



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 27, 2026 – 11:26 AM UTC

PDB ID : 6RA3 / pdb_00006ra3
Title : Structural basis for recognition and ring-cleavage of the Pseudomonas quinolone signal (PQS) by AqDC in complex with its product
Authors : Wullich, S.; Kobus, S.; Smits, S.H.; Fetzner, S.
Deposited on : 2019-04-05
Resolution : 2.00 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 ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	FAILED
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

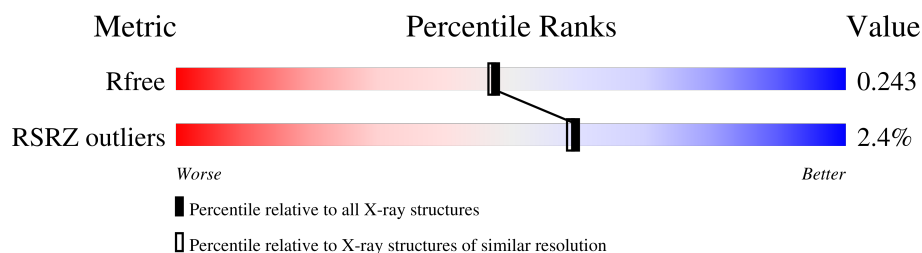
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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}	180053	10052 (2.00-2.00)
RSRZ outliers	180081	10067 (2.00-2.00)

MolProbity failed to run properly - the sequence quality summary graphics cannot be shown.

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	JWH	E	301	-	X	-	-

2 Entry composition [i](#)

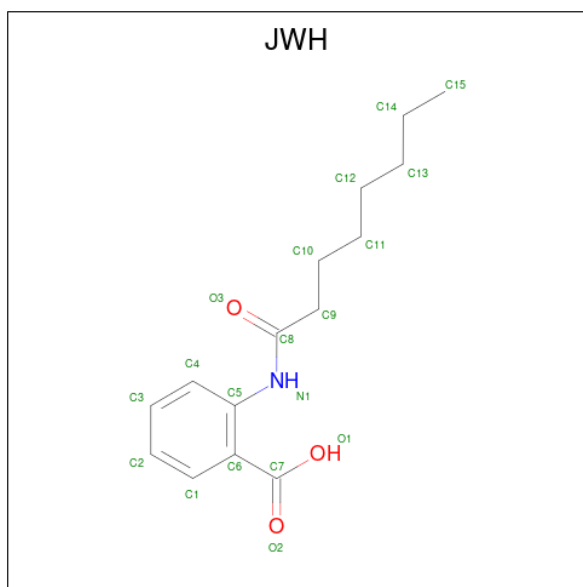
There are 3 unique types of molecules in this entry. The entry contains 12773 atoms, of which 5950 are hydrogens and 0 are deuteriums.

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 Putative dioxygenase (1H-3-hydroxy-4-oxoquinaldine 2,4-dioxygenase).

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	267	Total	C	H	N	O	S	0	0	0
			4056	1312	1982	378	375	9			
1	F	265	Total	C	H	N	O	S	0	0	0
			4006	1296	1956	374	371	9			
1	E	267	Total	C	H	N	O	S	0	0	0
			4070	1315	1992	379	375	9			

- Molecule 2 is 2-(octanoylamino)benzoic acid (CCD ID: JWH) (formula: C₁₅H₂₁NO₃).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	E	1	Total	C	H	N	O	0	0
			39	15	20	1	3		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	156	Total 156	O 156	0	0
3	F	221	Total 221	O 221	0	0
3	E	225	Total 225	O 225	0	0

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3 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α , β , γ	96.17Å 96.17Å 189.62Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.09 – 2.00 48.09 – 2.00	Depositor EDS
% Data completeness (in resolution range)	100.0 (48.09-2.00) 99.9 (48.09-2.00)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.71 (at 2.00Å)	Xtriage
Refinement program	PHENIX 1.12_2829	Depositor
R, R_{free}	0.189 , 0.242 0.191 , 0.243	Depositor DCC
R_{free} test set	4269 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å ²)	29.2	Xtriage
Anisotropy	0.193	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 43.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	12773	wwPDB-VP
Average B, all atoms (Å ²)	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.09% 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](#)

MolProbity failed to run properly - this section is therefore empty.

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

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

4.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

4.6 Ligand geometry [i](#)

1 ligand is 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	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	JWH	E	301	-	19,19,19	3.88	8 (42%)	23,23,23	2.73	10 (43%)

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
2	JWH	E	301	-	-	6/15/15/15	0/1/1/1

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	301	JWH	C1-C6	8.66	1.53	1.39
2	E	301	JWH	C4-C5	8.59	1.53	1.39
2	E	301	JWH	C2-C3	5.58	1.50	1.38
2	E	301	JWH	C6-C5	-5.26	1.32	1.41
2	E	301	JWH	C8-N1	4.59	1.45	1.35
2	E	301	JWH	C2-C1	-4.34	1.31	1.38
2	E	301	JWH	C5-N1	4.30	1.50	1.41
2	E	301	JWH	C3-C4	-3.29	1.33	1.38

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	301	JWH	C5-C6-C7	-7.01	113.90	121.72
2	E	301	JWH	C9-C8-N1	5.81	124.70	114.59
2	E	301	JWH	O3-C8-N1	-5.19	114.34	123.64
2	E	301	JWH	C4-C5-N1	3.43	129.76	121.82
2	E	301	JWH	C1-C6-C5	3.34	122.57	118.81
2	E	301	JWH	C4-C5-C6	-3.09	115.33	119.37
2	E	301	JWH	C6-C5-N1	-2.20	114.75	118.70
2	E	301	JWH	C1-C6-C7	2.13	123.53	118.64
2	E	301	JWH	C3-C2-C1	-2.12	117.62	120.24
2	E	301	JWH	C13-C12-C11	-2.03	104.12	114.37

There are no chirality outliers.

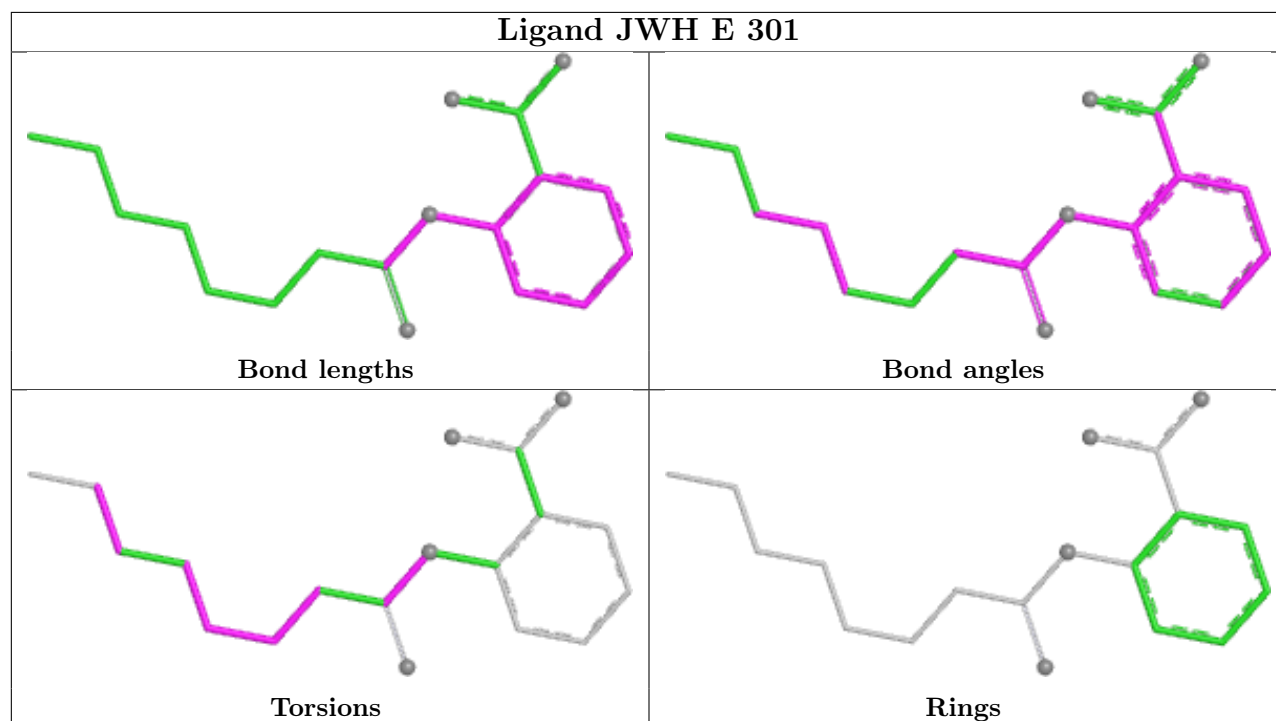
All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	E	301	JWH	O3-C8-N1-C5
2	E	301	JWH	C9-C8-N1-C5
2	E	301	JWH	C11-C10-C9-C8
2	E	301	JWH	C10-C11-C12-C13
2	E	301	JWH	C12-C13-C14-C15
2	E	301	JWH	C9-C10-C11-C12

There are no ring outliers.

No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



4.7 Other polymers [i](#)

There are no such residues in this entry.

4.8 Polymer linkage issues [i](#)

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	267/269 (99%)	0.58	8 (2%) 52 51	27, 47, 65, 90	0
1	E	267/269 (99%)	-0.35	2 (0%) 84 84	18, 29, 53, 92	0
1	F	265/269 (98%)	-0.01	9 (3%) 48 47	17, 35, 58, 91	0
All	All	799/807 (99%)	0.07	19 (2%) 59 59	17, 37, 61, 92	0

All (19) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	217	ILE	4.8
1	A	216	LYS	4.0
1	F	215	PRO	3.8
1	F	217	ILE	3.5
1	A	215	PRO	3.5
1	A	265	ALA	2.8
1	A	220	TYR	2.7
1	F	264	GLY	2.6
1	F	156	GLY	2.5
1	E	156	GLY	2.5
1	A	203	ALA	2.4
1	F	206	CYS	2.4
1	E	214	HIS	2.4
1	F	229	ALA	2.3
1	F	218	GLY	2.3
1	F	216	LYS	2.2
1	A	227	PHE	2.1
1	A	-1	MET	2.1
1	F	252	GLN	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](#)

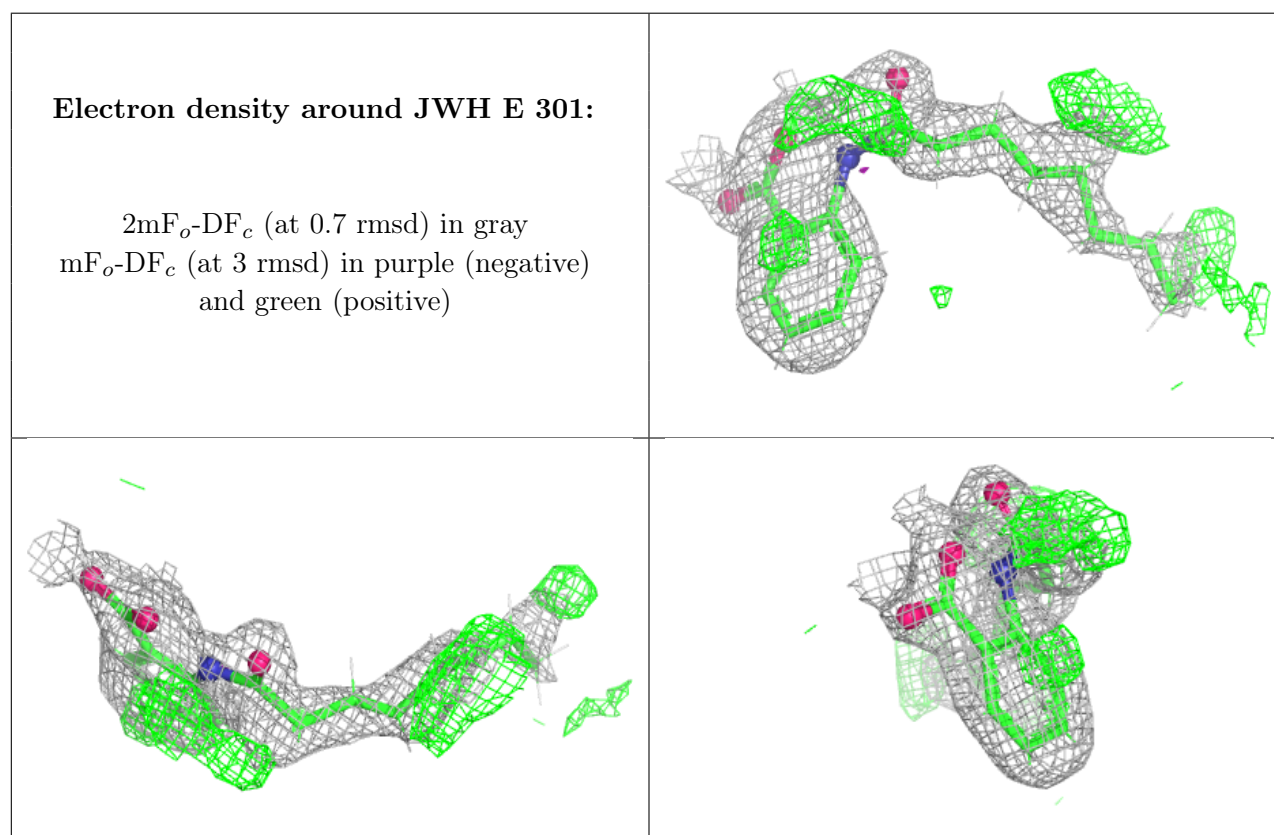
There are no oligosaccharides in this entry.

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. 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	B-factors($\text{\AA}^2$)	Q<0.9
2	JWH	E	301	19/19	0.81	0.16	24,35,43,48	39

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.



5.5 Other polymers [i](#)

There are no such residues in this entry.