Full wwPDB X-ray Structure Validation Report ⓘ

Dec 3, 2023 – 07:30 am GMT

PDB ID	:	2WFB
Title	:	High resolution structure of the apo form of the orange protein (ORP) from Desulfovibrio gigas
Authors	:	Najmudin, S.; Bonifacio, C.; Duarte, A.G.; Pereira, A.S.; Moura, I.; Moura, J.M.; Romao, M.J.
Deposited on	:	2009-04-03
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:

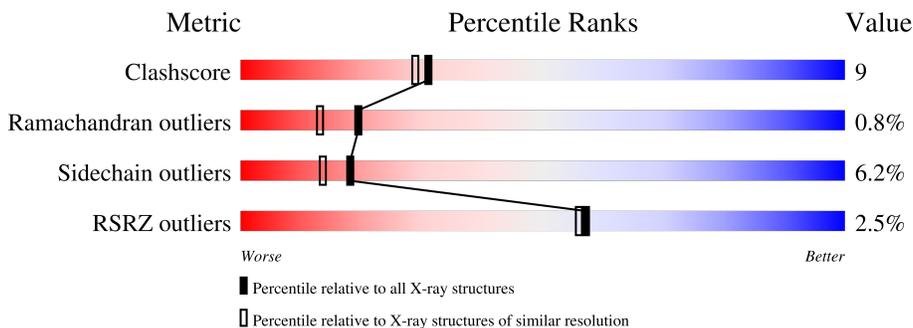|		
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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	Percentile Ranks	Value
Clashscore		9
Ramachandran outliers		0.8%
Sidechain outliers		6.2%
RSRZ outliers		2.5%

Worse   *Better*

■ Percentile relative to all X-ray structures
▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (2.00-2.00)

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
3	ACT	A	1124	-	-	X	-

2 Entity composition ⓘ

There are 4 unique types of molecules in this entry. The entry contains 958 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 PUTATIVE UNCHARACTERIZED PROTEIN ORP.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	120	Total 861	C 539	N 156	O 162	S 4	0	2	0

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	ALA	-	expression tag	UNP Q5DUA6
A	2	SER	-	expression tag	UNP Q5DUA6
A	3	HIS	-	expression tag	UNP Q5DUA6

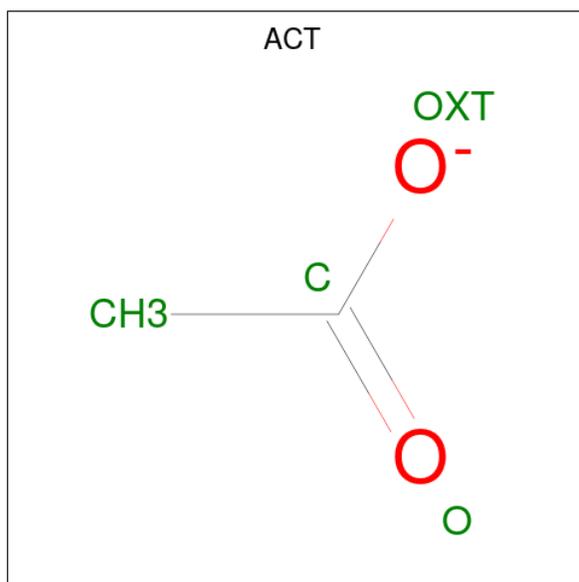- Molecule 2 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).
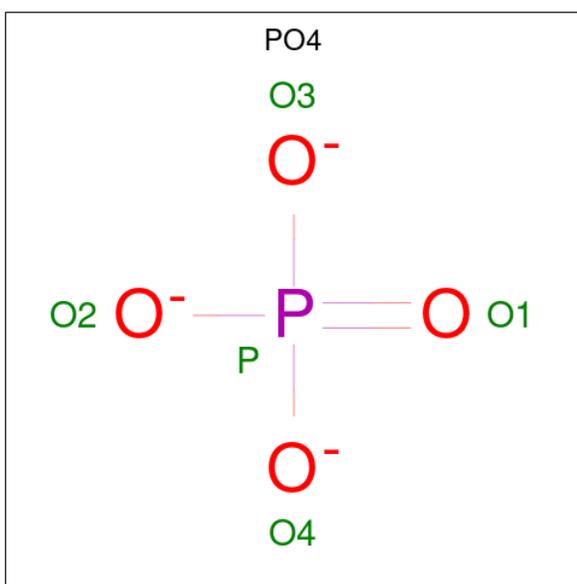
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total 5	O 4	P 1	0	0
2	A	1	Total 5	O 4	P 1	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total 5	O 4	P 1	0	0

- Molecule 3 is ACETATE ION (three-letter code: ACT) (formula: $C_2H_3O_2$).

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total 4	C 2	O 2	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	78	Total 78	O 78	0	0

SEQUENCE-PLOTS INFOmissingINFO

3 Data and refinement statistics ⓘ

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α, β, γ	43.08Å 43.08Å 106.08Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	106.00 – 2.00 106.09 – 1.79	Depositor EDS
% Data completeness (in resolution range)	90.5 (106.00-2.00) 73.6 (106.09-1.79)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.07 (at 1.79Å)	Xtriage
Refinement program	REFMAC 5.5.0036	Depositor
R, R_{free}	0.183 , 0.244 (Not available) , (Not available)	Depositor DCC
R_{free} test set	401 reflections (4.77%)	wwPDB-VP
Wilson B-factor (Å^2)	23.3	Xtriage
Anisotropy	0.112	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.44 , 58.5	EDS
L-test for twinning[2]	$< |L| > = 0.48, < L^2 > = 0.31$	Xtriage
Estimated twinning fraction	0.051 for -h,-k,l	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	958	wwPDB-VP
Average B, all atoms (Å^2)	22.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.84% of the height of the origin peak. No significant pseudotranslation is detected.*

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[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.

4 Model quality ⓘ

4.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: PO4, ACT

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	0.63	0/879	0.79	1/1190 (0.1%)

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	A	0	2

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	37	THR	N-CA-C	6.05	127.35	111.00

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	36	ALA	Peptide
1	A	37	THR	Peptide

4.2 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.

WORLDWIDE
wwPDB
PROTEIN DATA BANK

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	861	0	874	16	0
2	A	15	0	0	0	0
3	A	4	0	3	5	1
4	A	78	0	0	1	1
All	All	958	0	877	16	2

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 9.

All (16) 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:A:26:ARG:HD3	3:A:1124:ACT:H2	1.20	1.19
1:A:37:THR:HB	1:A:39:ALA:H	1.26	1.00
1:A:26:ARG:CD	3:A:1124:ACT:H2	2.01	0.89
1:A:26:ARG:HD3	3:A:1124:ACT:CH3	2.07	0.83
1:A:23:ARG:HH22	3:A:1124:ACT:H1	1.45	0.82
1:A:37:THR:HB	1:A:39:ALA:N	1.95	0.81
1:A:36:ALA:HA	1:A:37:THR:O	1.91	0.71
1:A:23:ARG:HH22	3:A:1124:ACT:CH3	2.09	0.64
1:A:63:LEU:HD11	1:A:71:LEU:HD13	1.81	0.63
1:A:33:VAL:HG12	1:A:40:ALA:HB2	1.83	0.61
1:A:106:ARG:NH2	4:A:2056:HOH:O	2.33	0.55
1:A:34:ASP:O	1:A:38:MET:HA	2.07	0.55
1:A:3:HIS:HB2	1:A:6:ARG:HG3	1.92	0.52
1:A:3:HIS:HB2	1:A:6:ARG:CG	2.46	0.45
1:A:63:LEU:CD1	1:A:71:LEU:HD13	2.48	0.44
1:A:33:VAL:HG21	1:A:104:VAL:HG21	2.02	0.42

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:1124:ACT:CH3	3:A:1124:ACT:CH3[6_555]	2.03	0.17
4:A:2026:HOH:O	4:A:2036:HOH:O[6_655]	2.16	0.04

4.3 Torsion angles ⓘ

4.3.1 Protein backbone ⓘ

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	120/120 (100%)	116 (97%)	3 (2%)	1 (1%)	19	13

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	37	THR

4.3.2 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	83/81 (102%)	78 (94%)	5 (6%)	19	14

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

Mol	Chain	Res	Type
1	A	6	ARG
1	A	37	THR
1	A	72	LEU
1	A	90	LYS
1	A	120	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	58	ASN

4.3.3 RNA ⓘ

There are no RNA molecules in this entry.

4.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

4.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

4.6 Ligand geometry ⓘ

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	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	PO4	A	1123	-	4,4,4	0.98	0	6,6,6	0.66	0
2	PO4	A	1122	-	4,4,4	1.00	0	6,6,6	0.92	0
3	ACT	A	1124	-	3,3,3	0.73	0	3,3,3	1.33	0
2	PO4	A	1121	-	4,4,4	1.49	0	6,6,6	0.61	0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1124	ACT	5	1

4.7 Other polymers ⓘ

There are no such residues in this entry.

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(Å²)	Q<0.9
1	A	120/120 (100%)	-0.61	3 (2%)	57	56	13, 20, 36, 44	0

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1	ALA	3.4
1	A	36	ALA	2.7
1	A	37	THR	2.0

5.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.4 Ligands ⓘ

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(Å²)	Q<0.9
3	ACT	A	1124	4/4	0.90	0.12	26,26,27,27	0
2	PO4	A	1123	5/5	0.96	0.14	37,38,40,42	0
2	PO4	A	1121	5/5	0.99	0.07	20,20,21,22	0
2	PO4	A	1122	5/5	0.99	0.07	28,29,30,31	0

5.5 Other polymers ⓘ

There are no such residues in this entry.