



wwPDB X-ray Structure Validation Summary Report ⓘ

Jan 31, 2016 – 08:15 PM GMT

PDB ID : 1JGY
Title : Photosynthetic Reaction Center Mutant With Tyr M 76 Replaced With Phe
Authors : Camara-Artigas, A.; Magee, C.L.; Williams, J.C.; Allen, J.P.
Deposited on : 2001-06-27
Resolution : 2.70 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

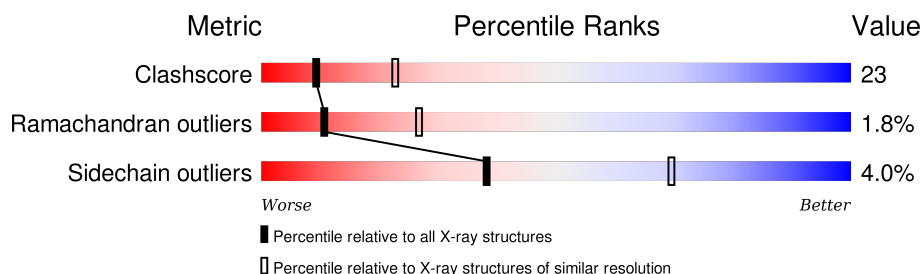
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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	102246	2422 (2.70-2.70)
Ramachandran outliers	100387	2382 (2.70-2.70)
Sidechain outliers	100360	2382 (2.70-2.70)

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 ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

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 10 unique types of molecules in this entry. The entry contains 7123 atoms, of which 0 are hydrogens and 0 are deuteriums.

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
1	L	281	Total	C	N	O	S	0	0	0
			2232	1507	355	362	8			

- Molecule 2 is a protein called Photosynthetic Reaction Center M Subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	M	302	Total	C	N	O	S	0	0	0
			2407	1607	394	396	10			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
M	76	PHE	TYR	ENGINEERED	UNP P02953

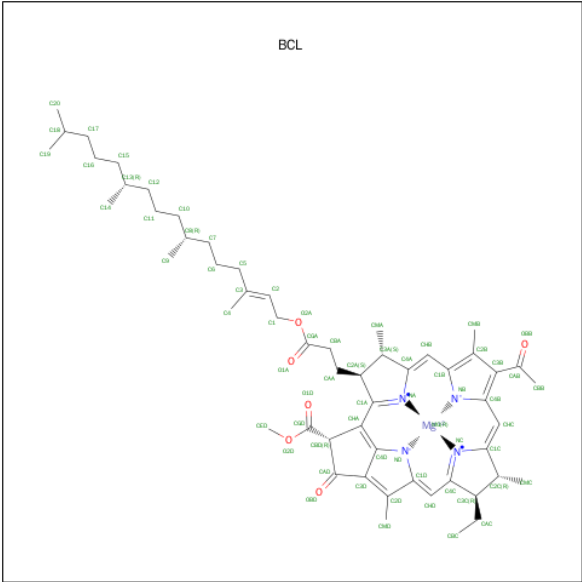
- Molecule 3 is a protein called Photosynthetic Reaction Center H Subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	H	240	Total	C	N	O	S	0	0	0
			1829	1169	314	337	9			

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

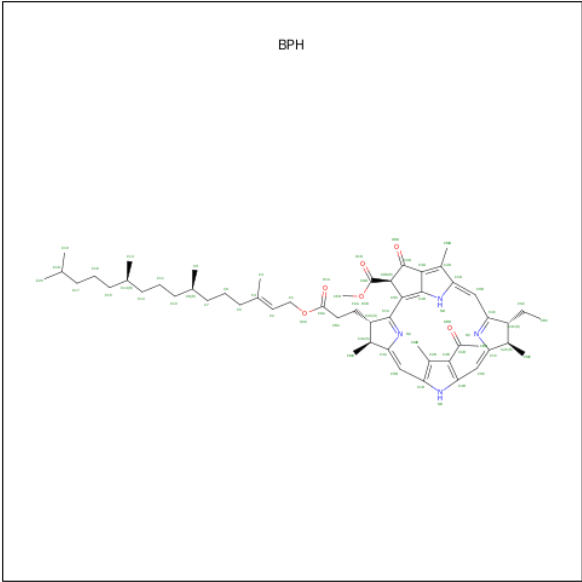
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	M	1	Total	Fe	0	0
			1	1		

- Molecule 5 is BACTERIOCHLOROPHYLL A (three-letter code: BCL) (formula: C₅₅H₇₄MgN₄O₆).



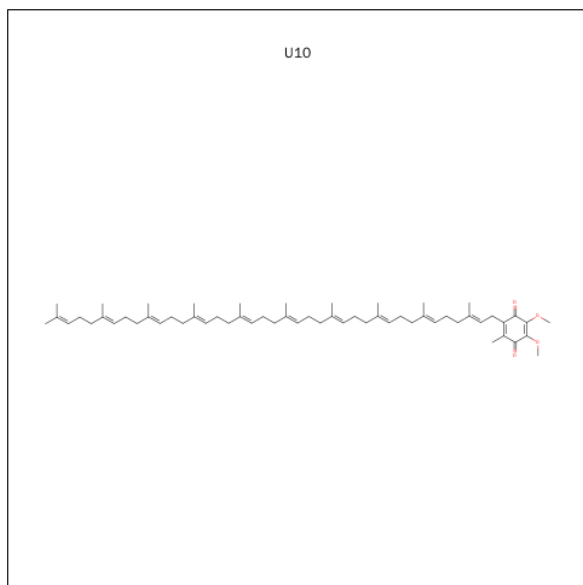
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	L	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
5	L	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
5	M	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
5	M	1	Total 66	C 55	Mg 1	N 4	O 6	0	0

- Molecule 6 is BACTERIOPHEOPHYTIN A (three-letter code: BPH) (formula: C₅₅H₇₆N₄O₆).



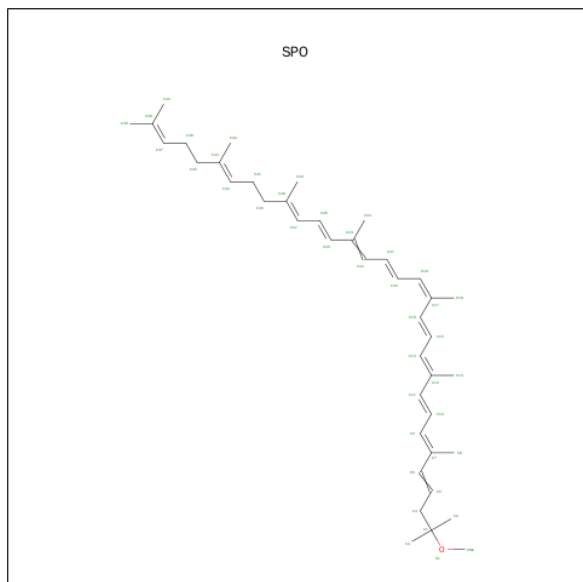
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	M	1	Total	C	N	O	0	0
			65	55	4	6		
6	L	1	Total	C	N	O	0	0
			65	55	4	6		

- Molecule 7 is UBIQUINONE-10 (three-letter code: U10) (formula: $C_{59}H_{90}O_4$).



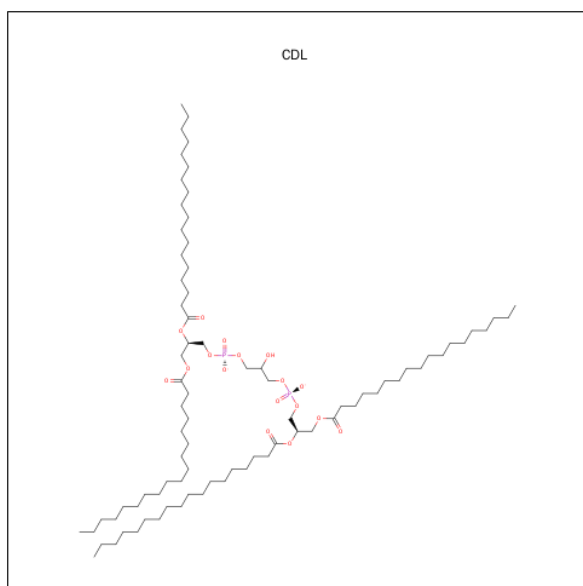
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	M	1	Total	C	O	0	0
			48	44	4		

- Molecule 8 is SPHEROIDENE (three-letter code: SPO) (formula: $C_{41}H_{60}O$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	M	1	Total	C	O	0	0
			42	41	1		

- Molecule 9 is CARDIOLIPIN (three-letter code: CDL) (formula: $C_{81}H_{156}O_{17}P_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
9	M	1	Total	C	O	P	0	0
			81	62	17	2		

- Molecule 10 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	H	40	Total	O	0	0
			40	40		
10	L	16	Total	O	0	0
			16	16		
10	M	33	Total	O	0	0
			33	33		

A207	L208	S209	S210	D211	L212		T219	K220	S221		V225	T226		E229	E230	D231	K232	I233	C234		V237		G240	L241	K242	Y243	A244	A245	P246	K247	R248	K249	S250	VAL	VAL	ALA	ALA	MET	LEU	ALA	GLU	TYR	ALA
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4 Data and refinement statistics

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

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α , β , γ	141.68Å 141.68Å 186.84Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	29.10 – 2.70	Depositor
% Data completeness (in resolution range)	62.6 (29.10-2.70)	Depositor
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.218 , 0.257	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	7123	wwPDB-VP
Average B, all atoms (Å ²)	49.0	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, CDL, BPH, FE, SPO, U10

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	0.41	0/2320	0.60	0/3175
2	M	0.42	0/2499	0.58	0/3411
3	H	0.40	0/1877	0.64	0/2553
All	All	0.41	0/6696	0.61	0/9139

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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 hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	L	2232	0	2187	99	0
2	M	2407	0	2321	150	0
3	H	1829	0	1836	88	0
4	M	1	0	0	0	0
5	L	132	0	148	11	0
5	M	132	0	148	11	0
6	L	65	0	76	4	0
6	M	65	0	76	10	0
7	M	48	0	63	5	0
8	M	42	0	60	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	M	81	0	106	2	0
10	H	40	0	0	4	0
10	L	16	0	0	0	0
10	M	33	0	0	9	0
All	All	7123	0	7021	321	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 23.

The worst 5 of 321 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:21:THR:HG23	2:M:26:LEU:HD21	1.39	1.05
3:H:249:LYS:HG3	3:H:250:SER:H	1.23	1.03
3:H:148:PRO:HA	3:H:151:LEU:HD12	1.43	1.00
2:M:114:LEU:HA	2:M:117:ILE:HD12	1.47	0.97
2:M:279:THR:HB	10:M:1024:HOH:O	1.65	0.95

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

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	279/281 (99%)	243 (87%)	33 (12%)	3 (1%)	17	42
2	M	300/307 (98%)	268 (89%)	30 (10%)	2 (1%)	26	55
3	H	238/260 (92%)	214 (90%)	14 (6%)	10 (4%)	3	7
All	All	817/848 (96%)	725 (89%)	77 (9%)	15 (2%)	11	27

5 of 15 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	H	210	SER
3	H	211	ASP
2	M	80	TRP
3	H	51	ALA
1	L	26	VAL

5.3.2 Protein sidechains ⓘ

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	220/220 (100%)	210 (96%)	10 (4%)	34	65
2	M	236/240 (98%)	224 (95%)	12 (5%)	29	59
3	H	195/208 (94%)	191 (98%)	4 (2%)	61	87
All	All	651/668 (98%)	625 (96%)	26 (4%)	38	69

5 of 26 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	M	51	TYR
2	M	133	THR
3	H	225	VAL
2	M	76	PHE
2	M	86	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 8 such sidechains are listed below:

Mol	Chain	Res	Type
2	M	202	HIS
3	H	206	ASN
2	M	299	GLN
2	M	28	ASN
2	M	259	ASN

5.3.3 RNA ⓘ

There are no RNA molecules 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 10 ligands modelled in this entry, 1 is monoatomic - leaving 9 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	850	2	53,74,74	1.39	7 (13%)	57,115,115	1.93	15 (26%)
5	BCL	L	851	1	53,74,74	1.52	9 (16%)	57,115,115	1.69	9 (15%)
6	BPH	L	855	-	64,70,70	1.22	9 (14%)	73,101,101	1.84	14 (19%)
9	CDL	M	3000	-	80,80,99	0.66	2 (2%)	82,92,111	0.92	4 (4%)
5	BCL	M	852	2	53,74,74	1.35	6 (11%)	57,115,115	1.77	9 (15%)
5	BCL	M	853	1	53,74,74	1.56	8 (15%)	57,115,115	2.00	13 (22%)
6	BPH	M	854	-	64,70,70	1.43	12 (18%)	73,101,101	1.69	13 (17%)
7	U10	M	857	-	48,48,63	2.23	14 (29%)	58,61,79	2.38	23 (39%)
8	SPO	M	859	-	40,41,41	3.51	23 (57%)	45,50,50	2.72	15 (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 Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	BCL	L	850	2	-	0/37/137/137	0/0/9/9
5	BCL	L	851	1	-	0/37/137/137	0/0/9/9
6	BPH	L	855	-	-	0/54/105/105	0/1/6/6
9	CDL	M	3000	-	-	0/91/91/110	0/0/0/0
5	BCL	M	852	2	-	0/37/137/137	0/0/9/9
5	BCL	M	853	1	-	0/37/137/137	0/0/9/9
6	BPH	M	854	-	-	0/54/105/105	0/1/6/6
7	U10	M	857	-	-	0/45/69/87	0/1/1/1
8	SPO	M	859	-	-	0/47/47/47	0/0/0/0

The worst 5 of 90 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	M	859	SPO	C4-C5	-3.82	1.44	1.50
7	M	857	U10	C7-C8	-3.71	1.45	1.50
8	M	859	SPO	C31-C32	-3.27	1.41	1.50
5	L	851	BCL	C3C-C4C	-2.98	1.47	1.51
8	M	859	SPO	C11-C12	-2.96	1.39	1.45

The worst 5 of 115 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	M	859	SPO	C25-C23-C22	-10.34	102.32	118.98
5	L	851	BCL	CMB-C2B-C1B	-6.09	118.30	128.36
5	M	853	BCL	CMB-C2B-C1B	-6.01	118.43	128.36
5	M	853	BCL	CAA-C2A-C1A	-5.90	91.66	112.47
5	L	850	BCL	CMB-C2B-C1B	-5.78	118.80	128.36

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

9 monomers are involved in 39 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	L	850	BCL	7	0
5	L	851	BCL	5	0
6	L	855	BPH	4	0
9	M	3000	CDL	2	0
5	M	852	BCL	9	0
5	M	853	BCL	3	0
6	M	854	BPH	10	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	M	857	U10	5	0
8	M	859	SPO	2	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

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

6.4 Ligands [i](#)

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

6.5 Other polymers [i](#)

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