



# Full wwPDB X-ray Structure Validation Report ⓘ

Jul 26, 2016 – 01:52 AM EDT

PDB ID : 5IOJ  
Title : Crystal structure of the Sphingobium sp. TCM1 phosphotriesterase without the binuclear manganese center  
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Deposited on : 2016-03-08  
Resolution : 1.76 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](mailto: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.

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

MolProbity	:	4.02b-467
Mogul	:	unknown
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20027939
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
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-20027939



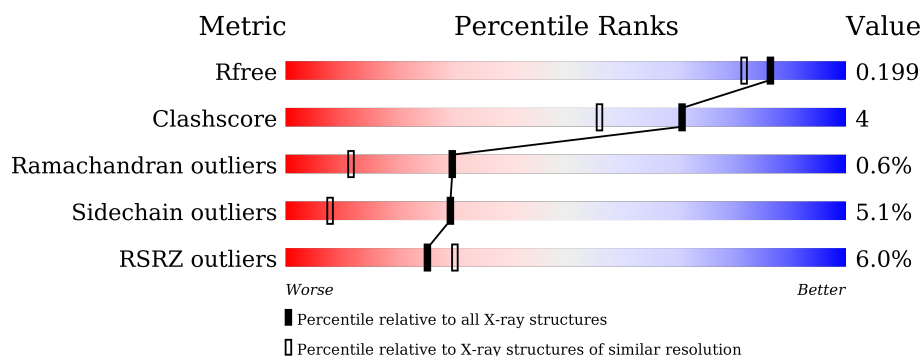
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.76 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))
$R_{free}$	91344	1609 (1.76-1.76)
Clashscore	102246	1730 (1.76-1.76)
Ramachandran outliers	100387	1711 (1.76-1.76)
Sidechain outliers	100360	1711 (1.76-1.76)
RSRZ outliers	91569	1610 (1.76-1.76)

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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  $\leq 5\%$ . 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	591	<div> <div>6%</div> <div> <div></div> <div>72%</div> <div>9%</div> <div>•</div> <div>16%</div> </div> </div>
1	B	591	<div> <div>4%</div> <div> <div></div> <div>75%</div> <div>7%</div> <div>•</div> <div>16%</div> </div> </div>



## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 8458 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 Haloalkylphosphorus hydrolase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	494	Total	C	N	O	S	0	1	0
			3753	2361	681	699	12			
1	B	495	Total	C	N	O	S	0	0	0
			3753	2361	681	699	12			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	584	LEU	-	expression tag	UNP A0A077JBW9
A	585	GLU	-	expression tag	UNP A0A077JBW9
A	586	HIS	-	expression tag	UNP A0A077JBW9
A	587	HIS	-	expression tag	UNP A0A077JBW9
A	588	HIS	-	expression tag	UNP A0A077JBW9
A	589	HIS	-	expression tag	UNP A0A077JBW9
A	590	HIS	-	expression tag	UNP A0A077JBW9
A	591	HIS	-	expression tag	UNP A0A077JBW9
B	584	LEU	-	expression tag	UNP A0A077JBW9
B	585	GLU	-	expression tag	UNP A0A077JBW9
B	586	HIS	-	expression tag	UNP A0A077JBW9
B	587	HIS	-	expression tag	UNP A0A077JBW9
B	588	HIS	-	expression tag	UNP A0A077JBW9
B	589	HIS	-	expression tag	UNP A0A077JBW9
B	590	HIS	-	expression tag	UNP A0A077JBW9
B	591	HIS	-	expression tag	UNP A0A077JBW9

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	445	Total	O	0	0
			445	445		
2	B	507	Total	O	0	0
			507	507		







## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	88.31Å 93.92Å 112.49Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.96 – 1.76 39.96 – 1.76	Depositor EDS
% Data completeness (in resolution range)	99.8 (39.96-1.76) 99.8 (39.96-1.76)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.87 (at 1.76Å)	Xtriage
Refinement program	REFMAC	Depositor
R, $R_{free}$	0.161 , 0.192 0.166 , 0.199	Depositor DCC
$R_{free}$ test set	2001 reflections (2.19%)	DCC
Wilson B-factor (Å <sup>2</sup> )	20.7	Xtriage
Anisotropy	0.754	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 55.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	8458	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 11.10% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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.



## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

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	0.35	0/3843	0.58	0/5233
1	B	0.38	0/3843	0.60	4/5233 (0.1%)
All	All	0.36	0/7686	0.59	4/10466 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	498	ARG	NE-CZ-NH2	-6.80	116.90	120.30
1	B	498	ARG	NE-CZ-NH1	6.10	123.35	120.30
1	B	211	ARG	NE-CZ-NH2	-5.54	117.53	120.30
1	B	214	LEU	CA-CB-CG	5.16	127.16	115.30

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	3753	0	3708	44	0
1	B	3753	0	3709	21	0
2	A	445	0	0	10	0
2	B	507	0	0	4	0
All	All	8458	0	7417	65	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 4.

All (65) 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:562:THR:HG23	1:A:565:HIS:HE1	1.42	0.84
1:A:516:PRO:HB2	1:A:562:THR:HG21	1.61	0.81
1:B:88:GLN:OE1	1:B:576:ARG:NH2	2.16	0.78
1:B:435:LEU:HD21	1:B:498:ARG:HD2	1.68	0.75
1:A:562:THR:HG23	1:A:565:HIS:CE1	2.24	0.73
1:B:211:ARG:NH2	1:B:290:ILE:O	2.24	0.69
1:A:274[B]:VAL:HG23	1:A:315:THR:HB	1.75	0.68
1:A:274[A]:VAL:HG12	1:A:278:LEU:HD23	1.78	0.66
1:A:375:PRO:HA	1:A:376:LYS:HB2	1.77	0.65
1:A:507:LYS:NZ	2:A:605:HOH:O	2.30	0.64
1:A:352:ASP:N	1:A:353:VAL:HG22	2.14	0.62
1:A:274[A]:VAL:HG13	1:A:315:THR:HB	1.81	0.61
1:A:151:THR:HG21	1:A:173:GLY:H	1.66	0.61
1:A:559:CYS:HB2	1:A:562:THR:HG22	1.85	0.58
1:A:452:LYS:NZ	2:A:606:HOH:O	2.33	0.58
1:B:498:ARG:HD3	1:B:510:GLU:OE1	2.05	0.57
1:B:326:ARG:NH2	1:B:370:ASP:OD1	2.38	0.57
1:A:146:CYS:SG	1:A:243:LEU:HD13	2.45	0.56
1:A:349:SER:O	2:A:601:HOH:O	2.18	0.55
1:A:378:ARG:NH1	2:A:609:HOH:O	2.38	0.55
1:B:194:ARG:NH2	2:B:606:HOH:O	2.39	0.54
1:A:487:LEU:HD21	1:A:569:LEU:HD11	1.88	0.54
1:B:350:ASP:HB3	1:B:451:ARG:HH12	1.72	0.54
1:A:421:ILE:HG22	1:A:427:PRO:HB3	1.89	0.53
1:B:372:ARG:HG2	1:B:373:SER:O	2.09	0.53
1:B:151:THR:HG21	1:B:173:GLY:H	1.73	0.53
1:A:367:ASP:HB3	1:A:375:PRO:HB3	1.91	0.53
1:A:444:ASP:OD1	2:A:602:HOH:O	2.19	0.52
1:A:151:THR:CG2	1:A:173:GLY:H	2.21	0.52
1:A:516:PRO:CB	1:A:562:THR:HG21	2.35	0.52
1:B:134:ARG:HB2	1:B:171:PRO:HG2	1.92	0.51
1:A:98:GLU:OE2	1:A:498:ARG:NH2	2.34	0.50
1:B:351:GLY:HA2	1:B:352:ASP:HB2	1.96	0.48
1:B:93:PRO:HA	1:B:94:GLY:HA2	1.67	0.48
1:A:435:LEU:HD21	1:A:498:ARG:HD2	1.94	0.47
1:B:288:LEU:HD11	1:B:296:PRO:HB2	1.95	0.47
1:B:272:THR:HB	1:B:316:PRO:O	2.14	0.47
1:A:428:LYS:HB3	1:A:428:LYS:HE3	1.57	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:274[B]:VAL:HG21	1:A:317:HIS:NE2	2.30	0.46
1:A:487:LEU:HD22	1:A:579:PHE:CZ	2.50	0.46
1:A:120:HIS:HE1	2:A:983:HOH:O	1.99	0.46
1:A:169:ARG:NH2	2:A:608:HOH:O	2.37	0.45
1:A:134:ARG:HB2	1:A:171:PRO:HG2	1.99	0.45
1:B:351:GLY:HA2	1:B:352:ASP:CB	2.46	0.45
1:B:444:ASP:OD2	2:B:601:HOH:O	2.21	0.45
1:B:132:TRP:CZ2	1:B:187:PRO:HB2	2.52	0.44
1:A:367:ASP:CG	1:A:378:ARG:HH12	2.20	0.44
1:A:451:ARG:NE	2:A:602:HOH:O	2.30	0.44
1:B:432:GLU:OE2	2:B:602:HOH:O	2.21	0.44
1:A:274[B]:VAL:HG22	1:A:278:LEU:HD23	1.99	0.43
1:A:449:THR:HG21	2:B:1025:HOH:O	2.18	0.43
1:A:554:HIS:HE1	2:A:624:HOH:O	2.01	0.43
1:A:367:ASP:OD1	1:A:372:ARG:HD2	2.19	0.42
1:A:151:THR:HG22	2:A:672:HOH:O	2.20	0.42
1:A:136:GLY:O	1:A:151:THR:HA	2.20	0.42
1:A:547:ARG:HB3	1:A:556:TRP:HB2	2.01	0.42
1:A:272:THR:HB	1:A:316:PRO:O	2.19	0.42
1:B:317:HIS:HB2	1:B:388:PHE:O	2.19	0.42
1:A:340:VAL:HA	1:A:341:PRO:HD3	1.88	0.42
1:A:551:GLU:CD	1:A:551:GLU:H	2.23	0.42
1:A:135:GLY:HA2	1:A:561:THR:HA	2.01	0.41
1:A:367:ASP:HA	1:A:372:ARG:HD2	2.02	0.41
1:B:435:LEU:CD2	1:B:498:ARG:HD2	2.45	0.41
1:B:358:GLY:HA3	1:B:388:PHE:HB3	2.03	0.41
1:A:357:ASN:HB2	1:A:385:GLN:OE1	2.21	0.41

There are no symmetry-related clashes.

## 5.3 Torsion angles ⓘ

### 5.3.1 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	493/591 (83%)	470 (95%)	19 (4%)	4 (1%)	24	8
1	B	493/591 (83%)	470 (95%)	21 (4%)	2 (0%)	39	19
All	All	986/1182 (83%)	940 (95%)	40 (4%)	6 (1%)	30	12

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	376	LYS
1	A	352	ASP
1	A	200	VAL
1	B	200	VAL
1	A	406	ALA
1	B	406	ALA

### 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	399/476 (84%)	377 (94%)	22 (6%)	27	7
1	B	399/476 (84%)	380 (95%)	19 (5%)	31	9
All	All	798/952 (84%)	757 (95%)	41 (5%)	29	8

All (41) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	90	VAL
1	A	91	ILE
1	A	138	LEU
1	A	166	LEU
1	A	188	VAL
1	A	243	LEU
1	A	247	LEU
1	A	310	LEU
1	A	314	PHE
1	A	349	SER

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Mol	Chain	Res	Type
1	A	352	ASP
1	A	353	VAL
1	A	408	LEU
1	A	417	ARG
1	A	428	LYS
1	A	449	THR
1	A	477	ASN
1	A	487	LEU
1	A	551	GLU
1	A	562	THR
1	A	572	ASP
1	A	581	THR
1	B	88	GLN
1	B	151	THR
1	B	158	ILE
1	B	166	LEU
1	B	186	LYS
1	B	206	ILE
1	B	211	ARG
1	B	214	LEU
1	B	295	ARG
1	B	314	PHE
1	B	339	ASP
1	B	352	ASP
1	B	373	SER
1	B	417	ARG
1	B	449	THR
1	B	477	ASN
1	B	487	LEU
1	B	577	LEU
1	B	582	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 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 [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

## 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

### 6.1 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	494/591 (83%)	0.53	34 (6%)	20 25	32, 41, 61, 115	0
1	B	495/591 (83%)	0.47	25 (5%)	32 37	31, 37, 59, 106	0
All	All	989/1182 (83%)	0.50	59 (5%)	25 30	31, 39, 60, 115	0

All (59) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	351	GLY	6.9
1	A	350	ASP	4.9
1	A	451	ARG	4.8
1	B	572	ASP	4.7
1	B	582	VAL	4.2
1	B	90	VAL	4.2
1	A	90	VAL	4.2
1	B	575	ALA	3.9
1	A	93	PRO	3.7
1	A	571	PRO	3.6
1	B	350	ASP	3.6
1	B	349	SER	3.5
1	A	581	THR	3.5
1	A	88	GLN	3.4
1	A	575	ALA	3.3
1	B	353	VAL	3.3
1	A	354	PRO	3.3
1	A	352	ASP	3.3
1	B	92	GLY	3.3
1	A	577	LEU	3.2
1	A	493	PHE	3.2
1	B	581	THR	3.2
1	B	93	PRO	3.1
1	B	546	VAL	3.1

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Mol	Chain	Res	Type	RSRZ
1	B	351	GLY	3.1
1	A	140	LEU	3.0
1	A	399	VAL	3.0
1	B	372	ARG	2.9
1	B	580	PRO	2.8
1	A	483	ARG	2.8
1	A	397	ASN	2.6
1	B	224	ALA	2.6
1	A	580	PRO	2.6
1	A	302	PHE	2.6
1	B	91	ILE	2.6
1	A	353	VAL	2.5
1	A	497	VAL	2.5
1	A	422	ALA	2.5
1	B	88	GLN	2.5
1	A	578	GLY	2.4
1	B	392	VAL	2.4
1	A	188	VAL	2.4
1	B	577	LEU	2.4
1	A	492	PHE	2.4
1	B	406	ALA	2.3
1	A	225	GLY	2.3
1	A	557	PHE	2.3
1	B	476	PHE	2.3
1	A	274[A]	VAL	2.2
1	B	571	PRO	2.2
1	A	546	VAL	2.1
1	B	185	PRO	2.1
1	B	261	THR	2.1
1	A	476	PHE	2.1
1	A	91	ILE	2.1
1	A	312	ALA	2.0
1	B	352	ASP	2.0
1	A	491	PRO	2.0
1	A	471	ALA	2.0

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

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



### 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

### 6.4 Ligands [i](#)

There are no ligands in this entry.

### 6.5 Other polymers [i](#)

There are no such residues in this entry.