



# Full wwPDB X-ray Structure Validation Report ⓘ

Apr 13, 2026 – 10:22 AM EDT

PDB ID : 9OUB / pdb\_00009oub  
Title : Structure of full-length Streptococcus mutans GtfD in complex with dextran 1000 in domain V  
Authors : Schormann, N.; Deivanayagam, C.  
Deposited on : 2025-05-28  
Resolution : 2.35 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](mailto: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>.

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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  
Buster-report : wwPDB partial adaption of 1.1.7 (2018)  
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

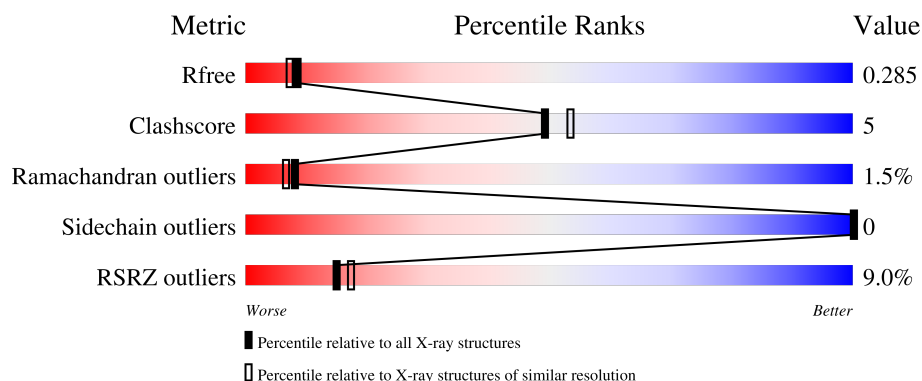
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.35 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))
$R_{free}$	180053	1596 (2.36-2.36)
Clashscore	190562	1663 (2.36-2.36)
Ramachandran outliers	187476	1646 (2.36-2.36)
Sidechain outliers	187428	1646 (2.36-2.36)
RSRZ outliers	180081	1598 (2.36-2.36)

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  $\geq 3$ , 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	1438	<div> <div>8%</div> <div>76%</div> <div>13%</div> <div>11%</div> </div>
2	B	6	<div> <div>83%</div> <div>17%</div> </div>
3	C	2	<div> <div>50%</div> <div>50%</div> </div>
3	D	2	<div> <div>100%</div> </div>

## 2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 10238 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 Glucosyltransferase-S.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1284	Total	C	N	O	S	0	0	0
			10056	6296	1728	2012	20			

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	33	MET	-	expression tag	UNP P49331
A	34	ALA	-	expression tag	UNP P49331
A	1463	LEU	-	expression tag	UNP P49331
A	1464	GLU	-	expression tag	UNP P49331
A	1465	HIS	-	expression tag	UNP P49331
A	1466	HIS	-	expression tag	UNP P49331
A	1467	HIS	-	expression tag	UNP P49331
A	1468	HIS	-	expression tag	UNP P49331
A	1469	HIS	-	expression tag	UNP P49331
A	1470	HIS	-	expression tag	UNP P49331

- Molecule 2 is an oligosaccharide called alpha-D-glucopyranose-(1-6)-alpha-D-glucopyranose-(1-6)-alpha-D-glucopyranose-(1-6)-alpha-D-glucopyranose-(1-6)-alpha-D-glucopyranose.



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
2	B	6	Total	C	O	0	0	0
			66	36	30			

- Molecule 3 is an oligosaccharide called alpha-D-glucopyranose-(1-6)-alpha-D-glucopyranose.

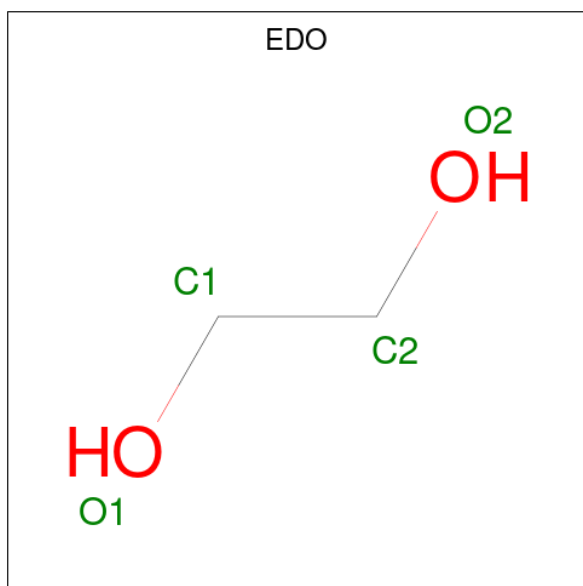


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
3	C	2	Total	C	O	0	0	0
			22	12	10			
3	D	2	Total	C	O	0	0	0
			22	12	10			

- Molecule 4 is CALCIUM ION (CCD ID: CA) (formula: Ca) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Ca	0	0
			1	1		

- Molecule 5 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C<sub>2</sub>H<sub>6</sub>O<sub>2</sub>) (labeled as "Ligand of Interest" by depositor).




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

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	63	Total 63	O 63	0	0



- Molecule 2: alpha-D-glucopyranose-(1-6)-alpha-D-glucopyranose-(1-6)-alpha-D-glucopyranose-(1-6)-alpha-D-glucopyranose-(1-6)-alpha-D-glucopyranose

Chain B:  83% 17%

GLC1  
GLC2  
GLC3  
GLC4  
GLC5  
GLC6

- Molecule 3: alpha-D-glucopyranose-(1-6)-alpha-D-glucopyranose

Chain C:  50% 50%

GLC1  
GLC2

- Molecule 3: alpha-D-glucopyranose-(1-6)-alpha-D-glucopyranose

Chain D:  100%

GLC1  
GLC2

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	77.84Å 95.48Å 175.33Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	64.58 – 2.35 64.58 – 2.35	Depositor EDS
% Data completeness (in resolution range)	94.8 (64.58-2.35) 94.8 (64.58-2.35)	Depositor EDS
$R_{merge}$	0.15	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.41 (at 2.34Å)	Xtriage
Refinement program	PHENIX (1.18.2_3874)	Depositor
R, $R_{free}$	0.238 , 0.284 0.239 , 0.285	Depositor DCC
$R_{free}$ test set	2577 reflections (4.67%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	40.7	Xtriage
Anisotropy	0.044	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.28 , 20.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	10238	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	46.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.35% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<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.



## 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: EDO, GLC, CA

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	0.15	0/10257	0.38	0/13887

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.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	652	ARG	Sidechain

### 5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	10056	0	9547	106	0
2	B	66	0	55	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	22	0	19	0	0
3	D	22	0	19	0	0
4	A	1	0	0	0	0
5	A	8	0	12	0	0
6	A	63	0	0	0	0
All	All	10238	0	9652	106	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 5.

All (106) 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:1320:ASN:HB2	1:A:1323:TYR:H	1.34	0.89
1:A:177:ILE:HB	1:A:181:TYR:HA	1.62	0.80
1:A:1280:PHE:HB3	1:A:1283:ASP:HA	1.63	0.80
1:A:189:GLN:O	1:A:191:LYS:N	2.19	0.76
1:A:366:SER:HA	1:A:370:LYS:HD3	1.66	0.75
1:A:1431:ASP:H	1:A:1435:GLY:HA2	1.52	0.73
1:A:203:LEU:HD12	1:A:212:LEU:HD11	1.73	0.71
1:A:220:PHE:HE1	1:A:1105:MET:HE3	1.57	0.69
1:A:730:SER:O	1:A:734:LYS:NZ	2.27	0.63
1:A:771:PRO:HD2	1:A:789:ALA:HB1	1.80	0.62
1:A:705:MET:HE1	1:A:710:THR:HG22	1.82	0.61
1:A:1320:ASN:HB2	1:A:1323:TYR:N	2.13	0.61
1:A:1356:VAL:HA	1:A:1365:TYR:HA	1.82	0.60
1:A:1436:ASN:OD1	1:A:1440:ASN:ND2	2.35	0.59
1:A:929:LEU:HB2	1:A:931:MET:HE3	1.85	0.58
1:A:864:GLY:HA3	1:A:898:PHE:CE1	2.40	0.57
1:A:1319:ASN:HD22	1:A:1324:PHE:HA	1.70	0.56
1:A:473:ASP:OD2	1:A:1034:SER:OG	2.21	0.56
1:A:769:TYR:N	1:A:794:ARG:O	2.35	0.55
1:A:864:GLY:HA3	1:A:898:PHE:HE1	1.71	0.55
1:A:440:TRP:HB2	1:A:926:ARG:HH21	1.71	0.55
1:A:193:ASN:ND2	1:A:1158:ARG:O	2.37	0.55
1:A:988:LYS:HD3	1:A:989:ASP:HB2	1.89	0.55
1:A:220:PHE:CE1	1:A:1105:MET:HE3	2.40	0.54
1:A:1419:VAL:HB	1:A:1427:LEU:HD11	1.88	0.54
1:A:532:LEU:HD22	1:A:537:ARG:HH12	1.74	0.53
1:A:178:ASP:HA	1:A:189:GLN:HB2	1.91	0.53
1:A:237:ILE:HB	1:A:1089:MET:HE2	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:332:THR:O	1:A:336:GLN:HG2	2.09	0.53
1:A:1301:PHE:C	1:A:1303:ALA:H	2.18	0.52
1:A:196:LEU:HD22	1:A:198:VAL:HG23	1.91	0.52
1:A:261:LYS:NZ	1:A:262:ASP:OD2	2.41	0.52
1:A:579:PHE:HB3	1:A:652:ARG:HB3	1.92	0.51
1:A:1245:ALA:HB1	1:A:1248:ARG:HE	1.75	0.51
1:A:913:LEU:O	1:A:917:ILE:HG12	2.11	0.51
1:A:1280:PHE:CE1	1:A:1285:LYS:HG2	2.46	0.51
1:A:1414:GLN:HG2	1:A:1416:LYS:HG3	1.92	0.51
1:A:1434:SER:OG	1:A:1435:GLY:N	2.44	0.50
1:A:740:VAL:HG22	1:A:823:VAL:HG22	1.93	0.50
1:A:1438:VAL:HA	1:A:1457:GLY:HA3	1.93	0.50
1:A:1280:PHE:HE1	1:A:1285:LYS:HG2	1.77	0.49
1:A:286:TRP:CD2	1:A:292:GLN:HG3	2.47	0.49
1:A:439:ASN:HB2	1:A:1017:LEU:HD21	1.94	0.49
1:A:1308:LEU:HA	1:A:1320:ASN:O	2.13	0.49
1:A:325:THR:O	1:A:328:VAL:HG22	2.13	0.49
1:A:1298:LEU:HG	1:A:1299:LYS:N	2.28	0.48
1:A:1438:VAL:HG23	1:A:1439:TYR:CD2	2.49	0.48
1:A:201:LYS:HE3	1:A:203:LEU:HD21	1.96	0.48
1:A:298:TYR:CD2	1:A:350:PHE:HB2	2.49	0.48
1:A:1169:LYS:HE3	1:A:1201:MET:HE2	1.96	0.48
1:A:428:ASN:OD1	1:A:437:GLN:NE2	2.34	0.48
1:A:433:VAL:O	1:A:437:GLN:HG2	2.13	0.47
1:A:430:ASN:HB3	1:A:433:VAL:HB	1.96	0.47
1:A:846:THR:OG1	1:A:851:GLU:OE2	2.24	0.47
1:A:1320:ASN:HB3	1:A:1322:TYR:H	1.80	0.47
1:A:493:LYS:HE3	1:A:497:ASN:OD1	2.15	0.47
1:A:1079:LYS:NZ	1:A:1082:GLN:OE1	2.45	0.47
1:A:463:ARG:HD2	1:A:899:GLU:OE2	2.14	0.47
1:A:844:ASN:ND2	1:A:848:GLN:O	2.44	0.47
1:A:1235:ARG:HD3	1:A:1244:MET:SD	2.54	0.46
1:A:777:LYS:HE2	1:A:812:TYR:HE1	1.80	0.46
1:A:532:LEU:O	1:A:536:THR:OG1	2.27	0.46
1:A:1019:GLU:HG2	1:A:1023:LYS:HZ2	1.80	0.46
1:A:400:PRO:HB3	1:A:512:TYR:CD2	2.50	0.46
1:A:412:ASP:HB3	1:A:508:ASN:ND2	2.31	0.45
1:A:226:LYS:HD3	1:A:1094:ALA:O	2.16	0.45
1:A:264:LEU:HD13	1:A:270:TRP:CE2	2.51	0.45
1:A:1094:ALA:HB1	1:A:1112:GLY:HA3	1.98	0.45
1:A:1344:PHE:O	1:A:1352:LYS:HG2	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1405:ARG:NE	1:A:1438:VAL:HG22	2.31	0.45
1:A:179:GLY:C	1:A:181:TYR:H	2.24	0.45
1:A:1309:ALA:HA	1:A:1318:GLN:HG3	1.99	0.45
1:A:214:ASP:OD1	1:A:216:SER:OG	2.34	0.44
1:A:175:LYS:H	1:A:186:SER:HB2	1.83	0.44
1:A:181:TYR:O	1:A:183:TYR:N	2.51	0.44
1:A:770:ARG:NE	1:A:786:ASP:OD1	2.48	0.44
1:A:1239:ASP:O	1:A:1241:SER:N	2.43	0.43
1:A:1431:ASP:HB3	1:A:1435:GLY:N	2.32	0.43
1:A:196:LEU:HD22	1:A:198:VAL:CG2	2.48	0.43
1:A:648:ASP:OD1	1:A:852:SER:OG	2.32	0.43
1:A:239:ASN:CG	1:A:241:GLU:HG3	2.43	0.43
1:A:480:ASP:HB3	1:A:1027:ILE:HG12	2.01	0.42
1:A:177:ILE:H	1:A:188:GLY:HA2	1.84	0.42
1:A:504:ALA:HB1	1:A:509:ASP:OD2	2.18	0.42
1:A:1307:GLU:HA	1:A:1307:GLU:OE1	2.19	0.42
1:A:1428:ARG:NH1	1:A:1456:TRP:O	2.50	0.42
1:A:891:LYS:HE2	1:A:953:SER:HB3	2.01	0.42
1:A:1441:LYS:HD2	1:A:1441:LYS:HA	1.83	0.42
1:A:324:GLN:O	1:A:328:VAL:HG13	2.20	0.42
1:A:1359:ASN:C	1:A:1359:ASN:OD1	2.62	0.42
1:A:208:ASN:C	1:A:210:GLY:H	2.28	0.42
1:A:1106:THR:HG22	1:A:1134:GLY:O	2.19	0.42
1:A:226:LYS:HG3	1:A:227:LEU:N	2.35	0.42
1:A:1248:ARG:HH22	2:B:1:GLC:H4	1.85	0.41
1:A:1244:MET:HE3	1:A:1264:GLY:HA3	2.01	0.41
1:A:1023:LYS:HE2	1:A:1024:TYR:CZ	2.56	0.41
1:A:1395:LEU:O	1:A:1412:GLY:HA2	2.21	0.41
1:A:206:ASP:O	1:A:210:GLY:HA2	2.21	0.41
1:A:380:TYR:CE1	1:A:975:VAL:HG21	2.56	0.41
1:A:1226:TRP:HE3	1:A:1234:LYS:HG2	1.85	0.41
1:A:1282:GLN:H	1:A:1282:GLN:HG3	1.76	0.41
1:A:1263:ASP:HB3	1:A:1265:ILE:HG12	2.03	0.41
1:A:586:GLU:HB3	1:A:633:GLN:NE2	2.37	0.40
1:A:912:PHE:O	1:A:916:ILE:HG13	2.21	0.40
1:A:1078:LEU:HA	1:A:1083:THR:HG23	2.03	0.40
1:A:1002:LYS:HA	1:A:1048:TRP:O	2.21	0.40

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	1278/1438 (89%)	1152 (90%)	107 (8%)	19 (2%)	8 7

All (19) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	565	SER
1	A	1344	PHE
1	A	182	TYR
1	A	265	LYS
1	A	1293	THR
1	A	1309	ALA
1	A	1310	ARG
1	A	1313	PHE
1	A	1365	TYR
1	A	190	PRO
1	A	199	ASN
1	A	1315	THR
1	A	269	THR
1	A	189	GLN
1	A	1287	ILE
1	A	1317	SER
1	A	1208	ILE
1	A	1240	GLY
1	A	1291	ILE

### 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	1055/1216 (87%)	1055 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	189	GLN
1	A	217	GLN
1	A	236	GLN
1	A	266	ASN
1	A	336	GLN
1	A	446	ASN
1	A	511	GLN
1	A	547	ASN
1	A	588	GLN
1	A	621	ASN
1	A	626	GLN
1	A	859	GLN
1	A	886	ASN
1	A	1121	GLN
1	A	1126	ASN
1	A	1366	HIS
1	A	1375	ASN
1	A	1384	ASN
1	A	1436	ASN
1	A	1440	ASN

### 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	GLC	B	1	2	11,11,12	0.18	0	15,15,17	0.42	0
2	GLC	B	2	2	11,11,12	0.23	0	15,15,17	0.55	0
2	GLC	B	3	2	11,11,12	0.20	0	15,15,17	0.41	0
2	GLC	B	4	2	11,11,12	0.24	0	15,15,17	0.54	0
2	GLC	B	5	2	11,11,12	0.17	0	15,15,17	0.41	0
2	GLC	B	6	2	11,11,12	0.28	0	15,15,17	0.25	0
3	GLC	C	1	3	11,11,12	0.34	0	15,15,17	0.88	1 (6%)
3	GLC	C	2	3	11,11,12	0.34	0	15,15,17	0.55	0
3	GLC	D	1	3	11,11,12	0.38	0	15,15,17	1.06	1 (6%)
3	GLC	D	2	3	11,11,12	0.24	0	15,15,17	0.74	1 (6%)

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	GLC	B	1	2	-	2/2/19/22	0/1/1/1
2	GLC	B	2	2	-	0/2/19/22	0/1/1/1
2	GLC	B	3	2	-	2/2/19/22	0/1/1/1
2	GLC	B	4	2	-	2/2/19/22	0/1/1/1
2	GLC	B	5	2	-	1/2/19/22	0/1/1/1
2	GLC	B	6	2	-	2/2/19/22	0/1/1/1
3	GLC	C	1	3	-	2/2/19/22	0/1/1/1
3	GLC	C	2	3	-	1/2/19/22	0/1/1/1
3	GLC	D	1	3	-	1/2/19/22	0/1/1/1
3	GLC	D	2	3	-	1/2/19/22	0/1/1/1

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
3	D	1	GLC	C1-O5-C5	3.40	116.75	112.19
3	D	2	GLC	C1-O5-C5	2.59	115.66	112.19
3	C	1	GLC	C1-C2-C3	2.23	112.89	109.64

There are no chirality outliers.

All (14) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	3	GLC	C4-C5-C6-O6
2	B	3	GLC	O5-C5-C6-O6
2	B	1	GLC	O5-C5-C6-O6
2	B	6	GLC	O5-C5-C6-O6
2	B	1	GLC	C4-C5-C6-O6
2	B	5	GLC	O5-C5-C6-O6
3	C	1	GLC	O5-C5-C6-O6
3	D	1	GLC	O5-C5-C6-O6
3	C	2	GLC	O5-C5-C6-O6
3	D	2	GLC	O5-C5-C6-O6
2	B	4	GLC	C4-C5-C6-O6
2	B	6	GLC	C4-C5-C6-O6
3	C	1	GLC	C4-C5-C6-O6
2	B	4	GLC	O5-C5-C6-O6

There are no ring outliers.

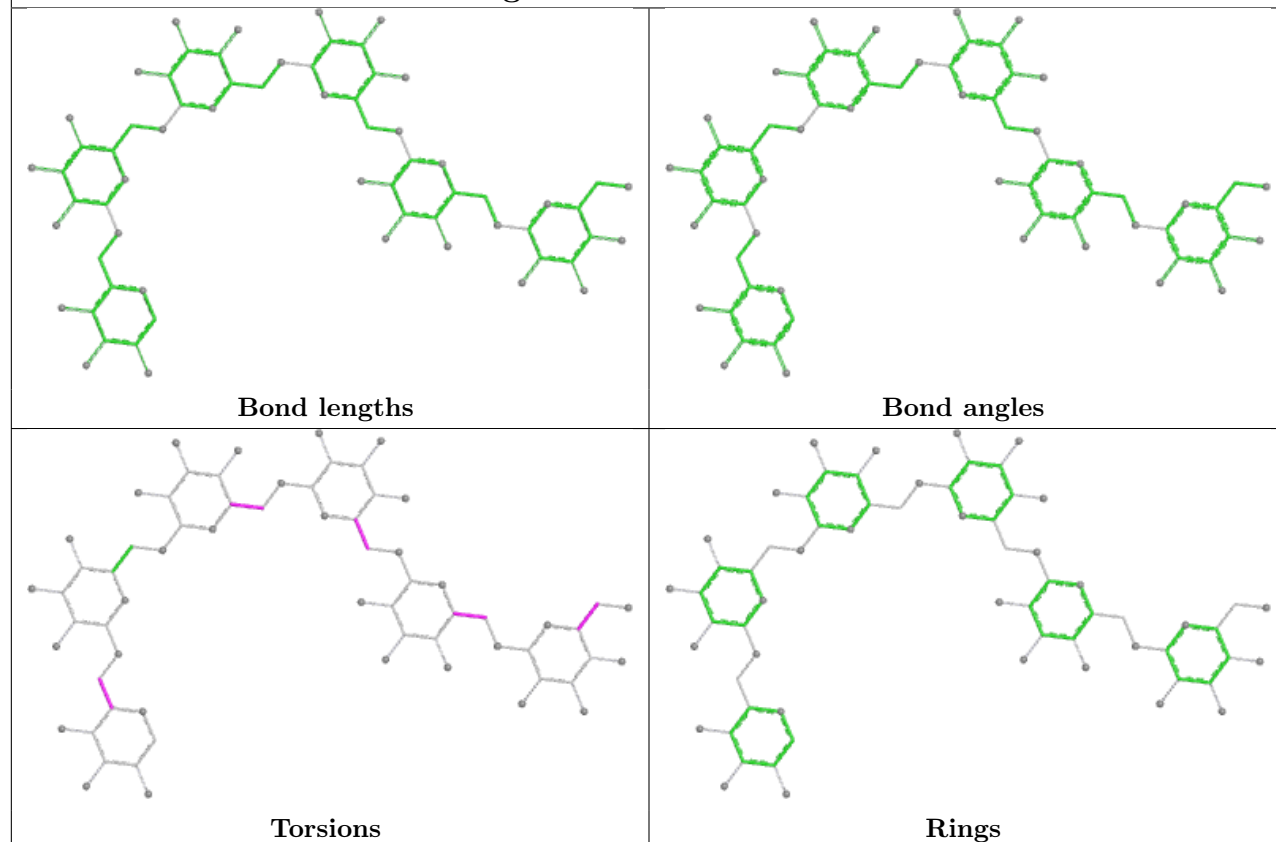
1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	1	GLC	1	0

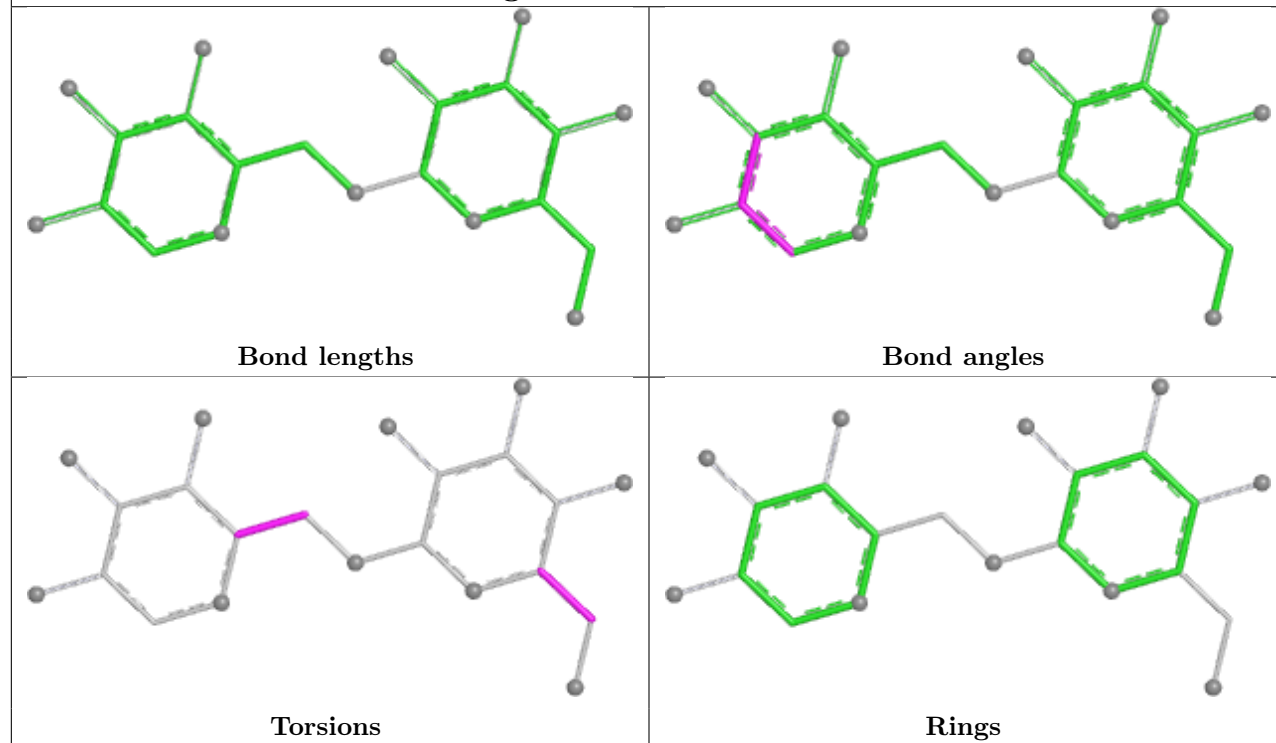
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

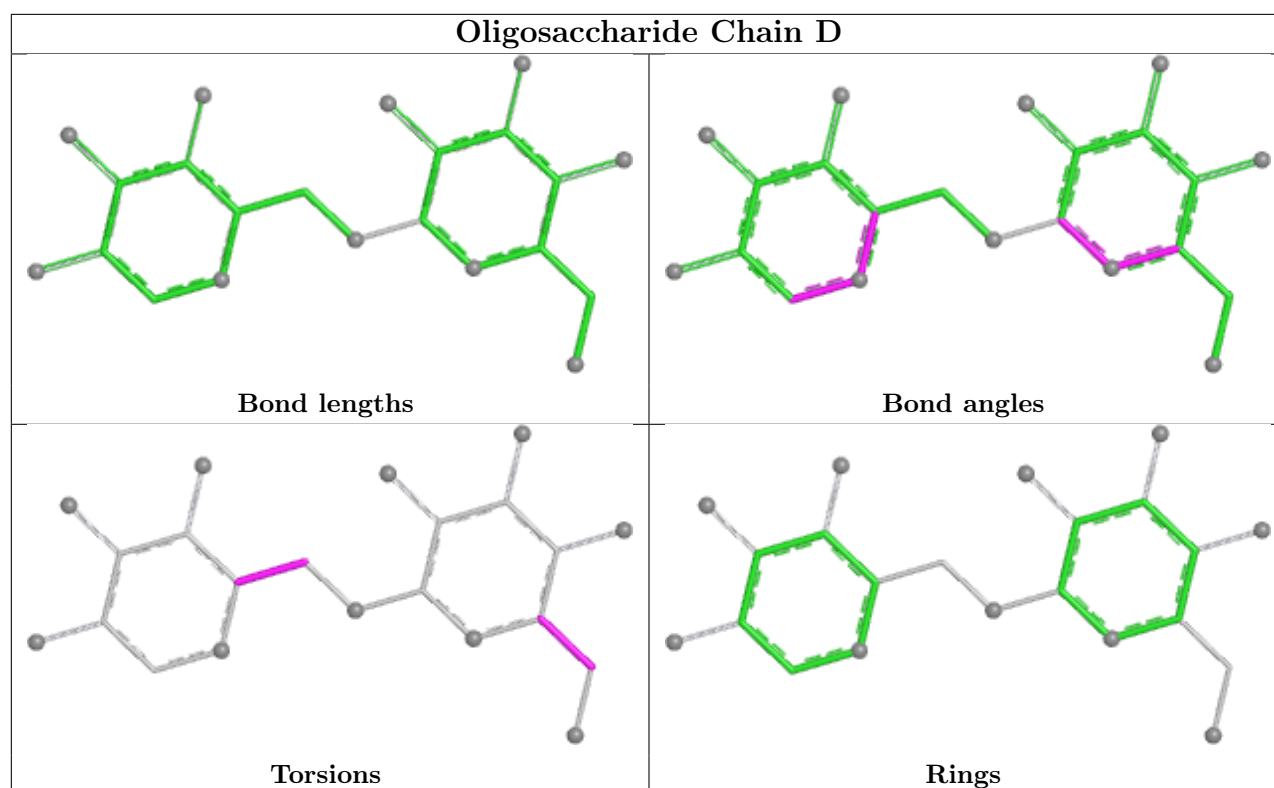


## Oligosaccharide Chain B



## Oligosaccharide Chain C





## 5.6 Ligand geometry [i](#)

Of 3 ligands modelled in this entry, 1 is 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
5	EDO	A	1503	-	3,3,3	0.42	0	2,2,2	0.38	0
5	EDO	A	1502	-	3,3,3	0.44	0	2,2,2	0.35	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	EDO	A	1503	-	-	0/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	EDO	A	1502	-	-	0/1/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

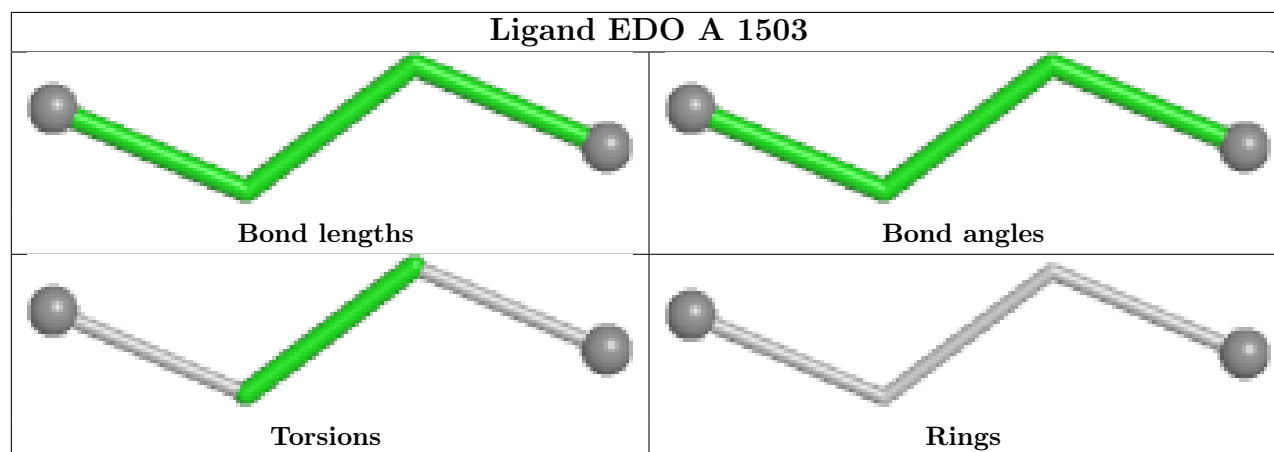
There are no chirality outliers.

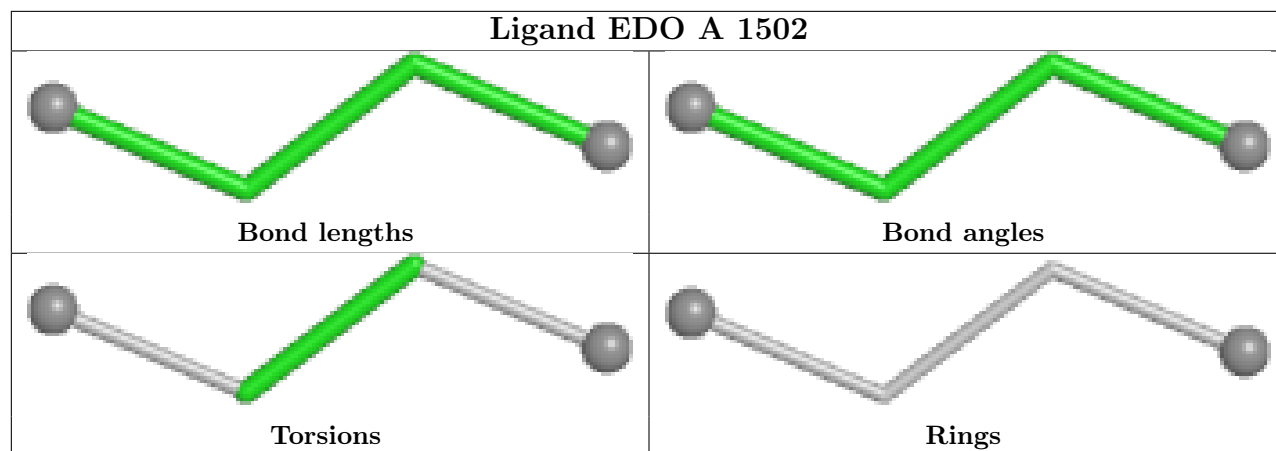
There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





## 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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	1284/1438 (89%)	0.58	116 (9%) <b>15</b> <b>17</b>	27, 42, 80, 98	0

All (116) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1312	ILE	6.9
1	A	1313	PHE	5.0
1	A	1443	VAL	4.8
1	A	1445	LEU	4.8
1	A	1368	ASP	4.6
1	A	1315	THR	4.5
1	A	1294	ASP	4.5
1	A	1439	TYR	4.4
1	A	1307	GLU	4.3
1	A	1347	ASP	4.2
1	A	190	PRO	4.2
1	A	1351	VAL	4.1
1	A	1308	LEU	4.0
1	A	1353	GLY	4.0
1	A	1316	ASP	4.0
1	A	1293	THR	4.0
1	A	177	ILE	4.0
1	A	1317	SER	3.9
1	A	265	LYS	3.8
1	A	1444	THR	3.8
1	A	1344	PHE	3.8
1	A	1338	ALA	3.7
1	A	1323	TYR	3.7
1	A	1438	VAL	3.7
1	A	1309	ALA	3.7
1	A	1446	ALA	3.7
1	A	1321	TRP	3.6

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Mol	Chain	Res	Type	RSRZ
1	A	1289	GLY	3.5
1	A	1369	SER	3.5
1	A	1287	ILE	3.5
1	A	1314	ALA	3.5
1	A	1327	ASP	3.5
1	A	1286	GLN	3.4
1	A	1318	GLN	3.4
1	A	1339	GLY	3.4
1	A	1345	ALA	3.3
1	A	1283	ASP	3.3
1	A	1437	MET	3.3
1	A	501	ILE	3.3
1	A	898	PHE	3.2
1	A	185	GLY	3.2
1	A	1363	HIS	3.2
1	A	1322	TYR	3.2
1	A	1304	ASN	3.1
1	A	181	TYR	3.1
1	A	1295	ASN	3.1
1	A	1356	VAL	3.1
1	A	1343	TYR	3.0
1	A	182	TYR	3.0
1	A	369	GLU	3.0
1	A	186	SER	3.0
1	A	845	ALA	3.0
1	A	1348	GLY	3.0
1	A	1336	THR	2.9
1	A	1357	THR	2.9
1	A	198	VAL	2.9
1	A	368	GLY	2.9
1	A	1298	LEU	2.9
1	A	1297	LYS	2.8
1	A	1442	VAL	2.8
1	A	1326	SER	2.8
1	A	1354	SER	2.8
1	A	1281	GLY	2.8
1	A	566	ALA	2.8
1	A	1337	ILE	2.7
1	A	1325	GLY	2.7
1	A	1364	TYR	2.7
1	A	1461	TYR	2.7
1	A	1409	THR	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	1448	GLY	2.7
1	A	275	GLU	2.7
1	A	1358	TYR	2.7
1	A	1303	ALA	2.6
1	A	543	ALA	2.6
1	A	266	ASN	2.6
1	A	1411	GLU	2.6
1	A	322	ALA	2.6
1	A	1300	TYR	2.6
1	A	203	LEU	2.5
1	A	1342	LEU	2.5
1	A	1089	MET	2.5
1	A	1285	LYS	2.5
1	A	1302	LEU	2.5
1	A	1284	GLY	2.5
1	A	1462	TYR	2.3
1	A	192	LYS	2.3
1	A	202	VAL	2.3
1	A	846	THR	2.3
1	A	1440	ASN	2.3
1	A	183	TYR	2.3
1	A	274	SER	2.3
1	A	1208	ILE	2.3
1	A	1335	GLN	2.2
1	A	1346	SER	2.2
1	A	174	VAL	2.2
1	A	196	LEU	2.2
1	A	1205	LEU	2.2
1	A	1260	LEU	2.2
1	A	1030	ARG	2.2
1	A	1435	GLY	2.2
1	A	1401	ILE	2.2
1	A	1301	PHE	2.2
1	A	1274	ASN	2.2
1	A	1306	GLY	2.2
1	A	1310	ARG	2.2
1	A	1355	PHE	2.2
1	A	1296	GLY	2.2
1	A	842	LYS	2.1
1	A	178	ASP	2.1
1	A	1456	TRP	2.1
1	A	1463	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	393	TYR	2.1
1	A	1311	ASN	2.1
1	A	267	GLY	2.1
1	A	1464	GLU	2.0
1	A	1392	GLY	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, 95<sup>th</sup> 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.

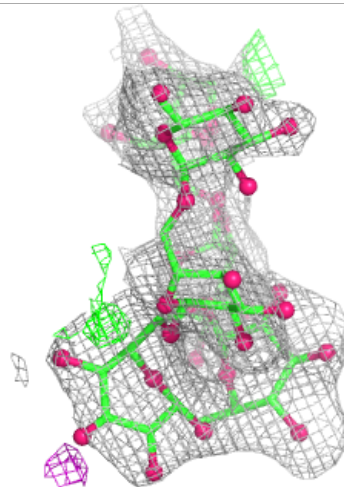
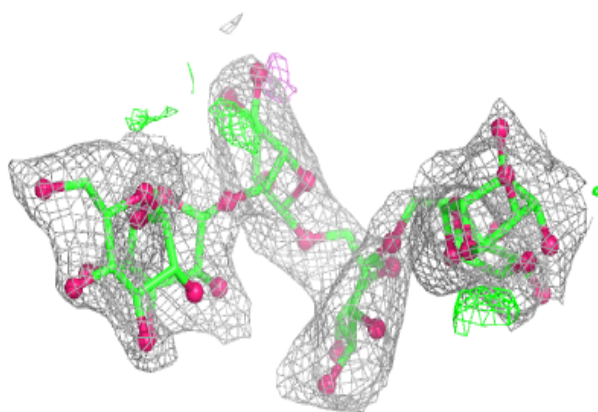
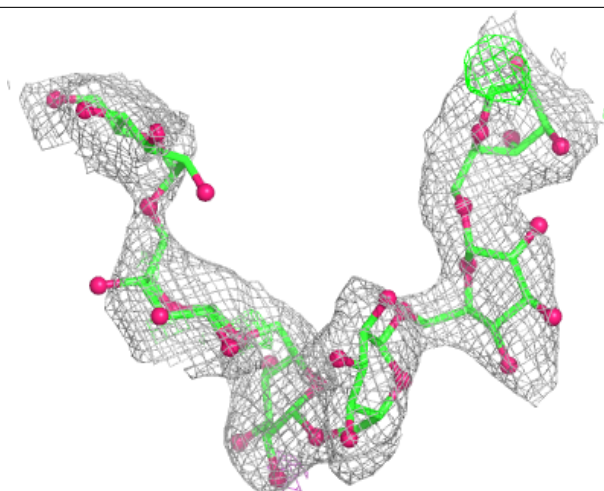
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
2	GLC	B	5	11/12	0.58	0.14	75,86,89,94	0
2	GLC	B	6	11/12	0.58	0.13	85,91,95,96	0
2	GLC	B	1	11/12	0.66	0.11	66,69,72,75	0
3	GLC	D	1	11/12	0.66	0.23	86,92,96,99	0
3	GLC	C	1	11/12	0.70	0.15	53,55,60,61	0
3	GLC	D	2	11/12	0.70	0.12	91,94,98,99	0
3	GLC	C	2	11/12	0.71	0.14	57,60,66,68	0
2	GLC	B	3	11/12	0.72	0.13	60,65,71,72	0
2	GLC	B	4	11/12	0.79	0.15	59,61,69,76	0
2	GLC	B	2	11/12	0.84	0.10	65,68,72,73	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.



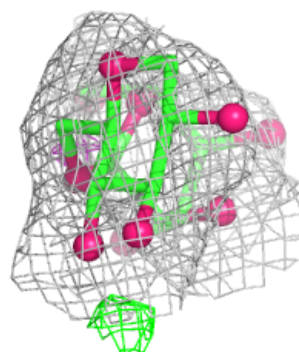
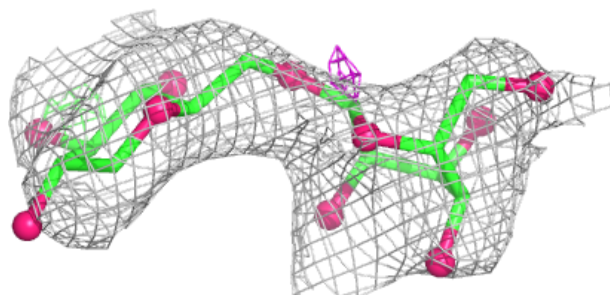
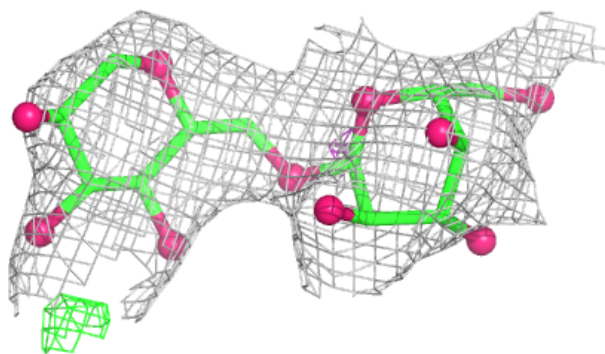
**Electron density around Chain B:**

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

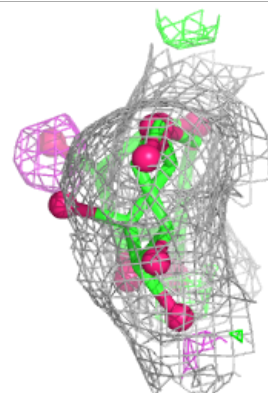
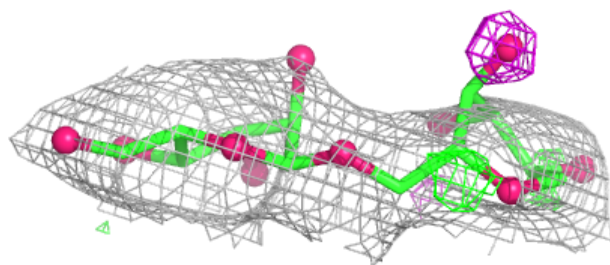
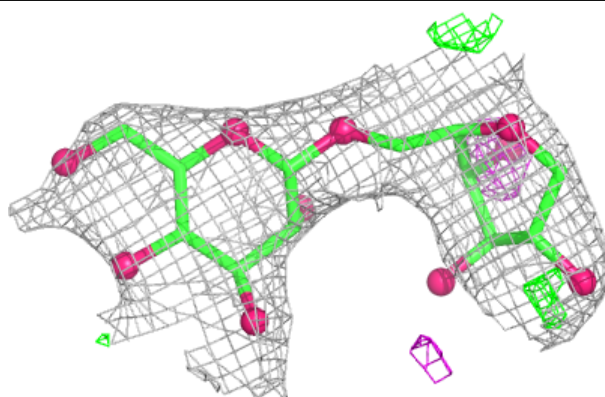


**Electron density around Chain C:**

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

**Electron density around Chain D:**

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

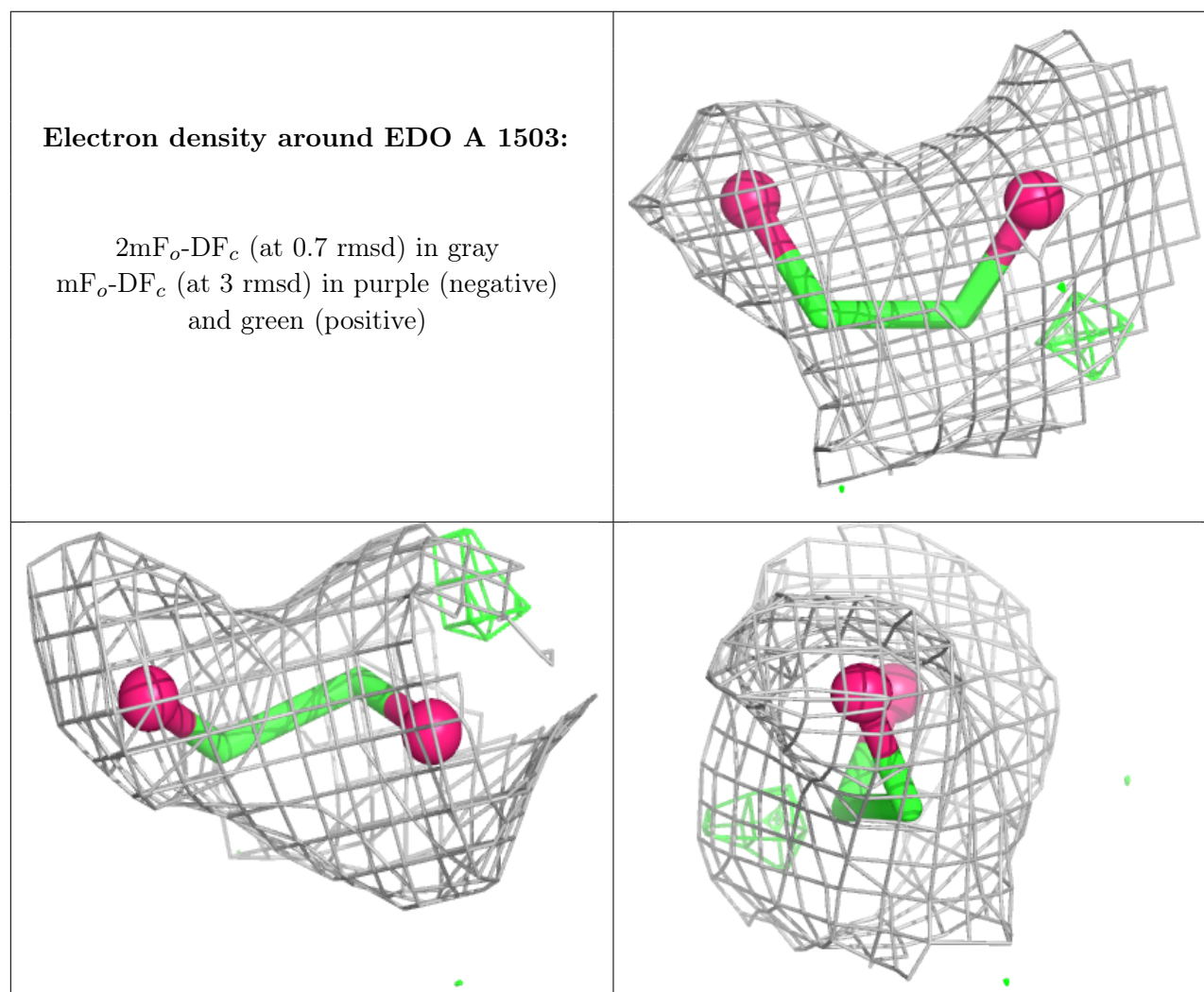


## 6.4 Ligands ⓘ

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<sup>th</sup> 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.

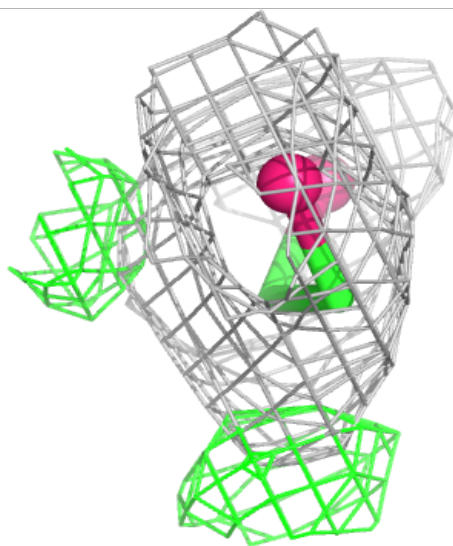
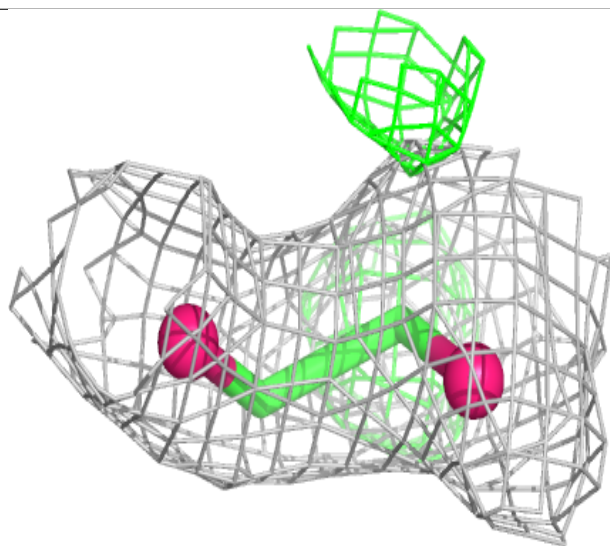
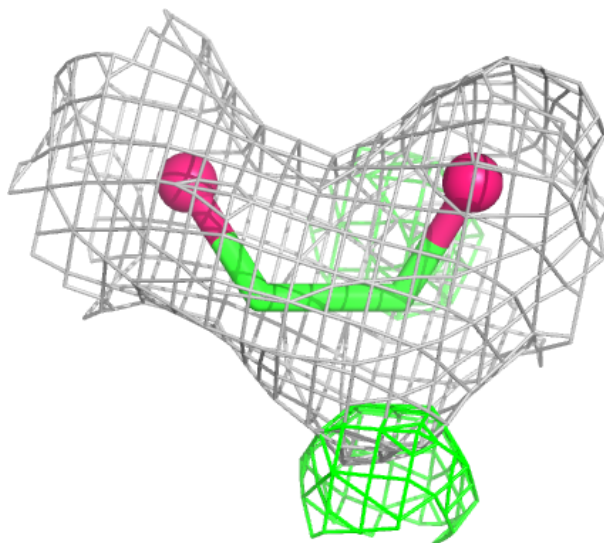
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
5	EDO	A	1503	4/4	0.59	0.17	65,67,69,71	0
5	EDO	A	1502	4/4	0.79	0.11	37,37,39,39	0
4	CA	A	1501	1/1	0.96	0.04	28,28,28,28	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.



**Electron density around EDO A 1502:**

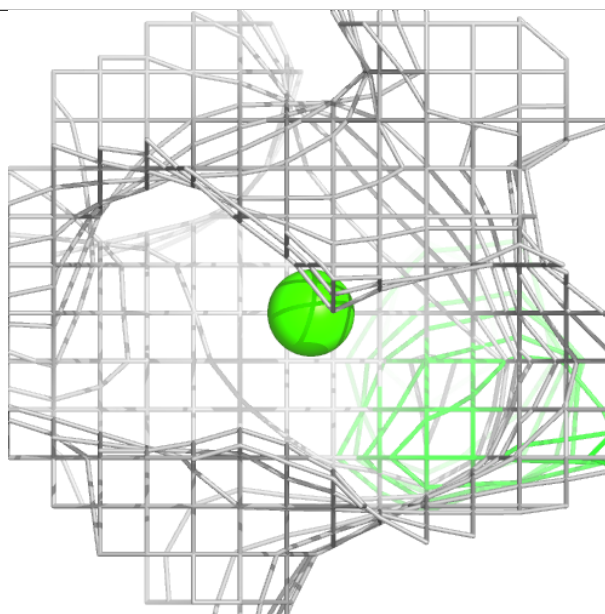
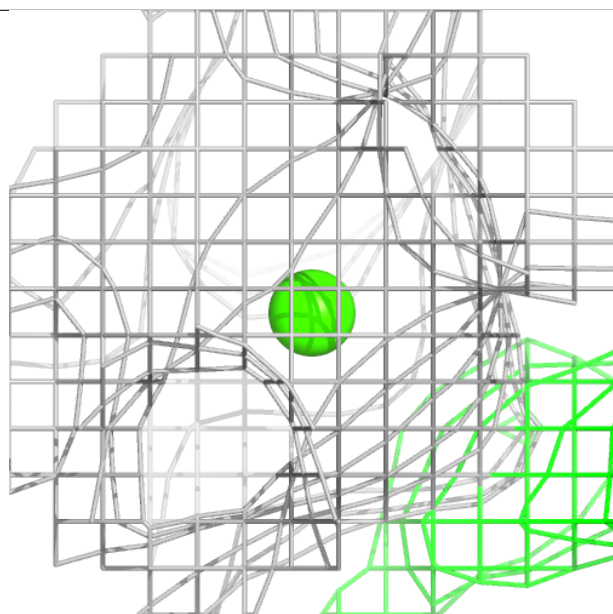
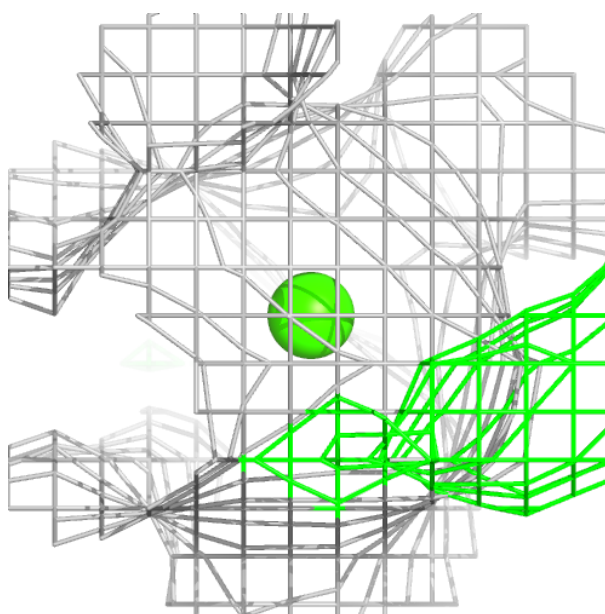
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





**Electron density around CA A 1501:**

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



## 6.5 Other polymers ⓘ

There are no such residues in this entry.