Full wwPDB X-ray Structure Validation Report ⓘ

Aug 8, 2020 – 10:16 PM BST

PDB ID	:	5W7C
Title	:	Human acyloxyacyl hydrolase (AOAH), proteolytically processed, S263A mutant, with LPS
Authors	:	Gorelik, A.; Illes, K.; Nagar, B.
Deposited on	:	2017-06-19
Resolution	:	2.23 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see references ①) were used in the production of this report:

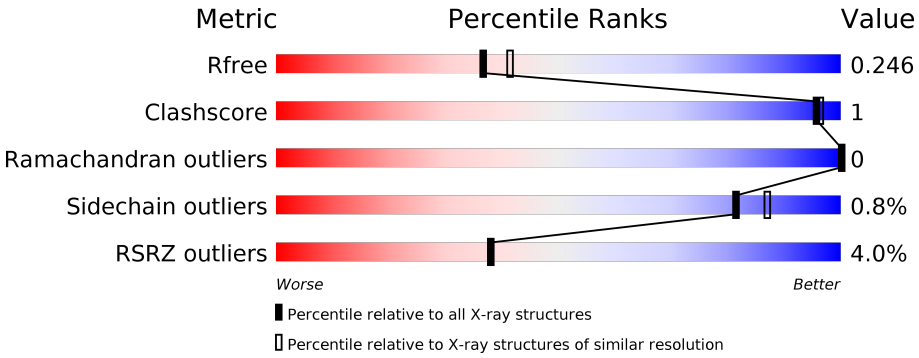
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.13.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.23 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	2391 (2.26-2.22)
Clashscore	141614	2539 (2.26-2.22)
Ramachandran outliers	138981	2489 (2.26-2.22)
Sidechain outliers	138945	2490 (2.26-2.22)
RSRZ outliers	127900	2353 (2.26-2.22)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	139	4% 79% . 20%
1	B	139	4% 80% 20%
2	C	423	2% 95% . .
2	D	423	6% 96% . .
3	E	2	100%
3	F	2	100%

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Mol	Chain	Length	Quality of chain
3	G	2	100%
3	H	2	100%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	NAG	F	2	-	-	-	X
4	NAG	C	608	-	-	-	X

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 17748 atoms, of which 8673 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 Acyloxyacyl hydrolase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	111	Total	C	H	N	O	S	0	0	0
			1760	558	889	146	158	9			
1	B	111	Total	C	H	N	O	S	0	0	0
			1760	558	889	146	158	9			

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	14	ASP	-	expression tag	UNP P28039
A	15	ARG	-	expression tag	UNP P28039
A	16	HIS	-	expression tag	UNP P28039
A	17	HIS	-	expression tag	UNP P28039
A	18	HIS	-	expression tag	UNP P28039
A	19	HIS	-	expression tag	UNP P28039
A	20	HIS	-	expression tag	UNP P28039
A	21	HIS	-	expression tag	UNP P28039
A	22	LYS	-	expression tag	UNP P28039
A	23	LEU	-	expression tag	UNP P28039
B	14	ASP	-	expression tag	UNP P28039
B	15	ARG	-	expression tag	UNP P28039
B	16	HIS	-	expression tag	UNP P28039
B	17	HIS	-	expression tag	UNP P28039
B	18	HIS	-	expression tag	UNP P28039
B	19	HIS	-	expression tag	UNP P28039
B	20	HIS	-	expression tag	UNP P28039
B	21	HIS	-	expression tag	UNP P28039
B	22	LYS	-	expression tag	UNP P28039
B	23	LEU	-	expression tag	UNP P28039

- Molecule 2 is a protein called Acyloxyacyl hydrolase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	C	420	Total	C	H	N	O	S	0	0	0
			6634	2145	3264	590	618	17			
2	D	419	Total	C	H	N	O	S	0	0	0
			6627	2143	3261	589	617	17			

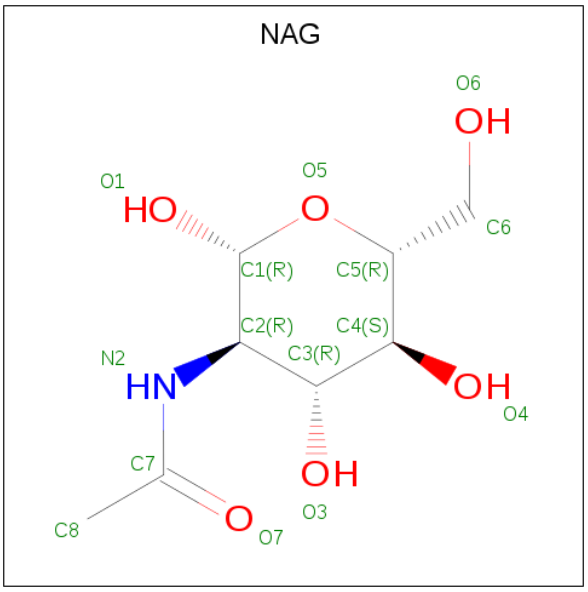
There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	263	ALA	SER	engineered mutation	UNP P28039
D	263	ALA	SER	engineered mutation	UNP P28039

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

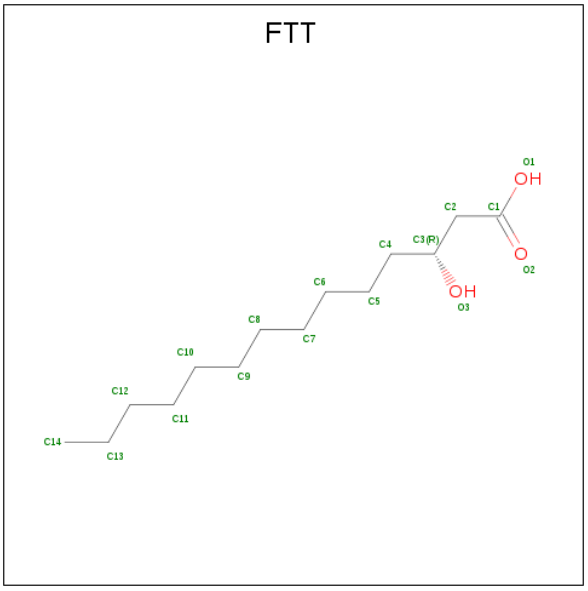
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	2	Total	C	H	N	O	0	0	0
			55	16	27	2	10			
3	F	2	Total	C	H	N	O	0	0	0
			55	16	27	2	10			
3	G	2	Total	C	H	N	O	0	0	0
			55	16	27	2	10			
3	H	2	Total	C	H	N	O	0	0	0
			55	16	27	2	10			

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



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	H	N	O	0	0
			28	8	14	1	5		
4	C	1	Total	C	H	N	O	0	0
			28	8	14	1	5		
4	B	1	Total	C	H	N	O	0	0
			28	8	14	1	5		
4	D	1	Total	C	H	N	O	0	0
			28	8	14	1	5		

- Molecule 5 is 3-HYDROXY-TETRADECANOIC ACID (three-letter code: FTT) (formula: $C_{14}H_{28}O_3$).

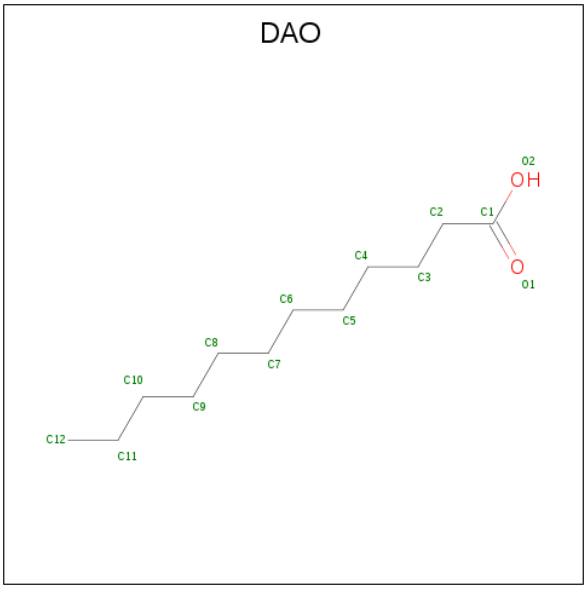


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C H O 44 14 27 3	0	0
5	C	1	Total C H O 43 14 26 3	0	0
5	C	1	Total C H O 44 14 27 3	0	0
5	B	1	Total C H O 44 14 27 3	0	0
5	D	1	Total C H O 43 14 26 3	0	0
5	D	1	Total C H O 44 14 27 3	0	0

- Molecule 6 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	D	3	Total Ca 3 3	0	0
6	C	3	Total Ca 3 3	0	0

- Molecule 7 is LAURIC ACID (three-letter code: DAO) (formula: $C_{12}H_{24}O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	C	1	Total C H O 36 12 23 1	0	0
7	D	1	Total C H O 36 12 23 1	0	0

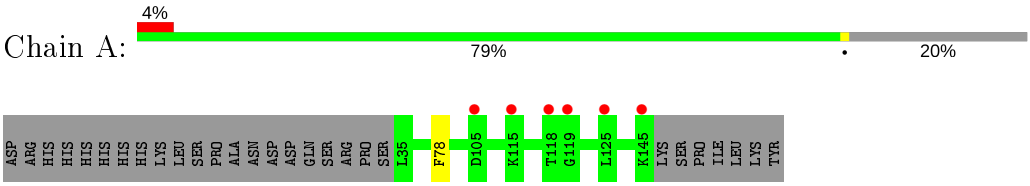
- Molecule 8 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	35	Total O 35 35	0	0
8	C	152	Total O 152 152	0	0
8	B	15	Total O 15 15	0	0
8	D	93	Total O 93 93	0	0

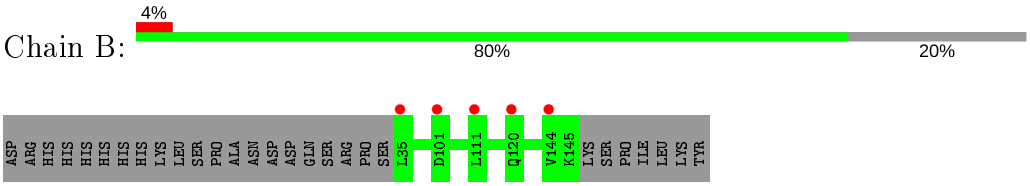
3 Residue-property plots (i)

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.

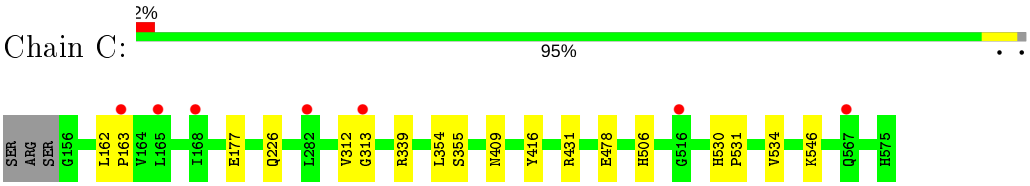
• Molecule 1: Acyloxyacyl hydrolase



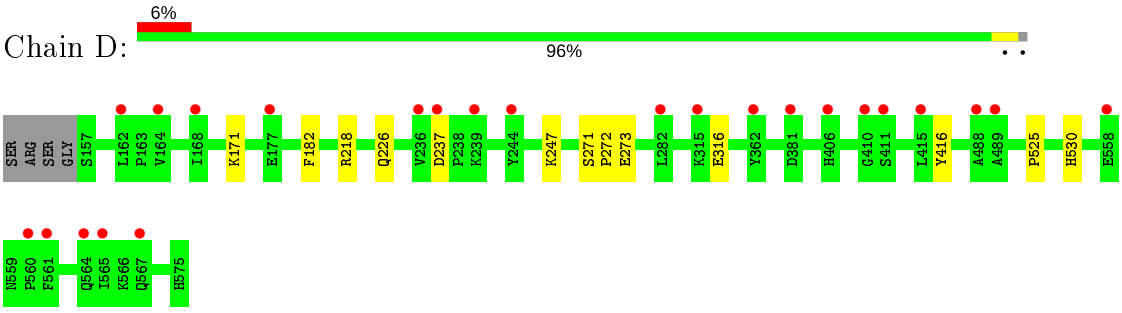
• Molecule 1: Acyloxyacyl hydrolase



• Molecule 2: Acyloxyacyl hydrolase

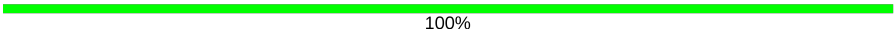


• Molecule 2: Acyloxyacyl hydrolase

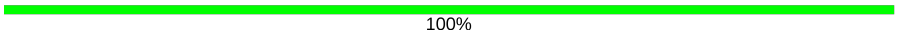


• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

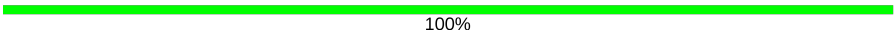
• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain F: 

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

Chain G: 

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

Chain H: 

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	88.17Å 104.08Å 145.28Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	44.82 – 2.23 44.82 – 2.23	Depositor EDS
% Data completeness (in resolution range)	99.9 (44.82-2.23) 100.0 (44.82-2.23)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.45 (at 2.22Å)	Xtriage
Refinement program	PHENIX (1.10.1_2155)	Depositor
R, R_{free}	0.211 , 0.245 0.213 , 0.246	Depositor DCC
R_{free} test set	3292 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	38.6	Xtriage
Anisotropy	0.464	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.38 , 42.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	17748	wwPDB-VP
Average B, all atoms (Å^2)	52.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.16% 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: CA, DAO, NAG, FTT

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	0.24	0/887	0.37	0/1202
1	B	0.23	0/887	0.38	0/1202
2	C	0.25	0/3466	0.43	0/4705
2	D	0.24	0/3462	0.42	0/4700
All	All	0.24	0/8702	0.41	0/11809

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	871	889	889	0	0
1	B	871	889	889	0	0
2	C	3370	3264	3264	9	0
2	D	3366	3261	3261	7	0
3	E	28	27	25	1	0
3	F	28	27	25	0	0
3	G	28	27	25	0	0
3	H	28	27	25	0	0
4	A	14	14	13	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	14	14	13	0	0
4	C	14	14	13	1	0
4	D	14	14	13	1	0
5	A	17	27	27	0	0
5	B	17	27	27	0	0
5	C	34	53	53	1	0
5	D	34	53	53	0	0
6	C	3	0	0	0	0
6	D	3	0	0	0	0
7	C	13	23	23	2	0
7	D	13	23	23	1	0
8	A	35	0	0	0	0
8	B	15	0	0	0	0
8	C	152	0	0	1	0
8	D	93	0	0	1	0
All	All	9075	8673	8661	19	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 1.

All (19) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:530:HIS:NE2	7:D:609:DAO:O1	2.12	0.82
2:C:530:HIS:NE2	7:C:609:DAO:O1	2.13	0.81
2:C:546:LYS:NZ	8:C:701:HOH:O	2.21	0.73
2:C:409:ASN:ND2	4:C:608:NAG:O7	2.24	0.69
2:C:177:GLU:O	2:C:339:ARG:NH2	2.31	0.64
2:D:316:GLU:OE1	2:D:316:GLU:N	2.33	0.61
2:D:237:ASP:OD2	2:D:247:LYS:NZ	2.38	0.56
4:D:608:NAG:O3	4:D:608:NAG:O7	2.18	0.53
2:C:312:VAL:HG21	2:C:534:VAL:HG22	1.94	0.48
2:D:271:SER:OG	2:D:273:GLU:OE1	2.30	0.47
2:C:312:VAL:HG22	2:C:313:GLY:N	2.31	0.45
2:C:531:PRO:HD3	7:C:609:DAO:H101	1.98	0.44
5:C:610:FTT:H62	5:C:611:FTT:H22	2.00	0.43
2:C:162:LEU:HB3	2:C:163:PRO:HD2	2.01	0.43
2:D:272:PRO:HG3	2:D:525:PRO:HG2	2.01	0.43
2:D:171:LYS:NZ	2:D:182:PHE:O	2.52	0.42
3:E:1:NAG:H62	3:E:2:NAG:O5	2.19	0.42
2:D:218:ARG:NH2	8:D:710:HOH:O	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:354:LEU:HD23	2:C:355:SER:N	2.35	0.41

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	109/139 (78%)	108 (99%)	1 (1%)	0	100	100
1	B	109/139 (78%)	108 (99%)	1 (1%)	0	100	100
2	C	418/423 (99%)	399 (96%)	19 (4%)	0	100	100
2	D	417/423 (99%)	397 (95%)	20 (5%)	0	100	100
All	All	1053/1124 (94%)	1012 (96%)	41 (4%)	0	100	100

There are no Ramachandran outliers to report.

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	102/129 (79%)	101 (99%)	1 (1%)	76	82
1	B	102/129 (79%)	102 (100%)	0	100	100
2	C	372/375 (99%)	367 (99%)	5 (1%)	69	76
2	D	372/375 (99%)	370 (100%)	2 (0%)	88	92

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	948/1008 (94%)	940 (99%)	8 (1%)	81 87

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

Mol	Chain	Res	Type
1	A	78	PHE
2	C	226	GLN
2	C	416	TYR
2	C	431	ARG
2	C	478	GLU
2	C	506	HIS
2	D	226	GLN
2	D	416	TYR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
2	C	446	GLN
2	C	495	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

8 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	NAG	E	1	3,2	14,14,15	0.70	1 (7%)	17,19,21	0.86	1 (5%)
3	NAG	E	2	3	14,14,15	0.47	0	17,19,21	0.78	1 (5%)
3	NAG	F	1	3,2	14,14,15	0.41	0	17,19,21	0.62	0
3	NAG	F	2	3	14,14,15	0.51	0	17,19,21	0.45	0
3	NAG	G	1	3,2	14,14,15	0.17	0	17,19,21	0.54	0
3	NAG	G	2	3	14,14,15	0.20	0	17,19,21	0.55	0
3	NAG	H	1	3,2	14,14,15	0.25	0	17,19,21	0.59	0
3	NAG	H	2	3	14,14,15	0.17	0	17,19,21	0.44	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
3	NAG	E	1	3,2	-	0/6/23/26	0/1/1/1
3	NAG	E	2	3	-	1/6/23/26	0/1/1/1
3	NAG	F	1	3,2	-	0/6/23/26	0/1/1/1
3	NAG	F	2	3	-	2/6/23/26	0/1/1/1
3	NAG	G	1	3,2	-	2/6/23/26	0/1/1/1
3	NAG	G	2	3	-	2/6/23/26	0/1/1/1
3	NAG	H	1	3,2	-	0/6/23/26	0/1/1/1
3	NAG	H	2	3	-	2/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	1	NAG	O5-C1	-2.19	1.40	1.43

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	E	1	NAG	O4-C4-C3	-2.14	105.40	110.35
3	E	2	NAG	C3-C4-C5	2.04	113.88	110.24

There are no chirality outliers.

All (9) torsion outliers are listed below:

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

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

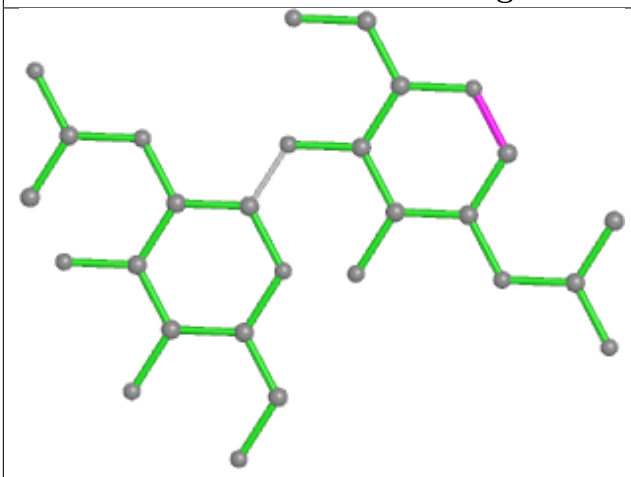
There are no ring outliers.

2 monomers are involved in 1 short contact:

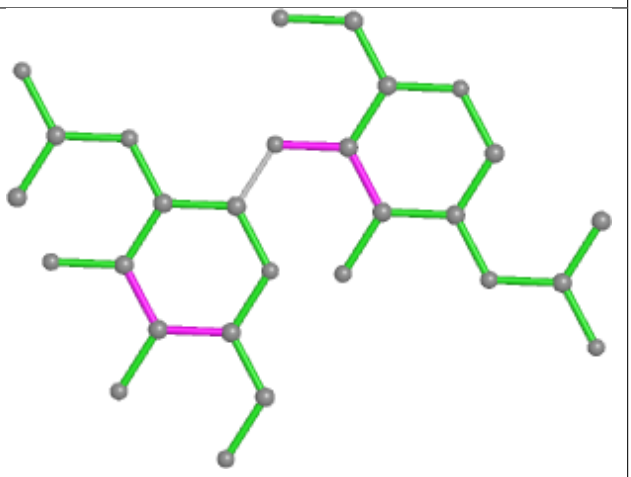
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	E	2	NAG	1	0
3	E	1	NAG	1	0

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

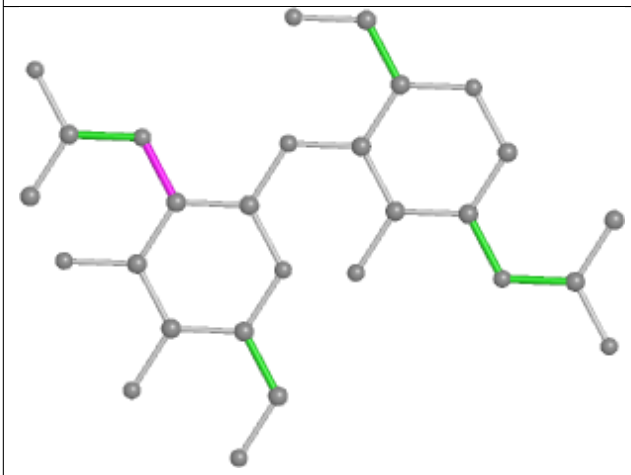
Oligosaccharide Chain E



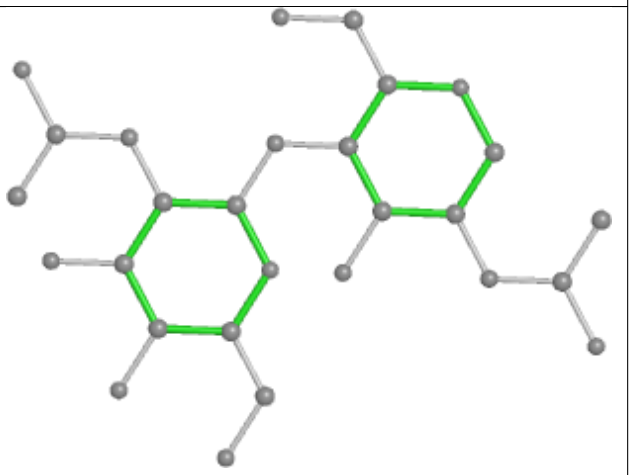
Bond lengths



Bond angles

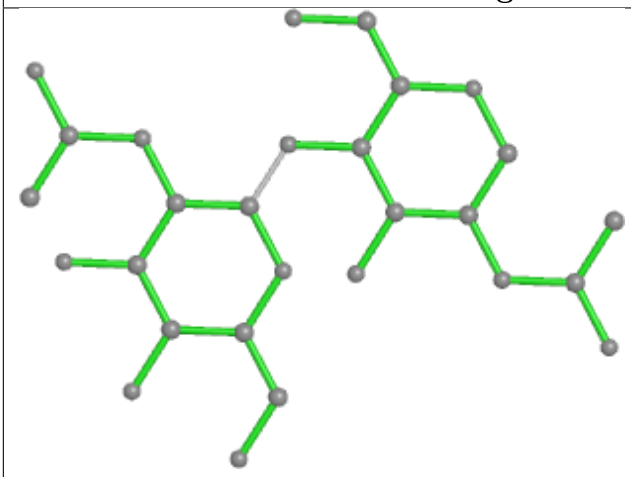


Torsions

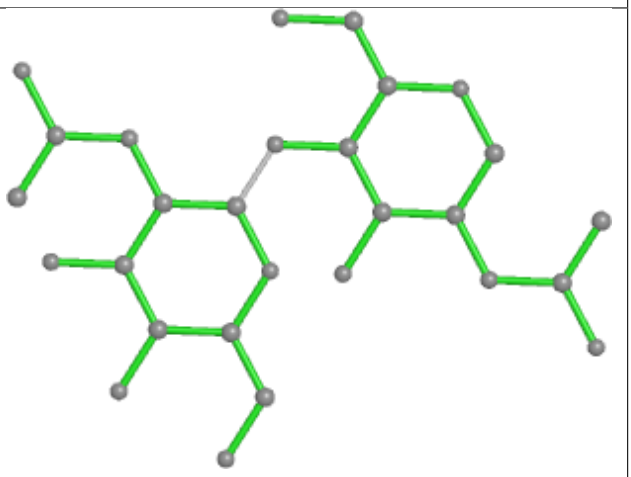


Rings

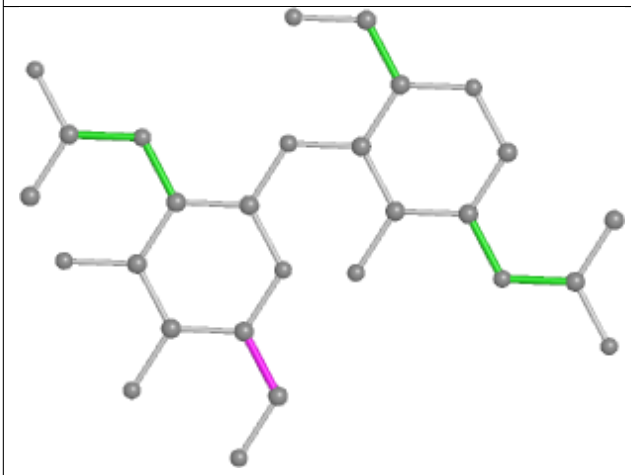
Oligosaccharide Chain F



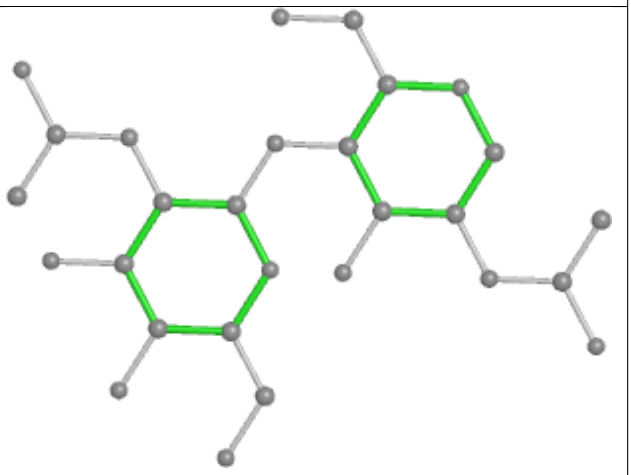
Bond lengths



Bond angles

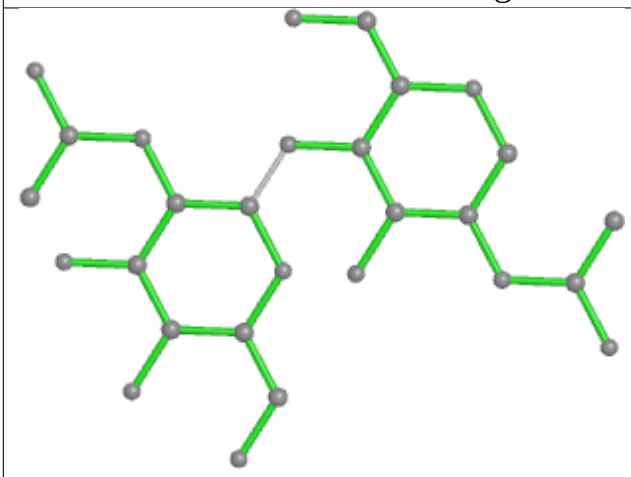


Torsions

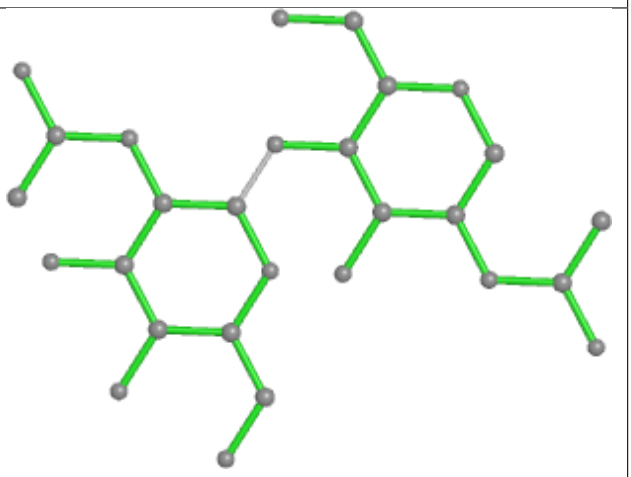


Rings

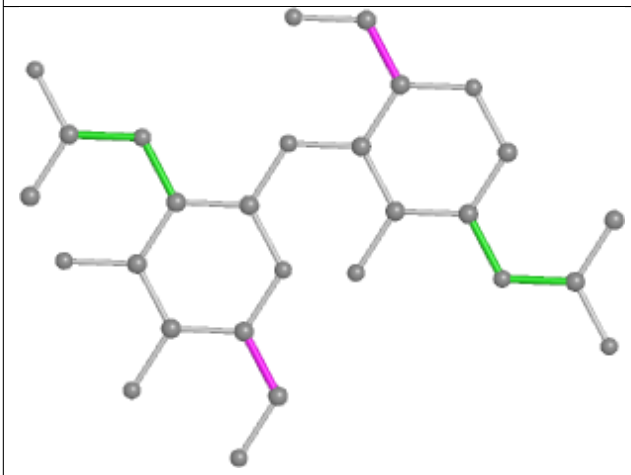
Oligosaccharide Chain G



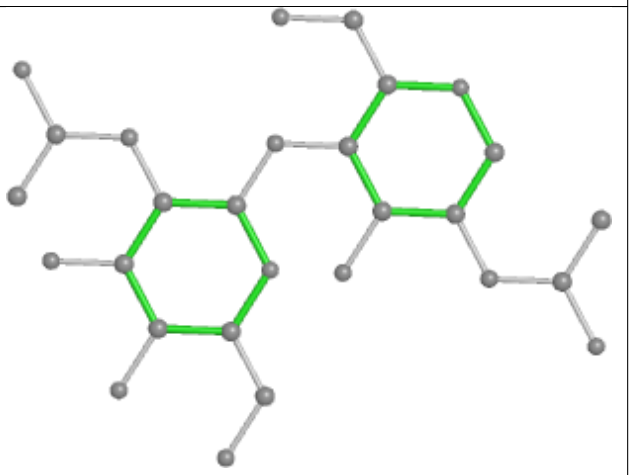
Bond lengths



Bond angles

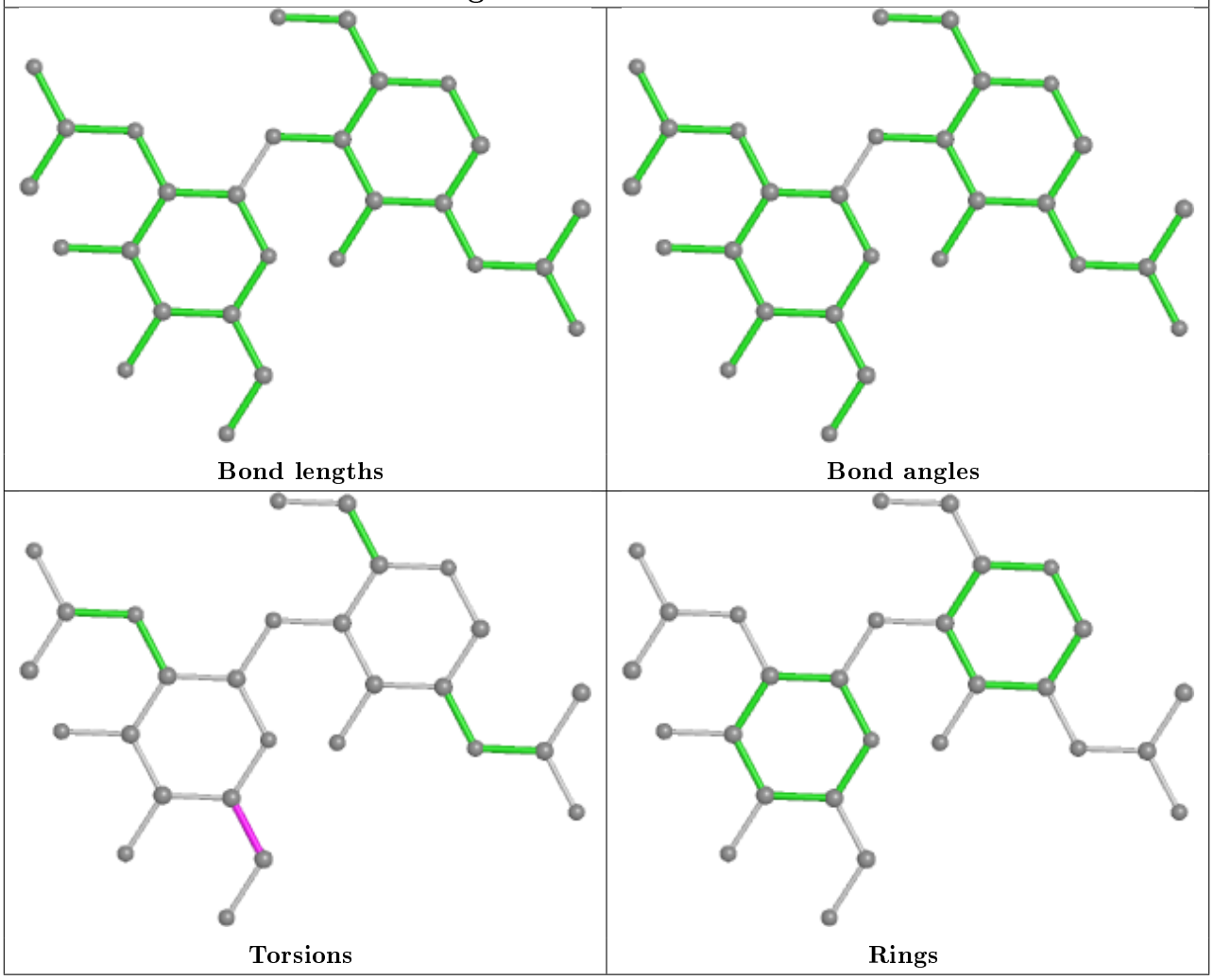


Torsions



Rings

Oligosaccharide Chain H



5.6 Ligand geometry (i)

Of 18 ligands modelled in this entry, 6 are monoatomic - leaving 12 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
5	FTT	D	611	-	13,16,16	0.41	0	13,17,17	0.89	0
4	NAG	B	201	1	14,14,15	0.25	0	17,19,21	0.47	0
5	FTT	C	611	-	13,16,16	0.42	0	13,17,17	0.82	0
5	FTT	C	610	7	13,16,16	0.45	0	13,17,17	0.96	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
5	FTT	A	202	-	13,16,16	0.40	0	13,17,17	0.90	0
4	NAG	C	608	2	14,14,15	0.98	2 (14%)	17,19,21	0.82	0
4	NAG	D	608	2	14,14,15	0.78	1 (7%)	17,19,21	0.96	1 (5%)
7	DAO	C	609	5	12,12,13	0.44	0	11,11,13	0.95	0
7	DAO	D	609	5	12,12,13	0.44	0	11,11,13	0.94	0
5	FTT	D	610	7	13,16,16	0.42	0	13,17,17	0.84	0
5	FTT	B	202	-	13,16,16	0.44	0	13,17,17	0.70	0
4	NAG	A	201	1	14,14,15	0.28	0	17,19,21	0.38	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
5	FTT	D	611	-	-	6/13/15/15	-
4	NAG	B	201	1	-	0/6/23/26	0/1/1/1
5	FTT	C	611	-	-	7/13/15/15	-
5	FTT	C	610	7	-	8/13/15/15	-
5	FTT	A	202	-	-	6/13/15/15	-
4	NAG	C	608	2	-	2/6/23/26	0/1/1/1
4	NAG	D	608	2	-	2/6/23/26	0/1/1/1
7	DAO	C	609	5	-	2/9/10/11	-
7	DAO	D	609	5	-	2/9/10/11	-
5	FTT	D	610	7	-	7/13/15/15	-
5	FTT	B	202	-	-	11/13/15/15	-
4	NAG	A	201	1	-	1/6/23/26	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	608	NAG	C1-C2	2.73	1.56	1.52
4	D	608	NAG	O5-C1	2.44	1.47	1.43
4	C	608	NAG	O5-C1	-2.30	1.40	1.43

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	D	608	NAG	C1-O5-C5	3.69	117.19	112.19

There are no chirality outliers.

All (54) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	C	611	FTT	C1-C2-C3-C4
5	C	611	FTT	C1-C2-C3-O3
4	D	608	NAG	C3-C2-N2-C7
5	D	610	FTT	C1-C2-C3-C4
5	D	610	FTT	C1-C2-C3-O3
5	B	202	FTT	C1-C2-C3-O3
4	C	608	NAG	C1-C2-N2-C7
5	C	610	FTT	O3-C3-C4-C5
5	D	610	FTT	C10-C11-C12-C13
5	C	611	FTT	C6-C7-C8-C9
5	D	611	FTT	C7-C8-C9-C10
5	C	610	FTT	C10-C11-C12-C13
5	B	202	FTT	C5-C6-C7-C8
5	B	202	FTT	C6-C7-C8-C9
5	D	611	FTT	O3-C3-C4-C5
5	C	610	FTT	C9-C10-C11-C12
5	C	611	FTT	C7-C8-C9-C10
7	D	609	DAO	C6-C7-C8-C9
5	A	202	FTT	C9-C10-C11-C12
4	D	608	NAG	C1-C2-N2-C7
5	B	202	FTT	C7-C8-C9-C10
5	D	610	FTT	C7-C8-C9-C10
5	B	202	FTT	C11-C10-C9-C8
5	A	202	FTT	C6-C7-C8-C9
7	D	609	DAO	C4-C5-C6-C7
5	B	202	FTT	C9-C10-C11-C12
5	D	610	FTT	C11-C12-C13-C14
5	C	611	FTT	O3-C3-C4-C5
5	D	610	FTT	O3-C3-C4-C5
5	D	611	FTT	C10-C11-C12-C13
5	C	610	FTT	C1-C2-C3-C4
5	B	202	FTT	C1-C2-C3-C4
5	A	202	FTT	C11-C12-C13-C14
5	D	611	FTT	C4-C5-C6-C7
5	D	611	FTT	C2-C3-C4-C5
5	C	611	FTT	C2-C3-C4-C5
5	C	610	FTT	C2-C3-C4-C5
5	C	610	FTT	C11-C12-C13-C14
5	A	202	FTT	C7-C8-C9-C10
5	C	610	FTT	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
5	C	610	FTT	C7-C8-C9-C10
5	B	202	FTT	O3-C3-C4-C5
5	D	611	FTT	C3-C4-C5-C6
5	D	610	FTT	C5-C6-C7-C8
4	A	201	NAG	C4-C5-C6-O6
7	C	609	DAO	C4-C5-C6-C7
5	B	202	FTT	C3-C4-C5-C6
7	C	609	DAO	C9-C10-C11-C12
5	B	202	FTT	C4-C5-C6-C7
5	C	611	FTT	C11-C12-C13-C14
5	A	202	FTT	C10-C11-C12-C13
4	C	608	NAG	O5-C5-C6-O6
5	B	202	FTT	C10-C11-C12-C13
5	A	202	FTT	C11-C10-C9-C8

There are no ring outliers.

6 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	C	611	FTT	1	0
5	C	610	FTT	1	0
4	C	608	NAG	1	0
4	D	608	NAG	1	0
7	C	609	DAO	2	0
7	D	609	DAO	1	0

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, 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	111/139 (79%)	0.55	6 (5%)	25	25	32, 43, 79, 96	0
1	B	111/139 (79%)	0.48	5 (4%)	33	33	39, 49, 76, 86	0
2	C	420/423 (99%)	0.31	7 (1%)	70	71	27, 42, 69, 94	0
2	D	419/423 (99%)	0.46	24 (5%)	23	23	30, 47, 65, 92	0
All	All	1061/1124 (94%)	0.41	42 (3%)	38	38	27, 45, 69, 96	0

All (42) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	118	THR	8.4
2	D	164	VAL	5.8
1	A	119	GLY	5.3
2	D	410	GLY	4.3
2	D	239	LYS	4.2
2	D	282	LEU	4.2
1	B	144	VAL	4.1
2	D	315	LYS	4.0
2	D	565	ILE	3.9
2	D	236	VAL	3.8
1	A	125	LEU	3.5
1	B	111	LEU	3.2
1	B	120	GLN	3.1
2	D	168	ILE	3.1
2	D	237	ASP	3.0
1	B	35	LEU	3.0
2	D	162	LEU	3.0
2	D	558	GLU	3.0
2	C	163	PRO	2.9
2	D	564	GLN	2.9
1	A	145	LYS	2.6

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Mol	Chain	Res	Type	RSRZ
2	D	381	ASP	2.6
1	A	105	ASP	2.6
2	C	165	LEU	2.6
2	C	516	GLY	2.6
1	B	101	ASP	2.5
2	C	567	GLN	2.5
2	D	406	HIS	2.4
2	D	560	PRO	2.4
2	C	282	LEU	2.4
2	D	561	PHE	2.4
2	D	177	GLU	2.3
2	D	244	TYR	2.3
2	D	362	TYR	2.2
2	C	168	ILE	2.2
2	C	313	GLY	2.2
1	A	115	LYS	2.1
2	D	411	SER	2.1
2	D	415	LEU	2.0
2	D	489	ALA	2.0
2	D	567	GLN	2.0
2	D	488	ALA	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
3	NAG	F	2	14/15	0.63	0.42	74,90,107,109	0
3	NAG	E	1	14/15	0.72	0.17	60,74,88,93	0
3	NAG	E	2	14/15	0.76	0.21	80,96,116,117	0
3	NAG	G	1	14/15	0.80	0.21	60,75,93,94	0
3	NAG	F	1	14/15	0.83	0.20	67,85,108,108	0
3	NAG	H	2	14/15	0.84	0.30	64,76,87,91	0
3	NAG	H	1	14/15	0.85	0.16	63,75,93,93	0

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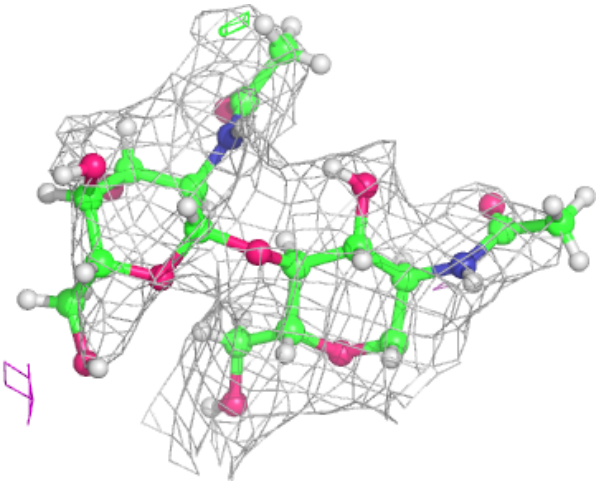
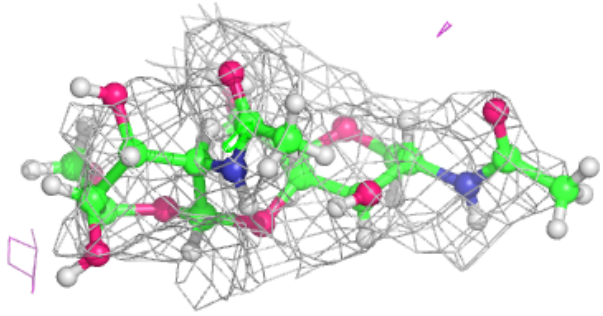
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	NAG	G	2	14/15	0.87	0.15	73,95,104,115	0

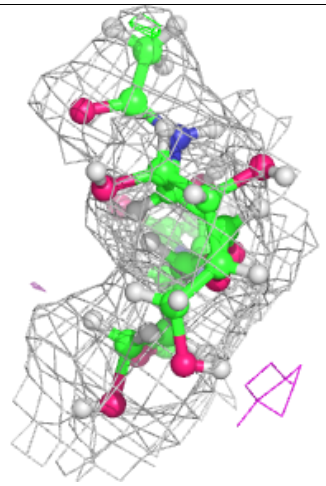
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around Chain E:

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

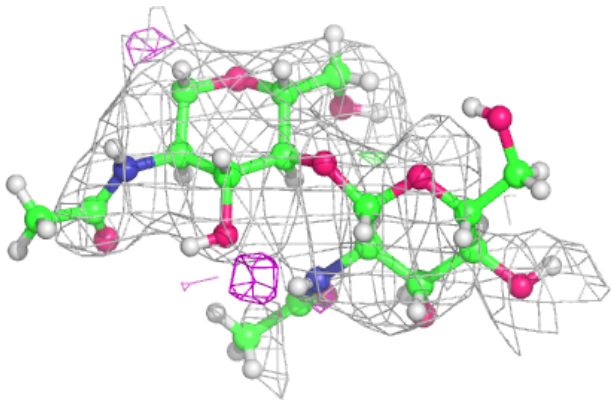


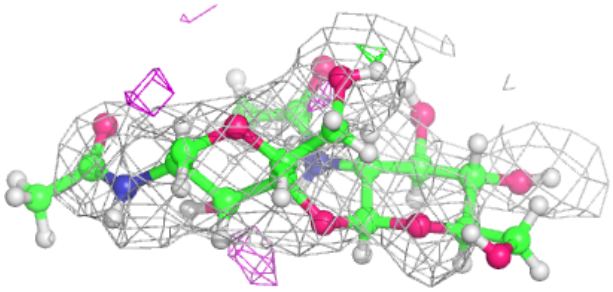


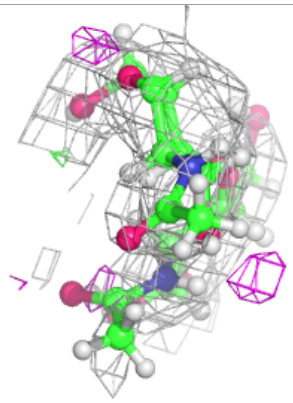


Electron density around Chain F:

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

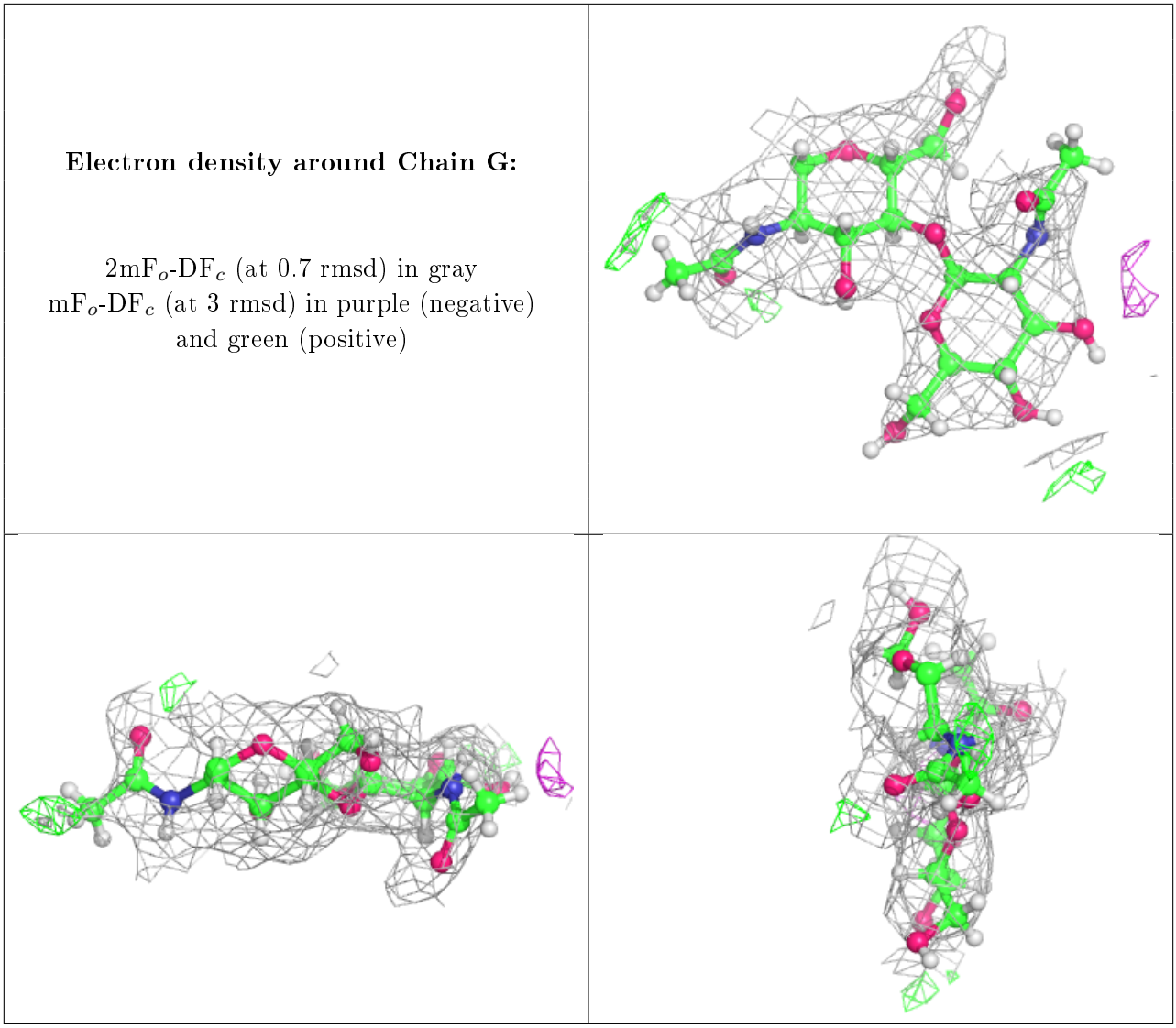


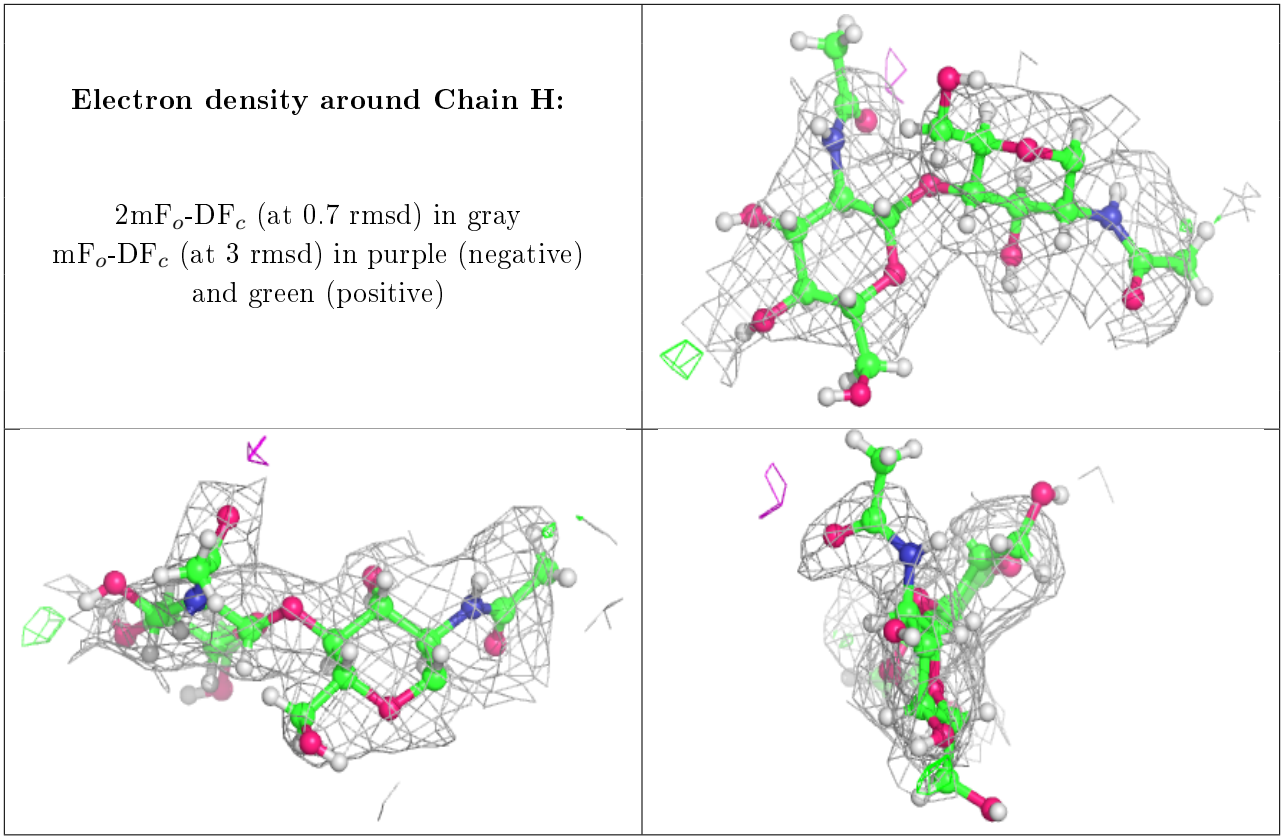




Electron density around Chain G:

$2mF_o$-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, 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	FTT	D	610	17/17	0.55	0.27	40,52,61,70	0
4	NAG	D	608	14/15	0.57	0.18	80,99,118,123	0
4	NAG	C	608	14/15	0.67	0.46	89,89,107,107	0
7	DAO	D	609	13/14	0.74	0.19	44,55,62,64	0
5	FTT	B	202	17/17	0.74	0.23	48,59,70,73	0
5	FTT	C	610	17/17	0.75	0.24	38,51,57,63	0
5	FTT	A	202	17/17	0.78	0.23	42,55,65,69	0
4	NAG	B	201	14/15	0.78	0.17	71,87,105,109	0
5	FTT	D	611	17/17	0.79	0.15	40,55,61,67	0
7	DAO	C	609	13/14	0.82	0.19	42,54,62,64	0
5	FTT	C	611	17/17	0.82	0.13	39,53,62,65	0
4	NAG	A	201	14/15	0.92	0.11	61,73,87,88	0
6	CA	D	603	1/1	0.97	0.12	36,36,36,36	0
6	CA	D	601	1/1	0.97	0.18	35,35,35,35	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
6	CA	C	603	1/1	0.98	0.11	35,35,35,35	0
6	CA	D	602	1/1	0.98	0.26	47,47,47,47	0
6	CA	C	602	1/1	0.99	0.08	33,33,33,33	0
6	CA	C	601	1/1	0.99	0.14	31,31,31,31	0

6.5 Other polymers (i)

There are no such residues in this entry.