

wwPDB X-ray Structure Validation Summary Report (i)

May 22, 2020 – 08:33 pm BST

PDB ID : 3WWD

Title: The complex of pOPH S172C with DMSO

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G.C.

Deposited on : 2014-06-17

Resolution : 1.65 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

Mogul: 1.8.5 (274361), CSD as541be (2020)

Xtriage (Phenix) : 1.13 EDS : 2.11

Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)

Refmac: 5.8.0158

 $\begin{array}{cccc} & CCP4 & : & 7.0.044 \; (Gargrove) \\ Ideal \; geometry \; (proteins) & : & Engh \; \& \; Huber \; (2001) \end{array}$

Ideal geometry (DNA, RNA) : Parkinson et al. (1996)

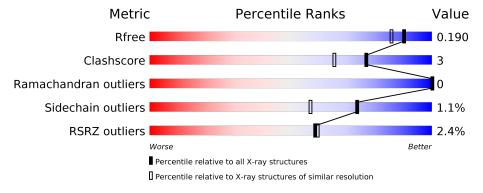
Validation Pipeline (wwPDB-VP) : 2.11

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 1.65 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	$\begin{array}{c} \text{Whole archive} \\ (\#\text{Entries}) \end{array}$	$\begin{array}{c} {\rm Similar \; resolution} \\ (\#{\rm Entries, \; resolution \; range(\AA)}) \end{array}$
R_{free}	130704	1827 (1.66-1.66)
Clashscore	141614	1931 (1.66-1.66)
Ramachandran outliers	138981	1891 (1.66-1.66)
Sidechain outliers	138945	1891 (1.66-1.66)
RSRZ outliers	127900	1791 (1.66-1.66)

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% 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		
			2%		
1	A	364	84%	8%	8%



2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 3121 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 Oxidized polyvinyl alcohol hydrolase.

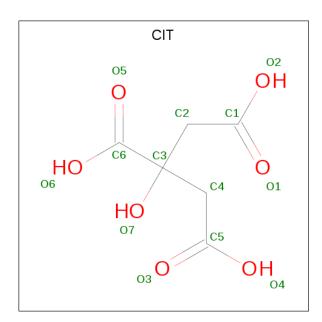
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace		
1	Λ	336	Total	С	N	О	S	0	0	0
1	Α	330	2580	1630	457	478	15	0	0	

There are 15 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-4	ALA	_	EXPRESSION TAG	UNP Q9LCQ7
A	-3	GLY	-	EXPRESSION TAG	UNP Q9LCQ7
A	-2	ALA	-	EXPRESSION TAG	UNP Q9LCQ7
A	172	OCS	SER	ENGINEERED MUTATION	UNP Q9LCQ7
A	349	ALA	_	EXPRESSION TAG	UNP Q9LCQ7
A	350	SER	_	EXPRESSION TAG	UNP Q9LCQ7
A	351	ALA	_	EXPRESSION TAG	UNP Q9LCQ7
A	352	TRP	_	EXPRESSION TAG	UNP Q9LCQ7
A	353	SER	-	EXPRESSION TAG	UNP Q9LCQ7
A	354	HIS	-	EXPRESSION TAG	UNP Q9LCQ7
A	355	PRO	-	EXPRESSION TAG	UNP Q9LCQ7
A	356	GLN	-	EXPRESSION TAG	UNP Q9LCQ7
A	357	PHE	=	EXPRESSION TAG	UNP Q9LCQ7
A	358	GLU	=	EXPRESSION TAG	UNP Q9LCQ7
A	359	LYS	-	EXPRESSION TAG	UNP Q9LCQ7

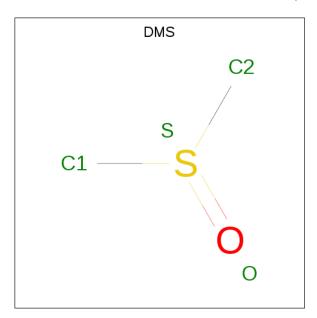
• Molecule 2 is CITRIC ACID (three-letter code: CIT) (formula: C₆H₈O₇).





Mol	Chain	Residues	Atoms		ZeroOcc	AltConf	
2	A	1	Total 13	C 6	O 7	0	0

 \bullet Molecule 3 is DIMETHYL SULFOXIDE (three-letter code: DMS) (formula: $\mathrm{C_2H_6OS}).$



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

• Molecule 4 is water.



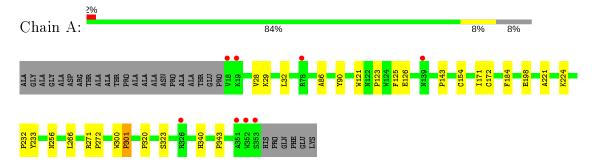
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	524	Total O 524 524	0	0



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 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: Oxidized polyvinyl alcohol hydrolase





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants	58.52Å 65.28Å 84.17Å	Depositor
a, b, c, α , β , γ	90.00° 90.00° 90.00°	Depositor
Resolution (Å)	25.00 - 1.65	Depositor
resolution (A)	24.02 - 1.65	EDS
% Data completeness	(Not available) (25.00-1.65)	Depositor
(in resolution range)	97.2 (24.02-1.65)	EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	4.36 (at 1.65Å)	Xtriage
Refinement program	CNS 1.21	Depositor
P. P.	0.167 , 0.193	Depositor
R, R_{free}	0.164 , 0.190	DCC
R_{free} test set	1975 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	10.3	Xtriage
Anisotropy	0.273	Xtriage
Bulk solvent $k_{sol}(e/Å^3)$, $B_{sol}(Å^2)$	0.34 , 41.7	EDS
L-test for twinning ²	$ < L > = 0.48, < L^2> = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	3121	wwPDB-VP
Average B, all atoms (Å ²)	13.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 7.13% of the height of the origin peak. No significant pseudotranslation is detected.

²Theoretical 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.



¹Intensities estimated from amplitudes.

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: OCS, DMS, CIT

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).

Mal	Chain	Bond	lengths	Bond angles		
MIOI	Mol Chain	RMSZ	# Z >5	RMSZ	# Z > 5	
1	A	0.29	0/2656	0.59	0/3626	

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	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	233	TYR	Sidechain

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	Α	2580	0	2431	15	0
2	A	13	0	5	0	0

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Mol	Chain	Non-H	H(model)	$\mathbf{H}(\mathbf{added})$	Clashes	Symm-Clashes	
3	A	4	0	6	0	0	
4	A	524	0	0	0	0	
All	All	3121	0	2442	15	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.

The worst 5 of 15 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	$egin{aligned} ext{Interatomic} \ ext{distance} \ (ext{Å}) \end{aligned}$	Clash overlap (Å)
1:A:125:PHE:CD2	1:A:143:PRO:HG2	2.33	0.63
1:A:121:TRP:CD1	1:A:123:PRO:HD2	2.36	0.60
1:A:86:ALA:HA	1:A:90:TYR:O	2.08	0.54
1:A:28:VAL:CG2	1:A:154:CYS:SG	2.99	0.51
1:A:256:ASN:HD22	1:A:266:LEU:HA	1.77	0.49

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	333/364 (92%)	321 (96%)	12 (4%)	0	100	100	

There are no Ramachandran outliers to report.

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	$269/285 \ (94\%)$	266 (99%)	3 (1%)	73 57	

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

Mol	Chain	Res	Type
1	A	126	GLU
1	A	198	GLU
1	A	301	PRO

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 9 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	256	ASN
1	A	340	HIS
1	A	306	GLN
1	A	139	ASN
1	A	302	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

1 non-standard protein/DNA/RNA residue 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	B	Bond lengths			Bond angles		
			nes		Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2	
1	OCS	A	172	1	7,8,9	0.71	0	6,11,13	1.38	1 (16%)	



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.

\mathbf{Mol}	Type	Chain	${f Res}$	Link	Chirals	Torsions	Rings
1	OCS	A	172	1	-	4/4/7/9	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	\mathbf{Z}	$\mathbf{Observed}(^o)$	$\operatorname{Ideal}({}^o)$
1	A	172	OCS	OD3-SG-CB	2.44	109.84	106.94

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	172	OCS	N-CA-CB-SG
1	A	172	OCS	CA-CB-SG-OD1
1	A	172	OCS	CA-CB-SG-OD2
1	A	172	OCS	CA-CB-SG-OD3

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	172	OCS	1	0

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

2 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	pe Chain	Dog	Res Link	B	Bond lengths			Bond angles		
MIOI	Type		nes		Counts	RMSZ	# Z >2	Counts	RMSZ	# Z > 2	
2	CIT	A	401	_	3,12,12	0.83	0	3,17,17	0.40	0	
3	DMS	A	402	-	3,3,3	2.16	2 (66%)	3,3,3	0.22	0	

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.

\mathbf{Mol}	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	CIT	A	401	_	-	0/6/16/16	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	\mathbf{Z}	${ m Observed}({ m \AA})$	$\mathbf{Ideal}(exttt{A})$
3	A	402	DMS	C1-S	2.65	1.95	1.75
3	A	402	DMS	C2-S	2.61	1.95	1.75

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, 95^{th} 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 $>$	$\#\mathrm{RSRZ}{>}2$		$OWAB(\AA^2)$	Q < 0.9	
1	A	335/364 (92%)	-0.16	8 (2%)	59	59	5, 9, 20, 40	0

The worst 5 of 8 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	19	LYS	4.2
1	A	351	ALA	3.9
1	A	353	SER	3.6
1	A	18	VAL	2.8
1	A	352	TRP	2.6

6.2 Non-standard residues in protein, DNA, RNA chains (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, 95^{th} 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	${f B\text{-factors}}({f \AA}^2)$	Q < 0.9
1	OCS	A	172	9/10	0.96	0.09	6,7,10,13	0

6.3 Carbohydrates (i)

There are no carbohydrates 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, 95^{th} 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	${f B\text{-factors}}({f \AA}^2)$	Q < 0.9
2	CIT	A	401	13/13	0.84	0.18	13,19,25,26	0
3	DMS	A	402	4/4	0.95	0.11	16,17,18,18	0

6.5 Other polymers (i)

There are no such residues in this entry.

