

# Full wwPDB X-ray Structure Validation Report (i)

Jan 8, 2024 - 01:40 am GMT

PDB ID	:	5MIE
Title	:	The study of the X-ray induced enzymatic reduction of molecular oxygen to
		water for laccase from Steccherinum murashkinskyi. The 15-th structure of the
		series with total exposition time 423 min.
Authors	:	Polyakov, K.M.; Gavryushov, S.; Fedorova, T.V.; Glazunova, O.A.; Popov,
		A.N.
Deposited on	:	2016-11-28
Resolution	:	1.35 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 (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:

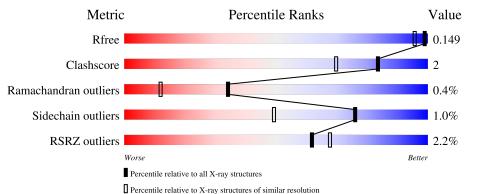
Xtriage (Phenix) EDS Percentile statistics Refmac	:::::::::::::::::::::::::::::::::::::::	1.8.4, CSD as541be (2020) 1.13 2.36 20191225.v01 (using entries in the PDB archive December 25th 2019) 5.8.0158
CCP4 Ideal geometry (proteins)		7.0.044 (Gargrove) Engh & Huber (2001)
Ideal geometry (DNA, RNA) Validation Pipeline (wwPDB-VP)	:	e ( )

# 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 1.35 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	$egin{array}{c} { m Whole \ archive} \ (\#{ m Entries}) \end{array}$	${f Similar\ resolution}\ (\#{ m Entries,\ resolution\ range}({ m \AA}))$
$R_{free}$	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	А	546	<sup>2%</sup> 85%	5% • 9%
2	В	2	50%	50%
2	С	2	10	0%



#### 5MIE

# 2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 8085 atoms, of which 3387 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	А	499	Total 7292	C 2466	H 3387	N 662	O 767	S 10	79	35	0

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



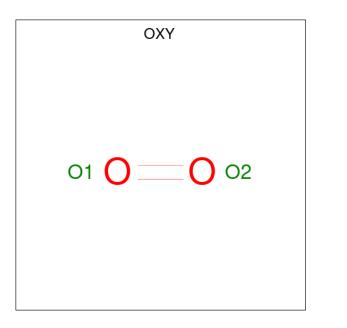
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
2	В	2	Total         C         N         O           28         16         2         10	0	0	0
2	С	2	Total         C         N         O           28         16         2         10	0	0	0

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

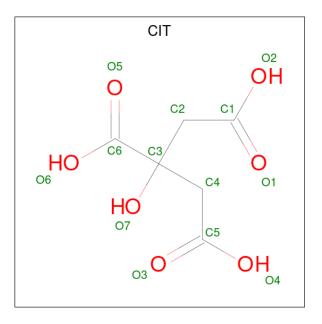
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	А	4	Total Cu 6 6	0	2

• Molecule 4 is OXYGEN MOLECULE (three-letter code: OXY) (formula: O<sub>2</sub>).





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



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

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



M	ol	Chain	Residues	Atoms		ZeroOcc	AltConf
6		А	1	Total 1	Na 1	0	0

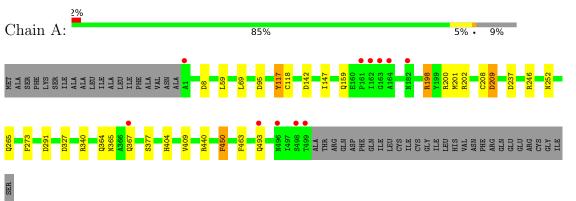
• Molecule 7 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	А	705	Total         O           715         715	0	10



# 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

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

Chain B:	50%	50%	
NAG1 NAG2			
• Molecule 2: opyranose	2-acetamido-2-deoxy-beta-D	D-glucopyranose-(1-4)-2-acetamid	.o-2-deoxy-beta-D-gluc

Chain C:

100%





## 4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants	56.33Å 84.38Å 112.43Å	Depositor
a, b, c, $\alpha$ , $\beta$ , $\gamma$	$90.00^{\circ}$ $90.00^{\circ}$ $90.00^{\circ}$	Depositor
Resolution (Å)	67.49 - 1.35	Depositor
Resolution (A)	19.46 - 1.35	EDS
% Data completeness	98.8 (67.49-1.35)	Depositor
(in resolution range)	98.8 (19.46-1.35)	EDS
R <sub>merge</sub>	0.04	Depositor
R <sub>sym</sub>	(Not available)	Depositor
$< I/\sigma(I) > 1$	$3.11 (at 1.35 \text{\AA})$	Xtriage
Refinement program	REFMAC 5.8.0049	Depositor
$R, R_{free}$	0.132 , $0.148$	Depositor
It, Itfree	0.133 , $0.149$	DCC
$R_{free}$ test set	5870 reflections $(5.03\%)$	wwPDB-VP
Wilson B-factor $(Å^2)$	9.2	Xtriage
Anisotropy	0.154	Xtriage
Bulk solvent $k_{sol}(e/Å^3)$ , $B_{sol}(Å^2)$	0.43, $51.9$	EDS
L-test for twinning <sup>2</sup>	$ < L >=0.48, < L^2>=0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.98	EDS
Total number of atoms	8085	wwPDB-VP
Average B, all atoms $(Å^2)$	11.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 5.48% of the height of the origin peak. No significant pseudotranslation is detected.

<sup>&</sup>lt;sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.



<sup>&</sup>lt;sup>1</sup>Intensities 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: CIT, OXY, CU, NA, 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).

Mal	Chain	Bo	Bond lengths		ond angles
Mol Chain	RMSZ	# Z  > 5	RMSZ	# Z  > 5	
1	А	0.93	2/4171~(0.0%)	1.00	22/5738~(0.4%)

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 out		#Planarity outliers
1	А	0	1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	А	377[A]	SER	CB-OG	-9.66	1.29	1.42
1	А	377[B]	SER	CB-OG	-9.66	1.29	1.42

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$\mathbf{Observed}(^{o})$	$Ideal(^{o})$
1	А	237	ASP	CB-CG-OD1	11.81	128.93	118.30
1	А	327	ASP	CB-CG-OD2	7.59	125.13	118.30
1	А	95	ASP	CB-CG-OD1	6.88	124.49	118.30
1	А	291	ASP	CB-CG-OD2	-6.86	112.13	118.30
1	А	200	ARG	NE-CZ-NH1	6.75	123.68	120.30
1	А	340	ARG	NE-CZ-NH2	-6.46	117.07	120.30
1	А	450	PHE	CB-CG-CD2	-6.31	116.39	120.80
1	А	202	ARG	NE-CZ-NH1	6.19	123.39	120.30
1	А	409[A]	VAL	CA-CB-CG2	6.14	120.10	110.90
1	А	409[B]	VAL	CA-CB-CG2	6.14	120.10	110.90
1	А	198[A]	ARG	NE-CZ-NH2	-6.12	117.24	120.30

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Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
1	А	198[B]	ARG	NE-CZ-NH2	-6.12	117.24	120.30
1	А	69	LEU	CB-CG-CD2	6.10	121.38	111.00
1	А	198[A]	ARG	NE-CZ-NH1	6.00	123.30	120.30
1	А	198[B]	ARG	NE-CZ-NH1	6.00	123.30	120.30
1	А	450	PHE	CB-CG-CD1	5.82	124.87	120.80
1	А	8	ASP	CB-CG-OD2	-5.68	113.19	118.30
1	А	209	ASP	CB-CG-OD1	5.63	123.37	118.30
1	А	340	ARG	CG-CD-NE	5.49	123.34	111.80
1	А	440	ARG	NE-CZ-NH2	-5.38	117.61	120.30
1	А	142	ASP	CB-CG-OD1	5.26	123.03	118.30
1	А	117	TYR	CA-CB-CG	5.05	122.99	113.40

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There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	А	404	HIS	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	А	3905	3387	3674	17	0
2	В	28	0	25	1	0
2	С	28	0	25	0	0
3	А	6	0	0	0	0
4	А	2	0	0	0	0
5	А	13	0	5	0	0
6	А	1	0	0	0	0
7	А	715	0	0	10	0
All	All	4698	3387	3729	18	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 2.

All (18) 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:364:GLN:OE1	7:A:706:HOH:O	1.71	1.06
1:A:159[B]:GLN:HG3	7:A:750:HOH:O	1.57	1.04
1:A:198[B]:ARG:CZ	7:A:707:HOH:O	2.25	0.85
1:A:265[C]:GLN:OE1	7:A:705:HOH:O	1.97	0.82
1:A:159[B]:GLN:CG	7:A:750:HOH:O	2.19	0.78
1:A:493:GLN:HG2	7:A:932:HOH:O	1.88	0.73
1:A:147:ILE:HD11	1:A:201[B]:MET:HE2	1.78	0.64
1:A:198[B]:ARG:NE	7:A:707:HOH:O	2.32	0.62
1:A:118:CYS:SG	1:A:208[B]:CYS:HB3	2.44	0.57
1:A:265[C]:GLN:CD	7:A:705:HOH:O	2.40	0.56
1:A:118:CYS:HA	1:A:208[B]:CYS:SG	2.47	0.55
1:A:198[B]:ARG:HG2	1:A:252[B]:ASN:ND2	2.24	0.52
1:A:147:ILE:HD11	1:A:201[B]:MET:CE	2.44	0.48
2:B:2:NAG:H83	2:B:2:NAG:H3	1.96	0.46
1:A:364:GLN:NE2	7:A:715[A]:HOH:O	2.50	0.45
1:A:265[B]:GLN:NE2	1:A:273:PHE:CZ	2.86	0.43
1:A:364:GLN:HB3	7:A:1037:HOH:O	2.19	0.43
1:A:365:ASN:HD21	1:A:367:GLN:HB2	1.84	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	А	535/546~(98%)	521 (97%)	12 (2%)	2 (0%)	34 12

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	А	209	ASP
1	А	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 side chain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	А	443/447~(99%)	439 (99%)	4 (1%)	78 53	

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	А	117	TYR
1	А	246	ARG
1	А	450	PHE
1	А	463	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	А	44	ASN
1	А	182	ASN
1	А	364	GLN
1	А	444	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).



Mal	Mol Type Chain		Res 1	Link	Bo	ond leng	$\mathbf{ths}$	Bond angles		
INIOI	туре	Unam	nes	LIIIK	Counts	RMSZ	# Z >2	Counts	RMSZ	# Z >2
2	NAG	С	1	2,1	14,14,15	0.95	1 (7%)	17,19,21	1.05	1 (5%)
2	NAG	В	2	2	14,14,15	1.50	2 (14%)	17,19,21	1.90	4 (23%)
2	NAG	В	1	2,1	14,14,15	1.58	3 (21%)	17,19,21	1.03	0
2	NAG	С	2	2	14,14,15	0.74	0	17,19,21	2.13	3 (17%)

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	С	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	В	2	2	-	3/6/23/26	0/1/1/1
2	NAG	В	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	С	2	2	-	0/6/23/26	0/1/1/1

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	$\mathrm{Ideal}(\mathrm{\AA})$
2	В	1	NAG	O5-C1	-4.08	1.37	1.43
2	В	2	NAG	C2-N2	3.93	1.53	1.46
2	В	1	NAG	C1-C2	2.38	1.55	1.52
2	В	2	NAG	C1-C2	2.27	1.55	1.52
2	С	1	NAG	C8-C7	2.16	1.55	1.50
2	В	1	NAG	O3-C3	2.00	1.47	1.43

All (6) bond length outliers are listed below:

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
2	С	2	NAG	C1-O5-C5	-7.40	102.17	112.19
2	В	2	NAG	O7-C7-C8	-4.19	114.27	122.06
2	В	2	NAG	C8-C7-N2	3.96	122.80	116.10
2	В	2	NAG	C3-C4-C5	3.36	116.23	110.24
2	В	2	NAG	C1-C2-N2	3.11	115.80	110.49
2	С	2	NAG	O4-C4-C3	-2.45	104.68	110.35
2	С	2	NAG	C1-C2-N2	2.16	114.18	110.49
2	С	1	NAG	O4-C4-C5	-2.12	104.03	109.30

There are no chirality outliers.

All (3) torsion outliers are listed below:



Mol	Chain	Res	Type	Atoms
2	В	2	NAG	C8-C7-N2-C2
2	В	2	NAG	O7-C7-N2-C2
2	В	2	NAG	C3-C2-N2-C7

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	В	2	NAG	1	0

### 5.5 Carbohydrates (i)

4 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).

Mal	Mol Type Chain R		Res	Res Link	Bo	ond leng	ths	Bond angles		
INIOI	туре	Chain	nes	LIIIK	Counts	RMSZ	# Z >2	Counts	RMSZ	# Z >2
2	NAG	В	1	2,1	14,14,15	1.58	3 (21%)	17,19,21	1.03	0
2	NAG	В	2	2	14,14,15	1.50	2 (14%)	17,19,21	1.90	4 (23%)
2	NAG	С	1	2,1	14,14,15	0.95	1 (7%)	17,19,21	1.05	1 (5%)
2	NAG	С	2	2	14,14,15	0.74	0	17,19,21	2.13	3 (17%)

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	В	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	В	2	2	-	3/6/23/26	0/1/1/1
2	NAG	С	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	С	2	2	-	0/6/23/26	0/1/1/1

All (6) bond length outliers are listed below:



Mol	Chain	Res	Type	Atoms	Z	$\operatorname{Observed}(\operatorname{\AA})$	Ideal(Å)
2	В	1	NAG	O5-C1	-4.08	1.37	1.43
2	В	2	NAG	C2-N2	3.93	1.53	1.46
2	В	1	NAG	C1-C2	2.38	1.55	1.52
2	В	2	NAG	C1-C2	2.27	1.55	1.52
2	С	1	NAG	C8-C7	2.16	1.55	1.50
2	В	1	NAG	O3-C3	2.00	1.47	1.43

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$\mathbf{Observed}(^{o})$	$Ideal(^{o})$
2	С	2	NAG	C1-O5-C5	-7.40	102.17	112.19
2	В	2	NAG	O7-C7-C8	-4.19	114.27	122.06
2	В	2	NAG	C8-C7-N2	3.96	122.80	116.10
2	В	2	NAG	C3-C4-C5	3.36	116.23	110.24
2	В	2	NAG	C1-C2-N2	3.11	115.80	110.49
2	С	2	NAG	O4-C4-C3	-2.45	104.68	110.35
2	С	2	NAG	C1-C2-N2	2.16	114.18	110.49
2	С	1	NAG	O4-C4-C5	-2.12	104.03	109.30

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	В	2	NAG	C8-C7-N2-C2
2	В	2	NAG	O7-C7-N2-C2
2	В	2	NAG	C3-C2-N2-C7

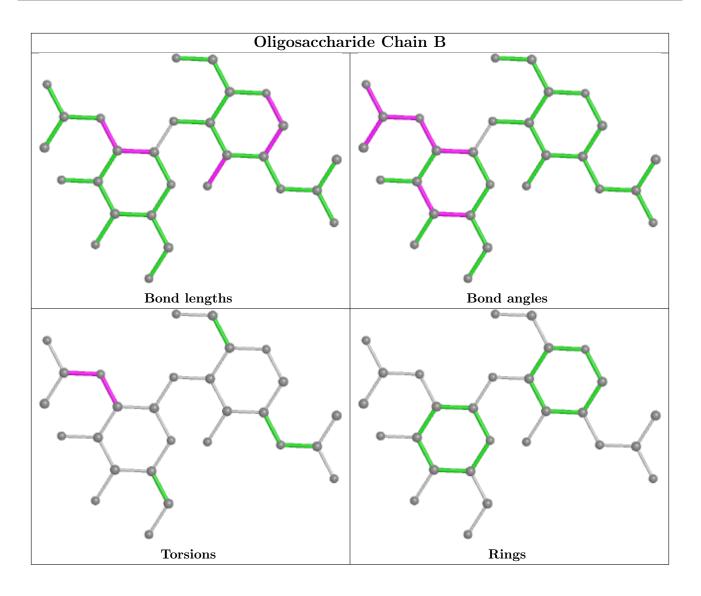
There are no ring outliers.

1 monomer is involved in 1 short contact:

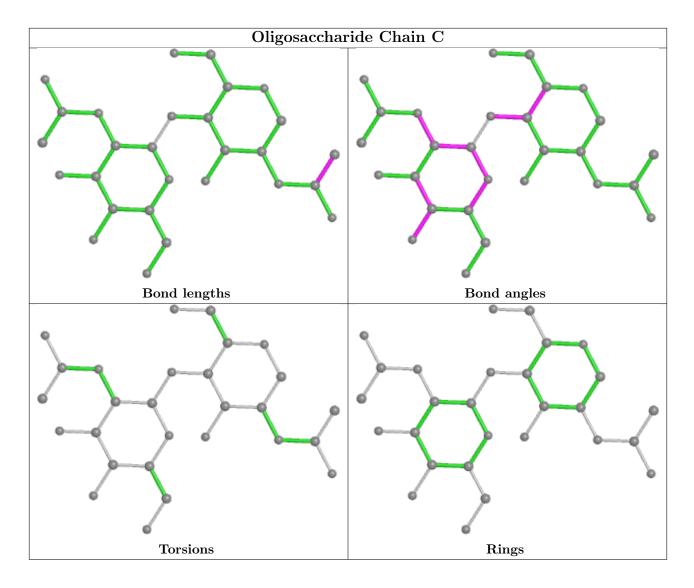
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	В	2	NAG	1	0

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









## 5.6 Ligand geometry (i)

Of 9 ligands modelled in this entry, 7 are monoatomic - leaving 2 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
4	OXY	А	609	3	1,1,1	0.16	0	-		
5	CIT	А	610	-	12,12,12	1.15	0	$17,\!17,\!17$	1.51	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
5	CIT	А	610	-	-	2/16/16/16	-

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
5	А	610	CIT	O6-C6-C3	4.30	120.52	113.05
5	А	610	CIT	O2-C1-C2	2.09	121.05	114.35

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	А	610	CIT	O1-C1-C2-C3
5	А	610	CIT	O2-C1-C2-C3

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 $>$	#RSRZ>2		$OWAB(Å^2)$	Q<0.9	
1	А	499/546~(91%)	-0.49	11 (2%)	62	68	5, 9, 19, 50	0

All (11) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	А	162[A]	ILE	5.8
1	А	499	THR	5.2
1	А	498	SER	4.9
1	А	1	ALA	4.2
1	А	163[A]	GLY	3.4
1	А	496	ASN	3.0
1	А	161[A]	PRO	2.3
1	А	182	ASN	2.3
1	А	367	GLN	2.3
1	А	164[A]	ALA	2.2
1	А	493	GLN	2.0

### 6.2 Non-standard residues in protein, DNA, RNA chains (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	$B-factors(Å^2)$	Q < 0.9
2	NAG	В	2	14/15	0.84	0.20	$19,\!27,\!33,\!35$	0
2	NAG	С	2	14/15	0.95	0.08	12,15,23,26	0
2	NAG	В	1	14/15	0.97	0.06	10,12,14,15	0
2	NAG	С	1	14/15	0.97	0.05	9,10,13,14	0

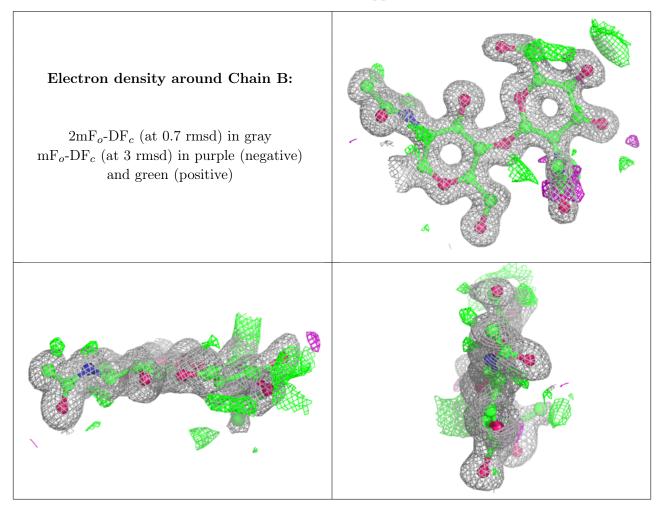


### 6.3 Carbohydrates (i)

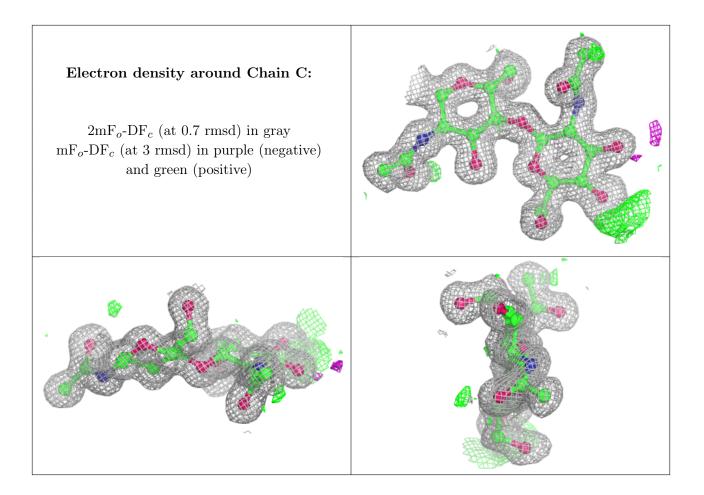
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median,  $95^{th}$  percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	$\mathbf{B} ext{-factors}(\mathrm{\AA}^2)$	Q<0.9
2	NAG	В	2	14/15	0.84	0.20	$19,\!27,\!33,\!35$	0
2	NAG	С	2	14/15	0.95	0.08	12,15,23,26	0
2	NAG	С	1	14/15	0.97	0.05	9,10,13,14	0
2	NAG	В	1	14/15	0.97	0.06	10,12,14,15	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.







### 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	$\operatorname{B-factors}(\operatorname{\AA}^2)$	Q<0.9
5	CIT	А	610	13/13	0.90	0.16	$19,\!24,\!33,\!36$	0
6	NA	А	611	1/1	0.98	0.07	$17,\!17,\!17,\!17$	1
3	CU	А	602[A]	1/1	1.00	0.03	$11,\!11,\!11,\!11$	1
3	CU	А	602[B]	1/1	1.00	0.03	5, 5, 5, 5	1
3	CU	А	603	1/1	1.00	0.04	$6,\!6,\!6,\!6$	1
3	CU	А	604	1/1	1.00	0.04	$6,\!6,\!6,\!6$	0
4	OXY	А	609	2/2	1.00	0.05	3,3,3,4	2
3	CU	А	601[A]	1/1	1.00	0.03	5, 5, 5, 5	1
3	CU	A	601[B]	1/1	1.00	0.03	$6,\!6,\!6,\!6$	1



## 6.5 Other polymers (i)

There are no such residues in this entry.

