

wwPDB X-ray Structure Validation Summary Report (i)

Jan 3, 2024 – 09:46 am GMT

PDB ID : 4UQA

Title: X-ray structure of glucuronoxylan-xylanohydrolase (Xyn30A) from Clostrid-

ium thermocellum

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Deposited on : 2014-06-22

Resolution : 1.52 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: 4.02b-467

Mogul : 1.8.4, CSD as541be (2020)

Xtriage (Phenix) : 1.13 EDS : 2.36

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

 $Refmac \quad : \quad 5.8.0158$

CCP4 : 7.0.044 (Gargrove)

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

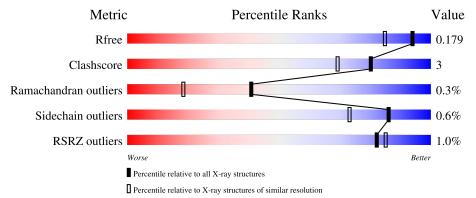
Validation Pipeline (wwPDB-VP) : 2.36

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 1.52 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 $(\#\text{Entries})$	Similar resolution $(\#\text{Entries, resolution range}(\text{\AA}))$
R_{free}	130704	4009 (1.54-1.50)
Clashscore	141614	4249 (1.54-1.50)
Ramachandran outliers	138981	4148 (1.54-1.50)
Sidechain outliers	138945	4146 (1.54-1.50)
RSRZ outliers	127900	3943 (1.54-1.50)

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 of 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		
			<u>%</u>		
1	A	409	91%	5%	-



2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 3472 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 CARBOHYDRATE BINDING FAMILY 6.

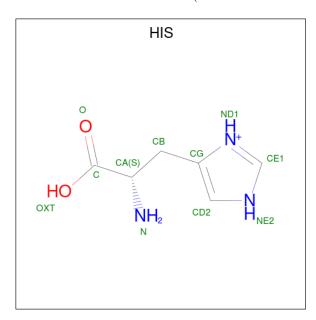
\mathbf{Mol}	Chain	Residues		At	oms			ZeroOcc	AltConf	Trace	
1	A	391	Total 3158	C 1994	N 556	O 591	S 17	0	3	0	

There are 26 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-22	MET	-	expression tag	UNP E6UTM3
A	-21	GLY	-	expression tag	UNP E6UTM3
A	-20	SER	-	expression tag	UNP E6UTM3
A	-19	SER	-	expression tag	UNP E6UTM3
A	-18	HIS	-	expression tag	UNP E6UTM3
A	-17	HIS	-	expression tag	UNP E6UTM3
A	-16	HIS	-	expression tag	UNP E6UTM3
A	-15	HIS	-	expression tag	UNP E6UTM3
A	-14	HIS	-	expression tag	UNP E6UTM3
A	-13	HIS	-	expression tag	UNP E6UTM3
A	-12	SER	-	expression tag	UNP E6UTM3
A	-11	SER	-	expression tag	UNP E6UTM3
A	-10	GLY	-	expression tag	UNP E6UTM3
A	-9	LEU	-	expression tag	UNP E6UTM3
A	-8	VAL	-	expression tag	UNP E6UTM3
A	-7	PRO	-	expression tag	UNP E6UTM3
A	-6	ARG	-	expression tag	UNP E6UTM3
A	-5	GLY	-	expression tag	UNP E6UTM3
A	-4	SER	-	expression tag	UNP E6UTM3
A	-3	HIS	-	expression tag	UNP E6UTM3
A	-2	MET	=	expression tag	UNP E6UTM3
A	-1	ALA	-	expression tag	UNP E6UTM3
A	0	SER	- expression tag		UNP E6UTM3
A	77	SER			UNP E6UTM3
A	163	ARG	ASN	conflict	UNP E6UTM3
A	315	CYS	TYR	engineered mutation	UNP E6UTM3



• Molecule 2 is HISTIDINE (three-letter code: HIS) (formula: $C_6H_{10}N_3O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C N O 11 6 3 2	0	0

• Molecule 3 is water.

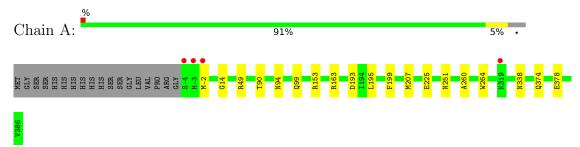
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	303	Total O 303 303	0	0



3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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: CARBOHYDRATE BINDING FAMILY 6





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants	46.73Å 50.37Å 58.87Å	Depositor
a, b, c, α , β , γ	65.00° 67.28° 76.84°	Depositor
Resolution (Å)	50.39 - 1.52	Depositor
resolution (A)	28.13 - 1.52	EDS
% Data completeness	96.5 (50.39-1.52)	Depositor
(in resolution range)	96.5 (28.13-1.52)	EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	2.46 (at 1.52Å)	Xtriage
Refinement program	REFMAC 5.0	Depositor
P.P.	0.135 , 0.171	Depositor
R, R_{free}	0.147 , 0.179	DCC
R_{free} test set	3274 reflections $(4.93%)$	wwPDB-VP
Wilson B-factor (Å ²)	16.6	Xtriage
Anisotropy	0.131	Xtriage
Bulk solvent $k_{sol}(e/Å^3)$, $B_{sol}(Å^2)$	0.36, 43.1	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	0.97	EDS
Total number of atoms	3472	wwPDB-VP
Average B, all atoms $(Å^2)$	22.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 7.75% 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)

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	Bond lengths		nd angles
Mol Chain		RMSZ $ \# Z > 5$		RMSZ $ $ # $ Z > 5$	
1	A	0.53	0/3247	0.75	2/4411 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$\mathbf{Observed}(^o)$	$\operatorname{Ideal}({}^{o})$
1	A	49	ARG	NE-CZ-NH1	6.92	123.76	120.30
1	A	49	ARG	NE-CZ-NH2	-6.81	116.89	120.30

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	3158	0	3058	16	0
2	A	11	0	6	2	0
3	A	303	0	0	8	0
All	All	3472	0	3064	17	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 17 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.



Atom-1	Atom-2	$\begin{array}{c} {\rm Interatomic} \\ {\rm distance} ({\rm \AA}) \end{array}$	$egin{aligned} ext{Clash} \ ext{overlap } (ext{Å}) \end{aligned}$
1:A:163[B]:ARG:HB2	1:A:163[B]:ARG:CZ	2.13	0.77
1:A:378:GLU:HG3	3:A:2265:HOH:O	1.87	0.74
1:A:94:ASN:HB2	3:A:2295:HOH:O	2.02	0.58
1:A:163[B]:ARG:HD3	3:A:2285:HOH:O	2.02	0.57
1:A:153:ARG:HD3	3:A:2121:HOH:O	2.06	0.56

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	392/409 (96%)	383 (98%)	8 (2%)	1 (0%)	41 18

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	264	TRP

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.

M	Iol	Chain	Analysed	nalysed Rotameric Outliers		Percentiles		
	1	A	341/353 (97%)	339 (99%)	2 (1%)		86	73

All (2) residues with a non-rotameric sidechain are listed below:



Mol	Chain	Res	Type
1	A	195	LEU
1	A	199	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type	
1	A	248	ASN	
1	A	321	ASN	
1	A	374	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 monosaccharides in this entry.

5.6 Ligand geometry (i)

1 ligand 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).

Mal	Type	Chain	Pos	Link	B	ond leng	$_{ m gths}$	В	ond ang	gles
IVIOI	туре	Chain	nes	Lilik	Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	HIS	A	1387	-	6,11,11	1.24	1 (16%)	7,14,14	1.56	2 (28%)

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.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	HIS	A	1387	-	-	2/8/8/8	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	\mathbf{Z}	Observed(A)	$\operatorname{Ideal}(ext{\AA})$
2	A	1387	HIS	OXT-C	-2.45	1.22	1.30

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	\mathbf{Z}	$\operatorname{Observed}(^{o})$	$Ideal(^{o})$
2	A	1387	HIS	OXT-C-O	-3.02	117.24	124.09
2	A	1387	HIS	CD2-NE2-CE1	2.12	109.09	105.78

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1387	HIS	OXT-C-CA-N
2	A	1387	HIS	O-C-CA-N

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1387	HIS	2	0

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></rsrz>	# RSRZ > 2	$OWAB(Å^2)$	Q < 0.9
1	A	391/409 (95%)	-0.00	4 (1%) 82 85	11, 20, 33, 78	0

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	-4	SER	9.3
1	A	-3	HIS	4.8
1	A	-2	MET	4.6
1	A	319	LYS	3.2

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 monosaccharides 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.

N	/Iol	Type	Chain	Res	Atoms	RSCC	RSR	$ m B ext{-}factors(\AA^2)$	Q<0.9
	2	HIS	A	1387	11/11	0.78	0.25	26,43,50,52	0



6.5 Other polymers (i)

There are no such residues in this entry.

