

wwPDB X-ray Structure Validation Summary Report (i)

Dec 3, 2023 - 10:45 pm GMT

PDB ID	:	1QOP
Title	:	CRYSTAL STRUCTURE OF WILD-TYPE TRYPTOPHAN SYNTHASE
		COMPLEXED WITH INDOLE PROPANOL PHOSPHATE
Authors	:	Weyand, M.; Schlichting, I.
Deposited on		
Resolution	:	1.40 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 types of validation reports are described at http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (1)) were used in the production of this report:

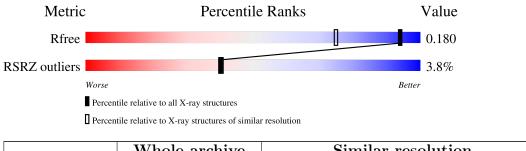
MolProbity	:	FAILED
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure: $X\text{-}RAY \, DIFFRACTION$

The reported resolution of this entry is 1.40 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	Similar resolution
Metric	$(\# { m Entries})$	$(\# { m Entries}, { m resolution} { m range}({ m \AA}))$
R_{free}	130704	1714 (1.40-1.40)
RSRZ outliers	127900	1674(1.40-1.40)

MolProbity failed to run properly - the sequence quality summary graphics cannot be shown.



2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 5878 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 TRYPTOPHAN SYNTHASE ALPHA CHAIN.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace		
1	А	265	Total 2039	C 1292	N 353	O 385	S 9	0	9	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
А	87	ILE	LEU	cloning artifact	UNP P00929

• Molecule 2 is a protein called TRYPTOPHAN SYNTHASE BETA CHAIN.

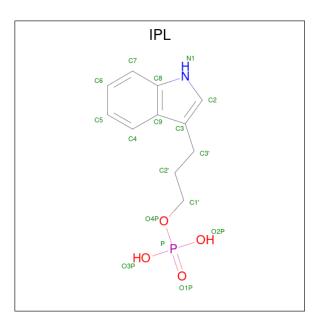
Mol	Chain	Residues		At	oms			ZeroOcc	AltConf	Trace
2	В	390	Total 3005	C 1890	N 528	O 567	S 20	0	15	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
В	34	SER	ARG	cloning artifact	UNP P00929

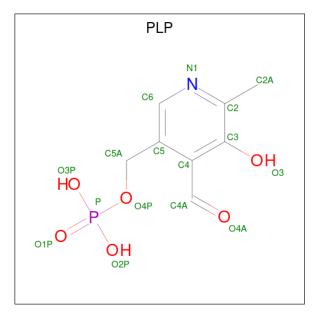
• Molecule 3 is INDOLE-3-PROPANOL PHOSPHATE (three-letter code: IPL) (formula: $C_{11}H_{14}NO_4P$).





Mol	Chain	Residues		Ato	oms			ZeroOcc	AltConf
2	Λ	1	Total	С	Ν	0	Р	0	0
3	A	1	17	11	1	4	1	U	U

• Molecule 4 is PYRIDOXAL-5'-PHOSPHATE (three-letter code: PLP) (formula: $C_8H_{10}NO_6P$).



Mol	Chain	Residues		Ate	oms			ZeroOcc	AltConf
4	В	1	Total	С	Ν	0	Р	0	0
4	D	1	15	8	1	5	1	0	0

• Molecule 5 is SODIUM ION (three-letter code: NA) (formula: Na).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	В	1	Total N 1	Va 1	0	0

• Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	А	288	Total O 288 288	0	0
6	В	513	Total O 513 513	0	1

MolProbity failed to run properly - this section is therefore empty.



3 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants	182.20Å 60.30Å 67.40Å	Depositor
a, b, c, α , β , γ	90.00° 94.70° 90.00°	Depositor
Resolution (Å)	20.00 - 1.40	Depositor
Resolution (A)	30.26 - 1.40	EDS
% Data completeness	95.0 (20.00-1.40)	Depositor
(in resolution range)	94.2 (30.26-1.40)	EDS
R _{merge}	(Not available)	Depositor
R_{sym}	0.06	Depositor
$< I/\sigma(I) > 1$	$1.54 (at 1.40 \text{\AA})$	Xtriage
Refinement program	REFMAC	Depositor
D D.	0.150 , 0.177	Depositor
R, R_{free}	0.151 , 0.180	DCC
R_{free} test set	6705 reflections $(5.01%)$	wwPDB-VP
Wilson B-factor $(Å^2)$	11.9	Xtriage
Anisotropy	0.666	Xtriage
Bulk solvent $k_{sol}(e/Å^3), B_{sol}(Å^2)$	0.39, 52.5	EDS
L-test for twinning ²	$ \langle L \rangle = 0.49, \langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	5878	wwPDB-VP
Average B, all atoms $(Å^2)$	17.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 4.99% of the height of the origin peak. No significant pseudotranslation is detected.

²Theoretical 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.



¹Intensities estimated from amplitudes.

4 Model quality (i)

4.1 Standard geometry (i)

MolProbity failed to run properly - this section is therefore empty.

4.2 Too-close contacts (i)

MolProbity failed to run properly - this section is therefore empty.

4.3 Torsion angles (i)

4.3.1 Protein backbone (i)

MolProbity failed to run properly - this section is therefore empty.

4.3.2 Protein sidechains (i)

MolProbity failed to run properly - this section is therefore empty.

4.3.3 RNA (i)

MolProbity failed to run properly - this section is therefore empty.

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

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

4.5 Carbohydrates (i)

There are no monosaccharides in this entry.

4.6 Ligand geometry (i)

Of 3 ligands modelled in this entry, 1 is monoatomic - leaving 2 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



4

PLP

В

4 (20%

20,22,23

1.72

]	RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).											
	Mol	Type	Chain	Res	Link		Bond lengths Counts $ RMSZ \# Z > 2$		Bond anglesCounts $RMSZ \mid \# Z > 2$			
ſ	3	IPL	А	300	-	17,18,18	0.69	0	20,25,25	1.23	1(5%)	

1.51

2(13%)

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).

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.

15,15,16

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	IPL	А	300	-	-	0/8/8/8	0/2/2/2
4	PLP	В	500	2	-	0/6/6/8	0/1/1/1

 $\mathbf{2}$

500

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$\operatorname{Observed}(\operatorname{\AA})$	Ideal(Å)
4	В	500	PLP	C3-C2	-3.83	1.37	1.40
4	В	500	PLP	P-O3P	-2.12	1.46	1.54

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
4	В	500	PLP	C2A-C2-C3	3.98	125.81	120.89
4	В	500	PLP	O4P-C5A-C5	3.73	116.47	109.35
3	А	300	IPL	C2'-C3'-C3	-2.72	106.21	114.15
4	В	500	PLP	C4-C3-C2	2.54	123.83	120.07
4	В	500	PLP	C6-C5-C4	-2.27	116.38	118.16

All (5) bond angle outliers are listed below:

There are no chirality outliers.

There are no torsion outliers.

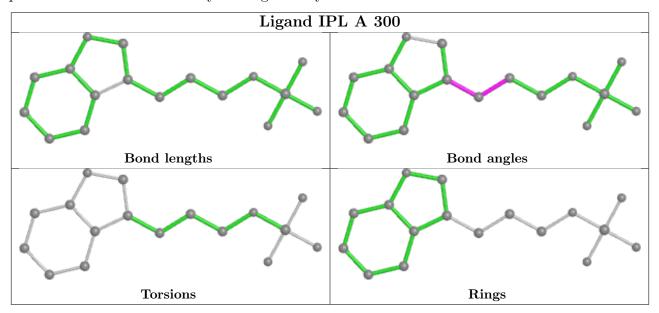
There are no ring outliers.

No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier.



Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



4.7 Other polymers (i)

There are no such residues in this entry.

4.8 Polymer linkage issues (i)

There are no chain breaks in this entry.



5 Fit of model and data (i)

5.1 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	$\langle RSRZ \rangle$	#RSRZ>2	$OWAB(Å^2)$	Q<0.9
1	А	265/268~(98%)	0.09	20 (7%) 14 13	10, 16, 33, 45	0
2	В	390/396~(98%)	-0.10	5 (1%) 77 75	8, 12, 24, 36	0
All	All	655/664~(98%)	-0.02	25 (3%) 40 40	8, 14, 28, 45	0

The worst 5 of 25 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	В	385	PHE	5.6
1	А	157[A]	ASN	5.3
1	А	186	GLU	4.4
1	А	194	HIS	4.3
1	А	192	PRO	3.7

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

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

5.3 Carbohydrates (i)

There are no monosaccharides in this entry.

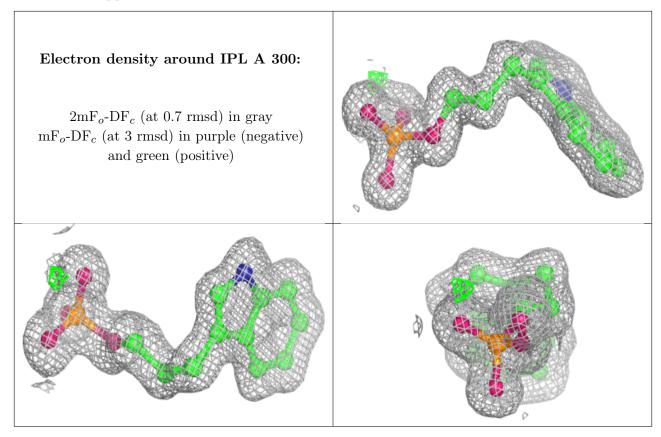
5.4 Ligands (i)

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	$\mathbf{B} ext{-factors}(\mathrm{\AA}^2)$	Q < 0.9
3	IPL	А	300	17/17	0.98	0.07	10,12,14,14	0
4	PLP	В	500	15/16	0.99	0.09	8,11,16,17	0
5	NA	В	501	1/1	1.00	0.05	10,10,10,10	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.



5.5 Other polymers (i)

There are no such residues in this entry.

