



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 08:40 AM UTC

PDB ID : 8CB6 / pdb_00008cb6
Title : Crystal structure of human lysosomal acid-alpha-glucosidase, GAA, in covalent complex with TAMRA tagged 1,6-Epi-cylcophellitol aziridine activity based probe
Authors : Sulzenbacher, G.; Roig-Zamboni, V.; Overkleeft, H.; Artola, M.
Deposited on : 2023-01-25
Resolution : 1.90 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

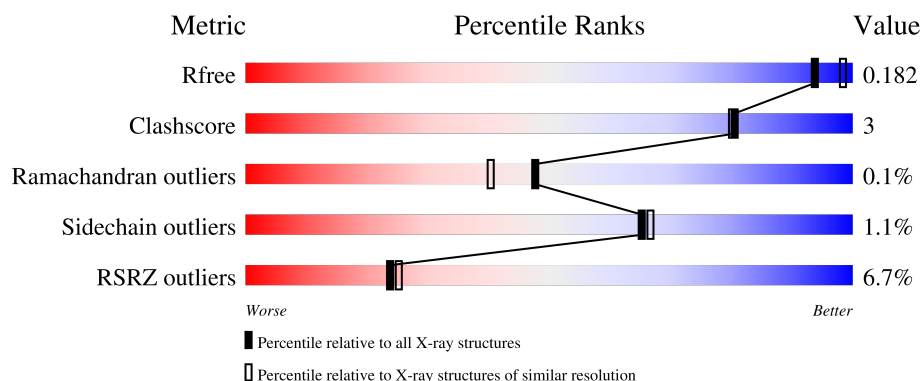
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 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	7789 (1.90-1.90)
Clashscore	190562	8410 (1.90-1.90)
Ramachandran outliers	187476	8333 (1.90-1.90)
Sidechain outliers	187428	8333 (1.90-1.90)
RSRZ outliers	180081	7790 (1.90-1.90)

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	F	123	18% 87% 11%
2	A	749	5% 92% 7%
3	B	3	67% 33%
4	C	2	50% 50%

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Mol	Chain	Length	Quality of chain
4	D	2	 100%
5	E	3	 33% 67%

2 Entry composition

There are 13 unique types of molecules in this entry. The entry contains 7632 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 (76 kDa).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	F	110	Total	C	N	O	S	0	6	0
			914	579	150	174	11			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	199	ARG	HIS	conflict	UNP P10253

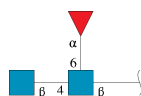
- Molecule 2 is a protein called Lysosomal alpha-glucosidase (70 kDa).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	A	741	Total	C	N	O	S	0	4	0
			5825	3746	978	1078	23			

There are 2 discrepancies between the modelled and reference sequences:

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

- Molecule 3 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.



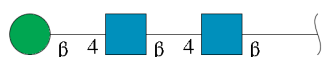
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	B	3	Total	C	N	O	0	0	0
			38	22	2	14			

- Molecule 4 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
4	C	2	Total	C	N	O	0	0	0
			28	16	2	10			
4	D	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 5 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
5	E	3	Total	C	N	O	0	0	0
			39	22	2	15			

- Molecule 6 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	F	3	Total	Cl	0	0
			3	3		
6	A	7	Total	Cl	0	0
			7	7		

- Molecule 7 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



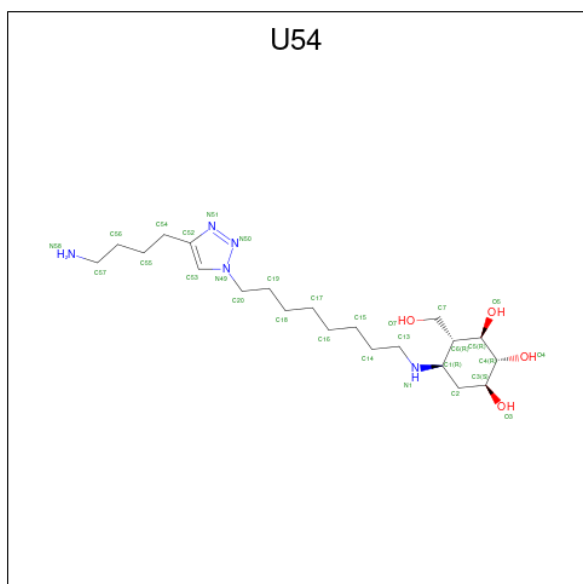
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	F	1	Total	C	O	0	0
			4	2	2		
7	F	1	Total	C	O	0	0
			4	2	2		
7	F	1	Total	C	O	0	0
			4	2	2		
7	A	1	Total	C	O	0	0
			4	2	2		
7	A	1	Total	C	O	0	0
			4	2	2		
7	A	1	Total	C	O	0	0
			4	2	2		
7	A	1	Total	C	O	0	0
			4	2	2		
7	A	1	Total	C	O	0	0
			4	2	2		

- Molecule 8 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



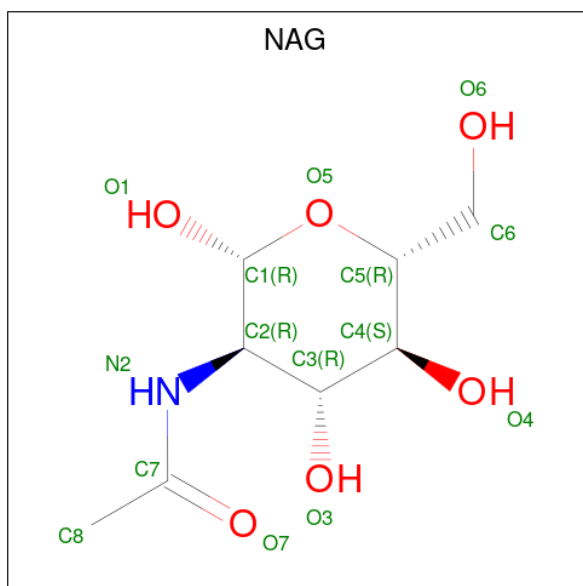
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	F	1	Total	C	O	0	0
			6	3	3		
8	A	1	Total	C	O	0	0
			6	3	3		
8	A	1	Total	C	O	0	0
			6	3	3		
8	A	1	Total	C	O	0	0
			6	3	3		

- Molecule 9 is (1S,2R,3R,4R,5R)-5-[8-[4-(4-azanylbtyl)-1,2,3-triazol-1-yl]octylamino]-4-(hydroxymethyl)cyclohexane-1,2,3-triol (CCD ID: U54) (formula: C₂₁H₄₁N₅O₄) (labeled as "Ligand of Interest" by depositor).



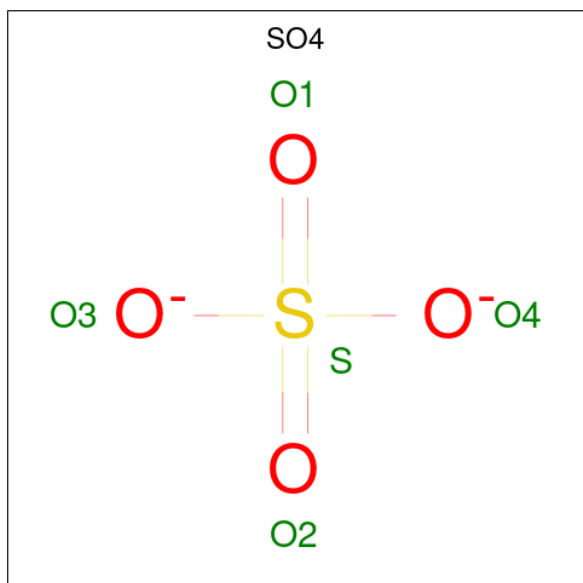
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
9	A	1	Total	C	N	O	0	0
			30	21	5	4		

- Molecule 10 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).



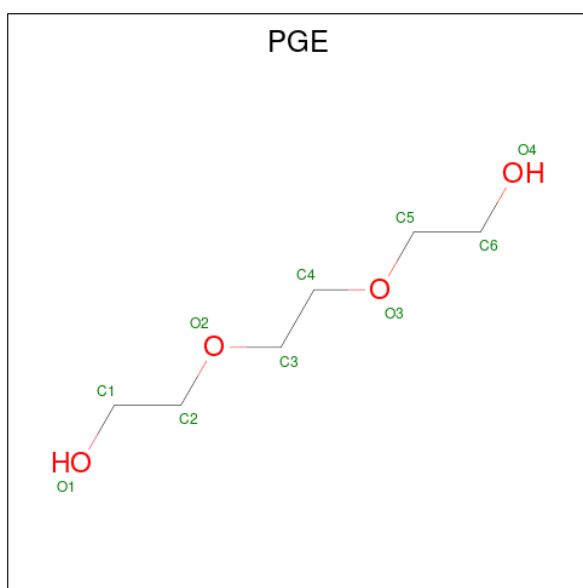
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
10	A	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 11 is SULFATE ION (CCD ID: SO4) (formula: O_4S).



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

- Molecule 12 is TRIETHYLENE GLYCOL (CCD ID: PGE) (formula: $C_6H_{14}O_4$).



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

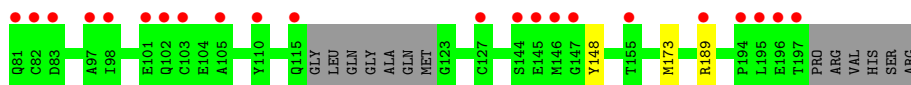
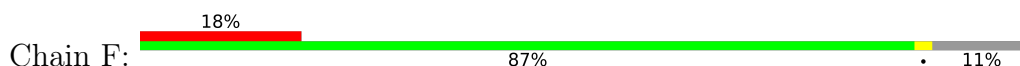
- Molecule 13 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
13	F	96	Total O 96 96	0	0
13	A	516	Total O 516 516	0	0

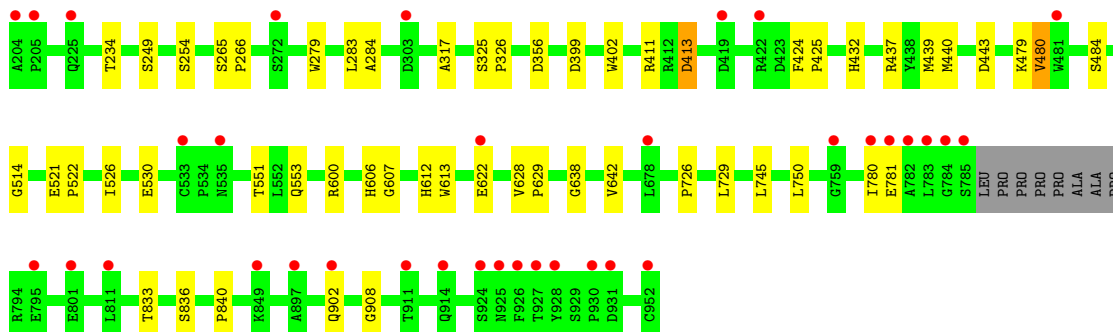
3 Residue-property plots [i](#)

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 (76 kDa)



- Molecule 2: Lysosomal alpha-glucosidase (70 kDa)



- Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose



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



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

Chain D:  100%

MAG1
MAG2

- Molecule 5: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain E:  33%  67%

MAG1
MAG2
BMA3

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	97.34Å 102.94Å 129.92Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.67 – 1.90 48.67 – 1.90	Depositor EDS
% Data completeness (in resolution range)	100.0 (48.67-1.90) 100.0 (48.67-1.90)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.96 (at 1.90Å)	Xtriage
Refinement program	REFMAC 7.1.015	Depositor
R, R_{free}	0.149 , 0.178 (Not available) , 0.182	Depositor DCC
R_{free} test set	5146 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å ²)	29.2	Xtriage
Anisotropy	0.049	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 46.6	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	0.97	EDS
Total number of atoms	7632	wwPDB-VP
Average B, all atoms (Å ²)	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.90% 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: EDO, FUC, CL, CSO, PGE, GOL, BMA, NAG, SO4, U54

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	F	0.98	0/953	1.15	0/1295
2	A	1.01	2/6004 (0.0%)	1.13	1/8209 (0.0%)
All	All	1.01	2/6957 (0.0%)	1.14	1/9504 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	606	HIS	CE1-NE2	5.41	1.38	1.32
2	A	726	PRO	C-O	5.01	1.29	1.23

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	413	ASP	CA-CB-CG	5.69	118.29	112.60

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	F	914	0	887	2	0
2	A	5825	0	5640	33	0
3	B	38	0	34	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	C	28	0	25	0	0
4	D	28	0	25	0	0
5	E	39	0	34	0	0
6	A	7	0	0	1	0
6	F	3	0	0	0	0
7	A	28	0	42	4	0
7	F	12	0	18	0	0
8	A	18	0	24	0	0
8	F	6	0	8	0	0
9	A	30	0	0	0	0
10	A	14	0	13	0	0
11	A	20	0	0	0	0
12	A	10	0	14	3	0
13	A	516	0	0	3	0
13	F	96	0	0	0	0
All	All	7632	0	6764	36	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 3.

All (36) 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)
2:A:284:ALA:H	12:A:1024:PGE:H3	1.33	0.90
6:A:1007:CL:CL	13:A:1537:HOH:O	2.44	0.72
2:A:908:GLY:HA2	7:A:1021:EDO:H21	1.74	0.69
2:A:551:THR:OG1	2:A:553[B]:GLN:OE1	2.11	0.67
2:A:840:PRO:HB3	2:A:902:GLN:HG3	1.76	0.66
2:A:840:PRO:HB3	2:A:902:GLN:CG	2.27	0.65
2:A:840:PRO:CB	2:A:902:GLN:HG3	2.29	0.61
2:A:356[A]:ASP:OD2	13:A:1101:HOH:O	2.18	0.55
2:A:283:LEU:HD12	12:A:1024:PGE:H32	1.89	0.55
2:A:325:SER:N	2:A:326:PRO:HA	2.23	0.53
2:A:439[A]:MET:SD	2:A:514:GLY:HA3	2.49	0.52
2:A:265:SER:HB2	2:A:266:PRO:HD2	1.93	0.51
2:A:234:THR:HA	2:A:249:SER:O	2.11	0.50
2:A:484:SER:OG	2:A:530:GLU:OE2	2.21	0.50
2:A:622:GLU:HG2	13:A:1240:HOH:O	2.13	0.48
1:F:148:TYR:CE2	1:F:173[A]:MET:HE3	2.49	0.48
2:A:479:LYS:HE2	2:A:530:GLU:OE2	2.14	0.47
2:A:628:VAL:HB	2:A:629:PRO:HD3	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:526:ILE:C	2:A:526:ILE:HD12	2.41	0.46
2:A:745:LEU:HA	2:A:750:LEU:O	2.16	0.46
2:A:612:HIS:O	2:A:642:VAL:HA	2.15	0.45
2:A:254:SER:HA	7:A:1015:EDO:H21	1.98	0.44
2:A:833:THR:HA	2:A:836:SER:OG	2.18	0.43
2:A:265:SER:HB2	2:A:266:PRO:CD	2.48	0.43
2:A:413:ASP:OD2	2:A:443:ASP:O	2.37	0.43
2:A:284:ALA:N	12:A:1024:PGE:H3	2.15	0.43
2:A:840:PRO:HB3	2:A:902:GLN:HG2	2.01	0.43
2:A:607:GLY:HA3	2:A:638:GLY:O	2.19	0.42
2:A:279:TRP:CE3	2:A:317:ALA:HB2	2.55	0.42
2:A:437:ARG:CZ	7:A:1022:EDO:H12	2.50	0.42
1:F:189:ARG:HH11	1:F:189:ARG:HG2	1.85	0.42
2:A:424:PHE:HB3	2:A:425:PRO:HD3	2.03	0.41
2:A:521:GLU:N	2:A:522:PRO:HA	2.35	0.41
2:A:600:ARG:O	2:A:612:HIS:CE1	2.74	0.41
2:A:432:HIS:HA	7:A:1022:EDO:H21	2.04	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	F	112/123 (91%)	110 (98%)	2 (2%)	0	100	100
2	A	740/749 (99%)	723 (98%)	16 (2%)	1 (0%)	48	40
All	All	852/872 (98%)	833 (98%)	18 (2%)	1 (0%)	48	40

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	A	480	VAL

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	F	107/111 (96%)	107 (100%)	0	100	100
2	A	628/630 (100%)	620 (99%)	8 (1%)	61	61
All	All	735/741 (99%)	727 (99%)	8 (1%)	65	67

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

Mol	Chain	Res	Type
2	A	399	ASP
2	A	411	ARG
2	A	440	MET
2	A	480	VAL
2	A	613	TRP
2	A	729	LEU
2	A	780	ILE
2	A	781	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
2	A	401	GLN
2	A	535	ASN
2	A	584	HIS
2	A	692	GLN
2	A	708	HIS
2	A	875	GLN
2	A	900	GLN
2	A	902	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	$\# Z > 2$
2	CSO	A	938	2	3,6,7	1.20	0	1,6,8	0.80	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	CSO	A	938	2	-	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 ⓘ

10 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	NAG	B	1	3,1	14,14,15	0.73	1 (7%)	17,19,21	1.32	1 (5%)
3	NAG	B	2	3	14,14,15	0.45	0	17,19,21	0.90	0
3	FUC	B	3	3	10,10,11	0.38	0	14,14,16	1.12	0
4	NAG	C	1	2,4	14,14,15	0.63	0	17,19,21	1.01	0
4	NAG	C	2	4	14,14,15	0.60	0	17,19,21	1.28	2 (11%)
4	NAG	D	1	2,4	14,14,15	0.54	0	17,19,21	1.21	1 (5%)
4	NAG	D	2	4	14,14,15	0.36	0	17,19,21	1.00	1 (5%)
5	NAG	E	1	2,5	14,14,15	0.72	0	17,19,21	0.92	0
5	NAG	E	2	5	14,14,15	0.59	0	17,19,21	1.27	2 (11%)
5	BMA	E	3	5	11,11,12	0.39	0	15,15,17	1.01	1 (6%)

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

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

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	1	NAG	C2-N2	-2.15	1.42	1.46

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	1	NAG	O5-C1-C2	-3.40	106.03	111.29
4	D	1	NAG	O5-C1-C2	-3.09	106.52	111.29
5	E	3	BMA	O5-C5-C6	2.80	113.11	107.66
5	E	2	NAG	O5-C5-C6	2.52	112.56	107.66

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	2	NAG	C1-O5-C5	2.45	115.47	112.19
4	C	2	NAG	C2-N2-C7	-2.33	119.78	122.90
5	E	2	NAG	C6-C5-C4	-2.14	107.75	113.02
4	C	2	NAG	O5-C5-C4	-2.09	105.73	110.83

There are no chirality outliers.

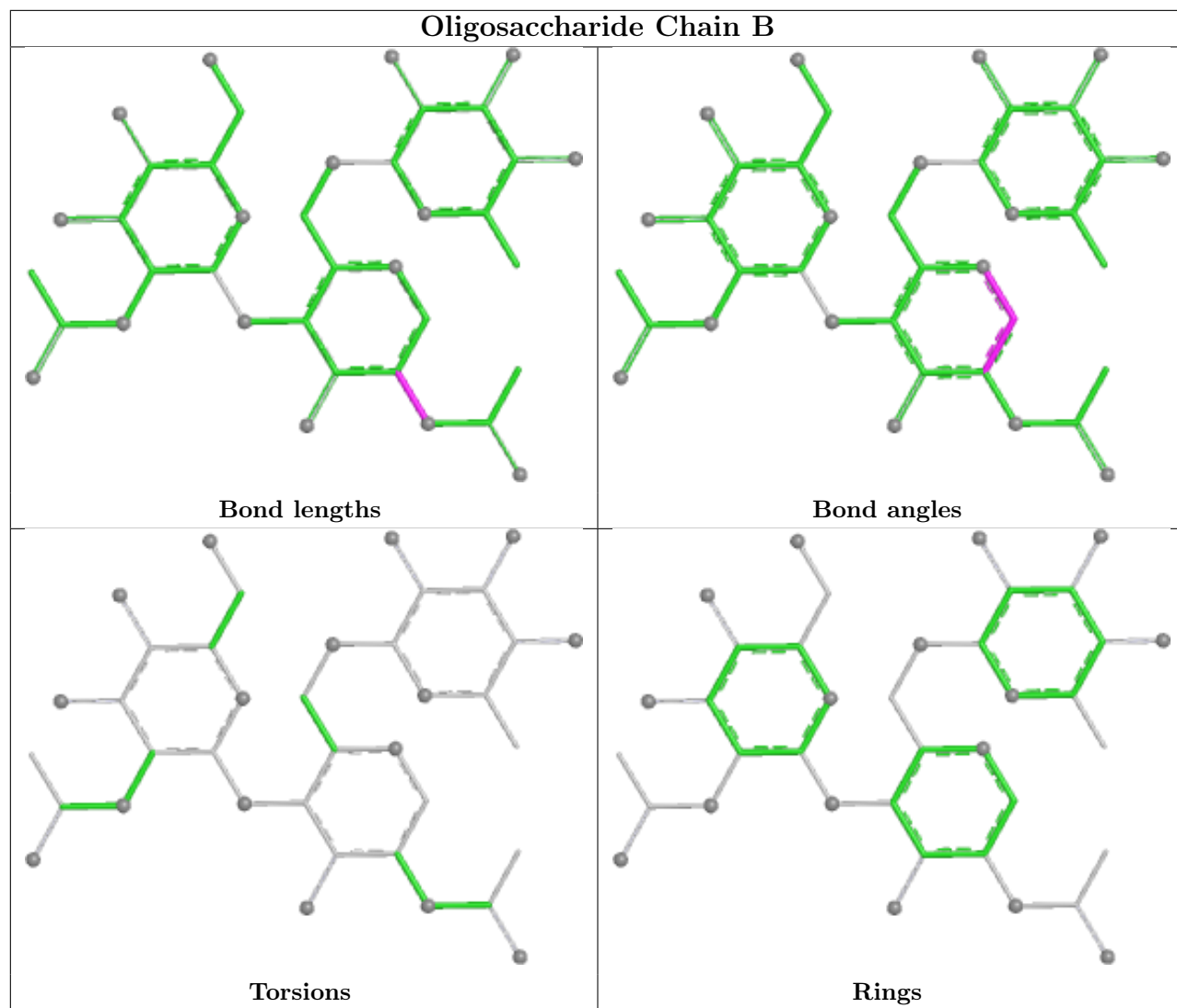
All (4) torsion outliers are listed below:

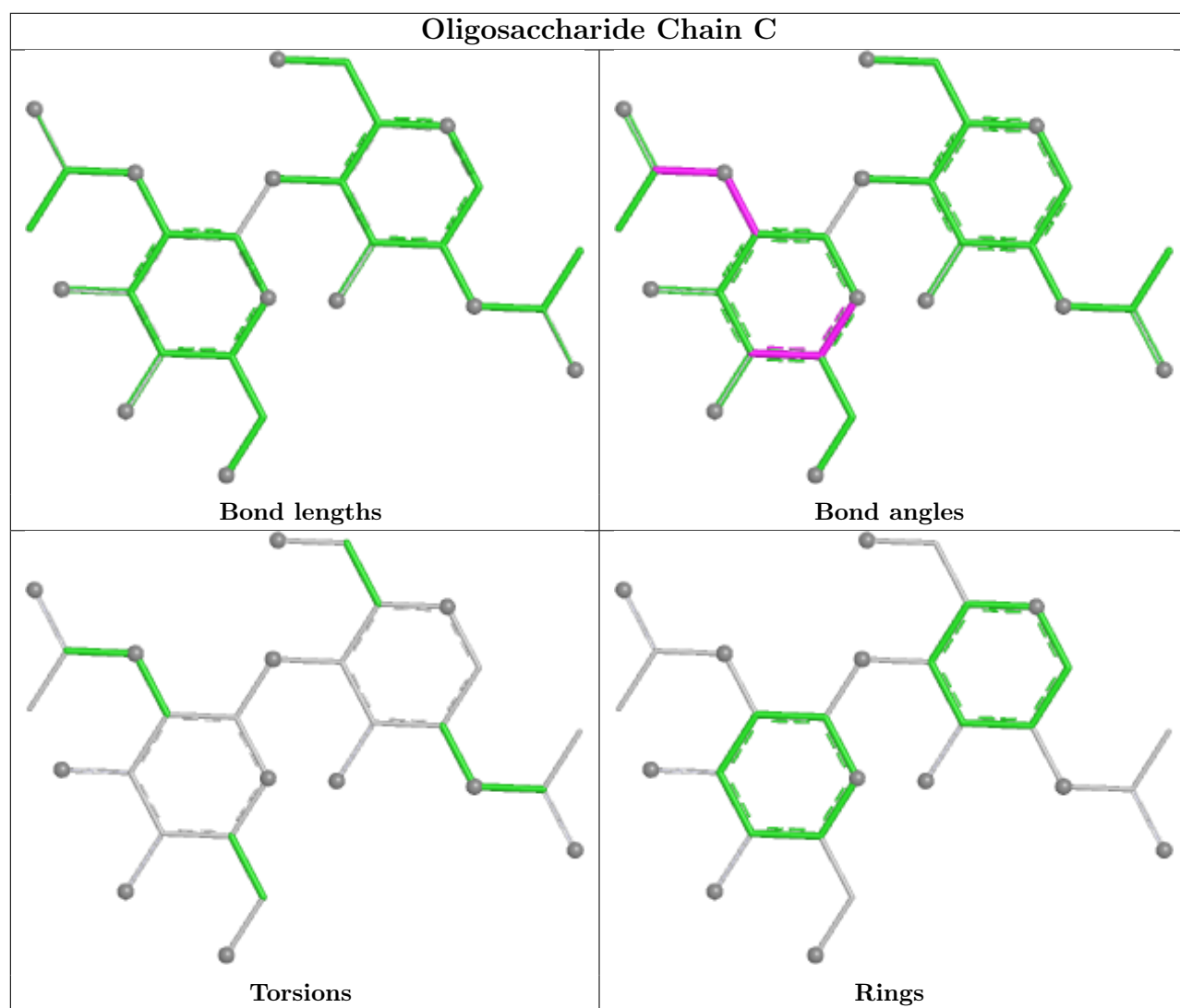
Mol	Chain	Res	Type	Atoms
5	E	3	BMA	O5-C5-C6-O6
5	E	3	BMA	C4-C5-C6-O6
4	D	2	NAG	C4-C5-C6-O6
4	D	2	NAG	O5-C5-C6-O6

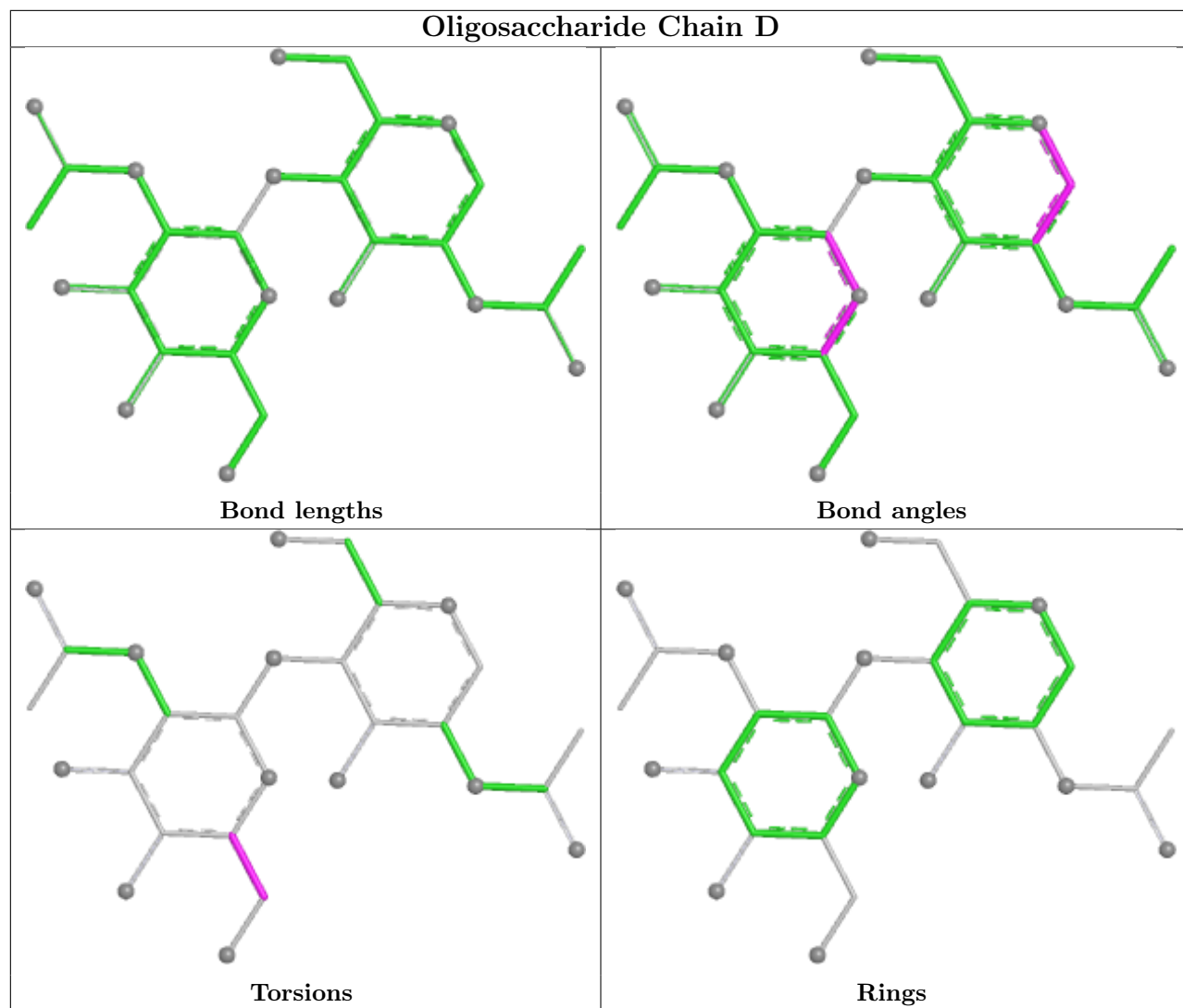
There are no ring outliers.

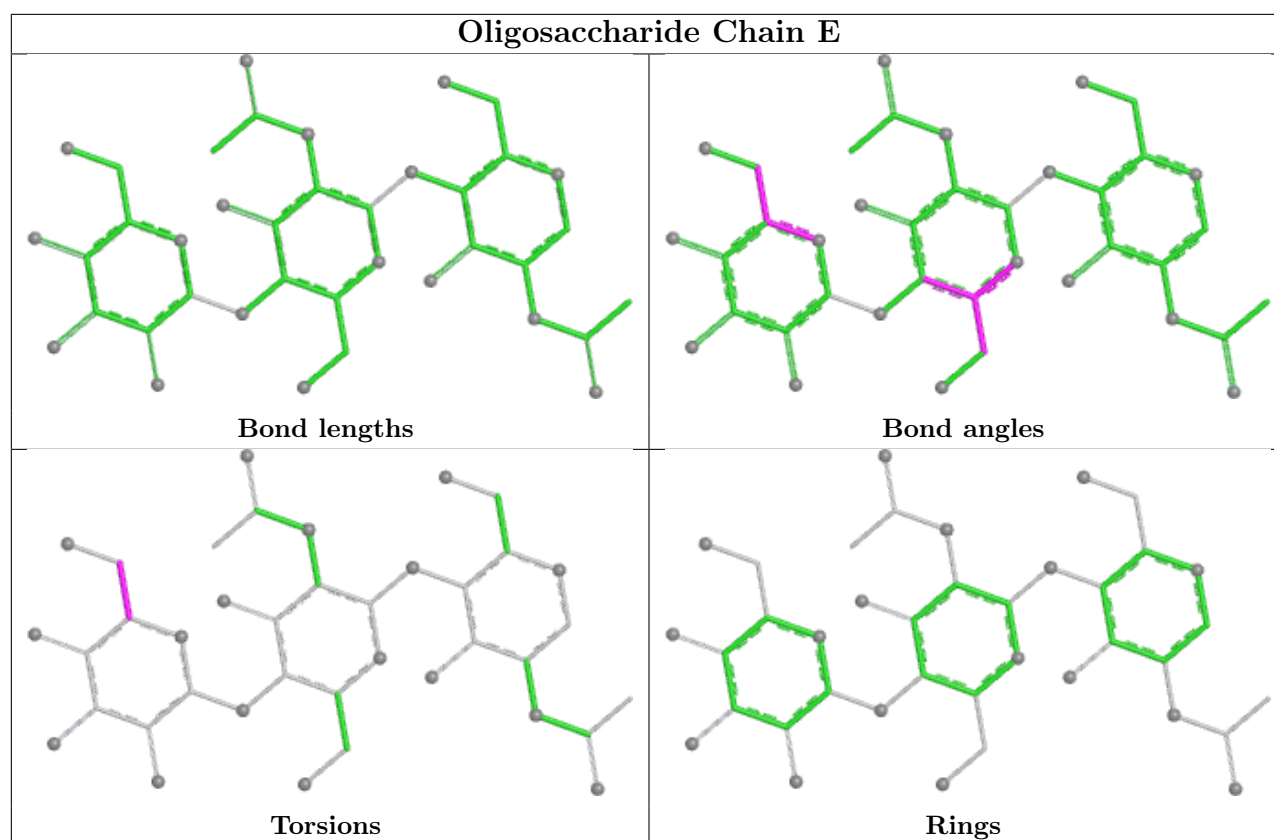
No monomer is involved in short contacts.

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









5.6 Ligand geometry [i](#)

Of 31 ligands modelled in this entry, 10 are monoatomic - leaving 21 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	$\# Z > 2$
11	SO4	A	1003	-	4,4,4	0.29	0	6,6,6	0.31	0
7	EDO	A	1023	-	3,3,3	0.12	0	2,2,2	0.28	0
8	GOL	F	305	-	5,5,5	0.14	0	5,5,5	0.28	0
7	EDO	A	1015	-	3,3,3	0.08	0	2,2,2	0.33	0
10	NAG	A	1002	2	14,14,15	0.47	0	17,19,21	0.93	2 (11%)
7	EDO	F	306	-	3,3,3	0.19	0	2,2,2	0.05	0
11	SO4	A	1004	-	4,4,4	0.40	0	6,6,6	0.22	0
11	SO4	A	1005	-	4,4,4	0.29	0	6,6,6	0.15	0
12	PGE	A	1024	-	9,9,9	0.49	0	8,8,8	0.55	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
8	GOL	A	1017	-	5,5,5	0.28	0	5,5,5	0.84	0
7	EDO	A	1018	-	3,3,3	0.28	0	2,2,2	0.06	0
7	EDO	A	1022	-	3,3,3	0.44	0	2,2,2	0.85	0
7	EDO	A	1016	-	3,3,3	0.13	0	2,2,2	0.11	0
11	SO4	A	1006	-	4,4,4	0.36	0	6,6,6	0.26	0
7	EDO	A	1014	-	3,3,3	0.03	0	2,2,2	0.09	0
8	GOL	A	1020	-	5,5,5	0.13	0	5,5,5	0.19	0
8	GOL	A	1019	-	5,5,5	0.25	0	5,5,5	0.40	0
7	EDO	F	304	-	3,3,3	0.08	0	2,2,2	0.28	0
7	EDO	F	307	-	3,3,3	0.56	0	2,2,2	0.31	0
7	EDO	A	1021	-	3,3,3	0.75	0	2,2,2	0.46	0
9	U54	A	1001	2	31,31,31	1.43	3 (9%)	38,39,39	1.41	5 (13%)

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
7	EDO	A	1018	-	-	0/1/1/1	-
8	GOL	A	1019	-	-	1/4/4/4	-
7	EDO	F	304	-	-	0/1/1/1	-
7	EDO	F	307	-	-	1/1/1/1	-
7	EDO	A	1022	-	-	1/1/1/1	-
7	EDO	A	1023	-	-	0/1/1/1	-
8	GOL	F	305	-	-	0/4/4/4	-
12	PGE	A	1024	-	-	0/7/7/7	-
7	EDO	A	1021	-	-	1/1/1/1	-
7	EDO	A	1015	-	-	1/1/1/1	-
7	EDO	A	1016	-	-	1/1/1/1	-
8	GOL	A	1020	-	-	0/4/4/4	-
9	U54	A	1001	2	-	5/19/39/39	0/2/2/2
10	NAG	A	1002	2	-	0/6/23/26	0/1/1/1
7	EDO	A	1014	-	-	1/1/1/1	-
8	GOL	A	1017	-	-	2/4/4/4	-
7	EDO	F	306	-	-	0/1/1/1	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	A	1001	U54	N51-N50	5.44	1.40	1.32
9	A	1001	U54	N49-N50	2.80	1.39	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	A	1001	U54	C53-C52	2.73	1.41	1.36

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	A	1001	U54	C20-N49-C53	3.98	136.27	128.83
9	A	1001	U54	C3-C2-C1	3.31	119.11	112.59
9	A	1001	U54	C20-N49-N50	-3.11	114.54	120.78
9	A	1001	U54	O4-C4-C3	-2.77	104.41	110.05
10	A	1002	NAG	O5-C5-C6	2.18	111.91	107.66
10	A	1002	NAG	O5-C1-C2	-2.16	107.95	111.29
9	A	1001	U54	C52-C53-N49	2.13	108.31	105.33

There are no chirality outliers.

All (14) torsion outliers are listed below:

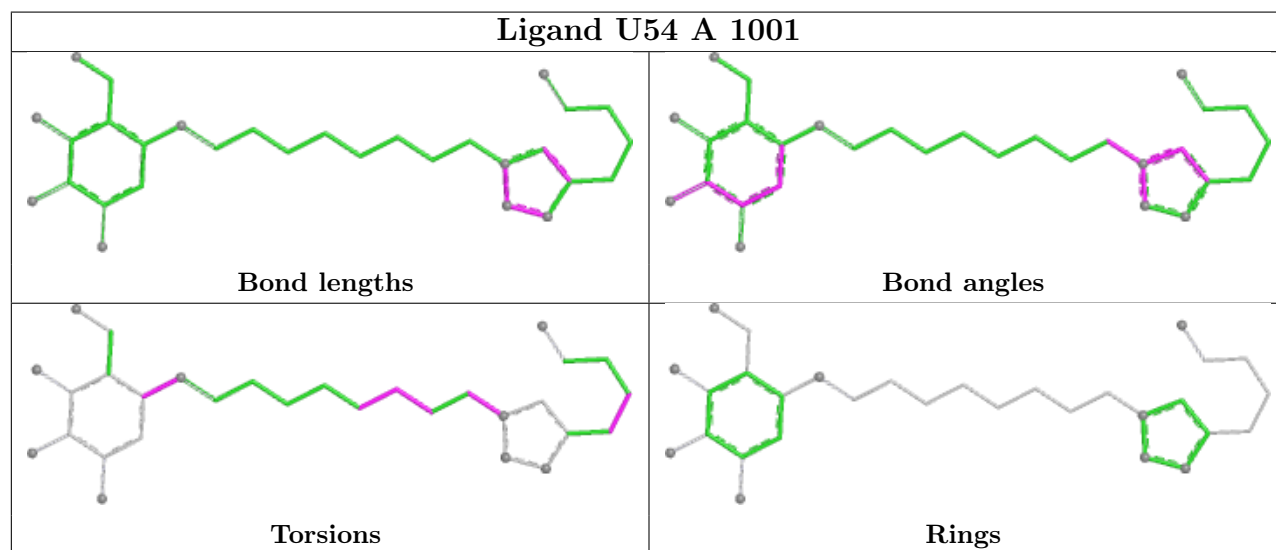
Mol	Chain	Res	Type	Atoms
8	A	1017	GOL	O1-C1-C2-C3
8	A	1017	GOL	O1-C1-C2-O2
7	A	1021	EDO	O1-C1-C2-O2
9	A	1001	U54	C52-C54-C55-C56
9	A	1001	U54	C16-C17-C18-C19
7	A	1014	EDO	O1-C1-C2-O2
9	A	1001	U54	C2-C1-N1-C13
7	A	1015	EDO	O1-C1-C2-O2
7	A	1016	EDO	O1-C1-C2-O2
9	A	1001	U54	C17-C18-C19-C20
7	F	307	EDO	O1-C1-C2-O2
7	A	1022	EDO	O1-C1-C2-O2
8	A	1019	GOL	O1-C1-C2-O2
9	A	1001	U54	C19-C20-N49-C53

There are no ring outliers.

4 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	A	1015	EDO	1	0
12	A	1024	PGE	3	0
7	A	1022	EDO	2	0
7	A	1021	EDO	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	F	110/123 (89%)	0.88	22 (20%) 3 2	20, 45, 69, 85	6 (5%)
2	A	740/749 (98%)	0.34	35 (4%) 36 39	23, 39, 58, 85	4 (0%)
All	All	850/872 (97%)	0.41	57 (6%) 24 25	20, 40, 60, 85	10 (1%)

All (57) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	A	783	LEU	7.3
2	A	782	ALA	6.9
1	F	197	THR	6.0
2	A	784	GLY	5.8
2	A	205	PRO	5.1
2	A	781	GLU	4.7
2	A	785	SER	4.5
1	F	195	LEU	4.4
2	A	204	ALA	4.1
1	F	144	SER	4.0
2	A	925	ASN	3.9
1	F	146	MET	3.9
2	A	678	LEU	3.8
2	A	780	ILE	3.8
1	F	82	CYS	3.5
2	A	897	ALA	3.2
2	A	481	TRP	3.2
2	A	931	ASP	3.1
2	A	533	CYS	3.0
2	A	535	ASN	2.9
1	F	105	ALA	2.9
1	F	115	GLN	2.9
1	F	194	PRO	2.8
1	F	189	ARG	2.8

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Mol	Chain	Res	Type	RSRZ
2	A	849	LYS	2.8
2	A	914	GLN	2.7
2	A	622	GLU	2.7
2	A	422	ARG	2.7
2	A	225	GLN	2.7
1	F	145	GLU	2.6
1	F	83	ASP	2.6
2	A	419	ASP	2.5
1	F	98	ILE	2.5
1	F	97	ALA	2.4
2	A	952	CYS	2.3
2	A	927	THR	2.3
2	A	930	PRO	2.3
2	A	759	GLY	2.3
2	A	911	THR	2.2
2	A	926	PHE	2.2
2	A	928	TYR	2.2
1	F	81	GLN	2.2
1	F	196	GLU	2.1
2	A	795	GLU	2.1
2	A	902	GLN	2.1
1	F	110	TYR	2.1
2	A	924	SER	2.1
2	A	801	GLU	2.1
1	F	155[A]	THR	2.1
1	F	103	CYS	2.1
1	F	101	GLU	2.0
1	F	102	GLN	2.0
1	F	127	CYS	2.0
2	A	811	LEU	2.0
2	A	303	ASP	2.0
2	A	272	SER	2.0
1	F	147	GLY	2.0

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

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($\text{\AA}^2$)	Q<0.9
2	CSO	A	938	7/8	0.93	0.11	45,45,60,72	0

6.3 Carbohydrates

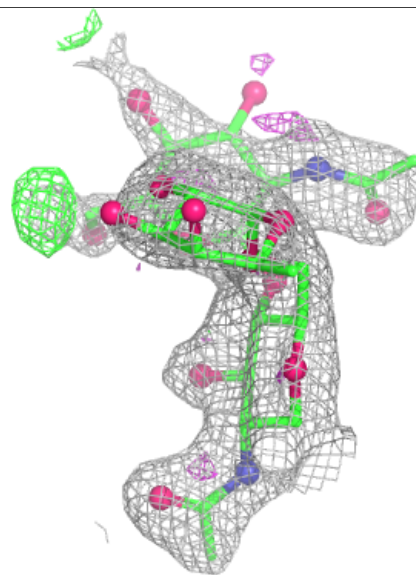
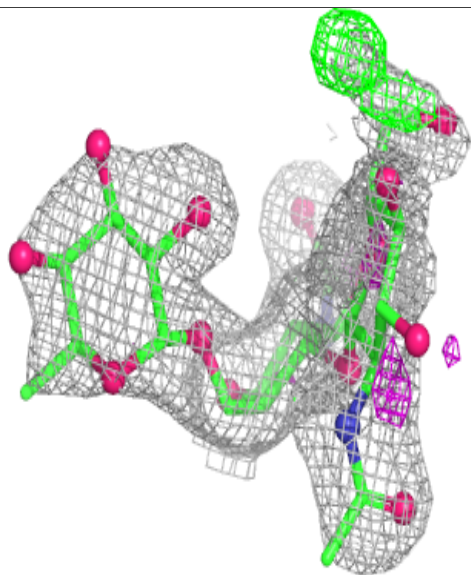
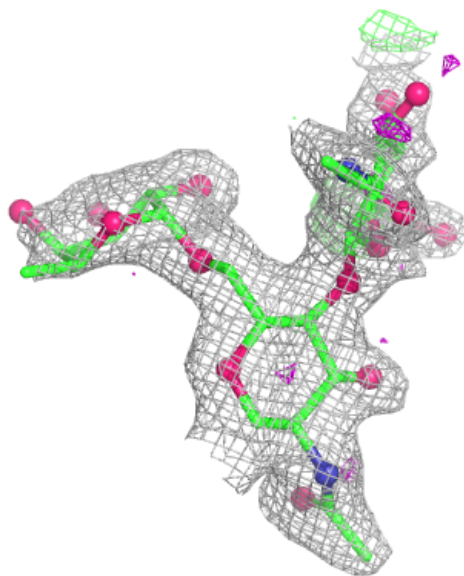
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	NAG	B	1	14/15	-	-	48,56,62,70	0
3	NAG	B	2	14/15	-	-	68,79,88,89	0
3	FUC	B	3	10/11	-	-	72,83,90,93	0
4	NAG	C	2	14/15	0.60	0.19	64,72,88,90	0
5	NAG	E	2	14/15	0.65	0.16	46,50,60,62	0
4	NAG	D	2	14/15	0.69	0.19	76,95,110,115	0
5	NAG	E	1	14/15	0.92	0.10	38,45,49,51	0
4	NAG	C	1	14/15	0.92	0.11	39,47,53,56	0
4	NAG	D	1	14/15	0.94	0.09	42,49,65,72	0
5	BMA	E	3	11/12	-	-	67,85,92,100	0

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

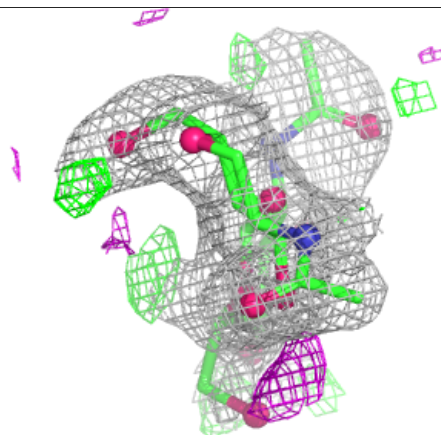
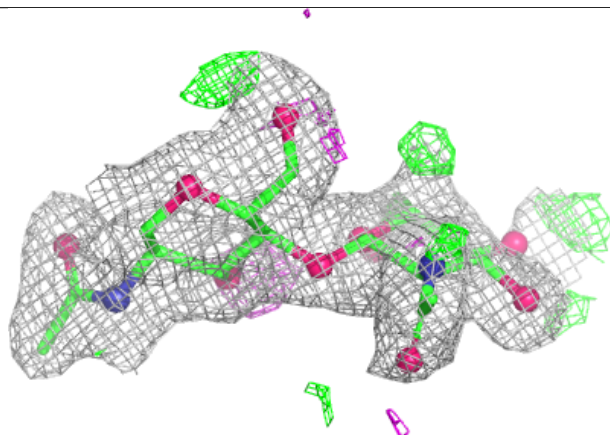
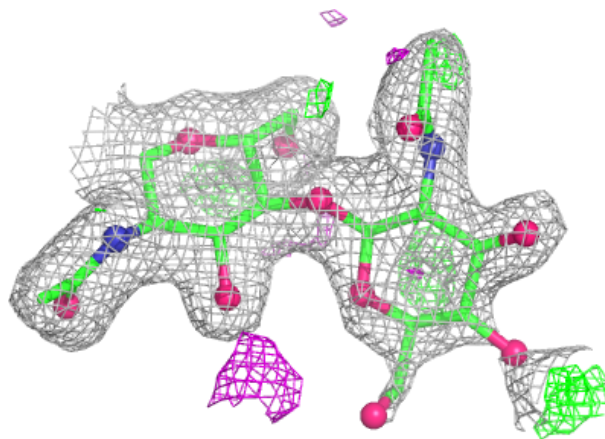
Electron density around Chain B:

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



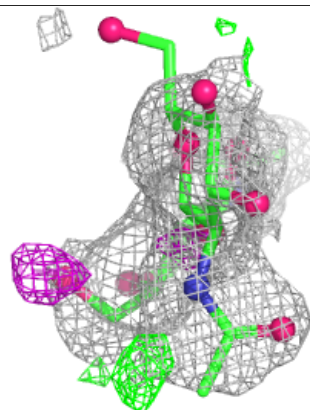
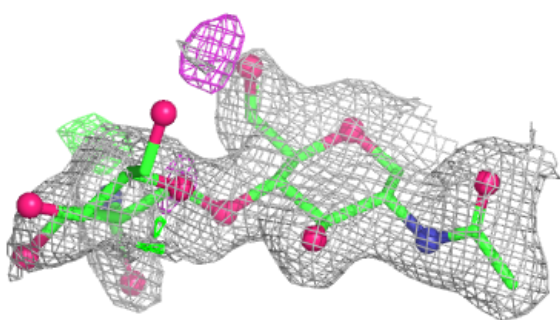
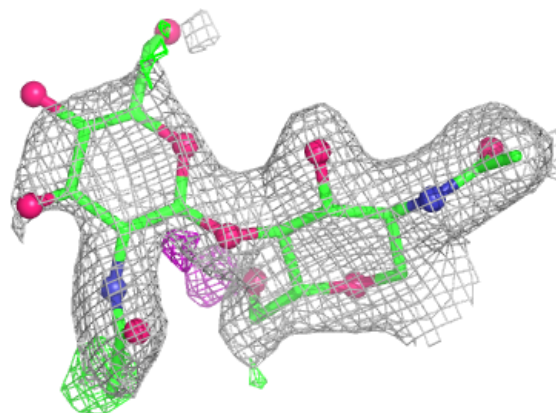
Electron density around Chain C:

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

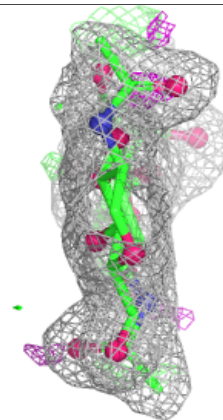
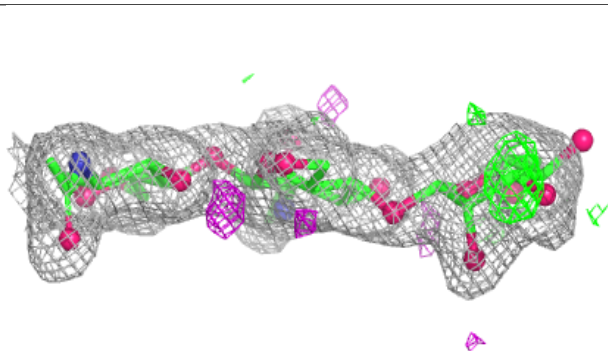
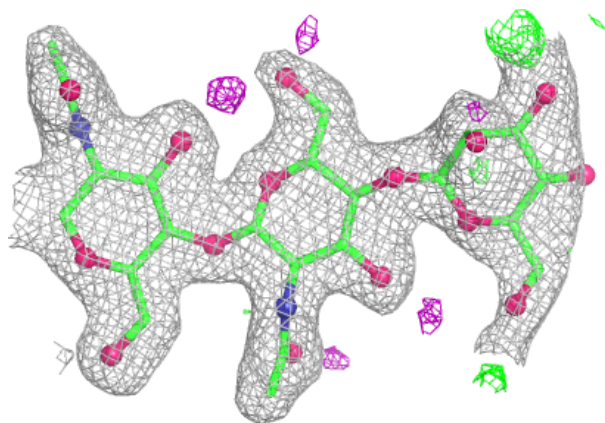


Electron density around Chain D:

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

**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)

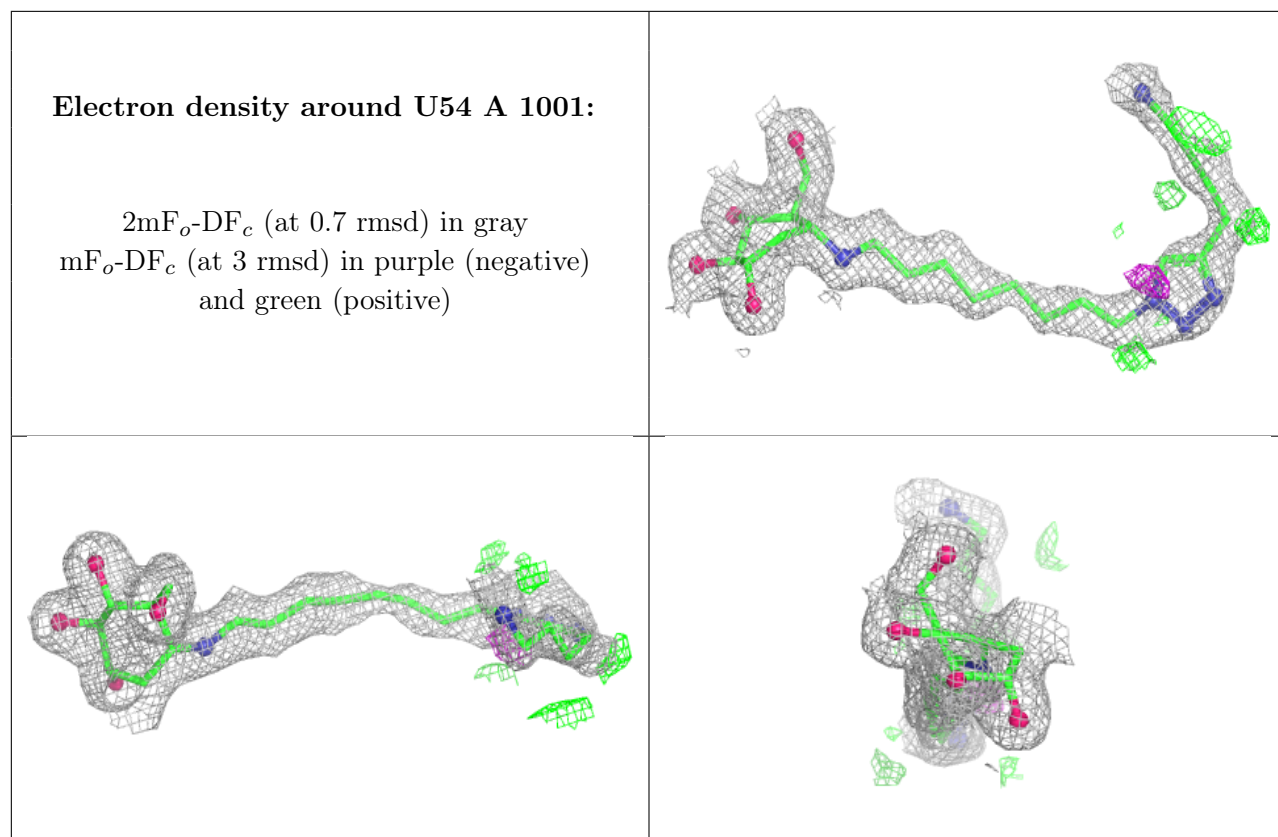


6.4 Ligands ⓘ

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
12	PGE	A	1024	10/10	0.62	0.27	44,57,65,71	0
10	NAG	A	1002	14/15	0.75	0.19	56,71,74,87	0
11	SO4	A	1005	5/5	0.77	0.14	65,72,84,91	0
6	CL	A	1013	1/1	0.80	0.37	94,94,94,94	0
7	EDO	A	1018	4/4	0.81	0.26	69,73,73,75	0
7	EDO	A	1023	4/4	0.83	0.20	45,56,62,63	0
7	EDO	F	307	4/4	0.83	0.21	53,54,56,58	0
6	CL	A	1012	1/1	0.84	0.31	77,77,77,77	0
8	GOL	A	1019	6/6	0.85	0.18	52,59,62,64	0
7	EDO	A	1016	4/4	0.85	0.21	46,67,71,76	0
7	EDO	A	1014	4/4	0.86	0.26	93,96,96,97	0
6	CL	A	1011	1/1	0.87	0.15	86,86,86,86	0
11	SO4	A	1006	5/5	0.87	0.14	73,75,84,85	0
6	CL	A	1009	1/1	0.87	0.20	93,93,93,93	0
6	CL	A	1007	1/1	0.89	0.15	84,84,84,84	0
7	EDO	A	1015	4/4	0.89	0.16	59,71,72,82	0
7	EDO	A	1021	4/4	0.89	0.27	51,52,53,57	0
6	CL	A	1010	1/1	0.90	0.23	91,91,91,91	0
6	CL	F	302	1/1	0.90	0.17	82,82,82,82	0
7	EDO	F	304	4/4	0.90	0.16	52,62,71,71	0
7	EDO	F	306	4/4	0.90	0.19	62,65,73,73	0
11	SO4	A	1003	5/5	0.91	0.12	46,48,58,61	0
7	EDO	A	1022	4/4	0.92	0.12	56,56,58,62	0
8	GOL	A	1017	6/6	0.92	0.14	35,50,61,61	0
8	GOL	A	1020	6/6	0.93	0.12	46,49,50,51	0
6	CL	F	301	1/1	0.93	0.14	82,82,82,82	0
6	CL	A	1008	1/1	0.94	0.19	93,93,93,93	0
9	U54	A	1001	30/30	0.95	0.14	32,53,86,87	0
8	GOL	F	305	6/6	0.95	0.11	45,54,58,59	0
11	SO4	A	1004	5/5	0.96	0.08	55,55,55,59	0
6	CL	F	303	1/1	0.96	0.10	77,77,77,77	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.



6.5 Other polymers [i](#)

There are no such residues in this entry.