



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 11:29 PM UTC

PDB ID : 6IQY / pdb_00006iqy
Title : High resolution structure of bilirubin oxidase from *Myrothecium verrucaria* - M467Q mutant, anaerobically prepared
Authors : Shibata, N.; Akter, M.; Higuchi, Y.
Deposited on : 2018-11-09
Resolution : 1.60 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	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

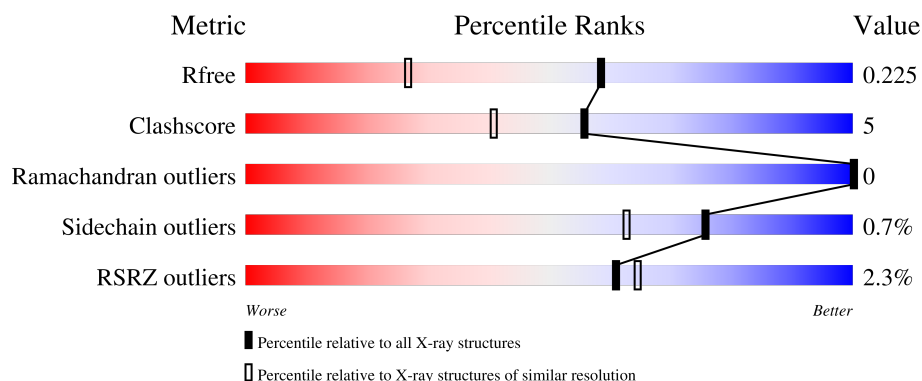
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.60 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}	180053	4673 (1.60-1.60)
Clashscore	190562	4931 (1.60-1.60)
Ramachandran outliers	187476	4831 (1.60-1.60)
Sidechain outliers	187428	4830 (1.60-1.60)
RSRZ outliers	180081	4672 (1.60-1.60)

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 $\leq 5\%$. 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	538	3% 90% 9%
1	B	538	2% 90% 9%
2	C	3	33% 67%
2	D	3	67% 33%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	ACT	B	609	-	-	X	-

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 10302 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.

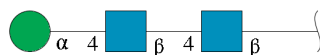
- Molecule 1 is a protein called Bilirubin oxidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	536	Total	C	N	O	S	0	7	0
			4309	2754	728	812	15			
1	B	536	Total	C	N	O	S	0	13	0
			4346	2780	735	816	15			

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-3	TYR	-	expression tag	UNP Q12737
A	-2	VAL	-	expression tag	UNP Q12737
A	-1	GLU	-	expression tag	UNP Q12737
A	0	PHE	-	expression tag	UNP Q12737
A	467	GLN	MET	engineered mutation	UNP Q12737
B	-3	TYR	-	expression tag	UNP Q12737
B	-2	VAL	-	expression tag	UNP Q12737
B	-1	GLU	-	expression tag	UNP Q12737
B	0	PHE	-	expression tag	UNP Q12737
B	467	GLN	MET	engineered mutation	UNP Q12737

- 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.

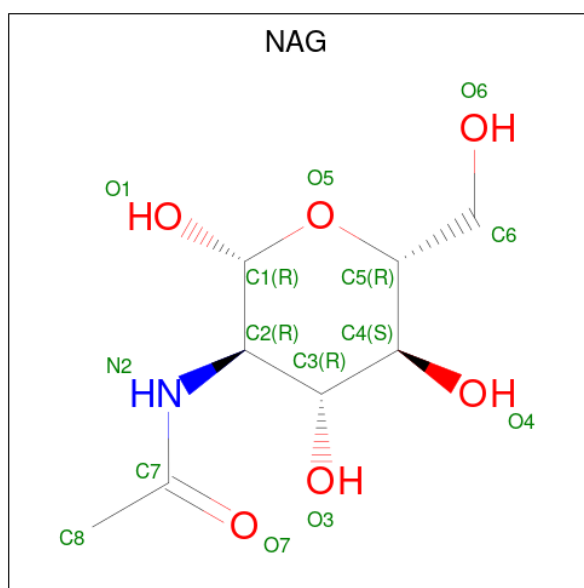


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	C	3	Total	C	N	O	0	0	0
			39	22	2	15			
2	D	3	Total	C	N	O	0	0	0
			39	22	2	15			

- Molecule 3 is COPPER (II) ION (CCD ID: CU) (formula: Cu).

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

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆).



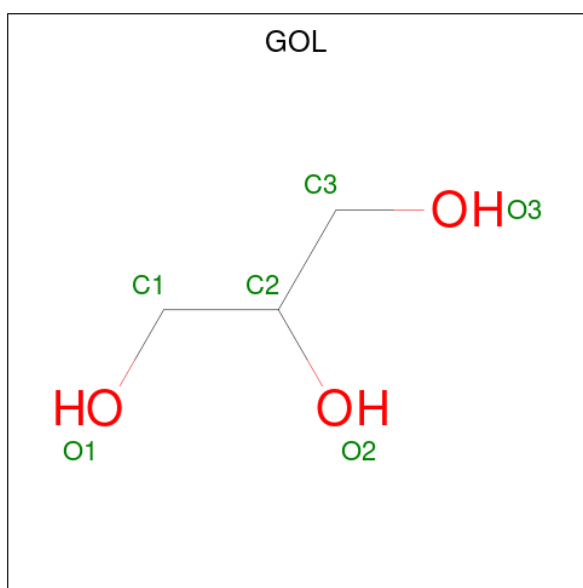
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			14	8	1	5		
4	B	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 5 is ACETATE ION (CCD ID: ACT) (formula: C₂H₃O₂).



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

- Molecule 6 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



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

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			6	3	3		
6	B	1	Total	C	O	0	0
			6	3	3		
6	B	1	Total	C	O	0	0
			6	3	3		
6	B	1	Total	C	O	0	0
			6	3	3		
6	B	1	Total	C	O	0	0
			6	3	3		

- Molecule 7 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	1	Total	Ca	0	0
			1	1		
7	B	1	Total	Ca	0	0
			1	1		

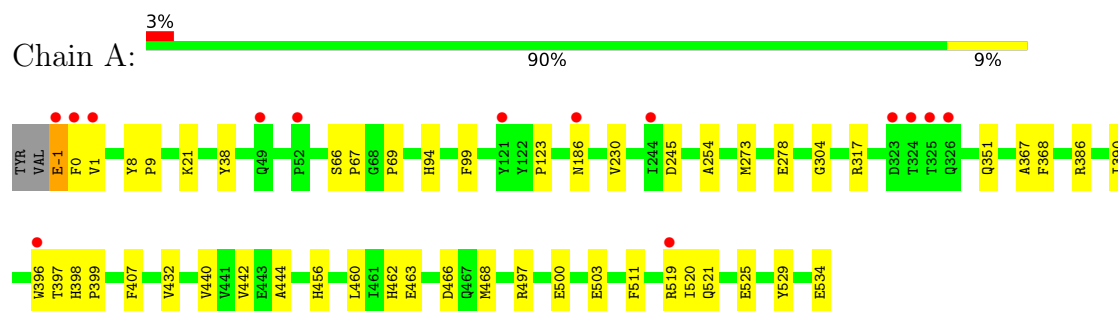
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	728	Total	O	0	0
			728	728		
8	B	753	Total	O	0	0
			753	753		

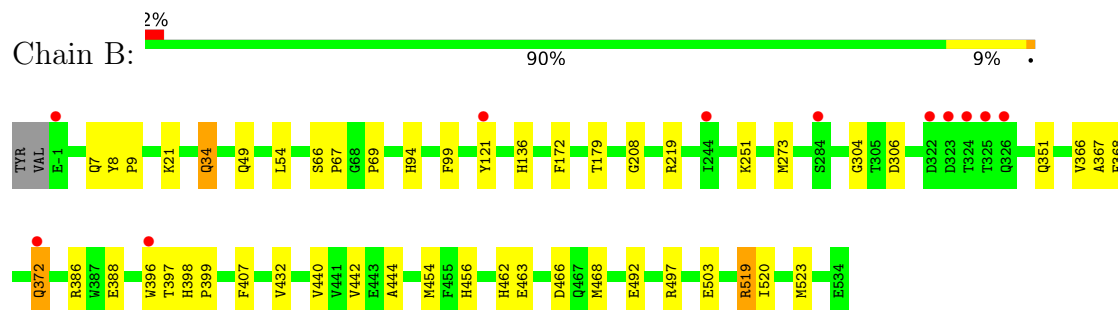
3 Residue-property plots [i](#)

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: Bilirubin oxidase



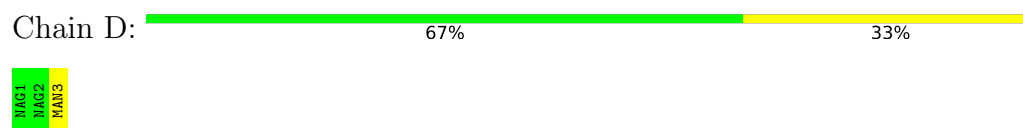
- Molecule 1: Bilirubin oxidase



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



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



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	59.30Å 152.25Å 69.91Å 90.00° 91.66° 90.00°	Depositor
Resolution (Å)	45.86 – 1.60 45.86 – 1.60	Depositor EDS
% Data completeness (in resolution range)	99.5 (45.86-1.60) 99.7 (45.86-1.60)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.20 (at 1.60Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.191 , 0.225 0.192 , 0.225	Depositor DCC
R_{free} test set	1996 reflections (1.23%)	wwPDB-VP
Wilson B-factor (Å ²)	11.9	Xtriage
Anisotropy	0.747	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 49.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.158 for h,-k,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	10302	wwPDB-VP
Average B, all atoms (Å ²)	15.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.67% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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.

5 Model quality

5.1 Standard geometry

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

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	0.44	0/4453	0.76	1/6089 (0.0%)
1	B	0.45	0/4505	0.77	3/6158 (0.0%)
All	All	0.45	0/8958	0.76	4/12247 (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	B	0	1

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	B	372	GLN	CG-CD-NE2	-6.94	105.99	116.40
1	B	372	GLN	N-CA-CB	-6.06	100.52	110.40
1	B	372	GLN	CA-CB-CG	-5.44	103.22	114.10
1	A	-1	GLU	CA-CB-CG	5.41	124.93	114.10

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	372	GLN	Sidechain

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	4309	0	4095	39	0
1	B	4346	0	4151	40	0
2	C	39	0	34	2	0
2	D	39	0	34	0	0
3	A	4	0	0	0	0
3	B	4	0	0	0	0
4	A	14	0	13	0	0
4	B	14	0	13	0	0
5	A	4	0	3	0	0
5	B	4	0	3	3	0
6	A	18	0	24	1	0
6	B	24	0	32	2	0
7	A	1	0	0	0	0
7	B	1	0	0	0	0
8	A	728	0	0	12	0
8	B	753	0	0	10	1
All	All	10302	0	8402	81	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 5.

All (81) 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:208:GLY:HA2	5:B:609:ACT:H3	1.70	0.74
1:A:186:ASN:ND2	8:A:708:HOH:O	2.30	0.64
1:B:492:GLU:OE2	8:B:701:HOH:O	2.14	0.63
1:A:519:ARG:NH1	8:A:709:HOH:O	2.31	0.62
1:B:179:THR:OG1	5:B:609:ACT:H2	1.99	0.62
1:B:7:GLN:NE2	8:B:708:HOH:O	2.30	0.62
1:B:34[A]:GLN:NE2	8:B:715:HOH:O	2.36	0.59
1:B:251:LYS:NZ	8:B:714:HOH:O	2.34	0.59
1:A:519:ARG:NH2	8:A:711:HOH:O	2.33	0.58
1:B:49:GLN:NE2	1:B:54:LEU:O	2.35	0.57
1:B:121:TYR:HD2	1:B:523[A]:MET:HE3	1.68	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:456:HIS:CD2	1:A:468[B]:MET:HE3	2.41	0.56
1:A:304:GLY:HA2	1:A:397:THR:HG21	1.88	0.55
1:B:8:TYR:CD1	1:B:9:PRO:HD2	2.43	0.54
1:B:407:PHE:HB3	1:B:444:ALA:HB2	1.90	0.54
1:A:463:GLU:N	8:A:716:HOH:O	2.41	0.54
1:B:366:VAL:HG21	6:B:612:GOL:H2	1.91	0.53
1:A:456:HIS:HB3	1:A:468[A]:MET:HG3	1.90	0.53
1:B:304:GLY:HA2	1:B:397:THR:HG21	1.89	0.52
1:B:21:LYS:HB2	1:B:69:PRO:HB2	1.90	0.52
1:A:500:GLU:O	1:A:503:GLU:HG2	2.10	0.52
1:B:368:PHE:HB2	1:B:468[B]:MET:HB2	1.90	0.52
1:B:463:GLU:N	8:B:723:HOH:O	2.43	0.52
1:B:396:TRP:CD1	1:B:398:HIS:HE2	2.28	0.51
1:A:368:PHE:HB2	1:A:468[B]:MET:HB2	1.93	0.51
1:A:317:ARG:NH2	8:A:717:HOH:O	2.43	0.51
1:A:503:GLU:HG3	1:A:511:PHE:CD1	2.46	0.50
1:A:407:PHE:HB3	1:A:444:ALA:HB2	1.93	0.50
1:A:21:LYS:HB2	1:A:69:PRO:HB2	1.94	0.49
8:A:785:HOH:O	2:C:1:NAG:H83	2.12	0.49
1:A:245:ASP:OD1	8:A:701:HOH:O	2.20	0.49
1:B:432:VAL:HG21	1:B:440:VAL:HG11	1.95	0.49
1:A:351[B]:GLN:HG3	1:A:390:ILE:HD12	1.94	0.48
1:B:136:HIS:CD2	8:B:716:HOH:O	2.65	0.48
1:B:456:HIS:CD2	1:B:468[B]:MET:HE3	2.49	0.48
1:A:456:HIS:CG	1:A:468[B]:MET:HE3	2.48	0.48
1:B:497:ARG:HD2	1:B:519:ARG:HH12	1.79	0.48
1:B:503:GLU:HG3	8:B:847:HOH:O	2.14	0.48
1:A:367:ALA:HB1	1:A:466:ASP:HB3	1.95	0.47
1:A:254:ALA:HB3	1:A:278:GLU:HB2	1.95	0.47
1:B:462:HIS:HB2	8:B:723:HOH:O	2.14	0.47
1:B:497:ARG:NH1	1:B:519:ARG:NH1	2.63	0.47
1:B:520:ILE:HA	1:B:523[A]:MET:HE2	1.95	0.47
1:A:273:MET:HE2	1:A:399:PRO:HG3	1.96	0.47
1:A:396:TRP:CD1	1:A:398:HIS:HE2	2.33	0.47
1:B:351:GLN:NE2	1:B:388:GLU:OE1	2.48	0.47
1:A:534:GLU:OE2	8:A:702:HOH:O	2.20	0.47
1:A:462:HIS:HB2	8:A:716:HOH:O	2.14	0.46
1:B:456:HIS:CG	1:B:468[B]:MET:HE3	2.50	0.46
1:B:368:PHE:HB2	1:B:468[A]:MET:HB3	1.97	0.46
1:A:503:GLU:HG3	1:A:511:PHE:HD1	1.81	0.46
8:A:1317:HOH:O	2:C:1:NAG:H81	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:136:HIS:HE1	1:B:468[B]:MET:HE1	1.80	0.45
1:B:497:ARG:CZ	1:B:519:ARG:HH12	2.30	0.45
1:A:432:VAL:HG21	1:A:440:VAL:HG11	1.99	0.45
1:B:172:PHE:CE1	1:B:219:ARG:HD3	2.52	0.44
1:A:-1:GLU:HG2	1:A:0:PHE:H	1.81	0.44
1:A:521:GLN:O	1:A:525:GLU:HG3	2.18	0.43
1:A:38:TYR:CD1	1:A:520:ILE:HD11	2.54	0.43
1:A:245:ASP:O	6:A:610:GOL:O3	2.35	0.43
1:B:367:ALA:HB1	1:B:466:ASP:HB3	2.01	0.43
1:A:351[B]:GLN:OE1	8:A:703:HOH:O	2.22	0.43
1:A:386:ARG:HA	1:A:442:VAL:O	2.19	0.42
1:B:94:HIS:HB2	8:B:716:HOH:O	2.18	0.42
1:B:208:GLY:HA2	5:B:609:ACT:CH3	2.46	0.42
1:A:468[B]:MET:HE2	1:A:468[B]:MET:HB3	1.94	0.42
1:B:66:SER:HA	1:B:67:PRO:C	2.44	0.42
1:B:454:MET:HE1	8:B:716:HOH:O	2.18	0.42
1:A:230:VAL:HG13	1:A:460:LEU:HB2	2.01	0.42
1:A:497:ARG:NH1	1:A:519:ARG:HD3	2.34	0.42
1:B:273:MET:HE2	1:B:399:PRO:HG3	2.02	0.42
1:B:366:VAL:CG2	6:B:612:GOL:H2	2.50	0.42
1:A:123:PRO:HB3	1:A:529:TYR:CG	2.55	0.41
1:A:8:TYR:CD1	1:A:9:PRO:HD2	2.56	0.41
1:B:386:ARG:HA	1:B:442:VAL:O	2.20	0.41
1:B:456:HIS:HB3	1:B:468[A]:MET:HG3	2.02	0.41
1:A:94:HIS:HB2	8:A:755:HOH:O	2.20	0.41
1:A:368:PHE:HB2	1:A:468[A]:MET:HB3	2.03	0.41
1:A:396:TRP:CD1	1:A:398:HIS:NE2	2.88	0.41
1:A:66:SER:HA	1:A:67:PRO:C	2.45	0.40
1:B:396:TRP:CD1	1:B:398:HIS:NE2	2.89	0.40

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)
8:B:1091:HOH:O	8:B:1266:HOH:O[1_655]	2.16	0.04

5.3 Torsion angles

5.3.1 Protein backbone

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	541/538 (101%)	516 (95%)	25 (5%)	0	100	100
1	B	547/538 (102%)	520 (95%)	27 (5%)	0	100	100
All	All	1088/1076 (101%)	1036 (95%)	52 (5%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains

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	462/457 (101%)	460 (100%)	2 (0%)	84	75
1	B	468/457 (102%)	463 (99%)	5 (1%)	65	46
All	All	930/914 (102%)	923 (99%)	7 (1%)	76	59

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	VAL
1	A	99	PHE
1	B	34[A]	GLN
1	B	34[B]	GLN
1	B	99	PHE
1	B	306	ASP
1	B	519	ARG

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

Mol	Chain	Res	Type
1	A	149	GLN
1	A	197	ASN
1	A	510	GLN
1	B	149	GLN

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 ⓘ

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	C	1	2,1	14,14,15	0.48	0	17,19,21	0.62	0
2	NAG	C	2	2	14,14,15	0.32	0	17,19,21	0.54	0
2	MAN	C	3	2	11,11,12	0.87	1 (9%)	15,15,17	1.23	2 (13%)
2	NAG	D	1	2,1	14,14,15	0.49	0	17,19,21	0.49	0
2	NAG	D	2	2	14,14,15	0.49	0	17,19,21	0.44	0
2	MAN	D	3	2	11,11,12	0.90	1 (9%)	15,15,17	1.24	2 (13%)

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	C	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	C	2	2	-	0/6/23/26	0/1/1/1
2	MAN	C	3	2	-	2/2/19/22	1/1/1/1
2	NAG	D	1	2,1	-	1/6/23/26	0/1/1/1
2	NAG	D	2	2	-	0/6/23/26	0/1/1/1
2	MAN	D	3	2	-	2/2/19/22	1/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	3	MAN	O5-C5	2.18	1.47	1.43
2	C	3	MAN	O5-C5	2.12	1.47	1.43

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	3	MAN	C1-O5-C5	3.67	117.11	112.19
2	C	3	MAN	C1-O5-C5	3.67	117.10	112.19
2	C	3	MAN	O2-C2-C3	-2.10	105.80	110.15
2	D	3	MAN	O2-C2-C3	-2.07	105.86	110.15

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	3	MAN	C4-C5-C6-O6
2	D	3	MAN	C4-C5-C6-O6
2	C	1	NAG	C8-C7-N2-C2
2	C	1	NAG	O7-C7-N2-C2
2	D	3	MAN	O5-C5-C6-O6
2	C	3	MAN	O5-C5-C6-O6
2	D	1	NAG	C4-C5-C6-O6

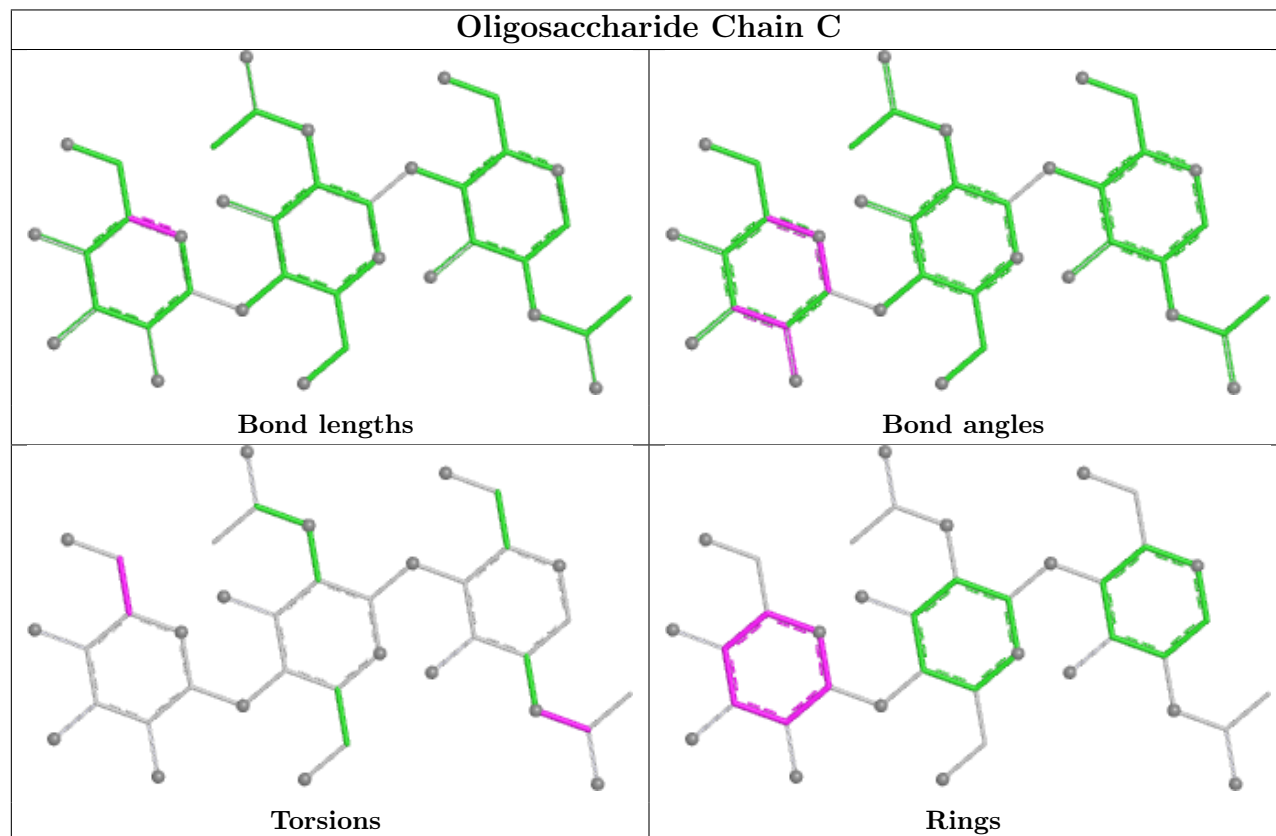
All (2) ring outliers are listed below:

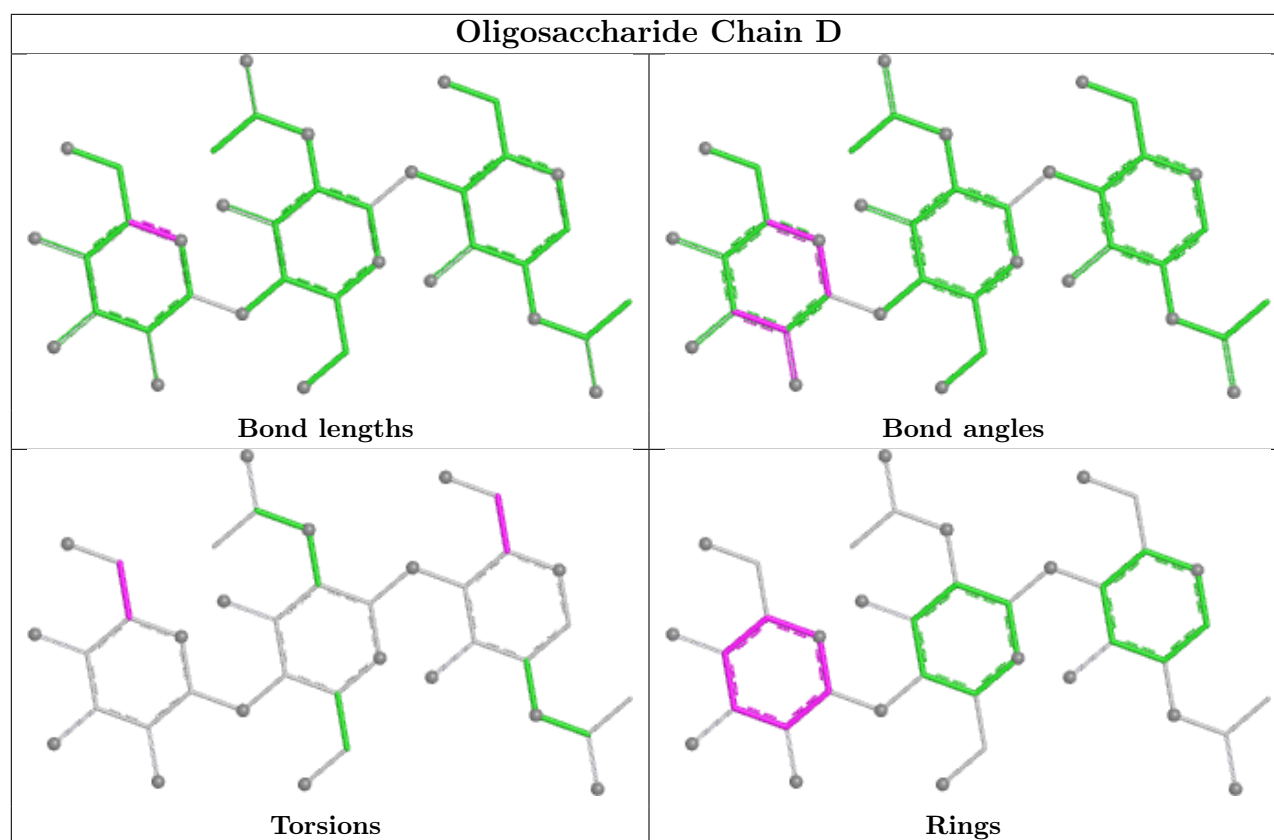
Mol	Chain	Res	Type	Atoms
2	C	3	MAN	C1-C2-C3-C4-C5-O5
2	D	3	MAN	C1-C2-C3-C4-C5-O5

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	1	NAG	2	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 21 ligands modelled in this entry, 10 are monoatomic - leaving 11 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	NAG	B	608	1	14,14,15	0.49	0	17,19,21	0.47	0
6	GOL	A	610	-	5,5,5	0.41	0	5,5,5	0.47	0
5	ACT	B	609	-	3,3,3	1.03	0	3,3,3	0.53	0
4	NAG	A	608	1	14,14,15	0.32	0	17,19,21	0.47	0
6	GOL	B	610	-	5,5,5	0.37	0	5,5,5	0.37	0
6	GOL	A	612	-	5,5,5	0.36	0	5,5,5	0.28	0
6	GOL	B	611	-	5,5,5	0.40	0	5,5,5	0.12	0
6	GOL	B	612	-	5,5,5	0.31	0	5,5,5	0.41	0
6	GOL	B	613	-	5,5,5	0.38	0	5,5,5	0.21	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	GOL	A	611	-	5,5,5	0.35	0	5,5,5	0.83	0
5	ACT	A	609	-	3,3,3	0.87	0	3,3,3	1.57	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
4	NAG	B	608	1	-	0/6/23/26	0/1/1/1
6	GOL	A	610	-	-	2/4/4/4	-
4	NAG	A	608	1	-	1/6/23/26	0/1/1/1
6	GOL	B	610	-	-	2/4/4/4	-
6	GOL	A	612	-	-	2/4/4/4	-
6	GOL	B	611	-	-	0/4/4/4	-
6	GOL	B	612	-	-	4/4/4/4	-
6	GOL	B	613	-	-	4/4/4/4	-
6	GOL	A	611	-	-	2/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (17) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	610	GOL	C1-C2-C3-O3
6	A	612	GOL	O1-C1-C2-C3
6	B	610	GOL	O1-C1-C2-C3
6	B	612	GOL	O1-C1-C2-C3
6	A	611	GOL	O1-C1-C2-C3
6	B	613	GOL	O1-C1-C2-C3
6	B	613	GOL	C1-C2-C3-O3
6	A	612	GOL	O1-C1-C2-O2
6	B	610	GOL	O1-C1-C2-O2
6	B	612	GOL	O1-C1-C2-O2
6	A	610	GOL	O2-C2-C3-O3
6	B	613	GOL	O1-C1-C2-O2
6	A	611	GOL	O1-C1-C2-O2
6	B	613	GOL	O2-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
6	B	612	GOL	O2-C2-C3-O3
4	A	608	NAG	C1-C2-N2-C7
6	B	612	GOL	C1-C2-C3-O3

There are no ring outliers.

3 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	610	GOL	1	0
5	B	609	ACT	3	0
6	B	612	GOL	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

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, 95th 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	536/538 (99%)	0.18	14 (2%) 57 60	6, 12, 24, 42	7 (1%)
1	B	536/538 (99%)	0.19	11 (2%) 63 67	4, 12, 24, 46	13 (2%)
All	All	1072/1076 (99%)	0.18	25 (2%) 61 64	4, 12, 24, 46	20 (1%)

All (25) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	372	GLN	4.1
1	B	396	TRP	3.7
1	B	325	THR	3.5
1	B	-1	GLU	3.4
1	A	519	ARG	3.1
1	A	396	TRP	3.0
1	B	323	ASP	2.9
1	A	-1	GLU	2.7
1	A	186	ASN	2.7
1	A	323	ASP	2.7
1	B	326	GLN	2.6
1	B	322	ASP	2.6
1	B	121	TYR	2.6
1	B	244	ILE	2.5
1	B	324	THR	2.5
1	A	121	TYR	2.4
1	A	52	PRO	2.3
1	A	1	VAL	2.3
1	A	325	THR	2.2
1	A	244	ILE	2.2
1	A	49	GLN	2.1
1	A	324	THR	2.1
1	B	284	SER	2.0
1	A	326	GLN	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	0	PHE	2.0

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](#)

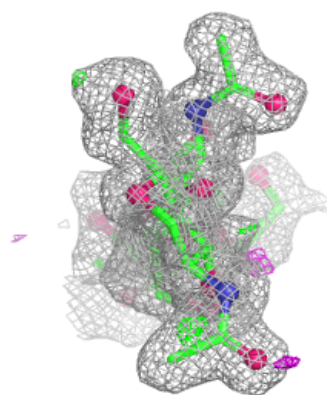
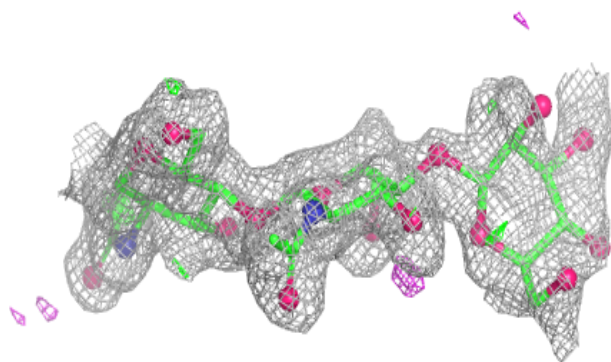
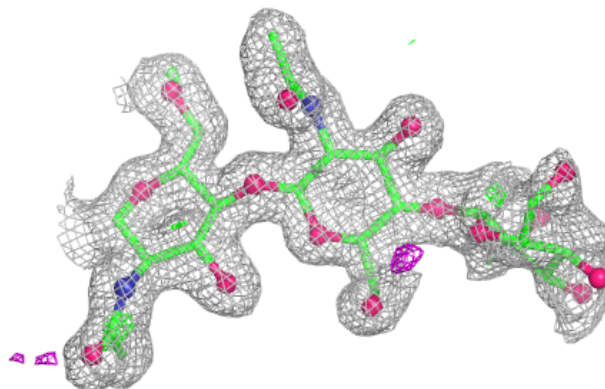
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

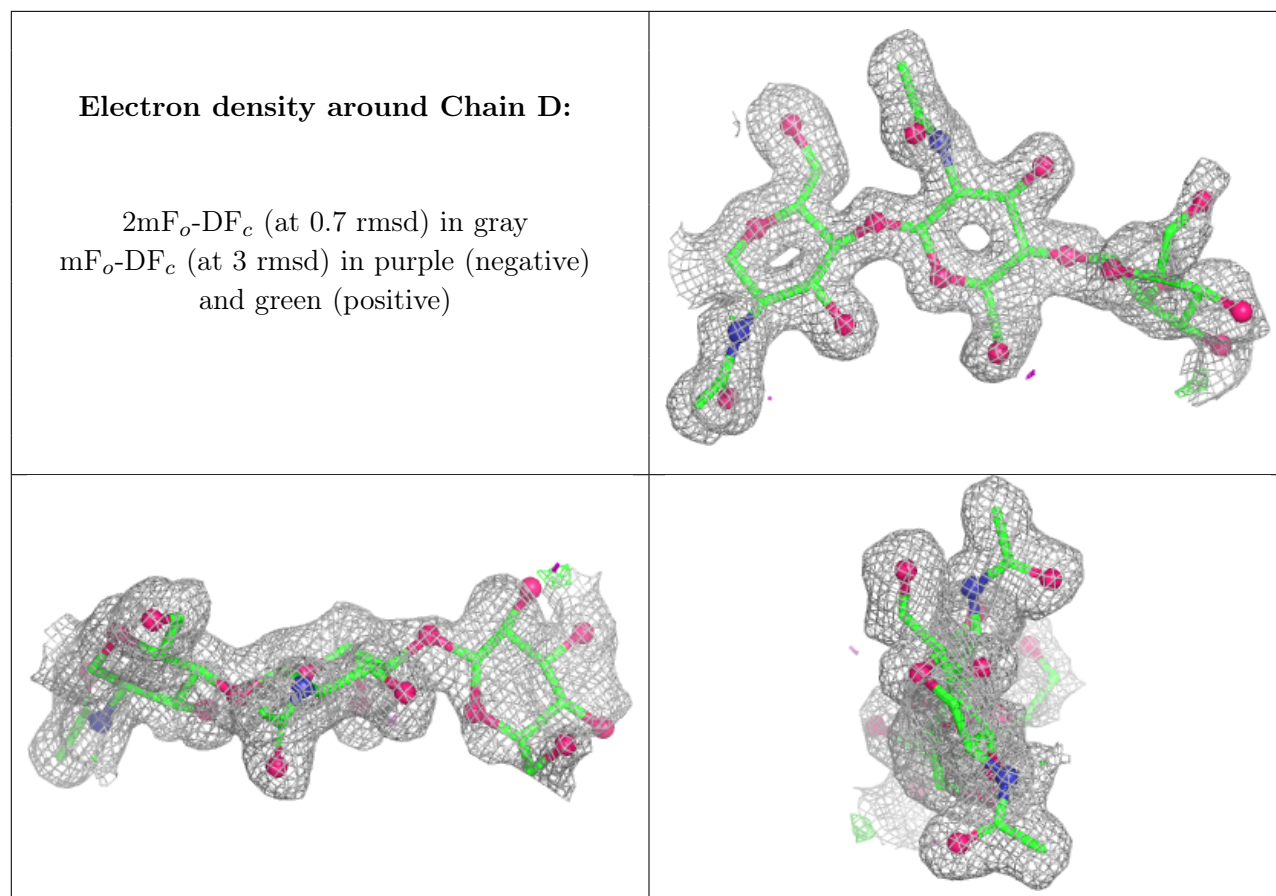
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	MAN	C	3	11/12	0.48	0.24	53,64,72,75	0
2	MAN	D	3	11/12	0.59	0.19	47,56,60,60	0
2	NAG	D	2	14/15	0.90	0.10	15,22,31,35	0
2	NAG	C	2	14/15	0.91	0.11	18,22,30,44	0
2	NAG	C	1	14/15	0.93	0.08	10,13,21,23	0
2	NAG	D	1	14/15	0.95	0.07	11,13,17,18	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 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, 95th 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
6	GOL	B	612	6/6	0.71	0.21	29,34,38,42	0
6	GOL	A	612	6/6	0.73	0.18	33,38,45,53	0
6	GOL	B	613	6/6	0.75	0.17	34,39,41,42	0
6	GOL	A	610	6/6	0.81	0.16	17,30,31,34	0
6	GOL	B	610	6/6	0.85	0.14	19,26,30,39	0
6	GOL	A	611	6/6	0.86	0.16	14,22,26,28	0
5	ACT	B	609	4/4	0.87	0.13	8,12,15,22	0
6	GOL	B	611	6/6	0.90	0.11	16,19,23,23	0
5	ACT	A	609	4/4	0.93	0.09	14,14,14,14	0
4	NAG	B	608	14/15	0.94	0.07	10,12,16,17	0
4	NAG	A	608	14/15	0.94	0.07	9,13,17,18	0
7	CA	A	613	1/1	0.98	0.04	18,18,18,18	1
7	CA	B	614	1/1	0.98	0.06	16,16,16,16	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	CU	B	603	1/1	0.99	0.02	11,11,11,11	1
3	CU	B	604	1/1	0.99	0.02	16,16,16,16	1
3	CU	A	602	1/1	0.99	0.03	12,12,12,12	0
3	CU	A	603	1/1	0.99	0.02	11,11,11,11	1
3	CU	B	602	1/1	0.99	0.03	11,11,11,11	0
3	CU	A	604	1/1	1.00	0.02	15,15,15,15	1
3	CU	B	601	1/1	1.00	0.02	10,10,10,10	0
3	CU	A	601	1/1	1.00	0.02	9,9,9,9	0

6.5 Other polymers [i](#)

There are no such residues in this entry.