

wwPDB X-ray Structure Validation Summary Report (i)

Jun 15, 2020 – 11:20 pm BST

PDB ID 3MO4

> Title The crystal structure of an alpha-(1-3,4)-fucosidase from Bifidobacterium

> > longum subsp. infantis ATCC 15697

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1.90 Å(reported) Resolution

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

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

Xtriage (Phenix) 1.13 EDS 2.11

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

> Refmac 5.8.0158

CCP4 7.0.044 (Gargrove)

Ideal geometry (proteins) Engh & Huber (2001) Ideal geometry (DNA, RNA) Parkinson et al. (1996)

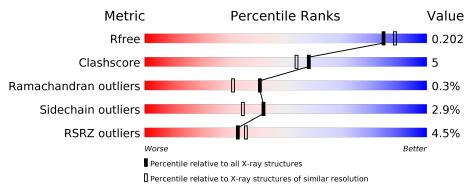
Validation Pipeline (wwPDB-VP) 2.11

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 1.90 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	6207 (1.90-1.90)
Clashscore	141614	6847 (1.90-1.90)
Ramachandran outliers	138981	6760 (1.90-1.90)
Sidechain outliers	138945	6760 (1.90-1.90)
RSRZ outliers	127900	6082 (1.90-1.90)

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		
1	A	480	5% 85%	9%	• 5%
1	В	480	82%	12%	•



2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 8073 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.

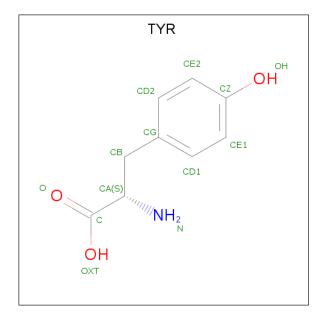
• Molecule 1 is a protein called Alpha-1,3/4-fucosidase.

Mol	Chain	Residues		Atoms				ZeroOcc	AltConf	Trace	
1	Δ	455	Total	С	N	О	S Se	Se	0	1	0
1	Λ	400	3578	2238	646	681	5	8	0	4	
1	D	459	Total	С	N	О	S	Se	0	1.4	0
1	D	409	3666	2302	654	696	5	9		14	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	${f Comment}$	Reference
A	-1	GLN	-	expression tag	UNP B7GNN8
A	0	GLY	-	expression tag	UNP B7GNN8
В	-1	GLN	-	expression tag	UNP B7GNN8
В	0	GLY	-	expression tag	UNP B7GNN8

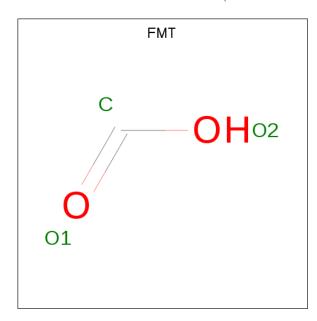
• Molecule 2 is TYROSINE (three-letter code: TYR) (formula: C₉H₁₁NO₃).





Mol	Chain	Residues	${f Atoms}$				ZeroOcc	AltConf
9	Λ	1	Total	С	Ν	О	0	0
	Λ	1	13	9	1	3	0	0

 \bullet Molecule 3 is FORMIC ACID (three-letter code: FMT) (formula: ${\rm CH_2O_2}).$



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf	
3	В	1	Total 3	C 1	O 2	0	0

• Molecule 4 is water.

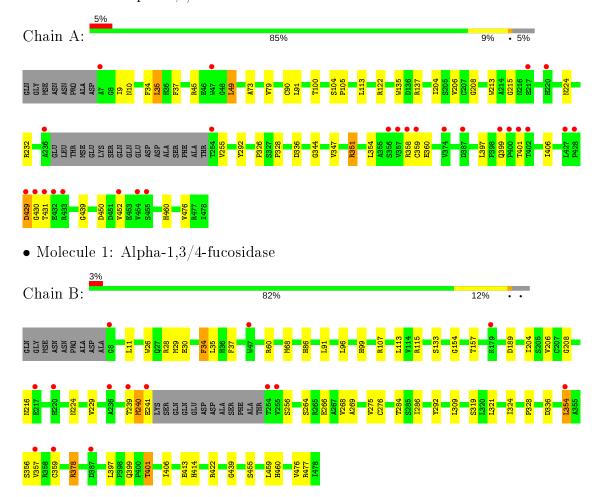
Mol	Chain	Residues	${f Atoms}$	ZeroOcc	AltConf
4	A	386	Total O 386 386	0	0
4	В	427	Total O 427 427	0	0



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: Alpha-1,3/4-fucosidase





4 Data and refinement statistics (i)

Property	Value	Source	
Space group	P 21 21 21	Depositor	
Cell constants	82.61Å 106.09Å 122.38Å	Depositor	
a, b, c, α , β , γ	90.00° 90.00° 90.00°	Depositor	
Resolution (Å)	41.93 - 1.90	Depositor	
Resolution (A)	44.61 - 1.90	EDS	
% Data completeness	94.2 (41.93-1.90)	Depositor	
(in resolution range)	99.3 (44.61-1.90)	EDS	
R_{merge}	0.12	Depositor	
R_{sym}	(Not available)	Depositor	
$< I/\sigma(I) > 1$	2.82 (at 1.89Å)	Xtriage	
Refinement program	PHENIX (phenix.refine: 1.5_2)	Depositor	
D D.	0.162 , 0.205	Depositor	
R, R_{free}	0.166 , 0.202	DCC	
R_{free} test set	4248 reflections $(5.01%)$	wwPDB-VP	
Wilson B-factor (Å ²)	22.5	Xtriage	
Anisotropy	0.575	Xtriage	
Bulk solvent $k_{sol}(e/Å^3)$, $B_{sol}(Å^2)$	0.35, 51.0	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	0.96	EDS	
Total number of atoms	8073	wwPDB-VP	
Average B, all atoms (Å ²)	27.0	wwPDB-VP	

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 3.93% 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: FMT

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		
IVIOI	Chain	RMSZ	# Z >5	RMSZ	# Z > 5	
1	A	0.32	0/3669	0.50	0/4976	
1	В	0.33	0/3786	0.51	0/5133	
All	All	0.33	0/7455	0.50	0/10109	

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	3578	0	3442	29	0
1	В	3666	0	3565	39	0
2	A	13	0	8	1	0
3	В	3	0	1	0	0
4	A	386	0	0	5	0
4	В	427	0	0	10	0
All	All	8073	0	7016	68	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 5.

The worst 5 of 68 close contacts within the same asymmetric unit are listed below, sorted by their



clash magnitude.

Atom-1	Atom-2	$egin{array}{l} ext{Interatomic} \ ext{distance } (ext{Å}) \end{array}$	$egin{array}{c} { m Clash} \ { m overlap} \ ({ m \AA}) \end{array}$
1:B:240:MSE:O	1:B:241:GLU:HB2	1.67	0.93
1:B:91[B]:LEU:HD13	1:B:113:LEU:HD23	1.59	0.82
1:A:35:LEU:HD22	1:A:79:VAL:HG21	1.60	0.81
1:B:216:ASN:HB3	4:B:539:HOH:O	1.81	0.80
1:A:232:ARG:NH1	1:A:255:VAL:HB	2.02	0.75

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	$455/480 \ (95\%)$	441 (97%)	12 (3%)	2 (0%)	34	24	
1	В	469/480 (98%)	457 (97%)	11 (2%)	1 (0%)	47	38	
All	All	924/960 (96%)	898 (97%)	23 (2%)	3 (0%)	41	31	

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	430	GLY
1	A	206	VAL
1	В	206	VAL

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	377/384 (98%)	366 (97%)	11 (3%)	42	35	
1	В	392/384 (102%)	380 (97%)	12 (3%)	40	32	
All	All	769/768 (100%)	746 (97%)	23 (3%)	42	33	

5 of 23 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	429	ASP
1	В	34	PHE
1	В	401	THR
1	В	11	LEU
1	В	107	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	${f Res}$	Type
1	A	437	GLN
1	В	86	HIS
1	В	99	HIS
1	В	294	GLN
1	В	460	HIS

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)

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	Chain Dag	n Dog	Chain Res	Dog	Pos	Pos	Pos	Pos	Thain Bog		Chain Ros Linl		Bond lengths			Bond angles		
	Type	Chain		$-\mathrm{es} \mid \mathrm{Link} \mid$	Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2								
3	FMT	В	479	-	0,2,2	0.00	-	0,1,1	0.00	-								

There are no bond length outliers.

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 $>$	$\#\mathrm{RSRZ}{>}2$	$OWAB(A^2)$	Q<0.9
1	A	447/480 (93%)	0.11	26 (5%) 23 25	12, 24, 62, 114	0
1	В	450/480 (93%)	0.04	14 (3%) 49 51	12, 21, 49, 106	0
All	All	897/960 (93%)	0.07	40 (4%) 33 36	12, 22, 56, 114	0

The worst 5 of 40 RSRZ outliers are listed below:

Mol	Chain	${f Res}$	Type	RSRZ
1	В	254	THR	6.9
1	A	427	LEU	5.3
1	В	255	VAL	5.3
1	A	431	THR	4.8
1	A	430	GLY	4.5

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)

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	$\mathbf{B} ext{-}\mathbf{factors}(\mathbf{\mathring{A}}^2)$	Q < 0.9
2	TYR	A	479	13/13	0.80	0.17	28,41,74,76	0
3	FMT	В	479	3/3	0.97	0.22	11,11,14,24	0

6.5 Other polymers (i)

There are no such residues in this entry.

