Full wwPDB X-ray Structure Validation Report ⓘ

Dec 22, 2022 – 06:02 PM EST

PDB ID	:	7T5E
Title	:	Neutron structure of Neurospora crassa Polysaccharide Monooxygenase 9D (NcLPMO9D) low pH vapor exchange
Authors	:	Schroder, G.C.; Meilleur, F.
Deposited on	:	2021-12-11
Resolution	:	1.90 Å(reported)

This is a Full wwPDB X-ray Structure Validation 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 ⓘ 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 ⓘ) were used in the production of this report:

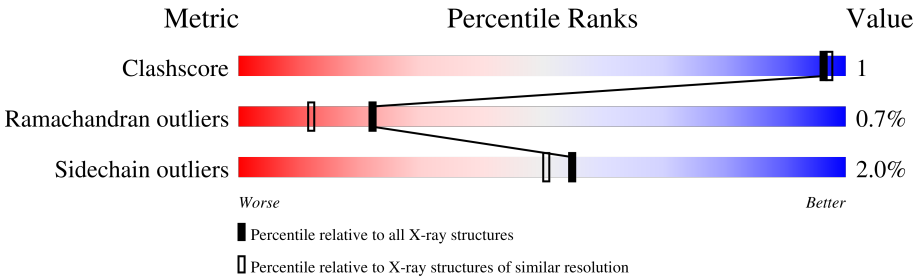
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	FAILED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.2

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION, NEUTRON 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	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	141614	6847 (1.90-1.90)
Ramachandran outliers	138981	6760 (1.90-1.90)
Sidechain outliers	138945	6760 (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 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%

Note EDS failed to run properly.

Mol	Chain	Length	Quality of chain
1	A	223	95% .
1	B	223	98% .
2	C	3	67% 33%
2	D	3	67% 33%

2 Entry composition

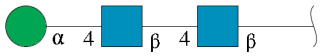
There are 4 unique types of molecules in this entry. The entry contains 8385 atoms, of which 3073 are hydrogens and 1461 are deuteriums.

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 Lytic polysaccharide monooxygenase.

Mol	Chain	Residues	Atoms							ZeroOcc	AltConf	Trace
1	A	223	Total	C	D	H	N	O	S	0	197	0
			3502	1058	330	1494	279	332	9			
1	B	223	Total	C	D	H	N	O	S	0	197	0
			3559	1077	333	1522	282	335	10			

- Molecule 2 is an oligosaccharide called alpha-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	C	3	Total	C	D	H	N	O	0	2	0
			77	22	10	28	2	15			
2	D	3	Total	C	D	H	N	O	0	2	0
			78	22	10	29	2	15			

- Molecule 3 is COPPER (II) ION (three-letter code: CU) (formula: Cu).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Cu	0	0
			1	1		
3	B	1	Total	Cu	0	0
			1	1		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	184	Total	D	O	0	1
			555	370	185		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	204	Total 612	D 408	O 204	0	0

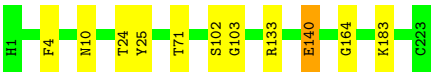
3 Residue-property plots (i)

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. 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. 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.

Note EDS failed to run properly.

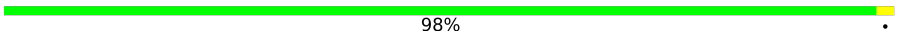
• Molecule 1: Lytic polysaccharide monooxygenase

Chain A:



• Molecule 1: Lytic polysaccharide monooxygenase

Chain B:



• Molecule 2: alpha-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain C:

• Molecule 2: alpha-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain D:

4 Data and refinement statistics (i)

EDS failed to run properly - this section is therefore incomplete.

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	68.30Å 42.27Å 70.41Å 90.00° 98.47° 90.00°	Depositor
Resolution (Å)	12.66 – 1.90	Depositor
% Data completeness (in resolution range)	98.0 (12.66-1.90)	Depositor
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	4.02 (at 1.90Å)	Xtriage
Refinement program	PHENIX 1.14_3260	Depositor
R, R_{free}	0.128 , 0.182	Depositor
Wilson B-factor (Å^2)	16.5	Xtriage
Anisotropy	0.598	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.017 for l,-k,h	Xtriage
Total number of atoms	8385	wwPDB-VP
Average B, all atoms (Å^2)	23.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 9.52% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical 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.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CU, MAN, NAG

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	0.67	0/2807	0.72	2/3832 (0.1%)
1	B	0.67	0/2778	0.79	0/3789
All	All	0.67	0/5585	0.75	2/7621 (0.0%)

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.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	133[A]	ARG	NE-CZ-NH2	-5.69	117.46	120.30
1	A	133[B]	ARG	NE-CZ-NH2	-5.69	117.46	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	102[B]	SER	Peptide

5.2 Too-close contacts

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	2008	1494	292	3	0
1	B	2037	1522	382	3	0
2	C	49	28	10	0	0
2	D	49	29	10	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	555	0	0	2	0
4	B	612	0	0	4	0
All	All	5312	3073	694	7	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 1.

All (7) 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:25[B]:TYR:CZ	4:B:401:HOH:O	1.71	1.34
1:B:25[B]:TYR:CE1	4:B:401:HOH:O	1.76	1.10
1:A:71:THR:O	4:A:401:HOH:O	2.19	0.60
1:A:140[A]:GLU:OE1	4:A:402:HOH:O	2.23	0.51
1:B:161[B]:ASN:ND2	4:B:417:HOH:O	2.52	0.41

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	369/223 (166%)	356 (96%)	10 (3%)	3 (1%)	19 9
1	B	365/223 (164%)	354 (97%)	9 (2%)	2 (0%)	29 18

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	734/446 (165%)	710 (97%)	19 (3%)	5 (1%)	22 12

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	103[A]	GLY
1	A	103[B]	GLY
1	A	164[B]	GLY
1	B	164[A]	GLY
1	B	164[B]	GLY

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	294/178 (165%)	285 (97%)	9 (3%)	40 32
1	B	298/178 (167%)	294 (99%)	4 (1%)	69 68
All	All	592/356 (166%)	579 (98%)	13 (2%)	55 47

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4[A]	PHE
1	A	4[B]	PHE
1	A	10[A]	ASN
1	A	10[B]	ASN
1	A	24	THR
1	A	140[A]	GLU
1	A	140[B]	GLU
1	A	183[A]	LYS
1	A	183[B]	LYS
1	B	4[A]	PHE
1	B	4[B]	PHE
1	B	146[A]	GLN
1	B	146[B]	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

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

5.5 Carbohydrates

10 monosaccharides 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	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	MAN	C	3	2	11,11,12	1.74	3 (27%)	15,15,17	1.30	2 (13%)
2	MAN	D	3	2	11,11,12	0.84	0	15,15,17	3.68	6 (40%)

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	MAN	C	3	2	-	2/2/19/22	0/1/1/1
2	MAN	D	3	2	-	2/2/19/22	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	3	MAN	C2-C3	2.93	1.56	1.52
2	C	3	MAN	C4-C3	2.52	1.58	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	3	MAN	C4-C5	2.36	1.58	1.53

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	3	MAN	O2-C2-C1	-7.56	93.69	109.15
2	D	3	MAN	C1-O5-C5	7.55	122.42	112.19
2	D	3	MAN	O5-C1-C2	6.60	120.97	110.77
2	D	3	MAN	C1-C2-C3	4.98	115.79	109.67
2	C	3	MAN	C1-O5-C5	3.44	116.86	112.19
2	D	3	MAN	O5-C5-C6	3.25	112.30	107.20
2	C	3	MAN	O5-C1-C2	2.37	114.42	110.77
2	D	3	MAN	O2-C2-C3	2.05	114.24	110.14

There are no chirality outliers.

All (4) torsion outliers are listed below:

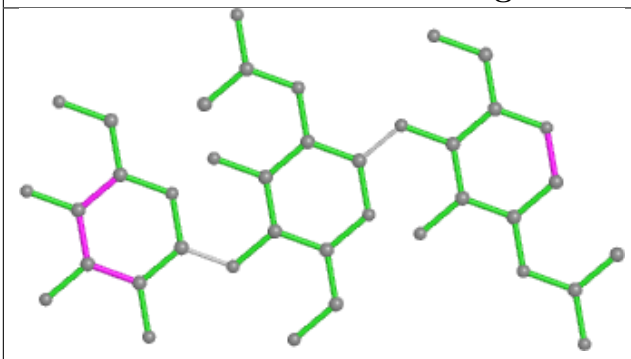
Mol	Chain	Res	Type	Atoms
2	D	3	MAN	O5-C5-C6-O6
2	C	3	MAN	O5-C5-C6-O6
2	D	3	MAN	C4-C5-C6-O6
2	C	3	MAN	C4-C5-C6-O6

There are no ring outliers.

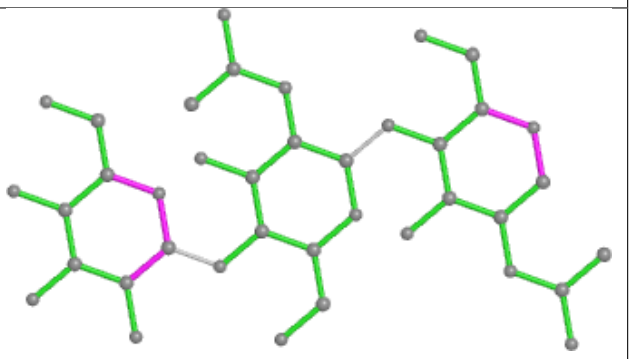
No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

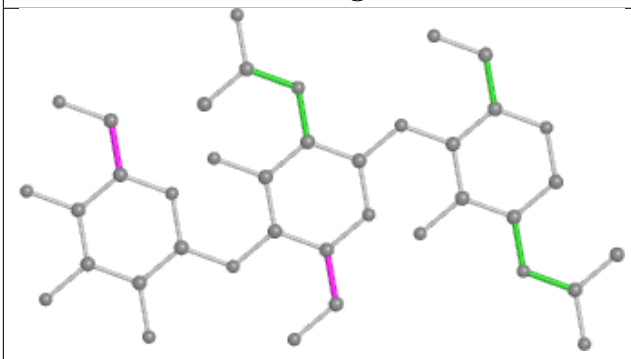
Oligosaccharide Chain C



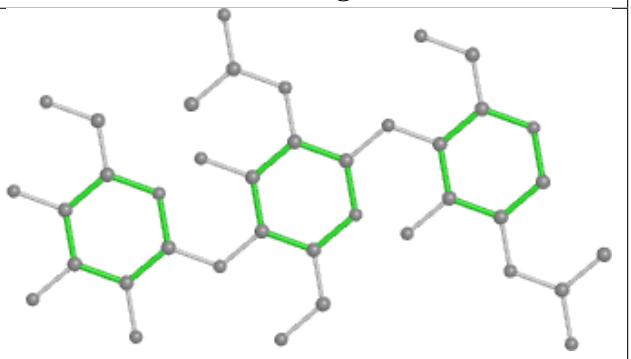
Bond lengths



Bond angles

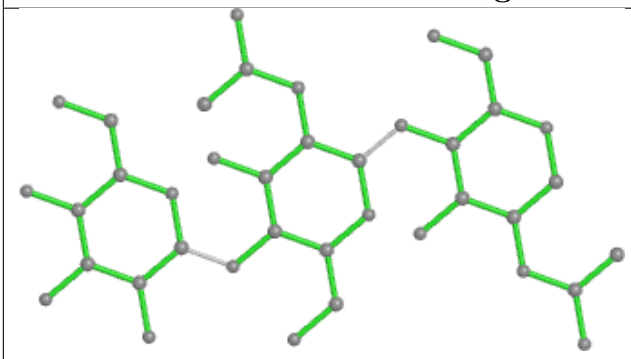


Torsions

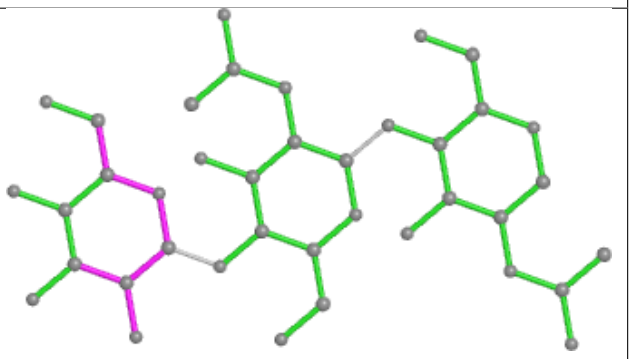


Rings

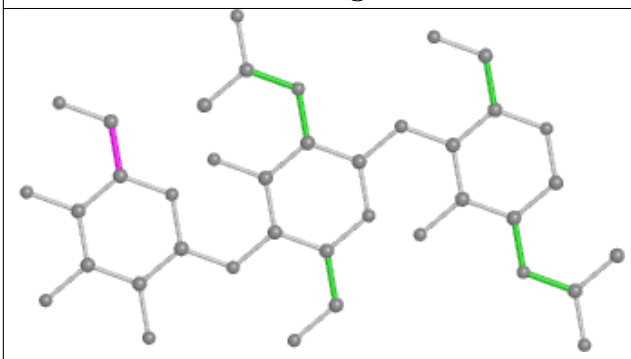
Oligosaccharide Chain D



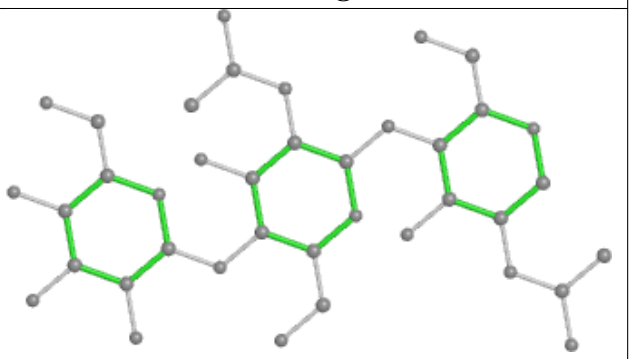
Bond lengths



Bond angles



Torsions



Rings

5.6 Ligand geometry (i)

Of 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

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

6.1 Protein, DNA and RNA chains

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

6.2 Non-standard residues in protein, DNA, RNA chains

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

6.3 Carbohydrates

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

6.4 Ligands

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

6.5 Other polymers

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