



Full wwPDB X-ray Structure Validation Report ⓘ

Sep 23, 2025 – 01:31 am BST

PDB ID : 9GTL / pdb_00009gtl
Title : Crystal structure of human lysosomal acid-alpha-glucosidase, GAA, in complex with iminosugar compound 4j
Authors : Sulzenbacher, G.; Roig-Zamboni, V.; Moracci, M.; Parenti, G.; Py, S.
Deposited on : 2024-09-18
Resolution : 2.00 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	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
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)	:	2.46

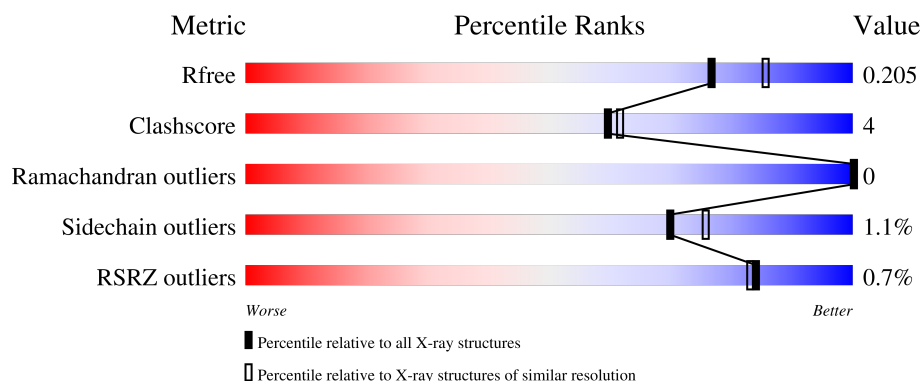
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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}	164625	9409 (2.00-2.00)
Clashscore	180529	10737 (2.00-2.00)
Ramachandran outliers	177936	10628 (2.00-2.00)
Sidechain outliers	177891	10627 (2.00-2.00)
RSRZ outliers	164620	9409 (2.00-2.00)

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	952	<div> <div>80%</div> <div>8%</div> <div>12%</div> </div>
2	B	3	<div> <div>33%</div> <div>67%</div> </div>
3	C	2	<div> <div>50%</div> <div>50%</div> </div>
4	D	4	<div> <div>25%</div> <div>75%</div> </div>
5	E	3	<div> <div>33%</div> <div>67%</div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
12	GOL	A	1018	-	-	X	-

2 Entry composition [i](#)

There are 13 unique types of molecules in this entry. The entry contains 7429 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 Lysosomal alpha-glucosidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	842	Total	C	N	O	S	0	11	0
			6706	4300	1124	1248	34			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	199	ARG	HIS	variant	UNP P10253
A	223	HIS	ARG	variant	UNP P10253
A	780	ILE	VAL	variant	UNP P10253

- Molecule 2 is an oligosaccharide called beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



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

- Molecule 3 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



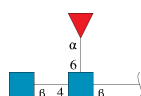
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	C	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 4 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



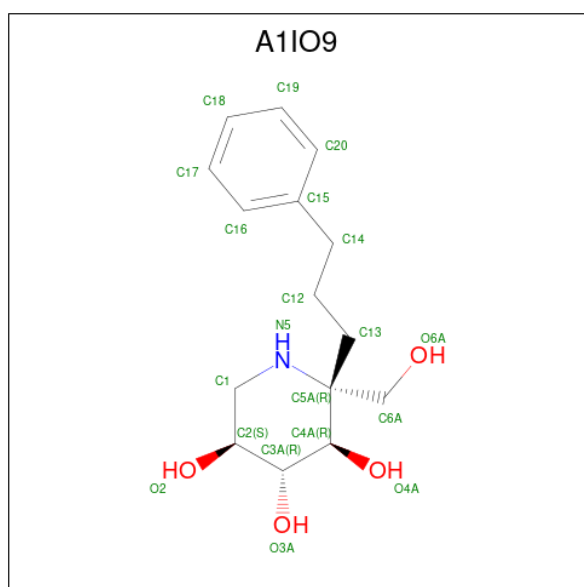
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	D	4	Total	C	N	O	0	0	0
			50	28	2	20			

- Molecule 5 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	E	3	Total	C	N	O	0	0	0
			38	22	2	14			

- Molecule 6 is (2 {R},3 {R},4 {R},5 {S})-2-(hydroxymethyl)-2-(3-phenylpropyl)piperidine-3,4,5-triol (CCD ID: A1IO9) (formula: C₁₅H₂₃NO₄).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	1	Total	C	N	O	0	0
			20	15	1	4		

- Molecule 7 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	O	S	0	0
			5	4	1		
7	A	1	Total	O	S	0	0
			5	4	1		
7	A	1	Total	O	S	0	0
			5	4	1		

- Molecule 8 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

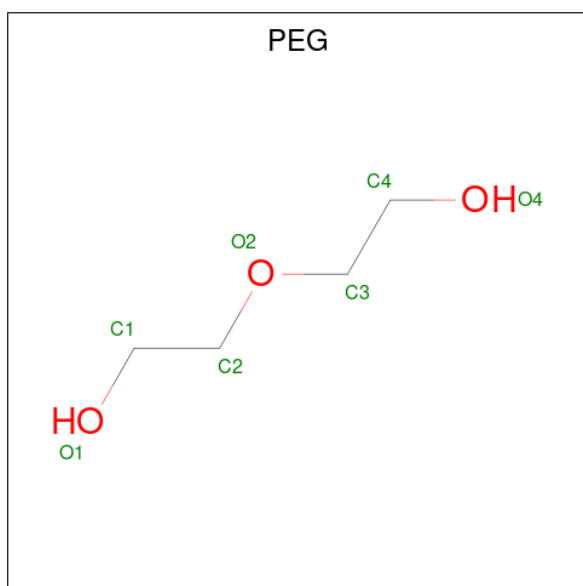
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	7	Total	Cl	0	0
			7	7		

- Molecule 9 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



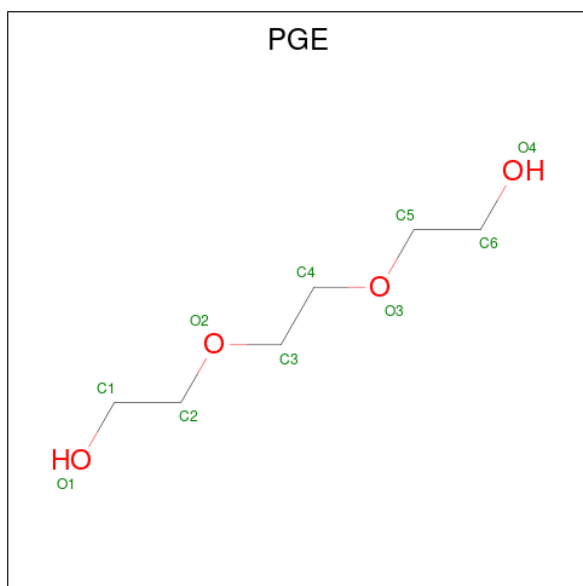
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	A	1	Total	C	O	0	0
			4	2	2		
9	A	1	Total	C	O	0	0
			4	2	2		
9	A	1	Total	C	O	0	0
			4	2	2		

- Molecule 10 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: $C_4H_{10}O_3$) (labeled as "Ligand of Interest" by depositor).



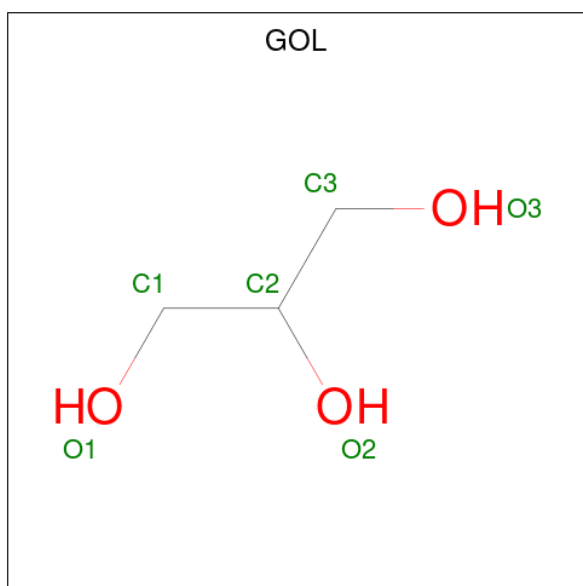
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
10	A	1	Total	C	O	0	0
			7	4	3		

- Molecule 11 is TRIETHYLENE GLYCOL (CCD ID: PGE) (formula: $C_6H_{14}O_4$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
11	A	1	Total	C	O	0	0
			10	6	4		

- Molecule 12 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



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

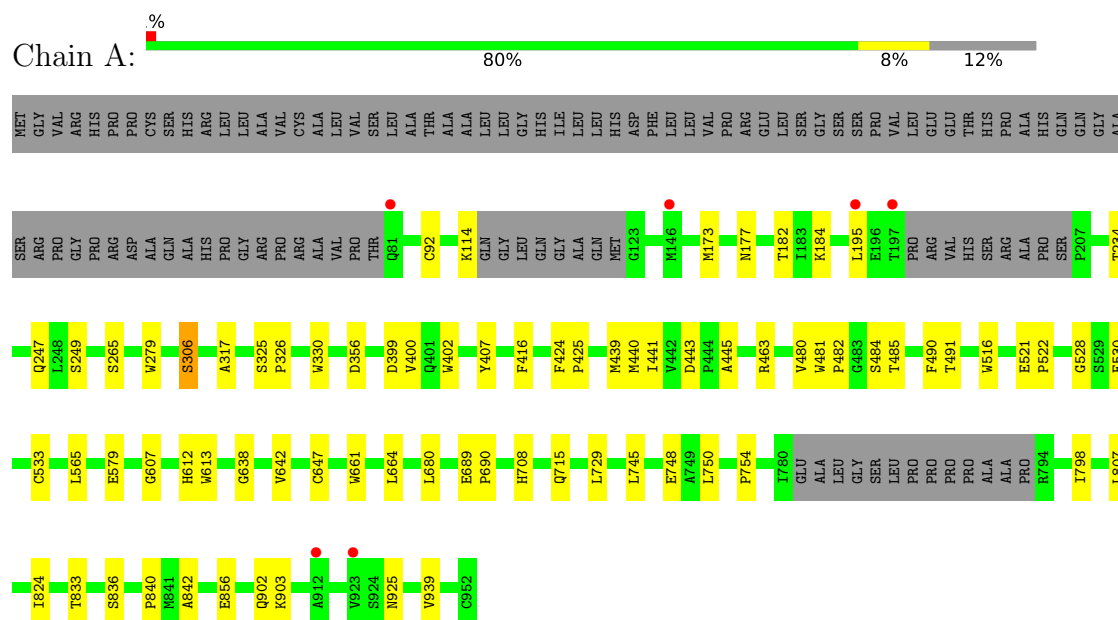
- Molecule 13 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
13	A	485	Total 485	O 485	0	0

3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: Lysosomal alpha-glucosidase



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



- Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 4: alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain D:  25% 75%

MAG1
MAG2
BGA3
MAN4

- Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain E:  33% 67%

MAG1
MAG2
FUC3

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	94.31Å 102.67Å 126.81Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.20 – 2.00 47.20 – 2.00	Depositor EDS
% Data completeness (in resolution range)	100.0 (47.20-2.00) 100.0 (47.20-2.00)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.57 (at 2.00Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.168 , 0.200 0.175 , 0.205	Depositor DCC
R_{free} test set	4183 reflections (2.71%)	wwPDB-VP
Wilson B-factor (Å ²)	36.9	Xtriage
Anisotropy	0.420	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 44.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	7429	wwPDB-VP
Average B, all atoms (Å ²)	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.75% 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: BMA, PEG, PGE, GOL, CSO, MAN, CL, NAG, FUC, SO4, EDO, A1IO9

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	0.97	0/6908	1.16	0/9435

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	748	GLU	Peptide

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	6706	0	6471	55	0
2	B	39	0	34	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	28	0	25	0	0
4	D	50	0	43	0	0
5	E	38	0	34	2	0
6	A	20	0	0	0	0
7	A	15	0	0	0	0
8	A	7	0	0	1	0
9	A	12	0	18	0	0
10	A	7	0	10	1	0
11	A	10	0	14	4	0
12	A	12	0	16	5	0
13	A	485	0	0	7	0
All	All	7429	0	6665	57	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 4.

All (57) 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:182:THR:HG21	11:A:1016:PGE:H5	1.71	0.72
1:A:840:PRO:HB3	1:A:902[B]:GLN:CG	2.22	0.68
1:A:463:ARG:HH22	12:A:1018:GOL:H12	1.59	0.68
1:A:840:PRO:HB3	1:A:902[B]:GLN:HG3	1.78	0.66
1:A:184:LYS:NZ	11:A:1016:PGE:H12	2.14	0.63
1:A:195:LEU:HD13	13:A:1498:HOH:O	1.99	0.62
1:A:925:ASN:HA	13:A:1407:HOH:O	1.99	0.62
1:A:325:SER:N	1:A:326:PRO:HA	2.14	0.62
1:A:177[A]:ASN:OD1	13:A:1101:HOH:O	2.16	0.61
1:A:306:SER:HB2	13:A:1169:HOH:O	2.02	0.59
1:A:521:GLU:N	1:A:522:PRO:HA	2.17	0.58
1:A:833:THR:HA	1:A:836:SER:OG	2.03	0.58
1:A:114:LYS:HE2	8:A:1007:CL:CL	2.40	0.58
1:A:715:GLN:NE2	1:A:856:GLU:OE1	2.33	0.57
13:A:1482:HOH:O	5:E:1:NAG:O7	2.17	0.56
1:A:114:LYS:C	12:A:1017:GOL:H31	2.33	0.54
1:A:840:PRO:HB3	1:A:902[B]:GLN:HG2	1.88	0.54
1:A:279:TRP:CE3	1:A:317:ALA:HB2	2.42	0.54
1:A:92:CYS:O	1:A:92:CYS:SG	2.67	0.52
1:A:400:VAL:HG11	1:A:439[B]:MET:HG3	1.92	0.52
1:A:840:PRO:CB	1:A:902[B]:GLN:HG3	2.39	0.51
1:A:833:THR:HA	1:A:836:SER:HG	1.75	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:463:ARG:HH22	12:A:1018:GOL:C1	2.24	0.50
1:A:481:TRP:N	1:A:482:PRO:HD2	2.27	0.50
1:A:445:ALA:HB1	1:A:485:THR:HB	1.95	0.49
1:A:689:GLU:HB3	1:A:690:PRO:HD3	1.95	0.48
1:A:234:THR:HA	1:A:249:SER:O	2.14	0.48
1:A:424:PHE:HB3	1:A:425:PRO:HD3	1.97	0.47
1:A:708:HIS:CE1	1:A:824:ILE:HD12	2.50	0.47
1:A:607:GLY:HA3	1:A:638:GLY:O	2.15	0.47
1:A:612:HIS:O	1:A:642:VAL:HA	2.15	0.47
1:A:443:ASP:HB3	13:A:1500:HOH:O	2.15	0.46
1:A:680:LEU:HD21	5:E:3:FUC:H5	1.96	0.46
1:A:484:SER:OG	1:A:530:GLU:OE2	2.28	0.46
1:A:491:THR:HB	1:A:565:LEU:HG	1.98	0.46
1:A:463:ARG:NH1	12:A:1018:GOL:H32	2.31	0.45
1:A:400:VAL:CG1	1:A:439[B]:MET:HG3	2.47	0.45
1:A:664:LEU:HD13	1:A:754:PRO:HG3	1.98	0.45
1:A:798:ILE:HD11	1:A:807:LEU:CD2	2.47	0.45
1:A:647:CYS:H	1:A:661:TRP:CG	2.35	0.45
1:A:184:LYS:HZ2	11:A:1016:PGE:H12	1.80	0.44
1:A:445:ALA:HB1	1:A:485:THR:CB	2.48	0.43
1:A:745:LEU:HA	1:A:750:LEU:O	2.18	0.43
1:A:356[B]:ASP:OD2	13:A:1102:HOH:O	2.22	0.43
1:A:247:GLN:HA	1:A:330:TRP:O	2.19	0.42
1:A:463:ARG:HH12	12:A:1018:GOL:H12	1.84	0.42
1:A:481:TRP:N	1:A:482:PRO:CD	2.83	0.42
10:A:1014:PEG:H41	10:A:1014:PEG:H22	1.87	0.42
1:A:902[A]:GLN:HA	1:A:939:VAL:O	2.19	0.42
1:A:689:GLU:N	1:A:690:PRO:CD	2.84	0.41
1:A:528:GLY:HA3	1:A:533:CYS:SG	2.60	0.41
1:A:441:ILE:HB	1:A:516:TRP:CE3	2.55	0.41
1:A:184:LYS:HZ3	11:A:1016:PGE:H12	1.84	0.41
1:A:842:ALA:HA	1:A:903:LYS:O	2.20	0.41
1:A:407:TYR:O	1:A:416:PHE:HA	2.21	0.40
1:A:490:PHE:CZ	1:A:579:GLU:HG3	2.57	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	844/952 (89%)	819 (97%)	25 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	730/805 (91%)	722 (99%)	8 (1%)	70	76

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	173	MET
1	A	265	SER
1	A	306	SER
1	A	399	ASP
1	A	440	MET
1	A	480	VAL
1	A	613	TRP
1	A	729	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	188	ASN
1	A	352	GLN
1	A	401	GLN
1	A	540	ASN
1	A	742	HIS
1	A	900	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

1 non-standard protein/DNA/RNA residue 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	$\# Z > 2$
1	CSO	A	938	1	3,6,7	0.54	0	0,6,8	-	-

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
1	CSO	A	938	1	-	0/1/5/7	-

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.

5.5 Carbohydrates ⓘ

12 monosaccharides are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
2	NAG	B	1	1,2	14,14,15	0.41	0	17,19,21	0.92	1 (5%)
2	NAG	B	2	2	14,14,15	0.43	0	17,19,21	1.14	2 (11%)
2	BMA	B	3	2	11,11,12	0.43	0	15,15,17	0.83	0
3	NAG	C	1	1,3	14,14,15	0.58	0	17,19,21	0.99	0
3	NAG	C	2	3	14,14,15	0.69	1 (7%)	17,19,21	1.08	1 (5%)
4	NAG	D	1	1,4	14,14,15	0.61	0	17,19,21	0.90	0
4	NAG	D	2	4	14,14,15	0.42	0	17,19,21	1.04	1 (5%)
4	BMA	D	3	4	11,11,12	0.39	0	15,15,17	1.07	1 (6%)
4	MAN	D	4	4	11,11,12	0.38	0	15,15,17	1.04	1 (6%)
5	NAG	E	1	1,5	14,14,15	0.54	0	17,19,21	1.24	1 (5%)
5	NAG	E	2	5	14,14,15	0.57	0	17,19,21	1.57	4 (23%)
5	FUC	E	3	5	10,10,11	0.58	0	14,14,16	1.01	1 (7%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	B	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	B	2	2	-	0/6/23/26	0/1/1/1
2	BMA	B	3	2	-	0/2/19/22	0/1/1/1
3	NAG	C	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	C	2	3	-	0/6/23/26	0/1/1/1
4	NAG	D	1	1,4	-	0/6/23/26	0/1/1/1
4	NAG	D	2	4	-	0/6/23/26	0/1/1/1
4	BMA	D	3	4	-	0/2/19/22	0/1/1/1
4	MAN	D	4	4	-	1/2/19/22	0/1/1/1
5	NAG	E	1	1,5	-	0/6/23/26	0/1/1/1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	E	2	5	-	0/6/23/26	0/1/1/1
5	FUC	E	3	5	-	-	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	2	NAG	C1-C2	2.04	1.55	1.52

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	E	2	NAG	C4-C3-C2	-3.65	105.67	111.02
5	E	1	NAG	O5-C5-C6	3.33	112.42	107.20
3	C	2	NAG	C4-C3-C2	3.04	115.48	111.02
5	E	2	NAG	C1-O5-C5	3.00	116.25	112.19
4	D	3	BMA	O5-C5-C6	2.93	111.79	107.20
5	E	2	NAG	C1-C2-N2	2.74	115.17	110.49
2	B	2	NAG	C4-C3-C2	2.46	114.63	111.02
4	D	2	NAG	C1-O5-C5	2.38	115.41	112.19
2	B	2	NAG	O5-C5-C4	-2.27	105.31	110.83
2	B	1	NAG	O4-C4-C3	-2.20	105.26	110.35
5	E	2	NAG	O5-C1-C2	-2.20	107.81	111.29
5	E	3	FUC	O5-C5-C4	2.16	113.39	109.52
4	D	4	MAN	C3-C4-C5	2.04	113.87	110.24

There are no chirality outliers.

All (1) torsion outliers are listed below:

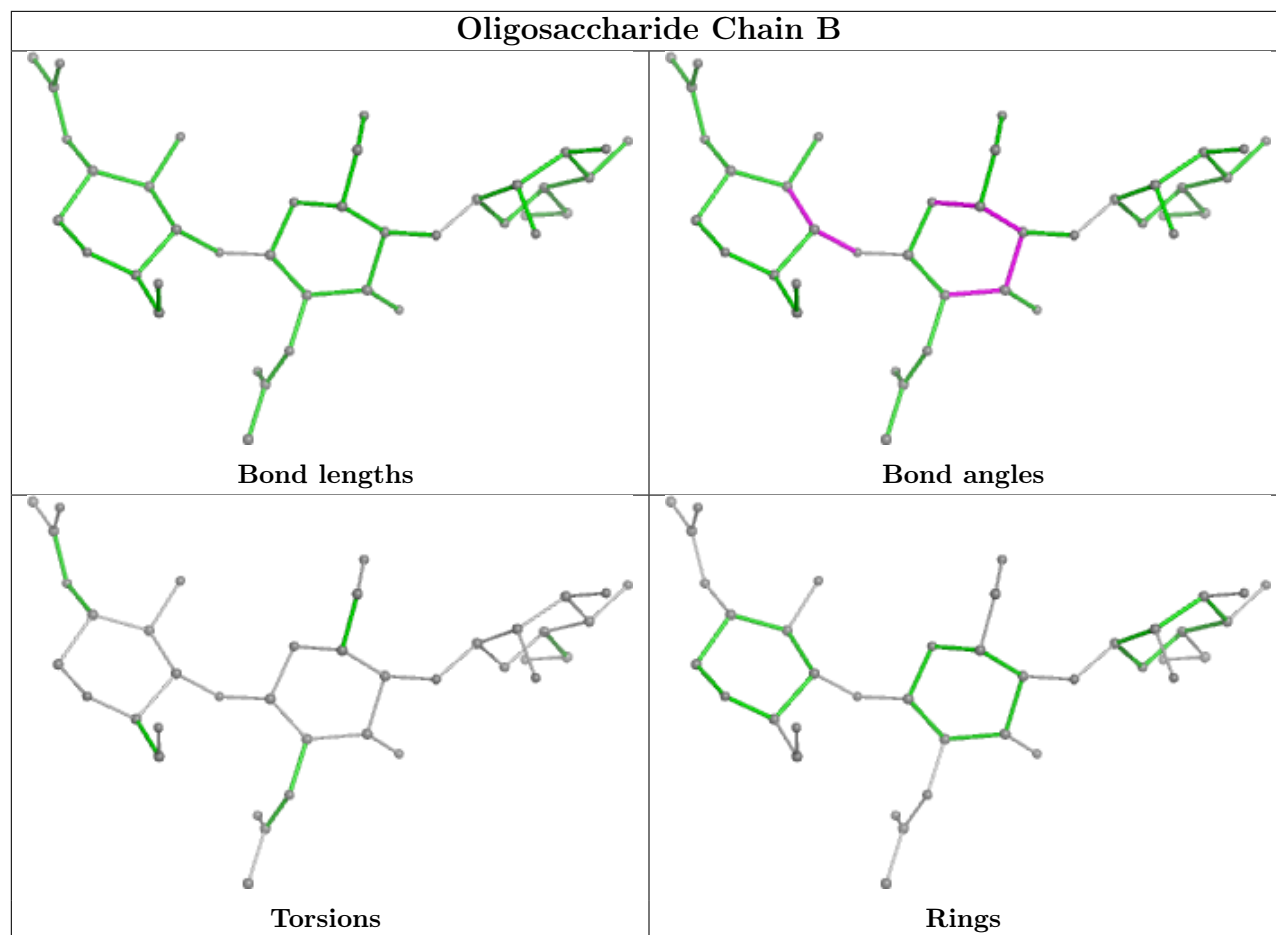
Mol	Chain	Res	Type	Atoms
4	D	4	MAN	O5-C5-C6-O6

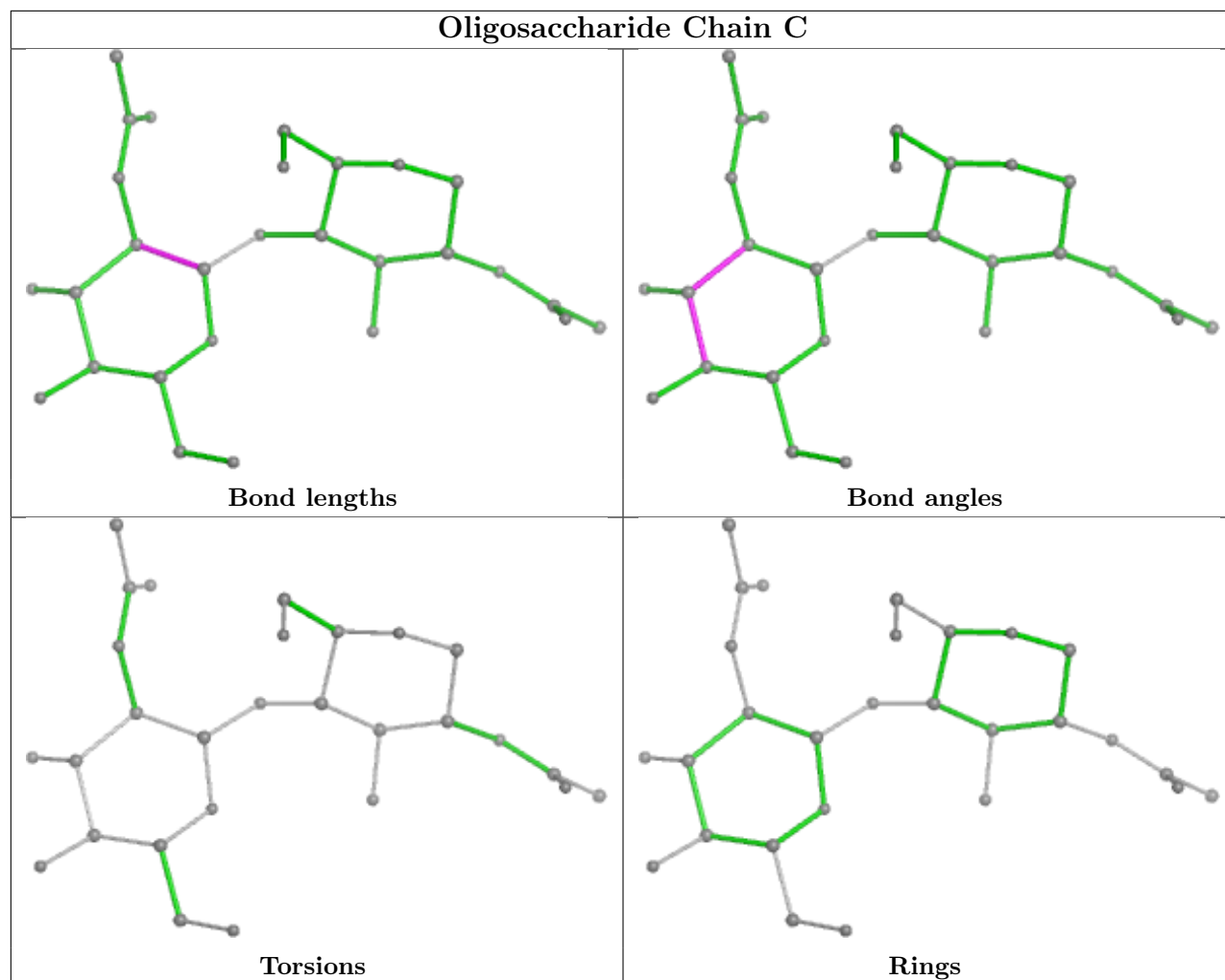
There are no ring outliers.

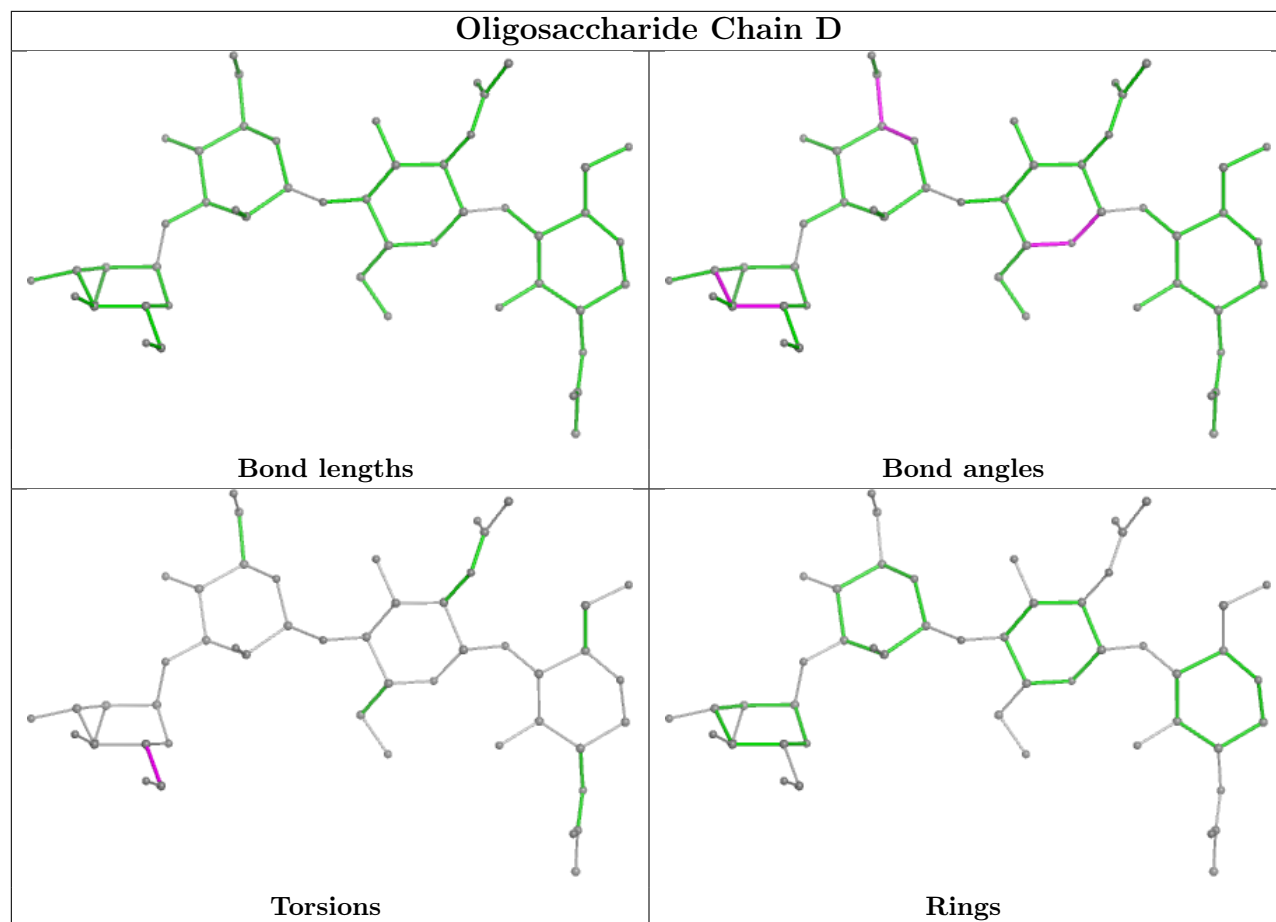
2 monomers are involved in 2 short contacts:

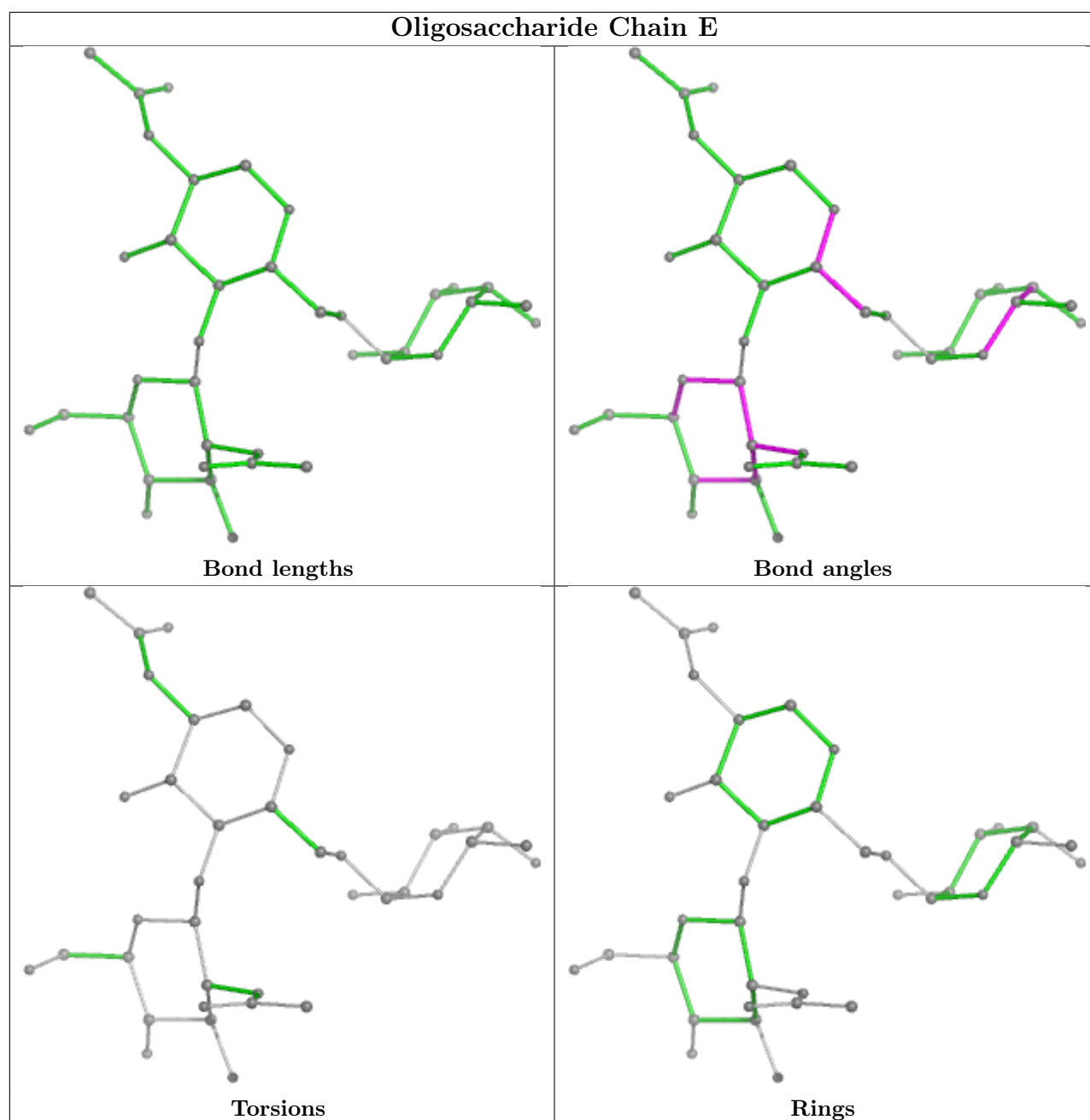
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	E	3	FUC	1	0
5	E	1	NAG	1	0

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 18 ligands modelled in this entry, 7 are monoatomic - leaving 11 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
12	GOL	A	1017	-	5,5,5	0.13	0	5,5,5	0.31	0
12	GOL	A	1018	-	5,5,5	0.23	0	5,5,5	0.44	0
7	SO4	A	1003	-	4,4,4	0.28	0	6,6,6	0.09	0
10	PEG	A	1014	-	6,6,6	0.43	0	5,5,5	0.16	0
9	EDO	A	1013	-	3,3,3	0.09	0	2,2,2	0.15	0
7	SO4	A	1004	-	4,4,4	0.38	0	6,6,6	0.07	0
6	A1IO9	A	1001	-	17,21,21	0.66	0	23,29,29	0.70	0
9	EDO	A	1012	-	3,3,3	0.14	0	2,2,2	0.33	0
11	PGE	A	1016	-	9,9,9	0.50	0	8,8,8	0.24	0
9	EDO	A	1015	-	3,3,3	0.11	0	2,2,2	0.04	0
7	SO4	A	1002	-	4,4,4	0.32	0	6,6,6	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
12	GOL	A	1017	-	-	0/4/4/4	-
12	GOL	A	1018	-	-	1/4/4/4	-
10	PEG	A	1014	-	-	1/4/4/4	-
9	EDO	A	1013	-	-	0/1/1/1	-
6	A1IO9	A	1001	-	-	0/10/30/30	0/2/2/2
9	EDO	A	1012	-	-	1/1/1/1	-
11	PGE	A	1016	-	-	2/7/7/7	-
9	EDO	A	1015	-	-	1/1/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (6) torsion outliers are listed below:

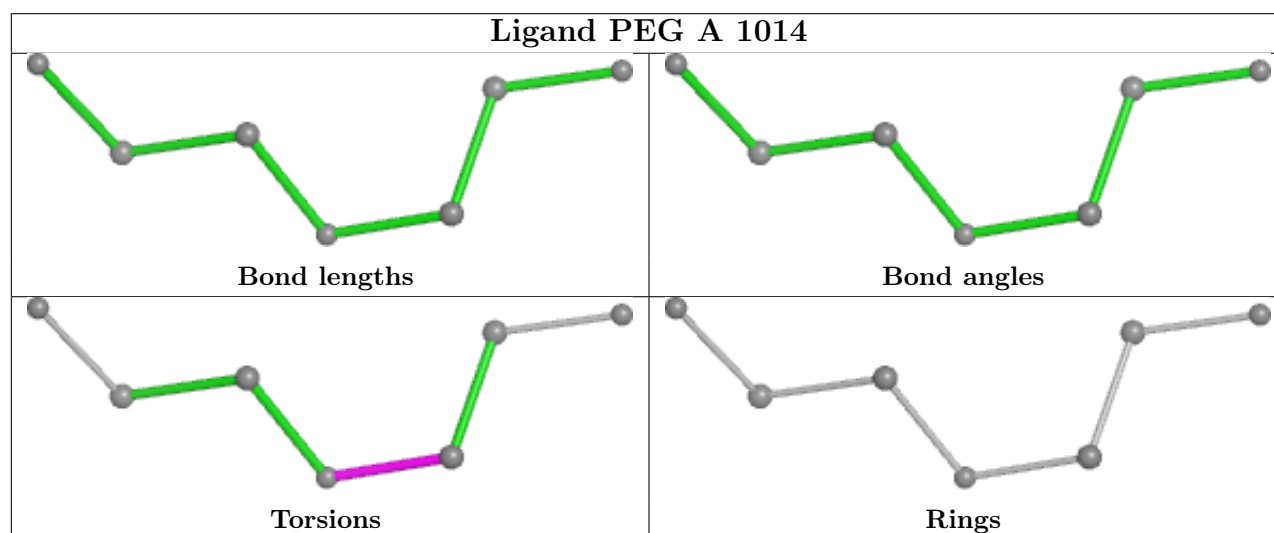
Mol	Chain	Res	Type	Atoms
10	A	1014	PEG	C4-C3-O2-C2
9	A	1012	EDO	O1-C1-C2-O2
11	A	1016	PGE	O1-C1-C2-O2
12	A	1018	GOL	O2-C2-C3-O3
9	A	1015	EDO	O1-C1-C2-O2
11	A	1016	PGE	O3-C5-C6-O4

There are no ring outliers.

4 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
12	A	1017	GOL	1	0
12	A	1018	GOL	4	0
10	A	1014	PEG	1	0
11	A	1016	PGE	4	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 [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, 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	841/952 (88%)	-0.21	6 (0%) 84 83	16, 40, 62, 111	11 (1%)

All (6) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	195	LEU	4.4
1	A	197	THR	3.2
1	A	146	MET	3.1
1	A	81	GLN	2.8
1	A	923	VAL	2.3
1	A	912	ALA	2.2

6.2 Non-standard residues in protein, DNA, RNA chains [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.

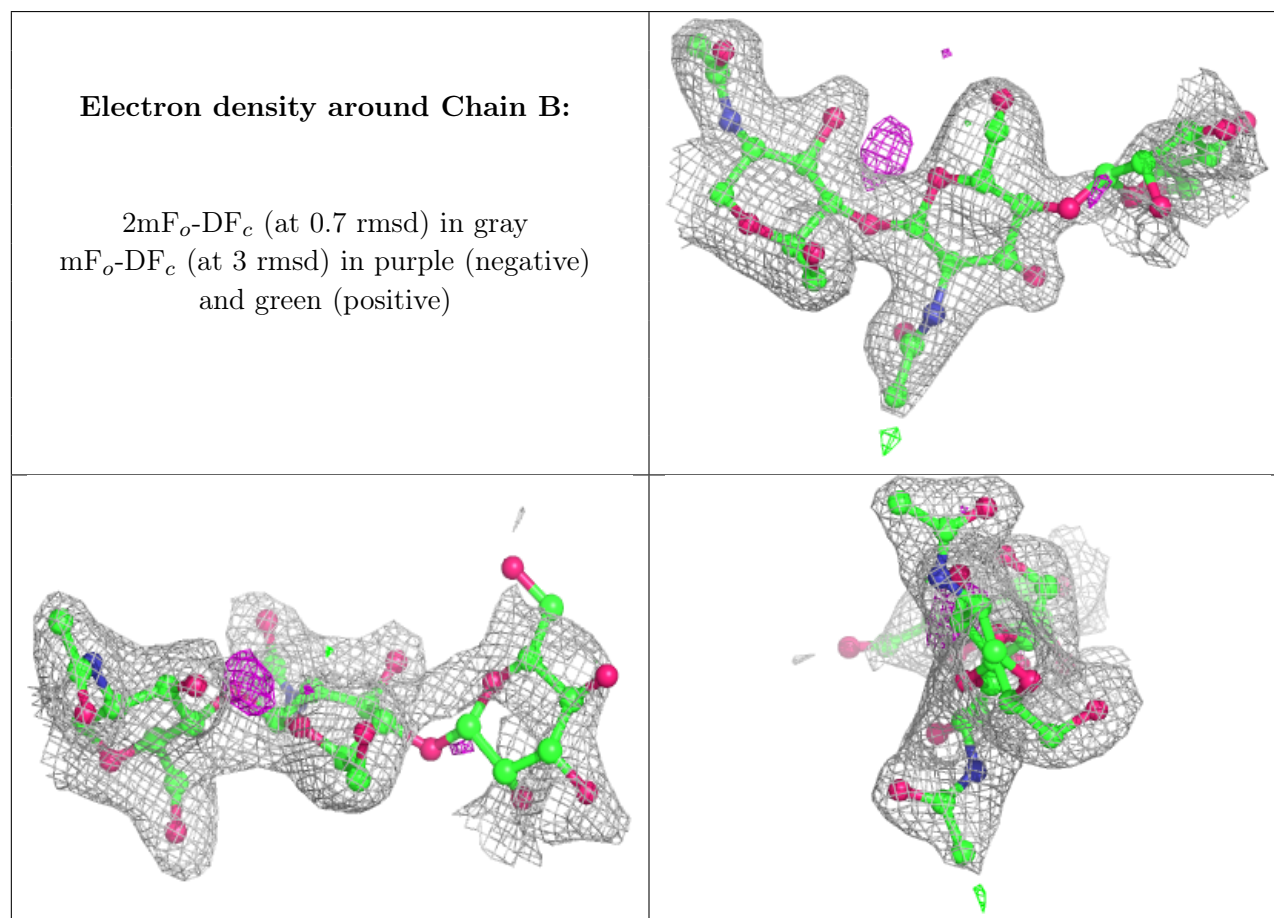
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
1	CSO	A	938	7/8	0.94	0.09	45,46,55,59	0

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.

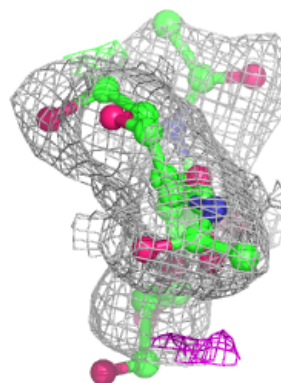
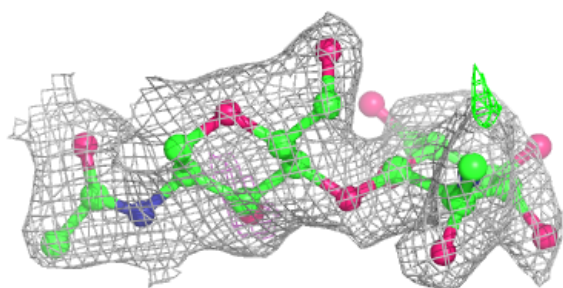
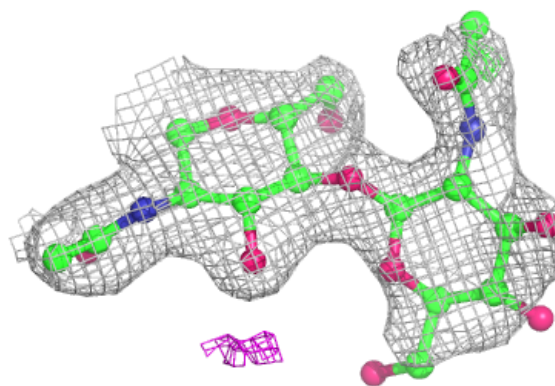
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	BMA	B	3	11/12	0.50	0.13	103,119,133,135	0
4	MAN	D	4	11/12	0.54	0.13	89,105,116,119	0
5	NAG	E	2	14/15	0.61	0.13	88,122,131,131	0
3	NAG	C	2	14/15	0.63	0.12	79,100,103,107	0
2	NAG	B	2	14/15	0.75	0.14	66,78,95,127	0
5	FUC	E	3	10/11	0.77	0.13	87,94,98,116	0
4	BMA	D	3	11/12	0.85	0.10	55,84,96,100	0
5	NAG	E	1	14/15	0.87	0.11	60,75,89,101	0
4	NAG	D	2	14/15	0.91	0.09	46,50,57,62	0
3	NAG	C	1	14/15	0.93	0.07	42,52,67,82	0
2	NAG	B	1	14/15	0.93	0.08	43,48,54,63	0
4	NAG	D	1	14/15	0.96	0.06	39,42,47,50	0

The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

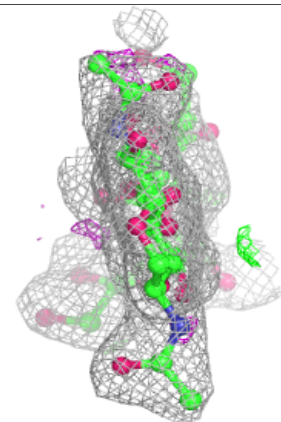
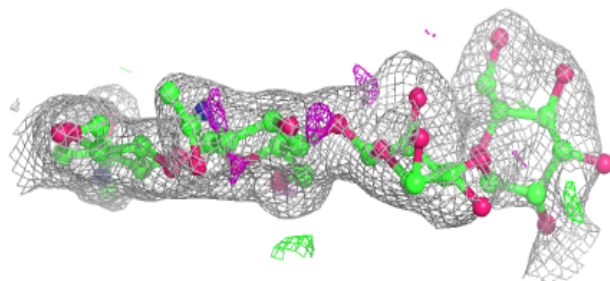
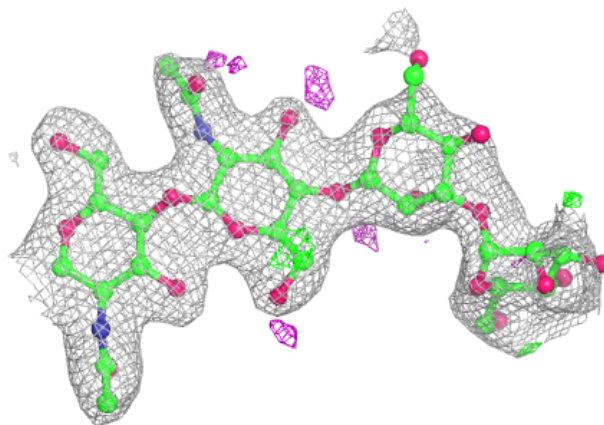


Electron density around Chain C:

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

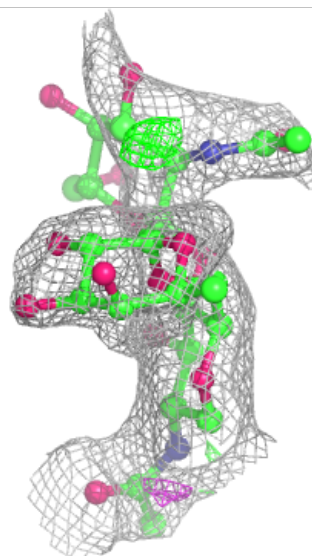
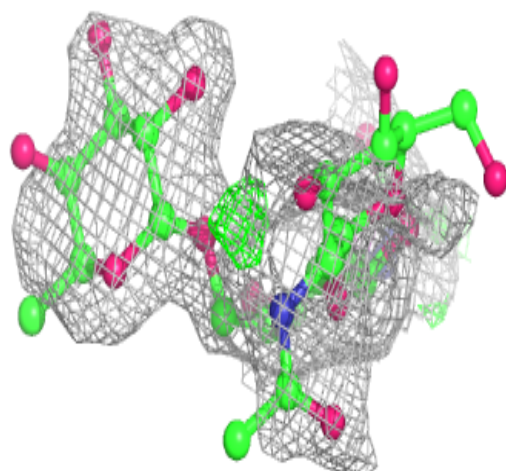
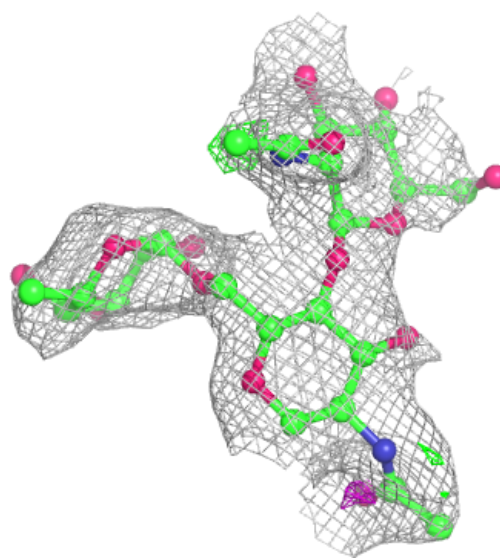
**Electron density around Chain D:**

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



Electron density around Chain E:

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** [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
7	SO4	A	1004	5/5	0.77	0.18	49,50,51,54	5
12	GOL	A	1018	6/6	0.78	0.14	50,56,63,65	0
12	GOL	A	1017	6/6	0.81	0.14	53,59,62,64	0

Continued on next page...

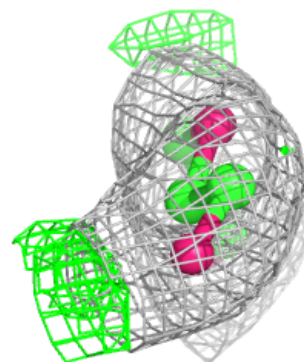
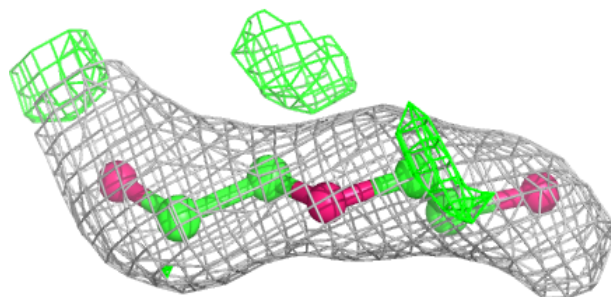
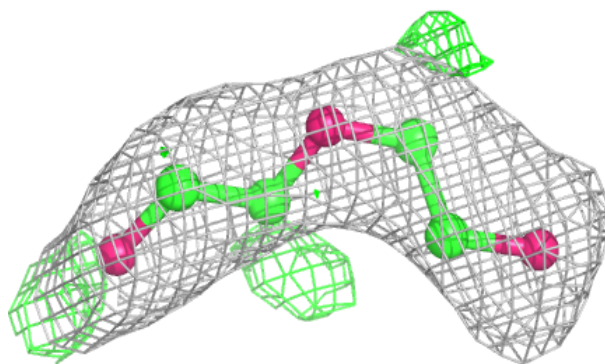
Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
10	PEG	A	1014	7/7	0.83	0.15	47,55,61,63	0
9	EDO	A	1013	4/4	0.86	0.22	45,48,50,51	4
11	PGE	A	1016	10/10	0.87	0.15	45,57,63,64	0
8	CL	A	1008	1/1	0.88	0.14	80,80,80,80	0
8	CL	A	1007	1/1	0.90	0.13	74,74,74,74	0
9	EDO	A	1015	4/4	0.91	0.10	50,50,56,60	0
8	CL	A	1005	1/1	0.93	0.13	81,81,81,81	0
8	CL	A	1006	1/1	0.93	0.13	74,74,74,74	0
8	CL	A	1009	1/1	0.94	0.10	82,82,82,82	0
8	CL	A	1010	1/1	0.94	0.10	76,76,76,76	0
9	EDO	A	1012	4/4	0.94	0.09	47,47,48,51	0
7	SO4	A	1003	5/5	0.95	0.07	58,59,69,71	0
7	SO4	A	1002	5/5	0.96	0.07	40,41,46,47	5
8	CL	A	1011	1/1	0.97	0.06	59,59,59,59	0
6	A1IO9	A	1001	20/20	0.97	0.07	30,34,49,50	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 PEG A 1014:

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.