wwPDB X-ray Structure Validation Summary Report (i)

Jun 22, 2024 – 11:48 AM EDT

PDB ID	:	5MHV
Title	:	The study of the X-ray induced enzymatic reduction of molecular oxygen to water for laccase from Steccherinum murashkinskyi.The fourth structure of the series with total exposition time 93 min.
Authors	:	Polyakov, K.M.; Gavryushov, S.; Fedorova, T.V.; Glazunova, O.A.; Popov, A.N.
Deposited on	:	2016-11-25
Resolution	:	1.35 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 (i)) were used in the production of this report:

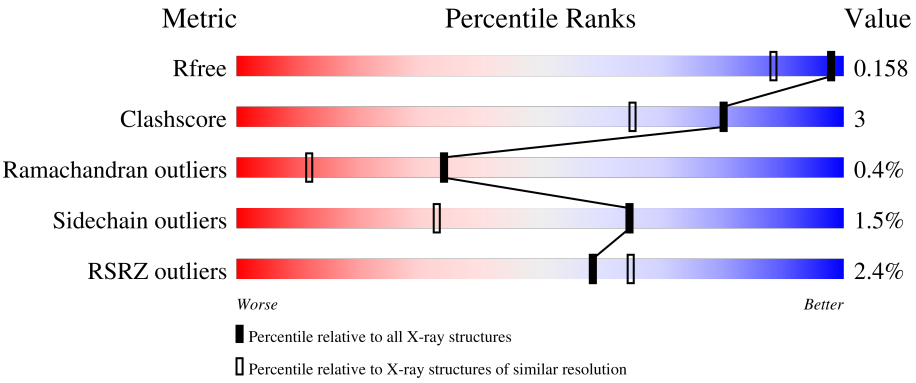
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.37.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

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 1.35 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}	130704	1509 (1.38-1.34)
Clashscore	141614	1551 (1.38-1.34)
Ramachandran outliers	138981	1530 (1.38-1.34)
Sidechain outliers	138945	1530 (1.38-1.34)
RSRZ outliers	127900	1487 (1.38-1.34)

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
1	A	499	2% 93% 6%
2	B	3	100%
2	C	3	100%

2 Entry composition (i)

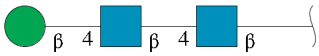
There are 7 unique types of molecules in this entry. The entry contains 8104 atoms, of which 3409 are hydrogens and 0 are deuteriums.

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 Laccase 2.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	499	Total	C	H	N	O	S	79	34	0
			7309	2464	3409	661	766	9			

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

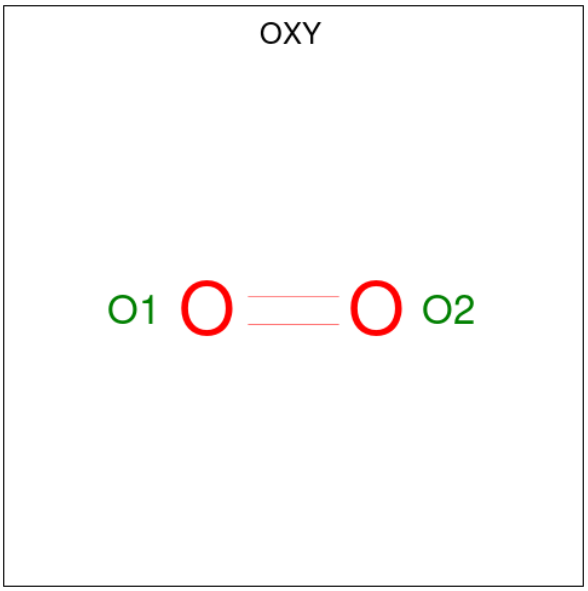


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	B	3	Total	C	N	O	0	0	0
			39	22	2	15			
2	C	3	Total	C	N	O	0	0	0
			39	22	2	15			

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

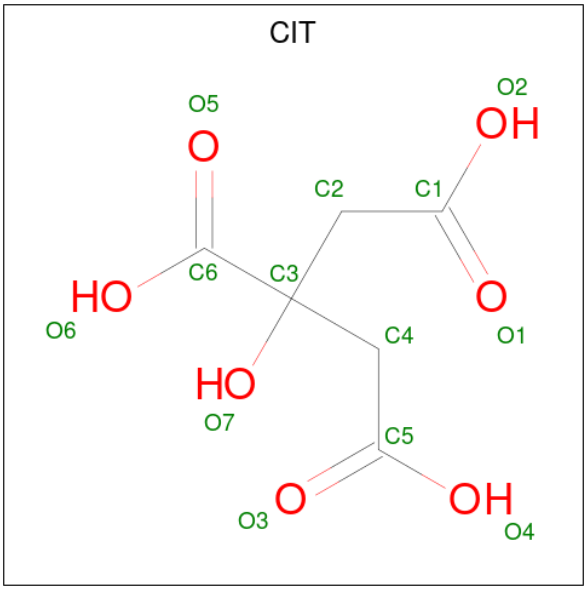
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	4	Total	Cu	0	2
			6	6		

- Molecule 4 is OXYGEN MOLECULE (three-letter code: OXY) (formula: O_2).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total O 2 2	0	0
4	A	1	Total O 2 2	0	0

- Molecule 5 is CITRIC ACID (three-letter code: CIT) (formula: $C_6H_8O_7$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C O 13 6 7	0	0

- Molecule 6 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total Na 1 1	0	0

- Molecule 7 is water.

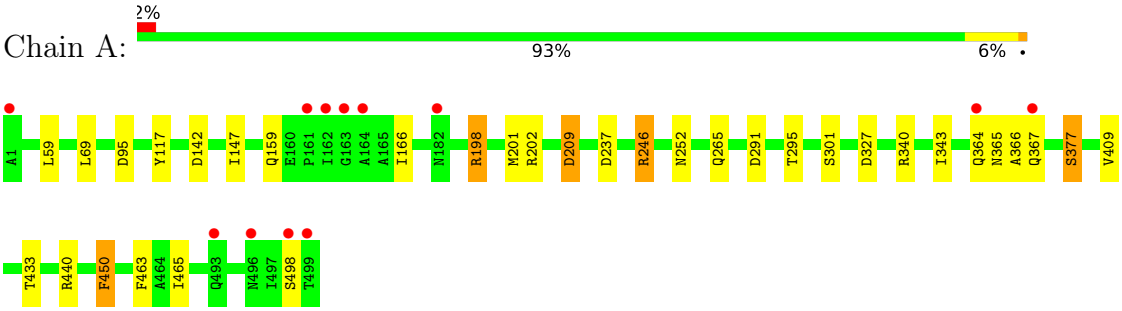
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	682	Total O 693 693	0	11

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.

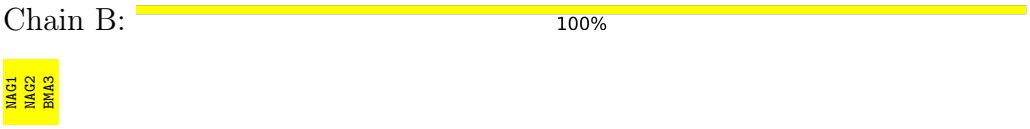
• Molecule 1: Laccase 2

Chain A:



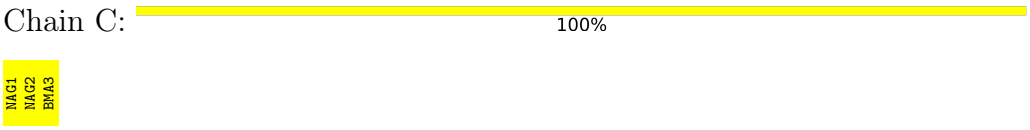
• Molecule 2: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain B:



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

Chain C:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	56.38Å 84.41Å 112.51Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	67.52 – 1.35 19.91 – 1.35	Depositor EDS
% Data completeness (in resolution range)	98.8 (67.52-1.35) 98.8 (19.91-1.35)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.18 (at 1.35Å)	Xtriage
Refinement program	REFMAC 5.8.0049	Depositor
R, R_{free}	0.133 , 0.151 0.143 , 0.158	Depositor DCC
R_{free} test set	5868 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å^2)	9.1	Xtriage
Anisotropy	0.153	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.44 , 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	0.98	EDS
Total number of atoms	8104	wwPDB-VP
Average B, all atoms (Å^2)	10.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.62% 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: BMA, NAG, CU, NA, OXY, CIT

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	0.97	3/4156 (0.1%)	1.03	17/5717 (0.3%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	377[A]	SER	CB-OG	-9.16	1.30	1.42
1	A	377[B]	SER	CB-OG	-9.16	1.30	1.42
1	A	301	SER	CB-OG	-5.30	1.35	1.42

The worst 5 of 17 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	237	ASP	CB-CG-OD1	12.32	129.38	118.30
1	A	209	ASP	CB-CG-OD1	7.78	125.30	118.30
1	A	202	ARG	NE-CZ-NH1	7.07	123.83	120.30
1	A	291	ASP	CB-CG-OD2	-6.90	112.09	118.30
1	A	95	ASP	CB-CG-OD1	6.80	124.42	118.30

There are no chirality outliers.

There are no planarity outliers.

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	3900	3409	3667	19	1
2	B	39	0	34	0	0
2	C	39	0	34	0	0
3	A	6	0	0	0	0
4	A	4	0	0	2	0
5	A	13	0	5	0	0
6	A	1	0	0	0	0
7	A	693	0	0	15	1
All	All	4695	3409	3740	21	1

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 21 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:A:265[B]:GLN:NE2	7:A:606:HOH:O	1.67	1.19
1:A:364:GLN:OE1	7:A:607:HOH:O	1.70	1.07
1:A:159[B]:GLN:CG	7:A:613:HOH:O	2.21	0.88
1:A:159[B]:GLN:HG3	7:A:613:HOH:O	1.72	0.88
1:A:295:THR:HG22	7:A:682:HOH:O	1.87	0.74

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:295:THR:CG2	7:A:1125:HOH:O[4_555]	1.90	0.30

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	533/499 (107%)	519 (97%)	12 (2%)	2 (0%)	34 12

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	209	ASP
1	A	59	LEU

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	441/409 (108%)	434 (98%)	7 (2%)	62 30

5 of 7 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	433[B]	THR
1	A	450	PHE
1	A	498	SER
1	A	463	PHE
1	A	433[A]	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 6 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	364	GLN
1	A	365	ASN
1	A	482	GLN
1	A	134	ASN
1	A	44	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

4 non-standard protein/DNA/RNA residues 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	NAG	B	2	2	14,14,15	1.95	5 (35%)	17,19,21	2.36	5 (29%)
2	NAG	C	1	1,2	14,14,15	0.96	0	17,19,21	1.16	1 (5%)
2	NAG	C	2	2	14,14,15	1.16	2 (14%)	17,19,21	1.84	4 (23%)
2	NAG	B	1	1,2	14,14,15	1.55	3 (21%)	17,19,21	1.28	2 (11%)

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	NAG	B	2	2	-	1/6/23/26	0/1/1/1
2	NAG	C	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	C	2	2	-	0/6/23/26	0/1/1/1
2	NAG	B	1	1,2	-	0/6/23/26	0/1/1/1

The worst 5 of 10 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	2	NAG	C2-N2	4.75	1.54	1.46
2	B	1	NAG	O5-C1	-3.07	1.38	1.43
2	B	1	NAG	C1-C2	3.00	1.56	1.52
2	B	2	NAG	C1-C2	2.78	1.56	1.52
2	C	2	NAG	O5-C1	-2.77	1.39	1.43

The worst 5 of 12 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	2	NAG	C1-O5-C5	-5.28	105.04	112.19
2	B	2	NAG	O7-C7-C8	-4.76	113.21	122.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	2	NAG	C3-C4-C5	4.29	117.88	110.24
2	B	2	NAG	C1-C2-N2	4.11	117.52	110.49
2	B	2	NAG	C2-N2-C7	-4.07	117.11	122.90

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	2	NAG	O5-C5-C6-O6

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

6 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	NAG	B	1	1,2	14,14,15	1.55	3 (21%)	17,19,21	1.28	2 (11%)
2	NAG	B	2	2	14,14,15	1.95	5 (35%)	17,19,21	2.36	5 (29%)
2	BMA	B	3	2	11,11,12	0.48	0	15,15,17	1.86	3 (20%)
2	NAG	C	1	1,2	14,14,15	0.96	0	17,19,21	1.16	1 (5%)
2	NAG	C	2	2	14,14,15	1.16	2 (14%)	17,19,21	1.84	4 (23%)
2	BMA	C	3	2	11,11,12	0.62	0	15,15,17	1.68	4 (26%)

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	NAG	B	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	B	2	2	-	1/6/23/26	0/1/1/1
2	BMA	B	3	2	-	0/2/19/22	0/1/1/1
2	NAG	C	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	C	2	2	-	0/6/23/26	0/1/1/1
2	BMA	C	3	2	-	0/2/19/22	0/1/1/1

The worst 5 of 10 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	2	NAG	C2-N2	4.75	1.54	1.46
2	B	1	NAG	O5-C1	-3.07	1.38	1.43
2	B	1	NAG	C1-C2	3.00	1.56	1.52
2	B	2	NAG	C1-C2	2.78	1.56	1.52
2	C	2	NAG	O5-C1	-2.77	1.39	1.43

The worst 5 of 19 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	2	NAG	C1-O5-C5	-5.28	105.04	112.19
2	B	2	NAG	O7-C7-C8	-4.76	113.21	122.06
2	B	2	NAG	C3-C4-C5	4.29	117.88	110.24
2	B	2	NAG	C1-C2-N2	4.11	117.52	110.49
2	B	2	NAG	C2-N2-C7	-4.07	117.11	122.90

There are no chirality outliers.

All (1) torsion outliers are listed below:

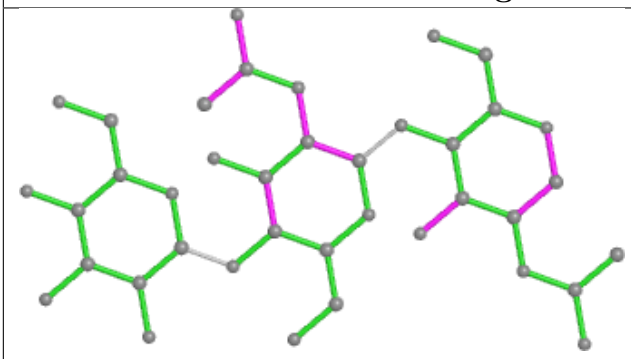
Mol	Chain	Res	Type	Atoms
2	B	2	NAG	O5-C5-C6-O6

There are no ring outliers.

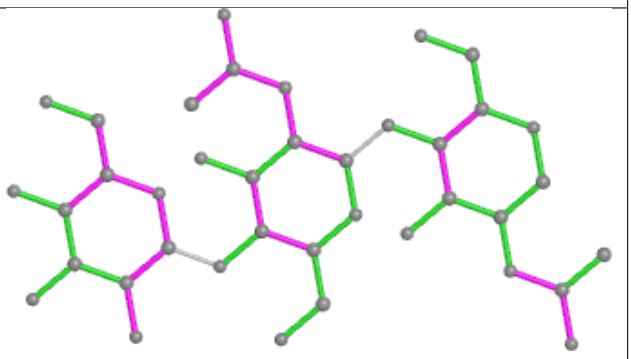
No monomer is involved in short contacts.

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

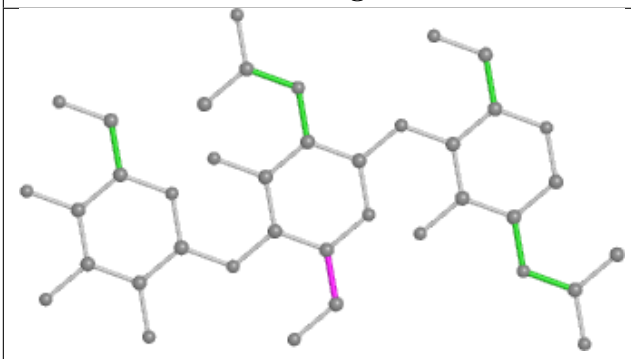
Oligosaccharide Chain B



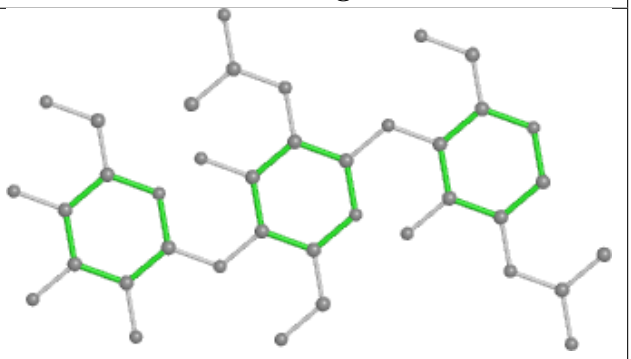
Bond lengths



Bond angles

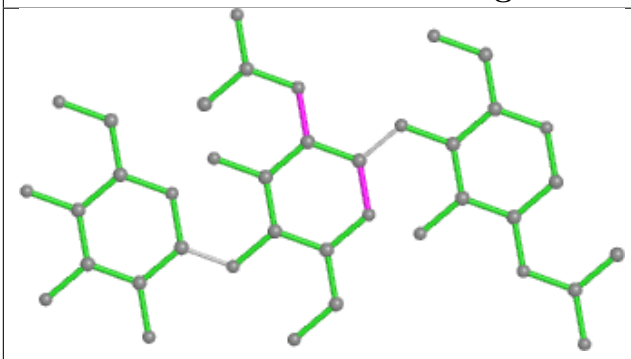


Torsions

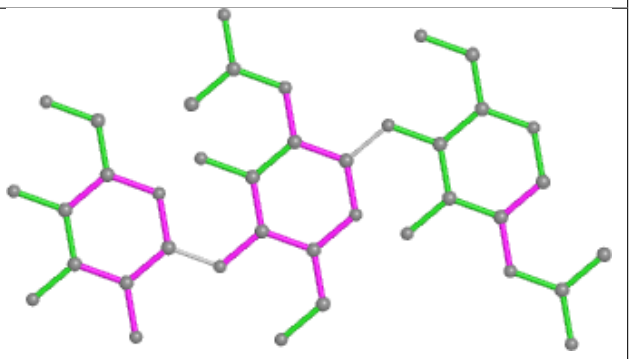


Rings

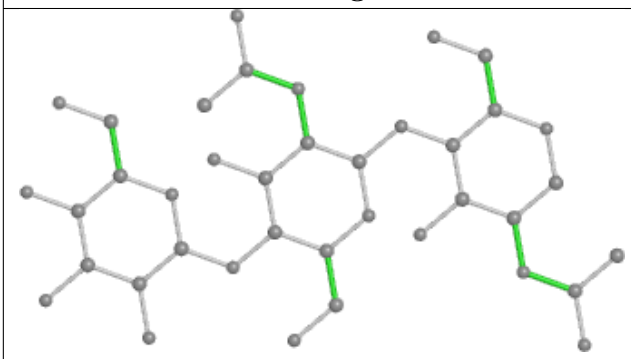
Oligosaccharide Chain C



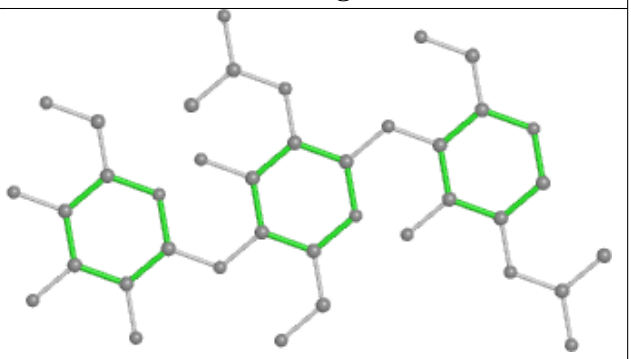
Bond lengths



Bond angles



Torsions



Rings

5.6 Ligand geometry (i)

Of 10 ligands modelled in this entry, 7 are monoatomic - leaving 3 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 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	$\#\|Z\| > 2$
5	CIT	A	513	-	12,12,12	1.18	0	17,17,17	1.68	3 (17%)
4	OXY	A	511	3	1,1,1	0.01	0	-		
4	OXY	A	512	-	1,1,1	0.06	0	-		

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
5	CIT	A	513	-	-	2/16/16/16	-

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	A	513	CIT	O6-C6-C3	4.40	120.69	113.05
5	A	513	CIT	O5-C6-C3	-2.66	118.49	122.25
5	A	513	CIT	C4-C3-C6	-2.30	105.16	110.11

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	513	CIT	O1-C1-C2-C3
5	A	513	CIT	O2-C1-C2-C3

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	511	OXY	1	0
4	A	512	OXY	1	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

6.1 Protein, DNA and RNA chains

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>2	OWAB(Å^2)	Q<0.9
1	A	499/499 (100%)	-0.41	12 (2%) 59 65	5, 9, 18, 48	0

The worst 5 of 12 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	162[A]	ILE	6.2
1	A	499	THR	5.6
1	A	498	SER	4.4
1	A	1	ALA	4.1
1	A	163[A]	GLY	4.0

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

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	B-factors(Å^2)	Q<0.9
2	NAG	B	2	14/15	0.80	0.21	19,25,30,34	0
2	NAG	C	2	14/15	0.95	0.09	11,14,23,26	0
2	NAG	B	1	14/15	0.96	0.07	10,11,15,15	0
2	NAG	C	1	14/15	0.97	0.05	8,10,13,14	0

6.3 Carbohydrates

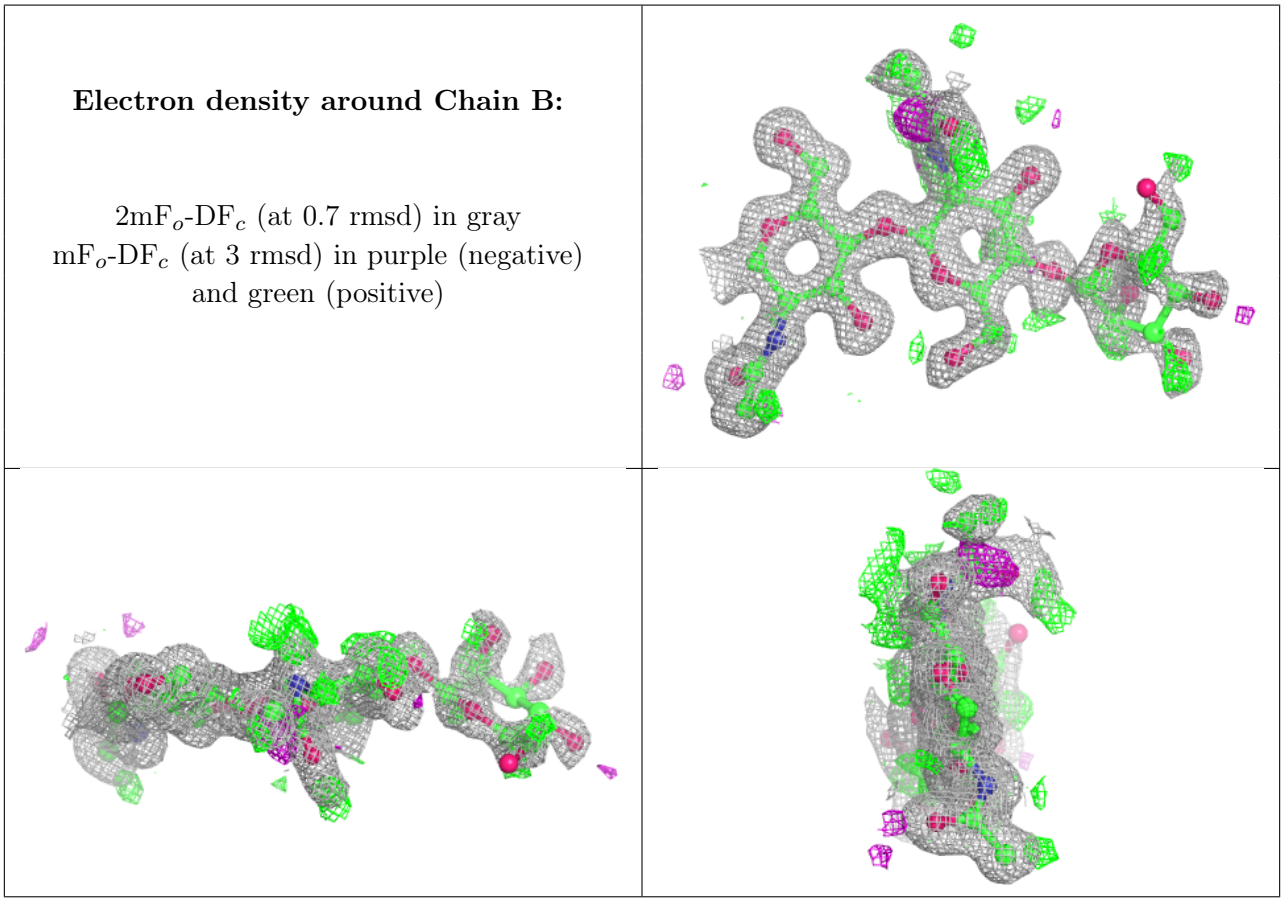
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	BMA	B	3	11/12	0.62	0.26	23,26,29,31	11
2	BMA	C	3	11/12	0.71	0.21	22,26,31,33	11
2	NAG	B	2	14/15	0.80	0.21	19,25,30,34	0
2	NAG	C	2	14/15	0.95	0.09	11,14,23,26	0
2	NAG	B	1	14/15	0.96	0.07	10,11,15,15	0
2	NAG	C	1	14/15	0.97	0.05	8,10,13,14	0

The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

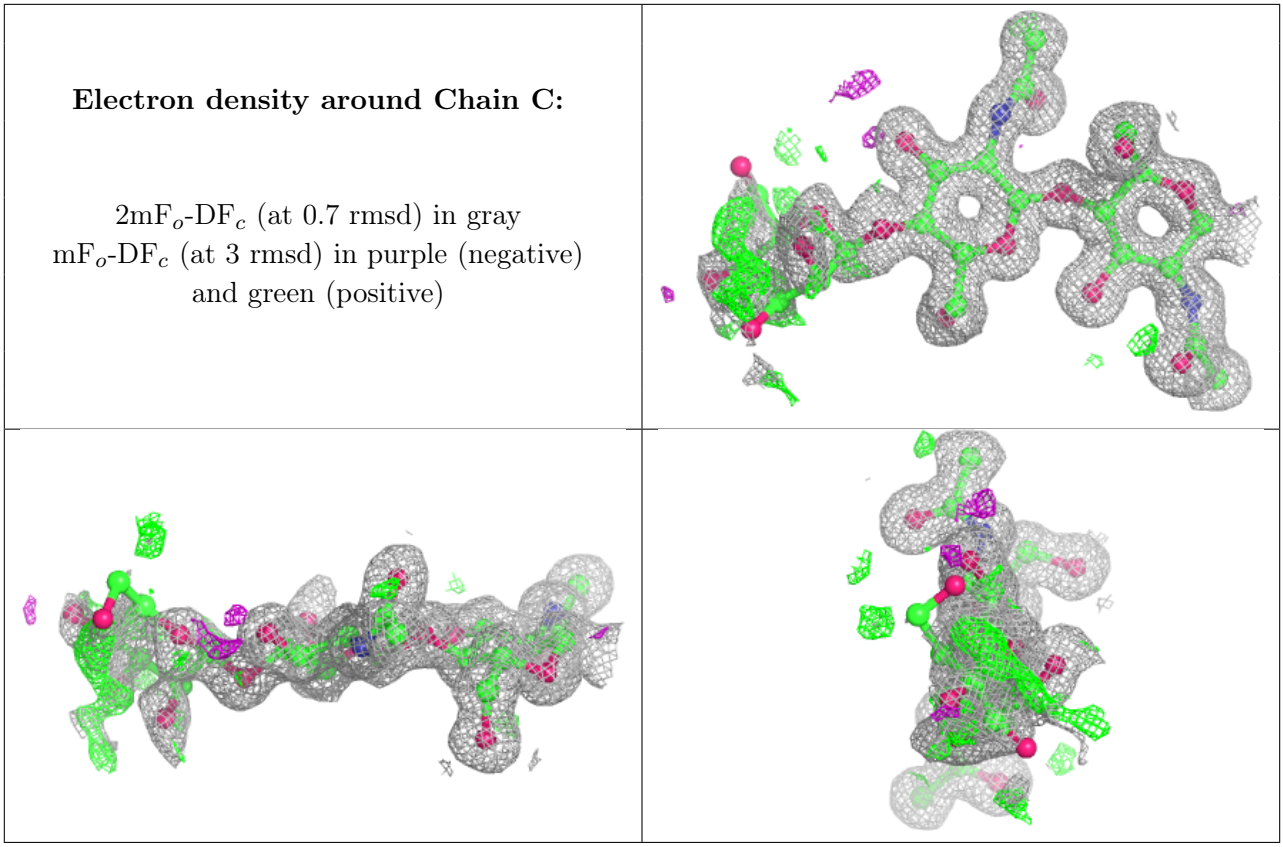
Electron density around Chain B:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



Electron density around Chain C:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



6.4 Ligands

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	B-factors(Å^2)	Q<0.9
5	CIT	A	513	13/13	0.91	0.14	18,24,30,34	0
4	OXY	A	512	2/2	0.96	0.07	10,10,10,11	2
6	NA	A	514	1/1	0.97	0.06	16,16,16,16	1
4	OXY	A	511	2/2	0.99	0.05	7,7,7,8	2
3	CU	A	503	1/1	1.00	0.05	6,6,6,6	1
3	CU	A	504	1/1	1.00	0.04	5,5,5,5	0
3	CU	A	501[A]	1/1	1.00	0.04	6,6,6,6	1
3	CU	A	501[B]	1/1	1.00	0.04	5,5,5,5	1
3	CU	A	502[A]	1/1	1.00	0.03	9,9,9,9	1
3	CU	A	502[B]	1/1	1.00	0.03	5,5,5,5	1

6.5 Other polymers

There are no such residues in this entry.