

# Full wwPDB X-ray Structure Validation Report (i)

May 24, 2020 – 04:47 am BST

PDB ID : 1UWP

Title : Initial Events in the Photocycle of Photoactive Yellow Protein

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Deposited on : 2004-02-11

Resolution : 1.20 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*A user guide is available at

https://www.wwpdb.org/validation/2017/XrayValidationReportHelp with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

MolProbity: 4.02b-467

Mogul : 1.8.5 (274361), CSD as541be (2020)

Xtriage (Phenix) : NOT EXECUTED EDS : NOT EXECUTED

Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)

Ideal geometry (proteins) : Engh & Huber (2001) Ideal geometry (DNA, RNA) : Parkinson et al. (1996)

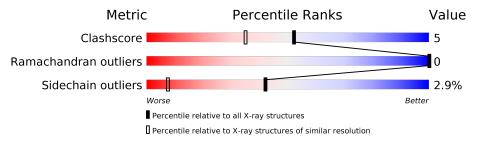
Validation Pipeline (wwPDB-VP) : 2.11

## 1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure: X-RAY DIFFRACTION

The reported resolution of this entry is 1.20 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	$\begin{array}{c} \textbf{Whole archive} \\ (\#\text{Entries}) \end{array}$	$\begin{array}{c} {\rm Similar \; resolution} \\ (\#{\rm Entries, \; resolution \; range(\AA)}) \end{array}$
Clashscore	141614	1286 (1.22-1.18)
Ramachandran outliers	138981	1240 (1.22-1.18)
Sidechain outliers	138945	1239 (1.22-1.18)

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 respectively. 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 <=5%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain		
1	X	125	90%	8%	•



## 2 Entry composition (i)

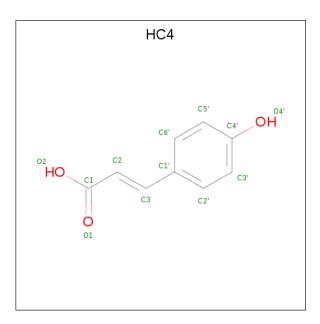
There are 4 unique types of molecules in this entry. The entry contains 1345 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 PHOTOACTIVE YELLOW PROTEIN.

Mol	Chain	Residues		Atoms			ZeroOcc	AltConf	Trace		
1	X	125	Total	C 746	N	0	S	Se	0	30	1
			1175	746	188	229	3	9			

• Molecule 2 is 4'-HYDROXYCINNAMIC ACID (three-letter code: HC4) (formula: C<sub>9</sub>H<sub>8</sub>O<sub>3</sub>).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf	
2	X	1	Total 22	C 18	O 4	0	1

• Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).





Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	X	1	Total O S 5 4 1	0	0
3	X	1	Total O S 5 4 1	0	0

• Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	X	138	Total O 138 138	0	0

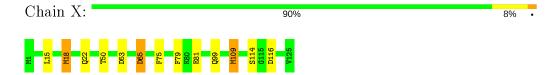


## 3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

Note EDS was not executed.

• Molecule 1: PHOTOACTIVE YELLOW PROTEIN





# 4 Data and refinement statistics (i)

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

Property	Value	Source	
Space group	P 63	Depositor	
Cell constants	65.92Å 65.92Å 40.58Å	Depositor	
a, b, c, $\alpha$ , $\beta$ , $\gamma$	$90.00^{\circ}$ $90.00^{\circ}$ $120.00^{\circ}$	Depositor	
Resolution (Å)	40.00 - 1.20	Depositor	
% Data completeness	98.2 (40.00-1.20)	Depositor	
(in resolution range)	30.2 (40.00 1.20)	Depositor	
$R_{merge}$	0.04	Depositor	
$R_{sym}$	(Not available)	Depositor	
Refinement program	REFMAC 5.1.24	Depositor	
$R, R_{free}$	0.136 , $0.157$	Depositor	
Estimated twinning fraction	No twinning to report.	Xtriage	
Total number of atoms	1345	wwPDB-VP	
Average B, all atoms (Å <sup>2</sup> )	13.0	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: SO4, HC4

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	Bo	nd angles
IVIOI	Chain	RMSZ	# Z >5	RMSZ	# Z  > 5
1	X	0.73	0/1257	0.96	9/1677~(0.5%)

There are no bond length outliers.

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	$\mathbf{Z}$	$Observed(^o)$	$Ideal(^{o})$
1	X	53[A]	ASP	CB-CG-OD2	7.00	124.60	118.30
1	X	53[B]	ASP	CB-CG-OD2	7.00	124.60	118.30
1	X	116	ASP	CB-CG-OD2	5.74	123.47	118.30
1	X	65[A]	ASP	CB-CG-OD2	5.62	123.36	118.30
1	X	65[B]	ASP	CB-CG-OD2	5.62	123.36	118.30
1	X	18[A]	MSE	CB-CG-SE	-5.38	96.58	112.70
1	X	18[B]	MSE	CB-CG-SE	-5.38	96.58	112.70
1	X	18[A]	MSE	CA-CB-CG	5.04	121.88	113.30
1	X	18[B]	MSE	CA-CB-CG	5.04	121.88	113.30

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	X	1175	0	1101	12	0
2	X	22	0	12	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	X	10	0	0	0	0
4	X	138	0	0	6	0
All	All	1345	0	1113	13	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 5.

All (13) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic	Clash
7100111 1		$\operatorname{distance}\left( \mathrm{\AA}\right)$	overlap (Å)
1:X:15:LEU:HA	1:X:18[B]:MSE:HE2	1.58	0.83
1:X:65[B]:ASP:OD1	4:X:2071:HOH:O	2.01	0.78
1:X:18[A]:MSE:HG2	1:X:22:GLN:HB2	1.64	0.77
1:X:79:PHE:HB2	1:X:109[C]:MSE:HE1	1.68	0.76
1:X:65[B]:ASP:CG	4:X:2071:HOH:O	2.26	0.73
1:X:18[A]:MSE:HG2	1:X:22:GLN:CB	2.19	0.71
1:X:65[A]:ASP:OD2	4:X:2070:HOH:O	2.10	0.69
1:X:99[B]:GLN:OE1	4:X:2103:HOH:O	2.16	0.63
2:X:1126[L]:HC4:O1	2:X:1126[L]:HC4:H6'	2.01	0.60
1:X:81[A]:GLU:HG3	4:X:2080:HOH:O	2.05	0.56
1:X:99[B]:GLN:HG3	4:X:2107:HOH:O	2.12	0.49
1:X:50:THR:HG21	2:X:1126[D]:HC4:C4'	2.48	0.44
1:X:18[A]:MSE:HG2	1:X:22:GLN:HB3	1.96	0.43

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	Percentile	es .
1	X	155/125 (124%)	149 (96%)	6 (4%)	0	100 100	)



There are no Ramachandran outliers to report.

#### 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	X	132/98 (135%)	127 (96%)	5 (4%)	33 4	

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	$\operatorname{Res}$	Type
1	X	75	PHE
1	X	109[A]	MSE
1	X	109[B]	MSE
1	X	109[C]	MSE
1	X	114	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

#### 5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

#### 5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

### 5.6 Ligand geometry (i)

4 ligands are modelled in this entry.



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	Mol Type Chain Res Link		Link	Bond lengths			Bond angles			
MIOI	Type	Chain	Res	LIIIK	Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	HC4	X	1126[D]	1	11,11,12	0.80	1 (9%)	13,13,15	0.66	0
2	HC4	X	1126[L]	1	11,11,12	1.29	1 (9%)	13,13,15	3.78	1 (7%)
3	SO4	X	1127	-	4,4,4	0.26	0	6,6,6	0.26	0
3	SO4	X	1128	-	4,4,4	0.14	0	6,6,6	0.15	0

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.

M	ol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	2	HC4	X	1126[D]	1	-	1/4/4/5	0/1/1/1
2	2	HC4	X	1126[L]	1	-	2/4/4/5	0/1/1/1

#### All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	$\mathbf{Z}$	$\operatorname{Observed}(\operatorname{\AA})$	$\operatorname{Ideal}(\operatorname{\AA})$
2	X	1126[L]	HC4	C2-C3	2.73	1.38	1.34
2	X	1126[D]	HC4	O4'-C4'	-2.21	1.31	1.37

#### All (1) bond angle outliers are listed below:

Mol	Chain	$\operatorname{Res}$	Type	Atoms	$\mathbf{Z}$	$\mathbf{Observed}(^o)$	$\operatorname{Ideal}({}^o)$
2	Χ	1126[L]	HC4	C1'-C3-C2	13.38	148.41	127.21

There are no chirality outliers.

All (3) torsion outliers are listed below:

$\mathbf{Mol}$	Chain	$\operatorname{Res}$	Type	Atoms
2	X	1126[D]	HC4	O1-C1-C2-C3
2	X	1126[L]	HC4	O1-C1-C2-C3
2	X	1126[L]	HC4	C1-C2-C3-C1'



There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	X	1126[D]	HC4	1	0
2	X	1126[L]	HC4	1	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 is therefore empty.

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

EDS was not executed - this section is therefore empty.

### 6.3 Carbohydrates (i)

EDS was not executed - this section is therefore empty.

### 6.4 Ligands (i)

EDS was not executed - this section is therefore empty.

### 6.5 Other polymers (i)

EDS was not executed - this section is therefore empty.

