Full wwPDB X-ray Structure Validation Report (i)

Mar 6, 2026 – 11:40 PM UTC

PDB ID	:	8PFI / pdb_00008pfi
Title	:	Crystal structure of human TLR8 in complex with compound 34
Authors	:	Faller, M.; Zink, F.
Deposited on	:	2023-06-16
Resolution	:	2.79 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 (i) 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 (i)) were used in the production of this report:

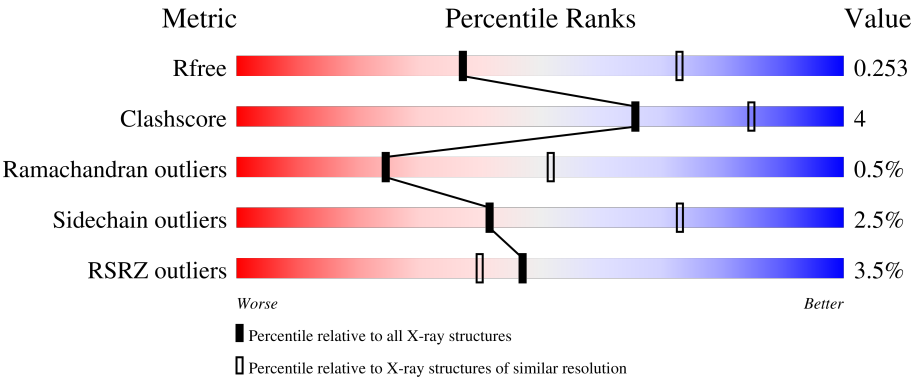
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.79 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	5248 (2.80-2.76)
Clashscore	190562	5693 (2.80-2.76)
Ramachandran outliers	187476	5590 (2.80-2.76)
Sidechain outliers	187428	5592 (2.80-2.76)
RSRZ outliers	180081	5251 (2.80-2.76)

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	807	3% 79% 12% 9%
1	B	807	3% 79% 12% • 9%
2	C	5	40% 60%
2	E	5	40% 60%
2	F	5	60% 40%

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Mol	Chain	Length	Quality of chain
2	H	5	40% 60%
3	D	3	33% 67%
3	G	3	33% 67%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 12696 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.

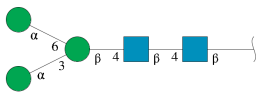
- Molecule 1 is a protein called Toll-like receptor 8.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	733	Total	C	N	O	S	0	0	0
			5765	3691	970	1085	19			
1	B	734	Total	C	N	O	S	0	0	0
			5865	3741	995	1110	19			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	828	GLU	-	expression tag	UNP Q9NR97
A	829	PHE	-	expression tag	UNP Q9NR97
A	830	LEU	-	expression tag	UNP Q9NR97
A	831	VAL	-	expression tag	UNP Q9NR97
A	832	PRO	-	expression tag	UNP Q9NR97
A	833	ARG	-	expression tag	UNP Q9NR97
B	828	GLU	-	expression tag	UNP Q9NR97
B	829	PHE	-	expression tag	UNP Q9NR97
B	830	LEU	-	expression tag	UNP Q9NR97
B	831	VAL	-	expression tag	UNP Q9NR97
B	832	PRO	-	expression tag	UNP Q9NR97
B	833	ARG	-	expression tag	UNP Q9NR97

- Molecule 2 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
2	C	5	Total	C	N	O	0	0	0
			61	34	2	25			

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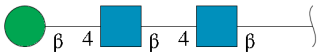
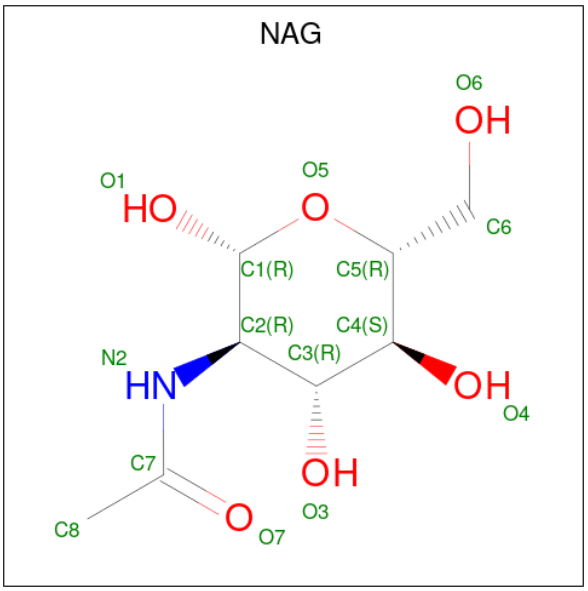
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
2	E	5	Total C N O 61 34 2 25	0	0	0
2	F	5	Total C N O 61 34 2 25	0	0	0
2	H	5	Total C N O 61 34 2 25	0	0	0

- 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 39 22 2 15	0	0	0
3	G	3	Total C N O 39 22 2 15	0	0	0

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).



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

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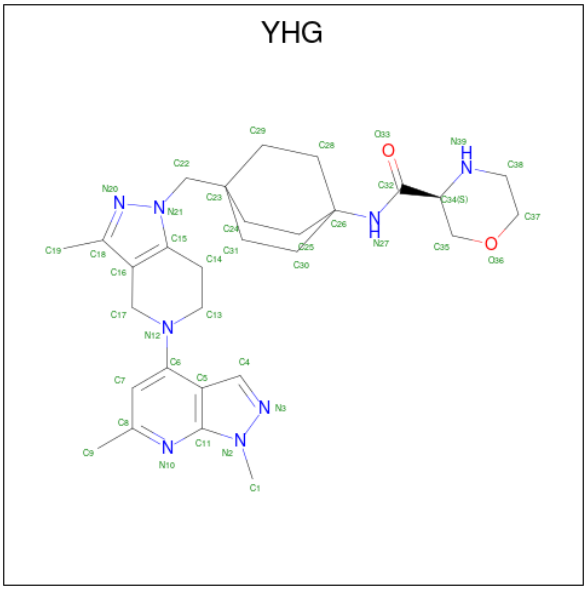
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C N O 14 8 1 5	0	0
4	A	1	Total C N O 14 8 1 5	0	0
4	A	1	Total C N O 14 8 1 5	0	0
4	A	1	Total C N O 14 8 1 5	0	0
4	A	1	Total C N O 14 8 1 5	0	0
4	B	1	Total C N O 14 8 1 5	0	0
4	B	1	Total C N O 14 8 1 5	0	0
4	B	1	Total C N O 14 8 1 5	0	0
4	B	1	Total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

- Molecule 5 is (3 {S})- {N}-[4-[[5-(1,6-dimethylpyrazolo[3,4-b]pyridin-4-yl)-3-methyl-6,7-dihydro-4 {H}-pyrazolo[4,3-c]pyridin-1-yl]methyl]-1-bicyclo[2.2.2]octanyl]morpholine-3-carboxamide (CCD ID: YHG) (formula: $C_{29}H_{40}N_8O_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C N O 39 29 8 2	0	0
5	B	1	Total C N O 39 29 8 2	0	0

- Molecule 6 is water.

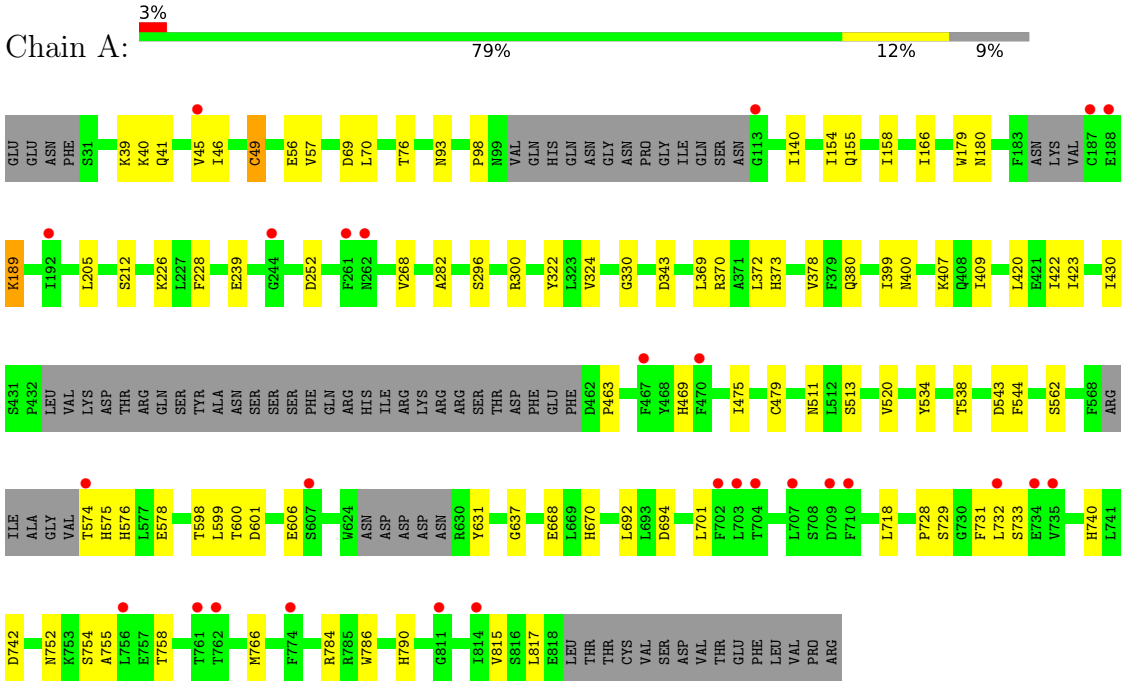
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	271	Total O 271 271	0	0
6	B	227	Total O 227 227	0	0

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.

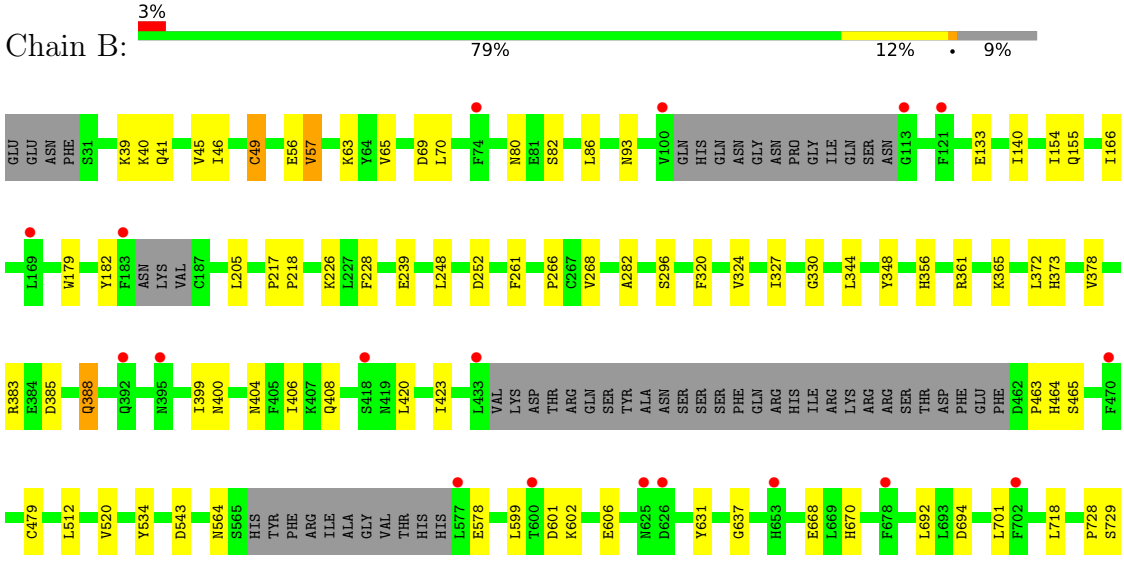
• Molecule 1: Toll-like receptor 8

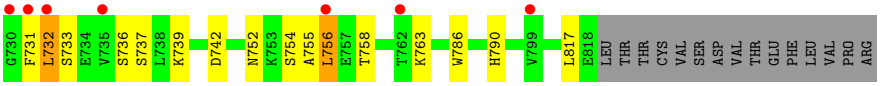
Chain A:



• Molecule 1: Toll-like receptor 8

Chain B:





• Molecule 2: alpha-D-mannopyranose-(1-3)-[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

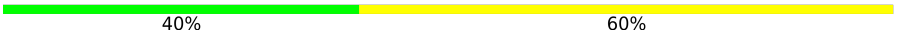
Chain C:





• Molecule 2: alpha-D-mannopyranose-(1-3)-[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 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 F:





• Molecule 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 H:





• 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:




NAG1
NAG2
BMA3

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	164.59Å 86.94Å 153.49Å 90.00° 120.63° 90.00°	Depositor
Resolution (Å)	66.04 – 2.79 66.04 – 2.79	Depositor EDS
% Data completeness (in resolution range)	99.0 (66.04-2.79) 99.0 (66.04-2.79)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.45 (at 2.77Å)	Xtriage
Refinement program	BUSTER 2.11.7	Depositor
R, R_{free}	0.216 , 0.250 0.222 , 0.253	Depositor DCC
R_{free} test set	2372 reflections (5.11%)	wwPDB-VP
Wilson B-factor (Å^2)	64.6	Xtriage
Anisotropy	0.362	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 51.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	0.000 for h,-k,-h-l	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	12696	wwPDB-VP
Average B, all atoms (Å^2)	76.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.32% 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, MAN, NAG, YHG

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	0.56	0/5883	0.90	0/8001
1	B	0.56	0/5979	0.90	0/8112
All	All	0.56	0/11862	0.90	0/16113

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	5765	0	5625	44	0
1	B	5865	0	5824	47	0
2	C	61	0	52	0	0
2	E	61	0	52	0	0
2	F	61	0	52	0	0
2	H	61	0	52	0	0
3	D	39	0	34	0	0
3	G	39	0	34	0	0
4	A	84	0	78	1	0
4	B	84	0	78	0	0
5	A	39	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	B	39	0	0	0	0
6	A	271	0	0	0	0
6	B	227	0	0	1	0
All	All	12696	0	11881	91	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 4.

All (91) 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:739:LYS:HD2	1:B:763:LYS:NZ	1.96	0.78
1:B:739:LYS:HD2	1:B:763:LYS:HZ2	1.50	0.77
1:B:520:VAL:HA	1:B:543:ASP:HB3	1.72	0.70
1:A:520:VAL:HA	1:A:543:ASP:HB3	1.72	0.69
1:A:574:THR:HB	1:A:576:HIS:NE2	2.14	0.62
1:B:57:VAL:HG11	1:B:82:SER:HB3	1.81	0.62
1:B:385:ASP:HA	1:B:388:GLN:HG3	1.83	0.60
1:B:733:SER:HB2	1:B:758:THR:HA	1.85	0.59
1:A:733:SER:HB2	1:A:758:THR:HA	1.84	0.58
1:A:373:HIS:HA	1:A:400:ASN:HB3	1.86	0.57
1:B:670:HIS:HA	1:B:694:ASP:HB3	1.87	0.56
1:A:599:LEU:HB2	1:A:631:TYR:HE1	1.71	0.56
1:A:670:HIS:HA	1:A:694:ASP:HB3	1.87	0.56
1:A:422:ILE:HG23	1:A:475:ILE:HD12	1.88	0.55
1:A:729:SER:HA	1:A:755:ALA:HA	1.89	0.54
1:A:538:THR:HG22	1:A:562:SER:HB2	1.90	0.54
1:B:729:SER:HA	1:B:755:ALA:HA	1.90	0.54
1:A:76:THR:HG22	1:A:98:PRO:HG3	1.89	0.53
1:B:752:ASN:ND2	1:B:754:SER:OG	2.41	0.53
1:A:668:GLU:HG3	1:A:692:LEU:HD23	1.91	0.53
1:B:373:HIS:HA	1:B:400:ASN:HB3	1.91	0.53
1:A:752:ASN:ND2	1:A:754:SER:OG	2.42	0.52
1:B:668:GLU:HG3	1:B:692:LEU:HD23	1.91	0.52
1:B:327:ILE:HG12	1:B:344:LEU:HD13	1.91	0.52
1:A:399:ILE:HD12	1:A:420:LEU:HD11	1.93	0.51
1:B:399:ILE:HD12	1:B:420:LEU:HD11	1.92	0.50
1:B:385:ASP:HA	1:B:388:GLN:CG	2.42	0.50
1:B:737:SER:HA	1:B:763:LYS:HE3	1.94	0.50
1:B:239:GLU:HA	1:B:282:ALA:HA	1.94	0.49
1:A:409:ILE:HD12	1:A:430:ILE:HD11	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:369:LEU:HD21	1:A:372:LEU:HD13	1.94	0.49
1:B:718:LEU:HA	1:B:742:ASP:HB3	1.95	0.48
1:B:728:PRO:HG2	1:B:731:PHE:HB2	1.96	0.48
1:A:239:GLU:HA	1:A:282:ALA:HA	1.95	0.48
1:A:786:TRP:CD1	1:A:790:HIS:CD2	3.02	0.48
1:A:300:ARG:HG2	1:A:322:TYR:HB2	1.95	0.48
1:B:786:TRP:CD1	1:B:790:HIS:CD2	3.02	0.48
1:A:718:LEU:HA	1:A:742:ASP:HB3	1.96	0.48
1:A:606:GLU:HG3	1:A:637:GLY:HA3	1.96	0.47
1:A:57:VAL:HG22	1:A:70:LEU:HD13	1.95	0.47
1:A:728:PRO:HG2	1:A:731:PHE:HB2	1.96	0.47
1:A:420:LEU:HD13	1:A:423:ILE:HG12	1.96	0.47
1:B:606:GLU:HG3	1:B:637:GLY:HA3	1.95	0.46
1:A:575:HIS:ND1	1:A:598:THR:HG23	2.31	0.46
1:B:736:SER:O	1:B:763:LYS:HG2	2.16	0.46
1:B:356:HIS:CD2	1:B:383:ARG:HE	2.33	0.46
1:A:228:PHE:HA	1:A:252:ASP:HB3	1.98	0.45
1:A:154:ILE:HG22	1:A:155:GLN:HG2	1.97	0.45
1:B:63:LYS:HA	1:B:86:LEU:HD23	1.99	0.45
1:B:154:ILE:HG22	1:B:155:GLN:HG2	1.96	0.45
1:A:574:THR:HG22	1:A:600:THR:HG21	1.99	0.45
1:A:511:ASN:OD1	1:A:513:SER:HB2	2.17	0.45
1:A:380:GLN:HB3	1:A:407:LYS:HD2	1.99	0.44
1:B:739:LYS:CD	1:B:763:LYS:HZ2	2.26	0.44
1:A:343:ASP:OD2	1:A:469:HIS:ND1	2.45	0.44
1:A:479:CYS:SG	1:A:534:TYR:CD1	3.11	0.44
1:A:575:HIS:ND1	1:A:598:THR:CG2	2.81	0.44
1:B:49:CYS:HB3	1:B:70:LEU:HD23	2.00	0.43
1:B:133:GLU:OE1	1:B:464:HIS:NE2	2.50	0.43
1:B:39:LYS:HE3	1:B:41:GLN:HB2	2.01	0.43
1:B:599:LEU:HB2	1:B:631:TYR:HE1	1.83	0.43
1:B:63:LYS:O	6:B:1001:HOH:O	2.22	0.43
1:B:205:LEU:HD12	1:B:226:LYS:HD2	2.00	0.43
1:A:179:TRP:NE1	1:A:463:PRO:HB3	2.34	0.43
1:B:404:ASN:HB3	1:B:406:ILE:HG13	2.00	0.43
1:A:39:LYS:HE3	1:A:41:GLN:HB2	2.01	0.43
1:A:69:ASP:HA	1:A:93:ASN:HB3	2.01	0.43
1:B:140:ILE:HD13	1:B:166:ILE:HD11	2.01	0.43
1:B:179:TRP:NE1	1:B:463:PRO:HB3	2.34	0.43
1:A:140:ILE:HD13	1:A:166:ILE:HD11	2.01	0.42
1:B:479:CYS:SG	1:B:534:TYR:CD1	3.12	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:69:ASP:HA	1:B:93:ASN:HB3	2.01	0.42
1:B:756:LEU:HD23	1:B:786:TRP:CG	2.55	0.42
1:B:228:PHE:HA	1:B:252:ASP:HB3	2.01	0.42
1:B:217:PRO:HA	1:B:218:PRO:HD3	1.94	0.42
1:B:732:LEU:HD13	1:B:756:LEU:HD11	2.01	0.41
1:A:205:LEU:HD12	1:A:226:LYS:HD2	2.02	0.41
1:A:370:ARG:HH22	4:A:903:NAG:H61	1.86	0.41
1:A:189:LYS:HA	1:A:212:SER:HB2	2.02	0.41
1:B:261:PHE:HE2	1:B:348:TYR:CE2	2.39	0.41
1:B:756:LEU:HD23	1:B:786:TRP:CD2	2.55	0.41
1:A:49:CYS:HB3	1:A:70:LEU:HD23	2.02	0.41
1:B:420:LEU:HD13	1:B:423:ILE:HG12	2.03	0.41
1:A:40:LYS:HA	1:A:45:VAL:HA	2.02	0.41
1:B:40:LYS:HA	1:B:45:VAL:HA	2.01	0.41
1:A:784:ARG:HD3	1:A:815:VAL:HA	2.03	0.41
1:A:158:ILE:O	1:A:180:ASN:HB3	2.21	0.40
1:B:45:VAL:HG12	1:B:65:VAL:HG12	2.03	0.40
1:A:740:HIS:HD2	1:A:766:MET:HB3	1.86	0.40
1:B:296:SER:HA	1:B:320:PHE:O	2.21	0.40
1:B:182:TYR:CE2	1:B:266:PRO:HD2	2.57	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	721/807 (89%)	675 (94%)	42 (6%)	4 (1%)	21	47
1	B	724/807 (90%)	675 (93%)	46 (6%)	3 (0%)	30	57
All	All	1445/1614 (90%)	1350 (93%)	88 (6%)	7 (0%)	24	52

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	330	GLY
1	B	330	GLY
1	A	601	ASP
1	B	601	ASP
1	A	189	LYS
1	A	378	VAL
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	647/751 (86%)	636 (98%)	11 (2%)	53 80
1	B	674/751 (90%)	652 (97%)	22 (3%)	33 66
All	All	1321/1502 (88%)	1288 (98%)	33 (2%)	42 73

All (33) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	46	ILE
1	A	49	CYS
1	A	56	GLU
1	A	268	VAL
1	A	296	SER
1	A	324	VAL
1	A	544	PHE
1	A	578	GLU
1	A	701	LEU
1	A	732	LEU
1	A	817	LEU
1	B	46	ILE
1	B	49	CYS
1	B	56	GLU
1	B	57	VAL
1	B	80	ASN
1	B	248	LEU

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Mol	Chain	Res	Type
1	B	268	VAL
1	B	324	VAL
1	B	361	ARG
1	B	365	LYS
1	B	372	LEU
1	B	388	GLN
1	B	408	GLN
1	B	465	SER
1	B	512	LEU
1	B	564	ASN
1	B	578	GLU
1	B	602	LYS
1	B	701	LEU
1	B	732	LEU
1	B	756	LEU
1	B	817	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (30) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	55	GLN
1	A	59	GLN
1	A	77	HIS
1	A	87	GLN
1	A	115	ASN
1	A	277	ASN
1	A	285	ASN
1	A	309	ASN
1	A	466	ASN
1	A	593	HIS
1	A	752	ASN
1	A	770	HIS
1	A	809	GLN
1	B	55	GLN
1	B	59	GLN
1	B	77	HIS
1	B	87	GLN
1	B	99	ASN
1	B	115	ASN
1	B	160	ASN
1	B	191	ASN
1	B	277	ASN

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Mol	Chain	Res	Type
1	B	285	ASN
1	B	309	ASN
1	B	388	GLN
1	B	593	HIS
1	B	594	ASN
1	B	629	ASN
1	B	752	ASN
1	B	809	GLN

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)

26 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	0.28	0	17,19,21	0.84	1 (5%)
2	NAG	C	2	2	14,14,15	0.28	0	17,19,21	0.58	0
2	BMA	C	3	2	11,11,12	0.24	0	15,15,17	0.53	0
2	MAN	C	4	2	11,11,12	0.33	0	15,15,17	0.89	1 (6%)
2	MAN	C	5	2	11,11,12	0.34	0	15,15,17	0.77	1 (6%)
3	NAG	D	1	3,1	14,14,15	0.30	0	17,19,21	0.53	0
3	NAG	D	2	3	14,14,15	0.33	0	17,19,21	0.70	1 (5%)
3	BMA	D	3	3	11,11,12	0.31	0	15,15,17	0.61	1 (6%)
2	NAG	E	1	1,2	14,14,15	0.29	0	17,19,21	0.77	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	NAG	E	2	2	14,14,15	0.29	0	17,19,21	0.43	0
2	BMA	E	3	2	11,11,12	0.29	0	15,15,17	0.38	0
2	MAN	E	4	2	11,11,12	0.33	0	15,15,17	0.72	1 (6%)
2	MAN	E	5	2	11,11,12	0.34	0	15,15,17	0.67	1 (6%)
2	NAG	F	1	1,2	14,14,15	0.28	0	17,19,21	0.49	0
2	NAG	F	2	2	14,14,15	0.31	0	17,19,21	0.58	0
2	BMA	F	3	2	11,11,12	0.27	0	15,15,17	0.52	0
2	MAN	F	4	2	11,11,12	0.31	0	15,15,17	0.89	1 (6%)
2	MAN	F	5	2	11,11,12	0.30	0	15,15,17	0.74	1 (6%)
3	NAG	G	1	3,1	14,14,15	0.27	0	17,19,21	0.52	0
3	NAG	G	2	3	14,14,15	0.29	0	17,19,21	0.64	1 (5%)
3	BMA	G	3	3	11,11,12	0.30	0	15,15,17	0.61	1 (6%)
2	NAG	H	1	1,2	14,14,15	0.30	0	17,19,21	0.69	1 (5%)
2	NAG	H	2	2	14,14,15	0.30	0	17,19,21	0.49	0
2	BMA	H	3	2	11,11,12	0.29	0	15,15,17	0.52	0
2	MAN	H	4	2	11,11,12	0.32	0	15,15,17	0.74	1 (6%)
2	MAN	H	5	2	11,11,12	0.34	0	15,15,17	0.71	1 (6%)

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

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

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

There are no bond length outliers.

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	4	MAN	C1-O5-C5	3.33	116.64	112.19
2	F	4	MAN	C1-O5-C5	3.32	116.64	112.19
2	C	5	MAN	C1-O5-C5	2.84	115.99	112.19
2	F	5	MAN	C1-O5-C5	2.79	115.92	112.19
2	H	4	MAN	C1-O5-C5	2.76	115.88	112.19
2	E	4	MAN	C1-O5-C5	2.69	115.79	112.19
2	E	1	NAG	C1-O5-C5	2.67	115.77	112.19
2	H	5	MAN	C1-O5-C5	2.53	115.58	112.19
3	D	2	NAG	C1-O5-C5	2.48	115.51	112.19
2	H	1	NAG	C1-O5-C5	2.42	115.44	112.19
2	E	5	MAN	C1-O5-C5	2.33	115.31	112.19
3	G	2	NAG	C1-O5-C5	2.30	115.27	112.19
3	D	3	BMA	C1-O5-C5	2.21	115.15	112.19
3	G	3	BMA	C1-O5-C5	2.18	115.11	112.19
2	C	1	NAG	C1-O5-C5	2.05	114.93	112.19

There are no chirality outliers.

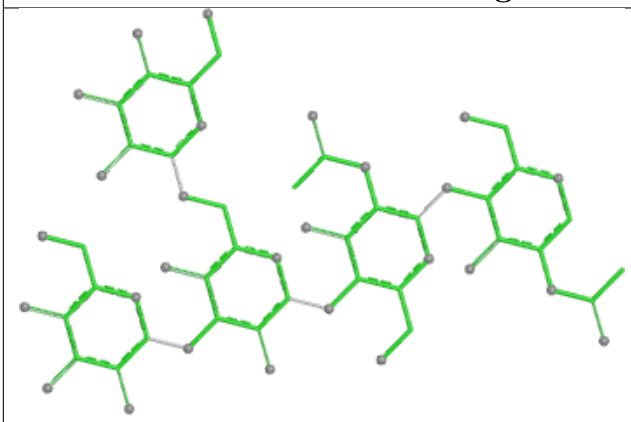
There are no torsion outliers.

There are no ring outliers.

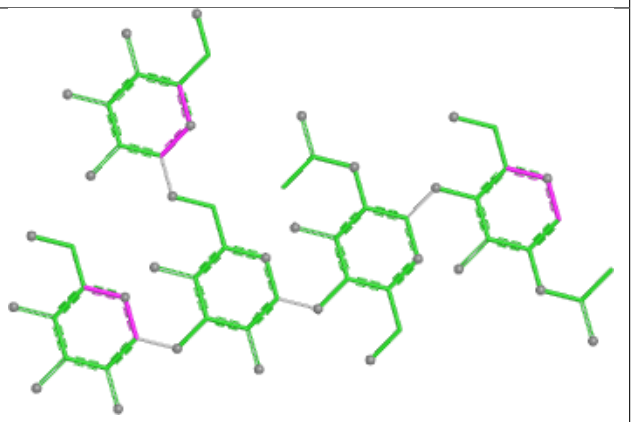
No monomer is involved in short contacts.

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

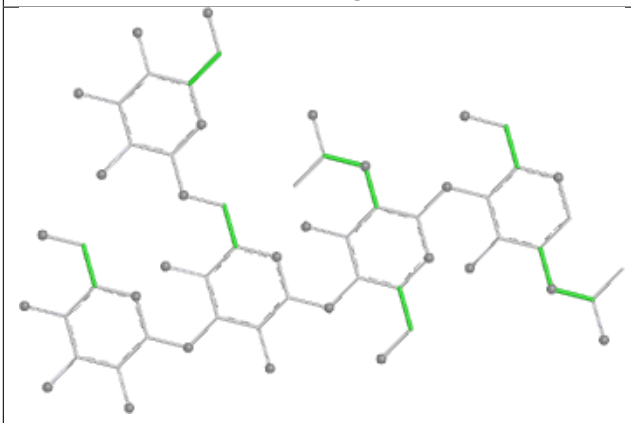
Oligosaccharide Chain C



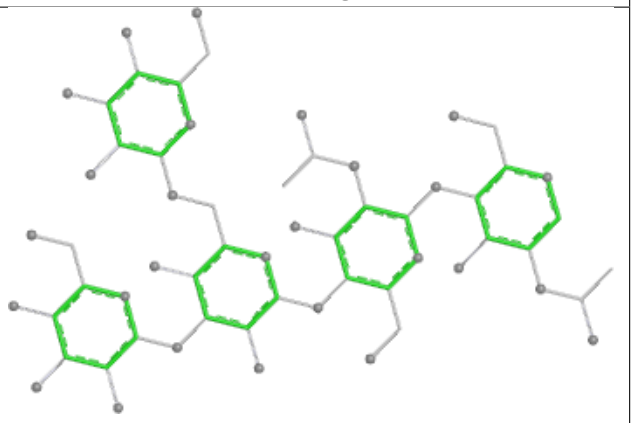
Bond lengths



Bond angles

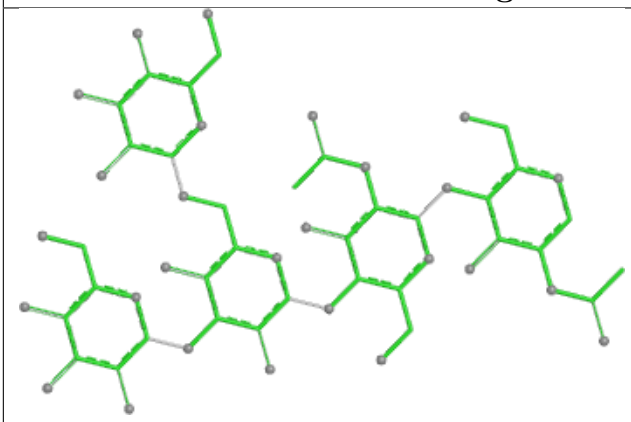


Torsions

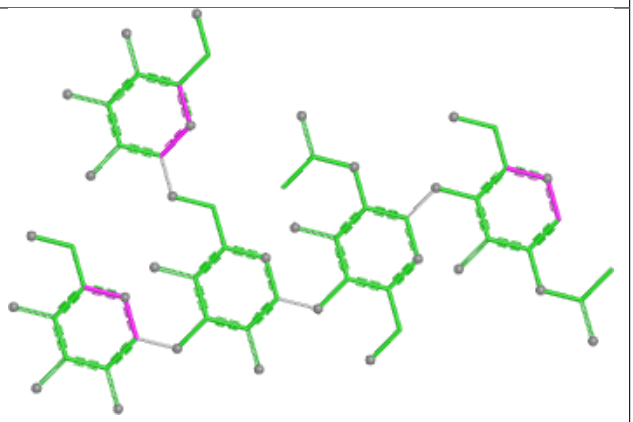


Rings

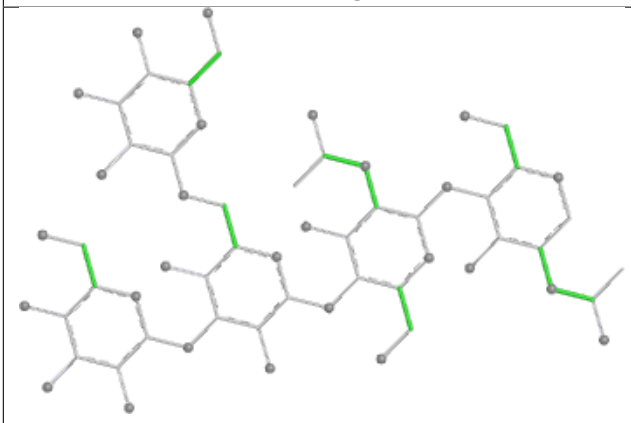
Oligosaccharide Chain E



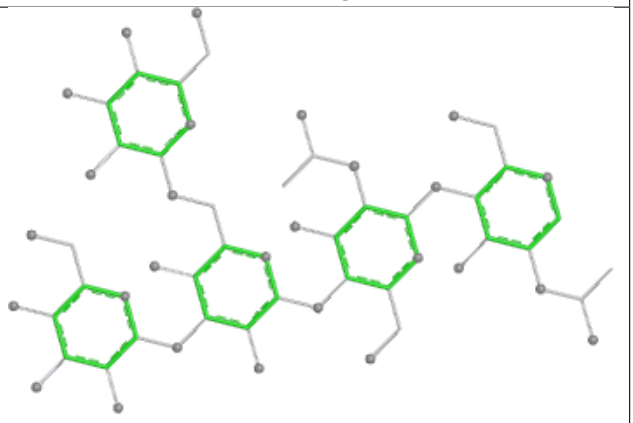
Bond lengths



Bond angles

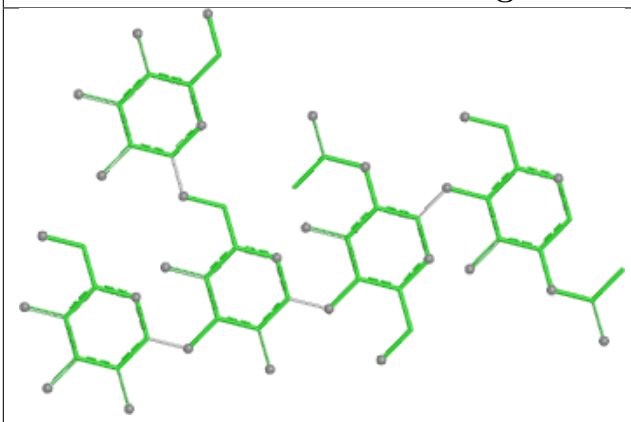


Torsions

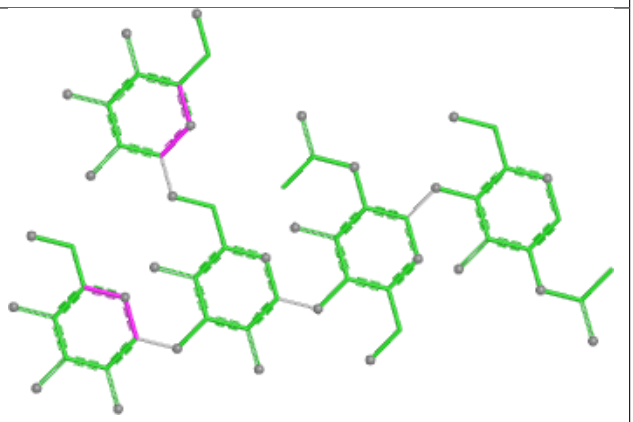


Rings

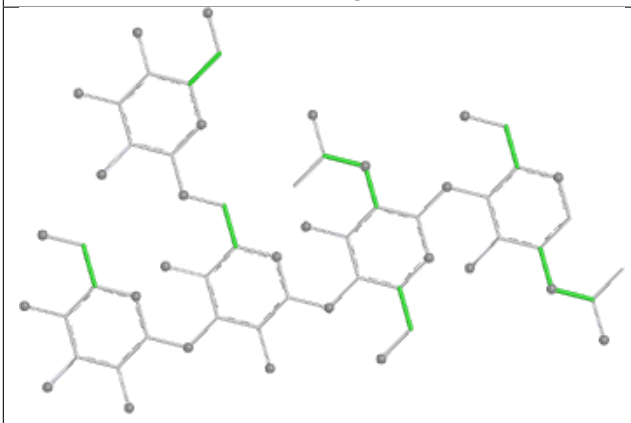
Oligosaccharide Chain F



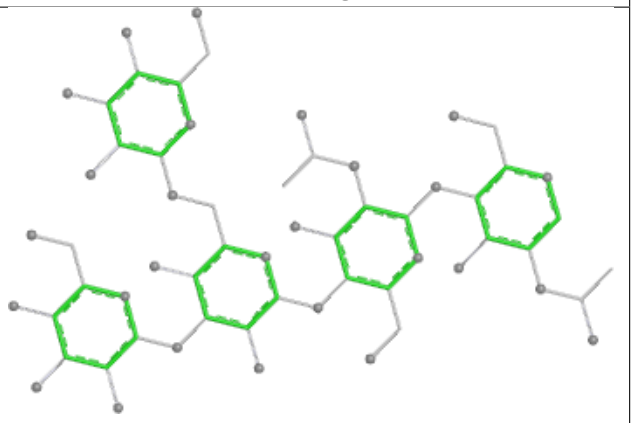
Bond lengths



Bond angles

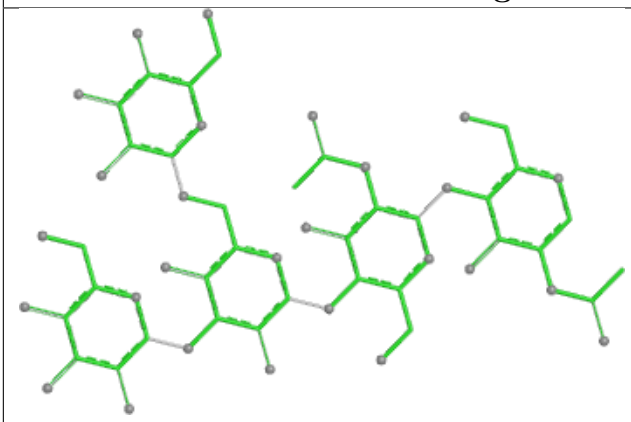


Torsions

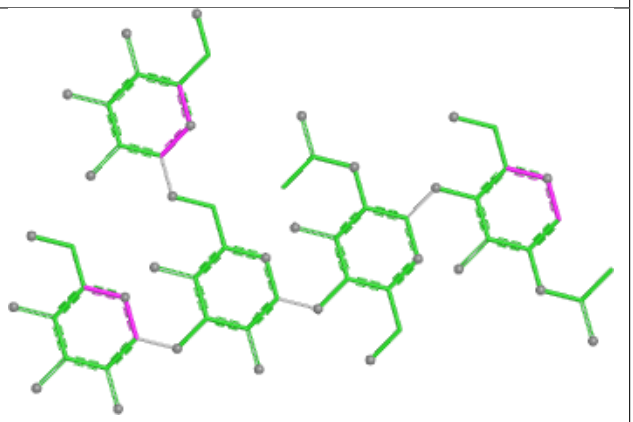


Rings

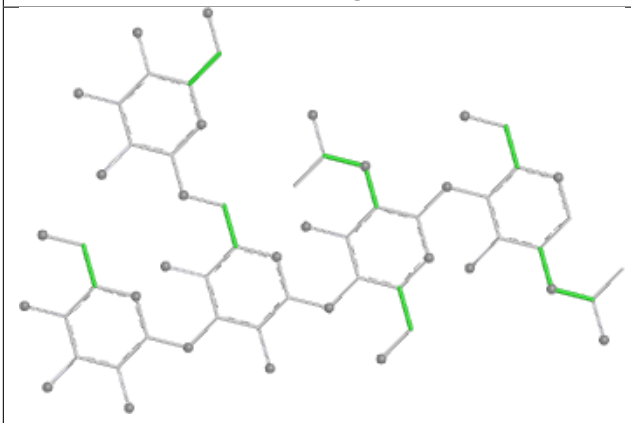
Oligosaccharide Chain H



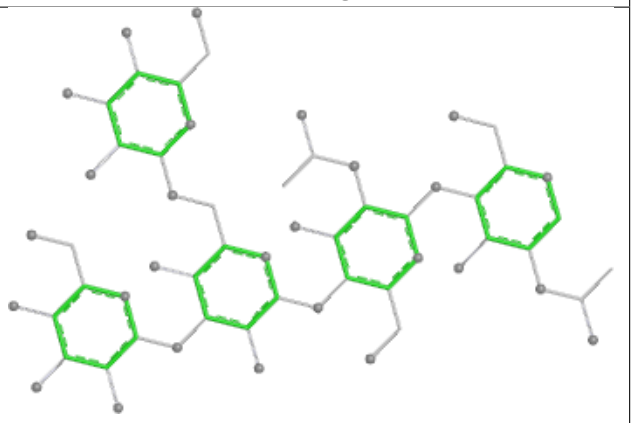
Bond lengths



Bond angles

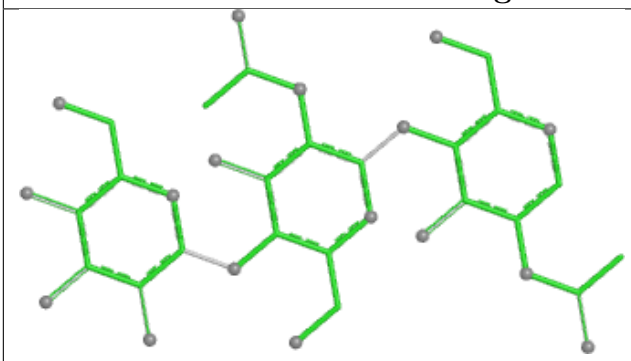


Torsions

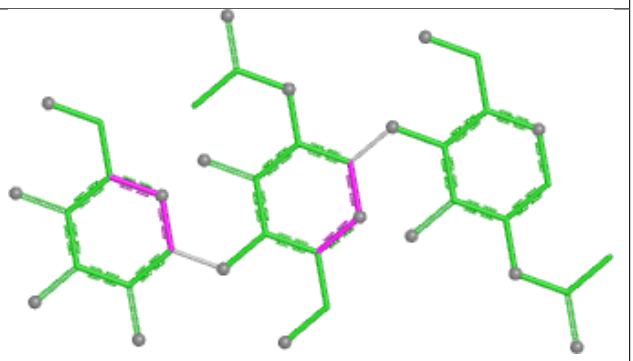


Rings

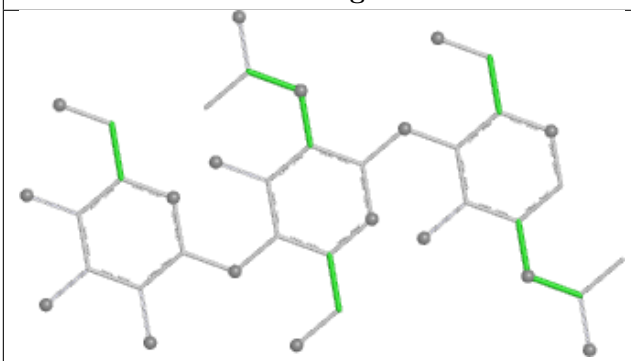
Oligosaccharide Chain D



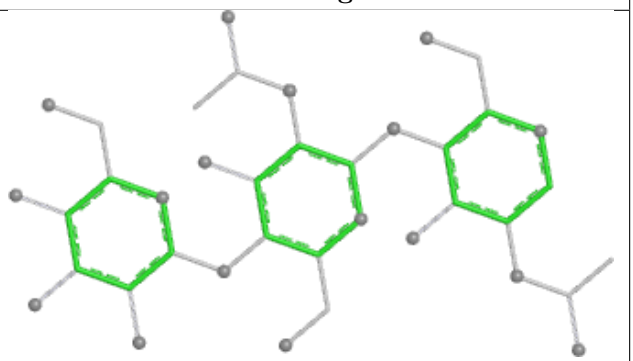
Bond lengths



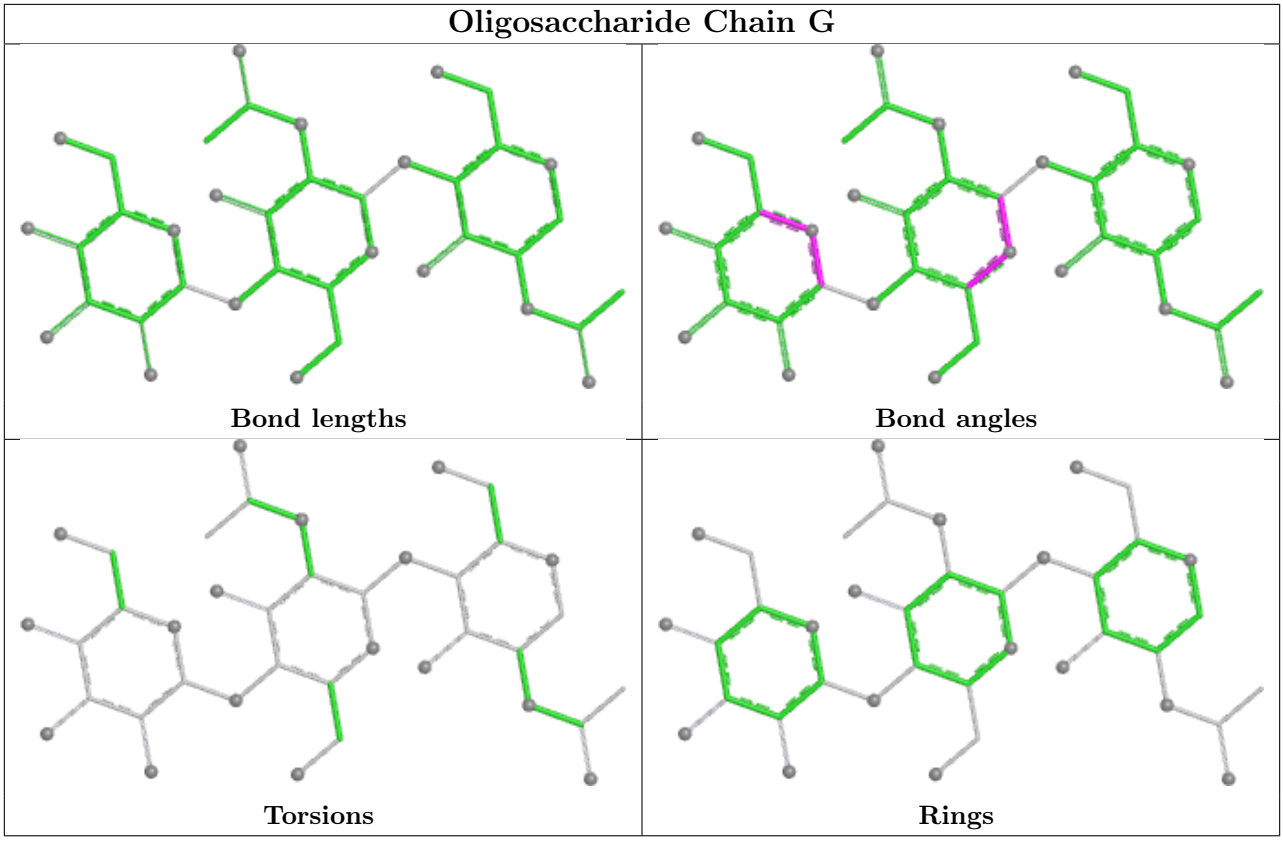
Bond angles



Torsions



Rings



5.6 Ligand geometry (i)

14 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	$\#\|Z\| > 2$
4	NAG	B	905	1	14,14,15	0.33	0	17,19,21	0.78	1 (5%)
4	NAG	A	903	1	14,14,15	0.34	0	17,19,21	0.74	1 (5%)
4	NAG	B	907	1	14,14,15	0.32	0	17,19,21	0.57	0
5	YHG	B	901	-	45,45,45	2.07	9 (20%)	54,69,69	2.93	20 (37%)
4	NAG	A	905	1	14,14,15	0.29	0	17,19,21	0.54	0
4	NAG	A	901	1	14,14,15	0.30	0	17,19,21	0.51	0
5	YHG	A	907	-	45,45,45	2.00	9 (20%)	54,69,69	2.99	19 (35%)
4	NAG	B	906	1	14,14,15	0.30	0	17,19,21	0.55	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
4	NAG	A	904	1	14,14,15	0.33	0	17,19,21	0.65	1 (5%)
4	NAG	B	904	1	14,14,15	0.32	0	17,19,21	0.72	1 (5%)
4	NAG	A	902	1	14,14,15	0.27	0	17,19,21	0.74	1 (5%)
4	NAG	A	906	1	14,14,15	0.30	0	17,19,21	0.56	0
4	NAG	B	903	1	14,14,15	0.30	0	17,19,21	0.72	1 (5%)
4	NAG	B	902	1	14,14,15	0.30	0	17,19,21	0.51	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
4	NAG	B	905	1	-	0/6/23/26	0/1/1/1
4	NAG	A	903	1	-	0/6/23/26	0/1/1/1
4	NAG	B	907	1	-	0/6/23/26	0/1/1/1
5	YHG	B	901	-	-	4/18/56/56	0/8/7/7
4	NAG	A	905	1	-	0/6/23/26	0/1/1/1
4	NAG	A	901	1	-	0/6/23/26	0/1/1/1
5	YHG	A	907	-	-	4/18/56/56	0/8/7/7
4	NAG	B	906	1	-	0/6/23/26	0/1/1/1
4	NAG	A	904	1	-	0/6/23/26	0/1/1/1
4	NAG	B	904	1	-	0/6/23/26	0/1/1/1
4	NAG	A	902	1	-	0/6/23/26	0/1/1/1
4	NAG	A	906	1	-	0/6/23/26	0/1/1/1
4	NAG	B	903	1	-	0/6/23/26	0/1/1/1
4	NAG	B	902	1	-	0/6/23/26	0/1/1/1

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	907	YHG	C5-C4	8.43	1.51	1.42
5	B	901	YHG	C5-C4	8.35	1.51	1.42
5	A	907	YHG	C4-N3	-4.51	1.27	1.32
5	B	901	YHG	C4-N3	-4.38	1.27	1.32
5	B	901	YHG	C35-C34	4.09	1.57	1.52
5	B	901	YHG	C15-N21	-3.52	1.31	1.35
5	B	901	YHG	N2-N3	-3.47	1.35	1.37
5	A	907	YHG	C35-C34	3.20	1.56	1.52
5	A	907	YHG	C15-N21	-3.14	1.31	1.35
5	A	907	YHG	N2-N3	-2.59	1.35	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	907	YHG	C18-N20	-2.58	1.27	1.32
5	B	901	YHG	C18-N20	-2.55	1.27	1.32
5	A	907	YHG	C25-C26	2.49	1.58	1.53
5	A	907	YHG	C16-C18	2.49	1.46	1.40
5	B	901	YHG	C16-C18	2.48	1.46	1.40
5	B	901	YHG	C28-C26	2.41	1.57	1.53
5	B	901	YHG	C25-C26	2.37	1.57	1.53
5	A	907	YHG	C28-C26	2.20	1.57	1.53

All (45) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	B	901	YHG	C5-C11-N10	-9.88	120.29	126.56
5	A	907	YHG	C5-C11-N10	-9.82	120.32	126.56
5	A	907	YHG	C4-N3-N2	7.03	111.34	106.36
5	B	901	YHG	C4-N3-N2	6.40	110.89	106.36
5	B	901	YHG	C5-C6-N12	6.23	124.80	118.92
5	A	907	YHG	C5-C6-N12	6.21	124.79	118.92
5	A	907	YHG	C7-C6-C5	-5.87	114.40	120.83
5	B	901	YHG	C7-C6-C5	-5.70	114.59	120.83
5	A	907	YHG	C15-N21-N20	-5.61	108.02	113.85
5	A	907	YHG	C18-N20-N21	5.47	111.05	104.95
5	A	907	YHG	C37-O36-C35	5.30	117.40	110.02
5	B	901	YHG	C15-N21-N20	-5.12	108.53	113.85
5	B	901	YHG	C18-N20-N21	5.12	110.65	104.95
5	B	901	YHG	C11-C5-C4	-4.93	100.25	104.42
5	B	901	YHG	C16-C18-N20	-4.70	106.00	111.37
5	A	907	YHG	C16-C18-N20	-4.69	106.00	111.37
5	A	907	YHG	C11-C5-C4	-4.58	100.55	104.42
5	B	901	YHG	C37-O36-C35	4.58	116.39	110.02
5	B	901	YHG	C14-C15-C16	-3.61	121.48	125.54
5	A	907	YHG	C1-N2-N3	3.57	124.48	120.05
5	B	901	YHG	C17-C16-C18	-3.50	129.86	133.45
5	A	907	YHG	C14-C15-C16	-3.47	121.64	125.54
5	A	907	YHG	C17-C16-C18	-3.42	129.95	133.45
5	B	901	YHG	C19-C18-N20	3.39	125.98	119.39
5	B	901	YHG	C1-N2-N3	3.37	124.23	120.05
5	A	907	YHG	C19-C18-N20	3.33	125.86	119.39
5	B	901	YHG	C30-C26-C25	-3.17	105.87	108.84
5	A	907	YHG	C11-N2-N3	-3.00	108.19	110.91
5	A	907	YHG	C5-C4-N3	-2.83	109.23	111.38
4	B	905	NAG	C1-O5-C5	2.80	115.94	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	B	901	YHG	C25-C26-N27	2.78	114.92	109.03
5	A	907	YHG	C30-C26-C25	-2.77	106.25	108.84
5	B	901	YHG	C11-N2-N3	-2.67	108.49	110.91
5	A	907	YHG	C25-C26-N27	2.47	114.27	109.03
4	A	903	NAG	C1-O5-C5	2.46	115.49	112.19
4	B	904	NAG	C1-O5-C5	2.38	115.38	112.19
5	B	901	YHG	C5-C4-N3	-2.37	109.58	111.38
4	A	904	NAG	C1-O5-C5	2.27	115.23	112.19
5	B	901	YHG	C16-C17-N12	2.25	112.81	110.06
5	A	907	YHG	C16-C17-N12	2.20	112.74	110.06
4	A	902	NAG	C1-O5-C5	2.10	115.00	112.19
4	B	903	NAG	C1-O5-C5	2.09	114.98	112.19
5	B	901	YHG	C31-C23-C22	2.09	112.59	109.02
5	B	901	YHG	O36-C35-C34	2.08	114.00	111.13
5	A	907	YHG	C31-C23-C22	2.02	112.47	109.02

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	907	YHG	C5-C6-N12-C13
5	B	901	YHG	C5-C6-N12-C13
5	A	907	YHG	C7-C6-N12-C13
5	B	901	YHG	C7-C6-N12-C13
5	A	907	YHG	N27-C32-C34-C35
5	A	907	YHG	O33-C32-C34-C35
5	B	901	YHG	N27-C32-C34-C35
5	B	901	YHG	O33-C32-C34-C35

There are no ring outliers.

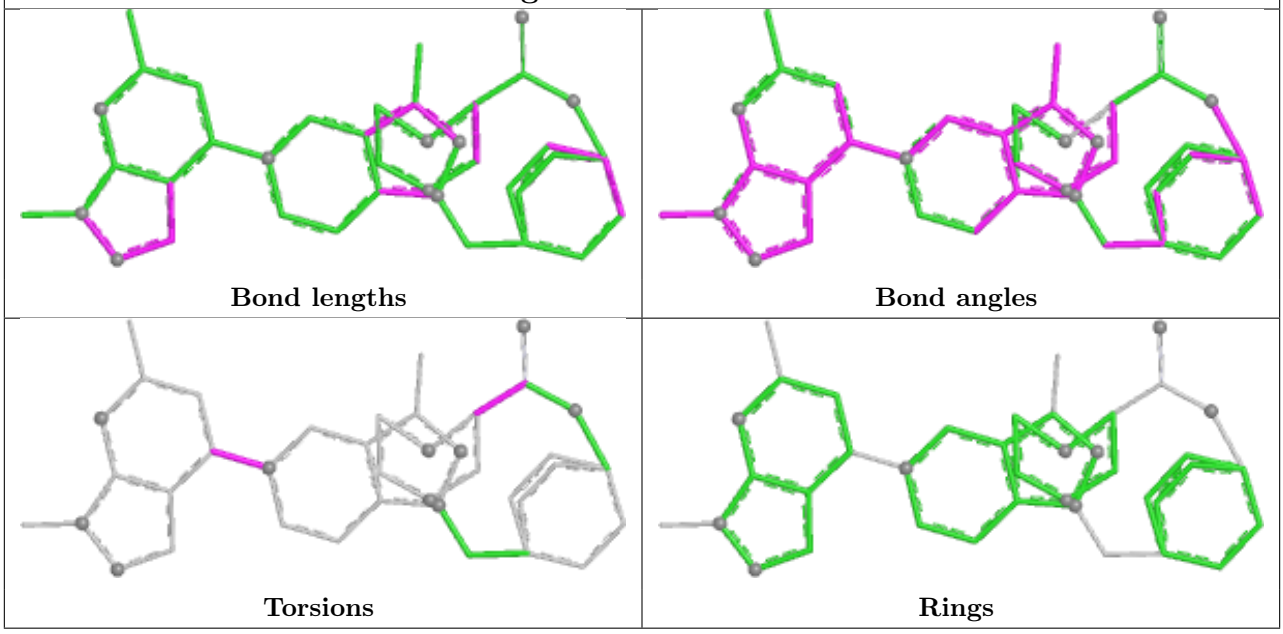
1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	903	NAG	1	0

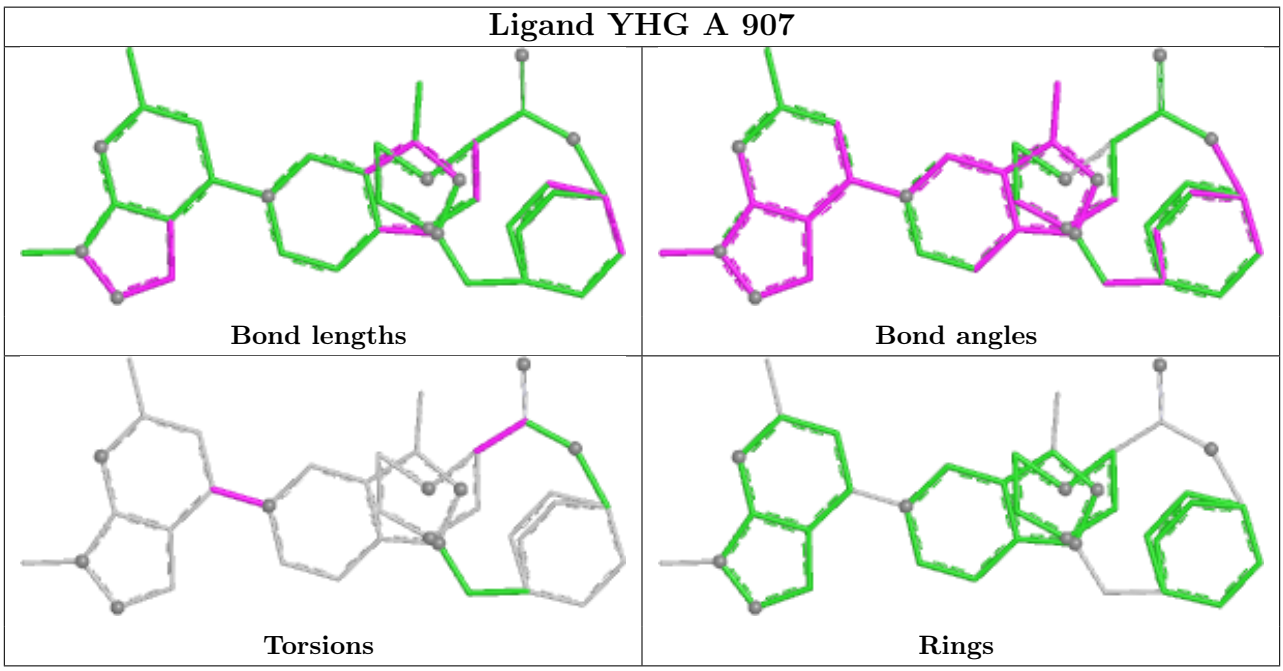
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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 YHG B 901



Ligand YHG A 907



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	733/807 (90%)	0.33	27 (3%)	45	38	40, 72, 96, 114	0
1	B	734/807 (90%)	0.40	25 (3%)	48	41	41, 80, 130, 153	0
All	All	1467/1614 (90%)	0.37	52 (3%)	47	40	40, 75, 119, 153	0

All (52) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	626	ASP	4.2
1	A	187	CYS	3.9
1	B	183	PHE	3.7
1	B	756	LEU	3.6
1	B	732	LEU	3.6
1	A	703	LEU	3.5
1	A	702	PHE	3.5
1	A	732	LEU	3.5
1	A	735	VAL	3.4
1	A	811	GLY	3.4
1	B	470	PHE	3.3
1	A	814	ILE	3.3
1	B	731	PHE	3.1
1	A	467	PHE	3.1
1	B	762	THR	3.1
1	B	625	ASN	2.8
1	B	730	GLY	2.7
1	B	100	VAL	2.6
1	B	121	PHE	2.6
1	A	704	THR	2.6
1	A	710	PHE	2.6
1	A	756	LEU	2.5
1	A	734	GLU	2.5
1	A	574	THR	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	653	HIS	2.5
1	A	45	VAL	2.5
1	A	261	PHE	2.5
1	A	470	PHE	2.5
1	B	169	LEU	2.4
1	B	74	PHE	2.4
1	A	244	GLY	2.4
1	B	392	GLN	2.3
1	B	735	VAL	2.3
1	A	762	THR	2.3
1	B	678	PHE	2.3
1	A	707	LEU	2.3
1	B	799	VAL	2.3
1	A	188	GLU	2.2
1	A	607	SER	2.2
1	B	433	LEU	2.2
1	A	709	ASP	2.2
1	B	418	SER	2.2
1	B	113	GLY	2.2
1	B	702	PHE	2.2
1	B	600	THR	2.1
1	A	262	ASN	2.1
1	B	577	LEU	2.1
1	A	113	GLY	2.1
1	A	774	PHE	2.1
1	A	761	THR	2.1
1	B	395	ASN	2.1
1	A	192	ILE	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)

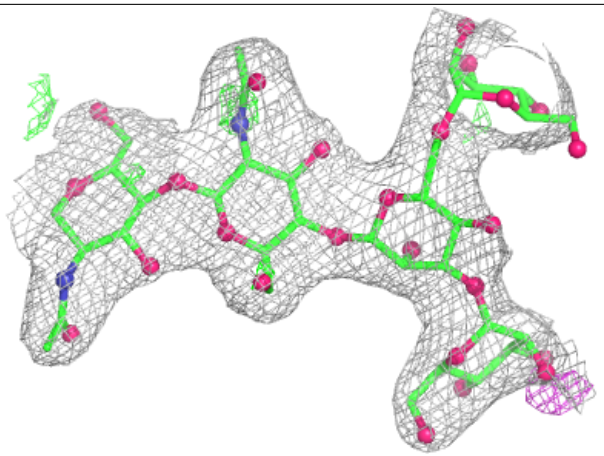
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

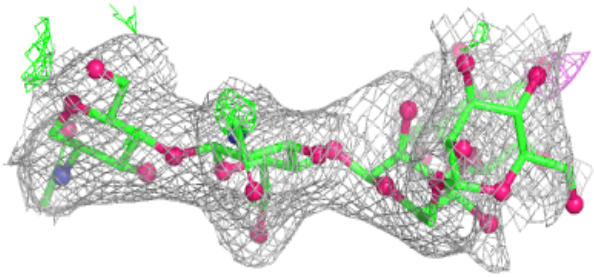
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	BMA	G	3	11/12	0.43	0.16	81,83,83,83	0
2	MAN	H	5	11/12	0.55	0.13	87,88,88,89	0
3	BMA	D	3	11/12	0.64	0.14	71,73,73,73	0
2	MAN	E	4	11/12	0.65	0.13	78,79,79,79	0
2	MAN	C	5	11/12	0.68	0.13	89,90,91,91	0
2	MAN	C	4	11/12	0.70	0.15	87,88,88,88	0
2	MAN	E	5	11/12	0.70	0.12	78,79,79,80	0
2	MAN	F	4	11/12	0.70	0.14	85,86,86,86	0
2	MAN	H	4	11/12	0.73	0.11	86,87,88,88	0
2	MAN	F	5	11/12	0.78	0.10	87,87,88,88	0
2	BMA	E	3	11/12	0.79	0.12	71,74,76,77	0
2	BMA	H	3	11/12	0.83	0.10	80,83,85,86	0
3	NAG	D	2	14/15	0.83	0.11	63,65,67,69	0
3	NAG	G	2	14/15	0.84	0.11	73,76,77,79	0
2	BMA	F	3	11/12	0.87	0.08	82,84,85,86	0
2	BMA	C	3	11/12	0.89	0.08	82,85,86,87	0
2	NAG	C	1	14/15	0.91	0.13	68,70,71,72	0
2	NAG	H	2	14/15	0.93	0.09	68,69,73,76	0
2	NAG	E	2	14/15	0.93	0.09	58,60,63,67	0
2	NAG	C	2	14/15	0.93	0.12	74,74,77,79	0
2	NAG	F	2	14/15	0.93	0.11	75,76,78,80	0
2	NAG	F	1	14/15	0.95	0.10	71,72,73,74	0
3	NAG	G	1	14/15	0.95	0.09	63,64,66,70	0
2	NAG	H	1	14/15	0.96	0.09	60,61,63,65	0
2	NAG	E	1	14/15	0.96	0.08	49,51,53,55	0
3	NAG	D	1	14/15	0.97	0.09	51,53,56,59	0

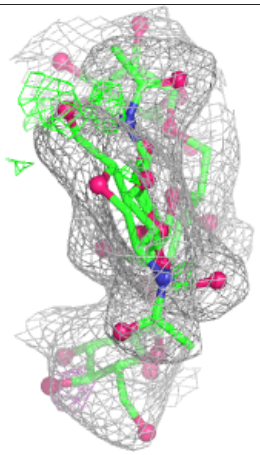
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

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)

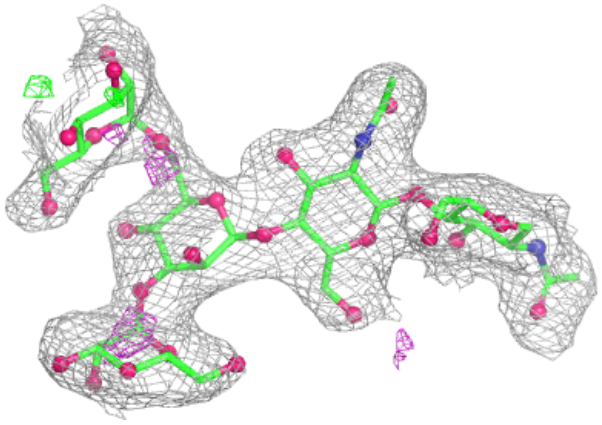


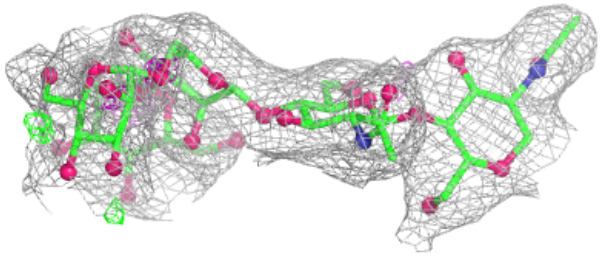


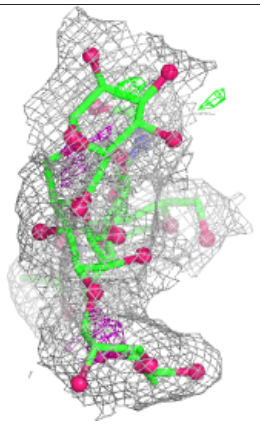


Electron density around Chain E:

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

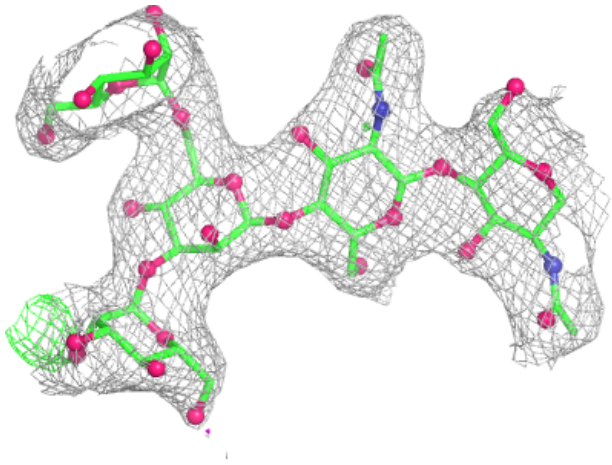


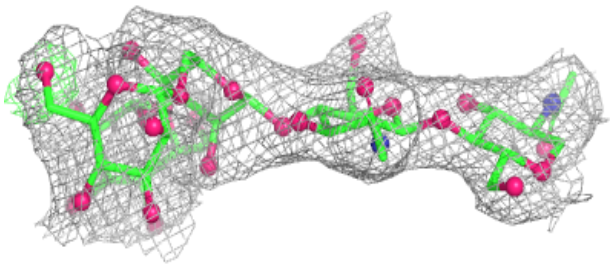


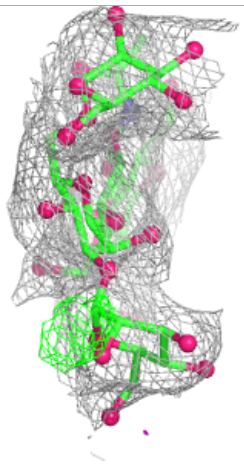


Electron density around Chain F:

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

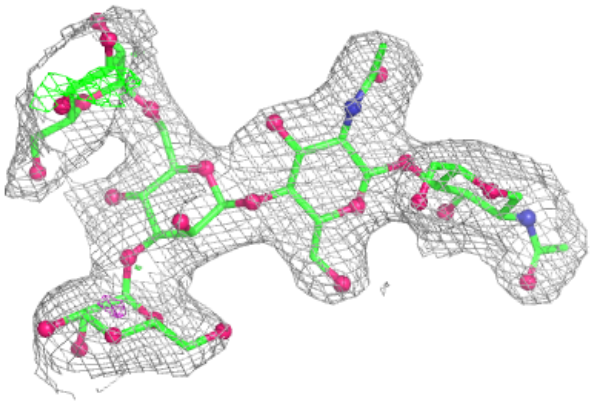


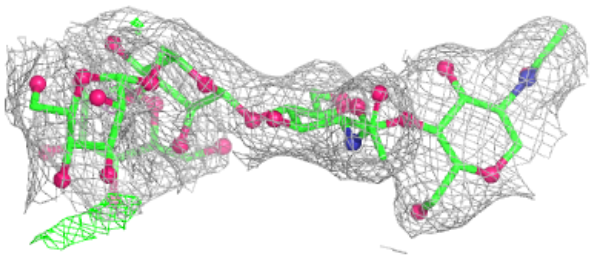


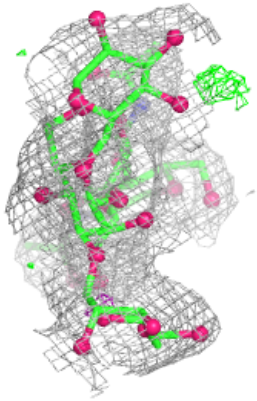


Electron density around Chain H:

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

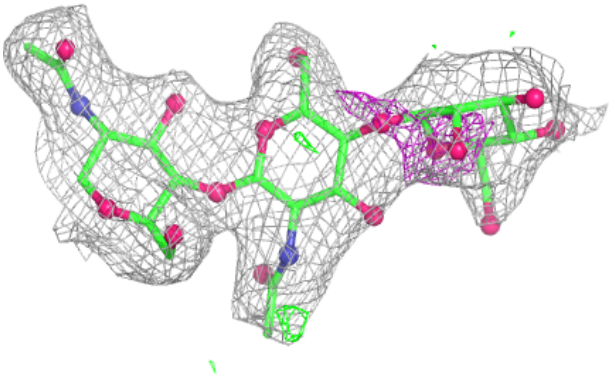


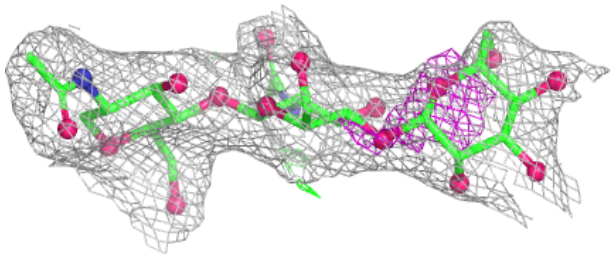


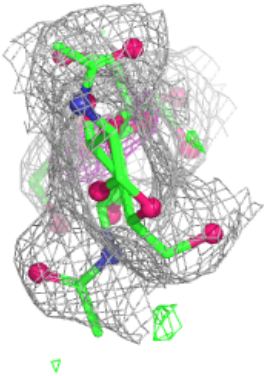


Electron density around Chain D:

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

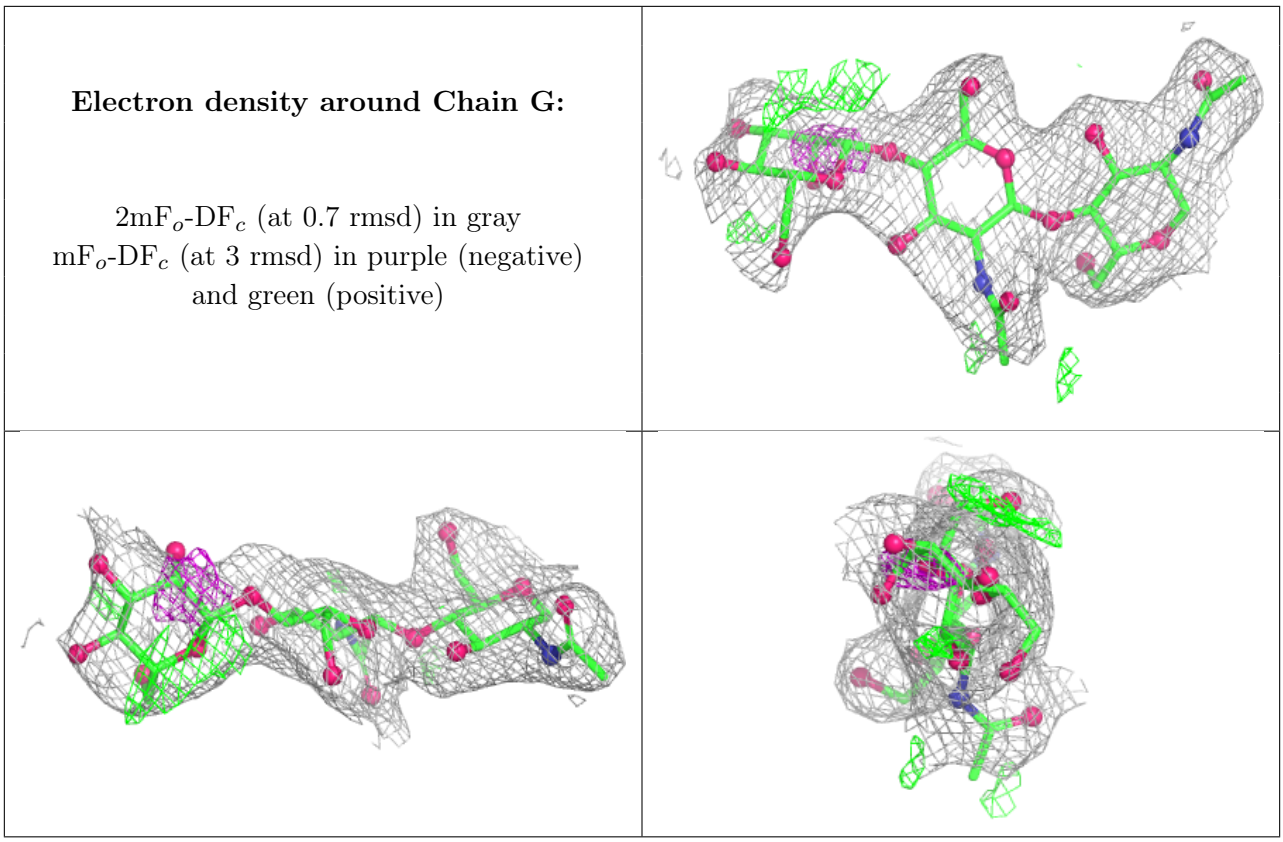






Electron density around Chain G:

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



6.4 Ligands

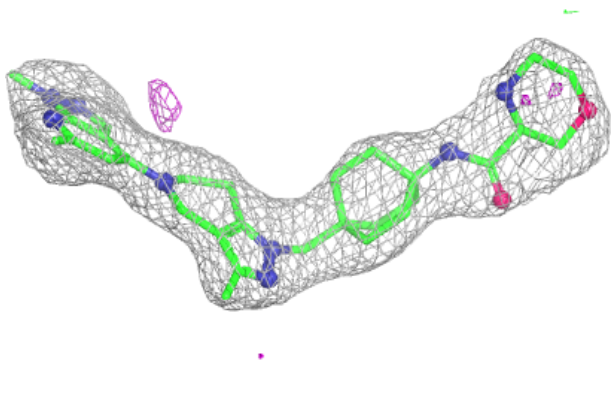
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

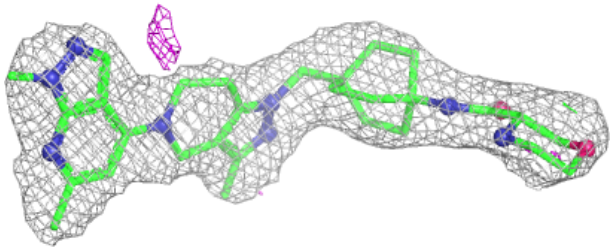
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	NAG	B	905	14/15	0.28	0.21	86,88,88,88	0
4	NAG	A	904	14/15	0.46	0.17	93,95,96,96	0
4	NAG	A	906	14/15	0.53	0.13	107,107,108,108	0
4	NAG	A	905	14/15	0.55	0.15	80,81,82,82	0
4	NAG	B	907	14/15	0.58	0.13	126,126,127,127	0
4	NAG	B	906	14/15	0.60	0.16	89,90,90,90	0
4	NAG	A	903	14/15	0.62	0.14	89,90,90,90	0
4	NAG	B	902	14/15	0.65	0.16	89,90,91,91	0
4	NAG	A	902	14/15	0.68	0.13	86,87,87,87	0
4	NAG	B	904	14/15	0.77	0.14	81,82,82,83	0
4	NAG	B	903	14/15	0.82	0.11	88,88,89,89	0
4	NAG	A	901	14/15	0.92	0.08	64,64,65,65	0
5	YHG	A	907	39/39	0.92	0.10	53,56,65,65	0
5	YHG	B	901	39/39	0.93	0.11	53,55,63,63	0

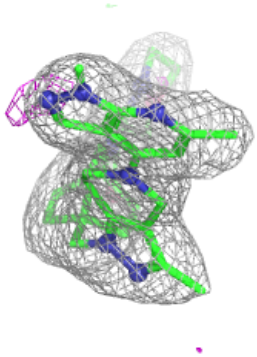
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around YHG A 907:

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

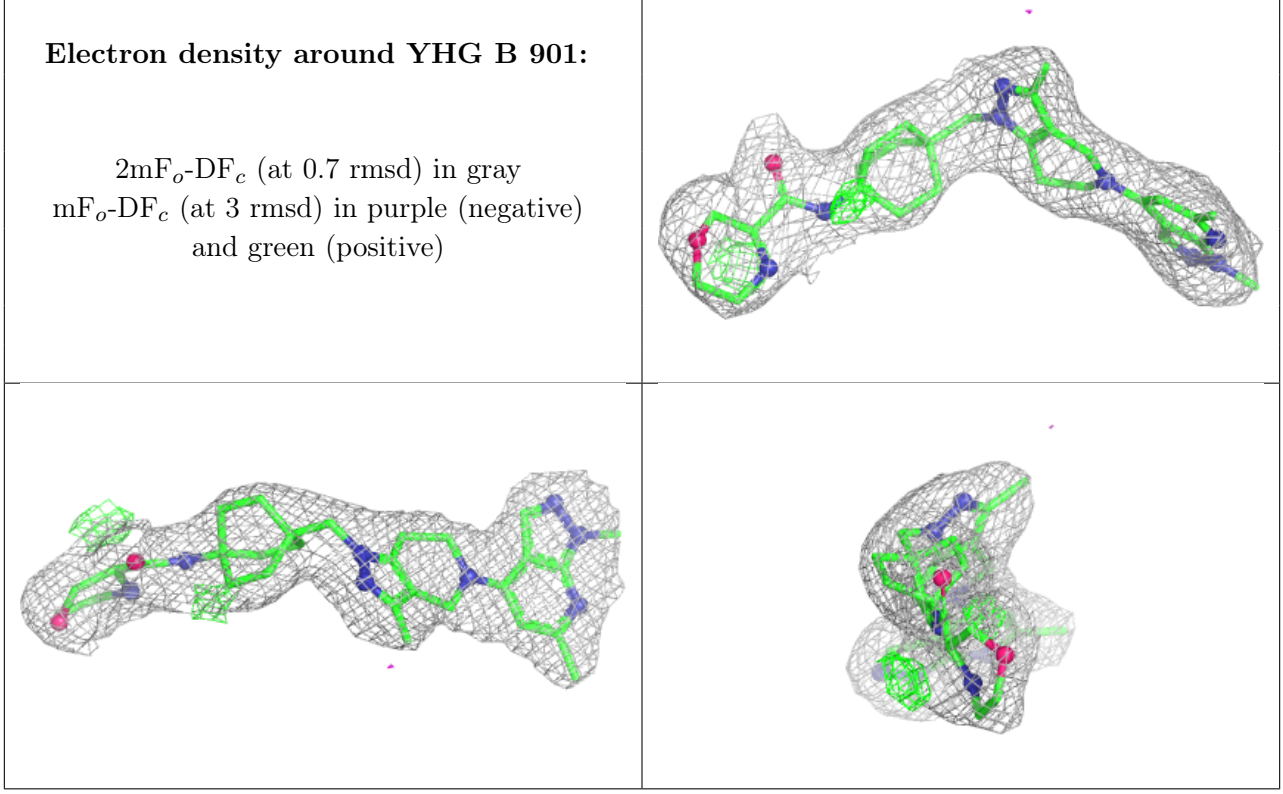






Electron density around YHG B 901:

$2mF_o$-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.