



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 11:25 AM GMT

PDB ID : 3OY2  
Title : Crystal structure of a putative glycosyltransferase from Paramecium bursaria  
Chlorella virus NY2A  
Authors : Xiang, Y.; Rossmann, M.G.  
Deposited on : 2010-09-22  
Resolution : 2.31 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](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 : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
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) : trunk26865

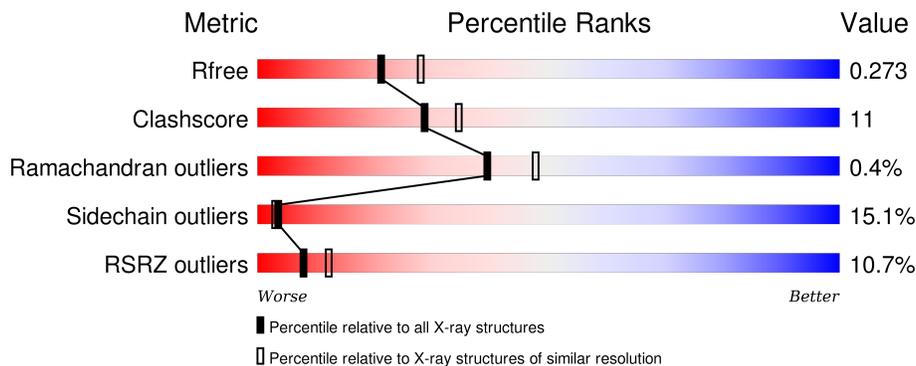
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.31 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	4425 (2.34-2.30)
Clashscore	102246	5057 (2.34-2.30)
Ramachandran outliers	100387	5008 (2.34-2.30)
Sidechain outliers	100360	5007 (2.34-2.30)
RSRZ outliers	91569	4432 (2.34-2.30)

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	413	
1	B	413	

## 2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 6309 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 Glycosyltransferase B736L.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	392	3101	1983	531	568	19	0	0	0
1	B	392	3101	1983	531	568	19	0	0	0

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	406	LEU	-	EXPRESSION TAG	UNP A7IXR1
A	407	GLU	-	EXPRESSION TAG	UNP A7IXR1
A	408	HIS	-	EXPRESSION TAG	UNP A7IXR1
A	409	HIS	-	EXPRESSION TAG	UNP A7IXR1
A	410	HIS	-	EXPRESSION TAG	UNP A7IXR1
A	411	HIS	-	EXPRESSION TAG	UNP A7IXR1
A	412	HIS	-	EXPRESSION TAG	UNP A7IXR1
A	413	HIS	-	EXPRESSION TAG	UNP A7IXR1
B	406	LEU	-	EXPRESSION TAG	UNP A7IXR1
B	407	GLU	-	EXPRESSION TAG	UNP A7IXR1
B	408	HIS	-	EXPRESSION TAG	UNP A7IXR1
B	409	HIS	-	EXPRESSION TAG	UNP A7IXR1
B	410	HIS	-	EXPRESSION TAG	UNP A7IXR1
B	411	HIS	-	EXPRESSION TAG	UNP A7IXR1
B	412	HIS	-	EXPRESSION TAG	UNP A7IXR1
B	413	HIS	-	EXPRESSION TAG	UNP A7IXR1

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	70	Total	O	0	0
			70	70		
2	B	37	Total	O	0	0
			37	37		



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	153.62Å 246.94Å 67.17Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	130.19 – 2.31 47.02 – 2.31	Depositor EDS
% Data completeness (in resolution range)	99.3 (130.19-2.31) 99.4 (47.02-2.31)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	0.07	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.45 (at 2.32Å)	Xtrriage
Refinement program	REFMAC 5.5.0088	Depositor
R, $R_{free}$	0.233 , 0.268 0.241 , 0.273	Depositor DCC
$R_{free}$ test set	2843 reflections (5.34%)	DCC
Wilson B-factor (Å <sup>2</sup> )	45.7	Xtrriage
Anisotropy	0.063	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 47.9	EDS
Estimated twinning fraction	No twinning to report.	Xtrriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtrriage
Outliers	1 of 56077 reflections (0.002%)	Xtrriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	6309	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	61.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.01% 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, 0.375 respectively for untwinned datasets, and 0.333, 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	0.82	4/3168 (0.1%)	0.97	13/4284 (0.3%)
1	B	0.72	1/3168 (0.0%)	0.88	5/4284 (0.1%)
All	All	0.77	5/6336 (0.1%)	0.92	18/8568 (0.2%)

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
1	B	0	3
All	All	0	4

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	388	ASN	CB-CG	12.44	1.79	1.51
1	A	328	VAL	CB-CG1	-6.58	1.39	1.52
1	A	332	ASP	CB-CG	-5.74	1.39	1.51
1	A	274	CYS	CB-SG	5.40	1.91	1.82
1	A	218	VAL	CB-CG2	-5.06	1.42	1.52

The worst 5 of 18 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	198	ARG	NE-CZ-NH2	-13.90	113.35	120.30
1	A	198	ARG	NE-CZ-NH2	-10.76	114.92	120.30
1	B	198	ARG	NE-CZ-NH1	8.93	124.77	120.30
1	A	196	ARG	NE-CZ-NH2	-7.31	116.64	120.30
1	A	332	ASP	CB-CG-OD1	-7.19	111.83	118.30

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	331	ARG	Peptide
1	B	262	LEU	Peptide
1	B	312	PHE	Peptide
1	B	331	ARG	Peptide

## 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	3101	0	3089	81	0
1	B	3101	0	3089	64	0
2	A	70	0	0	7	0
2	B	37	0	0	5	0
All	All	6309	0	6178	142	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 11.

The worst 5 of 142 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:B:388:ASN:CG	1:B:388:ASN:CB	1.79	1.46
1:A:262:LEU:O	1:A:262:LEU:HG	1.55	1.05
1:B:34:ILE:HD11	1:B:76:PHE:HZ	1.22	1.05
1:A:229:LYS:HE3	1:B:330:ASP:HB2	1.39	1.02
1:B:34:ILE:HD11	1:B:76:PHE:CZ	1.98	0.99

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	390/413 (94%)	379 (97%)	10 (3%)	1 (0%)	46	56
1	B	390/413 (94%)	376 (96%)	12 (3%)	2 (0%)	34	40
All	All	780/826 (94%)	755 (97%)	22 (3%)	3 (0%)	39	48

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	313	SER
1	B	290	SER
1	A	291	ALA

### 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	341/361 (94%)	290 (85%)	51 (15%)	3	3
1	B	341/361 (94%)	289 (85%)	52 (15%)	3	3
All	All	682/722 (94%)	579 (85%)	103 (15%)	3	3

5 of 103 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	356	GLU
1	B	64	ASN
1	B	346	LEU
1	A	366	VAL
1	B	34	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 12 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	162	HIS
1	A	251	HIS
1	B	89	ASN
1	A	131	HIS
1	B	55	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](#)

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 [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<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	392/413 (94%)	0.22	9 (2%) 64 72	27, 43, 67, 88	0
1	B	392/413 (94%)	1.02	75 (19%) 2 2	27, 72, 151, 192	0
All	All	784/826 (94%)	0.62	84 (10%) 8 12	27, 51, 136, 192	0

The worst 5 of 84 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	99	LEU	9.8
1	B	60	VAL	8.8
1	B	69	TYR	8.1
1	B	63	LEU	7.6
1	B	41	PHE	5.5

### 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 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.