60.3	20.5	22.1
	6	N1	62.4	20.4	21.9
	6	N2	60.4	18.7	23.3
	6	N3	58.6	20.9	23.1
	6	N4	60.5	22.6	21.7
	6	O1	54.9	23.6	23.6
	6	O2	55.3	24.0	21.3
	6	O3	56.5	25.9	20.7
	6	O4	62.5	27.0	23.9
	6	O5	61.6	26.2	25.7
	6	O6	66.8	19.0	21.5
	6	C1	63.2	21.3	21.3
	6	C2	64.5	20.8	21.2
	6	C3	64.5	19.5	21.7
	6	C4	63.1	19.2	22.2
	6	C5	62.7	18.1	22.9
	6	C6	61.4	17.8	23.3
	6	C7	61.1	16.5	23.9
	6	C8	59.7	16.7	24.4
	6	C9	59.3	18.1	23.9
	6	C10	58.1	18.7	24.1
	6	C11	57.7	20.3	23.8
	6	C12	56.5	20.7	24.0
	6	C13	56.6	22.0	23.5
	6	C14	57.9	22.0	22.9
	6	C15	58.3	23.3	22.3
	6	C16	59.5	23.5	21.7
	6	C17	59.8	24.9	21.1
	6	C18	61.2	24.5	20.4
	6	C19	61.5	23.2	21.3
	6	C20	62.8	22.6	20.9
	6	C21	65.7	21.4	20.5
	6	C22	65.7	18.6	21.8
	6	C23	65.5	17.3	22.5
	6	C24	61.4	15.3	23.1
	6	C25	59.7	16.6	25.9
	6	C26	59.6	18.0	26.6
	6	C27	55.3	20.1	24.7
	6	C28	56.0	23.2	23.3
	6	C29	57.0	24.1	22.5
	6	C30	60.3	26.3	22.0
	6	C31	60.6	25.7	23.4
	6	C32	61.1	24.4	18.9
	6	C33	56.2	24.8	21.4
	6	C34	56.5	25.7	19.3
	6	C35	61.6	26.4	24.3
	6	C36	62.7	26.7	26.5
	6	C37	62.5	26.5	28.0
	6	C38	63.3	25.7	28.8
	6	C39	63.0	25.2	30.2
	6	C40	62.1	23.9	30.2
	6	C41	60.6	24.3	30.4
	6	C42	59.9	23.2	31.2
	6	C43	58.5	23.8	31.5
	6	C44	58.3	23.9	33.1
	6	C45	56.9	23.9	33.5
	6	C46	56.6	24.1	35.0
	6	C47	56.0	25.5	35.2
	6	C48	56.0	26.4	34.0
	6	C49	55.3	27.8	34.3
	6	C50	56.1	29.0	34.1
	6	C51	55.5	30.2	34.8
	6	C52	64.4	24.9	28.1
	6	C53	59.7	21.9	30.4
	6	C54	55.6	23.0	35.4
	6	C55	56.1	29.3	32.6
BCHL	7	MG	63.4	14.0	32.5
	7	N1	63.8	14.0	30.4
	7	N2	62.0	15.5	32.2
	7	N3	63.5	14.7	34.4
	7	N4	65.4	13.1	32.7
	7	O1	65.0	13.9	38.7
	7	O2	68.2	12.7	37.4
	7	O3	67.6	14.7	36.7
	7	O4	69.4	8.8	35.8
	7	O5	70.3	10.8	36.1
	7	O6	61.9	13.3	26.3
	7	C1	64.7	13.2	29.8
	7	C2	64.4	13.1	28.4
	7	C3	63.3	13.8	28.2
	7	C4	62.9	14.4	29.5
	7	C5	61.8	15.2	29.7
	7	C6	61.4	15.8	31.0
	7	C7	60.3	16.9	31.1
	7	C8	60.3	17.2	32.6
	7	C9	61.3	16.1	33.1
	7	C10	61.5	16.1	34.5
	7	C11	62.6	15.4	35.1
	7	C12	62.9	15.3	36.5
	7	C13	64.0	14.5	36.6
	7	C14	64.4	14.1	35.2
	7	C15	65.5	13.3	35.1
	7	C16	66.0	12.8	34.0
	7	C17	67.2	11.9	33.8
	7	C18	67.4	11.9	32.2
	7	C19	66.1	12.5	31.7
	7	C20	65.8	12.5	30.4
	7	C21	65.1	12.3	27.3
	7	C22	62.6	14.1	26.9
	7	C23	62.8	15.5	26.3
	7	C24	61.0	18.1	30.4
	7	C25	59.0	17.1	33.3
	7	C26	58.5	18.5	33.8
	7	C27	62.2	16.0	37.6
	7	C28	64.9	13.8	37.4
	7	C29	66.0	13.0	36.6
	7	C30	67.0	10.5	34.3
	7	C31	67.8	10.4	35.6
	7	C32	68.6	12.7	31.8
	7	C33	67.3	13.3	37.1
	7	C34	68.8	15.2	37.2
	7	C35	69.2	10.0	35.8
	7	C36	70.4	11.4	37.3
	7	C37	71.5	12.5	37.2
	7	C38	72.7	12.3	36.6
	7	C39	73.4	13.4	35.9
	7	C40	72.6	13.9	34.7
	7	C41	73.2	15.2	34.2
	7	C42	72.9	15.3	32.6
	7	C43	74.1	15.9	32.0
	7	C44	73.8	16.4	30.5
	7	C45	73.3	17.9	30.5
	7	C46	73.2	18.4	29.0
	7	C47	72.5	19.8	29.0
	7	C48	71.0	19.9	29.2
	7	C49	70.7	21.1	30.1
	7	C50	69.6	22.0	29.4
	7	C51	68.3	21.4	29.6
	7	C52	73.5	11.0	36.5
	7	C53	72.6	13.9	32.1
	7	C54	74.6	18.5	28.4
	7	C55	70.0	22.0	27.9

dimensions $a = b = 112.4$ Å, $c = 98.4$ Å. The transformation giving the fractional crystallographic coordinates (x,y,z) in terms of the orthogonal coordinates (X,Y,Z) is as follows:

$$x = 0.01027\ X$$

$$y = 0.00890\ Y + 0.00514\ X$$

$$z = 0.01016\ Z$$

The three-fold axis relating the subunits of the bacteriochlorophyll-protein molecule is parallel to the Z axis and passes through the point X = 64.89 Å, Y = 0 Å (i.e., x = 2/3, y = 1/3). Rotations of the coordinates in Table I by 120° and 240° about this axis will generate the coordinates of the 21 bacteriochlorophyll molecules contained within a complete trimer.

We estimate that within the conjugated portions of each bacteriochlorophyll molecule the average error in the coordinates quoted in Table I is about 0.3 Å, and unlikely to exceed 0.5 Å. For the ring substituents, including the phytyl chains, the errors could be twice as large, and the detailed conformations of some of these groups are uncertain.

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