



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 13, 2026 – 10:19 AM EDT

PDB ID : 9OJH / pdb_00009ojh
Title : Structure of full-length Streptococcus mutans GtfD with inhibitor maltose in active site
Authors : Schormann, N.; Deivanayagam, C.
Deposited on : 2025-05-07
Resolution : 2.15 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

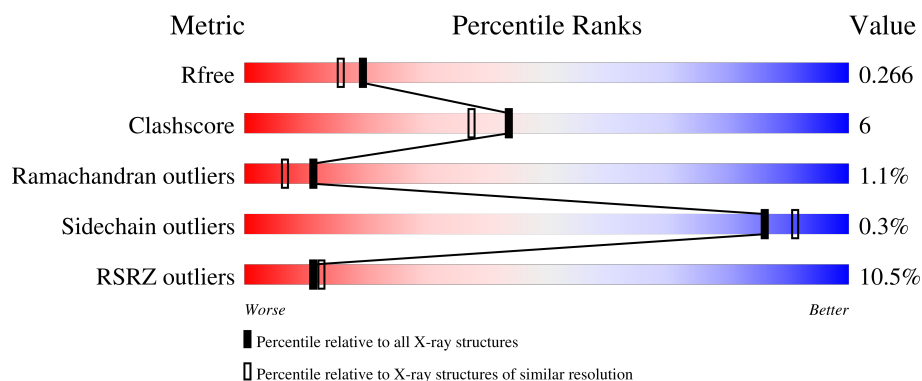
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.15 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	2057 (2.16-2.16)
Clashscore	190562	2159 (2.16-2.16)
Ramachandran outliers	187476	2134 (2.16-2.16)
Sidechain outliers	187428	2133 (2.16-2.16)
RSRZ outliers	180081	2059 (2.16-2.16)

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	1438	<div> <div>9%</div> <div> <div></div> <div>76%</div> <div>12%</div> <div>•</div> <div>11%</div> </div> </div>
2	B	2	<div> <div>50%</div> <div>50%</div> </div>

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 10491 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	1285	Total	C	N	O	S	0	0	0
			10101	6340	1723	2017	21			

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-(1-4)-alpha-D-glucopyranose.

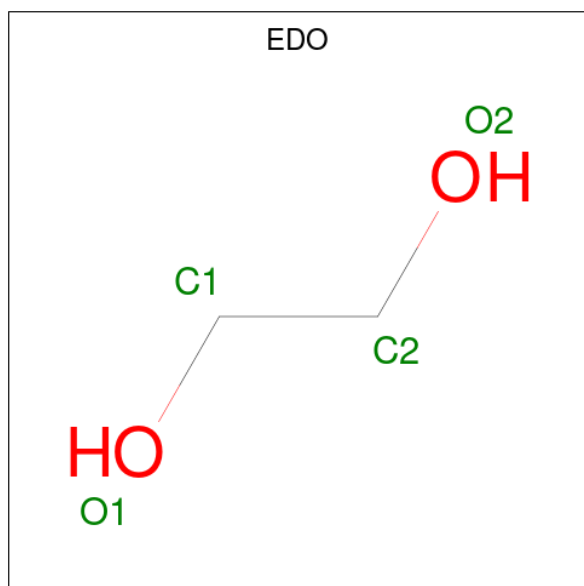


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
2	B	2	Total	C	O	0	0	0
			23	12	11			

- Molecule 3 is CALCIUM ION (CCD ID: CA) (formula: Ca) (labeled as "Ligand of Interest" by depositor).

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

- Molecule 4 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: $C_2H_6O_2$) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	362	Total	O	0	0
			362	362		



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	80.39Å 99.12Å 177.13Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.73 – 2.15 50.73 – 2.15	Depositor EDS
% Data completeness (in resolution range)	100.0 (50.73-2.15) 99.9 (50.73-2.15)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.87 (at 2.14Å)	Xtriage
Refinement program	PHENIX (1.18.2_3874: ???)	Depositor
R, R_{free}	0.226 , 0.266 0.227 , 0.266	Depositor DCC
R_{free} test set	3875 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	42.6	Xtriage
Anisotropy	0.085	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 32.4	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	0.95	EDS
Total number of atoms	10491	wwPDB-VP
Average B, all atoms (Å ²)	52.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.58% 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: GLC, CA, 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	0.18	0/10308	0.43	2/13946 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	1292	ILE	N-CA-C	-7.55	103.18	113.00
1	A	1422	ASP	N-CA-CB	5.59	118.50	110.45

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	10101	0	9612	121	0
2	B	23	0	21	1	0
3	A	1	0	0	0	0
4	A	4	0	6	0	0
5	A	362	0	0	1	0
All	All	10491	0	9639	121	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 6.

All (121) 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:1257:TRP:HB2	1:A:1285:LYS:HD3	1.56	0.86
1:A:1299:LYS:HB3	1:A:1310:ARG:HE	1.50	0.77
1:A:1376:ARG:HE	1:A:1378:GLU:HB2	1.49	0.77
1:A:1233:LYS:HB3	1:A:1235:ARG:HH12	1.51	0.75
1:A:177:ILE:HG23	1:A:179:GLY:H	1.51	0.74
1:A:1292:ILE:HA	1:A:1297:LYS:HA	1.70	0.73
1:A:1276:LYS:HD2	1:A:1308:LEU:HD23	1.70	0.72
1:A:1357:THR:HG23	1:A:1362:VAL:HB	1.69	0.72
1:A:1285:LYS:HB2	1:A:1307:GLU:OE1	1.94	0.68
1:A:1365:TYR:CE2	1:A:1367:ALA:HB2	2.31	0.65
1:A:1233:LYS:HB3	1:A:1235:ARG:NH1	2.13	0.64
1:A:1280:PHE:CD1	1:A:1285:LYS:HB3	2.34	0.63
1:A:1310:ARG:NH1	1:A:1324:PHE:O	2.34	0.61
1:A:1347:ASP:HB2	1:A:1349:LYS:NZ	2.16	0.61
1:A:1249:PHE:HA	1:A:1259:TYR:HA	1.82	0.60
1:A:1297:LYS:HB3	1:A:1332:THR:HG23	1.83	0.60
1:A:993:LYS:H	1:A:995:THR:HG23	1.67	0.60
1:A:1300:TYR:HB3	1:A:1307:GLU:HG3	1.84	0.59
1:A:1377:PHE:O	1:A:1379:ALA:N	2.36	0.58
1:A:1360:GLY:O	1:A:1362:VAL:HG13	2.04	0.58
1:A:1335:GLN:N	1:A:1345:ALA:O	2.37	0.58
1:A:1347:ASP:HB2	1:A:1349:LYS:HZ1	1.69	0.58
1:A:470:VAL:HG11	1:A:474:LEU:HD12	1.85	0.57
1:A:1376:ARG:NE	1:A:1378:GLU:HB2	2.17	0.57
1:A:305:GLY:HA2	1:A:326:VAL:HG12	1.87	0.56
1:A:1376:ARG:HE	1:A:1378:GLU:CB	2.18	0.56
1:A:1379:ALA:HB1	1:A:1386:TYR:HB2	1.87	0.56
1:A:913:LEU:O	1:A:917:ILE:HG12	2.06	0.56
1:A:1310:ARG:NH1	1:A:1325:GLY:O	2.40	0.55
1:A:790:LYS:HA	1:A:793:TYR:CE1	2.43	0.54
1:A:705:MET:HE1	1:A:710:THR:HG22	1.89	0.54
1:A:1235:ARG:HD3	1:A:1244:MET:SD	2.48	0.53
1:A:1297:LYS:HB3	1:A:1332:THR:CG2	2.39	0.53
1:A:1260:LEU:HD12	1:A:1264:GLY:O	2.10	0.52
1:A:1270:VAL:HG22	1:A:1279:TYR:CE1	2.45	0.52
1:A:299:MET:HE2	1:A:330:ILE:HD11	1.90	0.51
1:A:1287:ILE:HG23	1:A:1302:LEU:HA	1.92	0.51
1:A:854:SER:HA	1:A:857:ASP:HB2	1.90	0.51
1:A:1381:LYS:HG3	1:A:1382:ASP:N	2.25	0.51
1:A:1302:LEU:C	1:A:1306:GLY:HA2	2.35	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1364:TYR:HD1	1:A:1372:LEU:HD11	1.76	0.50
1:A:1381:LYS:HD2	1:A:1386:TYR:OH	2.13	0.49
1:A:1339:GLY:C	1:A:1341:LYS:H	2.21	0.49
1:A:537:ARG:NE	1:A:548:GLU:OE1	2.44	0.49
1:A:1381:LYS:HG2	1:A:1384:ASN:HB2	1.94	0.49
1:A:504:ALA:HB1	1:A:509:ASP:OD2	2.13	0.48
1:A:264:LEU:HD13	1:A:270:TRP:CE2	2.48	0.48
1:A:1279:TYR:HB2	1:A:1300:TYR:CZ	2.48	0.48
1:A:1355:PHE:HZ	1:A:1379:ALA:HA	1.77	0.48
1:A:1400:ARG:HA	1:A:1405:ARG:HA	1.95	0.48
1:A:702:LYS:HA	1:A:705:MET:HB2	1.96	0.48
1:A:1291:ILE:H	1:A:1291:ILE:HG12	1.42	0.48
1:A:1407:PHE:HB2	1:A:1430:TYR:CZ	2.49	0.47
1:A:1421:TYR:CE1	1:A:1427:LEU:HD12	2.50	0.47
1:A:182:TYR:HB3	1:A:190:PRO:HB3	1.96	0.47
1:A:1357:THR:HG23	1:A:1362:VAL:CB	2.42	0.47
1:A:1388:LEU:HD12	1:A:1392:GLY:O	2.15	0.47
1:A:1292:ILE:CA	1:A:1297:LYS:HA	2.42	0.46
1:A:268:LYS:HE2	1:A:268:LYS:HB3	1.69	0.46
1:A:1214:TYR:HB2	1:A:1237:PHE:CZ	2.50	0.46
1:A:1252:ASP:HB2	1:A:1258:TYR:HE1	1.80	0.46
1:A:584:ASP:OD2	2:B:1:GLC:O3	2.34	0.46
1:A:1416:LYS:HB3	1:A:1432:LYS:HA	1.97	0.45
1:A:280:PRO:HG2	1:A:283:MET:HB2	1.99	0.45
1:A:1185:SER:OG	1:A:1189:ASP:HA	2.16	0.44
1:A:418:TYR:O	1:A:469:ASN:HA	2.17	0.44
1:A:1248:ARG:O	1:A:1259:TYR:HA	2.17	0.44
1:A:171:ILE:HG21	1:A:181:TYR:CD1	2.53	0.44
1:A:865:PHE:CG	1:A:901:ALA:HB2	2.53	0.44
1:A:557:ILE:HG12	1:A:693:MET:HB3	1.99	0.44
1:A:524:ASP:HB3	1:A:578:ILE:HD13	1.98	0.44
1:A:685:LYS:HB3	1:A:686:TYR:CD2	2.53	0.44
1:A:762:THR:O	1:A:765:LYS:HE2	2.18	0.44
1:A:783:TYR:CD2	1:A:789:ALA:HB2	2.53	0.44
1:A:1285:LYS:HE2	1:A:1287:ILE:HD11	2.00	0.44
1:A:171:ILE:N	1:A:172:PRO:HD3	2.33	0.44
1:A:925:ASP:OD2	1:A:1007:ASP:HB2	2.19	0.43
1:A:579:PHE:HB3	1:A:652:ARG:HB3	2.00	0.43
1:A:1150:PHE:CE2	1:A:1156:GLN:HB2	2.53	0.43
1:A:867:ASN:O	1:A:917:ILE:HD12	2.18	0.43
1:A:1280:PHE:CE1	1:A:1285:LYS:HB3	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1300:TYR:CB	1:A:1307:GLU:HG3	2.48	0.43
1:A:814:ASN:HB3	1:A:816:GLN:H	1.83	0.43
1:A:1437:MET:HB3	1:A:1437:MET:HE2	1.82	0.43
1:A:1002:LYS:HA	1:A:1048:TRP:O	2.19	0.43
1:A:1291:ILE:C	1:A:1293:THR:N	2.76	0.43
1:A:523:ILE:HG12	1:A:577:TYR:CZ	2.53	0.42
1:A:470:VAL:CG1	1:A:474:LEU:HD12	2.47	0.42
1:A:1270:VAL:HG22	1:A:1279:TYR:HE1	1.83	0.42
1:A:1292:ILE:O	1:A:1293:THR:C	2.62	0.42
1:A:1311:ASN:OD1	1:A:1326:SER:HB3	2.20	0.42
1:A:171:ILE:HG21	1:A:181:TYR:CE1	2.55	0.42
1:A:1077:GLU:OE2	1:A:1079:LYS:HE3	2.19	0.42
1:A:1290:LYS:HB2	1:A:1290:LYS:HE3	1.80	0.42
1:A:1422:ASP:HB2	1:A:1424:ARG:H	1.84	0.42
1:A:1299:LYS:HB3	1:A:1310:ARG:NE	2.28	0.42
1:A:433:VAL:O	1:A:437:GLN:HG2	2.20	0.42
1:A:1027:ILE:H	1:A:1027:ILE:HG13	1.73	0.42
1:A:1261:ASN:HD21	1:A:1265:ILE:HG23	1.85	0.42
1:A:322:ALA:O	1:A:326:VAL:HG13	2.19	0.41
1:A:627:ALA:HB1	1:A:813:LEU:HG	2.03	0.41
1:A:1404:GLN:OE1	1:A:1436:ASN:HB2	2.19	0.41
1:A:173:ASN:C	1:A:175:LYS:H	2.29	0.41
1:A:454:ASP:OD2	1:A:948:LYS:NZ	2.42	0.41
1:A:1291:ILE:O	1:A:1298:LEU:N	2.49	0.41
1:A:583:HIS:N	1:A:863:GLU:OE2	2.47	0.41
1:A:688:ALA:HB2	1:A:835:VAL:HB	2.03	0.41
1:A:1261:ASN:ND2	1:A:1265:ILE:HG23	2.34	0.41
1:A:574:MET:HE2	1:A:574:MET:HB3	1.85	0.41
1:A:794:ARG:NH2	1:A:808:ASP:OD1	2.50	0.41
1:A:970:PRO:HD2	1:A:1003:SER:HA	2.03	0.41
1:A:1016:PHE:O	1:A:1020:LEU:HG	2.21	0.41
1:A:1351:VAL:HG11	1:A:1356:VAL:HG23	2.03	0.41
1:A:527:LEU:HB2	1:A:560:SER:HB2	2.03	0.41
1:A:928:ASP:OD2	1:A:932:SER:OG	2.33	0.40
1:A:699:GLU:HB2	1:A:751:ASN:HD21	1.86	0.40
1:A:702:LYS:O	1:A:703:SER:C	2.62	0.40
1:A:1431:ASP:OD1	1:A:1434:SER:OG	2.39	0.40
1:A:912:PHE:HB3	5:A:1757:HOH:O	2.21	0.40
1:A:929:LEU:O	1:A:931:MET:HG3	2.21	0.40
1:A:1272:THR:HA	1:A:1277:THR:HA	2.02	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	1275/1438 (89%)	1184 (93%)	77 (6%)	14 (1%)	11 7

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	172	PRO
1	A	1259	TYR
1	A	1283	ASP
1	A	1368	ASP
1	A	1322	TYR
1	A	1325	GLY
1	A	1378	GLU
1	A	1450	ARG
1	A	1250	ALA
1	A	1294	ASP
1	A	1344	PHE
1	A	1449	ARG
1	A	1382	ASP
1	A	1451	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	1063/1216 (87%)	1060 (100%)	3 (0%)	86 91

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1290	LYS
1	A	1291	ILE
1	A	1292	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	236	GLN
1	A	316	GLN
1	A	511	GLN
1	A	615	GLN
1	A	766	ASN
1	A	1209	ASN
1	A	1247	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 ⓘ

2 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	12,12,12	0.33	0	17,17,17	1.03	1 (5%)
2	GLC	B	2	2	11,11,12	0.28	0	15,15,17	0.56	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	-	1/2/22/22	0/1/1/1
2	GLC	B	2	2	-	0/2/19/22	0/1/1/1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
2	B	1	GLC	C4-C3-C2	-2.43	106.56	110.83

There are no chirality outliers.

All (1) torsion outliers are listed below:

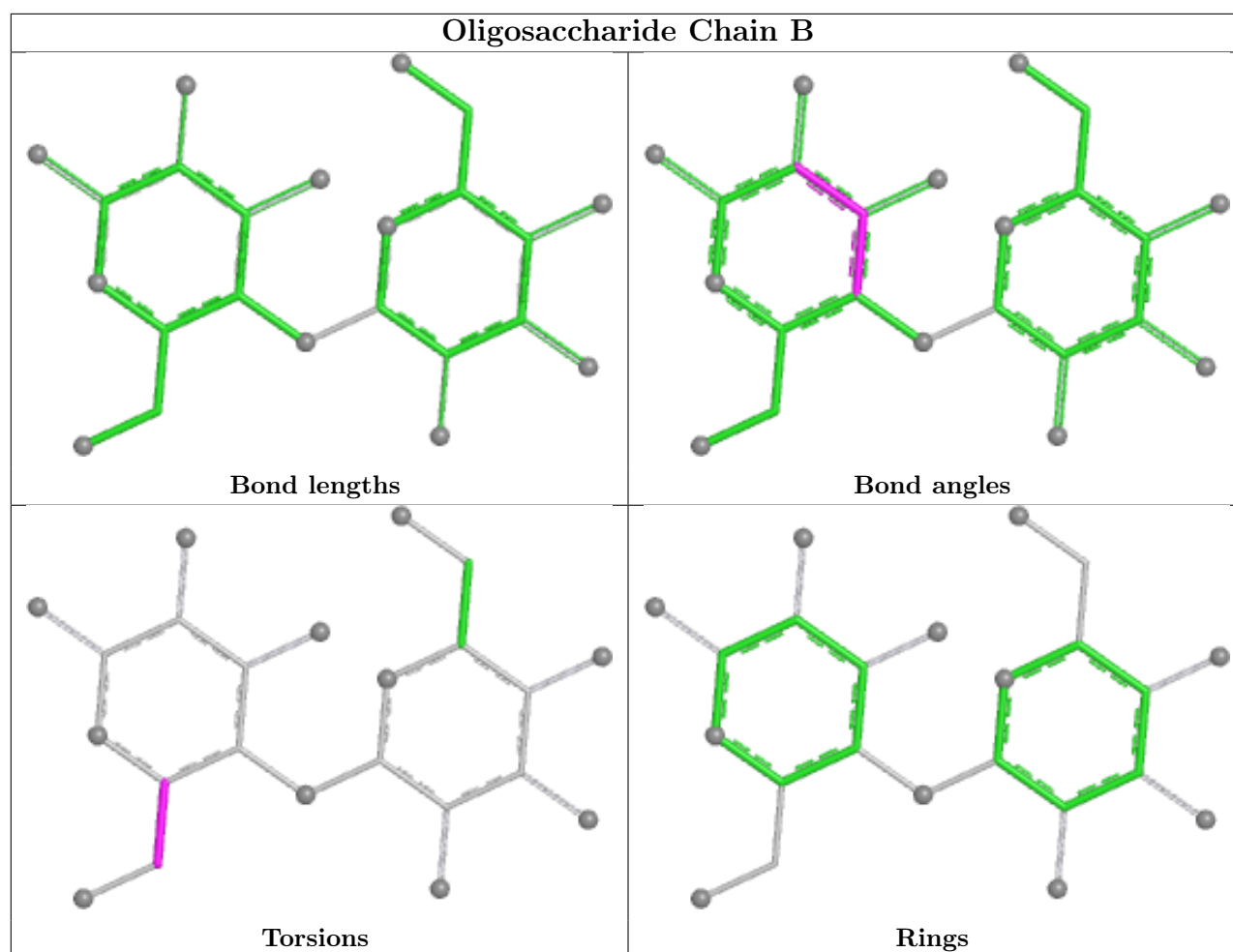
Mol	Chain	Res	Type	Atoms
2	B	1	GLC	O5-C5-C6-O6

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.



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	$\# Z > 2$
4	EDO	A	1502	-	3,3,3	0.43	0	2,2,2	0.34	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	EDO	A	1502	-	-	0/1/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

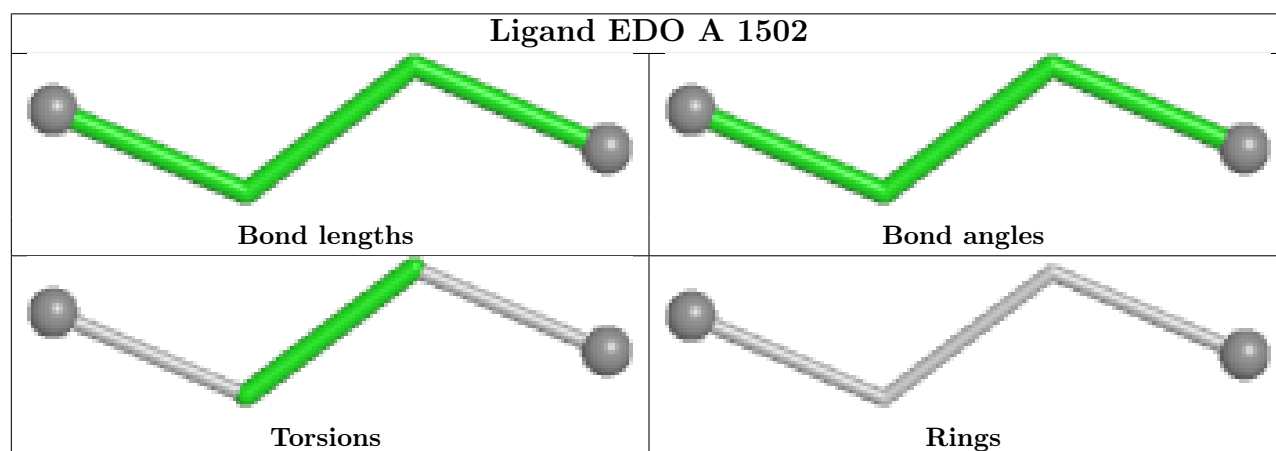
There are no chirality outliers.

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, 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	1285/1438 (89%)	0.57	135 (10%)	11 13	28, 47, 92, 109	0

All (135) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1446	ALA	6.8
1	A	1343	TYR	5.6
1	A	1310	ARG	5.5
1	A	1293	THR	4.9
1	A	1442	VAL	4.5
1	A	1328	GLY	4.4
1	A	1360	GLY	4.3
1	A	1448	GLY	4.3
1	A	1309	ALA	4.3
1	A	168	LEU	4.3
1	A	1363	HIS	4.1
1	A	171	ILE	4.0
1	A	1379	ALA	4.0
1	A	1459	ALA	4.0
1	A	1249	PHE	4.0
1	A	1257	TRP	3.9
1	A	1320	ASN	3.9
1	A	1337	ILE	3.9
1	A	1302	LEU	3.9
1	A	1362	VAL	3.9
1	A	1308	LEU	3.8
1	A	1301	PHE	3.8
1	A	1314	ALA	3.8
1	A	1367	ALA	3.8
1	A	174	VAL	3.8
1	A	1332	THR	3.7
1	A	1453	ILE	3.7

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Mol	Chain	Res	Type	RSRZ
1	A	169	ALA	3.6
1	A	1258	TYR	3.6
1	A	1440	ASN	3.6
1	A	1287	ILE	3.6
1	A	1275	GLY	3.6
1	A	1380	ASP	3.5
1	A	1300	TYR	3.5
1	A	1329	VAL	3.5
1	A	177	ILE	3.5
1	A	1333	GLY	3.5
1	A	1451	ILE	3.5
1	A	1267	LEU	3.5
1	A	1297	LYS	3.5
1	A	1321	TRP	3.4
1	A	1292	ILE	3.4
1	A	1338	ALA	3.4
1	A	1298	LEU	3.4
1	A	172	PRO	3.3
1	A	1342	LEU	3.3
1	A	1232	GLY	3.2
1	A	1339	GLY	3.2
1	A	1269	GLY	3.2
1	A	1445	LEU	3.2
1	A	1268	VAL	3.2
1	A	1401	ILE	3.1
1	A	1345	ALA	3.1
1	A	1444	THR	3.0
1	A	1344	PHE	3.0
1	A	1227	ILE	3.0
1	A	1372	LEU	2.9
1	A	1457	GLY	2.9
1	A	1312	ILE	2.9
1	A	752	GLN	2.9
1	A	1260	LEU	2.9
1	A	1458	ILE	2.8
1	A	1311	ASN	2.8
1	A	1439	TYR	2.8
1	A	1368	ASP	2.8
1	A	1324	PHE	2.8
1	A	1452	GLY	2.8
1	A	1331	VAL	2.8
1	A	179	GLY	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	1325	GLY	2.8
1	A	1364	TYR	2.8
1	A	1396	THR	2.8
1	A	1270	VAL	2.8
1	A	1347	ASP	2.7
1	A	1280	PHE	2.7
1	A	1421	TYR	2.7
1	A	1226	TRP	2.7
1	A	702	LYS	2.7
1	A	1289	GLY	2.7
1	A	1250	ALA	2.6
1	A	1317	SER	2.6
1	A	1322	TYR	2.6
1	A	1349	LYS	2.6
1	A	1285	LYS	2.6
1	A	1283	ASP	2.6
1	A	1438	VAL	2.6
1	A	173	ASN	2.6
1	A	1359	ASN	2.6
1	A	1234	LYS	2.6
1	A	1429	TYR	2.5
1	A	704	HIS	2.5
1	A	1400	ARG	2.5
1	A	1231	ASP	2.5
1	A	184	ILE	2.5
1	A	1290	LYS	2.5
1	A	789	ALA	2.5
1	A	1284	GLY	2.5
1	A	1306	GLY	2.5
1	A	1251	ASN	2.5
1	A	1295	ASN	2.5
1	A	1456	TRP	2.5
1	A	1427	LEU	2.4
1	A	1313	PHE	2.4
1	A	1233	LYS	2.4
1	A	1323	TYR	2.3
1	A	269	THR	2.3
1	A	783	TYR	2.3
1	A	1382	ASP	2.3
1	A	1422	ASP	2.3
1	A	1378	GLU	2.2
1	A	1291	ILE	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	229	ASN	2.2
1	A	792	LEU	2.2
1	A	170	ALA	2.2
1	A	772	LEU	2.2
1	A	440	TRP	2.2
1	A	1288	LYS	2.2
1	A	1255	GLY	2.2
1	A	1282	GLN	2.1
1	A	1449	ARG	2.1
1	A	753	ASN	2.1
1	A	1259	TYR	2.1
1	A	1336	THR	2.1
1	A	1265	ILE	2.1
1	A	1455	ARG	2.1
1	A	1315	THR	2.1
1	A	1358	TYR	2.1
1	A	1419	VAL	2.1
1	A	699	GLU	2.0
1	A	785	SER	2.1
1	A	1245	ALA	2.1
1	A	1248	ARG	2.0
1	A	1253	LYS	2.0
1	A	175	LYS	2.0
1	A	1279	TYR	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.

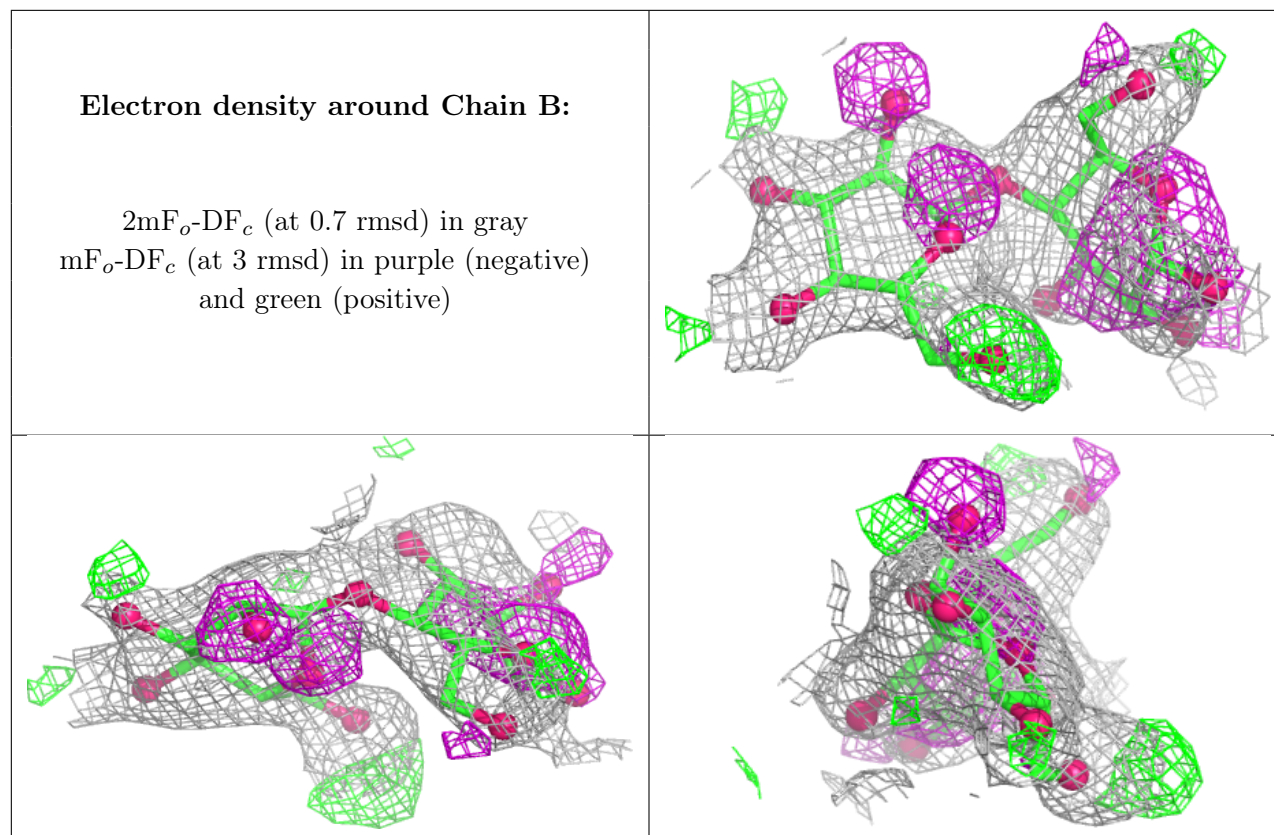
6.3 Carbohydrates [i](#)

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
2	GLC	B	2	11/12	0.47	0.21	52,59,66,66	0
2	GLC	B	1	12/12	0.70	0.17	49,56,62,63	0

The following is a graphical depiction of the model fit to experimental electron density for oligosac-

charide. Each fit is shown from different orientation to approximate a three-dimensional view.



6.4 Ligands [i](#)

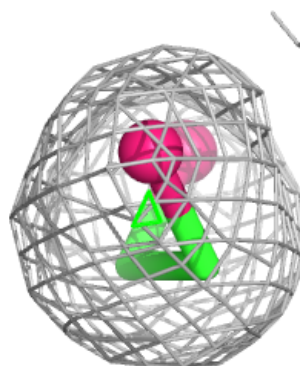
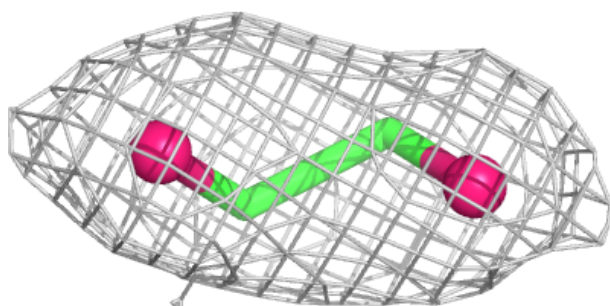
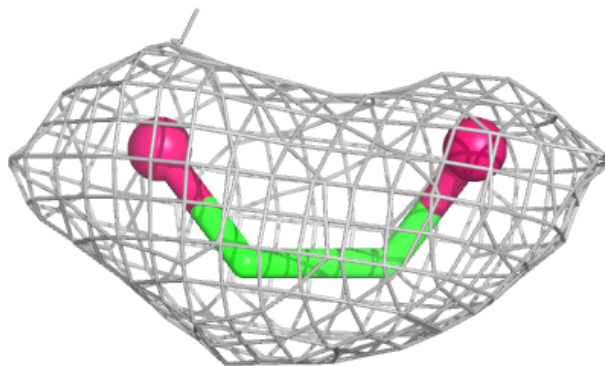
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q < 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	EDO	A	1502	4/4	0.94	0.10	41,44,44,51	0
3	CA	A	1501	1/1	0.98	0.04	38,38,38,38	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.

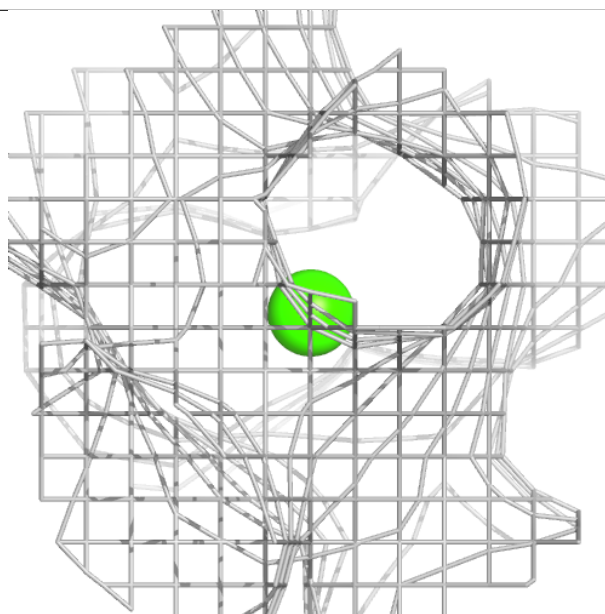
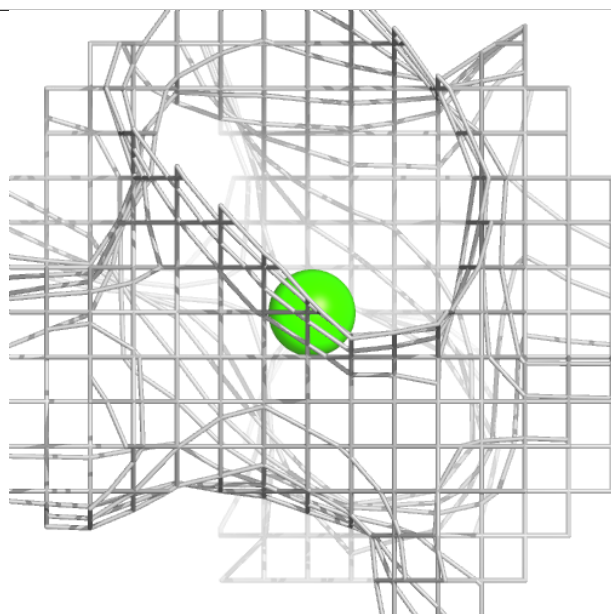
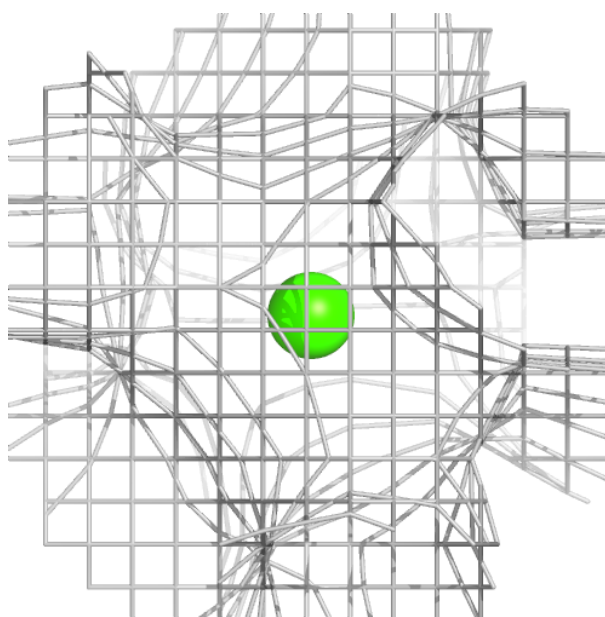
Electron density around EDO A 1502:

$2mF_o-DF_c$ (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 [i](#)

There are no such residues in this entry.