



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 6, 2020 – 04:15 PM BST

PDB ID : 1ONQ
Title : Crystal Structure of CD1a in Complex with a Sulfatide
Authors : Zajonc, D.M.; Elsliger, M.A.; Teyton, L.; Wilson, I.A.
Deposited on : 2003-02-28
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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.13.1
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.13.1

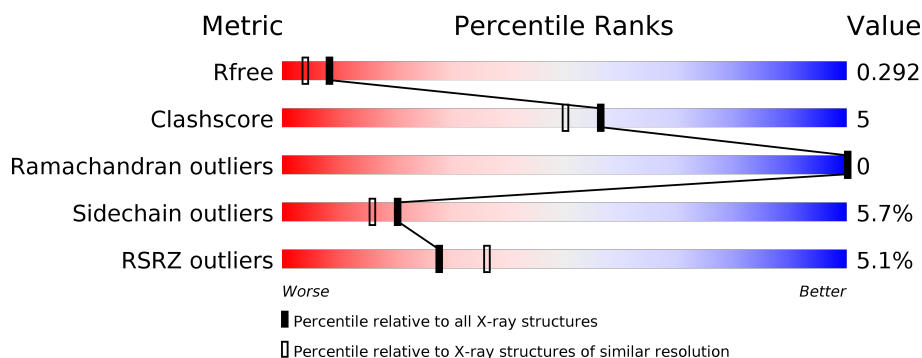
1 Overall quality at a glance

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.




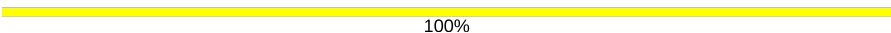
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1479 (2.16-2.16)
Clashscore	141614	1585 (2.16-2.16)
Ramachandran outliers	138981	1560 (2.16-2.16)
Sidechain outliers	138945	1559 (2.16-2.16)
RSRZ outliers	127900	1456 (2.16-2.16)

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 on 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	283	<div> <div>4%</div> <div> <div></div> <div>81%</div> <div>16%</div> <div>••</div> </div> </div>
1	C	283	<div> <div>8%</div> <div> <div></div> <div>85%</div> <div>11%</div> <div>•</div> </div> </div>
2	B	99	<div> <div></div> <div> <div></div> <div>81%</div> <div>17%</div> <div>•</div> </div> </div>
2	D	99	<div> <div>4%</div> <div> <div></div> <div>87%</div> <div>13%</div> </div> </div>
3	E	2	<div> <div></div> <div> <div></div> <div>100%</div> </div> </div>
3	G	2	<div> <div></div> <div> <div>50%</div> <div>50%</div> </div> </div>

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Mol	Chain	Length	Quality of chain
3	H	2	
4	F	2	

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
4	NAG	F	1	X	-	-	X
6	SLF	C	602	X	-	-	-

2 Entry composition [i](#)

There are 8 unique types of molecules in this entry. The entry contains 6791 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 T-cell surface glycoprotein CD1a.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	274	Total	C	N	O	S	0	0	0
			2228	1428	393	399	8			
1	C	273	Total	C	N	O	S	0	0	0
			2218	1422	390	398	8			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	278	HIS	-	expression tag	UNP P06126
A	279	HIS	-	expression tag	UNP P06126
A	280	HIS	-	expression tag	UNP P06126
A	281	HIS	-	expression tag	UNP P06126
A	282	HIS	-	expression tag	UNP P06126
A	283	HIS	-	expression tag	UNP P06126
C	278	HIS	-	expression tag	UNP P06126
C	279	HIS	-	expression tag	UNP P06126
C	280	HIS	-	expression tag	UNP P06126
C	281	HIS	-	expression tag	UNP P06126
C	282	HIS	-	expression tag	UNP P06126
C	283	HIS	-	expression tag	UNP P06126

- Molecule 2 is a protein called Beta-2-microglobulin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	99	Total	C	N	O	S	0	0	0
			829	528	140	158	3			
2	D	99	Total	C	N	O	S	0	0	0
			829	528	140	158	3			

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



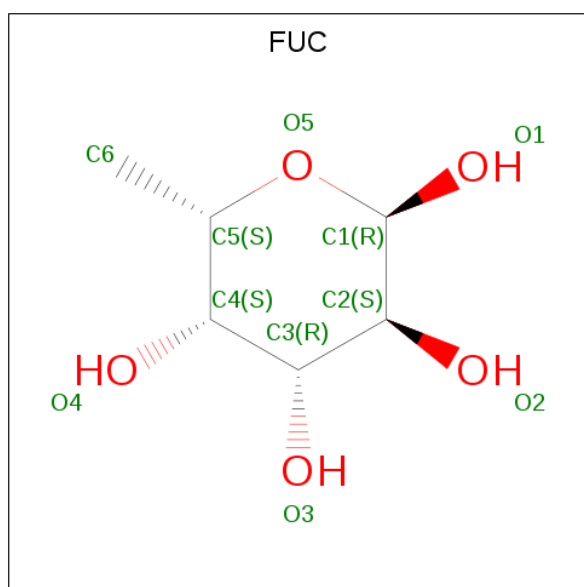
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	E	2	Total	C	N	O	0	0	0
			28	16	2	10			
3	G	2	Total	C	N	O	0	0	0
			28	16	2	10			
3	H	2	Total	C	N	O	0	0	0
			28	16	2	10			

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



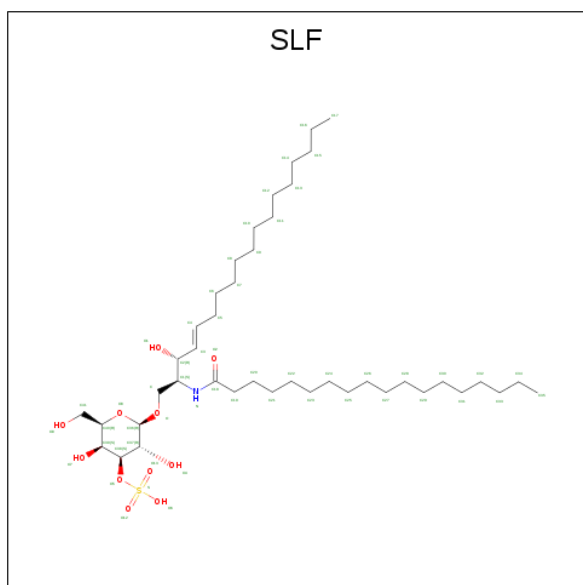
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	F	2	Total	C	N	O	0	0	0
			24	14	1	9			

- Molecule 5 is alpha-L-fucopyranose (three-letter code: FUC) (formula: C₆H₁₂O₅).



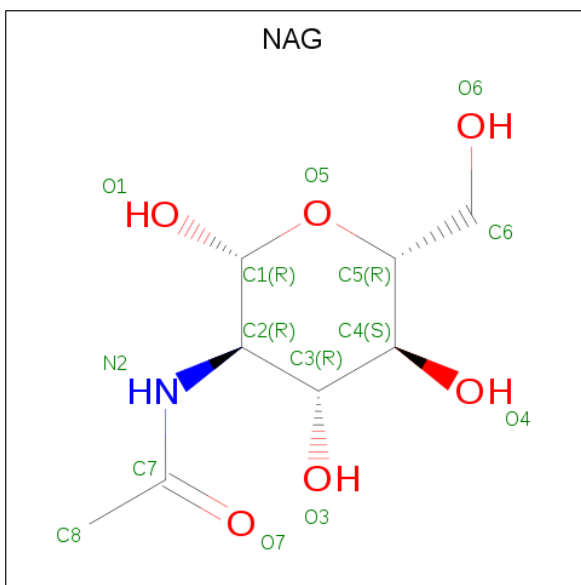
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			10	6	4		
5	C	1	Total	C	O	0	0
			10	6	4		

- Molecule 6 is SULFATE-3-D-GALACTOSYL-BETA-1-1-N-STEAROYL-D-SPHINGOSIN E (three-letter code: SLF) (formula: $C_{42}H_{81}NO_{11}S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	A	1	Total	C	N	O	S	0	0
			55	42	1	11	1		
6	C	1	Total	C	N	O		0	0
			40	36	1	3			

- Molecule 7 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



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

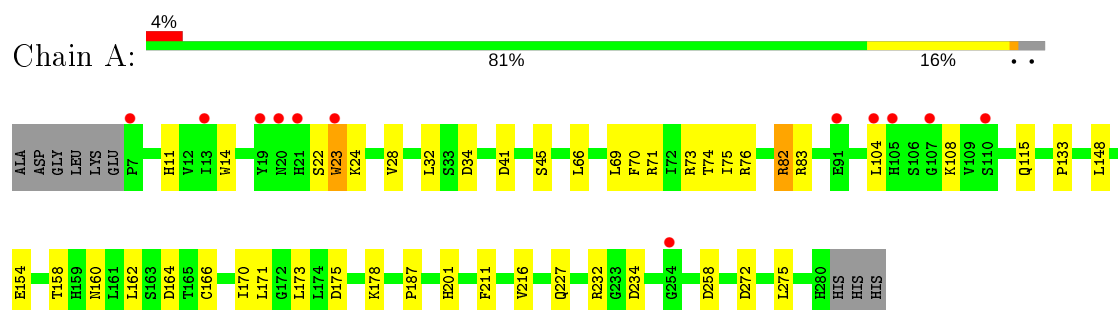
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	216	Total	O	0	0
			216	216		
8	B	82	Total	O	0	0
			82	82		
8	C	103	Total	O	0	0
			103	103		
8	D	49	Total	O	0	0
			49	49		

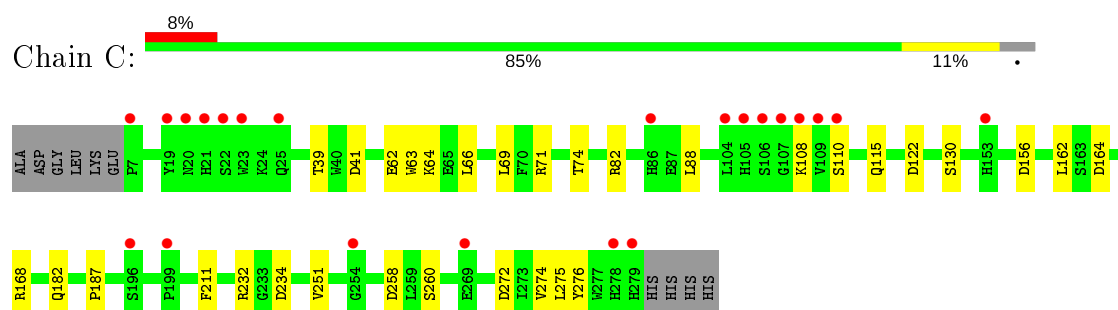
3 Residue-property plots [i](#)

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.

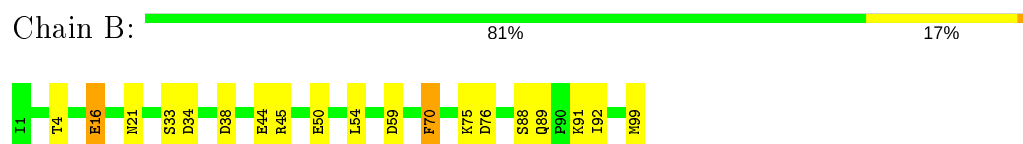
- Molecule 1: T-cell surface glycoprotein CD1a



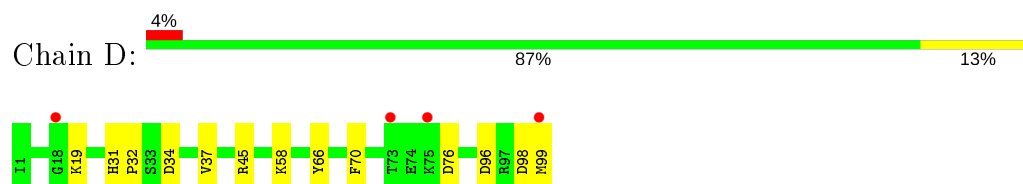
- Molecule 1: T-cell surface glycoprotein CD1a



- Molecule 2: Beta-2-microglobulin



- Molecule 2: Beta-2-microglobulin




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

Chain E:  100%


MAG1
MAG2

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

Chain G:  50% 50%

MAG1
MAG2

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

Chain H:  50% 50%

MAG1
MAG2

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

Chain F:  100%

MAG1
FUC2

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	55.41Å 42.71Å 204.22Å 90.00° 90.78° 90.00°	Depositor
Resolution (Å)	40.00 – 2.15 39.40 – 2.15	Depositor EDS
% Data completeness (in resolution range)	92.0 (40.00-2.15) 92.0 (39.40-2.15)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.50 (at 2.16Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, R_{free}	0.227 , 0.276 0.247 , 0.292	Depositor DCC
R_{free} test set	2236 reflections (4.60%)	wwPDB-VP
Wilson B-factor (Å ²)	31.9	Xtriage
Anisotropy	0.361	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 57.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.029 for h,-k,-l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	6791	wwPDB-VP
Average B, all atoms (Å ²)	17.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 12.92% 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 ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: SLF, NAG, FUC

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	0.62	0/2304	0.82	7/3136 (0.2%)
1	C	0.50	0/2293	0.74	7/3121 (0.2%)
2	B	0.68	1/852 (0.1%)	0.87	4/1152 (0.3%)
2	D	0.50	0/852	0.76	3/1152 (0.3%)
All	All	0.57	1/6301 (0.0%)	0.79	21/8561 (0.2%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	44	GLU	CD-OE2	5.25	1.31	1.25

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	34	ASP	CB-CG-OD2	6.90	124.51	118.30
2	B	38	ASP	CB-CG-OD2	6.26	123.93	118.30
1	C	41	ASP	CB-CG-OD2	6.22	123.90	118.30
1	A	164	ASP	CB-CG-OD2	6.11	123.80	118.30
1	C	156	ASP	CB-CG-OD2	6.07	123.76	118.30
1	C	234	ASP	CB-CG-OD2	6.01	123.71	118.30
2	B	34	ASP	CB-CG-OD2	5.99	123.69	118.30
1	A	258	ASP	CB-CG-OD2	5.99	123.69	118.30
1	A	272	ASP	CB-CG-OD2	5.94	123.65	118.30
1	A	175	ASP	CB-CG-OD2	5.91	123.62	118.30
1	C	272	ASP	CB-CG-OD2	5.83	123.54	118.30
1	A	41	ASP	CB-CG-OD2	5.73	123.45	118.30
1	A	234	ASP	CB-CG-OD2	5.58	123.32	118.30
1	C	164	ASP	CB-CG-OD2	5.34	123.10	118.30
2	B	59	ASP	CB-CG-OD2	5.28	123.06	118.30
2	D	34	ASP	CB-CG-OD2	5.25	123.02	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	76	ASP	CB-CG-OD2	5.20	122.98	118.30
2	D	76	ASP	CB-CG-OD2	5.11	122.89	118.30
2	D	98	ASP	CB-CG-OD2	5.04	122.84	118.30
1	C	122	ASP	CB-CG-OD2	5.03	122.83	118.30
1	C	258	ASP	CB-CG-OD2	5.00	122.81	118.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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	2228	0	2103	30	0
1	C	2218	0	2097	12	0
2	B	829	0	794	5	1
2	D	829	0	794	4	0
3	E	28	0	25	3	0
3	G	28	0	25	1	0
3	H	28	0	25	4	0
4	F	24	0	22	1	0
5	A	10	0	10	2	0
5	C	10	0	10	1	0
6	A	55	0	81	16	0
6	C	40	0	69	3	0
7	C	14	0	13	0	0
8	A	216	0	0	10	1
8	B	82	0	0	1	0
8	C	103	0	0	0	0
8	D	49	0	0	1	0
All	All	6791	0	6068	62	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

All (62) 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)
6:A:601:SLF:H312	6:A:601:SLF:HO9	1.40	0.86
6:A:601:SLF:O9	6:A:601:SLF:H312	1.77	0.85
5:A:531:FUC:C1	3:E:1:NAG:O6	2.26	0.83
1:A:73:ARG:CD	6:A:601:SLF:O4	2.36	0.74
5:C:532:FUC:C1	3:H:1:NAG:O6	2.38	0.72
2:B:50:GLU:OE2	8:B:137:HOH:O	2.09	0.71
1:A:73:ARG:NE	6:A:601:SLF:O4	2.28	0.65
1:A:11:HIS:ND1	8:A:751:HOH:O	2.29	0.64
1:A:73:ARG:NH1	6:A:601:SLF:H1A	2.13	0.63
2:D:31:HIS:ND1	2:D:32:PRO:HA	2.14	0.62
1:A:216:VAL:O	1:A:232:ARG:NH2	2.34	0.60
1:A:23:TRP:CZ3	4:F:2:FUC:H61	2.38	0.59
6:A:601:SLF:H211	6:A:601:SLF:HN	1.68	0.59
1:C:168:ARG:HD2	3:H:1:NAG:H83	1.84	0.59
1:A:32:LEU:HD13	1:A:173:LEU:HD23	1.86	0.57
1:A:187:PRO:HB3	1:A:211:PHE:HB3	1.85	0.57
1:C:74:THR:HG22	6:C:602:SLF:H221	1.85	0.57
1:C:62:GLU:O	1:C:66:LEU:HD23	2.05	0.57
6:A:601:SLF:O4	6:A:601:SLF:H2A	2.06	0.55
6:A:601:SLF:N	6:A:601:SLF:H211	2.22	0.55
1:A:158:THR:HG23	6:A:601:SLF:O1	2.09	0.53
1:A:45:SER:OG	1:A:71:ARG:HD3	2.09	0.53
1:C:260:SER:HB3	1:C:276:TYR:CD2	2.44	0.53
1:C:187:PRO:HB3	1:C:211:PHE:HB3	1.91	0.52
2:B:91:LYS:C	2:B:92:ILE:HD12	2.32	0.50
1:A:73:ARG:CG	6:A:601:SLF:O4	2.60	0.50
1:A:133:PRO:HB2	8:A:817:HOH:O	2.12	0.50
1:A:11:HIS:CE1	8:A:751:HOH:O	2.64	0.50
1:C:168:ARG:HH11	3:H:1:NAG:H81	1.77	0.49
1:C:274:VAL:HG12	1:C:276:TYR:CE1	2.47	0.49
1:A:148:LEU:CD2	6:A:601:SLF:O9	2.60	0.49
1:A:70:PHE:O	1:A:74:THR:HG23	2.12	0.48
2:D:96:ASP:HB3	2:D:99:MET:HB2	1.94	0.48
1:A:73:ARG:HD3	6:A:601:SLF:O4	2.13	0.48
1:A:69:LEU:HD11	1:A:73:ARG:HD2	1.96	0.48
1:A:154:GLU:HG2	6:A:601:SLF:O7	2.14	0.48
5:A:531:FUC:C1	3:E:1:NAG:HO6	2.26	0.48
2:B:33:SER:HB2	2:B:54:LEU:HD21	1.96	0.48
1:C:74:THR:HG22	6:C:602:SLF:C22	2.43	0.48
1:C:274:VAL:HG12	1:C:276:TYR:CZ	2.49	0.47
1:A:14:TRP:HD1	1:A:28:VAL:HG22	1.81	0.46
1:A:160:ASN:HB2	8:A:761:HOH:O	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:70:PHE:CD1	6:A:601:SLF:H201	2.50	0.46
1:A:104:LEU:HD13	1:A:170:ILE:HD13	1.98	0.46
6:A:601:SLF:C	6:A:601:SLF:O4	2.64	0.46
1:C:168:ARG:HH11	3:H:1:NAG:C8	2.29	0.46
8:A:715:HOH:O	3:G:1:NAG:H83	2.16	0.45
1:A:115:GLN:NE2	8:A:687:HOH:O	2.49	0.45
1:A:171:LEU:HD12	3:E:2:NAG:H82	1.98	0.45
1:A:71:ARG:O	1:A:75:ILE:HD12	2.17	0.45
1:A:227:GLN:NE2	8:A:680:HOH:O	2.25	0.44
1:C:274:VAL:CG1	1:C:276:TYR:CZ	3.01	0.44
1:A:82:ARG:NH1	8:A:730:HOH:O	2.51	0.43
1:A:14:TRP:CD1	1:A:28:VAL:HG22	2.55	0.42
2:D:58:LYS:HE3	8:D:142:HOH:O	2.20	0.42
2:D:37:VAL:HB	2:D:66:TYR:CZ	2.55	0.41
2:B:21:ASN:HB3	2:B:70:PHE:CE1	2.55	0.41
6:A:601:SLF:C21	6:A:601:SLF:HN	2.34	0.40
2:B:92:ILE:HD12	2:B:92:ILE:N	2.37	0.40
1:A:201:HIS:CD2	8:A:749:HOH:O	2.74	0.40
1:A:201:HIS:HD2	8:A:749:HOH:O	2.04	0.40
1:C:63:TRP:CZ3	6:C:602:SLF:H131	2.57	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:16:GLU:OE2	8:A:739:HOH:O[2_556]	2.15	0.05

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	272/283 (96%)	264 (97%)	8 (3%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	271/283 (96%)	264 (97%)	7 (3%)	0	100	100
2	B	97/99 (98%)	96 (99%)	1 (1%)	0	100	100
2	D	97/99 (98%)	96 (99%)	1 (1%)	0	100	100
All	All	737/764 (96%)	720 (98%)	17 (2%)	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	239/246 (97%)	227 (95%)	12 (5%)	24	21
1	C	238/246 (97%)	223 (94%)	15 (6%)	18	13
2	B	94/94 (100%)	86 (92%)	8 (8%)	10	6
2	D	94/94 (100%)	91 (97%)	3 (3%)	39	38
All	All	665/680 (98%)	627 (94%)	38 (6%)	20	16

All (38) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	22	SER
1	A	23	TRP
1	A	24	LYS
1	A	66	LEU
1	A	76	ARG
1	A	82	ARG
1	A	83	ARG
1	A	108	LYS
1	A	162	LEU
1	A	166	CYS
1	A	178	LYS
1	A	275	LEU
2	B	4	THR

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Mol	Chain	Res	Type
2	B	16	GLU
2	B	45	ARG
2	B	70	PHE
2	B	75	LYS
2	B	88	SER
2	B	89	GLN
2	B	99	MET
1	C	39	THR
1	C	64	LYS
1	C	69	LEU
1	C	71	ARG
1	C	82	ARG
1	C	88	LEU
1	C	108	LYS
1	C	110	SER
1	C	115	GLN
1	C	130	SER
1	C	162	LEU
1	C	182	GLN
1	C	232	ARG
1	C	251	VAL
1	C	275	LEU
2	D	19	LYS
2	D	45	ARG
2	D	70	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	11	HIS
1	A	25	GLN
1	A	184	GLN
1	A	228	GLN
1	C	115	GLN
1	C	143	HIS
1	C	150	GLN
1	C	180	HIS
1	C	184	GLN
1	C	193	HIS
1	C	225	GLN
1	C	227	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

8 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	E	1	1,3	14,14,15	0.82	1 (7%)	17,19,21	1.41	2 (11%)
3	NAG	E	2	3	14,14,15	1.17	1 (7%)	17,19,21	1.71	5 (29%)
4	NAG	F	1	1,4	14,14,15	0.62	0	17,19,21	1.15	2 (11%)
4	FUC	F	2	4	10,10,11	0.67	0	14,14,16	0.66	0
3	NAG	G	1	1,3	14,14,15	0.62	0	17,19,21	1.40	2 (11%)
3	NAG	G	2	3	14,14,15	0.68	0	17,19,21	1.21	2 (11%)
3	NAG	H	1	1,3	14,14,15	0.83	1 (7%)	17,19,21	1.81	6 (35%)
3	NAG	H	2	3	14,14,15	0.41	0	17,19,21	1.73	5 (29%)

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	E	1	1,3	-	1/6/23/26	0/1/1/1
3	NAG	E	2	3	-	2/6/23/26	0/1/1/1
4	NAG	F	1	1,4	1/1/5/7	2/6/23/26	0/1/1/1
4	FUC	F	2	4	-	-	0/1/1/1
3	NAG	G	1	1,3	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	G	2	3	-	2/6/23/26	0/1/1/1
3	NAG	H	1	1,3	-	3/6/23/26	0/1/1/1
3	NAG	H	2	3	-	1/6/23/26	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	2	NAG	C1-C2	3.25	1.57	1.52
3	H	1	NAG	C1-C2	2.33	1.55	1.52
3	E	1	NAG	C1-C2	2.11	1.55	1.52

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	H	2	NAG	C1-O5-C5	4.48	118.26	112.19
3	H	1	NAG	O7-C7-C8	-3.25	116.01	122.06
3	E	2	NAG	O5-C5-C6	3.22	112.26	107.20
3	G	1	NAG	C4-C3-C2	3.09	115.54	111.02
3	H	1	NAG	C2-N2-C7	3.04	127.23	122.90
4	F	1	NAG	O5-C5-C6	2.94	111.81	107.20
3	H	1	NAG	C1-O5-C5	2.76	115.93	112.19
3	H	2	NAG	O5-C1-C2	-2.66	107.08	111.29
3	G	2	NAG	O5-C5-C6	2.64	111.35	107.20
3	E	2	NAG	C1-C2-N2	2.49	114.74	110.49
3	H	1	NAG	O5-C1-C2	-2.46	107.40	111.29
3	G	2	NAG	C1-O5-C5	2.44	115.49	112.19
3	H	2	NAG	C6-C5-C4	-2.40	107.37	113.00
3	H	1	NAG	C8-C7-N2	2.36	120.10	116.10
3	H	1	NAG	C1-C2-N2	2.34	114.48	110.49
3	E	1	NAG	O5-C1-C2	-2.32	107.62	111.29
3	H	2	NAG	C3-C4-C5	2.32	114.38	110.24
3	E	2	NAG	O7-C7-C8	-2.29	117.81	122.06
3	E	2	NAG	O3-C3-C2	2.28	114.18	109.47
3	G	1	NAG	C2-N2-C7	2.21	126.05	122.90
3	E	2	NAG	O4-C4-C5	2.20	114.75	109.30
3	E	1	NAG	O3-C3-C4	-2.14	105.40	110.35
4	F	1	NAG	O5-C1-C2	-2.01	108.12	111.29
3	H	2	NAG	O5-C5-C4	2.01	115.70	110.83

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	F	1	NAG	C1

All (13) torsion outliers are listed below:

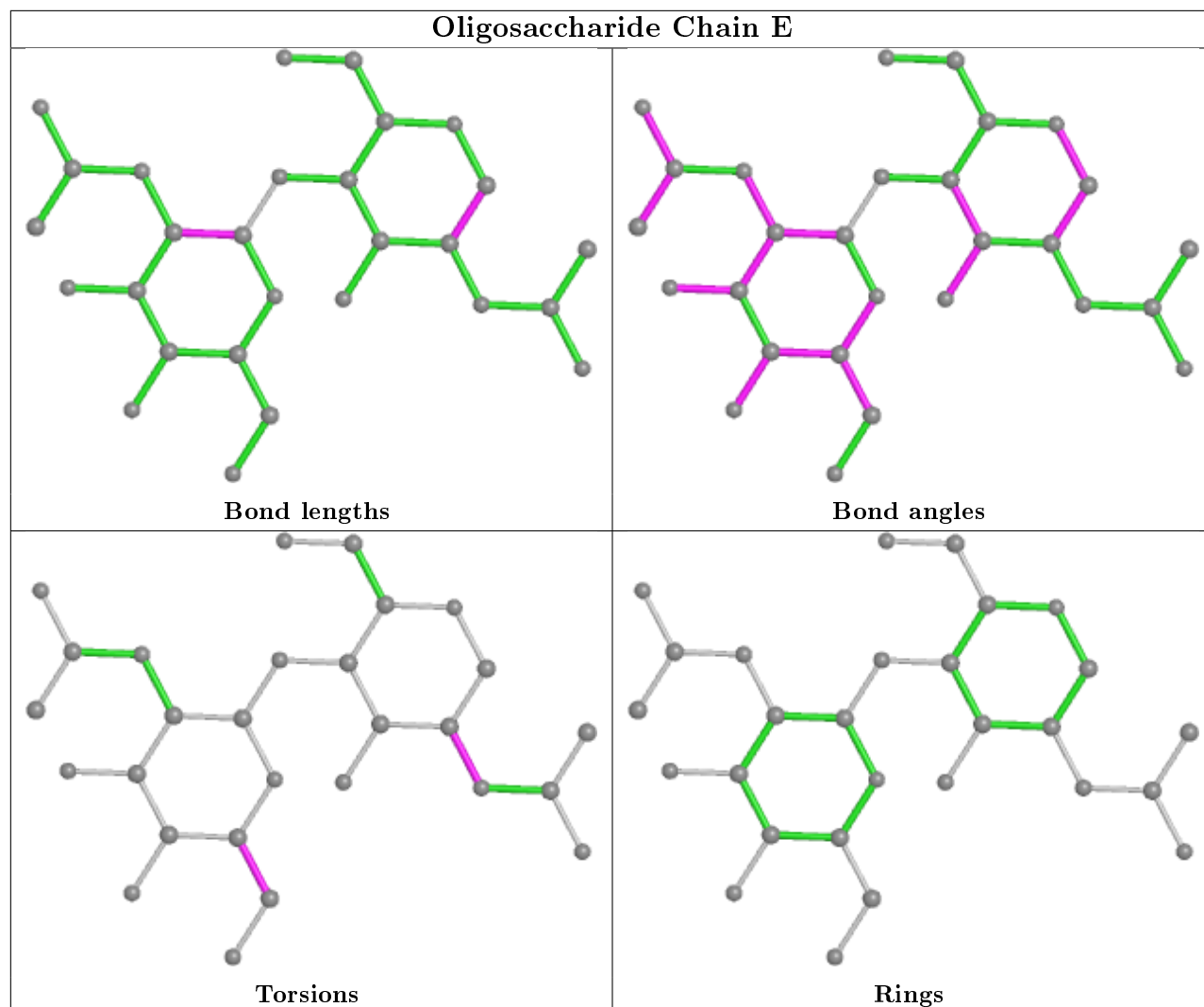
Mol	Chain	Res	Type	Atoms
3	H	1	NAG	C8-C7-N2-C2
3	H	1	NAG	O7-C7-N2-C2
3	E	2	NAG	O5-C5-C6-O6
3	E	2	NAG	C4-C5-C6-O6
4	F	1	NAG	C8-C7-N2-C2
4	F	1	NAG	O7-C7-N2-C2
3	H	2	NAG	O5-C5-C6-O6
3	G	2	NAG	C4-C5-C6-O6
3	G	2	NAG	O5-C5-C6-O6
3	G	1	NAG	C8-C7-N2-C2
3	G	1	NAG	O7-C7-N2-C2
3	E	1	NAG	C3-C2-N2-C7
3	H	1	NAG	C1-C2-N2-C7

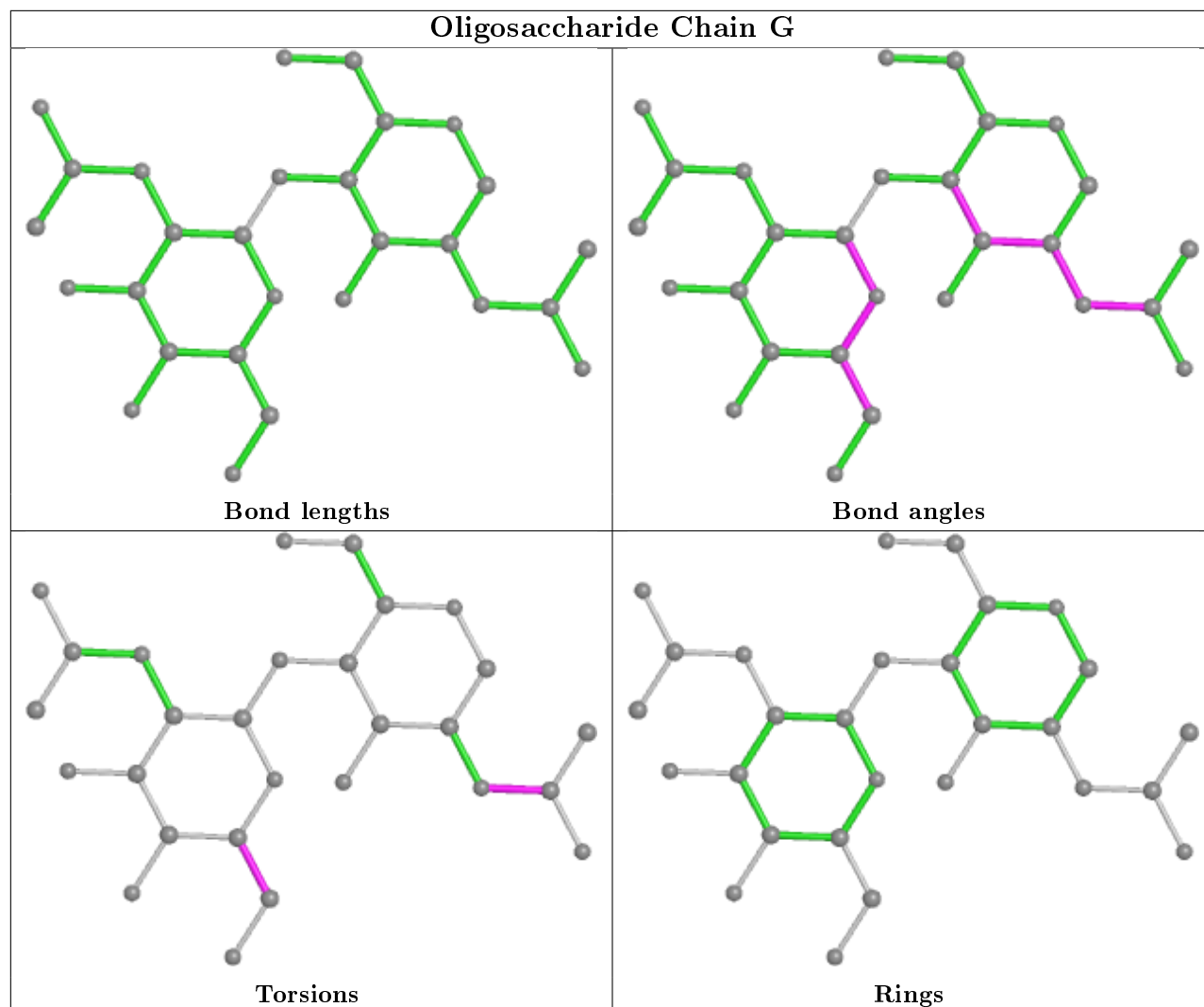
There are no ring outliers.

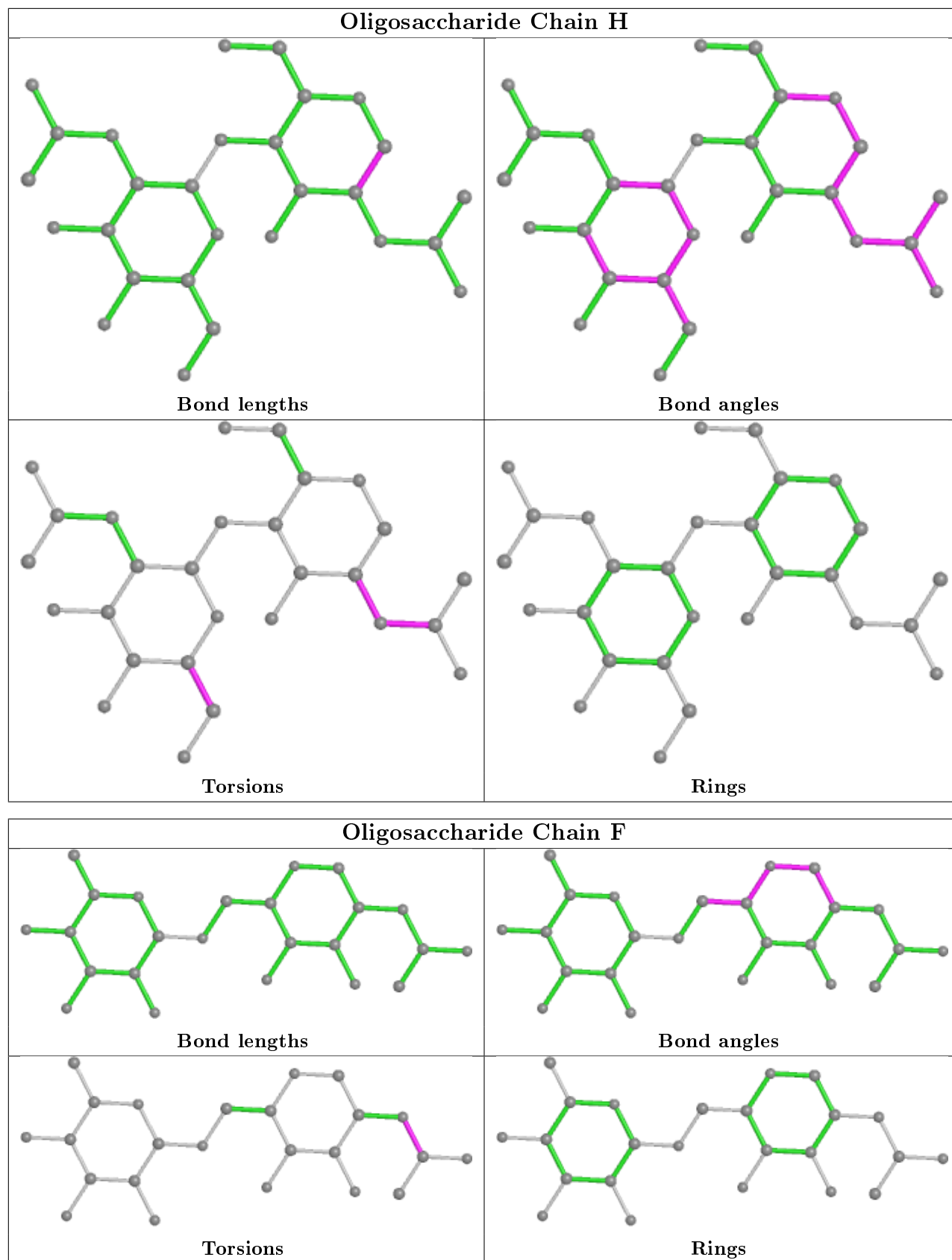
5 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	F	2	FUC	1	0
3	E	2	NAG	1	0
3	G	1	NAG	1	0
3	H	1	NAG	4	0
3	E	1	NAG	2	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

5 ligands 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$
5	FUC	A	531	-	10,10,11	0.56	0	14,14,16	1.28	2 (14%)
6	SLF	C	602	-	38,39,55	0.47	0	39,41,66	1.62	6 (15%)
5	FUC	C	532	-	10,10,11	0.65	0	14,14,16	1.20	2 (14%)
7	NAG	C	511	1	14,14,15	0.61	0	17,19,21	1.18	2 (11%)
6	SLF	A	601	-	54,55,55	1.01	3 (5%)	59,66,66	1.74	13 (22%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	FUC	A	531	-	-	-	0/1/1/1
6	SLF	C	602	-	1/1/3/12	20/42/42/72	-
5	FUC	C	532	-	-	-	0/1/1/1
7	NAG	C	511	1	-	3/6/23/26	0/1/1/1
6	SLF	A	601	-	-	21/52/72/72	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	601	SLF	O-C36	4.63	1.48	1.40
6	A	601	SLF	O5-S	3.27	1.66	1.57
6	A	601	SLF	C2-C3	2.05	1.53	1.50

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	C	602	SLF	C-C1-N	5.50	118.02	109.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	601	SLF	O-C36-C37	4.99	116.09	108.30
6	A	601	SLF	C41-C40-C39	-4.96	101.38	113.00
6	A	601	SLF	C2-C1-N	-4.11	102.56	110.01
6	A	601	SLF	C-C1-N	4.02	115.54	109.61
6	C	602	SLF	O1-C2-C3	-3.87	100.48	110.85
6	C	602	SLF	C19-C18-N	-3.86	109.13	115.83
6	A	601	SLF	C-O-C36	3.85	121.27	113.74
6	A	601	SLF	O8-C40-C41	3.75	115.76	106.44
6	C	602	SLF	C1-N-C18	3.75	129.80	123.48
6	A	601	SLF	C37-C38-C39	-3.22	106.22	110.85
5	A	531	FUC	C1-C2-C3	3.11	113.49	109.67
5	A	531	FUC	O5-C1-C2	2.82	115.12	110.77
7	C	511	NAG	C1-C2-N2	2.76	115.20	110.49
6	A	601	SLF	O8-C40-C39	2.71	114.62	109.69
6	A	601	SLF	C1-N-C18	2.70	128.04	123.48
5	C	532	FUC	C1-C2-C3	2.66	112.94	109.67
6	A	601	SLF	C20-C19-C18	-2.42	106.48	113.26
7	C	511	NAG	C2-N2-C7	2.41	126.33	122.90
6	C	602	SLF	C2-C1-N	2.36	114.28	110.01
6	A	601	SLF	C38-O5-S	2.26	123.24	118.88
5	C	532	FUC	O5-C1-C2	2.13	114.06	110.77
6	A	601	SLF	C36-C37-C38	2.06	113.69	110.07
6	C	602	SLF	O2-C18-C19	-2.04	118.28	122.02
6	A	601	SLF	O8-C36-C37	-2.01	106.10	110.35

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
6	C	602	SLF	C1

All (44) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	C	602	SLF	O-C-C1-C2
6	C	602	SLF	N-C1-C2-O1
6	C	602	SLF	N-C1-C2-C3
6	C	602	SLF	C1-C2-C3-C4
6	C	602	SLF	O1-C2-C3-C4
7	C	511	NAG	C1-C2-N2-C7
7	C	511	NAG	C8-C7-N2-C2
7	C	511	NAG	O7-C7-N2-C2
6	A	601	SLF	O-C-C1-N

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Mol	Chain	Res	Type	Atoms
6	A	601	SLF	O-C-C1-C2
6	A	601	SLF	O8-C36-O-C
6	A	601	SLF	C37-C36-O-C
6	A	601	SLF	C39-C38-O5-S
6	C	602	SLF	O2-C18-N-C1
6	A	601	SLF	C11-C12-C13-C14
6	A	601	SLF	C22-C23-C24-C25
6	C	602	SLF	C27-C28-C29-C30
6	A	601	SLF	C27-C28-C29-C30
6	C	602	SLF	N-C18-C19-C20
6	A	601	SLF	C-C1-N-C18
6	C	602	SLF	C11-C12-C13-C14
6	C	602	SLF	C12-C13-C14-C15
6	A	601	SLF	C9-C10-C11-C12
6	C	602	SLF	C4-C5-C6-C7
6	C	602	SLF	C21-C22-C23-C24
6	A	601	SLF	C11-C10-C9-C8
6	A	601	SLF	C24-C25-C26-C27
6	C	602	SLF	C3-C4-C5-C6
6	A	601	SLF	C2-C1-N-C18
6	C	602	SLF	C11-C10-C9-C8
6	C	602	SLF	C-C1-C2-C3
6	A	601	SLF	C37-C38-O5-S
6	C	602	SLF	C23-C24-C25-C26
6	C	602	SLF	C7-C8-C9-C10
6	A	601	SLF	C13-C14-C15-C16
6	A	601	SLF	C30-C31-C32-C33
6	A	601	SLF	O2-C18-C19-C20
6	C	602	SLF	O2-C18-C19-C20
6	A	601	SLF	C14-C15-C16-C17
6	C	602	SLF	C13-C14-C15-C16
6	A	601	SLF	N-C18-C19-C20
6	C	602	SLF	O-C-C1-N
6	A	601	SLF	C3-C4-C5-C6
6	A	601	SLF	C10-C11-C12-C13

There are no ring outliers.

4 monomers are involved in 22 short contacts:

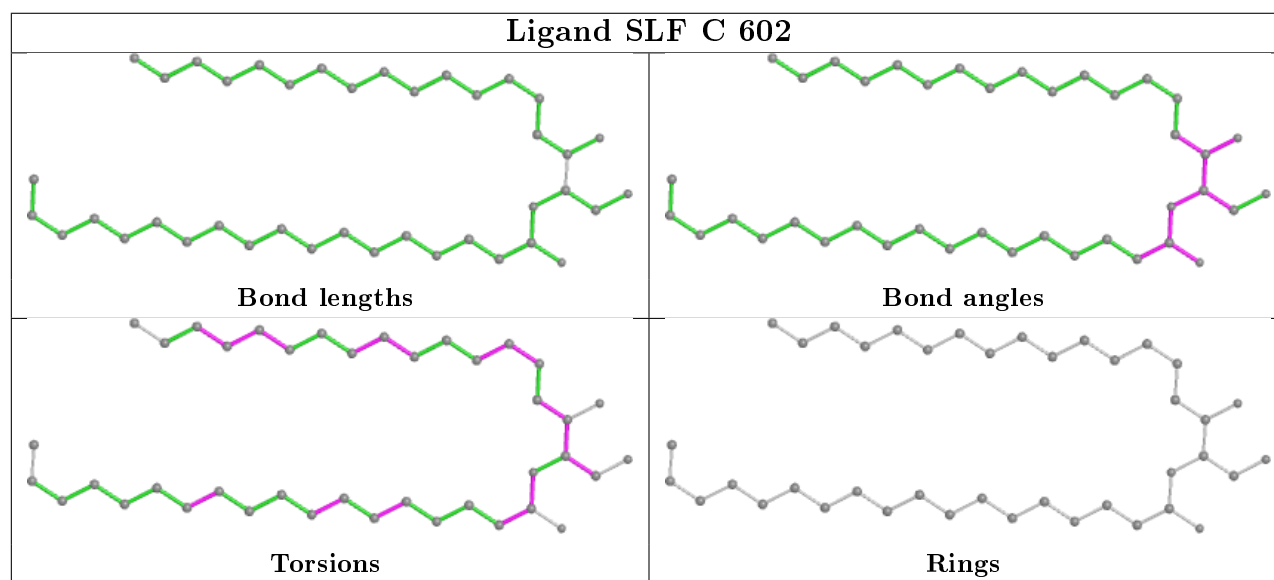
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	531	FUC	2	0
6	C	602	SLF	3	0

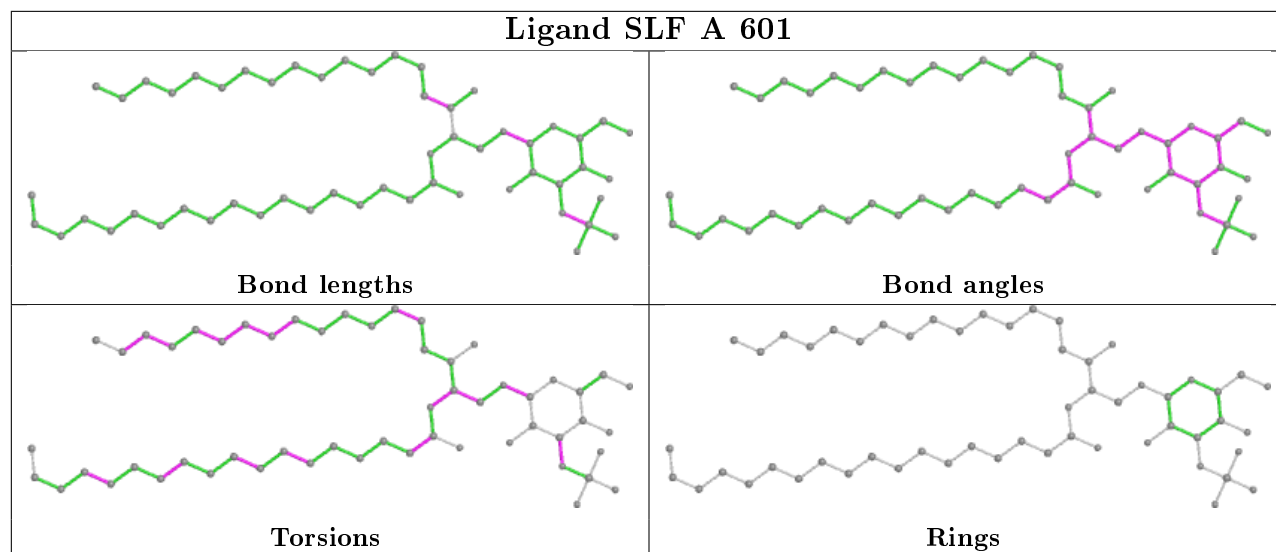
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	C	532	FUC	1	0
6	A	601	SLF	16	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	274/283 (96%)	0.43	12 (4%) 34 43	6, 14, 24, 29	0
1	C	273/283 (96%)	0.60	22 (8%) 12 16	7, 14, 21, 25	0
2	B	99/99 (100%)	0.14	0 100 100	10, 15, 21, 27	0
2	D	99/99 (100%)	0.44	4 (4%) 38 47	9, 15, 19, 25	0
All	All	745/764 (97%)	0.45	38 (5%) 28 36	6, 15, 22, 29	0

All (38) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	109	VAL	7.9
1	C	21	HIS	5.8
1	C	107	GLY	5.4
1	A	23	TRP	5.3
1	C	23	TRP	5.2
1	C	105	HIS	4.4
1	C	20	ASN	4.4
1	A	21	HIS	4.2
2	D	99	MET	4.1
1	A	110	SER	3.9
2	D	75	LYS	3.9
1	C	19	TYR	3.9
1	C	279	HIS	3.9
1	A	20	ASN	3.6
2	D	18	GLY	3.5
1	C	110	SER	3.5
1	C	106	SER	3.5
1	C	108	LYS	3.5
1	C	269	GLU	3.4
1	A	19	TYR	3.4
1	C	22	SER	3.3

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Mol	Chain	Res	Type	RSRZ
2	D	73	THR	3.3
1	C	254	GLY	3.3
1	C	196	SER	3.2
1	A	105	HIS	3.0
1	A	254	GLY	2.9
1	A	91	GLU	2.6
1	A	107	GLY	2.5
1	C	278	HIS	2.4
1	C	153	HIS	2.4
1	C	199	PRO	2.3
1	C	104	LEU	2.3
1	C	86	HIS	2.2
1	A	7	PRO	2.2
1	A	13	ILE	2.1
1	C	7	PRO	2.1
1	C	25	GLN	2.1
1	A	104	LEU	2.1

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

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

6.3 Carbohydrates ⓘ

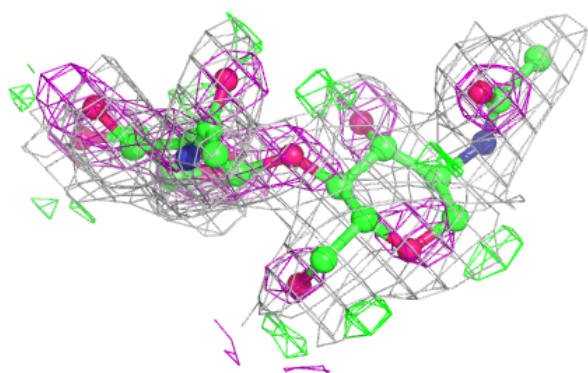
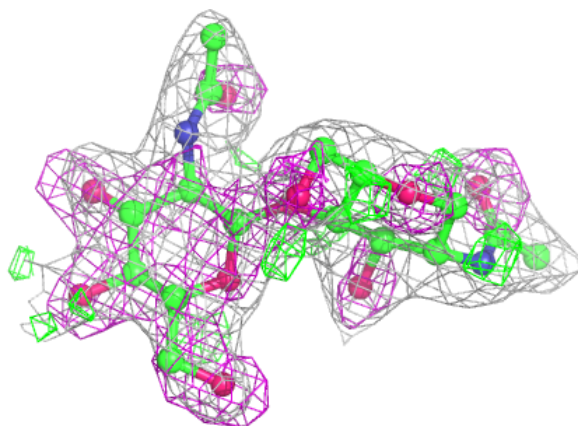
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	NAG	F	1	14/15	0.74	0.53	29,30,32,33	0
4	FUC	F	2	10/11	0.80	0.35	27,27,28,29	0
3	NAG	H	1	14/15	0.83	0.32	12,14,15,17	0
3	NAG	G	2	14/15	0.86	0.36	14,16,19,20	0
3	NAG	H	2	14/15	0.87	0.41	16,17,17,18	0
3	NAG	E	2	14/15	0.88	0.30	12,15,18,20	0
3	NAG	G	1	14/15	0.88	0.34	13,14,16,18	0
3	NAG	E	1	14/15	0.92	0.18	8,12,15,16	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.

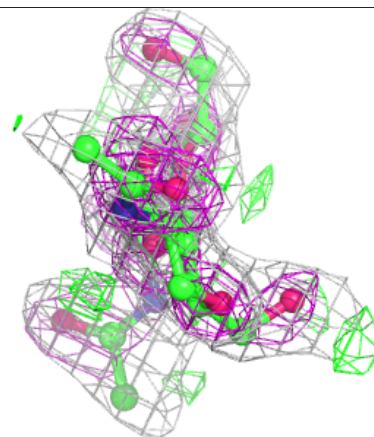
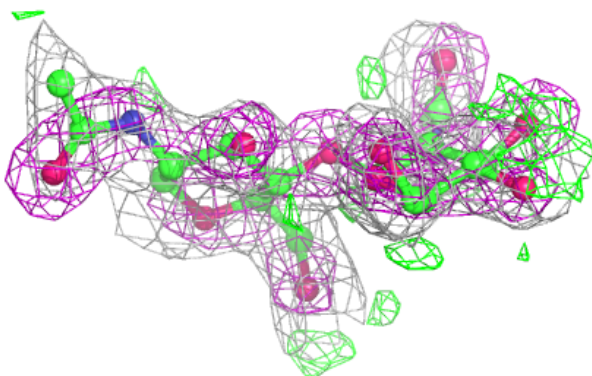
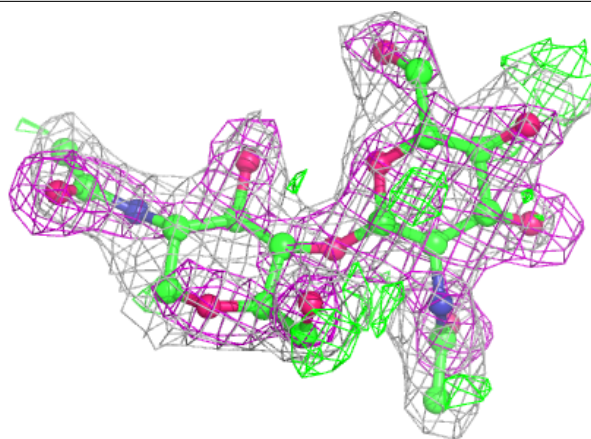
Electron density around Chain E:

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



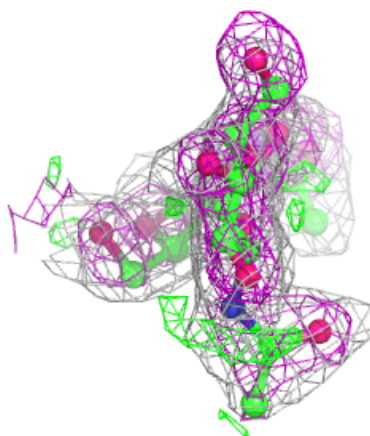
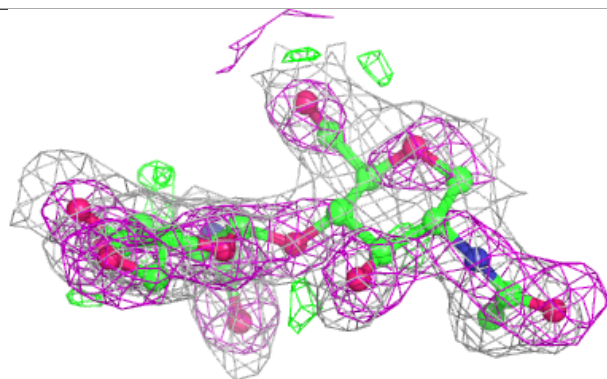
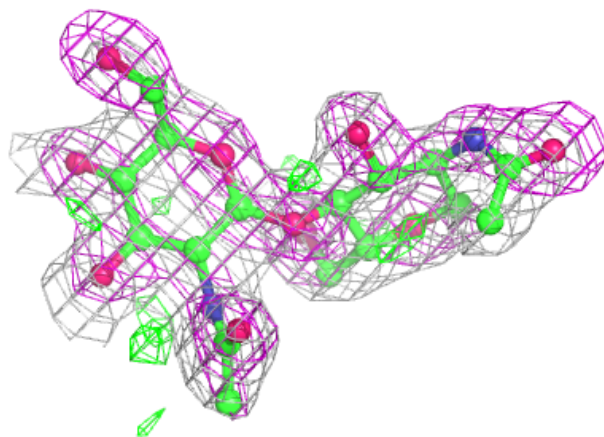
Electron density around Chain G:

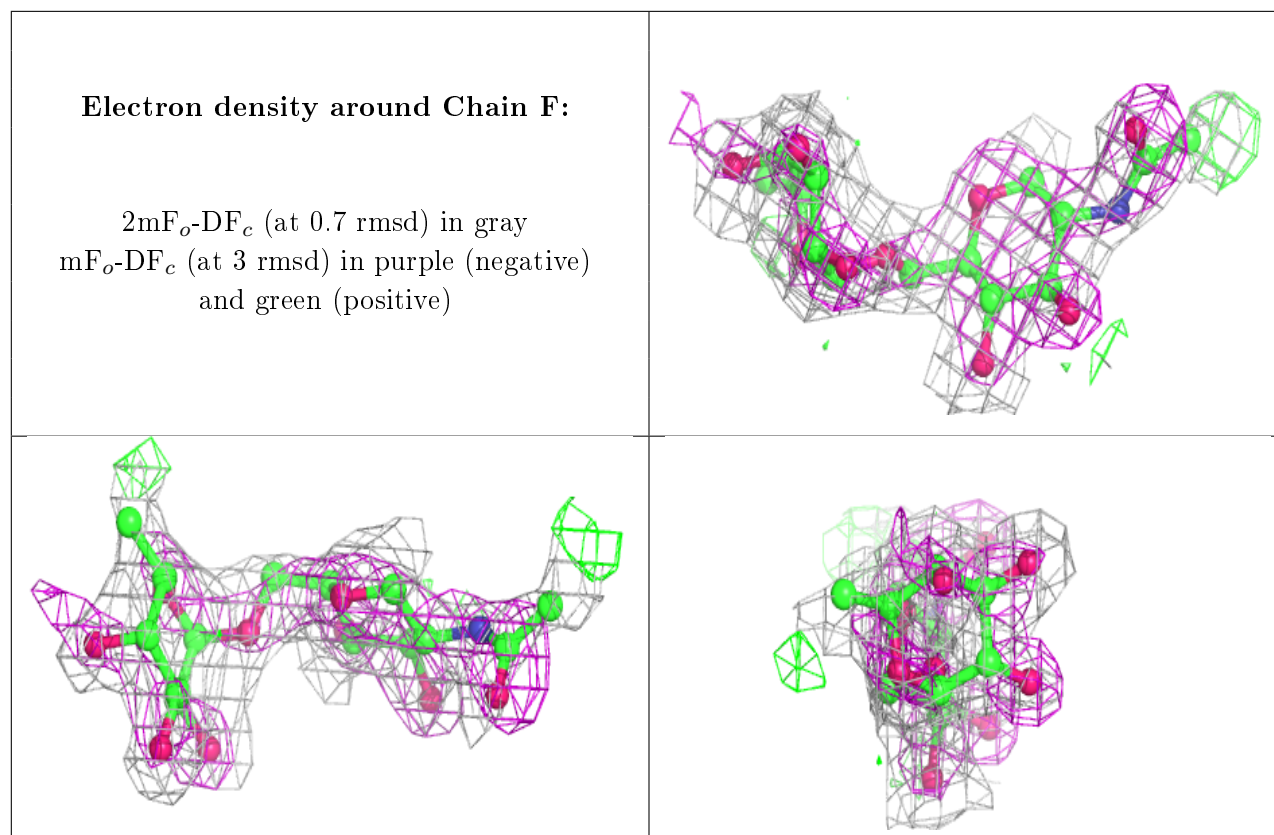
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around Chain H:

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





6.4 Ligands [i](#)

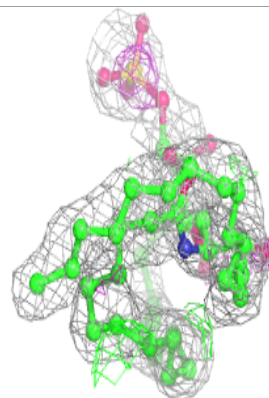
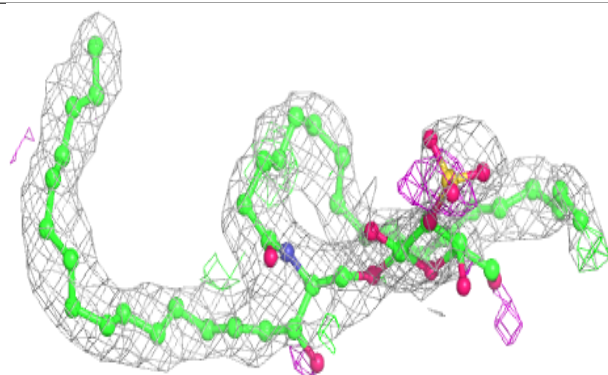
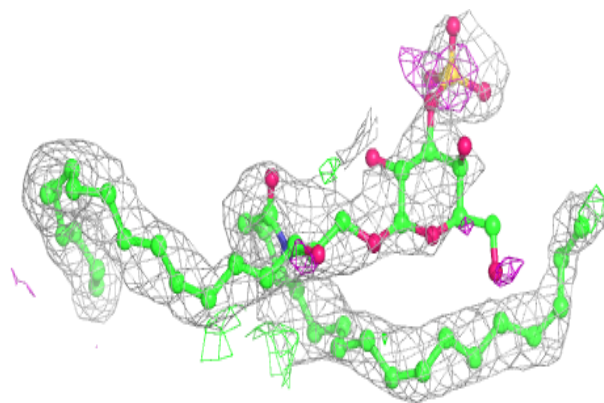
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
6	SLF	A	601	55/55	0.57	0.28	18,32,44,46	0
6	SLF	C	602	40/55	0.63	0.27	18,25,30,32	0
7	NAG	C	511	14/15	0.75	0.27	16,17,18,18	0
5	FUC	C	532	10/11	0.82	0.45	17,18,19,19	0
5	FUC	A	531	10/11	0.85	0.26	21,22,23,23	0

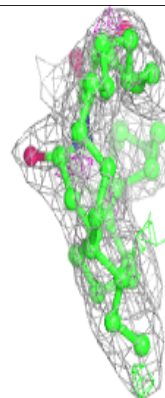
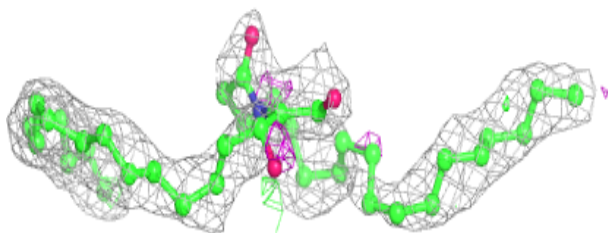
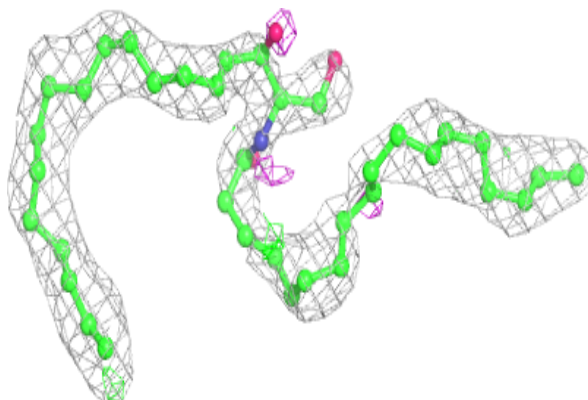
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around SLF A 601:

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

**Electron density around SLF C 602:**

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



6.5 Other polymers

There are no such residues in this entry.