wwPDB X-ray Structure Validation Summary Report (i)

May 21, 2020 – 03:09 pm BST

PDB ID	:	4XWS
Title	:	OxyR regulatory domain C199D mutant from pseudomonas aeruginosa
Authors	:	Jo, I.; Kim, J.S.; Ha, N.C.
Deposited on	:	2015-01-29
Resolution	:	3.01 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
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:

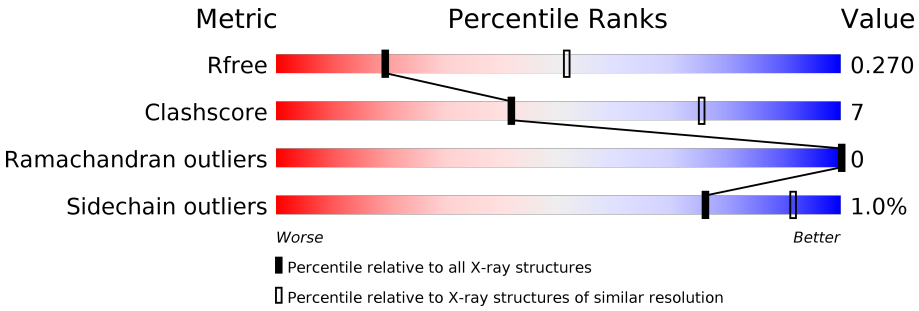
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation 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 3.01 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}	130704	2092 (3.00-3.00)
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)

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%

Mol	Chain	Length	Quality of chain
1	A	227	79% 14% 7%
1	B	227	66% 19% 15%
1	C	227	67% 16% • 16%
1	D	227	74% 12% 15%

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 6176 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 OxyR.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	212	Total	C	N	O	S	0	0	0
			1662	1074	285	298	5			
1	B	192	Total	C	N	O	S	0	0	0
			1506	980	254	268	4			
1	C	191	Total	C	N	O	S	0	0	0
			1490	969	251	266	4			
1	D	194	Total	C	N	O	S	0	0	0
			1518	990	255	269	4			

There are 20 discrepancies between the modelled and reference sequences:

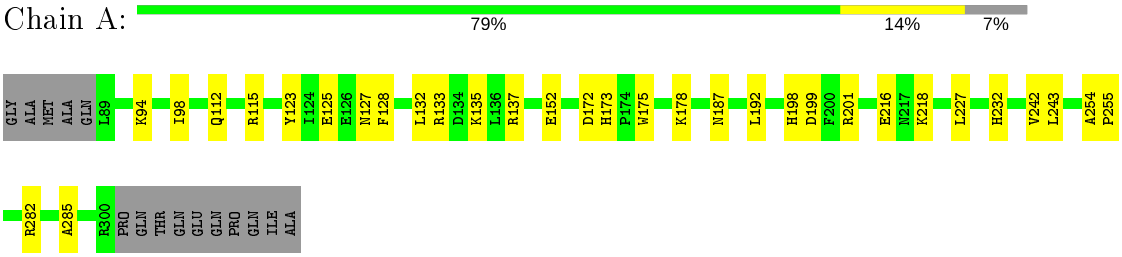
Chain	Residue	Modelled	Actual	Comment	Reference
A	84	GLY	-	expression tag	UNP Q9HTL4
A	85	ALA	-	expression tag	UNP Q9HTL4
A	86	MET	-	expression tag	UNP Q9HTL4
A	87	ALA	-	expression tag	UNP Q9HTL4
A	199	ASP	CYS	engineered mutation	UNP Q9HTL4
B	84	GLY	-	expression tag	UNP Q9HTL4
B	85	ALA	-	expression tag	UNP Q9HTL4
B	86	MET	-	expression tag	UNP Q9HTL4
B	87	ALA	-	expression tag	UNP Q9HTL4
B	199	ASP	CYS	engineered mutation	UNP Q9HTL4
C	84	GLY	-	expression tag	UNP Q9HTL4
C	85	ALA	-	expression tag	UNP Q9HTL4
C	86	MET	-	expression tag	UNP Q9HTL4
C	87	ALA	-	expression tag	UNP Q9HTL4
C	199	ASP	CYS	engineered mutation	UNP Q9HTL4
D	84	GLY	-	expression tag	UNP Q9HTL4
D	85	ALA	-	expression tag	UNP Q9HTL4
D	86	MET	-	expression tag	UNP Q9HTL4
D	87	ALA	-	expression tag	UNP Q9HTL4
D	199	ASP	CYS	engineered mutation	UNP Q9HTL4

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.

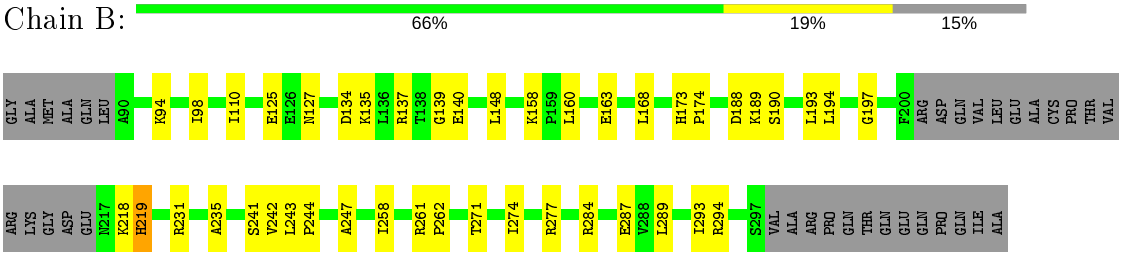
- Molecule 1: OxyR

Chain A:



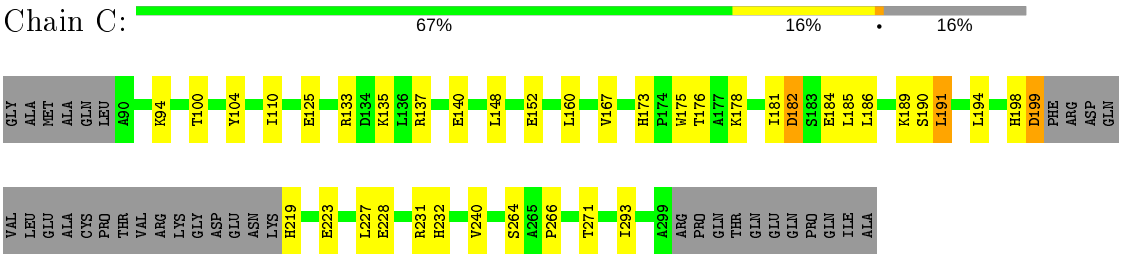
- Molecule 1: OxyR

Chain B:



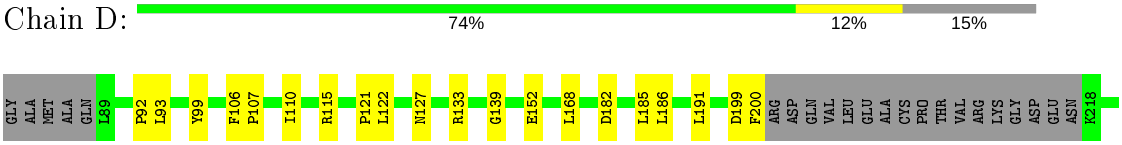
- Molecule 1: OxyR

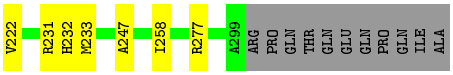
Chain C:



- Molecule 1: OxyR

Chain D:




V222
R231
H232
M233
A247
I258
R277
A299
ARG
PRO
GLN
THR
GLN
GLU
GLN
PRO
GLN
ILE
ALA

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 61	Depositor
Cell constants a, b, c, α, β, γ	129.94Å 129.94Å 135.69Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	19.99 – 3.01 43.31 – 3.01	Depositor EDS
% Data completeness (in resolution range)	97.4 (19.99-3.01) 98.1 (43.31-3.01)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.85 (at 3.01Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.4_1496)	Depositor
R, R_{free}	0.229 , 0.260 0.237 , 0.270	Depositor DCC
R_{free} test set	2004 reflections (7.88%)	wwPDB-VP
Wilson B-factor (Å^2)	61.3	Xtriage
Anisotropy	0.157	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 5.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.29$	Xtriage
Estimated twinning fraction	0.077 for h,-h-k,-l	Xtriage
F_o,F_c correlation	0.82	EDS
Total number of atoms	6176	wwPDB-VP
Average B, all atoms (Å^2)	60.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 23.83 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 4.3128e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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	A	0.23	0/1708	0.46	0/2333
1	B	0.22	0/1550	0.43	0/2118
1	C	0.25	0/1533	0.52	2/2097 (0.1%)
1	D	0.20	0/1562	0.39	0/2135
All	All	0.23	0/6353	0.45	2/8683 (0.0%)

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
1	C	0	1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	199	ASP	CB-CG-OD1	5.68	123.41	118.30
1	C	185	LEU	CA-CB-CG	5.32	127.52	115.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	182	ASP	Peptide

5.2 Too-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 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	A	1662	0	1677	20	0
1	B	1506	0	1515	28	0
1	C	1490	0	1501	27	0
1	D	1518	0	1534	15	0
All	All	6176	0	6227	87	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 7.

The worst 5 of 87 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)
1:B:158:LYS:HE2	1:B:294:ARG:HH12	1.33	0.91
1:C:100:THR:HG22	1:C:227:LEU:HD21	1.51	0.91
1:B:193:LEU:HD12	1:B:219:HIS:CD2	2.14	0.82
1:C:125:GLU:OE2	1:C:135:LYS:NZ	2.13	0.81
1:C:194:LEU:H	1:C:198:HIS:HD2	1.28	0.80

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	A	210/227 (92%)	198 (94%)	12 (6%)	0	100	100
1	B	188/227 (83%)	175 (93%)	13 (7%)	0	100	100
1	C	187/227 (82%)	176 (94%)	11 (6%)	0	100	100
1	D	190/227 (84%)	184 (97%)	6 (3%)	0	100	100
All	All	775/908 (85%)	733 (95%)	42 (5%)	0	100	100

There are no Ramachandran outliers to report.

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	A	182/193 (94%)	181 (100%)	1 (0%)	88 96
1	B	165/193 (86%)	164 (99%)	1 (1%)	86 95
1	C	163/193 (84%)	158 (97%)	5 (3%)	40 75
1	D	166/193 (86%)	166 (100%)	0	100 100
All	All	676/772 (88%)	669 (99%)	7 (1%)	76 91

5 of 7 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	190	SER
1	C	223	GLU
1	C	191	LEU
1	B	219	HIS
1	C	199	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	173	HIS
1	C	198	HIS

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

There are no ligands in this entry.

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

Unable to reproduce the depositors R factor - this section is therefore empty.

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

Unable to reproduce the depositors R factor - this section is therefore empty.

6.3 Carbohydrates

Unable to reproduce the depositors R factor - this section is therefore empty.

6.4 Ligands

Unable to reproduce the depositors R factor - this section is therefore empty.

6.5 Other polymers

Unable to reproduce the depositors R factor - this section is therefore empty.