Full wwPDB X-ray Structure Validation Report ⓘ

Jan 21, 2024 – 12:04 am GMT

PDB ID	:	6ZJZ
Title	:	Discovery of M5049: a novel selective TLR7/8 inhibitor for treatment of autoimmunity
Authors	:	Musil, D.; Lehman, M.; Strauss, J.
Deposited on	:	2020-06-29
Resolution	:	2.49 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:

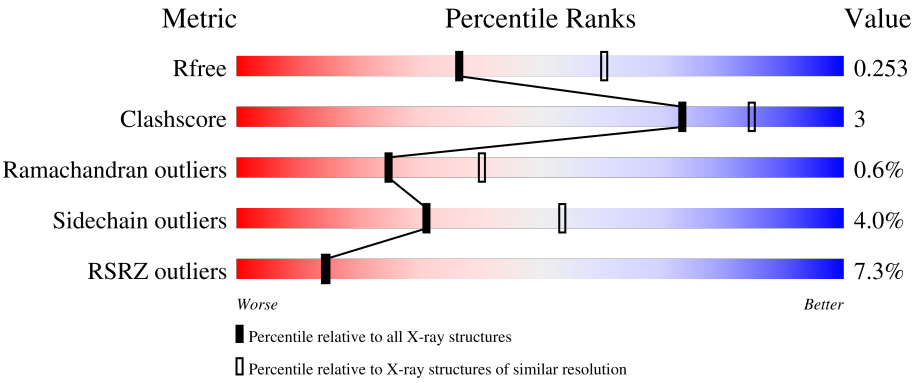
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.49 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	5857 (2.50-2.46)
Clashscore	141614	6594 (2.50-2.46)
Ramachandran outliers	138981	6469 (2.50-2.46)
Sidechain outliers	138945	6471 (2.50-2.46)
RSRZ outliers	127900	5738 (2.50-2.46)

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 <=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	801	5% 81% 9% · 8%
1	B	801	8% 80% 11% · 8%
2	C	6	33% 67%
2	E	6	50% 50%
3	D	3	33% 67%

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Mol	Chain	Length	Quality of chain
3	G	3	33% 67%
4	F	5	60% 40%
4	H	5	40% 60%

2 Entry composition

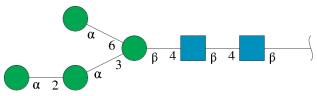
There are 8 unique types of molecules in this entry. The entry contains 12509 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Toll-like receptor 8.

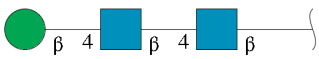
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	737	Total	C	N	O	S	156	0	0
			5937	3797	1011	1110	19			
1	B	740	Total	C	N	O	S	231	0	0
			5957	3817	1009	1111	20			

- Molecule 2 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



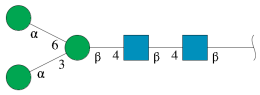
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	C	6	Total	C	N	O	0	0	0
			72	40	2	30			
2	E	6	Total	C	N	O	0	0	0
			72	40	2	30			

- Molecule 3 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.



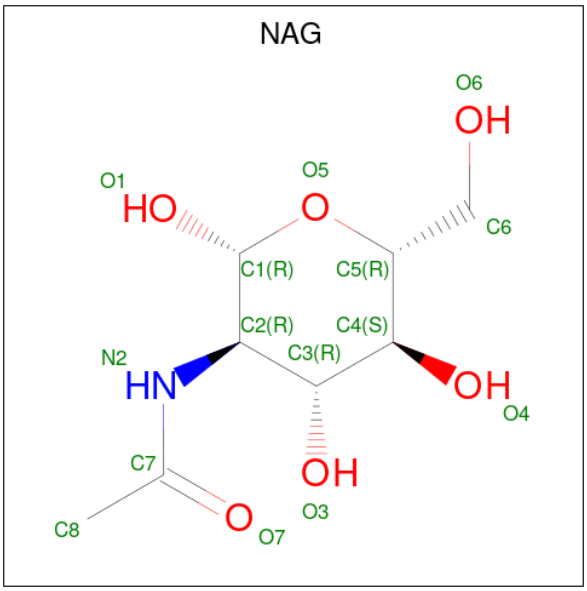
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	D	3	Total	C	N	O	0	0	0
			39	22	2	15			
3	G	3	Total	C	N	O	0	0	0
			39	22	2	15			

- Molecule 4 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	F	5	Total	C	N	O	0	0	0
			61	34	2	25			
4	H	5	Total	C	N	O	0	0	0
			61	34	2	25			

- Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



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

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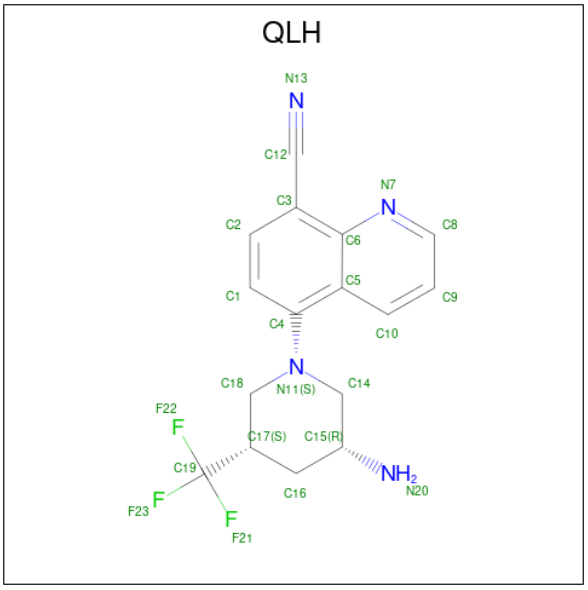
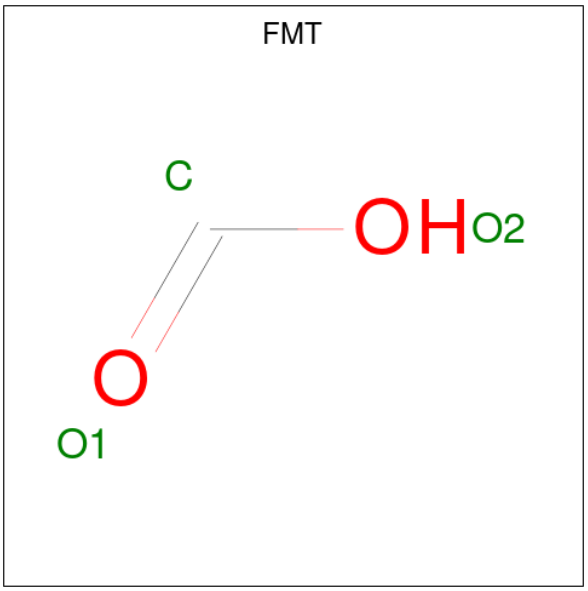
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	B	1	Total C N O 14 8 1 5	0	0
5	B	1	Total C N O 14 8 1 5	0	0
5	B	1	Total C N O 14 8 1 5	0	0
5	B	1	Total C N O 14 8 1 5	0	0

- Molecule 6 is 5-[(3 {R},5 {S})-3-azanyl-5-(trifluoromethyl)piperidin-1-yl]quinoline-8-carbonitrile (three-letter code: QLH) (formula: $C_{16}H_{15}F_3N_4$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total C F N 23 16 3 4	0	0
6	B	1	Total C F N 23 16 3 4	0	0

- Molecule 7 is FORMIC ACID (three-letter code: FMT) (formula: CH_2O_2).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	B	1	Total C O 3 1 2	0	0

- Molecule 8 is water.

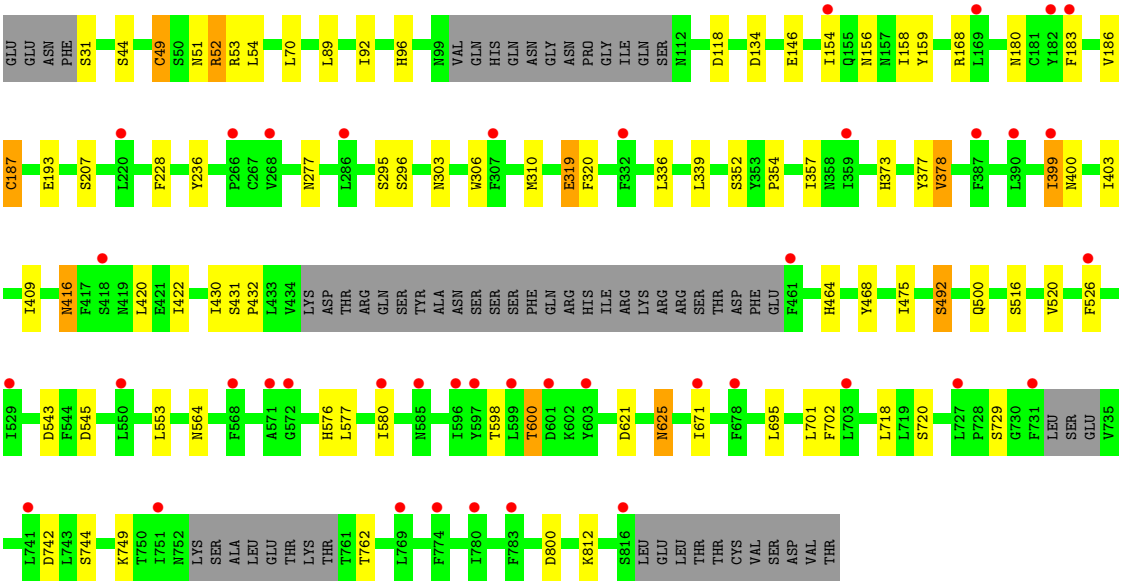
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	53	Total O 53 53	0	0
8	B	43	Total O 43 43	0	0

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.

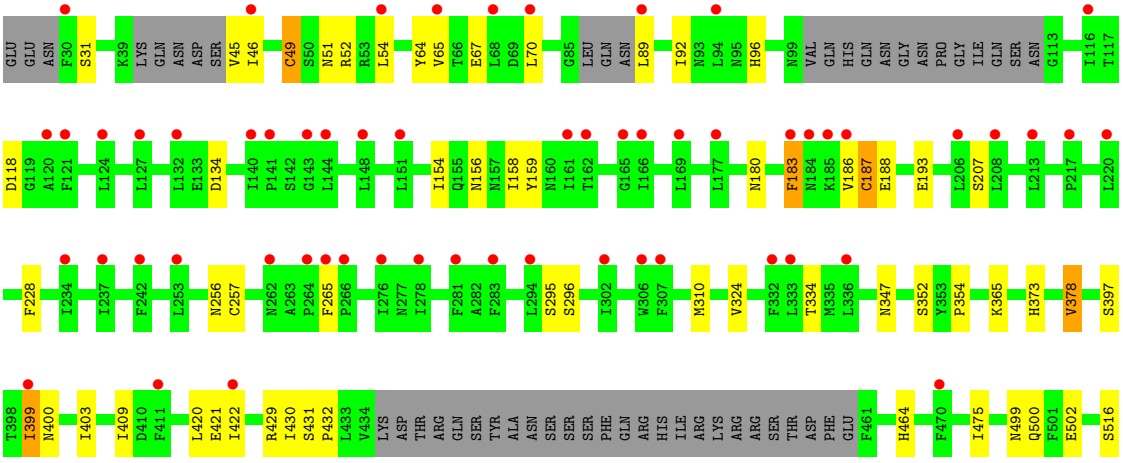
• Molecule 1: Toll-like receptor 8

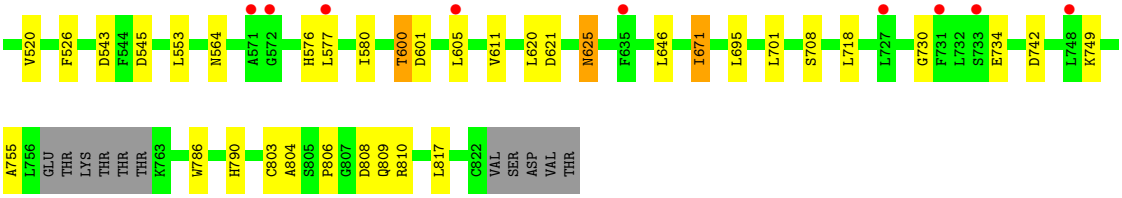
Chain A:



• Molecule 1: Toll-like receptor 8

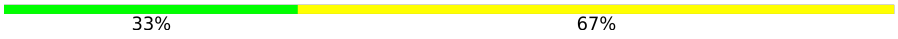
Chain B:





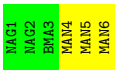
• Molecule 2: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain C:



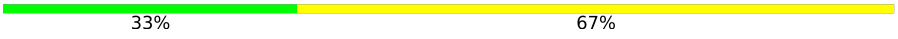
• Molecule 2: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain E:



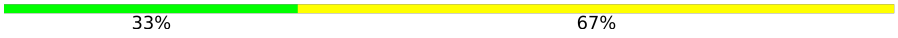
• Molecule 3: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain D:



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

Chain G:



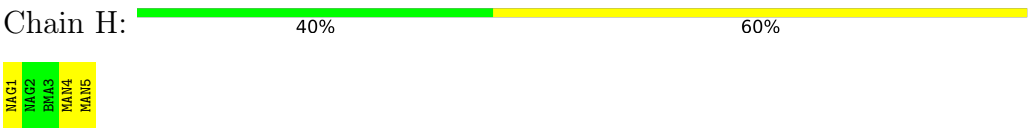
• Molecule 4: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain F:

• Molecule 4: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyra

nose

Chain H:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	146.36Å 98.25Å 141.09Å 90.00° 105.64° 90.00°	Depositor
Resolution (Å)	135.87 – 2.49 135.87 – 2.49	Depositor EDS
% Data completeness (in resolution range)	93.0 (135.87-2.49) 79.1 (135.87-2.49)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.53 (at 2.48Å)	Xtriage
Refinement program	BUSTER 2.11.7 (19-MAR-2020)	Depositor
R, R_{free}	0.204 , 0.243 0.212 , 0.253	Depositor DCC
R_{free} test set	2698 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å^2)	76.4	Xtriage
Anisotropy	0.041	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 63.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	12509	wwPDB-VP
Average B, all atoms (Å^2)	93.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.98% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: BMA, FMT, NAG, QLH, MAN

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	0.43	0/6059	0.60	0/8216
1	B	0.42	0/6079	0.59	0/8241
All	All	0.42	0/12138	0.60	0/16457

There are no bond length outliers.

There are no bond angle outliers.

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	5937	0	5919	34	0
1	B	5957	0	5948	45	0
2	C	72	0	61	0	0
2	E	72	0	61	0	0
3	D	39	0	34	0	0
3	G	39	0	34	0	0
4	F	61	0	52	0	0
4	H	61	0	52	0	0
5	A	70	0	65	0	0
5	B	56	0	52	0	0
6	A	23	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	B	23	0	0	0	0
7	B	3	0	2	0	0
8	A	53	0	0	0	0
8	B	43	0	0	0	0
All	All	12509	0	12280	78	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 (78) 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:B:621:ASP:O	1:B:625:ASN:HB2	1.90	0.72
1:A:621:ASP:O	1:A:625:ASN:HB2	1.92	0.69
1:B:397:SER:HB2	1:B:421:GLU:HG2	1.76	0.67
1:B:576:HIS:ND1	1:B:600:THR:OG1	2.25	0.67
1:A:373:HIS:HA	1:A:400:ASN:HB3	1.79	0.65
1:B:399:ILE:HG23	1:B:420:LEU:HD21	1.79	0.64
1:B:52:ARG:HB2	1:B:54:LEU:HG	1.79	0.63
1:B:373:HIS:HA	1:B:400:ASN:HB3	1.80	0.62
1:B:409:ILE:HD12	1:B:430:ILE:HD11	1.81	0.62
1:A:409:ILE:HD12	1:A:430:ILE:HD11	1.80	0.62
1:A:52:ARG:HB2	1:A:54:LEU:HG	1.82	0.60
1:B:158:ILE:H	1:B:180:ASN:HD22	1.51	0.58
1:A:158:ILE:H	1:A:180:ASN:HD22	1.51	0.57
1:A:492:SER:HB3	1:B:429:ARG:HH11	1.70	0.57
1:A:422:ILE:HG23	1:A:475:ILE:HD12	1.86	0.57
1:B:422:ILE:HG23	1:B:475:ILE:HD12	1.85	0.56
1:A:53:ARG:NH2	1:A:800:ASP:OD1	2.37	0.56
1:B:45:VAL:HG11	1:B:64:TYR:HD1	1.71	0.55
1:A:154:ILE:HD12	1:A:464:HIS:CE1	2.42	0.54
1:A:399:ILE:HG23	1:A:420:LEU:HD21	1.90	0.53
1:B:577:LEU:HB3	1:B:580:ILE:HD12	1.91	0.53
1:A:156:ASN:HB2	1:A:180:ASN:HD21	1.75	0.52
1:A:236:TYR:HD1	1:A:277:ASN:HB3	1.75	0.52
1:A:576:HIS:ND1	1:A:600:THR:OG1	2.43	0.52
1:B:526:PHE:HB3	1:B:553:LEU:HD21	1.92	0.51
1:B:499:ASN:HA	1:B:502:GLU:HG2	1.92	0.51
1:B:786:TRP:CE2	1:B:790:HIS:CD2	2.99	0.50
1:A:526:PHE:HB3	1:A:553:LEU:HD21	1.93	0.50
1:B:89:LEU:HD13	1:B:92:ILE:HD11	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:319:GLU:OE2	1:A:468:TYR:HB3	2.12	0.49
1:A:158:ILE:H	1:A:180:ASN:ND2	2.11	0.49
1:B:324:VAL:HG23	1:B:347:ASN:O	2.13	0.48
1:B:158:ILE:H	1:B:180:ASN:ND2	2.11	0.48
1:A:671:ILE:HD12	1:A:695:LEU:HD21	1.95	0.48
1:A:89:LEU:HD13	1:A:92:ILE:HD11	1.95	0.48
1:B:786:TRP:CE2	1:B:790:HIS:HD2	2.32	0.48
1:A:96:HIS:HD2	1:A:134:ASP:OD2	1.98	0.47
1:B:809:GLN:OE1	1:B:817:LEU:HD22	2.14	0.46
1:B:49:CYS:HB3	1:B:70:LEU:HD23	1.97	0.46
1:A:718:LEU:HA	1:A:742:ASP:HB3	1.97	0.46
1:B:46:ILE:HG13	1:B:67:GLU:HB2	1.97	0.46
1:A:399:ILE:O	1:A:399:ILE:HG13	2.16	0.46
1:B:96:HIS:HD2	1:B:134:ASP:OD2	1.99	0.46
1:B:718:LEU:HA	1:B:742:ASP:HB3	1.97	0.45
1:A:577:LEU:HB3	1:A:580:ILE:HD12	1.99	0.45
1:A:336:LEU:HD13	1:A:339:LEU:HD22	1.99	0.45
1:A:49:CYS:HB3	1:A:70:LEU:HD23	1.99	0.45
1:A:354:PRO:HD2	1:A:378:VAL:O	2.17	0.44
1:B:334:THR:HG22	1:B:365:LYS:HD3	1.98	0.44
1:B:399:ILE:O	1:B:399:ILE:HG13	2.17	0.44
1:B:154:ILE:HD12	1:B:464:HIS:CE1	2.53	0.44
1:B:730:GLY:H	1:B:755:ALA:HA	1.82	0.44
1:B:354:PRO:HD2	1:B:378:VAL:O	2.17	0.44
1:A:720:SER:HA	1:A:744:SER:O	2.17	0.44
1:B:520:VAL:HA	1:B:543:ASP:HB3	2.00	0.43
1:B:671:ILE:HD12	1:B:695:LEU:HD21	1.99	0.43
1:B:803:CYS:HB2	1:B:809:GLN:O	2.18	0.43
1:A:296:SER:HA	1:A:320:PHE:O	2.18	0.43
1:A:432:PRO:HA	1:A:500:GLN:OE1	2.19	0.43
1:B:45:VAL:HB	1:B:65:VAL:HA	2.01	0.43
1:B:786:TRP:NE1	1:B:790:HIS:CD2	2.87	0.43
1:B:620:LEU:CD1	1:B:646:LEU:HD22	2.49	0.42
1:B:708:SER:HB3	1:B:734:GLU:HB3	2.01	0.42
1:A:357:ILE:HG13	1:A:377:TYR:CZ	2.55	0.42
1:A:520:VAL:HA	1:A:543:ASP:HB3	2.01	0.42
1:A:159:TYR:CE1	1:A:187:CYS:HB2	2.55	0.41
1:A:336:LEU:HB3	1:A:339:LEU:HB2	2.02	0.41
1:B:156:ASN:HB2	1:B:180:ASN:HD21	1.85	0.41
1:B:207:SER:HA	1:B:228:PHE:HB2	2.02	0.41
1:B:804:ALA:O	1:B:810:ARG:HD2	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:207:SER:HA	1:A:228:PHE:HB2	2.02	0.41
1:B:256:ASN:O	1:B:257:CYS:HB2	2.21	0.41
1:A:303:ASN:HB3	1:A:306:TRP:CE2	2.56	0.40
1:B:432:PRO:HA	1:B:500:GLN:OE1	2.20	0.40
1:B:159:TYR:CE1	1:B:187:CYS:HB2	2.56	0.40
1:B:806:PRO:HD2	1:B:809:GLN:HB2	2.03	0.40
1:B:154:ILE:CD1	1:B:464:HIS:CE1	3.04	0.40
1:B:183:PHE:CE1	1:B:265:PHE:HB3	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	727/801 (91%)	688 (95%)	34 (5%)	5 (1%)	22	36
1	B	728/801 (91%)	686 (94%)	38 (5%)	4 (0%)	29	46
All	All	1455/1602 (91%)	1374 (94%)	72 (5%)	9 (1%)	25	40

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	186	VAL
1	A	729	SER
1	B	186	VAL
1	B	600	THR
1	A	600	THR
1	A	378	VAL
1	A	416	ASN
1	B	183	PHE
1	B	378	VAL

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	685/745 (92%)	655 (96%)	30 (4%)	28 49
1	B	687/745 (92%)	662 (96%)	25 (4%)	35 58
All	All	1372/1490 (92%)	1317 (96%)	55 (4%)	31 53

All (55) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	31	SER
1	A	44	SER
1	A	49	CYS
1	A	51	ASN
1	A	52	ARG
1	A	118	ASP
1	A	146	GLU
1	A	168	ARG
1	A	183	PHE
1	A	187	CYS
1	A	193	GLU
1	A	295	SER
1	A	310	MET
1	A	319	GLU
1	A	352	SER
1	A	399	ILE
1	A	403	ILE
1	A	416	ASN
1	A	431	SER
1	A	492	SER
1	A	516	SER
1	A	545	ASP
1	A	564	ASN
1	A	598	THR
1	A	625	ASN
1	A	701	LEU
1	A	702	PHE

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Mol	Chain	Res	Type
1	A	749	LYS
1	A	762	THR
1	A	812	LYS
1	B	31	SER
1	B	49	CYS
1	B	51	ASN
1	B	118	ASP
1	B	187	CYS
1	B	188	GLU
1	B	193	GLU
1	B	295	SER
1	B	296	SER
1	B	310	MET
1	B	352	SER
1	B	399	ILE
1	B	403	ILE
1	B	431	SER
1	B	516	SER
1	B	545	ASP
1	B	564	ASN
1	B	601	ASP
1	B	605	LEU
1	B	611	VAL
1	B	625	ASN
1	B	671	ILE
1	B	701	LEU
1	B	749	LYS
1	B	808	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	51	ASN
1	A	96	HIS
1	A	135	ASN
1	A	180	ASN
1	A	392	GLN
1	A	585	ASN
1	A	790	HIS
1	B	51	ASN
1	B	96	HIS
1	B	135	ASN

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Mol	Chain	Res	Type
1	B	180	ASN
1	B	585	ASN
1	B	790	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

28 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	NAG	C	1	1,2	14,14,15	0.36	0	17,19,21	0.52	0
2	NAG	C	2	2	14,14,15	0.30	0	17,19,21	0.54	0
2	BMA	C	3	2	11,11,12	0.25	0	15,15,17	0.86	1 (6%)
2	MAN	C	4	2	11,11,12	0.31	0	15,15,17	0.86	1 (6%)
2	MAN	C	5	2	11,11,12	0.39	0	15,15,17	0.72	1 (6%)
2	MAN	C	6	2	11,11,12	0.46	0	15,15,17	0.90	1 (6%)
3	NAG	D	1	1,3	14,14,15	0.32	0	17,19,21	0.67	0
3	NAG	D	2	3	14,14,15	0.32	0	17,19,21	0.87	1 (5%)
3	BMA	D	3	3	11,11,12	0.45	0	15,15,17	0.84	1 (6%)
2	NAG	E	1	1,2	14,14,15	0.30	0	17,19,21	0.73	0
2	NAG	E	2	2	14,14,15	0.32	0	17,19,21	0.63	0
2	BMA	E	3	2	11,11,12	0.26	0	15,15,17	0.52	0
2	MAN	E	4	2	11,11,12	0.32	0	15,15,17	0.92	1 (6%)
2	MAN	E	5	2	11,11,12	0.46	0	15,15,17	0.81	1 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	MAN	E	6	2	11,11,12	0.73	0	15,15,17	1.56	2 (13%)
4	NAG	F	1	1,4	14,14,15	0.31	0	17,19,21	0.57	0
4	NAG	F	2	4	14,14,15	0.32	0	17,19,21	0.48	0
4	BMA	F	3	4	11,11,12	0.35	0	15,15,17	0.98	1 (6%)
4	MAN	F	4	4	11,11,12	0.33	0	15,15,17	0.51	0
4	MAN	F	5	4	11,11,12	0.41	0	15,15,17	0.88	1 (6%)
3	NAG	G	1	1,3	14,14,15	0.30	0	17,19,21	0.67	0
3	NAG	G	2	3	14,14,15	0.32	0	17,19,21	0.97	1 (5%)
3	BMA	G	3	3	11,11,12	0.47	0	15,15,17	0.88	1 (6%)
4	NAG	H	1	1,4	14,14,15	0.28	0	17,19,21	0.80	1 (5%)
4	NAG	H	2	4	14,14,15	0.29	0	17,19,21	0.66	0
4	BMA	H	3	4	11,11,12	0.26	0	15,15,17	0.51	0
4	MAN	H	4	4	11,11,12	0.36	0	15,15,17	0.78	1 (6%)
4	MAN	H	5	4	11,11,12	0.75	0	15,15,17	1.38	2 (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
2	NAG	C	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	C	2	2	-	0/6/23/26	0/1/1/1
2	BMA	C	3	2	-	0/2/19/22	0/1/1/1
2	MAN	C	4	2	-	0/2/19/22	0/1/1/1
2	MAN	C	5	2	-	0/2/19/22	0/1/1/1
2	MAN	C	6	2	-	0/2/19/22	0/1/1/1
3	NAG	D	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	D	2	3	-	2/6/23/26	0/1/1/1
3	BMA	D	3	3	-	1/2/19/22	0/1/1/1
2	NAG	E	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	E	2	2	-	0/6/23/26	0/1/1/1
2	BMA	E	3	2	-	2/2/19/22	0/1/1/1
2	MAN	E	4	2	-	0/2/19/22	0/1/1/1
2	MAN	E	5	2	-	0/2/19/22	0/1/1/1
2	MAN	E	6	2	-	1/2/19/22	1/1/1/1
4	NAG	F	1	1,4	-	0/6/23/26	0/1/1/1
4	NAG	F	2	4	-	0/6/23/26	0/1/1/1
4	BMA	F	3	4	-	0/2/19/22	0/1/1/1
4	MAN	F	4	4	-	0/2/19/22	0/1/1/1

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

There are no bond length outliers.

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	E	6	MAN	C1-O5-C5	5.09	119.08	112.19
4	H	5	MAN	C1-O5-C5	4.39	118.14	112.19
3	G	2	NAG	C1-O5-C5	3.33	116.71	112.19
2	C	6	MAN	C1-O5-C5	3.10	116.39	112.19
4	F	5	MAN	C1-O5-C5	3.06	116.34	112.19
4	F	3	BMA	C1-O5-C5	3.00	116.25	112.19
2	C	4	MAN	C1-O5-C5	2.86	116.07	112.19
2	E	6	MAN	C1-C2-C3	2.65	112.92	109.67
3	G	3	BMA	C1-O5-C5	2.62	115.75	112.19
2	C	3	BMA	C1-O5-C5	2.45	115.51	112.19
3	D	3	BMA	C1-O5-C5	2.40	115.44	112.19
4	H	5	MAN	C1-C2-C3	2.36	112.57	109.67
4	H	1	NAG	C1-O5-C5	2.25	115.24	112.19
4	H	4	MAN	C1-O5-C5	2.20	115.17	112.19
2	C	5	MAN	C1-O5-C5	2.15	115.11	112.19
2	E	4	MAN	C1-O5-C5	2.09	115.03	112.19
3	D	2	NAG	C1-O5-C5	2.07	115.00	112.19
2	E	5	MAN	C1-O5-C5	2.06	114.98	112.19

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	G	2	NAG	O5-C5-C6-O6
3	D	2	NAG	O5-C5-C6-O6
3	G	2	NAG	C4-C5-C6-O6
3	D	2	NAG	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
4	H	5	MAN	C4-C5-C6-O6
2	E	6	MAN	C4-C5-C6-O6
4	H	3	BMA	C4-C5-C6-O6
2	E	3	BMA	C4-C5-C6-O6
4	H	3	BMA	O5-C5-C6-O6
2	E	3	BMA	O5-C5-C6-O6
3	G	3	BMA	C4-C5-C6-O6
3	D	3	BMA	C4-C5-C6-O6

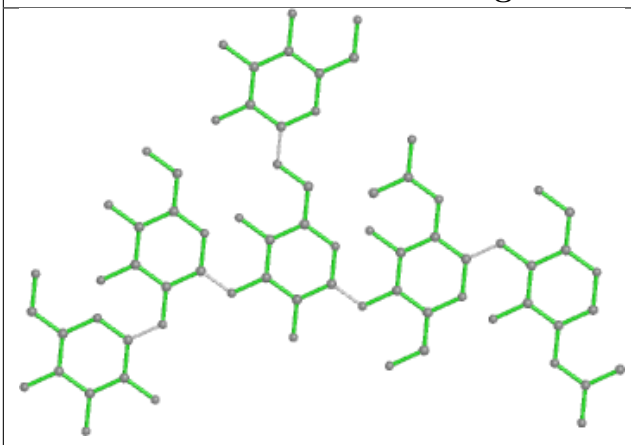
All (2) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	H	5	MAN	C1-C2-C3-C4-C5-O5
2	E	6	MAN	C1-C2-C3-C4-C5-O5

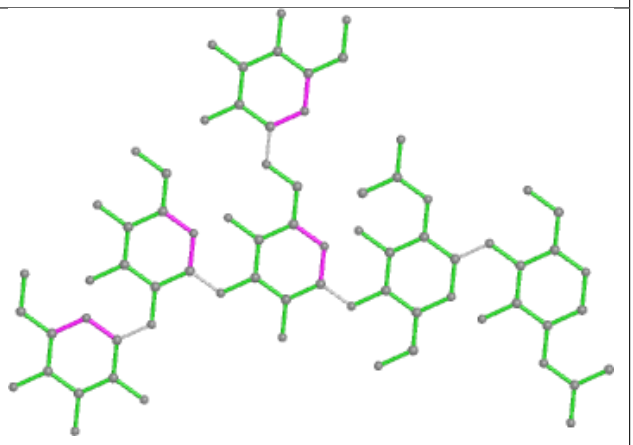
No monomer is involved in short contacts.

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

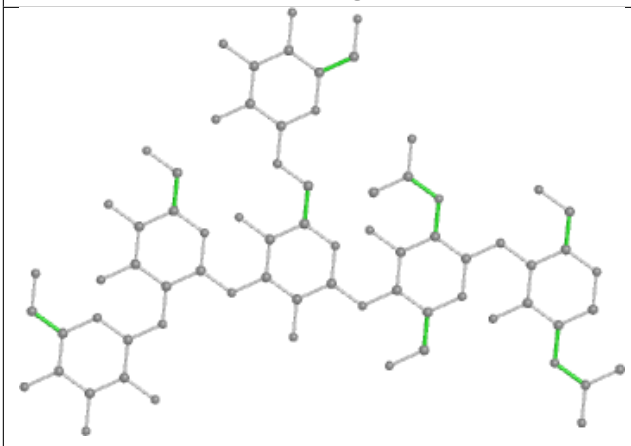
Oligosaccharide Chain C



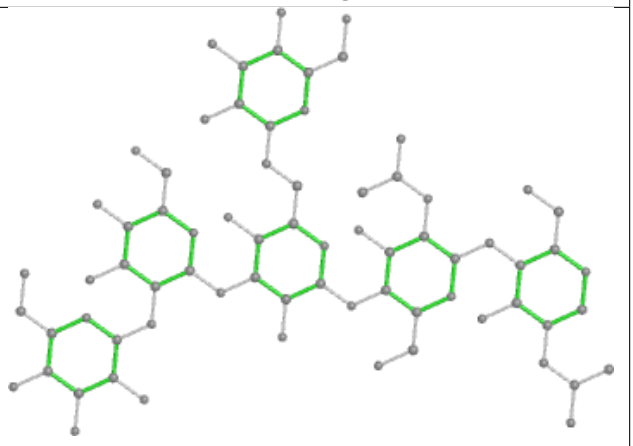
Bond lengths



Bond angles

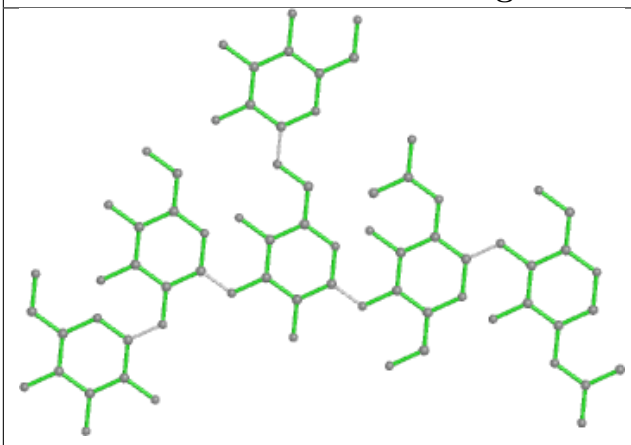


Torsions

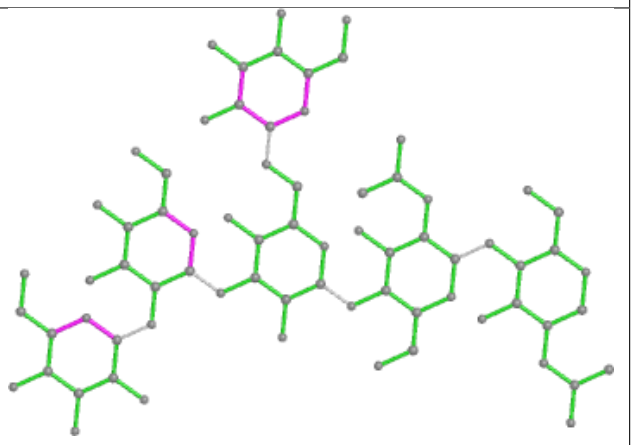


Rings

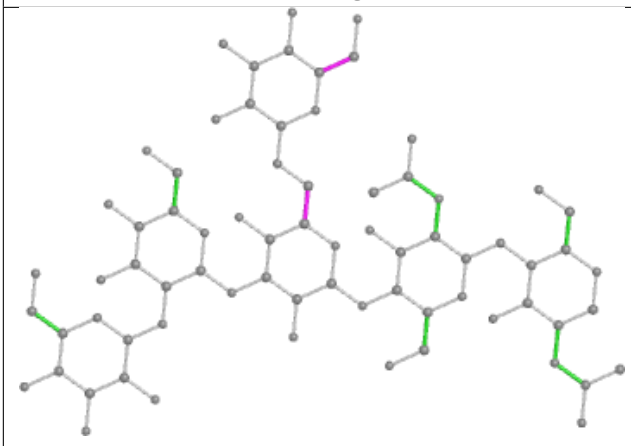
Oligosaccharide Chain E



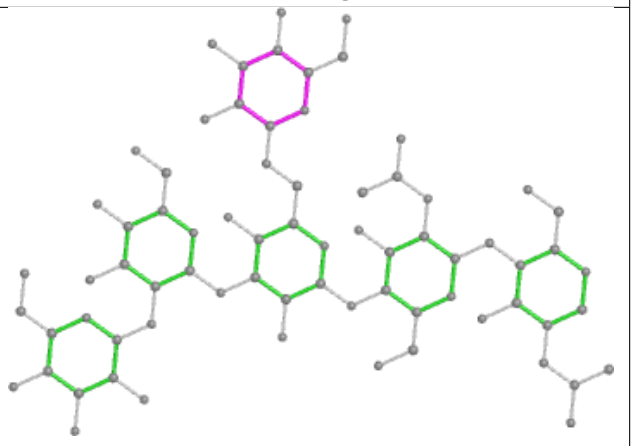
Bond lengths



Bond angles

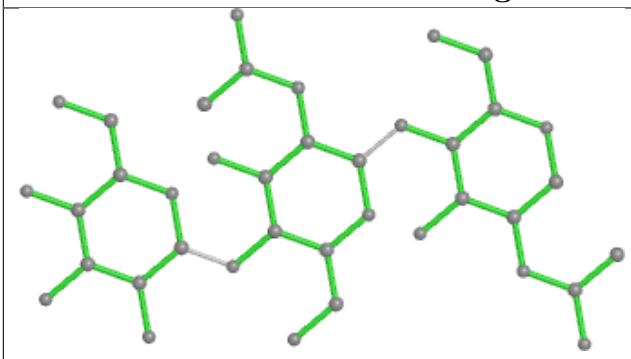


Torsions

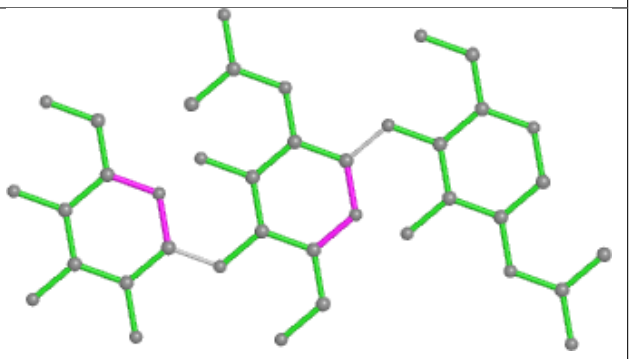


Rings

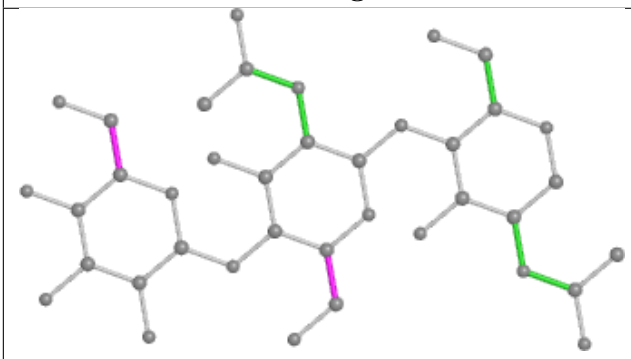
Oligosaccharide Chain D



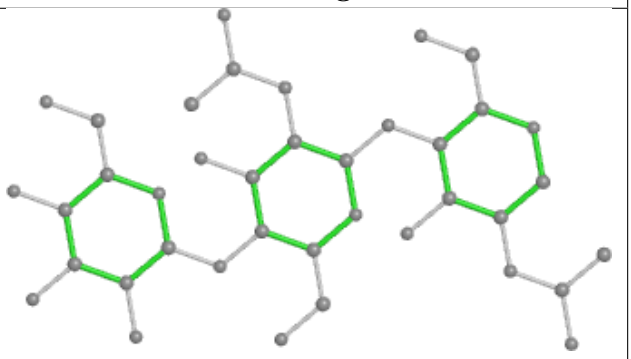
Bond lengths



Bond angles

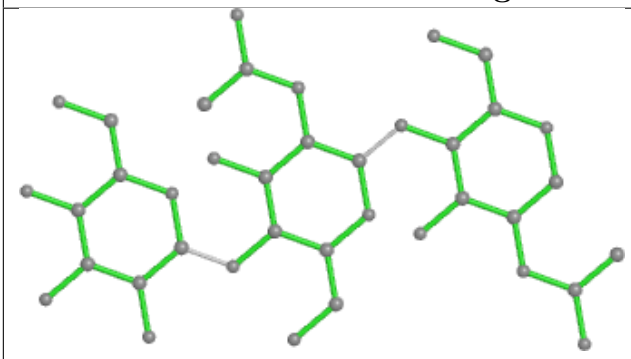


Torsions

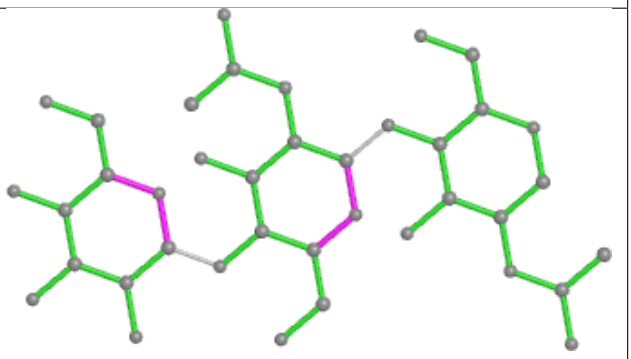


Rings

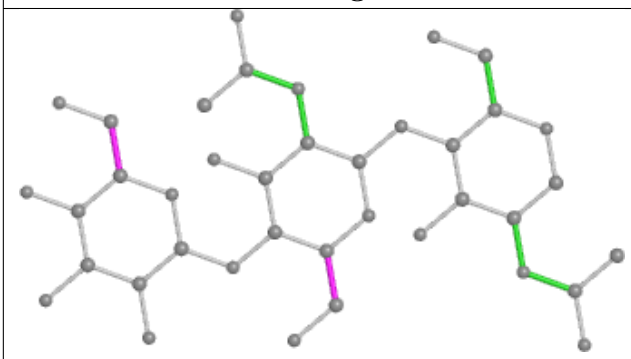
Oligosaccharide Chain G



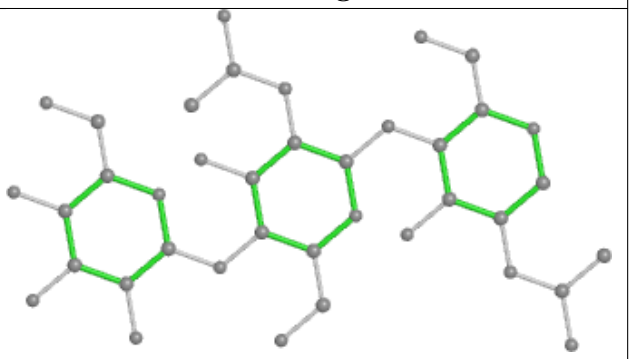
Bond lengths



Bond angles

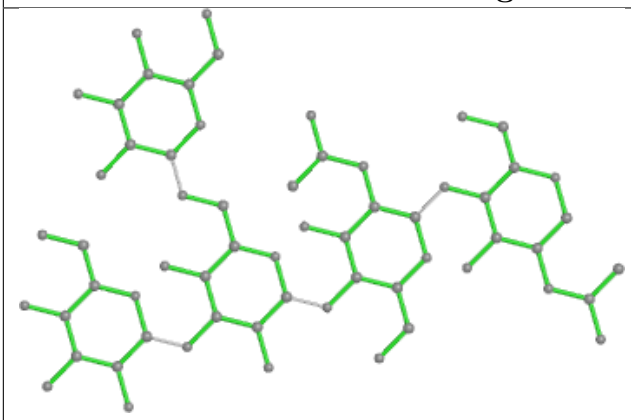


Torsions

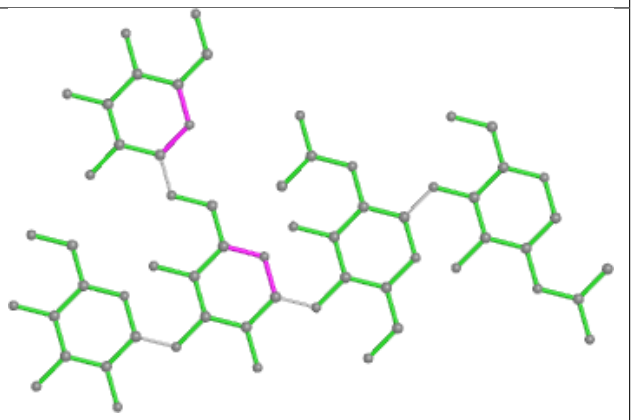


Rings

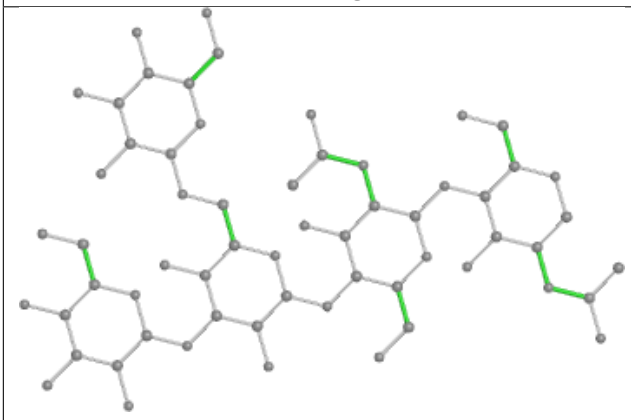
Oligosaccharide Chain F



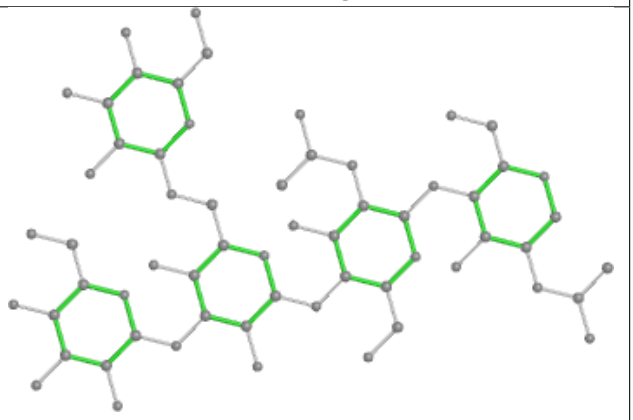
Bond lengths



Bond angles

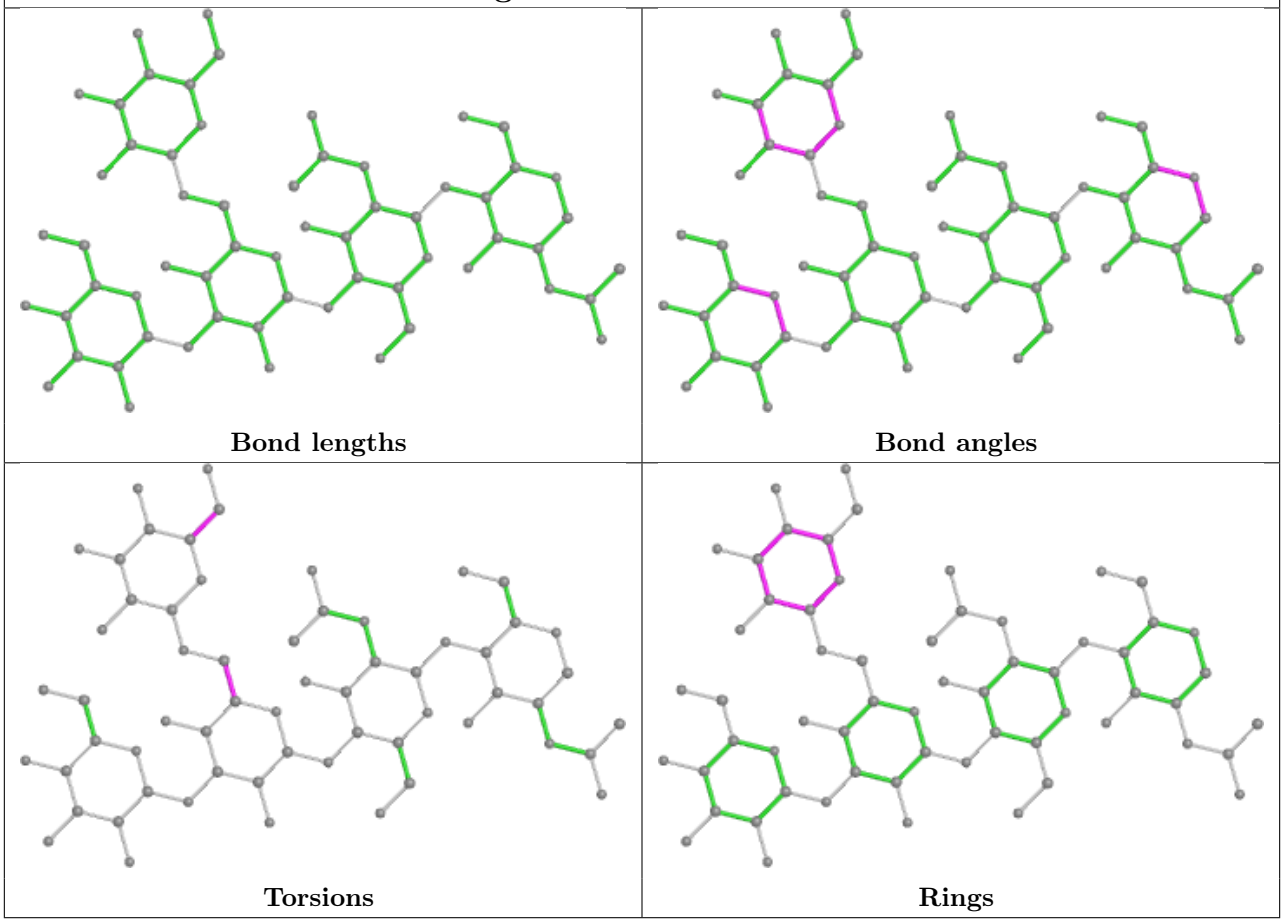


Torsions



Rings

Oligosaccharide Chain H



5.6 Ligand geometry (i)

12 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	$\#\|Z\| > 2$
6	QLH	B	918	-	25,25,25	1.24	5 (20%)	32,37,37	1.50	8 (25%)
5	NAG	A	904	1	14,14,15	0.35	0	17,19,21	1.12	2 (11%)
6	QLH	A	921	-	25,25,25	1.22	5 (20%)	32,37,37	1.45	7 (21%)
5	NAG	B	902	1	14,14,15	0.31	0	17,19,21	0.93	1 (5%)
5	NAG	B	901	1	14,14,15	0.26	0	17,19,21	0.68	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
5	NAG	A	901	1	14,14,15	0.32	0	17,19,21	0.71	1 (5%)
5	NAG	A	920	1	14,14,15	0.42	0	17,19,21	1.28	3 (17%)
5	NAG	A	902	1	14,14,15	0.31	0	17,19,21	0.84	1 (5%)
5	NAG	B	917	1	14,14,15	0.34	0	17,19,21	0.94	1 (5%)
5	NAG	B	903	1	14,14,15	0.27	0	17,19,21	0.69	1 (5%)
5	NAG	A	903	1	14,14,15	0.27	0	17,19,21	0.51	0
7	FMT	B	919	-	2,2,2	1.63	1 (50%)	1,1,1	0.89	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
6	QLH	B	918	-	-	1/12/24/24	0/3/3/3
5	NAG	A	904	1	-	1/6/23/26	0/1/1/1
6	QLH	A	921	-	-	0/12/24/24	0/3/3/3
5	NAG	B	902	1	-	2/6/23/26	0/1/1/1
5	NAG	B	901	1	-	0/6/23/26	0/1/1/1
5	NAG	A	901	1	-	0/6/23/26	0/1/1/1
5	NAG	A	920	1	-	1/6/23/26	0/1/1/1
5	NAG	A	902	1	-	2/6/23/26	0/1/1/1
5	NAG	B	917	1	-	2/6/23/26	0/1/1/1
5	NAG	B	903	1	-	2/6/23/26	0/1/1/1
5	NAG	A	903	1	-	2/6/23/26	0/1/1/1

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	B	918	QLH	C6-N7	-3.02	1.33	1.37
6	A	921	QLH	C6-N7	-2.93	1.33	1.37
6	A	921	QLH	C3-C6	2.80	1.46	1.43
6	B	918	QLH	C3-C6	2.62	1.46	1.43
6	B	918	QLH	F23-C19	2.36	1.39	1.33
6	B	918	QLH	F21-C19	2.34	1.39	1.33
6	B	918	QLH	F22-C19	2.32	1.39	1.33
6	A	921	QLH	F21-C19	2.31	1.39	1.33
7	B	919	FMT	O2-C	2.28	1.40	1.28
6	A	921	QLH	F22-C19	2.27	1.39	1.33
6	A	921	QLH	F23-C19	2.24	1.39	1.33

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	A	920	NAG	C2-N2-C7	3.78	128.28	122.90
5	B	902	NAG	C1-O5-C5	3.53	116.97	112.19
5	A	904	NAG	C1-C2-N2	3.39	116.29	110.49
6	A	921	QLH	C8-N7-C6	3.15	121.22	117.30
6	B	918	QLH	C8-N7-C6	3.13	121.20	117.30
5	A	902	NAG	C1-O5-C5	3.09	116.38	112.19
6	B	918	QLH	C3-C6-N7	3.01	121.29	119.12
6	A	921	QLH	C3-C6-N7	2.85	121.18	119.12
6	B	918	QLH	C16-C17-C19	-2.74	108.91	111.72
5	A	901	NAG	C1-O5-C5	2.67	115.81	112.19
5	B	917	NAG	C1-O5-C5	2.66	115.80	112.19
5	B	901	NAG	C1-O5-C5	2.52	115.61	112.19
5	A	920	NAG	C1-C2-N2	2.48	114.72	110.49
6	A	921	QLH	F22-C19-C17	-2.36	109.17	112.53
6	B	918	QLH	F23-C19-C17	-2.35	109.19	112.53
6	A	921	QLH	F23-C19-C17	-2.23	109.36	112.53
5	B	903	NAG	C1-O5-C5	2.17	115.13	112.19
6	A	921	QLH	C16-C17-C19	-2.17	109.50	111.72
5	A	904	NAG	C2-N2-C7	2.16	125.98	122.90
6	B	918	QLH	F22-C19-C17	-2.16	109.45	112.53
6	A	921	QLH	C4-C5-C6	2.10	119.69	117.14
6	B	918	QLH	C18-C17-C19	-2.08	107.93	111.34
6	B	918	QLH	C4-C5-C6	2.07	119.64	117.14
6	B	918	QLH	C9-C10-C5	-2.04	118.06	120.89
6	A	921	QLH	C9-C10-C5	-2.03	118.08	120.89
5	A	920	NAG	C1-O5-C5	2.03	114.94	112.19

There are no chirality outliers.

All (13) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	920	NAG	C3-C2-N2-C7
5	B	917	NAG	O5-C5-C6-O6
5	B	917	NAG	C4-C5-C6-O6
5	A	902	NAG	O5-C5-C6-O6
5	B	902	NAG	O5-C5-C6-O6
5	A	904	NAG	C1-C2-N2-C7
5	A	902	NAG	C4-C5-C6-O6
5	B	903	NAG	C4-C5-C6-O6
5	A	903	NAG	C4-C5-C6-O6
5	B	902	NAG	C4-C5-C6-O6

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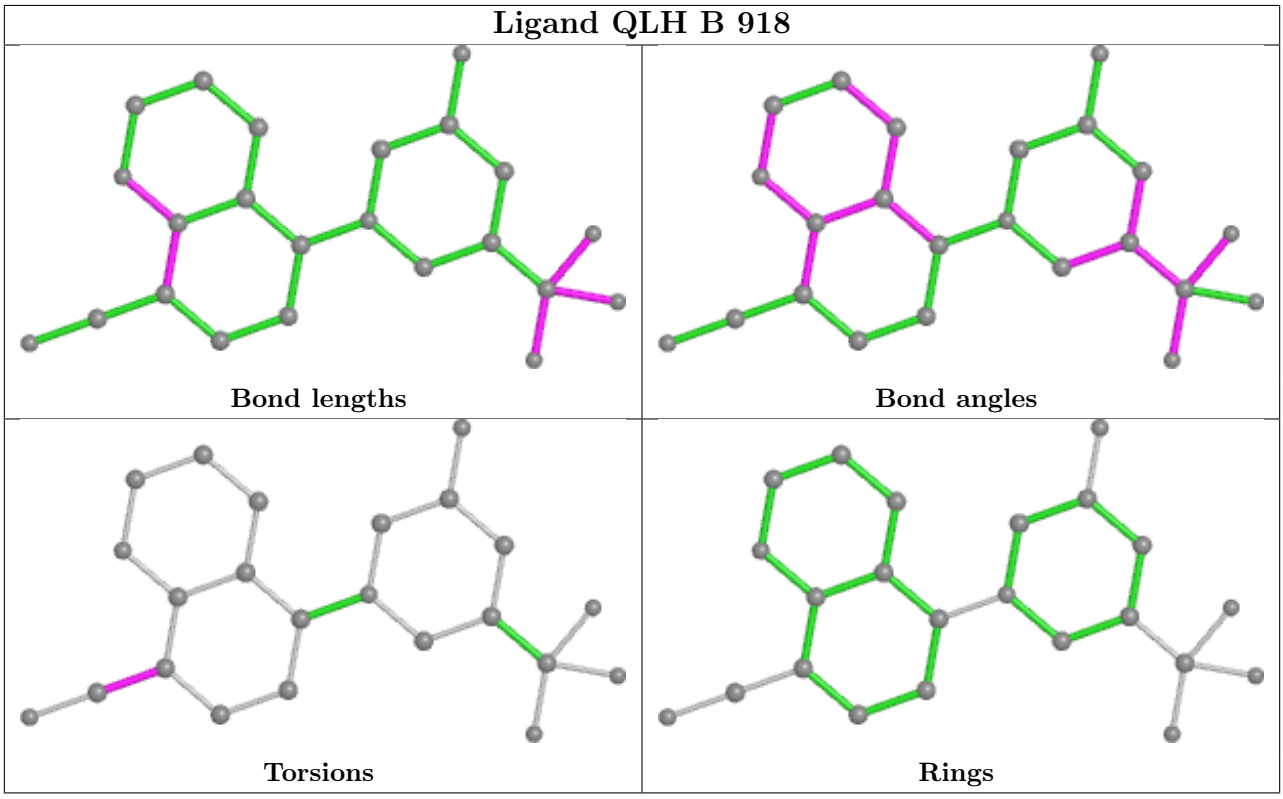
Mol	Chain	Res	Type	Atoms
5	B	903	NAG	O5-C5-C6-O6
5	A	903	NAG	O5-C5-C6-O6
6	B	918	QLH	N13-C12-C3-C6

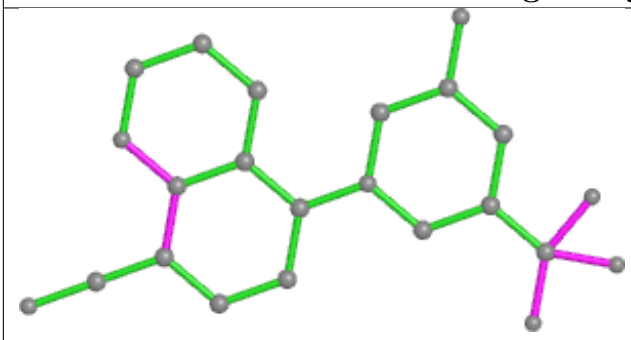
There are no ring outliers.

No monomer is involved in short contacts.

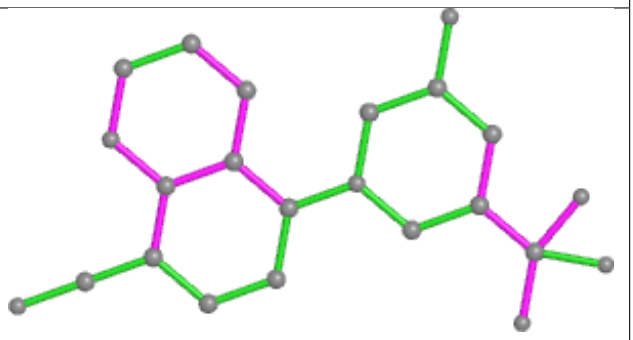
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 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.



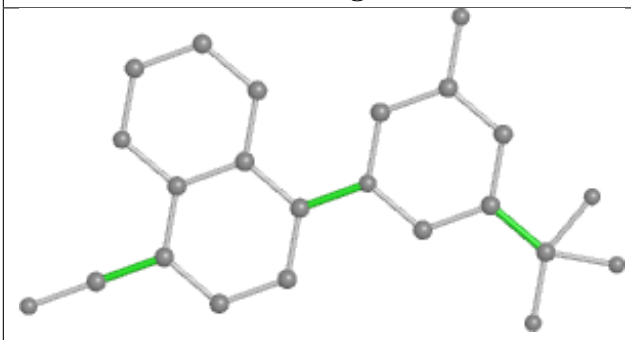
Ligand QLH A 921



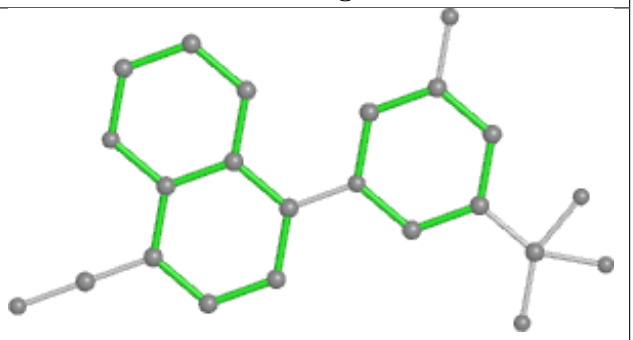
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers

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, 95^{th} 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	737/801 (92%)	0.50	41 (5%) 24 25	57, 86, 121, 136	50 (6%)
1	B	740/801 (92%)	0.60	67 (9%) 9 8	57, 92, 126, 141	71 (9%)
All	All	1477/1602 (92%)	0.55	108 (7%) 15 14	57, 89, 124, 141	121 (8%)

All (108) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	751	ILE	7.6
1	A	571	ALA	7.5
1	B	166	ILE	6.4
1	B	165	GLY	6.0
1	B	237	ILE	5.9
1	A	572	GLY	5.4
1	A	783	PHE	5.4
1	B	116	ILE	5.3
1	A	731	PHE	5.1
1	B	89	LEU	4.8
1	A	359	ILE	4.5
1	B	283	PHE	4.5
1	B	265	PHE	4.4
1	A	727	LEU	4.3
1	B	605	LEU	4.3
1	B	731	PHE	4.2
1	B	307	PHE	4.0
1	B	571	ALA	4.0
1	B	161	ILE	3.8
1	B	124	LEU	3.8
1	B	572	GLY	3.8
1	B	121	PHE	3.8
1	B	30	PHE	3.6
1	B	68	LEU	3.4

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Mol	Chain	Res	Type	RSRZ
1	A	568	PHE	3.3
1	A	769	LEU	3.2
1	B	120	ALA	3.2
1	B	234	ILE	3.2
1	A	774	PHE	3.2
1	B	141	PRO	3.2
1	A	399	ILE	3.1
1	A	268	VAL	3.1
1	A	671	ILE	3.1
1	B	208	LEU	3.1
1	A	286	LEU	3.1
1	B	169	LEU	3.0
1	A	678	PHE	3.0
1	A	461	PHE	3.0
1	B	206	LEU	2.9
1	A	387	PHE	2.9
1	B	70	LEU	2.9
1	B	127	LEU	2.9
1	B	470	PHE	2.8
1	A	169	LEU	2.8
1	A	390	LEU	2.8
1	B	264	PRO	2.8
1	A	596	ILE	2.8
1	A	183	PHE	2.8
1	B	162	THR	2.8
1	A	307	PHE	2.7
1	A	599	LEU	2.7
1	B	276	ILE	2.7
1	B	144	LEU	2.7
1	B	281	PHE	2.7
1	B	242	PHE	2.7
1	B	635	PHE	2.7
1	B	185	LYS	2.7
1	B	46	ILE	2.7
1	B	177	LEU	2.7
1	B	332	PHE	2.7
1	B	399	ILE	2.7
1	B	183	PHE	2.6
1	A	585	ASN	2.6
1	A	703	LEU	2.6
1	B	294	LEU	2.6
1	A	741	LEU	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	577	LEU	2.5
1	B	54	LEU	2.5
1	A	580	ILE	2.5
1	B	151	LEU	2.4
1	A	182	TYR	2.4
1	B	278	ILE	2.4
1	A	526	PHE	2.4
1	B	217	PRO	2.4
1	B	132	LEU	2.4
1	A	529	ILE	2.3
1	B	186	VAL	2.3
1	B	213	LEU	2.3
1	B	148	LEU	2.3
1	B	262	ASN	2.3
1	B	94	LEU	2.3
1	A	332	PHE	2.3
1	A	603	TYR	2.3
1	A	816	SER	2.2
1	B	302	ILE	2.2
1	B	411	PHE	2.2
1	B	253	LEU	2.2
1	B	143	GLY	2.2
1	A	780	ILE	2.2
1	A	601	ASP	2.2
1	B	266	PRO	2.1
1	B	333	LEU	2.1
1	B	336	LEU	2.1
1	B	748	LEU	2.1
1	A	154	ILE	2.1
1	B	306	TRP	2.1
1	B	422	ILE	2.1
1	B	220	LEU	2.1
1	A	418	SER	2.1
1	B	727	LEU	2.1
1	A	266	PRO	2.0
1	B	184	ASN	2.0
1	B	733	SER	2.0
1	B	65	VAL	2.0
1	A	220	LEU	2.0
1	A	550	LEU	2.0
1	B	140	ILE	2.0
1	A	597	TYR	2.0

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

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

6.3 Carbohydrates (i)

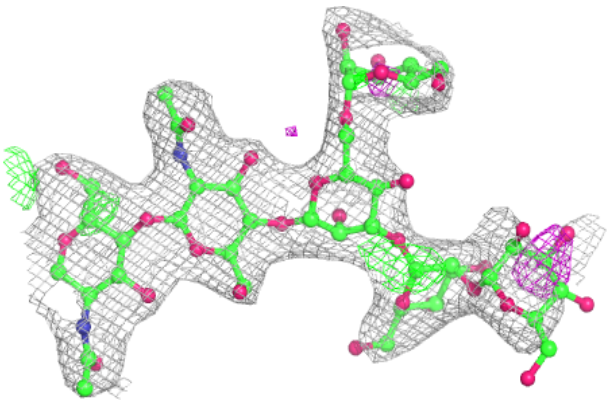
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

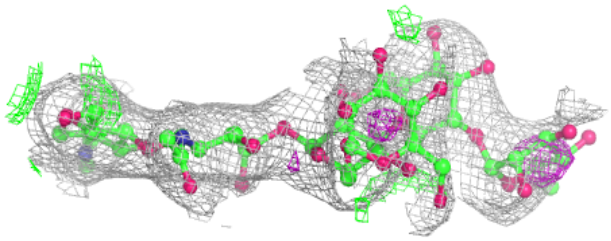
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	MAN	E	6	11/12	0.48	0.33	106,107,109,110	0
4	MAN	H	5	11/12	0.57	0.30	110,112,113,114	0
4	MAN	F	5	11/12	0.67	0.20	117,118,119,119	0
2	MAN	C	6	11/12	0.68	0.19	112,113,114,114	0
2	MAN	E	5	11/12	0.73	0.27	116,118,118,118	0
2	MAN	C	5	11/12	0.74	0.33	113,114,114,115	0
2	BMA	C	3	11/12	0.80	0.18	97,104,107,109	0
3	BMA	G	3	11/12	0.81	0.28	91,94,95,95	0
4	BMA	F	3	11/12	0.86	0.16	107,112,114,116	0
4	MAN	F	4	11/12	0.86	0.19	117,118,118,119	0
3	BMA	D	3	11/12	0.88	0.27	92,95,96,96	0
2	MAN	E	4	11/12	0.88	0.14	108,110,111,114	0
4	MAN	H	4	11/12	0.89	0.15	103,105,105,105	0
3	NAG	G	2	14/15	0.91	0.14	79,82,84,88	0
2	BMA	E	3	11/12	0.92	0.18	93,99,104,104	0
2	MAN	C	4	11/12	0.93	0.14	109,110,111,112	0
4	BMA	H	3	11/12	0.93	0.16	92,99,103,106	0
3	NAG	D	2	14/15	0.95	0.20	78,81,85,89	0
4	NAG	F	2	14/15	0.95	0.16	89,93,97,102	0
4	NAG	F	1	14/15	0.96	0.20	79,82,85,88	0
2	NAG	E	2	14/15	0.96	0.20	73,75,80,87	0
2	NAG	C	1	14/15	0.96	0.21	65,68,71,74	0
2	NAG	C	2	14/15	0.96	0.16	72,80,85,91	0
2	NAG	E	1	14/15	0.97	0.15	66,68,69,71	0
4	NAG	H	2	14/15	0.98	0.15	70,76,81,86	0
3	NAG	G	1	14/15	0.98	0.19	65,69,71,75	0
3	NAG	D	1	14/15	0.98	0.19	64,66,69,73	0
4	NAG	H	1	14/15	0.98	0.16	59,64,66,70	0

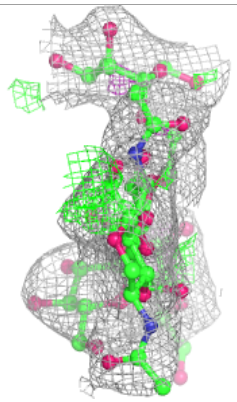
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around Chain C:

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

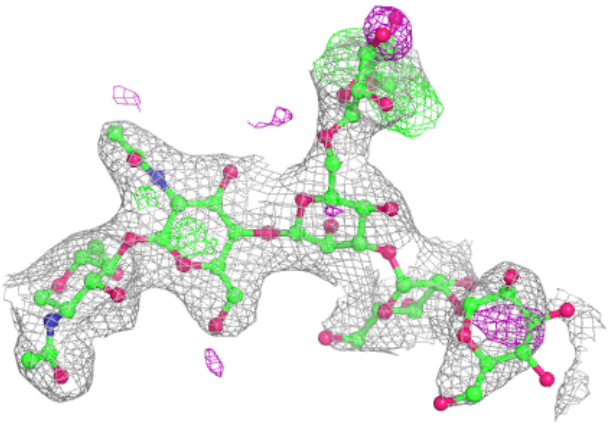


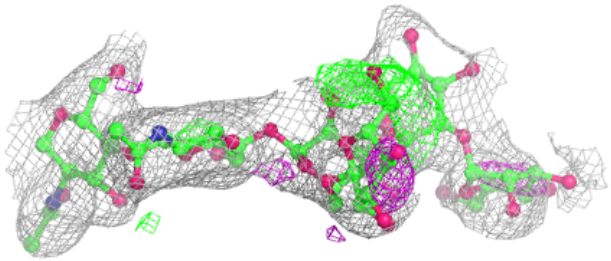


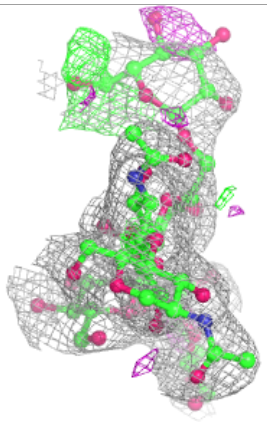


Electron density around Chain E:

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

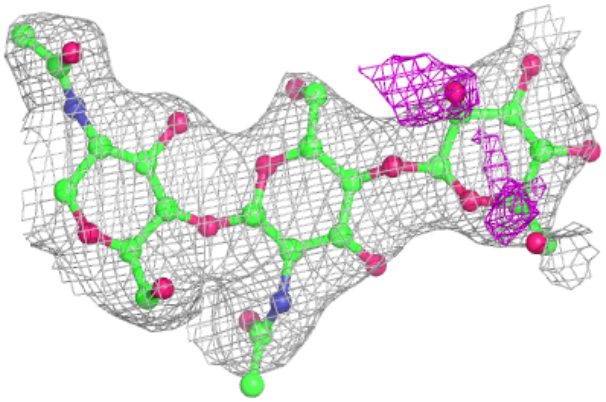


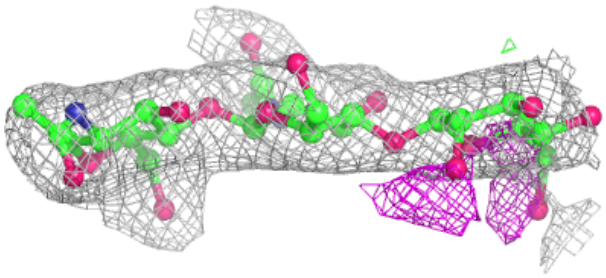


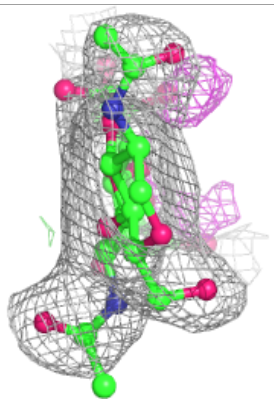


Electron density around Chain D:

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

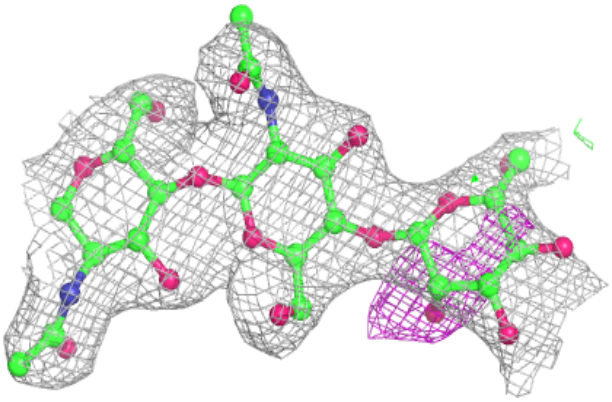


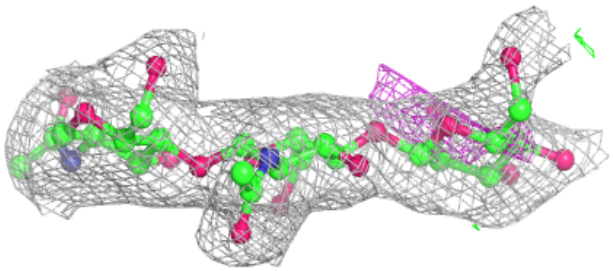


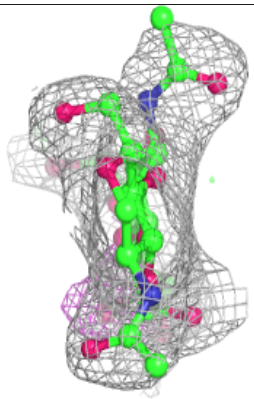


Electron density around Chain G:

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

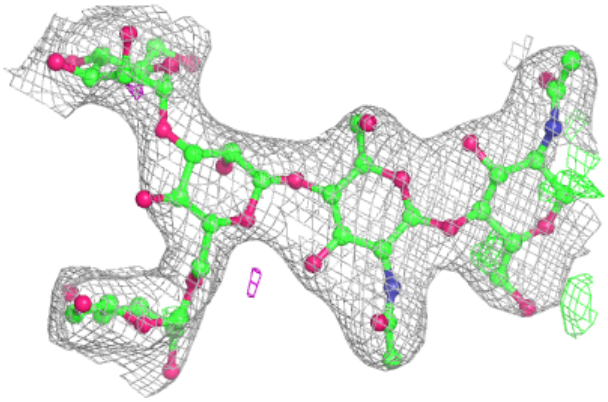


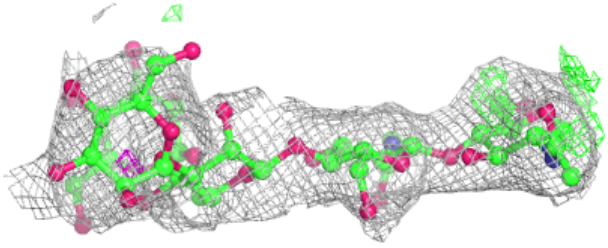


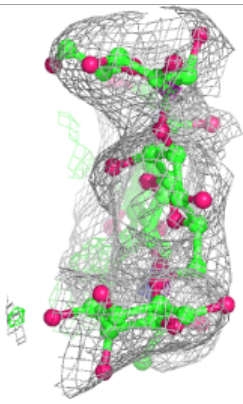


Electron density around Chain F:

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

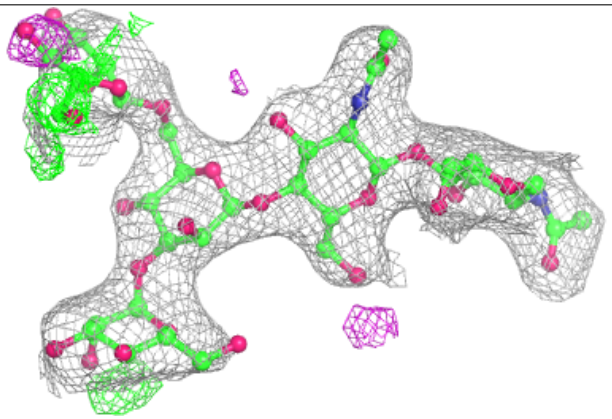


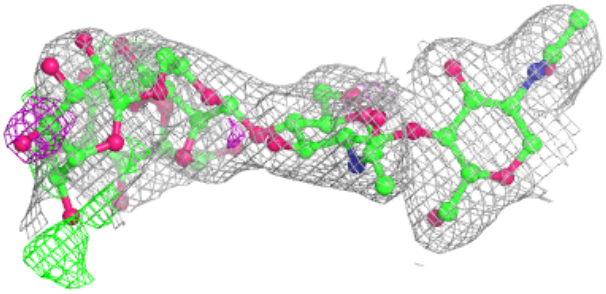


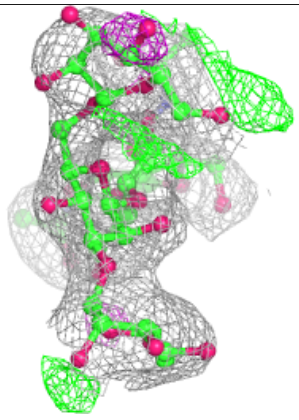


Electron density around Chain H:

$2mF_o$-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)

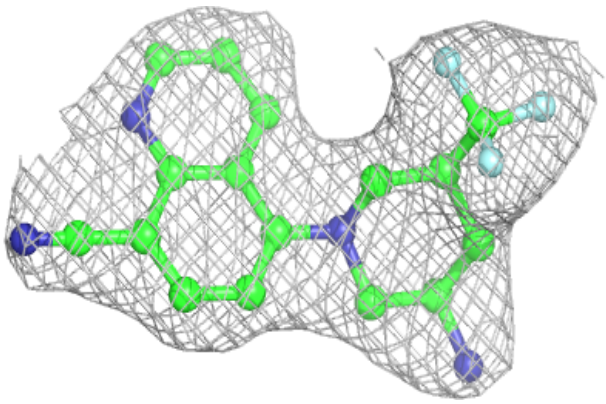
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

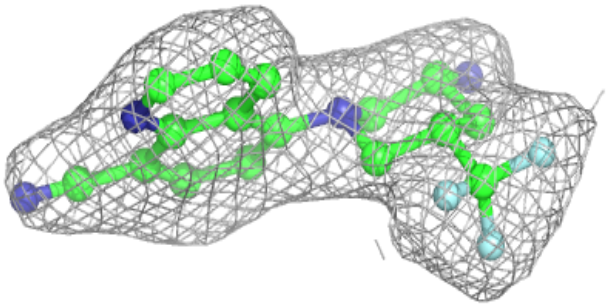
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	NAG	A	904	14/15	0.79	0.20	119,120,120,121	0
5	NAG	A	920	14/15	0.80	0.31	111,113,114,114	0
5	NAG	B	903	14/15	0.85	0.21	112,113,115,115	0
5	NAG	B	901	14/15	0.86	0.23	107,109,110,110	0
5	NAG	A	903	14/15	0.86	0.23	148,149,150,272	1
5	NAG	B	902	14/15	0.87	0.25	103,104,105,106	0
5	NAG	B	917	14/15	0.87	0.20	105,107,107,107	0
5	NAG	A	901	14/15	0.88	0.22	121,122,123,123	0
7	FMT	B	919	3/3	0.94	0.17	77,77,77,78	0
5	NAG	A	902	14/15	0.95	0.14	97,99,101,101	0
6	QLH	B	918	23/23	0.96	0.18	66,67,68,69	0
6	QLH	A	921	23/23	0.97	0.19	60,63,66,68	0

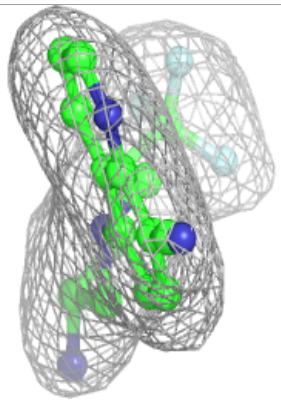
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around QLH B 918:

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

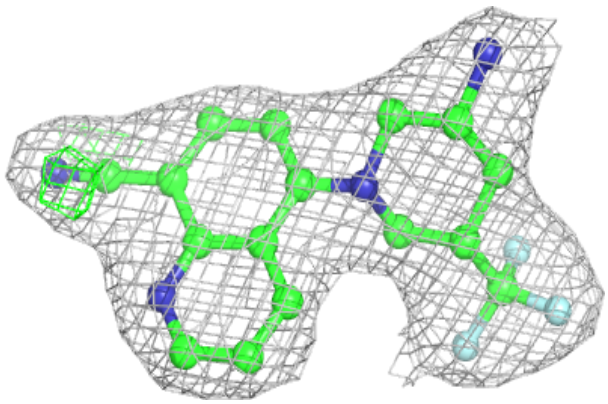


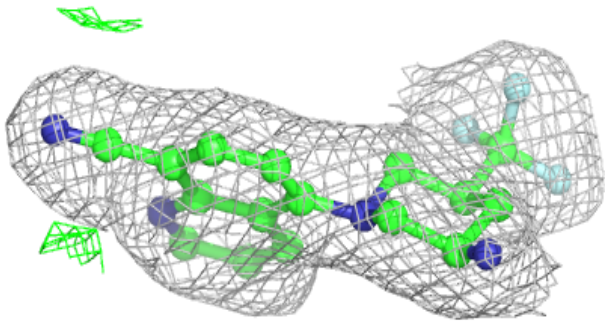


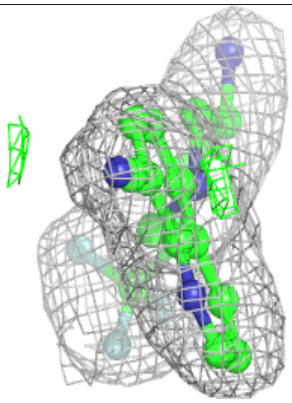


Electron density around QLH A 921:

$2mF_o$-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.