Full wwPDB X-ray Structure Validation Report (i)

Sep 3, 2023 – 07:05 PM EDT

PDB ID	:	3T00
Title	:	Crystal Structure of Phosphonoacetate hydrolase from Sinorhizobium meliloti 1021 in complex with vanadate
Authors	:	Agarwal, V.; Nair, S.K.
Deposited on	:	2011-07-19
Resolution	:	1.80 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 types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

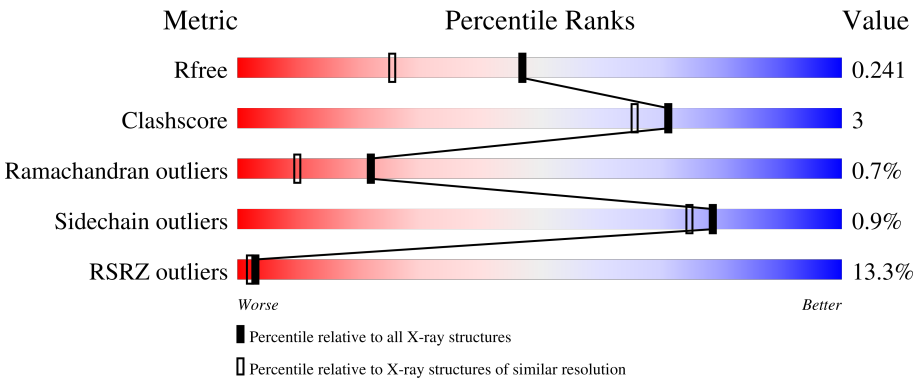
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

1 Overall quality at a glance (i)

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

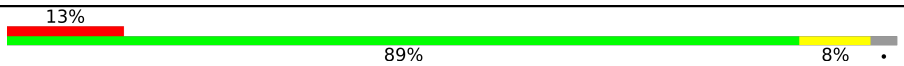
The reported resolution of this entry is 1.80 Å.

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	5950 (1.80-1.80)
Clashscore	141614	6793 (1.80-1.80)
Ramachandran outliers	138981	6697 (1.80-1.80)
Sidechain outliers	138945	6696 (1.80-1.80)
RSRZ outliers	127900	5850 (1.80-1.80)

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 of 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% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	427	

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 3553 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 phosphonoacetate hydrolase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	413	3194	2030	557	593	14	0	2	0

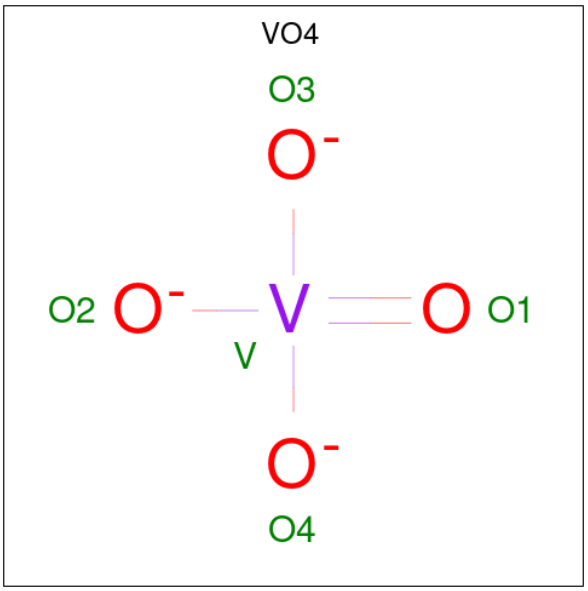
There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	GLY	-	expression tag	UNP Q92UV8
A	-1	SER	-	expression tag	UNP Q92UV8
A	0	HIS	-	expression tag	UNP Q92UV8

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Zn		
2	A	2	2	2	0	0

- Molecule 3 is VANADATE ION (three-letter code: VO4) (formula: O_4V).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total O V 5 4 1	0	0

- Molecule 4 is NICKEL (II) ION (three-letter code: NI) (formula: Ni).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total Ni 1 1	0	0

- Molecule 5 is water.

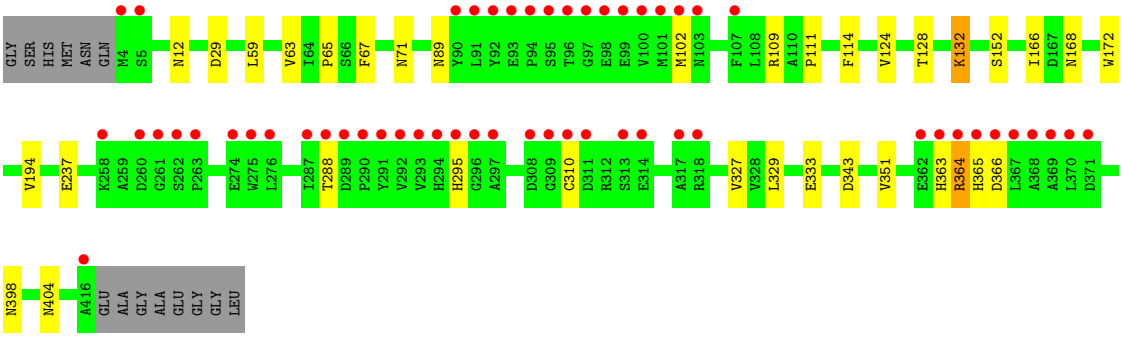
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	351	Total O 351 351	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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 and electron density. 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. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). 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: phosphonoacetate hydrolase

Chain A:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α, β, γ	111.12Å 111.12Å 72.44Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	25.00 – 1.80 34.54 – 1.80	Depositor EDS
% Data completeness (in resolution range)	98.1 (25.00-1.80) 98.1 (34.54-1.80)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.27 (at 1.79Å)	Xtriage
Refinement program	REFMAC 5.5.0056	Depositor
R, R_{free}	0.205 , 0.241 0.205 , 0.241	Depositor DCC
R_{free} test set	2111 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å^2)	23.6	Xtriage
Anisotropy	0.059	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 46.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	3553	wwPDB-VP
Average B, all atoms (Å^2)	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.89% of the height of the origin peak. No significant pseudotranslation is detected.*

[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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: VO4, NI, ZN

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	0.40	0/3273	0.54	0/4451

There are no bond length outliers.

There are no bond angle outliers.

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	A	3194	0	3166	22	0
2	A	2	0	0	0	0
3	A	5	0	0	0	0
4	A	1	0	0	0	0
5	A	351	0	0	2	0
All	All	3553	0	3166	22	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 3.

All (22) 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:63:VAL:H	1:A:71:ASN:HD21	1.23	0.83
1:A:89:ASN:HD22	1:A:288:THR:HA	1.44	0.81
1:A:363:HIS:O	1:A:364:ARG:HB2	1.90	0.71
1:A:132:LYS:HG3	5:A:486:HOH:O	1.94	0.67
1:A:114:PHE:HB3	1:A:124:VAL:HG11	1.86	0.57
1:A:71:ASN:HD22	1:A:404:ASN:HD21	1.53	0.57
1:A:63:VAL:N	1:A:71:ASN:HD21	2.01	0.54
1:A:63:VAL:H	1:A:71:ASN:ND2	1.99	0.54
1:A:109:ARG:NH2	1:A:343:ASP:OD2	2.40	0.53
1:A:12:ASN:HD21	1:A:111:PRO:HD2	1.75	0.51
1:A:166:ILE:HD11	1:A:172:TRP:CD2	2.47	0.50
1:A:71:ASN:ND2	1:A:404:ASN:HD21	2.09	0.50
1:A:65:PRO:HB2	1:A:67:PHE:CD2	2.49	0.48
1:A:329:LEU:HD22	1:A:333:GLU:HG2	1.98	0.46
1:A:29:ASP:HB2	5:A:581:HOH:O	2.16	0.46
1:A:59:LEU:H	1:A:398:ASN:HD21	1.64	0.45
1:A:194:VAL:HG11	1:A:237:GLU:CD	2.39	0.44
1:A:166:ILE:HD11	1:A:172:TRP:CG	2.55	0.42
1:A:365:HIS:CG	1:A:366:ASP:H	2.38	0.41
1:A:327:VAL:HB	1:A:351:VAL:HB	2.02	0.41
1:A:365:HIS:CD2	1:A:366:ASP:H	2.39	0.41
1:A:128:THR:O	1:A:152:SER:HA	2.20	0.41

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	413/427 (97%)	401 (97%)	9 (2%)	3 (1%)	22 10

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	295	HIS
1	A	364	ARG
1	A	168	ASN

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	A	335/341 (98%)	332 (99%)	3 (1%)	78 75

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	102	MET
1	A	132	LYS
1	A	310	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	12	ASN
1	A	71	ASN
1	A	72	ASN
1	A	89	ASN
1	A	257	HIS
1	A	398	ASN

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 monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 4 ligands modelled in this entry, 3 are monoatomic - leaving 1 for Mogul analysis.

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	$\#\|Z\| > 2$
3	VO4	A	503	1,2	1,4,4	4.62	1 (100%)	-		

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	503	VO4	O1-V	4.62	1.90	1.63

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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)

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	413/427 (96%)	0.95	55 (13%) 3 2	13, 22, 60, 67	0

All (55) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	292	VAL	24.5
1	A	291	TYR	16.2
1	A	293	VAL	14.0
1	A	290	PRO	12.5
1	A	367	LEU	12.2
1	A	294	HIS	12.1
1	A	370	LEU	12.1
1	A	295	HIS	11.3
1	A	371	ASP	11.1
1	A	363	HIS	10.7
1	A	369	ALA	10.6
1	A	296	GLY	8.8
1	A	96	THR	8.8
1	A	364	ARG	8.1
1	A	368	ALA	7.3
1	A	90	TYR	6.4
1	A	94	PRO	6.3
1	A	107	PHE	5.2
1	A	101	MET	5.2
1	A	366	ASP	5.1
1	A	365	HIS	5.1
1	A	289	ASP	5.0
1	A	100	VAL	5.0
1	A	91	LEU	5.0
1	A	260	ASP	4.4
1	A	288	THR	4.4
1	A	98	GLU	4.2

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Mol	Chain	Res	Type	RSRZ
1	A	310	CYS	4.1
1	A	95	SER	4.0
1	A	308	ASP	3.7
1	A	4	MET	3.7
1	A	309	GLY	3.6
1	A	103	ASN	3.5
1	A	97	GLY	3.5
1	A	275	TRP	3.3
1	A	99	GLU	3.1
1	A	92	TYR	3.0
1	A	93	GLU	2.9
1	A	102	MET	2.9
1	A	362	GLU	2.7
1	A	311	ASP	2.7
1	A	314	GLU	2.7
1	A	313	SER	2.7
1	A	317	ALA	2.6
1	A	258	LYS	2.5
1	A	318	ARG	2.5
1	A	274	GLU	2.4
1	A	261	GLY	2.4
1	A	262	SER	2.4
1	A	297	ALA	2.3
1	A	287	ILE	2.3
1	A	263	PRO	2.3
1	A	5	SER	2.3
1	A	276	LEU	2.2
1	A	416	ALA	2.1

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 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(Å^2)	Q<0.9
3	VO4	A	503	5/5	0.92	0.13	29,31,32,33	0
2	ZN	A	501	1/1	0.98	0.07	33,33,33,33	0
2	ZN	A	502	1/1	0.99	0.05	30,30,30,30	0
4	NI	A	504	1/1	1.00	0.04	26,26,26,26	0

6.5 Other polymers (i)

There are no such residues in this entry.