WORLDWIDE PDB PROTEIN DATA BANK

wwPDB X-ray Structure Validation Summary Report (i)

Aug 8, 2020 – 02:43 PM BST

PDB ID	:	4FNU
Title	:	Crystal structure of GH36 alpha-galactosidase AgaA A355E D478A from Geobacillus stearothermophilus in complex with stachyose
Authors	:	Merceron, R.; Foucault, M.; Haser, R.; Mattes, R.; Watzlawick, H.; Gouet, P.
Deposited on	:	2012-06-20
Resolution	:	3.60 Å(reported)

The following versions of software and data (see references (i)) 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 ⓘ

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

The reported resolution of this entry is 3.60 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.
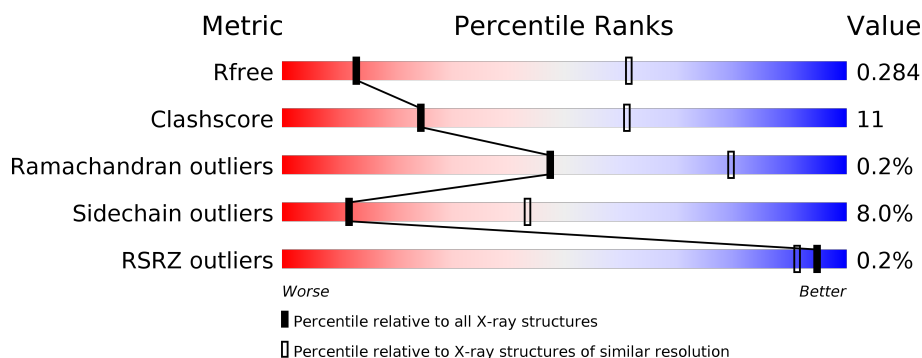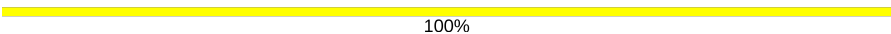

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1257 (3.70-3.50)
Clashscore	141614	1353 (3.70-3.50)
Ramachandran outliers	138981	1307 (3.70-3.50)
Sidechain outliers	138945	1307 (3.70-3.50)
RSRZ outliers	127900	1161 (3.70-3.50)

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	729	66% 28% · ·
1	B	729	69% 26% · ·
1	C	729	69% 27% · ·
1	D	729	71% 26% · ·
2	E	4	50% 50%
2	F	4	100%

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Mol	Chain	Length	Quality of chain
2	G	4	50% 50%
2	H	4	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
2	FRU	E	4	-	-	-	X
2	GLC	G	3	-	-	-	X
2	FRU	G	4	-	-	-	X

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 23332 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 Alpha-galactosidase AgaA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	718	Total 5788	C 3675	N 1020	O 1070	S 23	0	0	0
1	B	718	Total 5788	C 3675	N 1020	O 1070	S 23	0	0	0
1	C	718	Total 5788	C 3675	N 1020	O 1070	S 23	0	0	0
1	D	718	Total 5788	C 3675	N 1020	O 1070	S 23	0	0	0

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	355	GLU	ALA	engineered mutation	UNP Q9ALJ4
A	478	ALA	ASP	engineered mutation	UNP Q9ALJ4
B	355	GLU	ALA	engineered mutation	UNP Q9ALJ4
B	478	ALA	ASP	engineered mutation	UNP Q9ALJ4
C	355	GLU	ALA	engineered mutation	UNP Q9ALJ4
C	478	ALA	ASP	engineered mutation	UNP Q9ALJ4
D	355	GLU	ALA	engineered mutation	UNP Q9ALJ4
D	478	ALA	ASP	engineered mutation	UNP Q9ALJ4

- Molecule 2 is an oligosaccharide called beta-D-fructofuranose-(2-1)-alpha-D-glucopyranose-(1-6)-alpha-D-galactopyranose-(1-6)-alpha-D-galactopyranose.
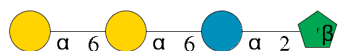
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
2	E	4	Total 45	C 24	O 21	0	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
2	F	4	Total 45	C 24	O 21	0	0	0
2	G	4	Total 45	C 24	O 21	0	0	0
2	H	4	Total 45	C 24	O 21	0	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 propo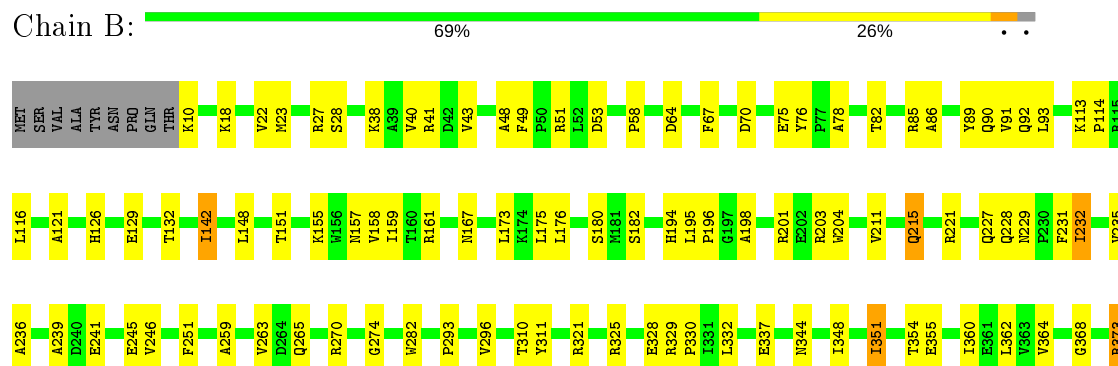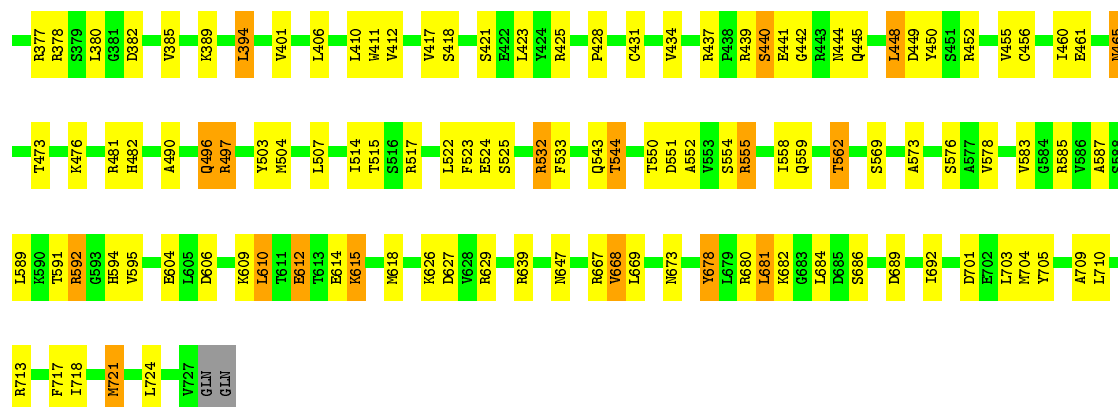rtions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, 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.
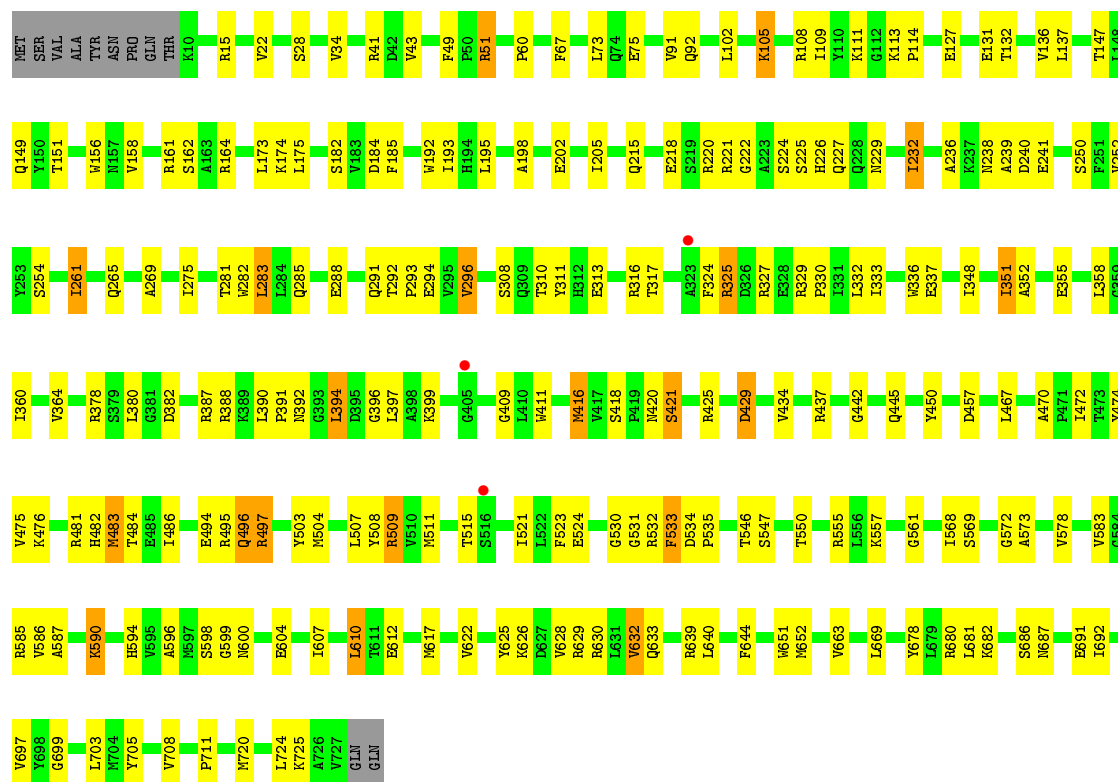
• Molecule 1: Alpha-galactosidase AgaA
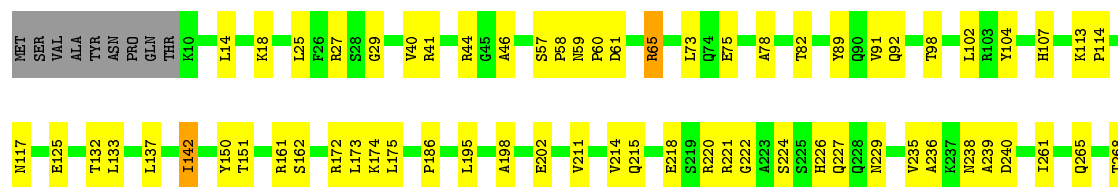
Chain A:

• Molecule 1: Alpha-galactosidase AgaA
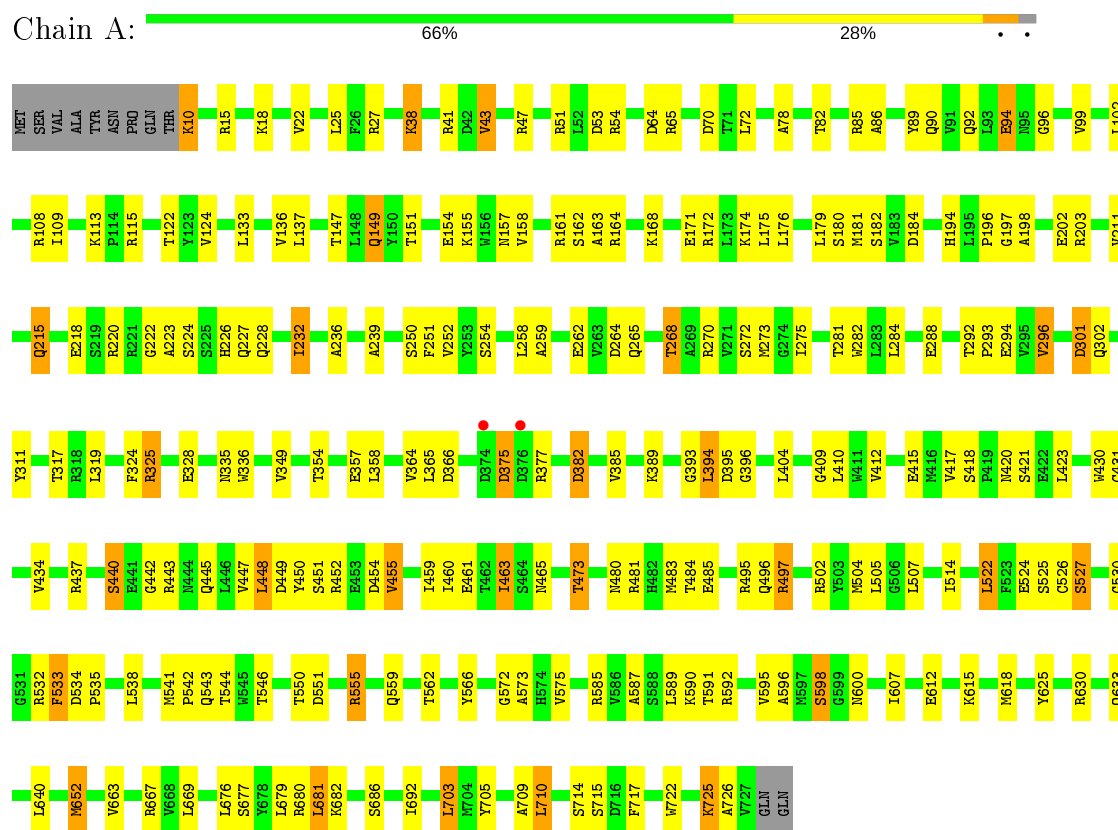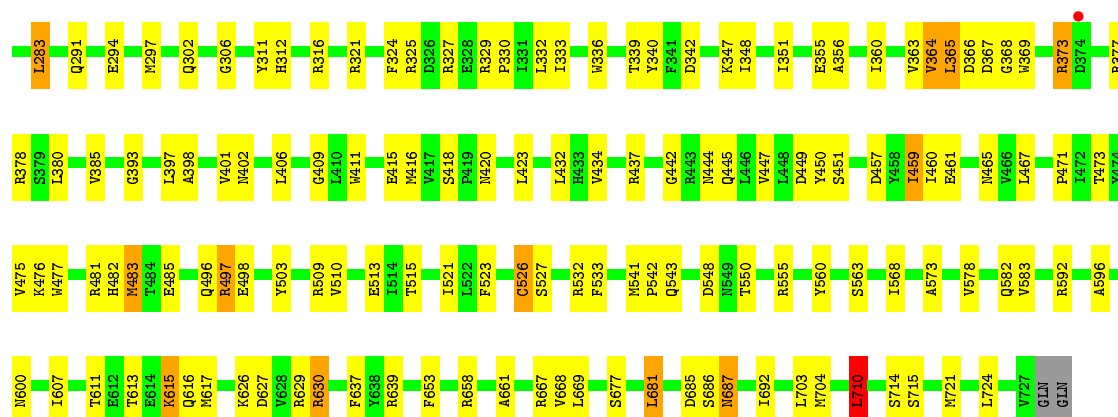
Chain B:

• Molecule 1: Alpha-galactosidase AgaA

• Molecule 1: Alpha-galactosidase AgaA

L283 Q291 E294 M297 Q302 G306 Y311 H312 R316 R321 F324 R325 D326 R327 E328 R329 P330 I331 L332 I333 W336 T339 Y340 F341 D342 K347 I348 I351 E355 A356 I360 V363 V364 L365 D366 D367 G368 W369 R373 D374 R377

R378 S379 L380 V385 G393 L397 A398 V401 M402 L406 G409 L410 W411 E415 M416 V417 S418 P419 N420 L423 L432 H433 V434 R437 G442 R443 N444 Q445 L446 V447 L448 D449 Y450 S451 D457 Y458 I459 I460 E461 N465 V466 L467 P471 I472 T473 Y474

V475 K476 W477 R481 H482 M483 T484 E485 Q496 R497 E498 Y503 R509 V510 E513 I514 T515 I521 L522 F523 C526 S527 R532 F533 M541 P542 Q543 D548 N549 T550 R555 Y560 S563 I568 A573 V578 Q582 V583 R592 A596

N600 I607 T611 E612 T613 E614 K615 Q616 M617 K626 D627 V628 R629 R630 F637 Y638 R639 F653 R658 A661 R667 V668 L669 S677 L681 D685 S686 N687 I692 L703 M704 L710 S714 S715 M721 L724 V727 GLN GLN

● Molecule 2: beta-D-fructofuranose-(2-1)-alpha-D-glucopyranose-(1-6)-alpha-D-galactopyranose-(1-6)-alpha-D-galactopyranose

Chain E:

GLA1 GLA2 GLC3 FRU4

● Molecule 2: beta-D-fructofuranose-(2-1)-alpha-D-glucopyranose-(1-6)-alpha-D-galactopyranose-(1-6)-alpha-D-galactopyranose

Chain F:

GLA1 GLA2 GLC3 FRU4

● Molecule 2: beta-D-fructofuranose-(2-1)-alpha-D-glucopyranose-(1-6)-alpha-D-galactopyranose-(1-6)-alpha-D-galactopyranose

Chain G:

GLA1 GLA2 GLC3 FRU4

● Molecule 2: beta-D-fructofuranose-(2-1)-alpha-D-glucopyranose-(1-6)-alpha-D-galactopyranose-(1-6)-alpha-D-galactopyranose

Chain H:

GLA1 GLA2 GLC3 FRU4

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α, β, γ	154.07Å 154.07Å 238.02Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	19.92 – 3.60 19.92 – 3.60	Depositor EDS
% Data completeness (in resolution range)	99.7 (19.92-3.60) 99.7 (19.92-3.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.09	Depositor
$<I/\sigma(I)>$ [1]	3.07 (at 3.62Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8_1069)	Depositor
R, R_{free}	0.238 , 0.282 0.238 , 0.284	Depositor DCC
R_{free} test set	1906 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	93.0	Xtriage
Anisotropy	0.223	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.23 , 19.4	EDS
L-test for twinning[2]	$<|L|>=0.49, <L^2>=0.33$	Xtriage
Estimated twinning fraction	0.024 for -h,-k,l	Xtriage
F_o,F_c correlation	0.90	EDS
Total number of atoms	23332	wwPDB-VP
Average B, all atoms (Å^2)	101.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.35% of the height of the origin peak. No significant pseudotranslation is detected.*

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[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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: GLA, GLC, FRU

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	0.22	0/5935	0.42	0/8046
1	B	0.22	0/5935	0.40	0/8046
1	C	0.22	0/5935	0.41	0/8046
1	D	0.22	0/5935	0.42	1/8046 (0.0%)
All	All	0.22	0/23740	0.41	1/32184 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	710	LEU	CA-CB-CG	5.87	128.81	115.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5788	0	5621	147	0
1	B	5788	0	5621	130	0
1	C	5788	0	5621	139	0
1	D	5788	0	5621	124	0
2	E	45	0	39	4	0
2	F	45	0	39	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	G	45	0	39	2	0
2	H	45	0	39	0	0
All	All	23332	0	22640	501	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 11.

The worst 5 of 501 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:681:LEU:HD11	1:B:703:LEU:HB3	1.61	0.81
1:B:684:LEU:H	1:B:704:MET:HE3	1.45	0.81
1:B:113:LYS:HD2	1:B:151:THR:HG21	1.66	0.78
1:A:113:LYS:HD2	1:A:151:THR:HG21	1.66	0.77
1:C:348:ILE:HD11	1:C:397:LEU:HD11	1.65	0.76

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	716/729 (98%)	683 (95%)	32 (4%)	1 (0%)	51	83
1	B	716/729 (98%)	685 (96%)	30 (4%)	1 (0%)	51	83
1	C	716/729 (98%)	683 (95%)	32 (4%)	1 (0%)	51	83
1	D	716/729 (98%)	682 (95%)	32 (4%)	2 (0%)	41	75
All	All	2864/2916 (98%)	2733 (95%)	126 (4%)	5 (0%)	47	79

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	496	GLN
1	B	496	GLN
1	C	496	GLN
1	D	496	GLN
1	D	526	CYS

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	608/618 (98%)	545 (90%)	63 (10%)	7	33
1	B	608/618 (98%)	555 (91%)	53 (9%)	10	41
1	C	608/618 (98%)	567 (93%)	41 (7%)	16	50
1	D	608/618 (98%)	570 (94%)	38 (6%)	18	53
All	All	2432/2472 (98%)	2237 (92%)	195 (8%)	12	43

5 of 195 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	440	SER
1	B	667	ARG
1	D	532	ARG
1	B	465	ASN
1	B	562	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 7 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	291	GLN
1	D	580	ASN
1	C	445	GLN
1	A	291	GLN
1	C	621	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)

16 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	GLA	E	1	2	11,11,12	2.57	2 (18%)	15,15,17	0.94	0
2	GLA	E	2	2	11,11,12	2.51	2 (18%)	15,15,17	1.73	2 (13%)
2	GLC	E	3	2	11,11,12	2.38	2 (18%)	15,15,17	1.34	1 (6%)
2	FRU	E	4	2	11,12,12	1.69	4 (36%)	10,18,18	1.65	2 (20%)
2	GLA	F	1	2	11,11,12	2.63	2 (18%)	15,15,17	1.15	1 (6%)
2	GLA	F	2	2	11,11,12	2.46	3 (27%)	15,15,17	2.43	7 (46%)
2	GLC	F	3	2	11,11,12	2.60	4 (36%)	15,15,17	1.58	4 (26%)
2	FRU	F	4	2	11,12,12	1.70	4 (36%)	10,18,18	1.96	4 (40%)
2	GLA	G	1	2	11,11,12	2.62	2 (18%)	15,15,17	1.30	1 (6%)
2	GLA	G	2	2	11,11,12	2.47	2 (18%)	15,15,17	2.24	5 (33%)
2	GLC	G	3	2	11,11,12	2.33	2 (18%)	15,15,17	2.14	7 (46%)
2	FRU	G	4	2	11,12,12	1.67	2 (18%)	10,18,18	1.89	4 (40%)
2	GLA	H	1	2	11,11,12	2.56	3 (27%)	15,15,17	1.29	1 (6%)
2	GLA	H	2	2	11,11,12	2.38	3 (27%)	15,15,17	2.28	6 (40%)
2	GLC	H	3	2	11,11,12	2.43	3 (27%)	15,15,17	1.77	5 (33%)
2	FRU	H	4	2	11,12,12	1.70	3 (27%)	10,18,18	2.03	4 (40%)

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	GLA	E	1	2	-	1/2/19/22	0/1/1/1
2	GLA	E	2	2	-	2/2/19/22	0/1/1/1
2	GLC	E	3	2	-	2/2/19/22	0/1/1/1
2	FRU	E	4	2	-	3/5/24/24	0/1/1/1
2	GLA	F	1	2	-	1/2/19/22	0/1/1/1
2	GLA	F	2	2	-	2/2/19/22	0/1/1/1
2	GLC	F	3	2	-	2/2/19/22	0/1/1/1
2	FRU	F	4	2	-	3/5/24/24	0/1/1/1
2	GLA	G	1	2	-	0/2/19/22	0/1/1/1
2	GLA	G	2	2	-	0/2/19/22	0/1/1/1
2	GLC	G	3	2	-	1/2/19/22	0/1/1/1
2	FRU	G	4	2	-	5/5/24/24	0/1/1/1
2	GLA	H	1	2	-	1/2/19/22	0/1/1/1
2	GLA	H	2	2	-	1/2/19/22	0/1/1/1
2	GLC	H	3	2	-	0/2/19/22	0/1/1/1
2	FRU	H	4	2	-	5/5/24/24	0/1/1/1

The worst 5 of 43 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	G	1	GLA	C2-C3	-7.38	1.41	1.52
2	F	1	GLA	C2-C3	-7.35	1.41	1.52
2	E	1	GLA	C2-C3	-7.27	1.41	1.52
2	E	2	GLA	C2-C3	-7.14	1.42	1.52
2	H	1	GLA	C2-C3	-7.04	1.42	1.52

The worst 5 of 54 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	G	3	GLC	C1-C2-C3	5.17	116.02	109.67
2	G	2	GLA	O5-C5-C6	4.97	114.99	107.20
2	F	2	GLA	C1-C2-C3	4.87	115.65	109.67
2	H	2	GLA	O5-C5-C6	4.54	114.33	107.20
2	F	2	GLA	O5-C5-C6	4.40	114.11	107.20

There are no chirality outliers.

5 of 29 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	E	4	FRU	O1-C1-C2-C3
2	E	4	FRU	O1-C1-C2-O2
2	E	4	FRU	O1-C1-C2-O5
2	G	4	FRU	O1-C1-C2-C3
2	G	4	FRU	O1-C1-C2-O2

There are no ring outliers.

4 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	E	1	GLA	2	0
2	G	2	GLA	1	0
2	E	2	GLA	2	0
2	G	4	FRU	2	0

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

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

Bond lengths

Bond angles

Torsions

Rings
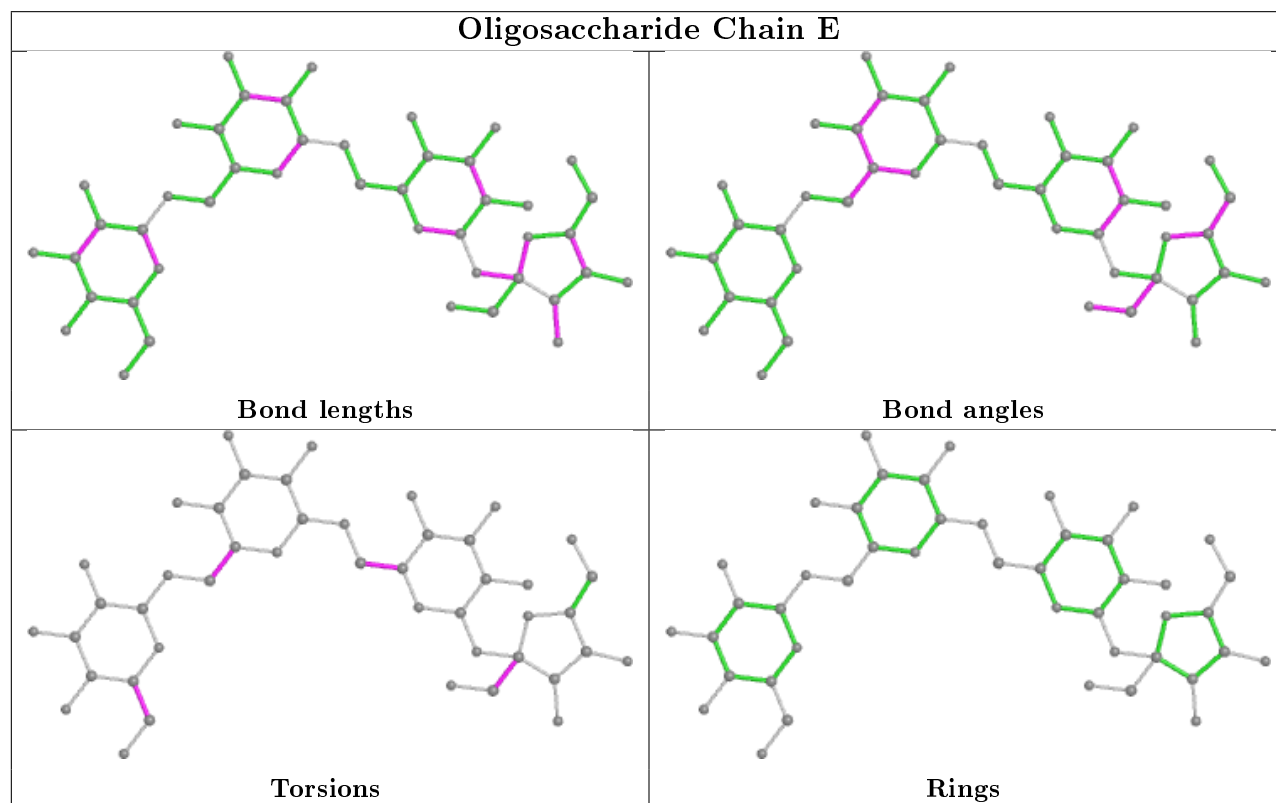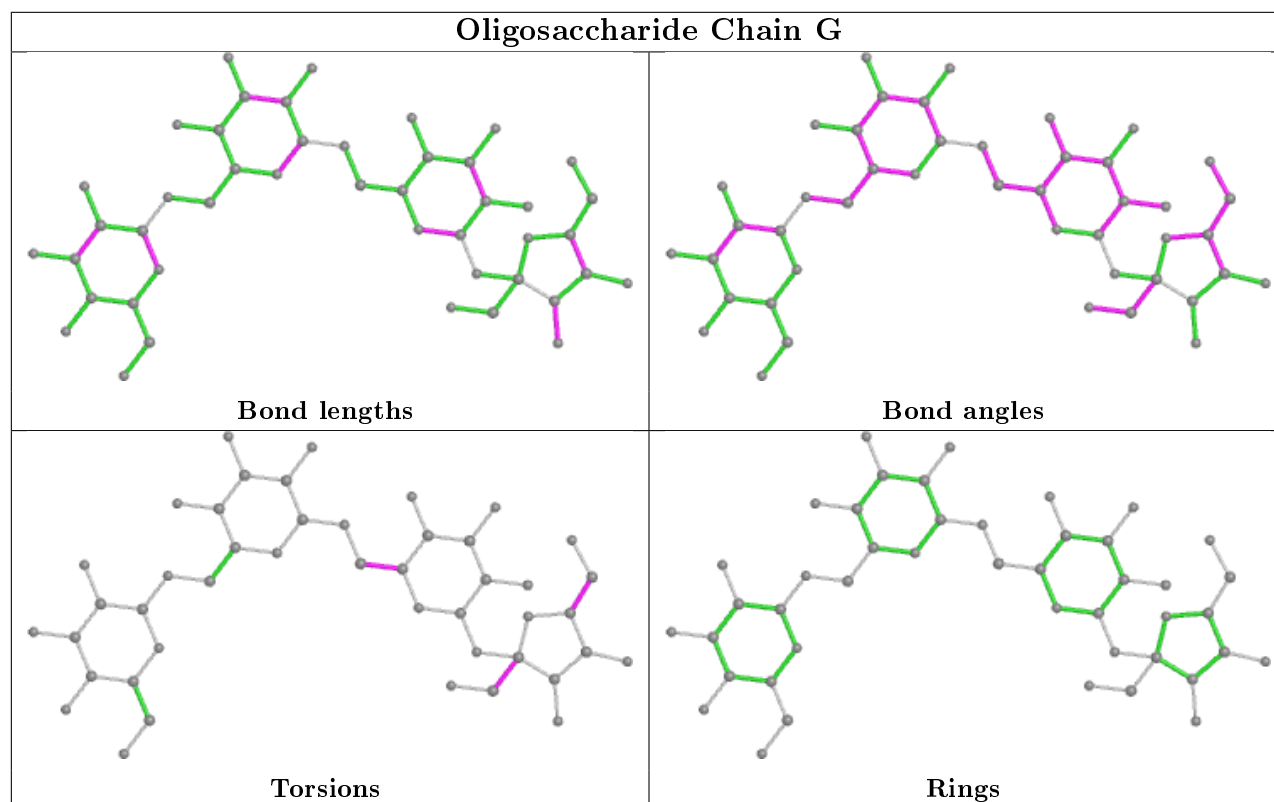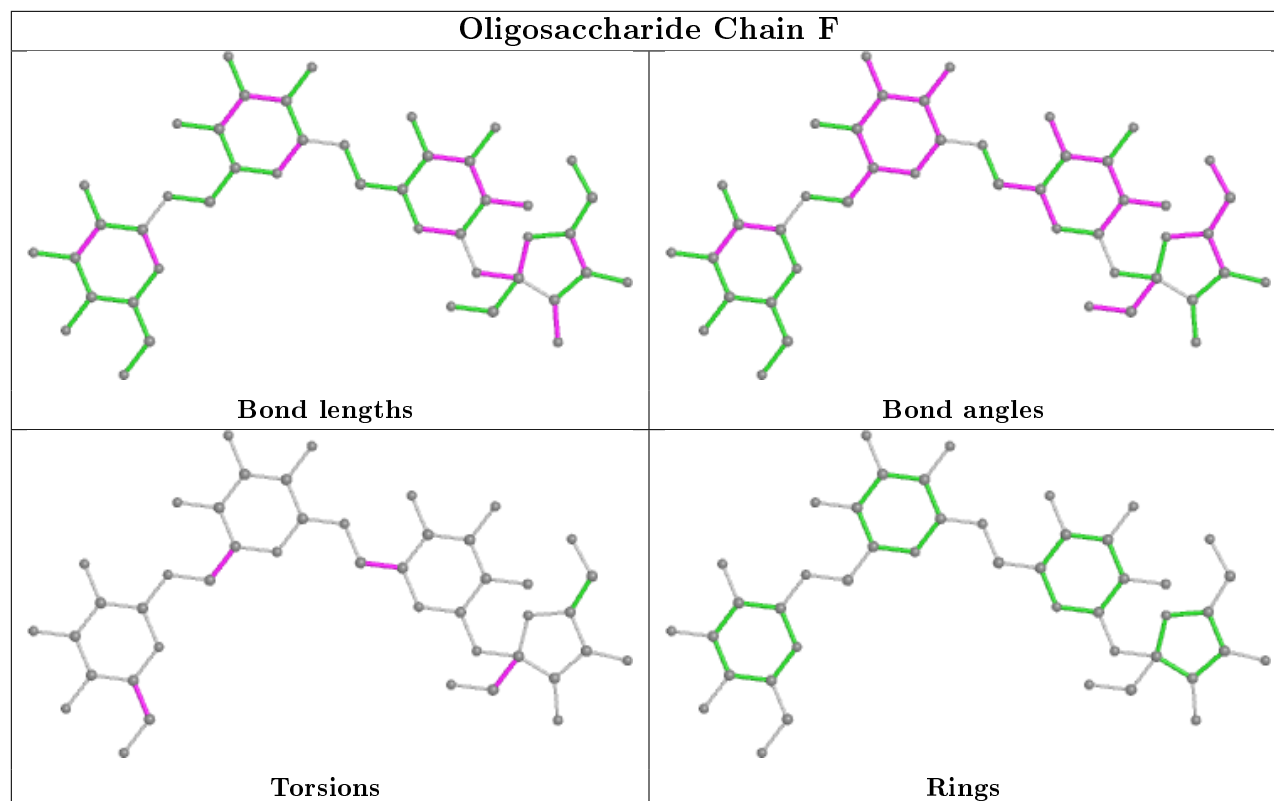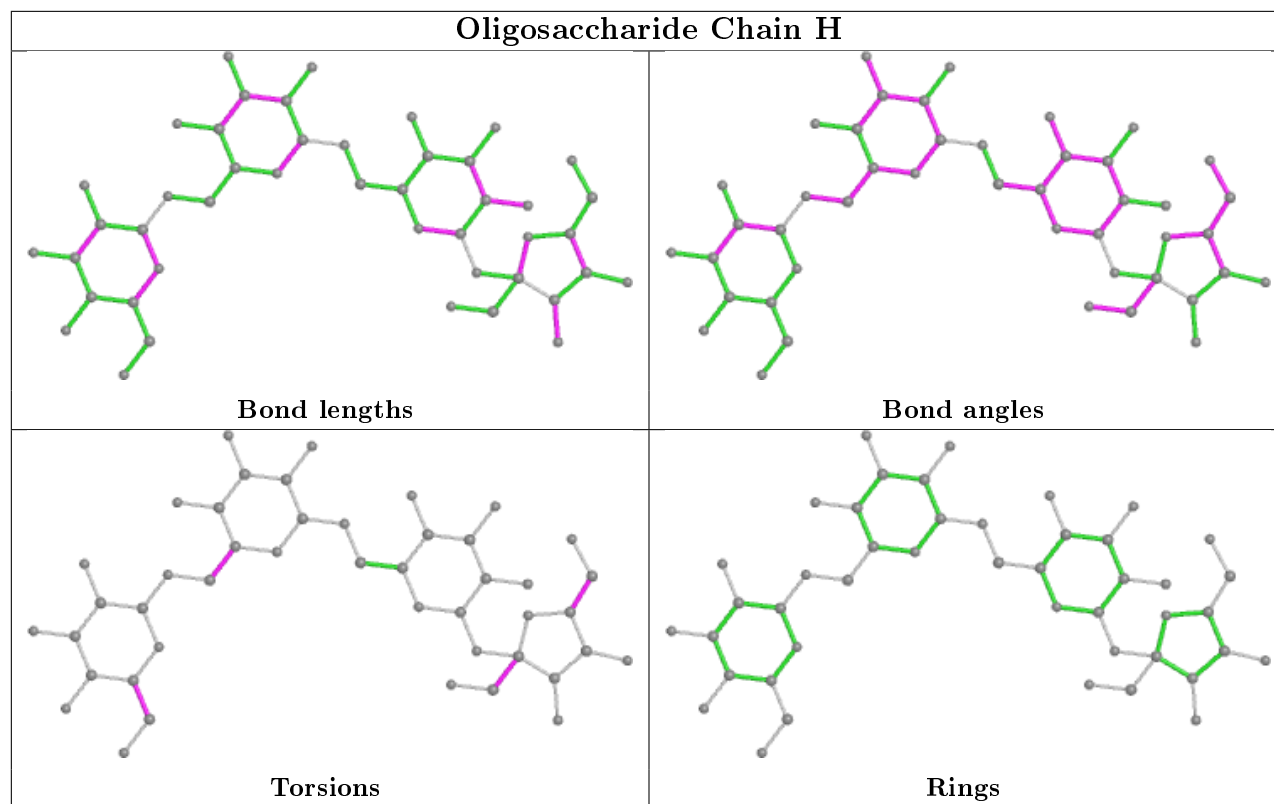
5.6 Ligand geometry (i)

There are no ligands in this entry.

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 (i)

6.1 Protein, DNA and RNA chains (i)

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	718/729 (98%)	-0.36	2 (0%)	94	88	61, 101, 145, 173	0
1	B	718/729 (98%)	-0.51	0	100	100	56, 90, 127, 144	0
1	C	718/729 (98%)	-0.31	3 (0%)	92	86	71, 113, 139, 163	0
1	D	718/729 (98%)	-0.45	1 (0%)	95	93	62, 93, 126, 151	0
All	All	2872/2916 (98%)	-0.41	6 (0%)	95	91	56, 100, 136, 173	0

The worst 5 of 6 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	516	SER	2.7
1	C	323	ALA	2.6
1	A	376	ASP	2.5
1	A	374	ASP	2.1
1	C	405	GLY	2.1

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.
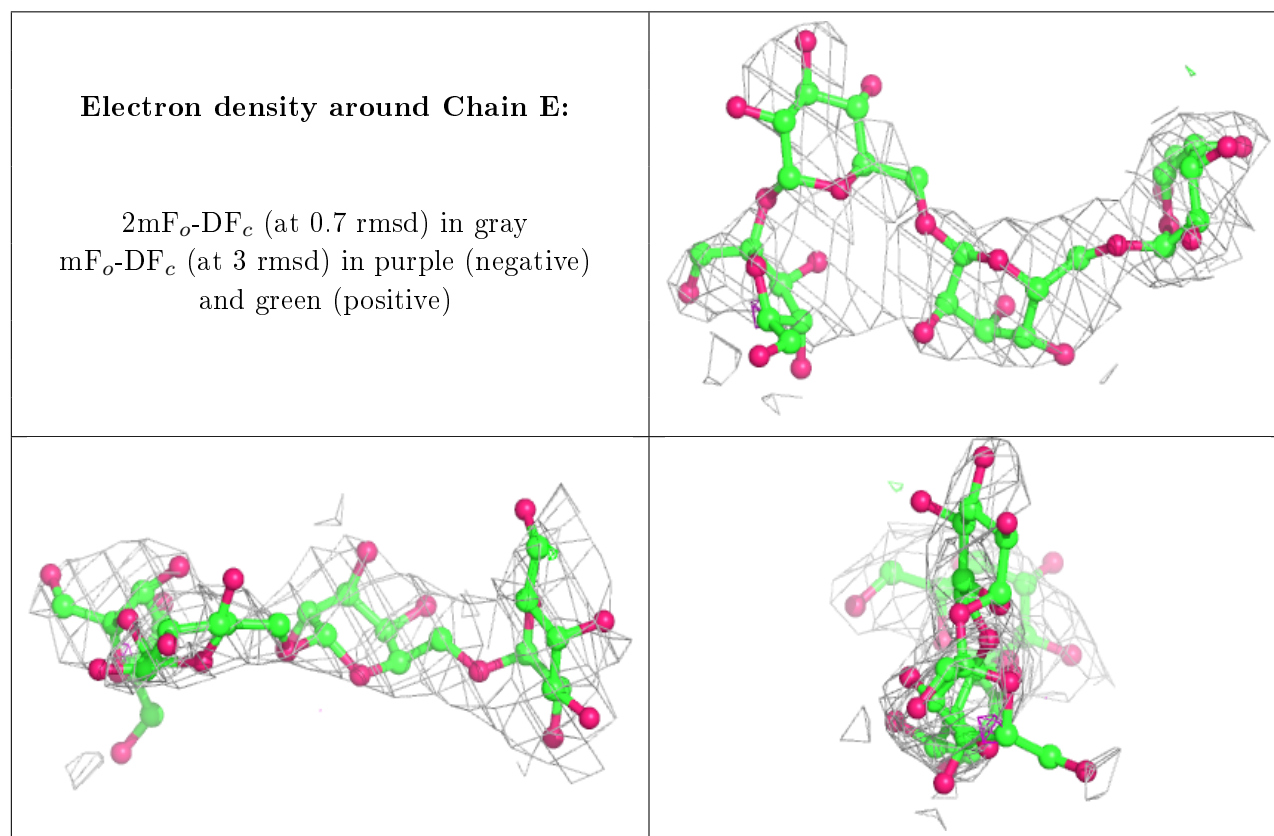
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	FRU	G	4	12/12	0.68	0.52	99,131,142,146	0
2	FRU	E	4	12/12	0.70	0.50	117,138,149,157	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å²)	Q<0.9
2	GLC	H	3	11/12	0.73	0.34	109,129,137,138	0
2	GLC	G	3	11/12	0.73	0.63	124,139,148,150	0
2	FRU	F	4	12/12	0.81	0.38	104,131,137,140	0
2	GLA	E	2	11/12	0.81	0.30	106,116,119,121	0
2	GLC	E	3	11/12	0.82	0.45	125,141,146,151	0
2	GLA	G	1	11/12	0.85	0.25	114,119,123,125	0
2	GLA	E	1	11/12	0.87	0.26	105,123,130,131	0
2	GLA	F	2	11/12	0.87	0.28	104,109,124,127	0
2	FRU	H	4	12/12	0.87	0.30	102,121,135,143	0
2	GLC	F	3	11/12	0.88	0.39	122,129,136,138	0
2	GLA	G	2	11/12	0.88	0.27	99,110,115,119	0
2	GLA	F	1	11/12	0.89	0.23	95,103,109,110	0
2	GLA	H	2	11/12	0.91	0.18	94,102,110,110	0
2	GLA	H	1	11/12	0.93	0.19	87,98,102,103	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.
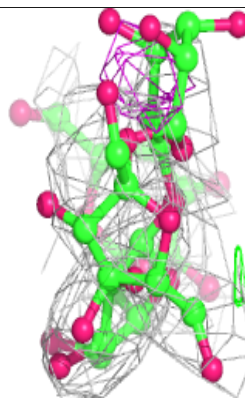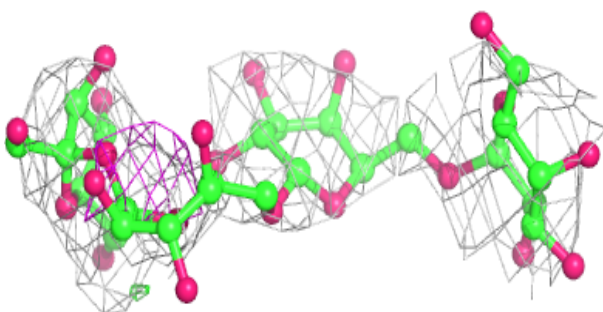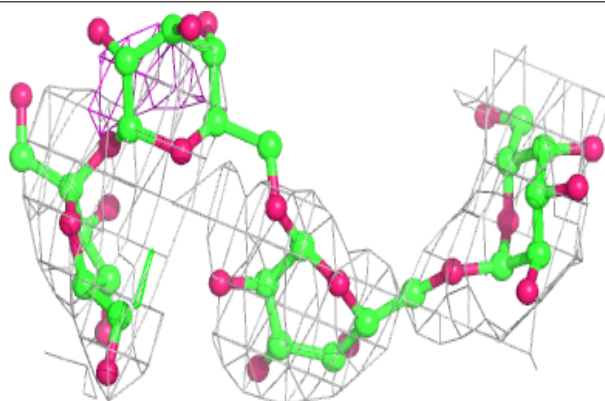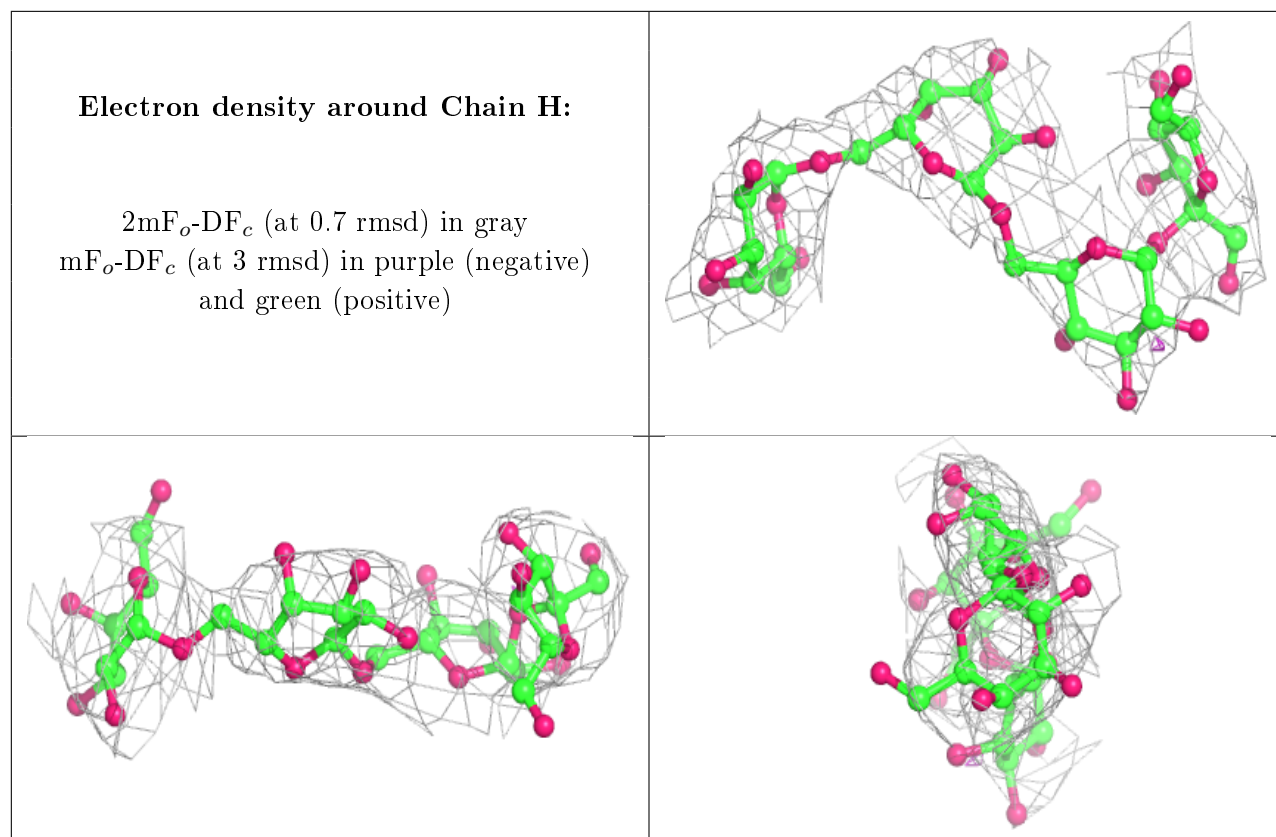
Electron density around Chain E:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (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)
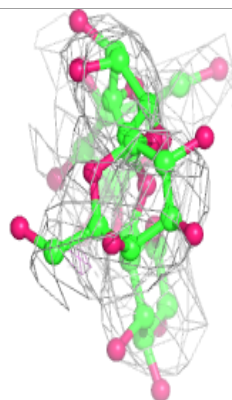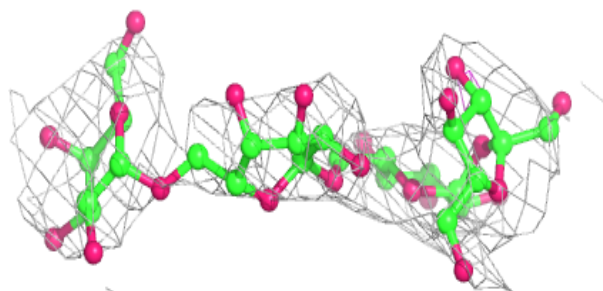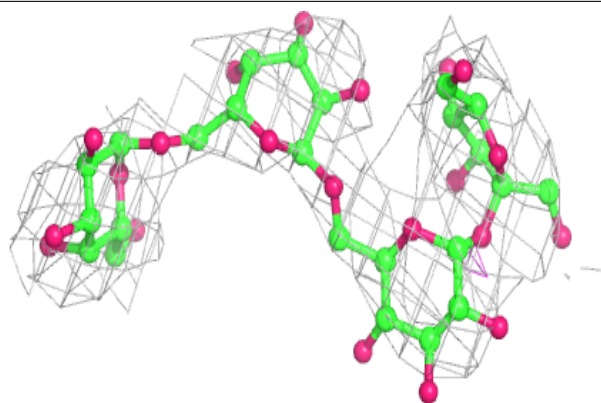
Electron density around Chain G:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)

Electron density around Chain H:

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

6.4 Ligands ⓘ

There are no ligands in this entry.

6.5 Other polymers ⓘ

There are no such residues in this entry.