



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 13, 2026 – 10:23 AM EDT

PDB ID : 9OUE / pdb_00009oue
Title : Structure of full-length Streptococcus mutans GtfD in complex with dextran 5000 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

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
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

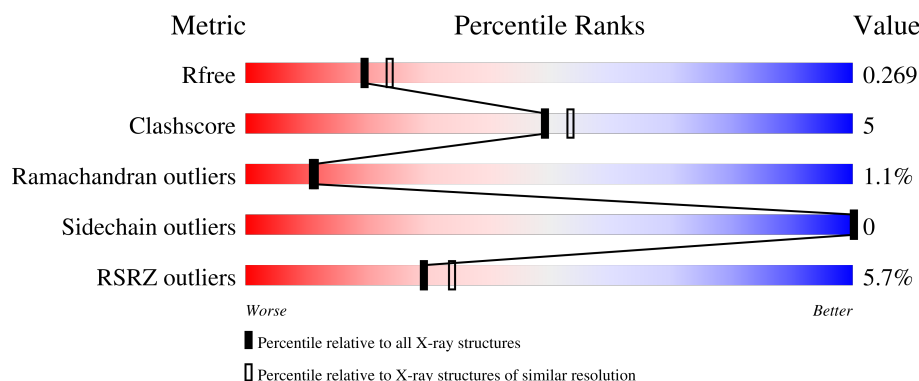
1 Overall quality at a glance

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 ≥ 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	1303	 6% 85% 14% .
2	B	23	 48% 48% .
3	C	3	 100%

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	1292	Total	C	N	O	S	0	0	0
			10192	6393	1740	2038	21			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
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

- [illegible]



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
2	B	23	Total 253	C 138	O 115	0	0	0

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

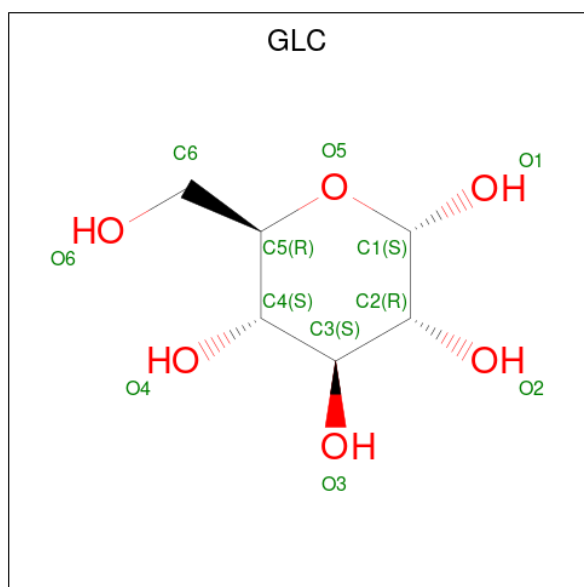


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
3	C	3	Total	C	O	0	0	0
			33	18	15			

- 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 alpha-D-glucopyranose (CCD ID: GLC) (formula: C₆H₁₂O₆) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			12	6	6		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	161	Total 161	O 161	0	0

Chain B:

48%

48%



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

Chain C:

100%



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	88.30Å 94.88Å 182.76Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	63.50 – 2.35 63.50 – 2.35	Depositor EDS
% Data completeness (in resolution range)	99.3 (63.50-2.35) 99.6 (63.50-2.35)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.61 (at 2.34Å)	Xtriage
Refinement program	PHENIX (1.18.2_3874)	Depositor
R, R_{free}	0.218 , 0.267 0.221 , 0.269	Depositor DCC
R_{free} test set	3036 reflections (4.69%)	wwPDB-VP
Wilson B-factor (Å ²)	50.0	Xtriage
Anisotropy	0.586	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 36.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	10652	wwPDB-VP
Average B, all atoms (Å ²)	59.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.25% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: CA, GLC

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	0.20	0/10404	0.43	0/14082

There are no bond length outliers.

There are no bond angle outliers.

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	10192	0	9729	110	0
2	B	253	0	208	8	0
3	C	33	0	28	0	0
4	A	1	0	0	0	0
5	A	12	0	12	1	0
6	A	161	0	0	1	0
All	All	10652	0	9977	110	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 (110) 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:1290:LYS:HZ2	1:A:1322:TYR:HD1	1.19	0.85
1:A:1316:ASP:OD1	1:A:1317:SER:N	2.20	0.74
1:A:1183:TYR:HE2	1:A:1221:GLN:HE22	1.35	0.73
1:A:514:LYS:HD2	1:A:574:MET:HE3	1.73	0.70
1:A:251:TYR:OH	1:A:385:LYS:HE3	1.92	0.70
1:A:993:LYS:H	1:A:995:THR:HG23	1.59	0.68
1:A:1453:ILE:HG12	1:A:1457:GLY:H	1.58	0.68
1:A:387:ALA:HA	1:A:390:ASN:ND2	2.09	0.67
1:A:1297:LYS:HB3	1:A:1330:ALA:HB3	1.78	0.66
1:A:1290:LYS:NZ	1:A:1322:TYR:HD1	1.95	0.62
1:A:305:GLY:HA2	1:A:326:VAL:HG12	1.79	0.62
1:A:1401:ILE:O	1:A:1404:GLN:HB2	2.00	0.61
1:A:1324:PHE:HA	1:A:1330:ALA:HA	1.82	0.61
1:A:513:ASN:ND2	1:A:520:GLN:O	2.31	0.61
1:A:543:ALA:O	1:A:546:LYS:NZ	2.34	0.60
1:A:1277:THR:OG1	1:A:1308:LEU:HB2	2.02	0.60
1:A:1014:GLY:HA3	1:A:1044:LYS:HG2	1.84	0.58
1:A:259:ARG:HD2	1:A:275:GLU:HA	1.85	0.58
1:A:739:ALA:HB2	1:A:760:MET:HE1	1.87	0.57
1:A:880:ASN:HD22	1:A:943:MET:HA	1.72	0.54
1:A:264:LEU:HD13	1:A:270:TRP:CE2	2.43	0.54
1:A:790:LYS:HA	1:A:793:TYR:CE1	2.42	0.54
1:A:1316:ASP:HB2	1:A:1322:TYR:HE1	1.72	0.54
1:A:913:LEU:O	1:A:917:ILE:HG12	2.09	0.53
1:A:325:THR:O	1:A:328:VAL:HG22	2.09	0.53
1:A:1434:SER:O	2:B:22:GLC:O3	2.23	0.53
1:A:418:TYR:CD1	1:A:982:ASP:HB3	2.44	0.52
1:A:1233:LYS:HB3	1:A:1265:ILE:HD12	1.91	0.52
1:A:748:LEU:O	1:A:749:LYS:HE2	2.09	0.52
1:A:1233:LYS:CB	1:A:1265:ILE:HD12	2.40	0.52
1:A:1377:PHE:O	2:B:20:GLC:H4	2.10	0.52
1:A:794:ARG:HD3	1:A:802:LEU:HD22	1.92	0.52
1:A:208:ASN:O	1:A:209:THR:OG1	2.24	0.52
1:A:456:GLU:O	1:A:456:GLU:HG2	2.10	0.52
1:A:914:ASP:OD2	5:A:1502:GLC:O4	2.28	0.51
1:A:366:SER:HA	1:A:370:LYS:HE3	1.93	0.51
1:A:1402:ASN:C	1:A:1404:GLN:H	2.19	0.51
1:A:274:SER:C	1:A:276:SER:H	2.18	0.51
1:A:382:ASN:HA	1:A:390:ASN:OD1	2.09	0.50
1:A:705:MET:HE3	1:A:748:LEU:HA	1.94	0.50
1:A:527:LEU:HB2	1:A:560:SER:HB2	1.93	0.50
1:A:1297:LYS:O	1:A:1329:VAL:HA	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1121:GLN:NE2	1:A:1125:GLY:O	2.45	0.49
1:A:1261:ASN:HB3	1:A:1267:LEU:HD21	1.95	0.49
1:A:790:LYS:HA	1:A:793:TYR:CD1	2.48	0.48
1:A:1309:ALA:HB1	1:A:1312:ILE:HG21	1.95	0.48
1:A:433:VAL:O	1:A:437:GLN:HG2	2.13	0.48
1:A:768:GLU:HG2	1:A:795:LYS:HG2	1.96	0.48
1:A:730:SER:OG	1:A:731:GLU:N	2.46	0.48
1:A:879:THR:O	1:A:883:ILE:HG13	2.14	0.47
1:A:492:GLU:HG2	1:A:839:ALA:HB1	1.96	0.47
1:A:1353:GLY:HA2	1:A:1366:HIS:O	2.14	0.47
1:A:796:THR:HG22	1:A:802:LEU:HG	1.97	0.47
1:A:186:SER:HB2	1:A:1217:GLN:NE2	2.30	0.47
1:A:523:ILE:HG12	1:A:577:TYR:CZ	2.50	0.47
1:A:268:LYS:HG3	1:A:269:THR:OG1	2.14	0.46
1:A:1286:GLN:N	1:A:1286:GLN:OE1	2.48	0.46
1:A:1285:LYS:NZ	2:B:4:GLC:O3	2.41	0.46
1:A:198:VAL:HG12	1:A:203:LEU:HD13	1.97	0.46
1:A:268:LYS:HG3	1:A:269:THR:N	2.30	0.46
1:A:584:ASP:OD1	1:A:585:SER:N	2.48	0.45
1:A:929:LEU:H	1:A:931:MET:HE3	1.81	0.45
1:A:1287:ILE:HG13	1:A:1302:LEU:HA	1.97	0.45
1:A:1436:ASN:OD1	1:A:1436:ASN:N	2.50	0.45
1:A:298:TYR:O	1:A:302:GLN:HG2	2.16	0.45
1:A:1333:GLY:H	1:A:1344:PHE:HB2	1.81	0.45
1:A:1259:TYR:HD2	1:A:1267:LEU:HD23	1.81	0.45
1:A:404:THR:HG21	1:A:408:LYS:HE2	1.98	0.45
1:A:998:ALA:O	1:A:1061:ARG:NH1	2.48	0.45
1:A:529:LEU:HD12	1:A:533:TYR:HE2	1.81	0.45
1:A:1233:LYS:HB3	1:A:1265:ILE:HG23	1.99	0.45
1:A:542:ASP:OD1	1:A:542:ASP:N	2.49	0.44
1:A:1279:TYR:HB2	1:A:1300:TYR:CZ	2.52	0.44
1:A:354:GLN:NE2	6:A:1624:HOH:O	2.51	0.44
1:A:458:ASN:O	1:A:951:HIS:HE1	2.01	0.44
1:A:1061:ARG:O	1:A:1065:TYR:HB2	2.18	0.44
1:A:473:ASP:OD2	1:A:1034:SER:OG	2.33	0.44
1:A:1136:MET:HE3	1:A:1136:MET:HB2	1.88	0.44
1:A:1293:THR:OG1	1:A:1298:LEU:HD12	2.18	0.44
1:A:1270:VAL:HG22	1:A:1279:TYR:HD1	1.83	0.44
1:A:238:VAL:HG23	1:A:261:LYS:HA	1.99	0.43
1:A:544:SER:HB3	1:A:630:LYS:NZ	2.32	0.43
1:A:865:PHE:CG	1:A:901:ALA:HB2	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:798:ASP:OD1	1:A:798:ASP:N	2.51	0.43
1:A:650:ILE:HD13	1:A:859:GLN:HB2	2.01	0.43
1:A:1405:ARG:HD2	1:A:1439:TYR:OH	2.19	0.43
1:A:1421:TYR:CE1	1:A:1427:LEU:HD13	2.53	0.43
1:A:904:TYR:OH	1:A:960:ASP:O	2.27	0.43
1:A:1226:TRP:CD2	1:A:1236:TYR:HB2	2.53	0.43
1:A:1249:PHE:O	2:B:2:GLC:H5	2.19	0.43
1:A:176:GLN:HA	1:A:181:TYR:HA	2.01	0.42
1:A:422:LEU:HD23	1:A:422:LEU:HA	1.96	0.42
1:A:1414:GLN:OE1	2:B:22:GLC:O4	2.35	0.42
1:A:1214:TYR:HB2	1:A:1237:PHE:CZ	2.55	0.42
1:A:265:LYS:O	1:A:268:LYS:HG2	2.20	0.42
1:A:274:SER:O	1:A:276:SER:N	2.50	0.41
1:A:677:ASP:OD1	1:A:681:LYS:NZ	2.50	0.41
1:A:1411:GLU:OE2	1:A:1413:LYS:NZ	2.53	0.41
1:A:693:MET:HE2	1:A:693:MET:HB3	1.97	0.41
1:A:622:GLU:O	1:A:626:GLN:HG2	2.20	0.41
1:A:699:GLU:HB3	1:A:751:ASN:HD21	1.85	0.41
1:A:1385:TRP:CE2	2:B:22:GLC:H61	2.56	0.41
1:A:1122:ASP:OD2	1:A:1126:ASN:HB2	2.21	0.41
1:A:913:LEU:HD12	1:A:914:ASP:N	2.35	0.41
1:A:1279:TYR:CZ	1:A:1291:ILE:HG21	2.56	0.41
1:A:418:TYR:O	1:A:469:ASN:HA	2.21	0.41
1:A:1352:LYS:NZ	2:B:13:GLC:H4	2.36	0.41
1:A:1002:LYS:HA	1:A:1048:TRP:O	2.21	0.40
1:A:1368:ASP:OD1	2:B:17:GLC:O2	2.39	0.40
1:A:748:LEU:C	1:A:749:LYS:HE2	2.47	0.40

There are no symmetry-related clashes.

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	1290/1303 (99%)	1214 (94%)	62 (5%)	14 (1%)	11	11

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1236	TYR
1	A	1274	ASN
1	A	1366	HIS
1	A	423	ALA
1	A	1334	SER
1	A	1367	ALA
1	A	1440	ASN
1	A	706	ASP
1	A	1304	ASN
1	A	1208	ILE
1	A	1293	THR
1	A	1337	ILE
1	A	1305	SER
1	A	172	PRO

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	1081/1101 (98%)	1081 (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 (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	316	GLN
1	A	324	GLN
1	A	354	GLN
1	A	446	ASN
1	A	626	GLN

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Mol	Chain	Res	Type
1	A	810	GLN
1	A	859	GLN
1	A	1126	ASN
1	A	1132	ASN
1	A	1221	GLN
1	A	1373	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 ⓘ

26 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	0.35	0	15,15,17	0.61	0
2	GLC	B	10	2	11,11,12	0.23	0	15,15,17	0.66	1 (6%)
2	GLC	B	11	2	11,11,12	0.21	0	15,15,17	0.56	0
2	GLC	B	12	2	11,11,12	0.21	0	15,15,17	1.02	1 (6%)
2	GLC	B	13	2	11,11,12	0.22	0	15,15,17	0.46	0
2	GLC	B	14	2	11,11,12	0.25	0	15,15,17	0.48	0
2	GLC	B	15	2	11,11,12	0.28	0	15,15,17	0.68	1 (6%)
2	GLC	B	16	2	11,11,12	0.18	0	15,15,17	0.54	0
2	GLC	B	17	2	11,11,12	0.25	0	15,15,17	0.57	1 (6%)
2	GLC	B	18	2	11,11,12	0.39	0	15,15,17	1.26	1 (6%)
2	GLC	B	19	2	11,11,12	0.21	0	15,15,17	0.56	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	GLC	B	2	2	11,11,12	0.25	0	15,15,17	0.66	0
2	GLC	B	20	2	11,11,12	0.22	0	15,15,17	0.59	0
2	GLC	B	21	2	11,11,12	0.23	0	15,15,17	1.00	1 (6%)
2	GLC	B	22	2	11,11,12	0.22	0	15,15,17	0.52	0
2	GLC	B	23	2	11,11,12	0.25	0	15,15,17	0.56	0
2	GLC	B	3	2	11,11,12	0.22	0	15,15,17	0.82	1 (6%)
2	GLC	B	4	2	11,11,12	0.21	0	15,15,17	0.50	0
2	GLC	B	5	2	11,11,12	0.21	0	15,15,17	0.51	0
2	GLC	B	6	2	11,11,12	0.30	0	15,15,17	0.42	0
2	GLC	B	7	2	11,11,12	0.19	0	15,15,17	0.39	0
2	GLC	B	8	2	11,11,12	0.20	0	15,15,17	0.38	0
2	GLC	B	9	2	11,11,12	0.17	0	15,15,17	0.38	0
3	GLC	C	1	3	11,11,12	0.21	0	15,15,17	0.39	0
3	GLC	C	2	3	11,11,12	0.24	0	15,15,17	0.43	0
3	GLC	C	3	3	11,11,12	0.25	0	15,15,17	0.46	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	-	2/2/19/22	0/1/1/1
2	GLC	B	10	2	-	2/2/19/22	0/1/1/1
2	GLC	B	11	2	-	2/2/19/22	0/1/1/1
2	GLC	B	12	2	-	0/2/19/22	0/1/1/1
2	GLC	B	13	2	-	0/2/19/22	0/1/1/1
2	GLC	B	14	2	-	2/2/19/22	0/1/1/1
2	GLC	B	15	2	-	0/2/19/22	0/1/1/1
2	GLC	B	16	2	-	2/2/19/22	0/1/1/1
2	GLC	B	17	2	-	2/2/19/22	0/1/1/1
2	GLC	B	18	2	-	0/2/19/22	0/1/1/1
2	GLC	B	19	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	20	2	-	2/2/19/22	0/1/1/1
2	GLC	B	21	2	-	0/2/19/22	0/1/1/1
2	GLC	B	22	2	-	2/2/19/22	0/1/1/1
2	GLC	B	23	2	-	0/2/19/22	0/1/1/1
2	GLC	B	3	2	-	1/2/19/22	0/1/1/1
2	GLC	B	4	2	-	2/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	GLC	B	5	2	-	2/2/19/22	0/1/1/1
2	GLC	B	6	2	-	0/2/19/22	0/1/1/1
2	GLC	B	7	2	-	2/2/19/22	0/1/1/1
2	GLC	B	8	2	-	0/2/19/22	0/1/1/1
2	GLC	B	9	2	-	0/2/19/22	0/1/1/1
3	GLC	C	1	3	-	1/2/19/22	0/1/1/1
3	GLC	C	2	3	-	2/2/19/22	0/1/1/1
3	GLC	C	3	3	-	2/2/19/22	0/1/1/1

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	18	GLC	C1-O5-C5	3.96	117.49	112.19
2	B	12	GLC	C1-O5-C5	3.80	117.28	112.19
2	B	21	GLC	C1-O5-C5	3.71	117.15	112.19
2	B	3	GLC	C1-O5-C5	3.08	116.32	112.19
2	B	15	GLC	C1-O5-C5	2.35	115.33	112.19
2	B	10	GLC	C1-O5-C5	2.27	115.23	112.19
2	B	17	GLC	C1-O5-C5	2.02	114.89	112.19

There are no chirality outliers.

All (30) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	7	GLC	C4-C5-C6-O6
2	B	16	GLC	C4-C5-C6-O6
2	B	19	GLC	C4-C5-C6-O6
2	B	11	GLC	C4-C5-C6-O6
2	B	16	GLC	O5-C5-C6-O6
3	C	3	GLC	C4-C5-C6-O6
2	B	7	GLC	O5-C5-C6-O6
2	B	11	GLC	O5-C5-C6-O6
2	B	20	GLC	O5-C5-C6-O6
2	B	19	GLC	O5-C5-C6-O6
3	C	3	GLC	O5-C5-C6-O6
3	C	2	GLC	C4-C5-C6-O6
2	B	5	GLC	O5-C5-C6-O6
2	B	1	GLC	C4-C5-C6-O6
2	B	20	GLC	C4-C5-C6-O6

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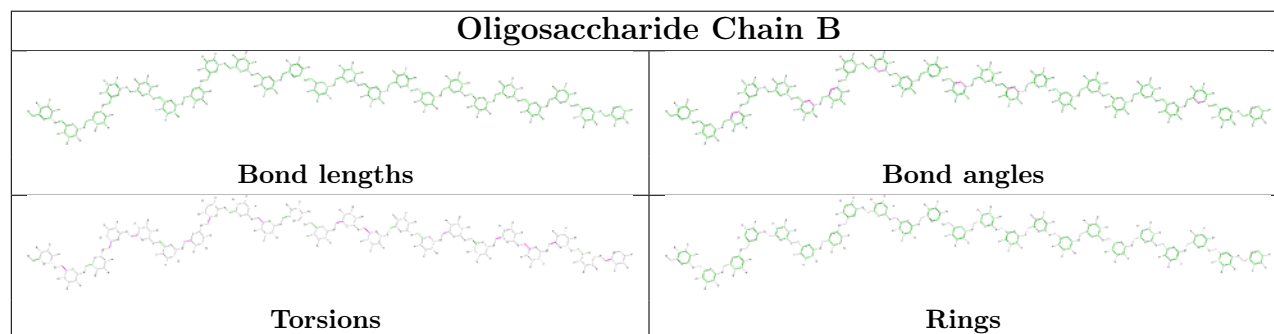
Mol	Chain	Res	Type	Atoms
2	B	5	GLC	C4-C5-C6-O6
2	B	17	GLC	C4-C5-C6-O6
2	B	1	GLC	O5-C5-C6-O6
3	C	2	GLC	O5-C5-C6-O6
2	B	4	GLC	C4-C5-C6-O6
2	B	17	GLC	O5-C5-C6-O6
2	B	4	GLC	O5-C5-C6-O6
3	C	1	GLC	O5-C5-C6-O6
2	B	14	GLC	C4-C5-C6-O6
2	B	10	GLC	C4-C5-C6-O6
2	B	22	GLC	C4-C5-C6-O6
2	B	14	GLC	O5-C5-C6-O6
2	B	22	GLC	O5-C5-C6-O6
2	B	3	GLC	O5-C5-C6-O6
2	B	10	GLC	O5-C5-C6-O6

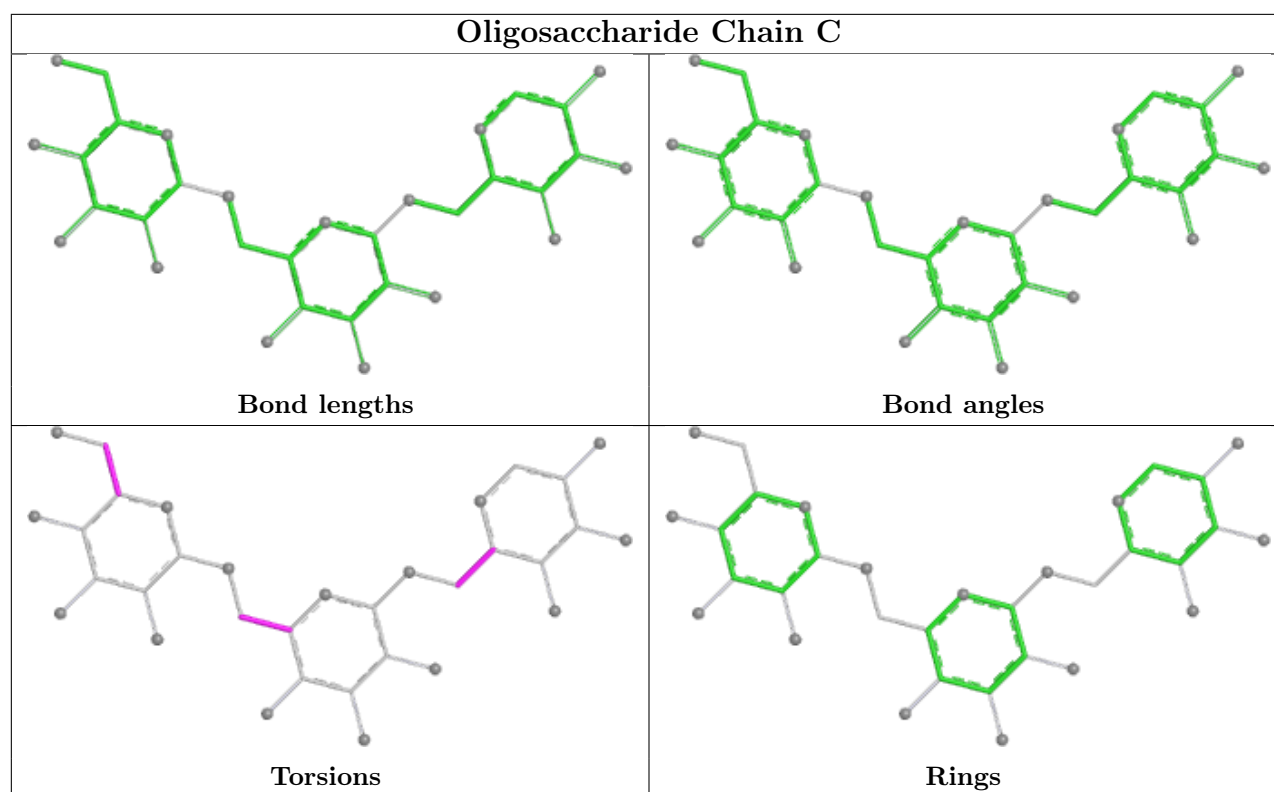
There are no ring outliers.

6 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	2	GLC	1	0
2	B	13	GLC	1	0
2	B	17	GLC	1	0
2	B	22	GLC	3	0
2	B	20	GLC	1	0
2	B	4	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.





5.6 Ligand geometry [i](#)

Of 2 ligands modelled in this entry, 1 is monoatomic - leaving 1 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	GLC	A	1502	-	12,12,12	0.17	0	17,17,17	0.58	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	GLC	A	1502	-	-	2/2/22/22	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) torsion outliers are listed below:

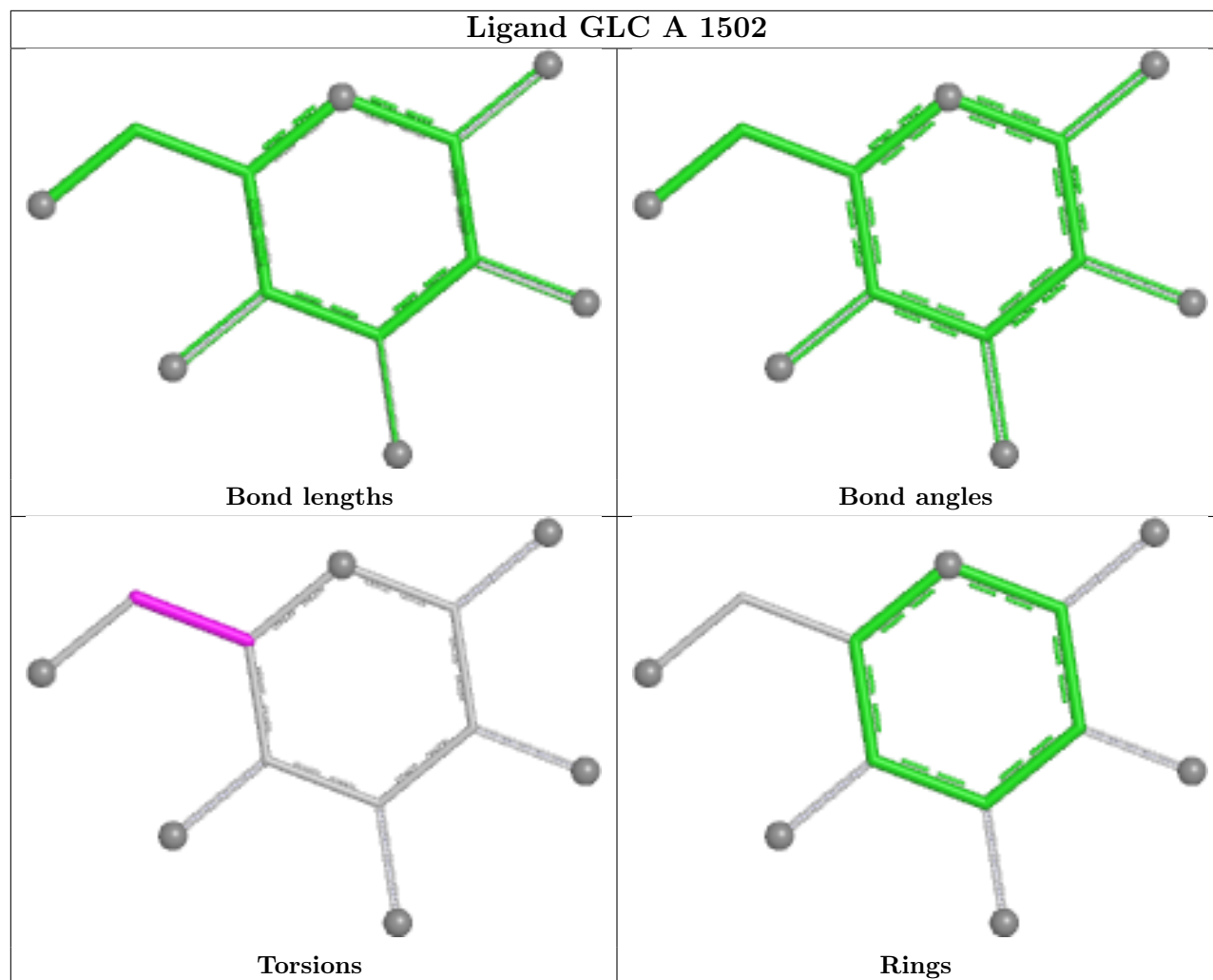
Mol	Chain	Res	Type	Atoms
5	A	1502	GLC	C4-C5-C6-O6
5	A	1502	GLC	O5-C5-C6-O6

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	1502	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 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, 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	1292/1303 (99%)	0.52	73 (5%)	29 34	40, 56, 83, 111	0

All (73) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1462	TYR	6.2
1	A	1293	THR	5.7
1	A	1287	ILE	5.5
1	A	1281	GLY	5.0
1	A	1303	ALA	4.9
1	A	1446	ALA	4.6
1	A	1442	VAL	4.3
1	A	1304	ASN	4.1
1	A	1231	ASP	4.0
1	A	1450	ARG	3.9
1	A	1451	ILE	3.6
1	A	1297	LYS	3.6
1	A	1298	LEU	3.5
1	A	1315	THR	3.4
1	A	1417	GLY	3.4
1	A	1461	TYR	3.4
1	A	1039	ILE	3.4
1	A	1443	VAL	3.4
1	A	1457	GLY	3.2
1	A	440	TRP	3.2
1	A	1286	GLN	3.2
1	A	1274	ASN	3.2
1	A	1366	HIS	3.2
1	A	1313	PHE	3.2
1	A	1275	GLY	3.2
1	A	1284	GLY	3.1
1	A	1240	GLY	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	1452	GLY	3.0
1	A	1290	LYS	2.9
1	A	1305	SER	2.9
1	A	1301	PHE	2.8
1	A	1404	GLN	2.8
1	A	1445	LEU	2.8
1	A	1453	ILE	2.7
1	A	1459	ALA	2.7
1	A	1276	LYS	2.7
1	A	1288	LYS	2.6
1	A	340	THR	2.6
1	A	1249	PHE	2.6
1	A	1226	TRP	2.6
1	A	422	LEU	2.5
1	A	1292	ILE	2.5
1	A	1277	THR	2.5
1	A	1395	LEU	2.5
1	A	1291	ILE	2.4
1	A	1351	VAL	2.4
1	A	1402	ASN	2.4
1	A	1296	GLY	2.4
1	A	1306	GLY	2.4
1	A	1438	VAL	2.4
1	A	1283	ASP	2.3
1	A	1339	GLY	2.3
1	A	1346	SER	2.3
1	A	1441	LYS	2.3
1	A	1295	ASN	2.2
1	A	1444	THR	2.2
1	A	189	GLN	2.2
1	A	1279	TYR	2.1
1	A	630	LYS	2.1
1	A	1258	TYR	2.1
1	A	1282	GLN	2.1
1	A	1280	PHE	2.1
1	A	1259	TYR	2.1
1	A	1255	GLY	2.1
1	A	1235	ARG	2.1
1	A	456	GLU	2.0
1	A	1225	ALA	2.0
1	A	1338	ALA	2.0
1	A	1426	LEU	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	1449	ARG	2.0
1	A	1289	GLY	2.0
1	A	1316	ASP	2.0
1	A	1265	ILE	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.

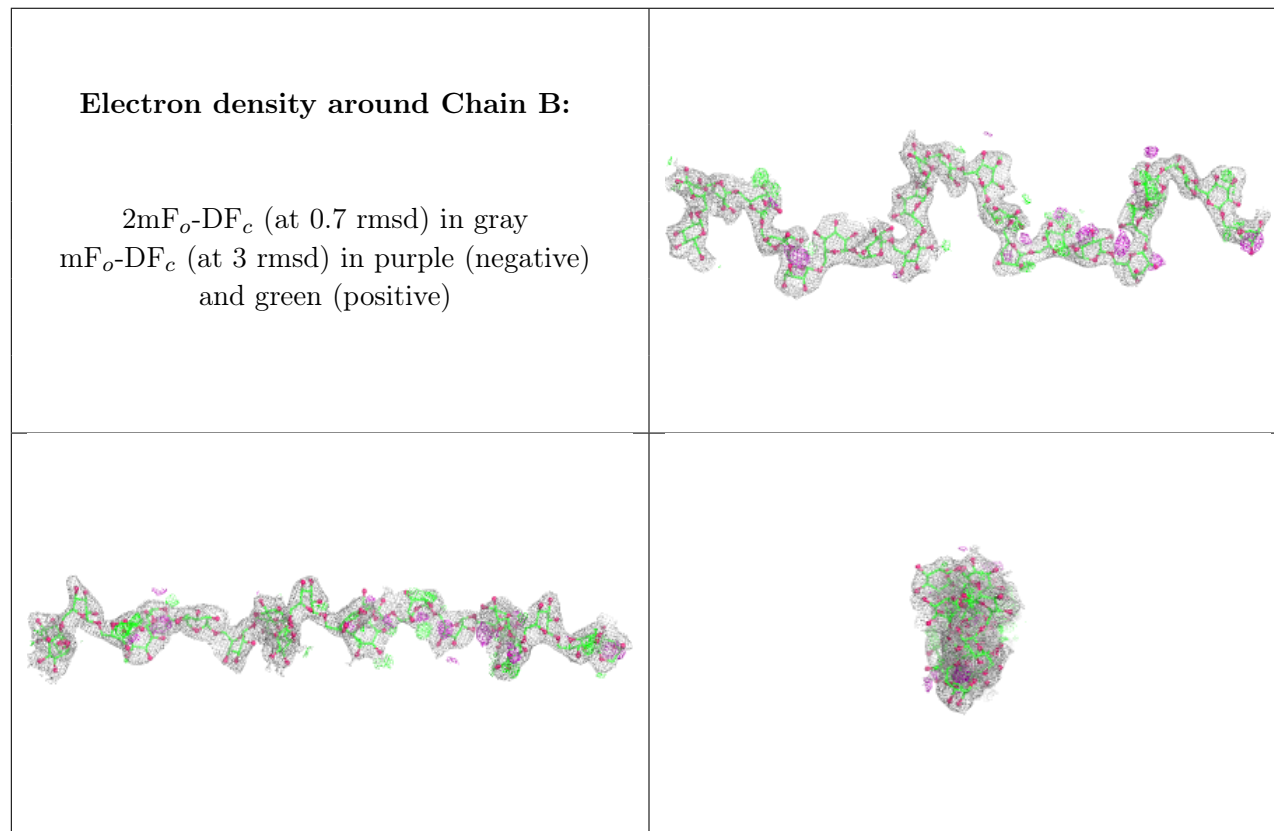
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	GLC	C	3	11/12	0.37	0.24	75,79,90,94	0
2	GLC	B	6	11/12	0.58	0.20	92,98,103,112	0
2	GLC	B	18	11/12	0.63	0.17	79,85,91,93	0
2	GLC	B	1	11/12	0.64	0.19	74,81,86,95	0
2	GLC	B	8	11/12	0.64	0.18	82,95,100,101	0
2	GLC	B	9	11/12	0.67	0.17	89,97,102,104	0
2	GLC	B	7	11/12	0.68	0.17	81,91,94,95	0
3	GLC	C	1	11/12	0.71	0.18	62,83,90,96	0
2	GLC	B	20	11/12	0.72	0.18	68,73,86,92	0
2	GLC	B	15	11/12	0.74	0.13	78,84,92,92	0
2	GLC	B	11	11/12	0.76	0.15	76,80,84,87	0
2	GLC	B	4	11/12	0.77	0.19	71,75,79,79	0
2	GLC	B	5	11/12	0.77	0.14	83,93,100,102	0
2	GLC	B	12	11/12	0.80	0.11	65,77,81,86	0
2	GLC	B	23	11/12	0.81	0.14	63,70,75,75	0
2	GLC	B	2	11/12	0.82	0.15	62,71,84,88	0
2	GLC	B	19	11/12	0.82	0.13	71,78,86,88	0
2	GLC	B	16	11/12	0.83	0.12	74,76,82,85	0
2	GLC	B	10	11/12	0.83	0.14	74,79,91,96	0
2	GLC	B	21	11/12	0.83	0.11	65,74,80,85	0
2	GLC	B	17	11/12	0.85	0.13	66,73,77,78	0
2	GLC	B	14	11/12	0.86	0.12	62,71,79,80	0
3	GLC	C	2	11/12	0.89	0.13	67,74,78,78	0
2	GLC	B	3	11/12	0.89	0.09	66,71,78,79	0

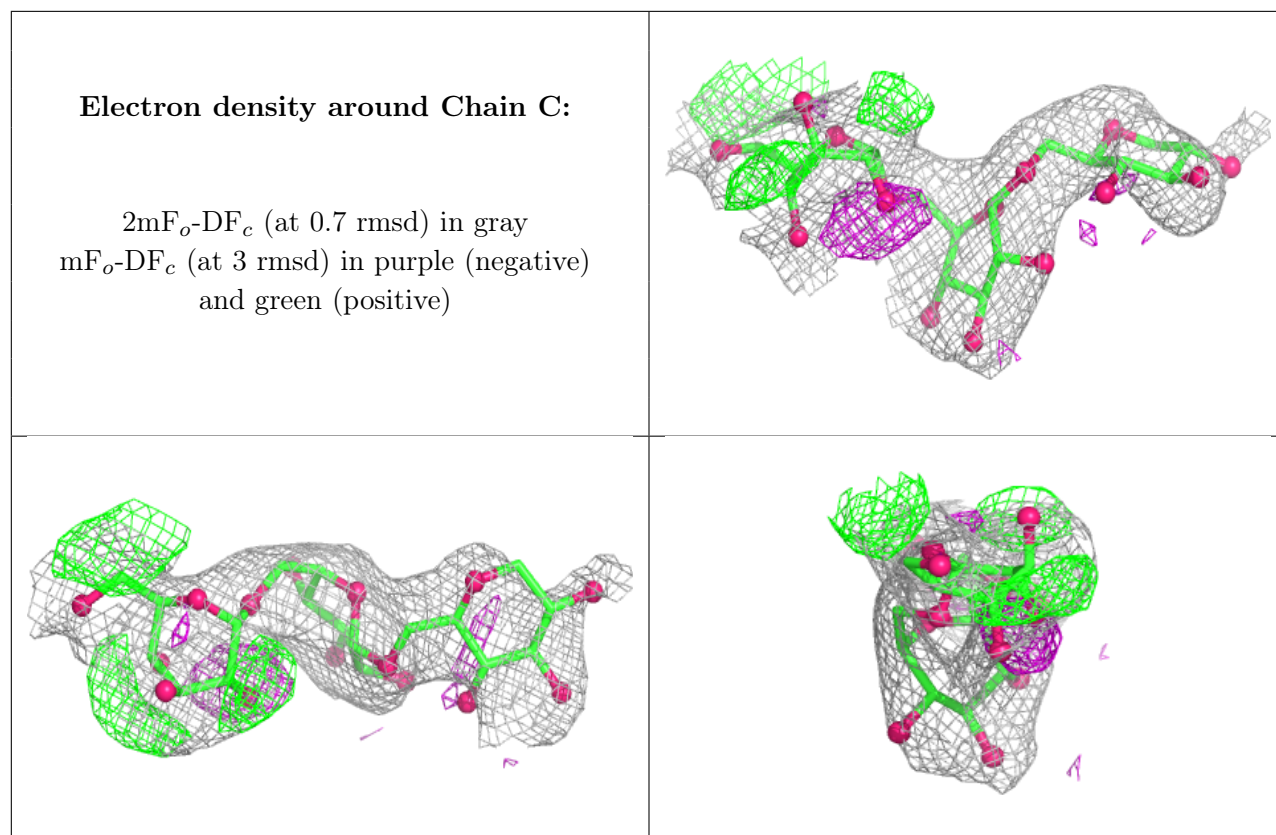
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	GLC	B	13	11/12	0.90	0.11	66,71,74,78	0
2	GLC	B	22	11/12	0.90	0.09	63,69,76,81	0

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](#)

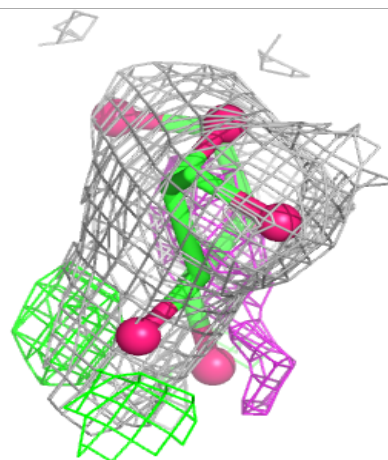
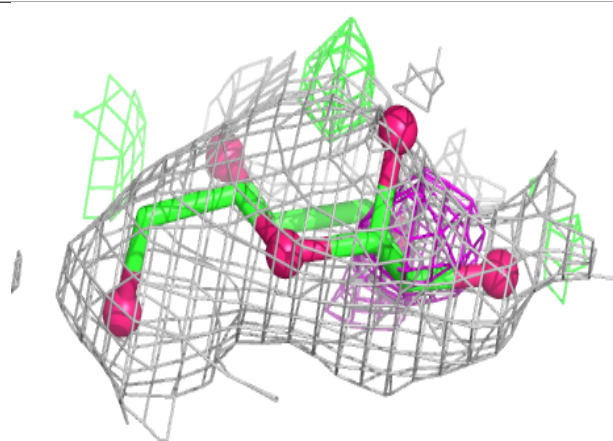
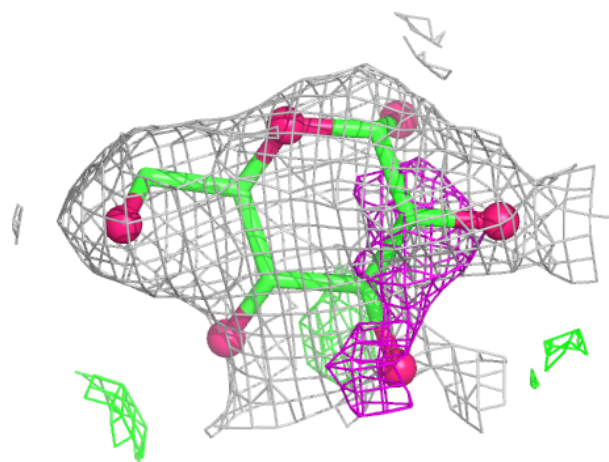
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	GLC	A	1502	12/12	0.78	0.15	48,65,76,78	0
4	CA	A	1501	1/1	0.91	0.10	63,63,63,63	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.

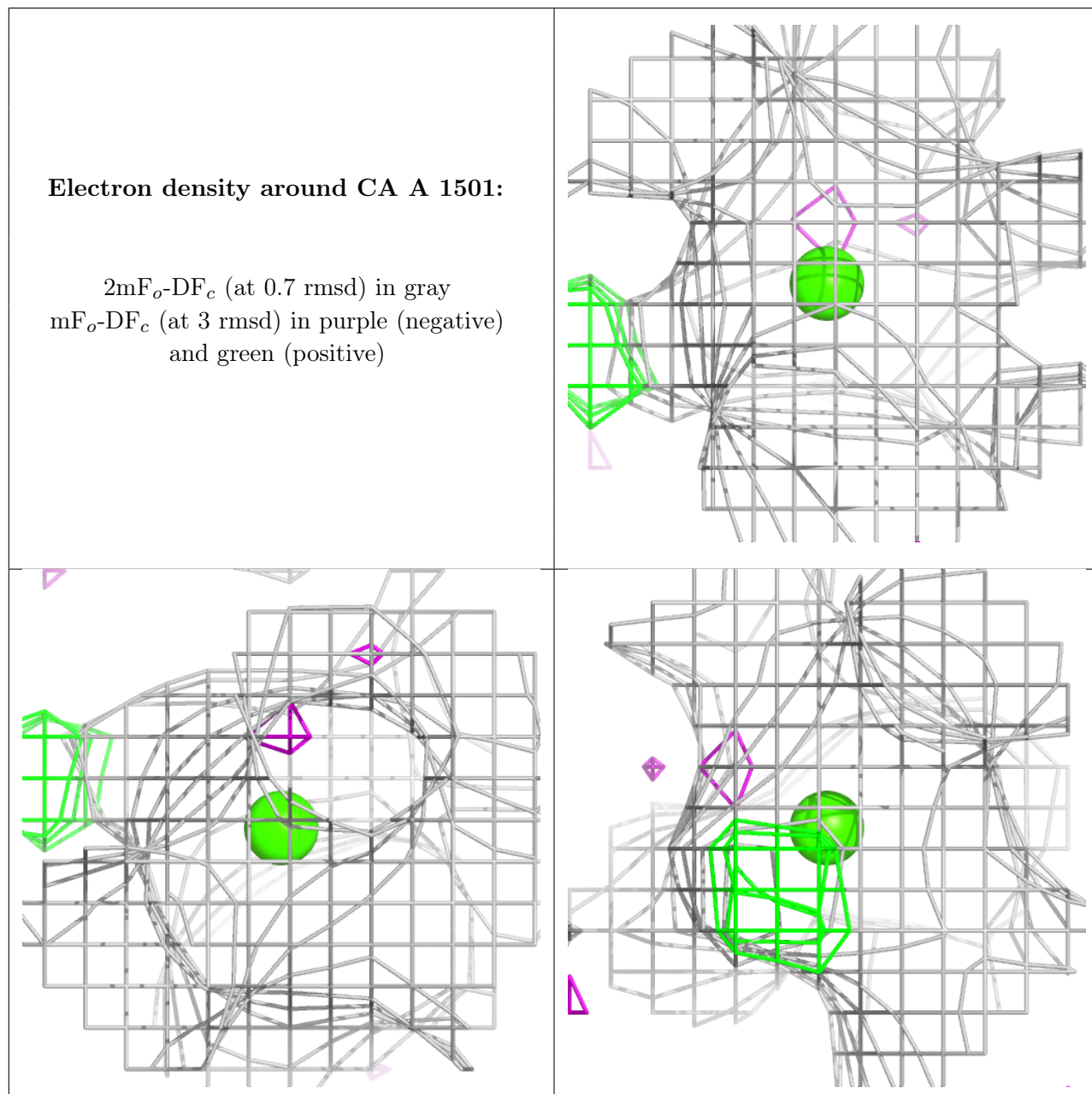
Electron density around GLC A 1502:

$2mF_o-DF_c$ (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.