



# Full wwPDB X-ray Structure Validation Report ⓘ

Apr 13, 2026 – 10:21 AM EDT

PDB ID : 9OGX / pdb\_00009ogx  
Title : Structure of full-length Streptococcus mutans GtfD active site mutant (D465A, D584A) in complex with sucrose  
Authors : Schormann, N.; Deivanayagam, C.  
Deposited on : 2025-05-02  
Resolution : 2.85 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

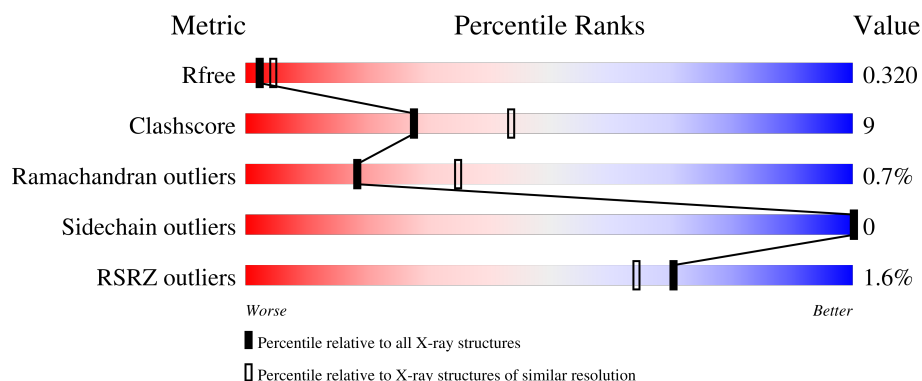
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*


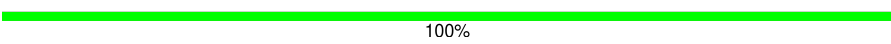
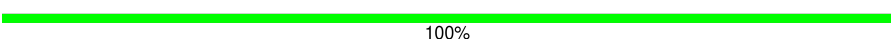
The reported resolution of this entry is 2.85 Å.

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	1407 (2.88-2.84)
Clashscore	190562	1446 (2.88-2.84)
Ramachandran outliers	187476	1406 (2.88-2.84)
Sidechain outliers	187428	1407 (2.88-2.84)
RSRZ outliers	180081	1408 (2.88-2.84)

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	 68% 18% 14%
2	B	2	 100%
2	C	2	 100%

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 9753 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.

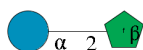
- Molecule 1 is a protein called Glucosyltransferase-S.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	1237	9703	6099	1642	1941	21	0	0	0

There are 12 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	465	ALA	ASP	engineered mutation	UNP P49331
A	584	ALA	ASP	engineered mutation	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

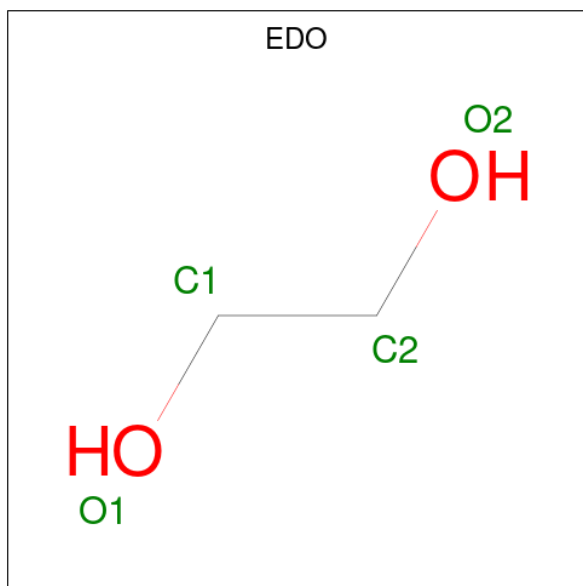
- Molecule 2 is an oligosaccharide called beta-D-fructofuranose-(2-1)-alpha-D-glucopyranose.



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
2	B	2	Total	C	O	0	0	0
			23	12	11			
2	C	2	Total	C	O	0	0	0
			23	12	11			

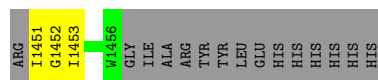
- Molecule 3 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C<sub>2</sub>H<sub>6</sub>O<sub>2</sub>) (labeled as "Ligand

of Interest" by depositor).



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





- GLC1  
FRU2

- GLC1
- 
- FRU2

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	83.44Å 96.99Å 181.56Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	75.93 – 2.85 75.93 – 2.85	Depositor EDS
% Data completeness (in resolution range)	71.0 (75.93-2.85) 71.0 (75.93-2.85)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.53 (at 2.86Å)	Xtriage
Refinement program	REFMAC 5.8.0425	Depositor
R, $R_{free}$	0.278 , 0.326 0.278 , 0.320	Depositor DCC
$R_{free}$ test set	1265 reflections (3.60%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	92.4	Xtriage
Anisotropy	0.012	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 60.6	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	9753	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	98.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.42% 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: FRU, GLC, EDO

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	0.45	0/9897	0.84	3/13392 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1236	TYR	N-CA-CB	6.17	120.92	110.49
1	A	963	PRO	N-CA-CB	-5.14	97.86	103.25
1	A	1237	PHE	CB-CA-C	5.10	118.57	109.38

There are no chirality outliers.

There are no planarity outliers.

### 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	9703	0	9174	171	0
2	B	23	0	21	0	0
2	C	23	0	21	0	0
3	A	4	0	6	0	0
All	All	9753	0	9222	171	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 9.



All (171) 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:876:SER:O	1:A:882:LYS:NZ	2.12	0.81
1:A:218:TYR:HH	1:A:1138:TYR:HH	1.38	0.70
1:A:1203:VAL:O	1:A:1206:LYS:NZ	2.26	0.69
1:A:644:LEU:HD12	1:A:683:ARG:HD2	1.74	0.68
1:A:1129:TYR:CD2	1:A:1143:LEU:HD11	2.30	0.67
1:A:555:PRO:O	1:A:559:ASN:HB2	1.95	0.66
1:A:1098:PHE:HB3	1:A:1105:MET:HE3	1.78	0.66
1:A:624:MET:O	1:A:629:LYS:NZ	2.29	0.65
1:A:883:ILE:HG22	1:A:950:LEU:HD21	1.78	0.65
1:A:283:MET:HE2	1:A:327:GLN:HG3	1.78	0.64
1:A:680:LEU:O	1:A:683:ARG:HG2	1.97	0.64
1:A:1001:THR:OG1	1:A:1002:LYS:NZ	2.32	0.63
1:A:1201:MET:HE2	1:A:1219:GLY:HA3	1.82	0.61
1:A:633:GLN:O	1:A:636:ILE:HD11	1.99	0.61
1:A:1249:PHE:HA	1:A:1259:TYR:HA	1.82	0.61
1:A:304:LEU:HD13	1:A:330:ILE:HG22	1.84	0.59
1:A:766:ASN:N	1:A:796:THR:OG1	2.33	0.59
1:A:419:ASP:OD2	1:A:1054:ASN:ND2	2.32	0.59
1:A:939:SER:H	1:A:942:ASP:HB2	1.67	0.58
1:A:1126:ASN:HB3	1:A:1155:VAL:HG13	1.85	0.58
1:A:1244:MET:HE3	1:A:1264:GLY:HA3	1.85	0.57
1:A:197:THR:HG22	1:A:202:VAL:HG22	1.87	0.57
1:A:503:GLU:HA	1:A:523:ILE:HD11	1.86	0.57
1:A:1129:TYR:CD2	1:A:1143:LEU:CD1	2.89	0.56
1:A:305:GLY:HA2	1:A:326:VAL:HG12	1.89	0.55
1:A:665:TYR:CE2	1:A:666:MET:HE3	2.41	0.55
1:A:677:ASP:HA	1:A:680:LEU:HG	1.87	0.55
1:A:794:ARG:NH1	1:A:795:LYS:O	2.40	0.54
1:A:974:VAL:HG12	1:A:996:LEU:HD12	1.89	0.54
1:A:431:PRO:HB3	1:A:1039:ILE:HA	1.90	0.54
1:A:653:LEU:HD21	1:A:658:MET:HE2	1.89	0.54
1:A:673:TYR:CE1	1:A:677:ASP:OD2	2.61	0.54
1:A:566:ALA:HB2	1:A:694:LYS:HE2	1.90	0.54
1:A:673:TYR:CD1	1:A:677:ASP:OD2	2.61	0.54
1:A:766:ASN:H	1:A:796:THR:HG1	1.53	0.53
1:A:973:GLU:OE1	1:A:1002:LYS:NZ	2.41	0.53
1:A:666:MET:HE1	1:A:890:PHE:CZ	2.43	0.53
1:A:198:VAL:C	1:A:200:ASN:H	2.17	0.53
1:A:629:LYS:NZ	1:A:672:TYR:OH	2.28	0.52
1:A:1336:THR:HA	1:A:1344:PHE:HA	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:248:ILE:HG22	1:A:974:VAL:HG23	1.92	0.52
1:A:447:TYR:OH	1:A:931:MET:SD	2.66	0.52
1:A:558:THR:HG22	1:A:565:SER:HB3	1.92	0.52
1:A:308:GLU:HB2	1:A:310:TYR:HE1	1.75	0.51
1:A:614:LYS:NZ	1:A:662:ASP:OD2	2.43	0.51
1:A:899:GLU:HA	1:A:958:ILE:HB	1.92	0.51
1:A:350:PHE:O	1:A:353:THR:HG22	2.10	0.51
1:A:1261:ASN:OD1	1:A:1265:ILE:N	2.39	0.51
1:A:198:VAL:HG12	1:A:198:VAL:O	2.11	0.51
1:A:591:ILE:O	1:A:595:ILE:HG13	2.11	0.50
1:A:554:GLU:N	1:A:555:PRO:HD2	2.27	0.50
1:A:590:VAL:O	1:A:594:ILE:HD12	2.11	0.50
1:A:889:LEU:O	1:A:892:SER:OG	2.26	0.50
1:A:1129:TYR:CE2	1:A:1143:LEU:HD22	2.46	0.50
1:A:1303:ALA:HB3	1:A:1306:GLY:HA2	1.94	0.50
1:A:636:ILE:HD13	1:A:672:TYR:CZ	2.47	0.49
1:A:1129:TYR:CE2	1:A:1143:LEU:CD2	2.95	0.49
1:A:484:ALA:HB1	1:A:1024:TYR:CD1	2.47	0.49
1:A:672:TYR:O	1:A:673:TYR:C	2.55	0.49
1:A:1257:TRP:HB2	1:A:1285:LYS:HE3	1.95	0.49
1:A:882:LYS:N	1:A:882:LYS:HD2	2.28	0.49
1:A:639:ALA:O	1:A:643:MET:HG3	2.13	0.49
1:A:421:LEU:HD12	1:A:469:ASN:CG	2.37	0.49
1:A:590:VAL:HG21	1:A:633:GLN:NE2	2.28	0.49
1:A:702:LYS:HA	1:A:705:MET:HB3	1.95	0.49
1:A:766:ASN:N	1:A:796:THR:HG1	2.09	0.48
1:A:393:TYR:CE2	1:A:431:PRO:HD3	2.48	0.48
1:A:334:ILE:HD12	1:A:340:THR:HG22	1.95	0.48
1:A:627:ALA:HB1	1:A:813:LEU:HG	1.96	0.48
1:A:773:LEU:HB3	1:A:780:LEU:HD21	1.94	0.48
1:A:393:TYR:HE2	1:A:431:PRO:HD3	1.79	0.48
1:A:183:TYR:HB2	1:A:205:PHE:CE2	2.49	0.47
1:A:205:PHE:HB3	1:A:210:GLY:O	2.14	0.47
1:A:218:TYR:OH	1:A:1138:TYR:OH	2.11	0.47
1:A:238:VAL:HB	1:A:261:LYS:HA	1.96	0.47
1:A:679:LEU:HD22	1:A:772:LEU:HD23	1.97	0.47
1:A:1332:THR:HB	1:A:1348:GLY:HA2	1.96	0.47
1:A:281:LEU:HD23	1:A:285:TRP:HB3	1.97	0.47
1:A:362:GLU:OE1	1:A:1061:ARG:N	2.48	0.47
1:A:550:ARG:HD3	1:A:744:ASN:HB2	1.97	0.47
1:A:872:VAL:HG21	1:A:878:TYR:HE1	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1230:SER:O	1:A:1231:ASP:CB	2.63	0.47
1:A:198:VAL:O	1:A:200:ASN:N	2.48	0.46
1:A:509:ASP:N	1:A:510:PRO:CD	2.78	0.46
1:A:1395:LEU:HD13	1:A:1399:GLN:HB2	1.97	0.46
1:A:677:ASP:O	1:A:681:LYS:HG2	2.15	0.46
1:A:633:GLN:N	1:A:633:GLN:CD	2.74	0.46
1:A:872:VAL:HG21	1:A:878:TYR:CE1	2.51	0.46
1:A:594:ILE:CG1	1:A:631:TYR:HD2	2.29	0.46
1:A:677:ASP:HA	1:A:680:LEU:CG	2.46	0.46
1:A:1140:LEU:HD21	1:A:1142:HIS:HE1	1.80	0.45
1:A:555:PRO:HA	1:A:559:ASN:OD1	2.16	0.45
1:A:1358:TYR:CE2	1:A:1359:ASN:HB2	2.51	0.45
1:A:636:ILE:HB	1:A:637:PRO:HD3	1.99	0.45
1:A:974:VAL:CG1	1:A:996:LEU:HD12	2.46	0.45
1:A:769:TYR:N	1:A:794:ARG:O	2.49	0.45
1:A:480:ASP:HB3	1:A:1027:ILE:HG12	1.99	0.45
1:A:219:GLN:HB3	1:A:1124:LYS:CE	2.46	0.45
1:A:636:ILE:HD13	1:A:672:TYR:CE2	2.52	0.45
1:A:860:LEU:HD23	1:A:895:VAL:HG12	1.98	0.45
1:A:1213:GLN:HG3	1:A:1242:GLY:O	2.16	0.45
1:A:704:HIS:O	1:A:704:HIS:ND1	2.49	0.45
1:A:1415:VAL:HG11	1:A:1420:ALA:HB2	1.99	0.45
1:A:395:LEU:HD11	1:A:1035:ASN:HA	1.99	0.45
1:A:630:LYS:C	1:A:631:TYR:HD1	2.25	0.45
1:A:392:ASP:O	1:A:393:TYR:C	2.59	0.44
1:A:504:ALA:O	1:A:505:TRP:HB2	2.17	0.44
1:A:1185:SER:OG	1:A:1189:ASP:HA	2.17	0.44
1:A:1127:TRP:CD1	1:A:1158:ARG:HD2	2.52	0.44
1:A:609:THR:OG1	1:A:612:GLU:HG3	2.16	0.44
1:A:1333:GLY:HA2	1:A:1347:ASP:HA	1.98	0.44
1:A:879:THR:N	1:A:937:TYR:O	2.49	0.44
1:A:890:PHE:HD1	1:A:893:TRP:CZ3	2.35	0.44
1:A:1249:PHE:HB3	1:A:1257:TRP:CE3	2.53	0.44
1:A:219:GLN:HB3	1:A:1124:LYS:HE2	1.98	0.44
1:A:234:HIS:ND1	1:A:262:ASP:OD2	2.48	0.44
1:A:653:LEU:HD11	1:A:680:LEU:HD11	2.00	0.44
1:A:1129:TYR:CG	1:A:1143:LEU:CD1	3.00	0.44
1:A:979:ARG:NH1	1:A:980:VAL:O	2.51	0.43
1:A:397:ASN:H	1:A:419:ASP:HB2	1.83	0.43
1:A:454:ASP:O	1:A:456:GLU:N	2.51	0.43
1:A:883:ILE:CG2	1:A:950:LEU:HD21	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1404:GLN:HB3	1:A:1436:ASN:OD1	2.17	0.43
1:A:264:LEU:HD13	1:A:270:TRP:CE2	2.53	0.43
1:A:476:GLN:OE1	1:A:476:GLN:N	2.51	0.43
1:A:849:VAL:HG13	1:A:850:TYR:HD1	1.82	0.43
1:A:939:SER:O	1:A:943:MET:N	2.46	0.43
1:A:228:ASN:ND2	1:A:1092:LYS:O	2.41	0.43
1:A:693:MET:HA	1:A:714:THR:O	2.18	0.43
1:A:878:TYR:CD2	1:A:938:GLY:HA2	2.54	0.43
1:A:356:ASN:HA	1:A:361:THR:HG21	2.01	0.43
1:A:248:ILE:HD13	1:A:253:THR:HG21	2.01	0.42
1:A:600:ASN:OD1	1:A:603:THR:HG23	2.18	0.42
1:A:280:PRO:HG2	1:A:283:MET:HB2	2.02	0.42
1:A:770:ARG:HB2	1:A:771:PRO:HD2	2.01	0.42
1:A:675:ALA:HB2	1:A:780:LEU:HD22	2.02	0.42
1:A:533:TYR:O	1:A:551:SER:N	2.51	0.42
1:A:986:TYR:CZ	1:A:993:LYS:HD2	2.54	0.42
1:A:183:TYR:HB2	1:A:205:PHE:HE2	1.83	0.42
1:A:308:GLU:HB2	1:A:310:TYR:CE1	2.54	0.42
1:A:913:LEU:O	1:A:917:ILE:HG12	2.19	0.42
1:A:224:LEU:HG	1:A:1099:VAL:HB	2.01	0.42
1:A:488:VAL:HB	1:A:849:VAL:HG21	2.01	0.42
1:A:1216:ASP:OD1	1:A:1220:TYR:N	2.52	0.42
1:A:756:VAL:O	1:A:756:VAL:HG23	2.19	0.41
1:A:1234:LYS:HB2	1:A:1266:ALA:HB2	2.01	0.41
1:A:1278:TYR:HD1	1:A:1306:GLY:O	2.03	0.41
1:A:289:LYS:HD3	1:A:1123:ALA:HB2	2.02	0.41
1:A:678:THR:HG22	1:A:772:LEU:HG	2.02	0.41
1:A:438:LEU:HD21	1:A:1020:LEU:HG	2.02	0.41
1:A:1142:HIS:HA	1:A:1146:GLU:O	2.20	0.41
1:A:446:ASN:O	1:A:447:TYR:C	2.63	0.41
1:A:635:ASN:HB3	1:A:638:THR:HB	2.03	0.41
1:A:300:ASN:HA	1:A:305:GLY:HA3	2.02	0.41
1:A:454:ASP:C	1:A:456:GLU:H	2.28	0.41
1:A:1339:GLY:O	1:A:1340:LYS:HB2	2.21	0.41
1:A:189:GLN:HB3	1:A:190:PRO:HD2	2.03	0.41
1:A:591:ILE:HG22	1:A:595:ILE:HD11	2.01	0.41
1:A:1000:ASN:OD1	1:A:1061:ARG:NH2	2.54	0.41
1:A:263:ILE:HG22	1:A:265:LYS:HA	2.02	0.41
1:A:967:TYR:O	1:A:968:ASN:C	2.63	0.41
1:A:257:TRP:CD1	1:A:280:PRO:HA	2.56	0.41
1:A:424:ASN:HB2	1:A:966:ILE:O	2.21	0.41

*Continued on next page...*

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:459:PHE:CD2	1:A:959:ALA:HB2	2.56	0.40
1:A:636:ILE:H	1:A:636:ILE:HD12	1.86	0.40
1:A:583:HIS:N	1:A:863:GLU:OE1	2.53	0.40
1:A:741:ILE:HD11	1:A:820:TYR:HE2	1.87	0.40
1:A:1342:LEU:HD22	1:A:1372:LEU:HD13	2.03	0.40
1:A:1451:ILE:O	1:A:1453:ILE:N	2.55	0.40
1:A:290:GLN:H	1:A:290:GLN:HG2	1.74	0.40
1:A:265:LYS:O	1:A:335:SER:OG	2.38	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	1211/1438 (84%)	1066 (88%)	136 (11%)	9 (1%)	18	35

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1307	GLU
1	A	1289	GLY
1	A	1329	VAL
1	A	1452	GLY
1	A	187	ASP
1	A	269	THR
1	A	673	TYR
1	A	214	ASP
1	A	455	PRO

### 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	1017/1214 (84%)	1017 (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 (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	316	GLN
1	A	356	ASN
1	A	494	ASN
1	A	513	ASN
1	A	598	GLN
1	A	626	GLN
1	A	633	GLN
1	A	867	ASN
1	A	956	GLN
1	A	1141	GLN
1	A	1156	GLN
1	A	1164	ASN
1	A	1170	ASN
1	A	1359	ASN
1	A	1384	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](#)

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

## 5.5 Carbohydrates

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).

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	0.39	0	15,15,17	0.57	0
2	FRU	B	2	2	11,12,12	0.39	0	10,18,18	0.37	0
2	GLC	C	1	2	11,11,12	0.32	0	15,15,17	0.61	0
2	FRU	C	2	2	11,12,12	0.49	0	10,18,18	0.50	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
2	GLC	B	1	2	-	0/2/19/22	0/1/1/1
2	FRU	B	2	2	-	2/5/24/24	0/1/1/1
2	GLC	C	1	2	-	1/2/19/22	0/1/1/1
2	FRU	C	2	2	-	3/5/24/24	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

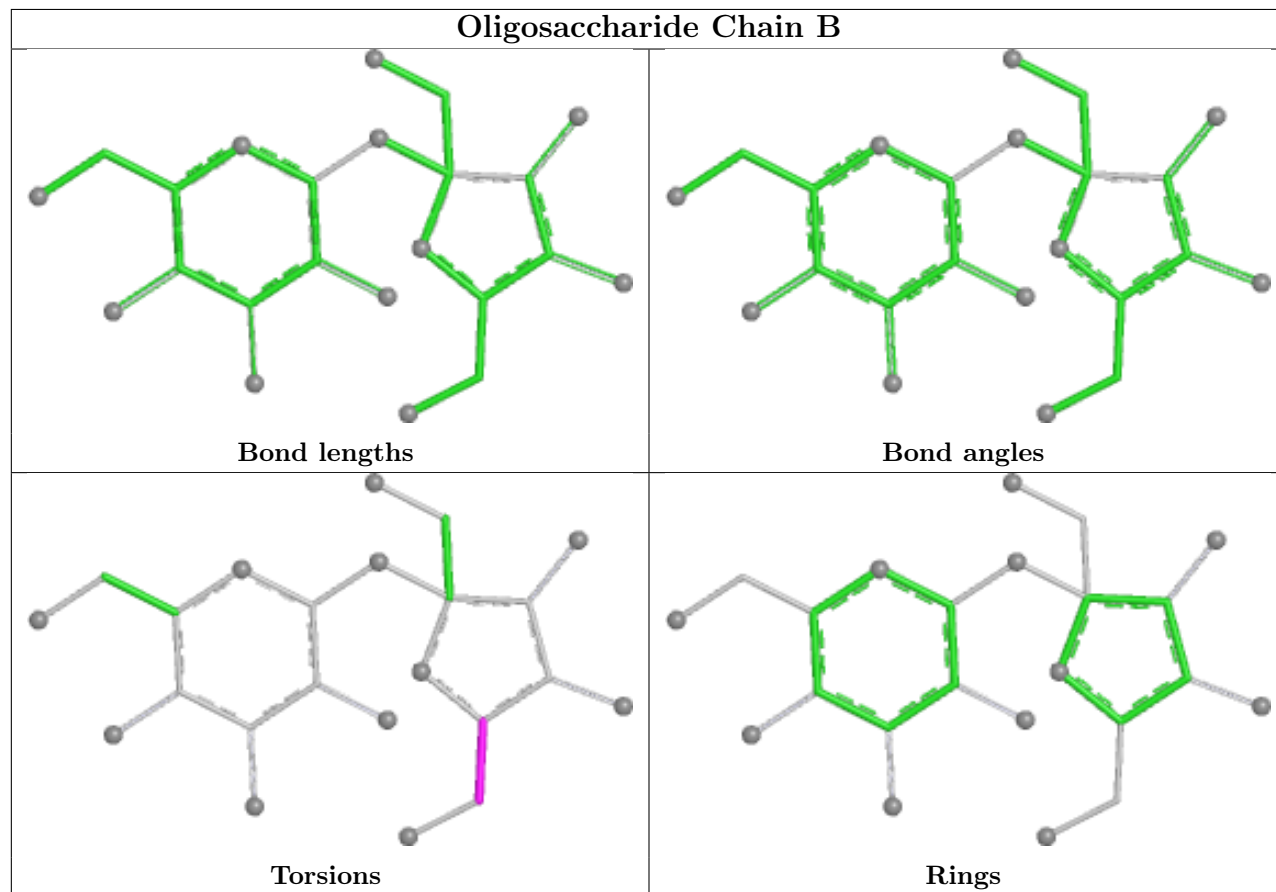
All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	2	FRU	O1-C1-C2-C3
2	C	2	FRU	O1-C1-C2-O2
2	B	2	FRU	O5-C5-C6-O6
2	C	1	GLC	O5-C5-C6-O6
2	B	2	FRU	C4-C5-C6-O6
2	C	2	FRU	O1-C1-C2-O5

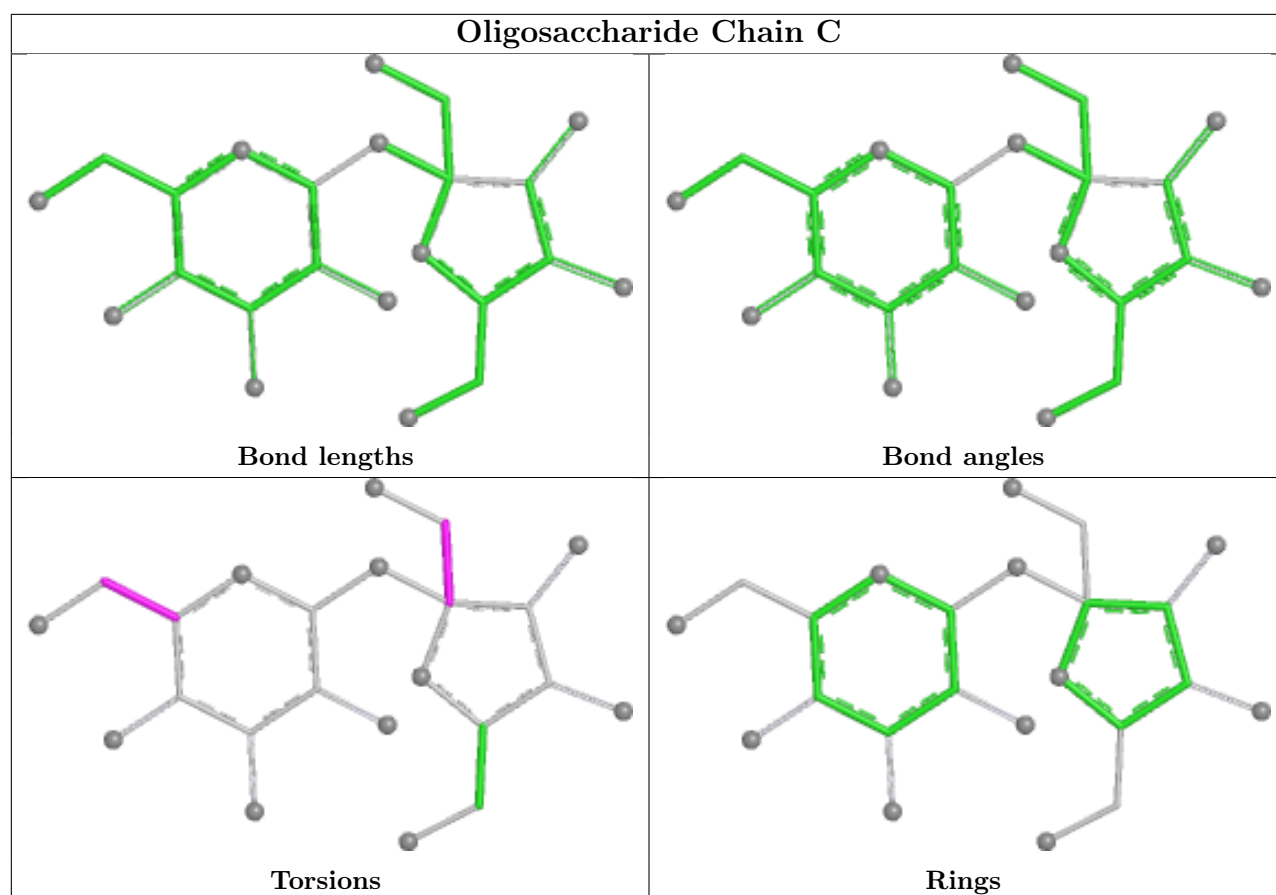
There are no ring outliers.

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.







## 5.6 Ligand geometry [i](#)

1 ligand is 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	$\# Z  > 2$
3	EDO	A	1501	-	3,3,3	0.07	0	2,2,2	0.14	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
3	EDO	A	1501	-	-	0/1/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

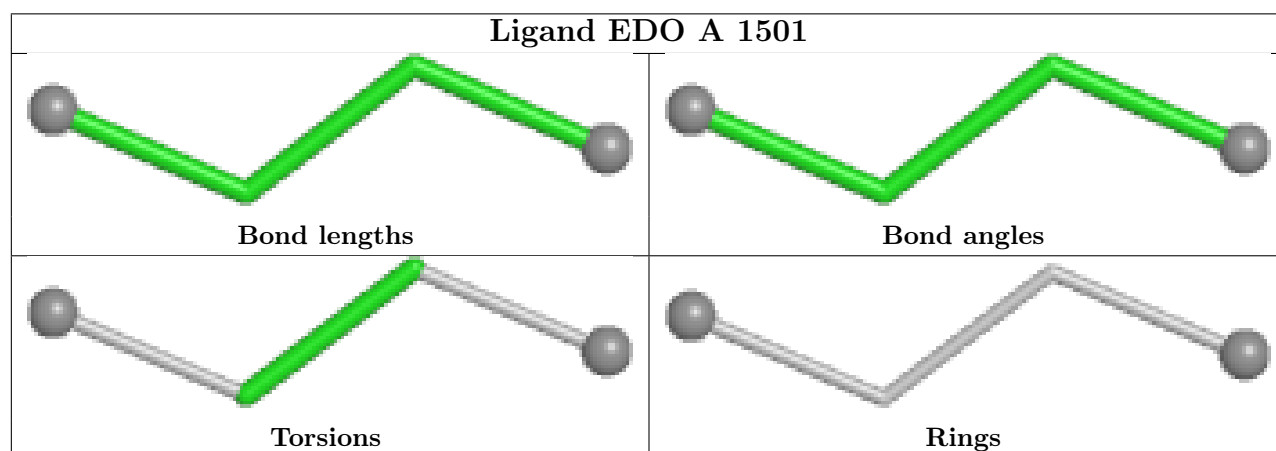
There are no chirality outliers.

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 [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<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	1237/1438 (86%)	0.11	20 (1%) 70 64	61, 96, 137, 168	0

All (20) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1304	ASN	5.3
1	A	911	SER	3.6
1	A	177	ILE	3.6
1	A	1305	SER	3.1
1	A	896	THR	2.8
1	A	330	ILE	2.7
1	A	459	PHE	2.6
1	A	1303	ALA	2.4
1	A	366	SER	2.4
1	A	1240	GLY	2.3
1	A	1143	LEU	2.3
1	A	1351	VAL	2.3
1	A	605	GLY	2.2
1	A	1083	THR	2.2
1	A	920	GLY	2.1
1	A	1321	TRP	2.1
1	A	1345	ALA	2.1
1	A	792	LEU	2.1
1	A	1300	TYR	2.1
1	A	808	ASP	2.0

### 6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

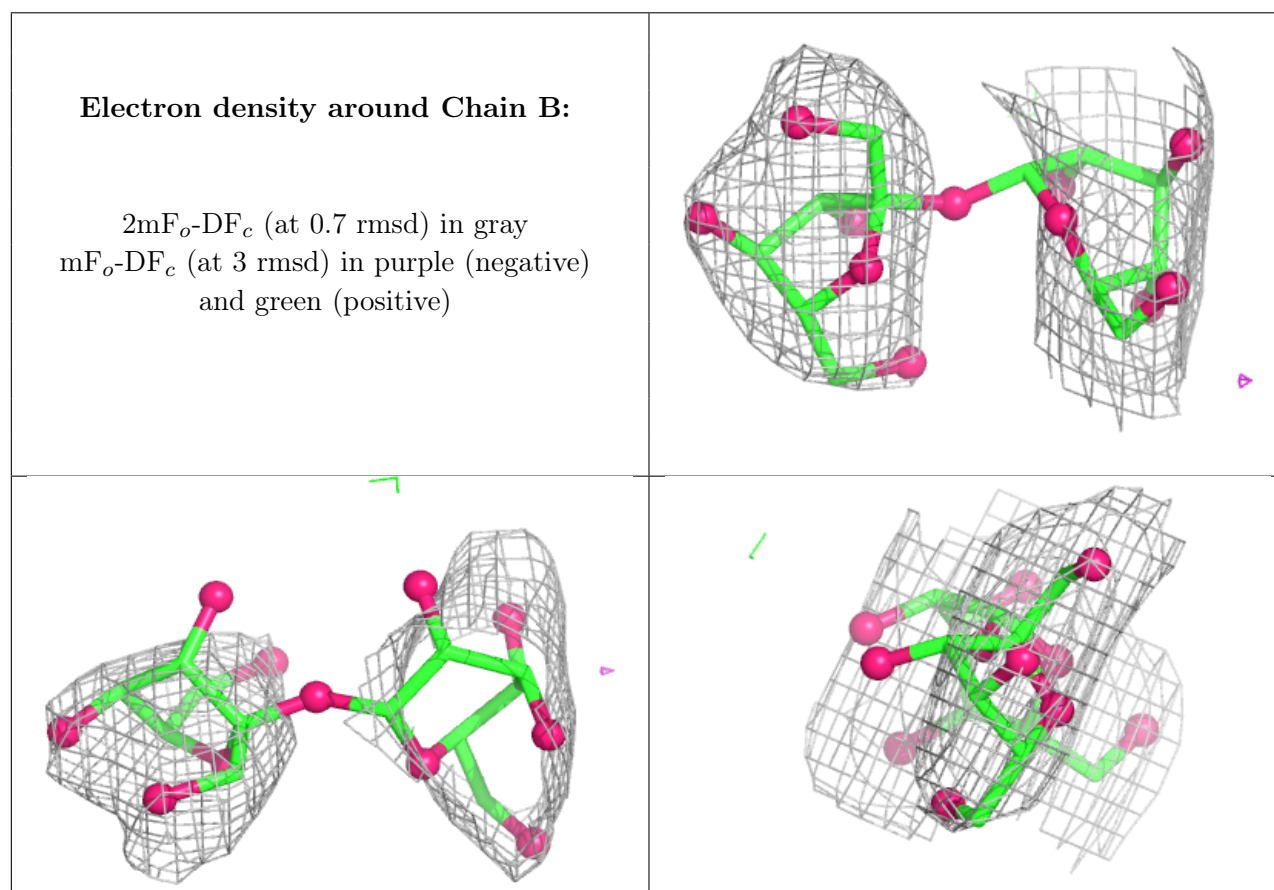
There are no non-standard protein/DNA/RNA residues in this entry.

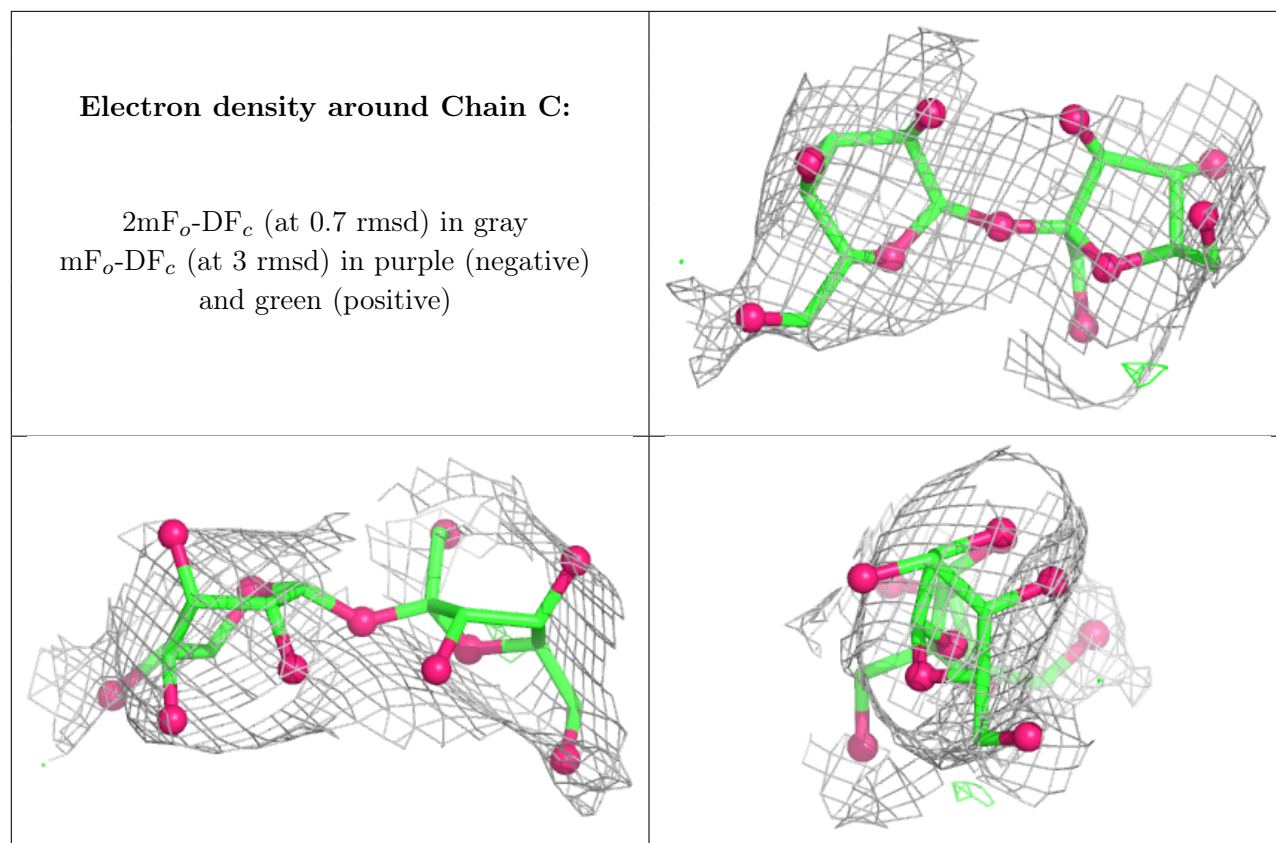
### 6.3 Carbohydrates ⓘ

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	C	1	11/12	0.82	0.10	108,112,116,116	0
2	FRU	C	2	12/12	0.82	0.12	106,108,114,115	0
2	FRU	B	2	12/12	0.85	0.12	80,84,88,90	0
2	GLC	B	1	11/12	0.89	0.14	67,71,78,80	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](#)

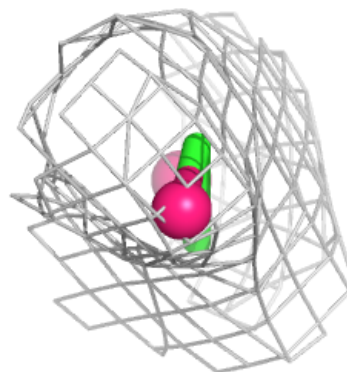
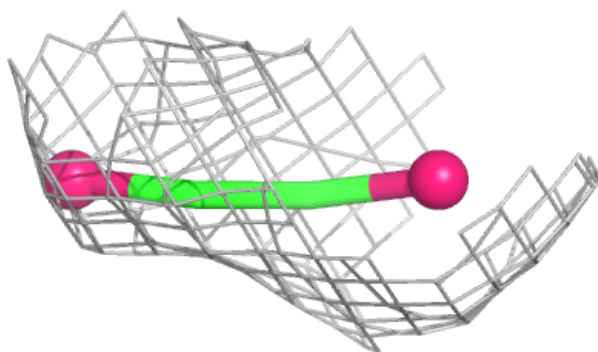
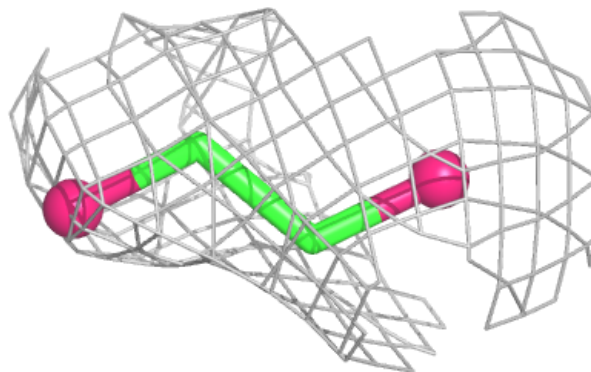
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 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
3	EDO	A	1501	4/4	0.87	0.11	96,98,99,99	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 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 [i](#)

There are no such residues in this entry.