



Full wwPDB X-ray Structure Validation Report ⓘ

Sep 19, 2020 – 09:40 AM BST

PDB ID : 6V7Z
Title : Human CD1d presenting alpha-Galactosylceramide in complex with VHH nanobody 1D22
Authors : Shahine, A.; Rossjohn, J.
Deposited on : 2019-12-10
Resolution : 2.75 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 : 2.14.6
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) : 2.14.6

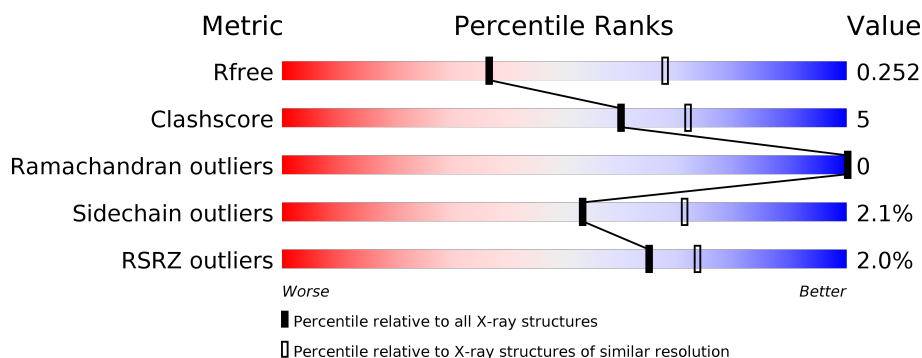
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.75 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.



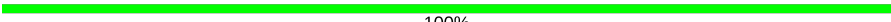
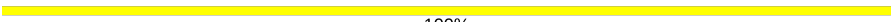


Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1235 (2.78-2.74)
Clashscore	141614	1277 (2.78-2.74)
Ramachandran outliers	138981	1257 (2.78-2.74)
Sidechain outliers	138945	1257 (2.78-2.74)
RSRZ outliers	127900	1207 (2.78-2.74)

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	347	<div> <div>%</div> <div> <div></div> <div>72%</div> <div>7%</div> <div>21%</div> </div> </div>
1	C	347	<div> <div>3%</div> <div> <div></div> <div>66%</div> <div>10%</div> <div>24%</div> </div> </div>
2	B	100	<div> <div>%</div> <div> <div></div> <div>89%</div> <div>9%</div> <div>..</div> </div> </div>
2	D	100	<div> <div>2%</div> <div> <div></div> <div>80%</div> <div>15%</div> <div>..</div> </div> </div>
3	E	118	<div> <div></div> <div> <div></div> <div>94%</div> <div>5%</div> <div>.</div> </div> </div>
3	F	118	<div> <div>3%</div> <div> <div></div> <div>87%</div> <div>12%</div> <div>.</div> </div> </div>

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Mol	Chain	Length	Quality of chain
4	G	2	 100%
4	J	2	 100%
5	H	2	 50%50%
6	I	3	 67%33%

2 Entry composition

There are 14 unique types of molecules in this entry. The entry contains 7908 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 Antigen-presenting glycoprotein CD1d.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	275	Total	C	N	O	S	0	0	0
			2181	1396	376	401	8			
1	C	263	Total	C	N	O	S	0	0	0
			2052	1319	344	382	7			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	4	MET	-	initiating methionine	UNP P15813
C	4	MET	-	initiating methionine	UNP P15813

- 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	1	0
			817	522	141	151	3			
2	D	96	Total	C	N	O	S	0	0	0
			752	485	124	141	2			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	0	MET	-	initiating methionine	UNP P61769
D	0	MET	-	initiating methionine	UNP P61769

- Molecule 3 is a protein called Nanobody VHH ID22.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	117	Total	C	N	O	S	0	1	0
			884	551	156	173	4			
3	F	117	Total	C	N	O	S	0	1	0
			864	537	150	173	4			

- 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	G	2	Total	C	N	O	0	0	0
			28	16	2	10			
4	J	2	Total	C	N	O	0	0	0
			28	16	2	10			

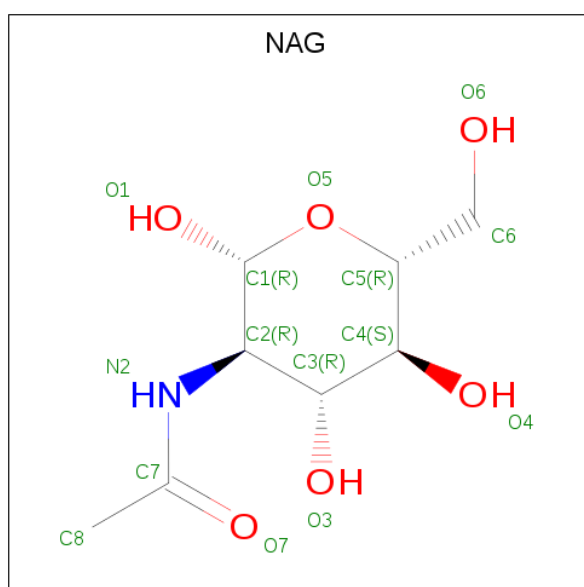
- Molecule 5 is an oligosaccharide called beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	H	2	Total	C	N	O	0	0	0
			25	14	1	10			

- Molecule 6 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.

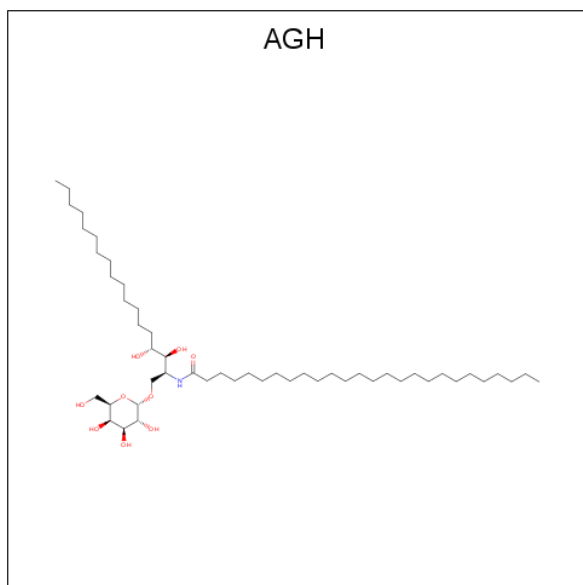
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
6	I	3	Total	C	N	O	0	0	0
			39	22	2	15			

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



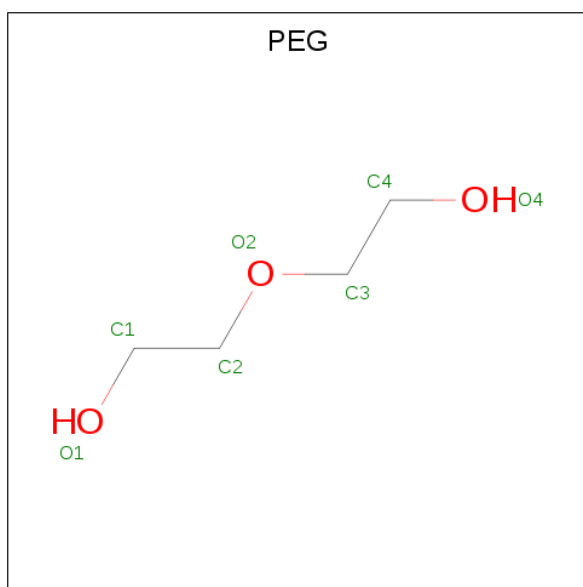
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	A	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 8 is N-{(1S,2R,3S)-1-[(ALPHA-D-GALACTOPYRANOSYLOXY)METHYL]-2,3-DIHYDROXYHEPTADECYL}HEXACOSANAMIDE (three-letter code: AGH) (formula: C₅₀H₉₉NO₉) (labeled as "Ligand of Interest" by author).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	A	1	Total	C	N	O	0	0
			60	50	1	9		
8	C	1	Total	C	N	O	0	0
			60	50	1	9		

- Molecule 9 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: C₄H₁₀O₃).

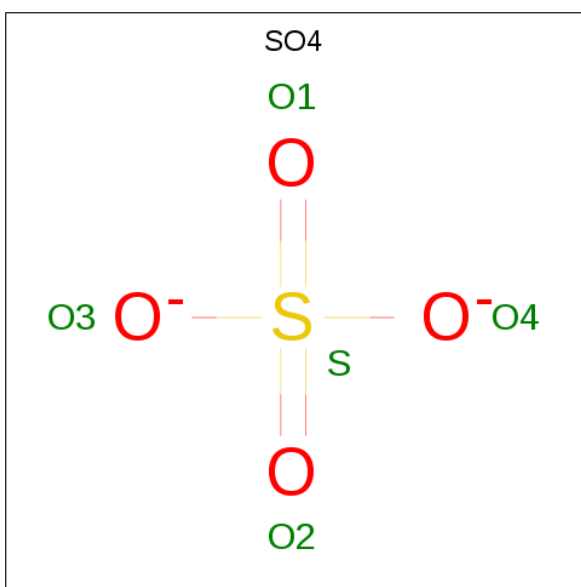


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	A	1	Total	C	O	0	0
			7	4	3		
9	A	1	Total	C	O	0	0
			7	4	3		
9	E	1	Total	C	O	0	0
			7	4	3		

- Molecule 10 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

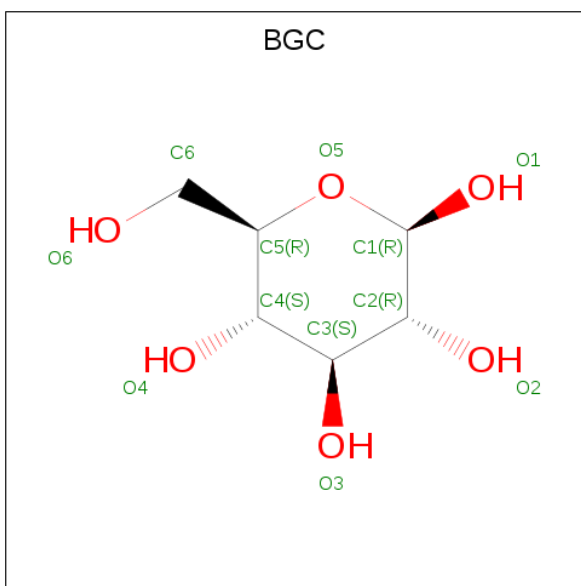
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	1	Total	Cl	0	0
			1	1		

- Molecule 11 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



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

- Molecule 12 is beta-D-glucopyranose (three-letter code: BGC) (formula: C₆H₁₂O₆).



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

- Molecule 13 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
13	D	1	Total Na 1 1	0	0

- Molecule 14 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
14	A	13	Total O 13 13	0	0
14	B	17	Total O 17 17	0	0
14	C	19	Total O 19 19	0	0
14	D	5	Total O 5 5	0	0
14	E	4	Total O 4 4	0	0
14	F	6	Total O 6 6	0	0



- Molecule 3: Nanobody VHH ID22

Chain E: 94% 5%



- Molecule 3: Nanobody VHH ID22

Chain F: 3% 87% 12%



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

Chain G: 100%



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

Chain J: 100%



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

Chain H: 50% 50%



- Molecule 6: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain I: 67% 33%



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	67.72Å 121.93Å 172.14Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	45.31 – 2.75 48.78 – 2.75	Depositor EDS
% Data completeness (in resolution range)	99.9 (45.31-2.75) 100.0 (48.78-2.75)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.04 (at 2.77Å)	Xtriage
Refinement program	PHENIX 1.14 _3260	Depositor
R, R_{free}	0.186 , 0.252 0.188 , 0.252	Depositor DCC
R_{free} test set	1860 reflections (4.91%)	wwPDB-VP
Wilson B-factor (Å ²)	71.1	Xtriage
Anisotropy	0.361	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 54.6	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	0.95	EDS
Total number of atoms	7908	wwPDB-VP
Average B, all atoms (Å ²)	78.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.28% 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: BGC, NAG, CL, NA, AGH, BMA, SO4, PEG

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	0.46	0/2246	0.65	0/3061
1	C	0.44	0/2113	0.65	1/2888 (0.0%)
2	B	0.49	0/843	0.66	0/1144
2	D	0.42	0/774	0.60	0/1057
3	E	0.48	0/903	0.66	0/1221
3	F	0.42	0/883	0.61	0/1199
All	All	0.45	0/7762	0.64	1/10570 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	191	LEU	CB-CG-CD1	-7.10	98.94	111.00

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2181	0	2087	16	0
1	C	2052	0	1900	28	0
2	B	817	0	775	7	0
2	D	752	0	674	12	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	E	884	0	850	2	0
3	F	864	0	802	11	0
4	G	28	0	25	0	0
4	J	28	0	25	0	0
5	H	25	0	22	0	0
6	I	39	0	34	0	0
7	A	14	0	13	0	0
8	A	60	0	99	3	0
8	C	60	0	99	7	0
9	A	14	0	20	0	0
9	E	7	0	10	0	0
10	A	1	0	0	0	0
11	B	5	0	0	0	0
12	B	12	0	12	0	0
13	D	1	0	0	0	0
14	A	13	0	0	0	0
14	B	17	0	0	0	0
14	C	19	0	0	1	0
14	D	5	0	0	0	0
14	E	4	0	0	0	0
14	F	6	0	0	0	0
All	All	7908	0	7447	70	0

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

All (70) 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:C:61:GLN:OE1	14:C:501:HOH:O	1.98	0.80
1:A:154:THR:HG23	8:A:402:AGH:HAB2	1.69	0.74
1:C:154:THR:HG23	8:C:401:AGH:HAB2	1.73	0.70
2:B:0:MET:HB3	3:F:104:GLU:OE2	1.93	0.68
1:A:187:PRO:HB3	1:A:211:PHE:HB3	1.78	0.65
1:A:47:VAL:HG11	8:A:402:AGH:HAQ1	1.78	0.65
3:F:23:ALA:HA	3:F:77:THR:HG22	1.78	0.64
2:D:4:THR:HG22	2:D:86:THR:HB	1.82	0.62
2:D:21:ASN:HB3	2:D:70:PHE:HE2	1.64	0.62
1:C:190:TRP:CE3	2:D:14:PRO:HG3	2.35	0.61
1:C:70:PHE:HE1	8:C:401:AGH:HAH1	1.67	0.59
1:A:30:ALA:HB2	8:A:402:AGH:HAP2	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:76:ASP:N	2:D:76:ASP:OD2	2.37	0.57
3:F:1:GLN:N	3:F:1:GLN:OE1	2.36	0.57
1:C:191:LEU:N	1:C:191:LEU:HD12	2.21	0.56
2:B:45:ARG:HH12	2:B:47:GLU:HG2	1.71	0.55
1:C:49:SER:HB3	1:C:54:SER:HB2	1.88	0.55
1:A:49:SER:HB3	1:A:54:SER:HB2	1.89	0.55
2:D:19:LYS:O	2:D:72:PRO:HD2	2.06	0.55
1:C:275:LEU:HD12	1:C:275:LEU:C	2.27	0.55
2:B:0:MET:H2	1:C:68:HIS:CE1	2.25	0.55
1:C:217:TRP:CE3	1:C:264:LYS:HD2	2.43	0.54
1:C:94:LEU:HD22	1:C:118:PHE:HE1	1.72	0.54
2:B:4:THR:HG22	2:B:86:THR:HB	1.89	0.54
1:C:221:MET:SD	1:C:226:GLU:HG2	2.49	0.53
1:C:191:LEU:HD11	1:C:275:LEU:CD1	2.39	0.53
1:C:148:LEU:HD23	3:F:1:GLN:NE2	2.24	0.53
3:F:90:THR:HG23	3:F:115:THR:HA	1.91	0.53
2:D:21:ASN:HB3	2:D:70:PHE:CE2	2.42	0.52
3:F:84:SER:OG	3:F:84:SER:O	2.26	0.52
1:C:61:GLN:O	1:C:65:THR:HG23	2.11	0.51
1:A:161:LEU:HA	1:A:165:THR:HB	1.94	0.50
1:C:219:LYS:HA	1:C:230:THR:HG21	1.92	0.49
1:A:146:GLN:OE1	3:F:58:ASN:HB2	2.12	0.49
2:D:70:PHE:C	2:D:70:PHE:CD2	2.85	0.49
1:A:61:GLN:O	1:A:65:THR:HG23	2.13	0.49
1:C:191:LEU:HD12	1:C:191:LEU:H	1.76	0.49
2:D:21:ASN:O	2:D:70:PHE:HD2	1.96	0.49
1:C:105:HIS:HB3	1:C:106:PRO:HD2	1.94	0.49
1:A:249:LEU:HG	1:A:251:VAL:HG13	1.95	0.48
1:C:191:LEU:HD11	1:C:275:LEU:HD13	1.95	0.47
1:A:239:ALA:HB3	2:B:12[B]:ARG:NH2	2.29	0.47
1:C:70:PHE:CE1	8:C:401:AGH:HAH1	2.49	0.46
3:F:102:PHE:HD1	3:F:105[B]:TYR:HH	1.62	0.45
1:A:217:TRP:HB3	1:A:264:LYS:HB2	2.00	0.44
1:C:55:GLN:NE2	1:C:58:PHE:O	2.46	0.44
1:A:190:TRP:CD2	2:B:14:PRO:HG3	2.52	0.44
1:C:96:LEU:HD21	8:C:401:AGH:H172	1.99	0.44
2:D:41:LYS:HB2	2:D:46:ILE:HD11	1.99	0.44
2:D:70:PHE:CD2	2:D:70:PHE:O	2.71	0.43
1:C:7:LEU:HD23	1:C:7:LEU:HA	1.74	0.43
1:A:166:CYS:O	1:A:170:VAL:HG12	2.18	0.43
3:E:82:MET:HE2	3:E:85:LEU:HD21	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:42:GLY:O	3:E:43:LYS:HD2	2.19	0.43
3:F:1:GLN:N	3:F:1:GLN:CD	2.72	0.43
2:D:51:HIS:HB3	2:D:66:TYR:CD1	2.54	0.42
1:C:94:LEU:HD22	1:C:118:PHE:CE1	2.53	0.42
1:C:40:TRP:CH2	1:C:70:PHE:HB3	2.55	0.42
1:C:187:PRO:HB3	1:C:211:PHE:HB3	2.02	0.41
1:A:189:ALA:HA	1:A:207:HIS:O	2.21	0.41
2:D:37:VAL:HB	2:D:66:TYR:CE2	2.55	0.41
3:F:75:LYS:O	3:F:77:THR:HG23	2.20	0.41
1:A:197:PRO:HG3	1:A:203:LEU:HB2	2.02	0.41
3:F:38:ARG:HB3	3:F:48:LEU:HD11	2.02	0.41
8:C:401:AGH:HAU1	8:C:401:AGH:HAX2	1.52	0.41
1:C:76:SER:HB3	8:C:401:AGH:O3	2.21	0.41
1:A:203:LEU:HD12	1:A:203:LEU:HA	1.88	0.41
2:B:7:ILE:HB	2:B:93:VAL:HG21	2.02	0.41
1:C:50:LEU:HD23	1:C:50:LEU:HA	1.76	0.41
1:C:73:TYR:CE1	8:C:401:AGH:H72	2.56	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	273/347 (79%)	264 (97%)	9 (3%)	0	100	100
1	C	255/347 (74%)	247 (97%)	8 (3%)	0	100	100
2	B	98/100 (98%)	97 (99%)	1 (1%)	0	100	100
2	D	92/100 (92%)	91 (99%)	1 (1%)	0	100	100
3	E	116/118 (98%)	115 (99%)	1 (1%)	0	100	100
3	F	116/118 (98%)	115 (99%)	1 (1%)	0	100	100
All	All	950/1130 (84%)	929 (98%)	21 (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	234/302 (78%)	231 (99%)	3 (1%)	69	81
1	C	215/302 (71%)	210 (98%)	5 (2%)	50	69
2	B	90/95 (95%)	88 (98%)	2 (2%)	52	70
2	D	78/95 (82%)	74 (95%)	4 (5%)	24	41
3	E	91/92 (99%)	89 (98%)	2 (2%)	52	70
3	F	86/92 (94%)	85 (99%)	1 (1%)	71	82
All	All	794/978 (81%)	777 (98%)	17 (2%)	53	71

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	161	LEU
1	A	192	SER
1	A	246	ARG
2	B	0	MET
2	B	70	PHE
1	C	89	ARG
1	C	110	SER
1	C	191	LEU
1	C	260	SER
1	C	262	ARG
2	D	3	ARG
2	D	11	SER
2	D	57	SER
2	D	70	PHE
3	E	62	SER
3	E	73	ASN
3	F	30	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such

sidechains are listed below:

Mol	Chain	Res	Type
1	C	68	HIS

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 ⓘ

9 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	$\# Z > 2$
4	NAG	G	1	1,4	14,14,15	0.37	0	17,19,21	0.52	0
4	NAG	G	2	4	14,14,15	0.23	0	17,19,21	0.46	0
5	NAG	H	1	1,5	14,14,15	0.35	0	17,19,21	0.59	0
5	BMA	H	2	5	11,11,12	1.52	2 (18%)	15,15,17	1.25	1 (6%)
6	NAG	I	1	1,6	14,14,15	0.64	1 (7%)	17,19,21	0.54	0
6	NAG	I	2	6	14,14,15	0.34	0	17,19,21	0.55	0
6	BMA	I	3	6	11,11,12	1.01	0	15,15,17	0.76	0
4	NAG	J	1	1,4	14,14,15	0.60	0	17,19,21	0.89	1 (5%)
4	NAG	J	2	4	14,14,15	1.61	1 (7%)	17,19,21	1.13	1 (5%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	G	1	1,4	-	2/6/23/26	0/1/1/1
4	NAG	G	2	4	-	0/6/23/26	0/1/1/1
5	NAG	H	1	1,5	-	1/6/23/26	0/1/1/1
5	BMA	H	2	5	-	0/2/19/22	0/1/1/1
6	NAG	I	1	1,6	-	2/6/23/26	0/1/1/1
6	NAG	I	2	6	-	2/6/23/26	0/1/1/1
6	BMA	I	3	6	-	1/2/19/22	0/1/1/1
4	NAG	J	1	1,4	-	0/6/23/26	0/1/1/1
4	NAG	J	2	4	-	2/6/23/26	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	J	2	NAG	O5-C1	5.70	1.52	1.43
5	H	2	BMA	C1-C2	3.21	1.59	1.52
5	H	2	BMA	C2-C3	2.89	1.56	1.52
6	I	1	NAG	O5-C1	2.18	1.47	1.43

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	J	2	NAG	C1-O5-C5	4.47	118.25	112.19
4	J	1	NAG	C1-O5-C5	2.82	116.02	112.19
5	H	2	BMA	C1-C2-C3	2.19	112.36	109.67

There are no chirality outliers.

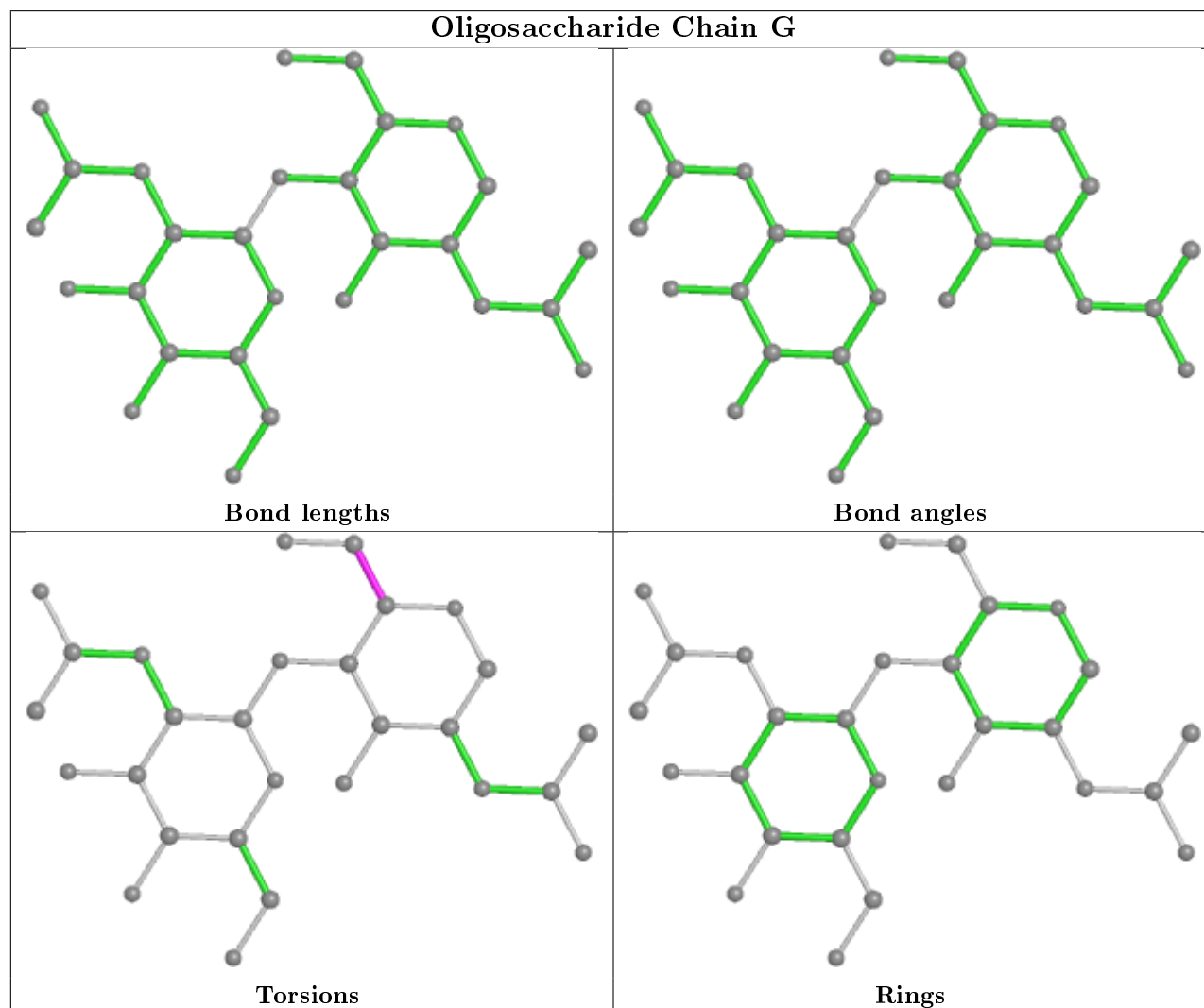
All (10) torsion outliers are listed below:

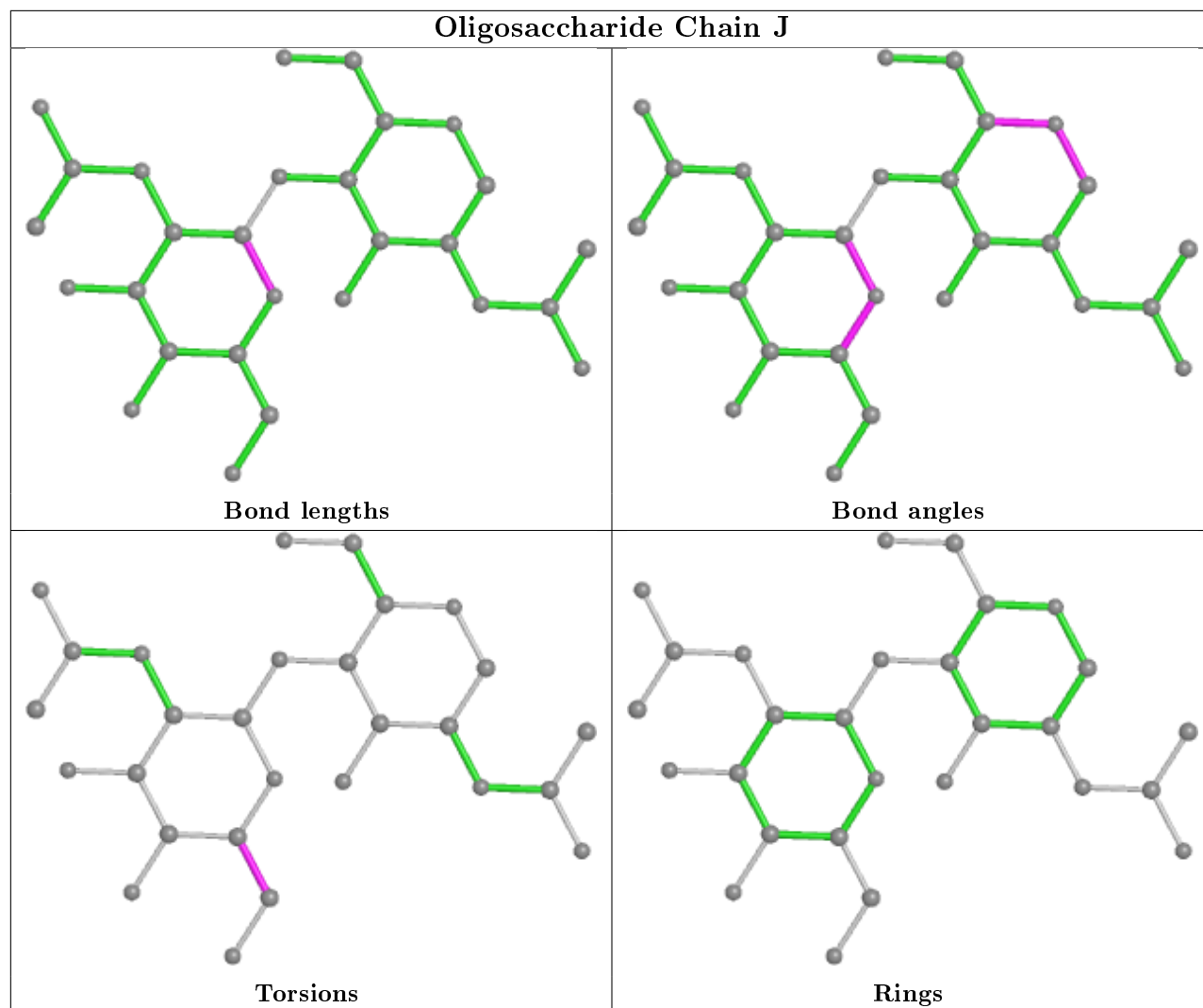
Mol	Chain	Res	Type	Atoms
4	G	1	NAG	O5-C5-C6-O6
4	G	1	NAG	C4-C5-C6-O6
6	I	2	NAG	O5-C5-C6-O6
4	J	2	NAG	C4-C5-C6-O6
6	I	3	BMA	O5-C5-C6-O6
6	I	1	NAG	C4-C5-C6-O6
6	I	1	NAG	O5-C5-C6-O6
4	J	2	NAG	O5-C5-C6-O6
6	I	2	NAG	C4-C5-C6-O6
5	H	1	NAG	O5-C5-C6-O6

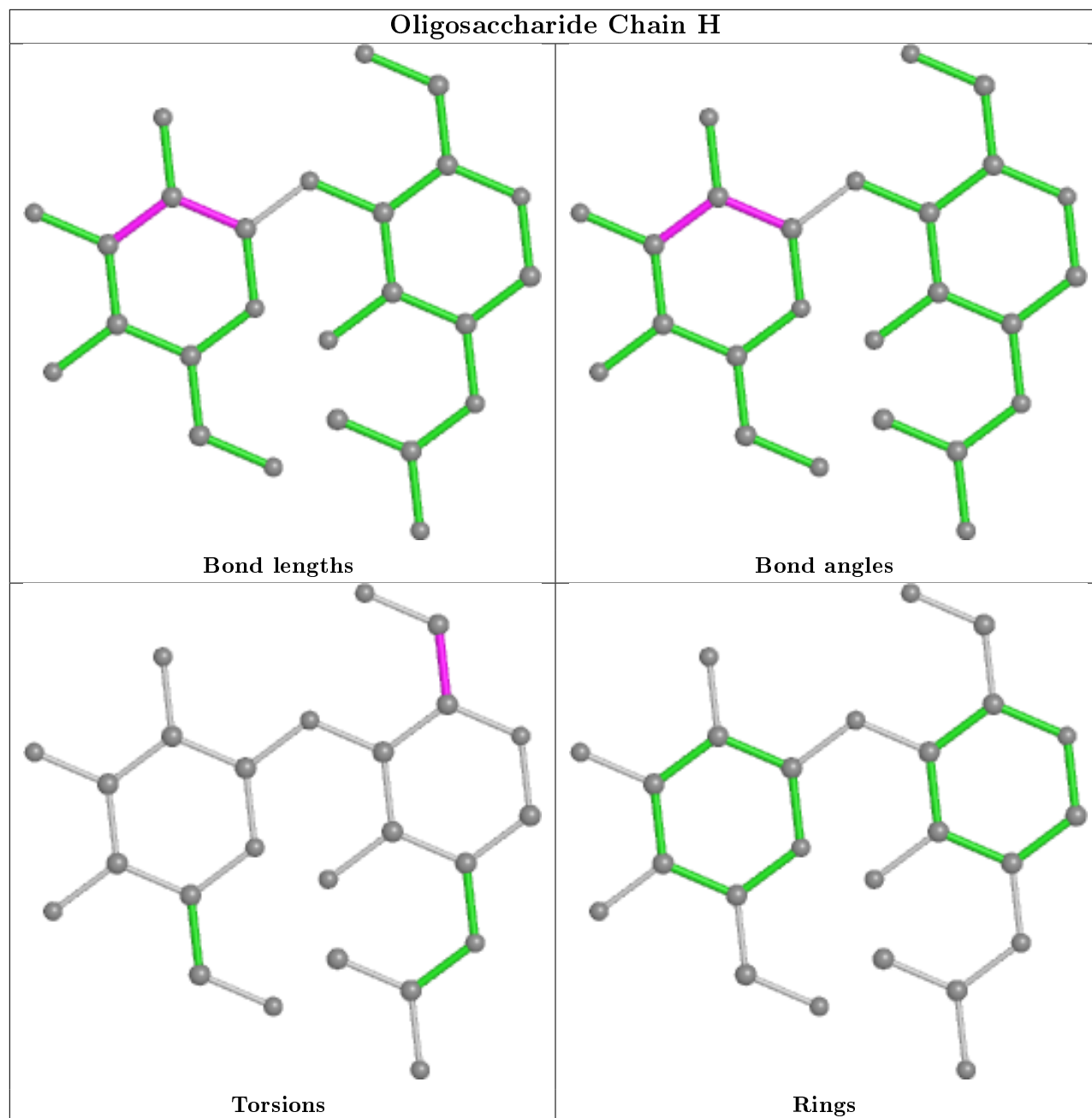
There are no ring outliers.

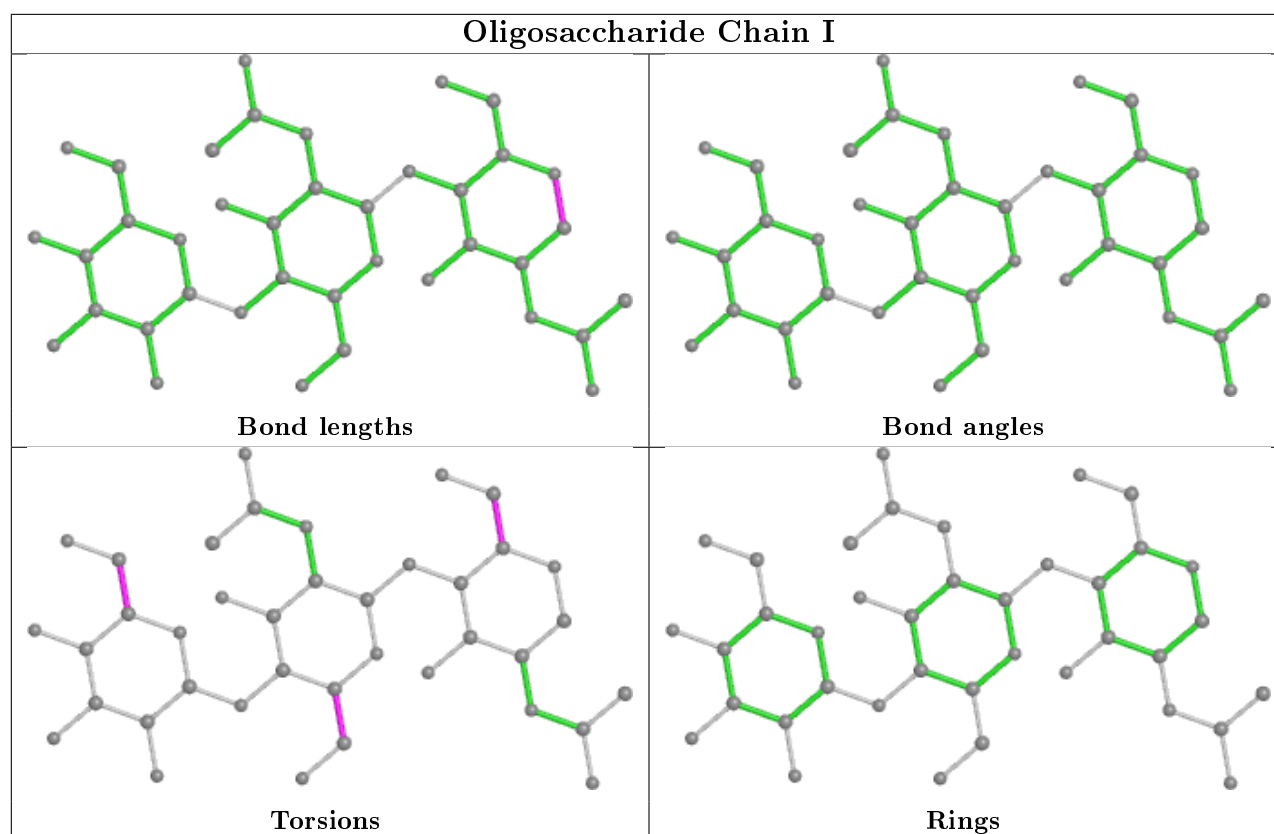
No monomer is involved in short contacts.

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 10 ligands modelled in this entry, 2 are monoatomic - leaving 8 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	$\# Z > 2$
9	PEG	A	403	-	6,6,6	0.48	0	5,5,5	0.44	0
8	AGH	C	401	-	60,60,60	1.36	5 (8%)	65,69,69	1.75	8 (12%)
11	SO4	B	101	-	4,4,4	0.11	0	6,6,6	0.16	0
8	AGH	A	402	-	60,60,60	1.43	5 (8%)	65,69,69	1.01	3 (4%)
9	PEG	E	201	-	6,6,6	0.52	0	5,5,5	0.35	0
7	NAG	A	401	1	14,14,15	0.63	1 (7%)	17,19,21	0.66	0
9	PEG	A	404	-	6,6,6	0.53	0	5,5,5	0.39	0
12	BGC	B	102	-	12,12,12	1.24	1 (8%)	17,17,17	1.79	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
9	PEG	A	403	-	-	1/4/4/4	-
8	AGH	C	401	-	-	22/58/78/78	0/1/1/1
8	AGH	A	402	-	-	18/58/78/78	0/1/1/1
9	PEG	E	201	-	-	3/4/4/4	-
7	NAG	A	401	1	-	0/6/23/26	0/1/1/1
9	PEG	A	404	-	-	2/4/4/4	-
12	BGC	B	102	-	-	2/2/22/22	0/1/1/1

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	A	402	AGH	CAA-N2	6.85	1.48	1.34
8	C	401	AGH	CAA-N2	6.06	1.47	1.34
8	A	402	AGH	OAA-CAA	-3.13	1.16	1.23
8	C	401	AGH	OAA-CAA	-3.06	1.17	1.23
12	B	102	BGC	O5-C1	2.98	1.50	1.42
8	C	401	AGH	O6A-C1A	2.53	1.48	1.41
8	A	402	AGH	O6A-C1A	2.40	1.47	1.41
8	A	402	AGH	CAB-CAA	2.15	1.55	1.51
8	C	401	AGH	O3A-C3A	2.11	1.48	1.43
7	A	401	NAG	C1-C2	2.11	1.55	1.52
8	C	401	AGH	CAB-CAA	2.06	1.55	1.51
8	A	402	AGH	O6A-C5M	2.06	1.49	1.44

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	C	401	AGH	C6-C5-C4	-9.88	97.93	114.18
12	B	102	BGC	C4-C3-C2	3.66	117.21	110.82
8	C	401	AGH	C2-N2-CAA	-3.21	118.06	123.48
12	B	102	BGC	O3-C3-C4	-3.12	103.14	110.35
8	C	401	AGH	O6A-C5M-C4A	2.67	114.55	109.69
8	A	402	AGH	C1-O1A-C1A	2.64	118.91	113.74
12	B	102	BGC	O1-C1-C2	2.64	116.47	109.03
8	C	401	AGH	OAA-CAA-N2	-2.55	118.64	122.95
12	B	102	BGC	O3-C3-C2	2.38	115.85	110.35
8	C	401	AGH	C8-C7-C6	-2.35	102.52	114.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	C	401	AGH	CAE-CAD-CAC	-2.32	102.64	114.42
8	C	401	AGH	CAC-CAB-CAA	-2.29	106.84	113.26
12	B	102	BGC	C1-O5-C5	-2.23	109.46	113.66
8	A	402	AGH	O3-C3-C4	2.20	114.12	108.81
8	C	401	AGH	CAB-CAA-N2	2.05	119.38	115.83
8	A	402	AGH	O6A-C5M-C6A	2.04	111.51	106.44

There are no chirality outliers.

All (48) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	C	401	AGH	CAA-CAB-CAC-CAD
12	B	102	BGC	O5-C5-C6-O6
8	A	402	AGH	CAJ-CAK-CAL-CAM
8	C	401	AGH	CAU-CAV-CAW-CAX
12	B	102	BGC	C4-C5-C6-O6
8	C	401	AGH	C4A-C5M-C6A-O5A
9	A	404	PEG	O1-C1-C2-O2
8	C	401	AGH	C14-C15-C16-C17
8	A	402	AGH	CAS-CAT-CAU-CAV
8	C	401	AGH	CAK-CAL-CAM-CAN
8	A	402	AGH	CAQ-CAR-CAS-CAT
8	C	401	AGH	CAC-CAD-CAE-CAF
8	C	401	AGH	CAJ-CAK-CAL-CAM
8	C	401	AGH	C7-C8-C9-C10
8	A	402	AGH	CAU-CAV-CAW-CAX
8	C	401	AGH	CAH-CAI-CAJ-CAK
8	A	402	AGH	CAG-CAH-CAI-CAJ
8	A	402	AGH	CAF-CAG-CAH-CAI
8	A	402	AGH	C4-C5-C6-C7
8	A	402	AGH	CAT-CAU-CAV-CAW
8	C	401	AGH	CAF-CAG-CAH-CAI
8	A	402	AGH	C14-C15-C16-C17
8	C	401	AGH	CAT-CAU-CAV-CAW
8	C	401	AGH	CAB-CAC-CAD-CAE
9	A	404	PEG	O2-C3-C4-O4
8	C	401	AGH	CAP-CAQ-CAR-CAS
8	C	401	AGH	CAM-CAN-CAO-CAP
8	C	401	AGH	CAR-CAS-CAT-CAU
8	C	401	AGH	C9-C10-C11-C12
8	C	401	AGH	CAV-CAW-CAX-CAY
9	E	201	PEG	C1-C2-O2-C3

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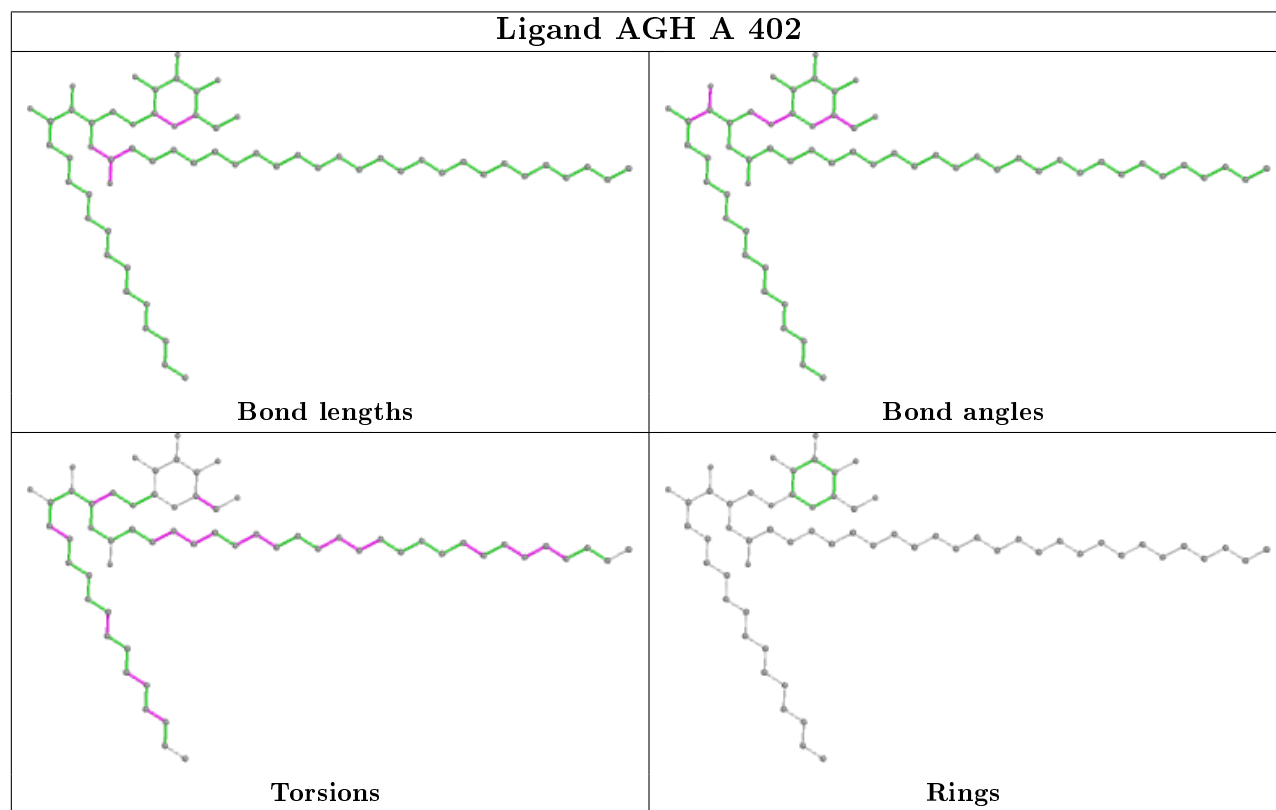
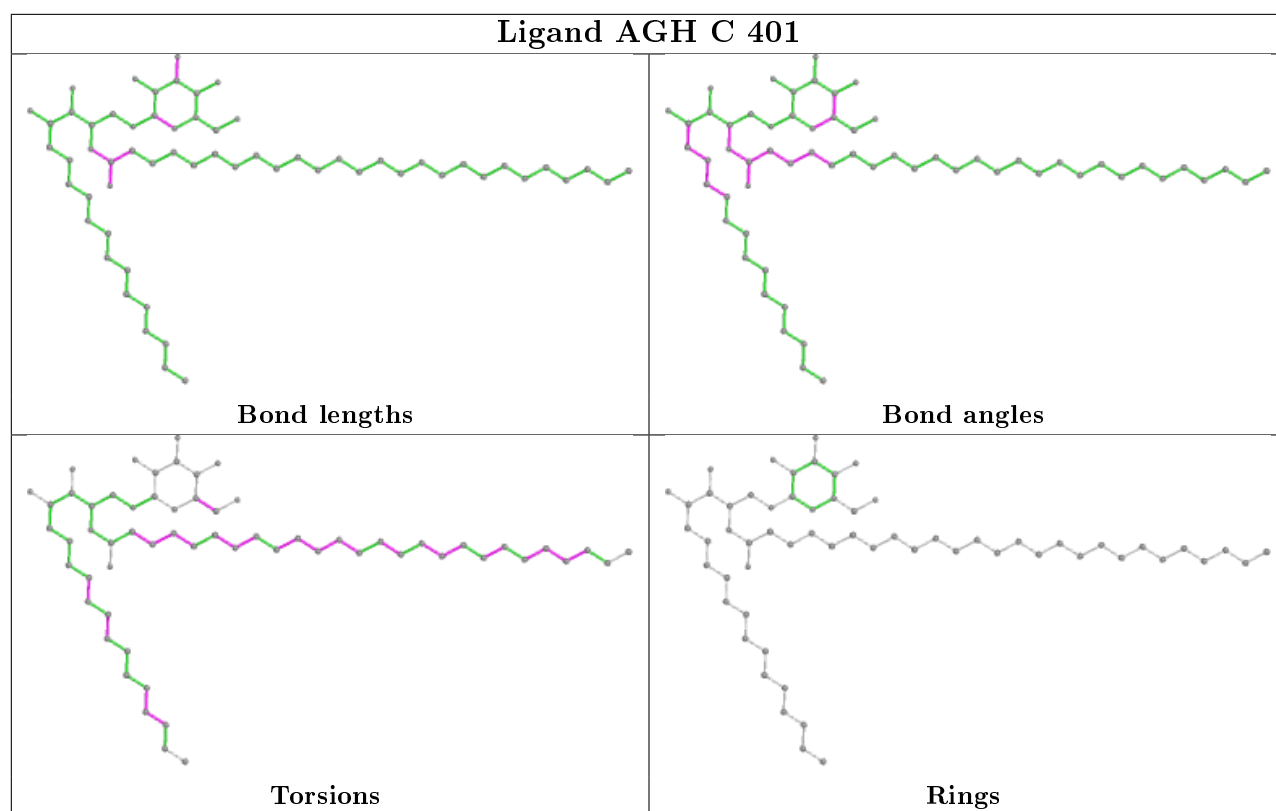
Mol	Chain	Res	Type	Atoms
8	C	401	AGH	C13-C14-C15-C16
8	A	402	AGH	C12-C13-C14-C15
8	A	402	AGH	O1A-C1-C2-C3
8	A	402	AGH	CAL-CAM-CAN-CAO
8	A	402	AGH	CAC-CAD-CAE-CAF
8	A	402	AGH	CAB-CAC-CAD-CAE
9	A	403	PEG	C1-C2-O2-C3
8	C	401	AGH	CAO-CAP-CAQ-CAR
8	A	402	AGH	CAD-CAE-CAF-CAG
8	A	402	AGH	C9-C10-C11-C12
8	C	401	AGH	CAI-CAJ-CAK-CAL
9	E	201	PEG	O1-C1-C2-O2
9	E	201	PEG	O2-C3-C4-O4
8	A	402	AGH	CAK-CAL-CAM-CAN
8	C	401	AGH	CAE-CAF-CAG-CAH
8	C	401	AGH	O6A-C5M-C6A-O5A
8	A	402	AGH	O6A-C5M-C6A-O5A

There are no ring outliers.

2 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	C	401	AGH	7	0
8	A	402	AGH	3	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 ⓘ

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	275/347 (79%)	-0.15	2 (0%) 87 91	42, 64, 103, 143	0
1	C	263/347 (75%)	0.09	11 (4%) 36 43	43, 79, 144, 185	0
2	B	99/100 (99%)	-0.03	1 (1%) 82 87	39, 66, 107, 122	0
2	D	96/100 (96%)	-0.03	2 (2%) 63 72	57, 102, 145, 167	0
3	E	117/118 (99%)	-0.10	0 100 100	39, 69, 106, 136	0
3	F	117/118 (99%)	-0.03	3 (2%) 56 65	47, 84, 130, 141	0
All	All	967/1130 (85%)	-0.04	19 (1%) 65 73	39, 74, 132, 185	0

All (19) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	260	SER	4.4
1	C	259	LEU	3.7
1	C	109	ALA	3.6
1	C	197	PRO	3.6
1	C	204	LEU	3.5
2	B	72	PRO	3.3
1	C	220	TRP	3.2
2	D	40	LEU	3.0
3	F	25	SER	3.0
1	C	104	VAL	2.7
1	C	107	GLY	2.6
3	F	1	GLN	2.5
1	C	249	LEU	2.5
1	A	202	LEU	2.4
3	F	85	LEU	2.4
2	D	35	ILE	2.2
1	C	277	TRP	2.2
1	C	203	LEU	2.1
1	A	106	PRO	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 ⓘ

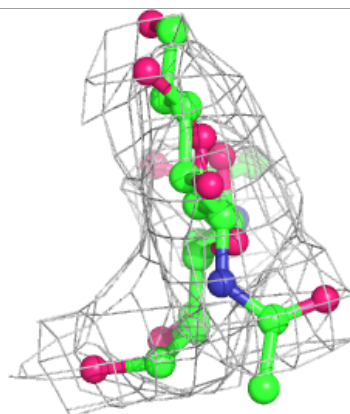
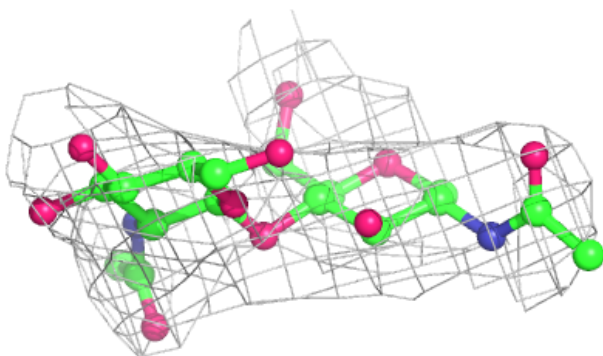
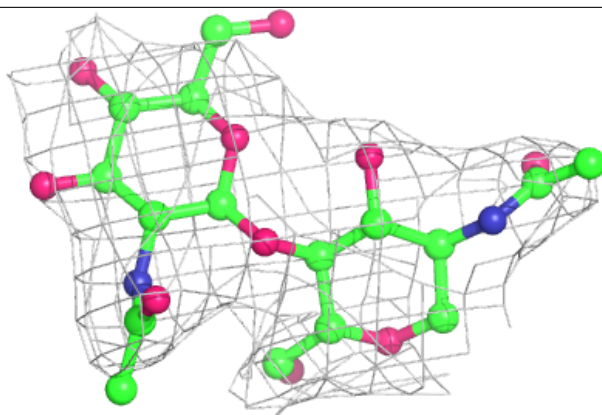
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
6	BMA	I	3	11/12	0.69	0.31	149,155,159,160	0
5	BMA	H	2	11/12	0.84	0.23	95,106,126,139	0
6	NAG	I	2	14/15	0.88	0.17	89,118,133,146	0
4	NAG	G	2	14/15	0.91	0.18	98,109,126,128	0
6	NAG	I	1	14/15	0.92	0.14	72,91,107,107	0
4	NAG	J	2	14/15	0.92	0.14	97,105,112,116	0
4	NAG	G	1	14/15	0.93	0.17	78,90,95,96	0
4	NAG	J	1	14/15	0.98	0.15	47,67,91,92	0
5	NAG	H	1	14/15	0.98	0.13	54,73,87,88	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.

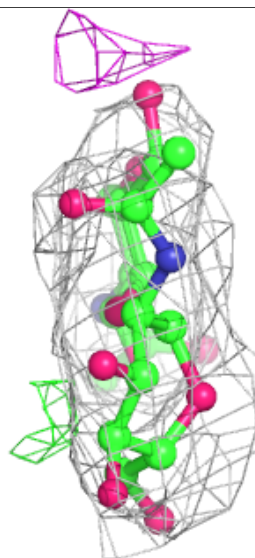
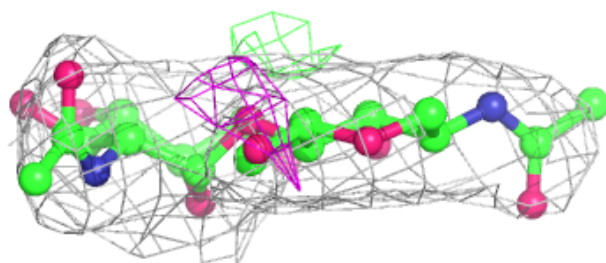
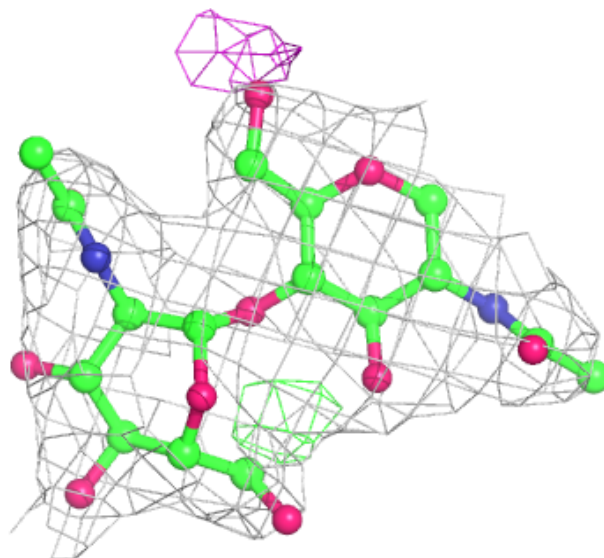
Electron density around Chain G:

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



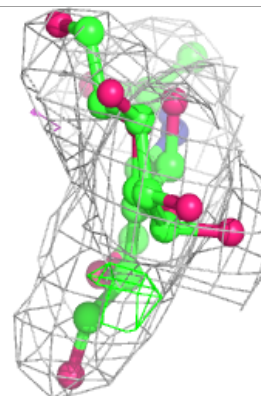
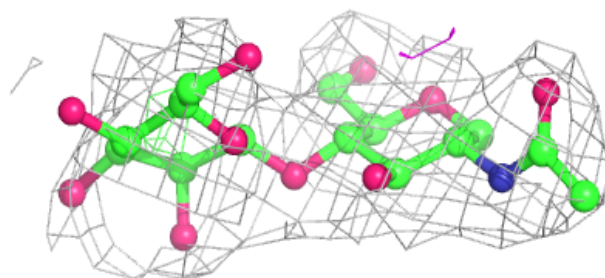
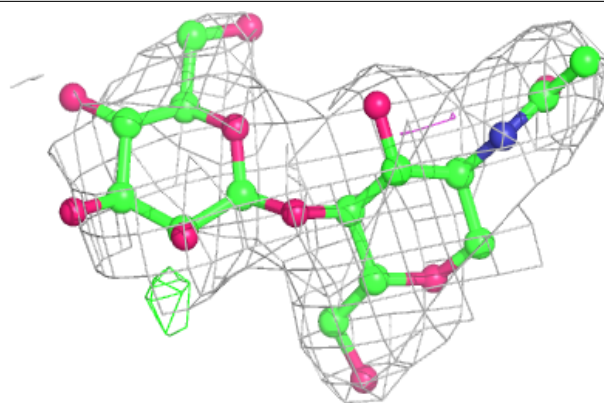
Electron density around Chain J:

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

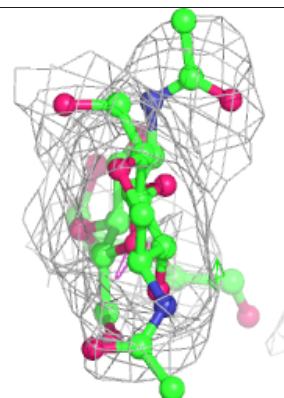
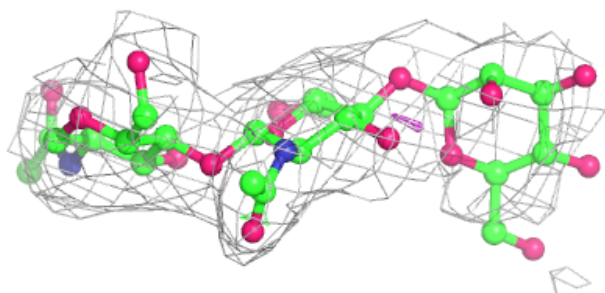
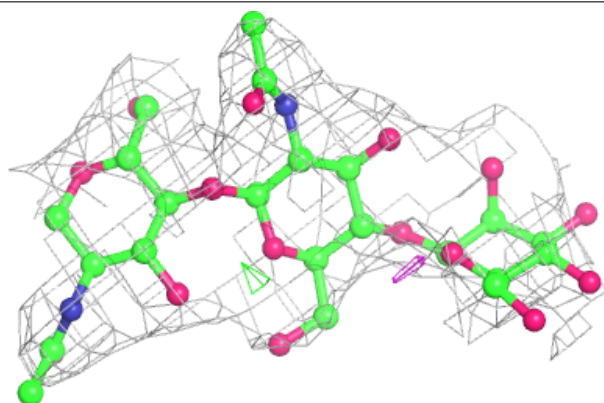


Electron density around Chain H:

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

**Electron density around Chain I:**

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



6.4 Ligands

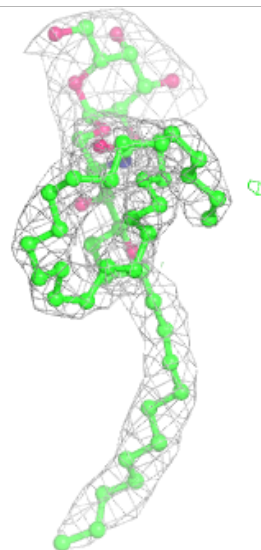
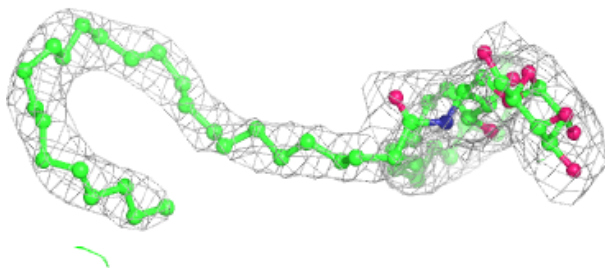
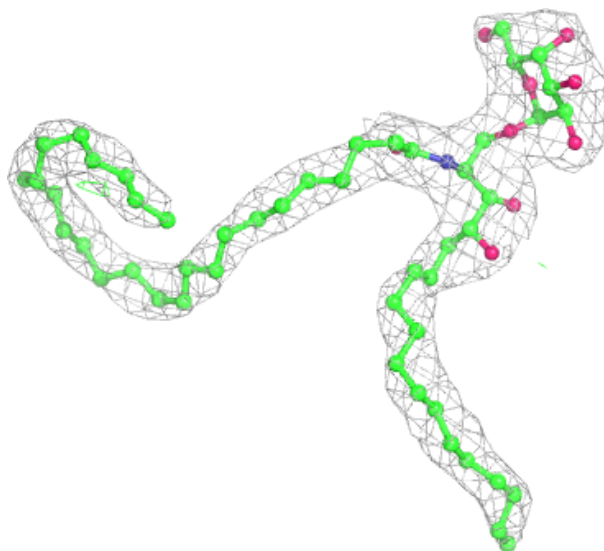
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
7	NAG	A	401	14/15	0.71	0.18	85,117,133,134	0
9	PEG	E	201	7/7	0.81	0.16	95,105,110,111	0
10	CL	A	405	1/1	0.83	0.24	96,96,96,96	0
9	PEG	A	404	7/7	0.91	0.29	85,86,94,95	0
12	BGC	B	102	12/12	0.91	0.19	54,77,87,91	0
11	SO4	B	101	5/5	0.92	0.19	114,119,123,123	0
9	PEG	A	403	7/7	0.93	0.18	49,58,69,75	0
8	AGH	A	402	60/60	0.95	0.21	48,63,78,84	0
8	AGH	C	401	60/60	0.96	0.23	44,65,79,83	0
13	NA	D	101	1/1	0.97	0.42	68,68,68,68	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.

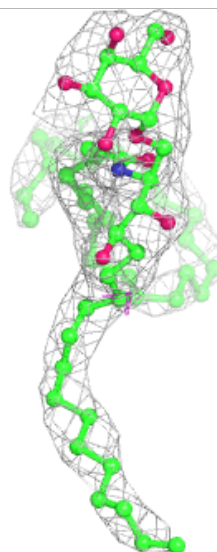
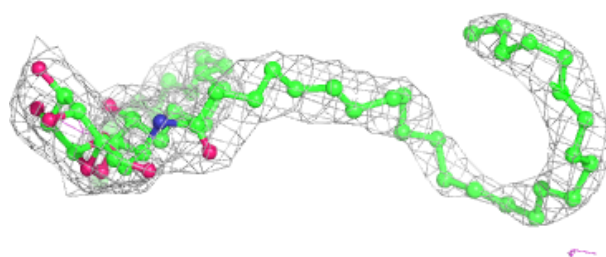
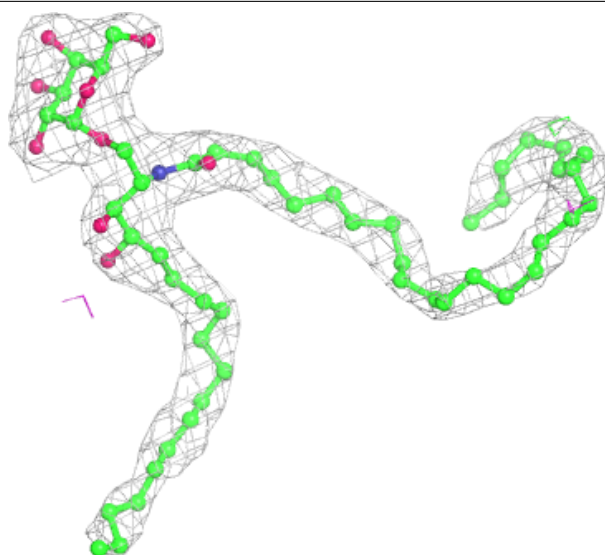
Electron density around AGH A 402:

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



Electron density around AGH C 401:

$2mF_o-DF_c$ (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.