



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 9, 2017 – 08:19 PM EDT

PDB ID : 2OOL
Title : Crystal structure of the chromophore-binding domain of an unusual bacterio-
phytochrome RpBphP3 from *R. palustris*
Authors : Yang, X.; Stojkovic, E.A.; Kuk, J.; Moffat, K.
Deposited on : unknown
Resolution : 2.20 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

<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 : **FAILED**
Mogul : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20030345
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20030345

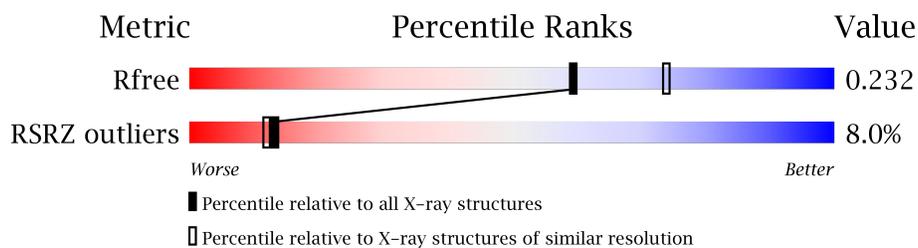
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	100719	4002 (2.20-2.20)
RSRZ outliers	101464	4033 (2.20-2.20)

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2 Entry composition [i](#)

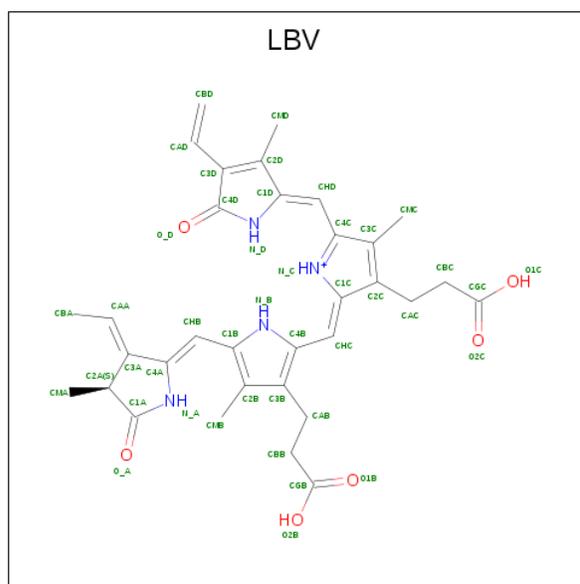
There are 3 unique types of molecules in this entry. The entry contains 5101 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Sensor protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	304	Total 2431	C 1542	N 435	O 445	S 9	15	5	0
1	B	298	Total 2368	C 1501	N 428	O 430	S 9	5	3	0

- Molecule 2 is 3-[2-[(Z)-[3-(2-carboxyethyl)-5-[(Z)-(4-ethenyl-3-methyl-5-oxidanylidene-pyrro-2-ylidene)methyl]-4-methyl-pyrrol-1-ium-2-ylidene]methyl]-5-[(Z)-[(3E)-3-ethylidene-4-methyl-5-oxidanylidene-pyrrolidin-2-ylidene]methyl]-4-methyl-1H-pyrrol-3-yl]propanoic acid (three-letter code: LBV) (formula: C₃₃H₃₇N₄O₆).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
2	A	1	Total 44	C 34	N 4	O 6	0	1
2	B	1	Total 43	C 33	N 4	O 6	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	161	Total 161	O 161	0	0
3	B	54	Total 54	O 54	0	0

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3 Data and refinement statistics

Property	Value	Source
Space group	P 3 2 1	Depositor
Cell constants a, b, c, α , β , γ	151.87Å 151.87Å 76.00Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	49.75 – 2.20 49.73 – 2.11	Depositor EDS
% Data completeness (in resolution range)	93.3 (49.75-2.20) 91.0 (49.73-2.11)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.37 (at 2.10Å)	Xtrriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.188 , 0.231 0.191 , 0.232	Depositor DCC
R_{free} test set	3599 reflections (8.18%)	DCC
Wilson B-factor (Å ²)	41.8	Xtrriage
Anisotropy	0.398	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 58.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	0.033 for -h,-k,l	Xtrriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	5101	wwPDB-VP
Average B, all atoms (Å ²)	58.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.26% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

4 Model quality [i](#)

4.1 Standard geometry [i](#)

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4.2 Too-close contacts [i](#)

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4.3 Torsion angles [i](#)

4.3.1 Protein backbone [i](#)

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4.3.2 Protein sidechains [i](#)

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4.3.3 RNA [i](#)

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

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4.5 Carbohydrates [i](#)

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4.6 Ligand geometry [i](#)

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4.7 Other polymers [i](#)

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4.8 Polymer linkage issues

There are no chain breaks in this entry.

5 Fit of model and data

5.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	304/337 (90%)	0.58	14 (4%) 33 32	49, 56, 69, 78	2 (0%)
1	B	298/337 (88%)	0.63	34 (11%) 6 5	49, 59, 71, 87	1 (0%)
All	All	602/674 (89%)	0.60	48 (7%) 13 12	49, 57, 71, 87	3 (0%)

All (48) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	210	PHE	5.5
1	B	112	PRO	5.1
1	B	162	LEU	5.0
1	A	333	ILE	4.4
1	B	67	ARG	4.2
1	B	114	GLY	4.1
1	B	211	HIS	3.7
1	B	191	TRP	3.5
1	B	185	TYR	3.2
1	B	110	VAL	3.2
1	B	212	PHE	3.1
1	B	81	TYR	3.1
1	B	28	CYS	3.1
1	B	165	ALA	3.1
1	A	261	VAL	3.1
1	B	194	GLN	3.0
1	B	82	LEU	2.8
1	A	314	CYS	2.8
1	B	87	ALA	2.7
1	B	236	ILE	2.7
1	B	187	PHE	2.7
1	B	196	ILE	2.6
1	B	202	SER	2.6
1	B	65	LEU	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	262	LEU	2.6
1	B	275	ASN	2.5
1	A	305	PHE	2.5
1	A	118	PHE	2.4
1	B	239	ARG	2.4
1	A	230	VAL	2.4
1	B	206	SER	2.4
1	B	330	GLU	2.4
1	B	69	PRO	2.3
1	A	282	MET	2.3
1	A	310	VAL	2.3
1	B	207	LEU	2.3
1	A	105[A]	ILE	2.2
1	A	135	PRO	2.2
1	A	298	CYS	2.2
1	B	107	LEU	2.2
1	B	200	ARG	2.2
1	B	52	ASP	2.2
1	A	101	ALA	2.2
1	B	95	HIS	2.1
1	A	281	ALA	2.1
1	B	203	GLY	2.1
1	B	44	TYR	2.1
1	B	189	ALA	2.0

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

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

5.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q < 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
2	LBV	B	400	43/43	0.82	0.19	0.23	61,75,81,82	0
2	LBV	A	400[B]	43/43	0.95	0.12	-1.35	32,44,55,58	1
2	LBV	A	400[A]	43/43	0.95	0.12	-1.35	32,44,55,58	1

5.5 Other polymers [i](#)

There are no such residues in this entry.