



# wwPDB X-ray Structure Validation Summary Report i

Feb 27, 2014 – 07:54 AM GMT

PDB ID : 2RCR  
Title : STRUCTURE OF THE MEMBRANE-BOUND PROTEIN PHOTOSYN-  
THETIC REACTION CENTER FROM RHODOBACTER SPHAEROIDES  
Authors : Chang, C.-H.; Norris, J.; Schiffer, M.  
Deposited on : 1991-02-04  
Resolution : 3.10 Å(reported)

This is a wwPDB validation summary report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

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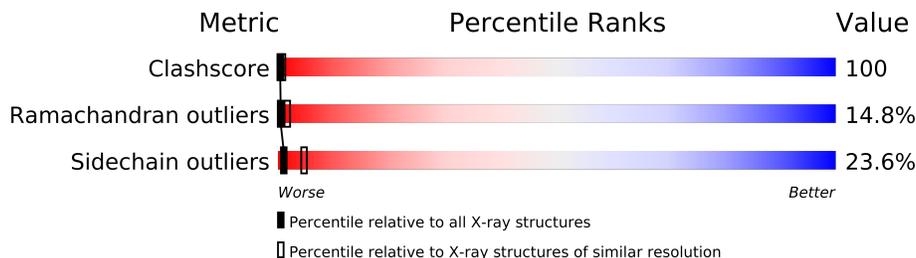
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
Percentile statistics : 21963  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable22683

# 1 Overall quality at a glance

The reported resolution of this entry is 3.10 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	79885	1078 (3.16-3.04)
Ramachandran outliers	78287	1044 (3.16-3.04)
Sidechain outliers	78261	1044 (3.16-3.04)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	L	281	
2	M	307	
3	H	260	

## 2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 7049 atoms, of which 0 are hydrogen and 0 are deuterium.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called PHOTOSYNTHETIC REACTION CENTER (L SUBUNIT).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	L	278	2203	1491	349	355	8	0	0	0

- Molecule 2 is a protein called PHOTOSYNTHETIC REACTION CENTER (M SUBUNIT).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	M	305	2428	1620	397	400	11	0	0	0

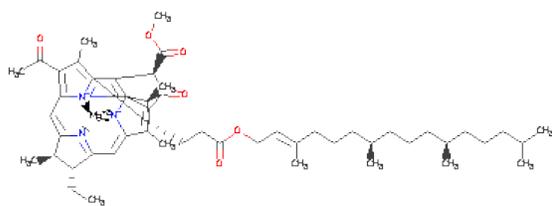
- Molecule 3 is a protein called PHOTOSYNTHETIC REACTION CENTER (H SUBUNIT).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	H	255	1927	1232	330	354	11	73	0	0

- Molecule 4 is FE (III) ION (three-letter code: FE) (formula: Fe).

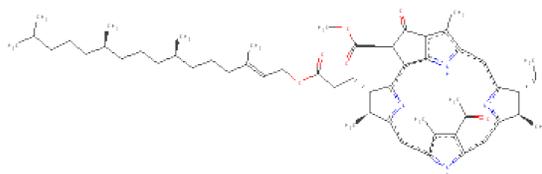
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	M	1	Total	Fe	0	0
			1	1		

- Molecule 5 is BACTERIOCHLOROPHYLL A (three-letter code: BCL) (formula: C<sub>55</sub>H<sub>74</sub>MgN<sub>4</sub>O<sub>6</sub>).



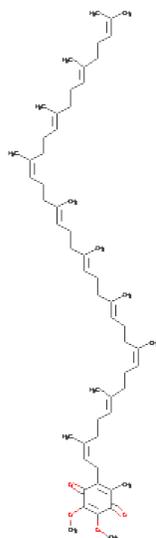
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	Mg	N	O		
5	M	1	66	55	1	4	6	7	0
5	L	1	66	55	1	4	6	0	0
5	M	1	66	55	1	4	6	3	0
5	L	1	66	55	1	4	6	6	0

- Molecule 6 is BACTERIOPHEOPHYTIN A (three-letter code: BPH) (formula:  $C_{55}H_{76}N_4O_6$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
6	M	1	65	55	4	6	7	0
6	L	1	65	55	4	6	0	0

- Molecule 7 is COENZYME Q10, (2Z,6E,10Z,14E,18E,22E,26Z)-ISOMER (three-letter code: UQ) (formula: C<sub>59</sub>H<sub>90</sub>O<sub>4</sub>).

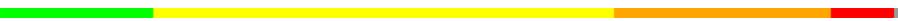


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
7	M	1	48	44	4	16	0
7	L	1	48	44	4	16	0



H299
G300
H301
A302
P303
LEU
ASN

- Molecule 3: PHOTOSYNTHETIC REACTION CENTER (H SUBUNIT)

Chain H: 

M1	V2	G3	V4	T5	A6	F7	G8	N9	F10	D11	L12	A13	S14	L15	A16	I17	F20	W21	L22	F23	L24	A25	G26	L27	L28	Y29	Y30	L31	Q32	T33	E34	M35	M36	R37	E38	G39	Y40	P41	E45	T48	P49	M52	Q53	G54	P55	F56	P57	L58	P59	K60	P61	K62	T63	F64	I65
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L66	P67	H68	G69	R70	G71	T72	L73	T74	V75	P76	G77	P78	E79	S80	E81	R82	R83	P84	L87	A88	R89	T90	A91	Y92	S93	G94	G95	F96	P97	H98	A99	P100	D103	P104	M105	K106	D107	G108	G109	G110	P111	A112	S113	W114	V115	A116	R117	R118	D119	L120	P121	E122	L123	D124	L128	M129
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K130	I131	K132	P133	M134	K135	F140	H141	V142	S143	A144	G145	K146	M147	P148	E149	G150	L151	P152	V153	R154	G155	C156	D157	L158	E159	I160	A161	G162	K163	V164	V165	D166	I167	W168	V169	D170	I171	P172	E173	Q174	M175	A176	R177	F178	L179	E180	V181	E182	L183	K184	D185	G186	S187	T188	R189	L190	P192
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M193	Q194	M195	V196	K197	V198	Q199	S200	M201	R202	V203	H204	V205	M206	A207	L208	S209	S210	D211	L212	F213	A214	G215	T216	P217	T218	T219	K220	S221	P222	T223	E224	V225	T226	L227	L228	E229	E230	D231	K232	L233	C234	G235	Y236	Y237	A238	G239	G240	L241	M242	Y243	A244	A245	R248	K249	S250	Y251	A252	A253
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A254
M255
LEU
ALA
GLU
TYR
ALA

## 4 Data and refinement statistics

Xtrriage (Phenix) and EDS were not executed - this section will therefore be incomplete.

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	142.20Å 139.60Å 78.70Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	(Not available) – 3.10	Depositor
% Data completeness (in resolution range)	(Not available) ((Not available)-3.10)	Depositor
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	PROLSQ	Depositor
R, $R_{free}$	0.220 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtrriage
Total number of atoms	7049	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	0.0	wwPDB-VP

## 5 Model quality (i)

### 5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: BCL, BPH, UQ, FE

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	L	1.00	2/2291 (0.1%)	1.47	24/3137 (0.8%)
2	M	1.21	6/2521 (0.2%)	1.57	36/3442 (1.0%)
3	H	0.96	4/1977 (0.2%)	1.52	23/2689 (0.9%)
All	All	1.07	12/6789 (0.2%)	1.52	83/9268 (0.9%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	M	0	5

The worst 5 of 12 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	M	250	TRP	CA-CB	-17.94	1.14	1.53
2	M	93	LEU	C-O	16.21	1.54	1.23
2	M	93	LEU	CA-C	-12.85	1.19	1.52
2	M	93	LEU	C-N	10.05	1.57	1.34
2	M	112	LEU	C-N	8.74	1.54	1.34

The worst 5 of 83 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	M	112	LEU	O-C-N	-24.12	84.11	122.70
1	L	166	ASN	CA-CB-CG	18.90	154.98	113.40
1	L	166	ASN	N-CA-CB	17.93	142.88	110.60
2	M	109	GLU	CA-C-N	-15.78	84.64	116.20
2	M	112	LEU	CA-C-N	13.93	147.85	117.20

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	M	109	GLU	Mainchain,Peptide
2	M	112	LEU	Mainchain,Peptide
2	M	265	ARG	Sidechain

## 5.2 Close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	L	2203	0	2156	482	1
2	M	2428	0	2342	596	1
3	H	1927	0	1927	364	2
4	M	1	0	0	0	0
5	L	132	0	148	46	0
5	M	132	0	148	63	0
6	L	65	0	76	16	0
6	M	65	0	76	33	0
7	L	48	0	59	21	0
7	M	48	0	63	33	0
All	All	7049	0	6995	1373	2

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 100.

The worst 5 of 1373 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
7:M:750:UQ:C13	7:M:750:UQ:C12	1.84	1.50
1:L:183:ASN:ND2	1:L:236:LEU:HB2	1.24	1.48
2:M:96:PRO:HG2	2:M:170:SER:CA	1.57	1.33
1:L:183:ASN:HD22	1:L:236:LEU:CB	1.44	1.30
2:M:96:PRO:CG	2:M:170:SER:HA	1.75	1.17

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:M:293:TYR:OH	3:H:166:ASP:OD1[4.445]	1.59	0.61
1:L:265:TRP:CB	3:H:49:PRO:O[1.556]	2.17	0.03

## 5.3 Torsion angles

### 5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	L	276/281 (98%)	187 (68%)	52 (19%)	37 (13%)	0 2
2	M	303/307 (99%)	189 (62%)	72 (24%)	42 (14%)	0 2
3	H	253/260 (97%)	144 (57%)	65 (26%)	44 (17%)	0 0
All	All	832/848 (98%)	520 (62%)	189 (23%)	123 (15%)	0 2

5 of 123 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	L	7	ARG
1	L	20	ASN
1	L	55	LEU
1	L	60	ASN
1	L	74	GLY

### 5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	L	216/220 (98%)	169 (78%)	47 (22%)	1 6
2	M	238/240 (99%)	179 (75%)	59 (25%)	1 3
3	H	203/208 (98%)	154 (76%)	49 (24%)	1 4
All	All	657/668 (98%)	502 (76%)	155 (24%)	1 5

5 of 155 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	M	134	ARG
2	M	210	SER
3	H	193	MET
2	M	142	LYS
2	M	161	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 20 such sidechains are listed below:

Mol	Chain	Res	Type
2	M	43	ASN
2	M	45	GLN
3	H	9	ASN
2	M	25	ASN
2	M	28	ASN

### 5.3.3 RNA ⓘ

There are no RNA chains in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

Of 9 ligands modelled in this entry, 1 is monoatomic - leaving 8 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
5	BCL	L	350	-	74,74,74	1.63	14 (18%)	97,115,115	1.50	17 (17%)
5	BCL	L	450	-	74,74,74	1.41	12 (16%)	97,115,115	1.43	17 (17%)
6	BPH	L	550	-	70,70,70	1.38	11 (15%)	94,101,101	1.34	14 (14%)
7	UQ	L	800	-	48,48,63	2.28	15 (31%)	59,61,79	2.64	25 (42%)
5	BCL	M	400	2	74,74,74	1.73	13 (17%)	97,115,115	1.41	15 (15%)
6	BPH	M	500	-	70,70,70	1.49	10 (14%)	94,101,101	1.25	11 (11%)
5	BCL	M	601	2	74,74,74	1.48	15 (20%)	97,115,115	1.43	16 (16%)
7	UQ	M	750	-	48,48,63	2.31	12 (25%)	59,61,79	2.20	20 (33%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsions and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	BCL	L	350	-	-	0/41/137/137	0/0/9/9
5	BCL	L	450	-	-	0/41/137/137	0/0/9/9
6	BPH	L	550	-	2/2/18/22	0/49/105/105	0/0/6/6
7	UQ	L	800	-	-	0/45/69/87	0/1/1/1
5	BCL	M	400	2	-	0/41/137/137	0/0/9/9
6	BPH	M	500	-	2/2/18/22	0/49/105/105	0/0/6/6
5	BCL	M	601	2	-	0/41/137/137	0/0/9/9
7	UQ	M	750	-	-	1/45/69/87	0/1/1/1

The worst 5 of 102 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	M	750	UQ	C12-C13	11.50	1.84	1.50
7	L	800	UQ	C16-C17	-8.19	1.24	1.53
5	M	400	BCL	MG-NA	6.73	2.27	2.07
7	L	800	UQ	C7-C8	6.03	1.60	1.50
6	L	550	BPH	C1D-CHD	5.24	1.41	1.35

The worst 5 of 135 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	L	800	UQ	C37-C38-C39	-6.39	113.13	128.63
7	M	750	UQ	C11-C12-C13	6.11	129.08	111.62
7	L	800	UQ	C20-C19-C21	5.92	124.39	115.39
7	L	800	UQ	C30-C29-C28	-5.81	112.01	123.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	L	800	UQ	C10-C9-C11	5.66	123.99	115.39

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
6	L	550	BPH	C8
6	L	550	BPH	C13
6	M	500	BPH	C8
6	M	500	BPH	C13

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	M	750	UQ	C24-C23-C22-C21

There are no ring outliers.

## 5.7 Other polymers

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

EDS was not executed - this section will therefore be empty.

### 6.2 Non-standard residues in protein, DNA, RNA chains

EDS was not executed - this section will therefore be empty.

### 6.3 Carbohydrates

EDS was not executed - this section will therefore be empty.

### 6.4 Ligands

EDS was not executed - this section will therefore be empty.

### 6.5 Other polymers

EDS was not executed - this section will therefore be empty.