wwPDB X-ray Structure Validation Summary Report (i)

Oct 23, 2023 – 12:06 AM EDT

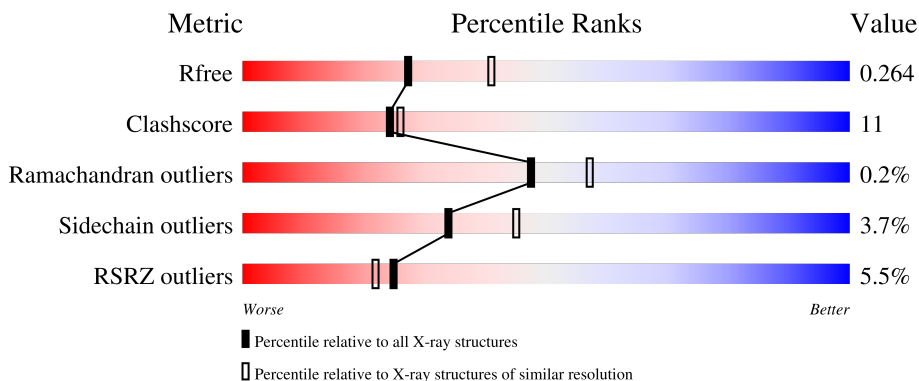|		
PDB ID	:	3FHQ
Title	:	Structure of endo-beta-N-acetylglucosaminidase A
Authors	:	Jie, Y.; Li, L.; Shaw, N.; Li, Y.; Song, J.; Zhang, W.; Xia, C.; Zhang, R.; Joachimiak, A.; Zhang, H.-C.; Wang, L.-X.; Wang, P.; Liu, Z.-J.
Deposited on	:	2008-12-10
Resolution	:	2.45 Å(reported)

1　Overall quality at a glance　ⓘ

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

The reported resolution of this entry is 2.45 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	Percentile Ranks	Value
Rfree		0.264
Clashscore		11
Ramachandran outliers		0.2%
Sidechain outliers		3.7%
RSRZ outliers		5.5%

Worse ………………………………………………………… *Better*

▮ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1544 (2.48-2.44)
Clashscore	141614	1613 (2.48-2.44)
Ramachandran outliers	138981	1598 (2.48-2.44)
Sidechain outliers	138945	1598 (2.48-2.44)
RSRZ outliers	127900	1523 (2.48-2.44)

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	621	4% / 77% / 18% · ·
1	B	621	6% / 77% / 18% · ·
1	D	621	4% / 76% / 18% · ·
1	F	621	8% / 75% / 19% · ·
2	C	3	67% / 33%

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Mol	Chain	Length	Quality of chain
2	E	3	33% 67%
2	G	3	33% 67%
2	H	3	67% 33%

2   Entry composition ⓘ

There are 4 unique types of molecules in this entry. The entry contains 20045 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.
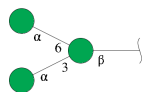
- Molecule 1 is a protein called Endo-beta-N-acetylglucosaminidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	601	Total 4781	C 3031	N 801	O 938	S 11	0	0	0
1	B	599	Total 4757	C 3017	N 797	O 932	S 11	0	0	0
1	D	597	Total 4746	C 3011	N 793	O 931	S 11	0	0	0
1	F	596	Total 4736	C 3003	N 793	O 929	S 11	0	0	0

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	43	ASP	ASN	engineered mutation	UNP Q9ZB22
A	455	ASP	GLY	engineered mutation	UNP Q9ZB22
A	518	THR	ILE	engineered mutation	UNP Q9ZB22
A	583	ILE	LEU	engineered mutation	UNP Q9ZB22
B	43	ASP	ASN	engineered mutation	UNP Q9ZB22
B	455	ASP	GLY	engineered mutation	UNP Q9ZB22
B	518	THR	ILE	engineered mutation	UNP Q9ZB22
B	583	ILE	LEU	engineered mutation	UNP Q9ZB22
D	43	ASP	ASN	engineered mutation	UNP Q9ZB22
D	455	ASP	GLY	engineered mutation	UNP Q9ZB22
D	518	THR	ILE	engineered mutation	UNP Q9ZB22
D	583	ILE	LEU	engineered mutation	UNP Q9ZB22
F	43	ASP	ASN	engineered mutation	UNP Q9ZB22
F	455	ASP	GLY	engineered mutation	UNP Q9ZB22
F	518	THR	ILE	engineered mutation	UNP Q9ZB22
F	583	ILE	LEU	engineered mutation	UNP Q9ZB22

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

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
2	C	3	Total 33	C 18	O 15	0	0	0
2	E	3	Total 33	C 18	O 15	0	0	0
2	G	3	Total 33	C 18	O 15	0	0	0
2	H	3	Total 33	C 18	O 15	0	0	0

- Molecule 3 is 3AR,5R,6S,7R,7AR-5-HYDROXYMETHYL-2-METHYL-5,6,7,7A-TETRA HYDRO-3AH-PYRANO[3,2-D]THIAZOLE-6,7-DIOL (three-letter code: NGT) (formula: $C_8H_{13}NO_4S$).
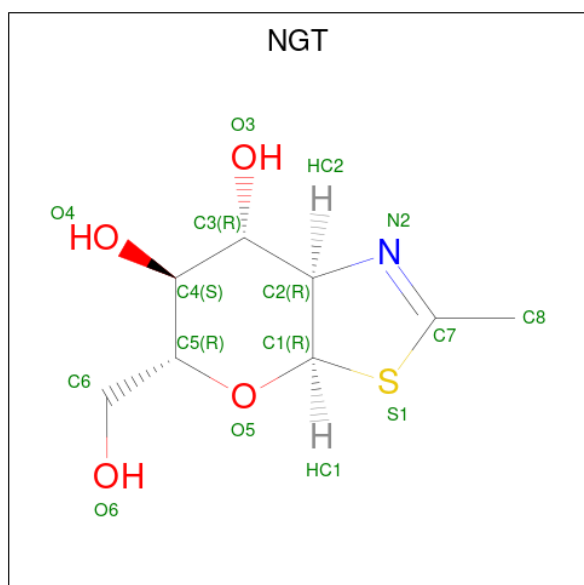
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total 14	C 8	N 1	O 4	S 1	0	0
3	B	1	Total 14	C 8	N 1	O 4	S 1	0	0
3	D	1	Total 14	C 8	N 1	O 4	S 1	0	0
3	F	1	Total 14	C 8	N 1	O 4	S 1	0	0

• Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	244	Total 244	O 244	0	0
4	B	182	Total 182	O 182	0	0
4	D	236	Total 236	O 236	0	0
4	F	175	Total 175	O 175	0	0

3 Residue-property plots ⓘ

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: Endo-beta-N-acetylglucosaminidase
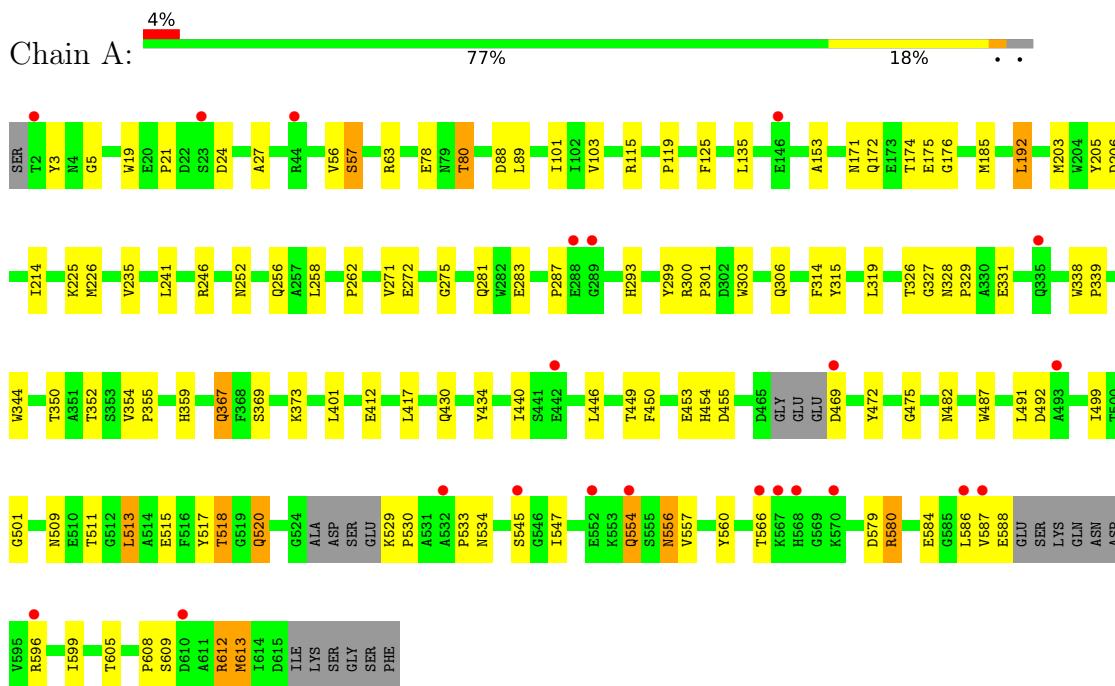
- Molecule 1: Endo-beta-N-acetylglucosaminidase
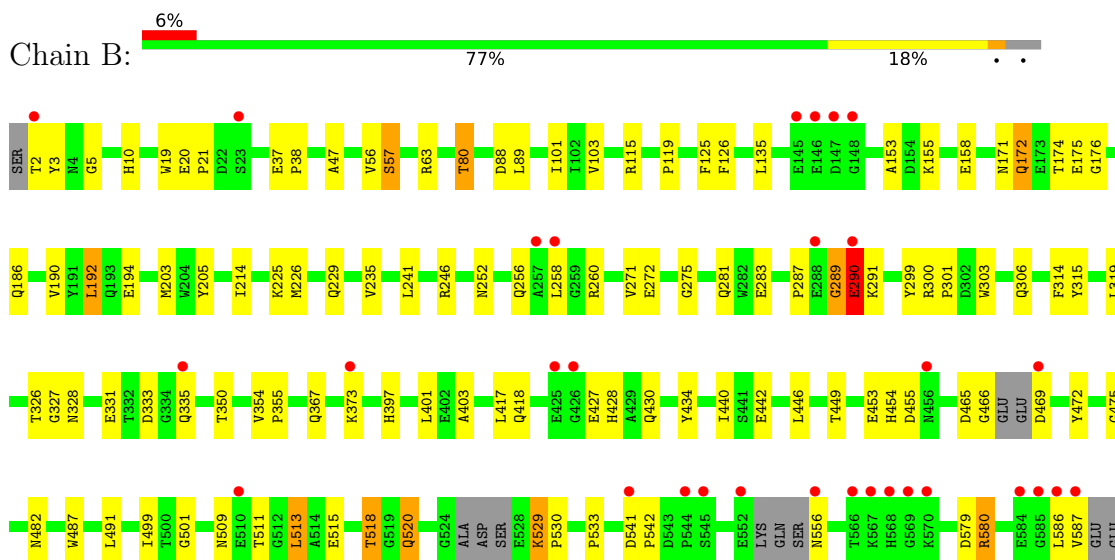
• Molecule 1: Endo-beta-N-acetylglucosaminidase
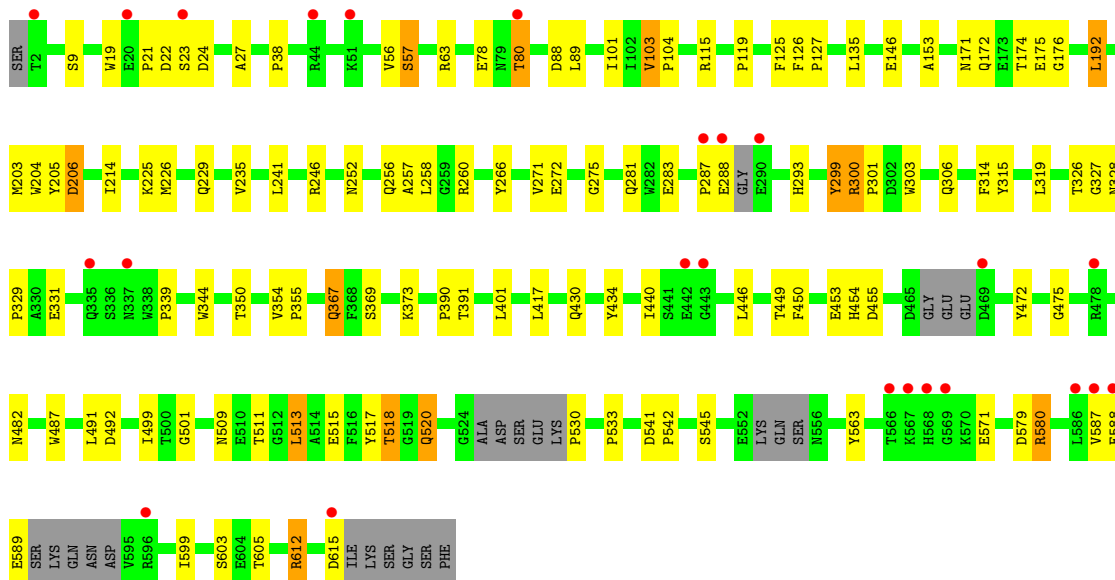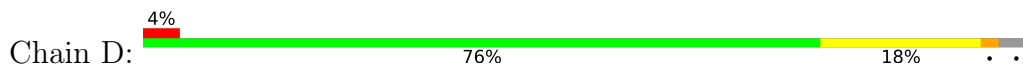
Chain D:

• Molecule 1: Endo-beta-N-acetylglucosaminidase
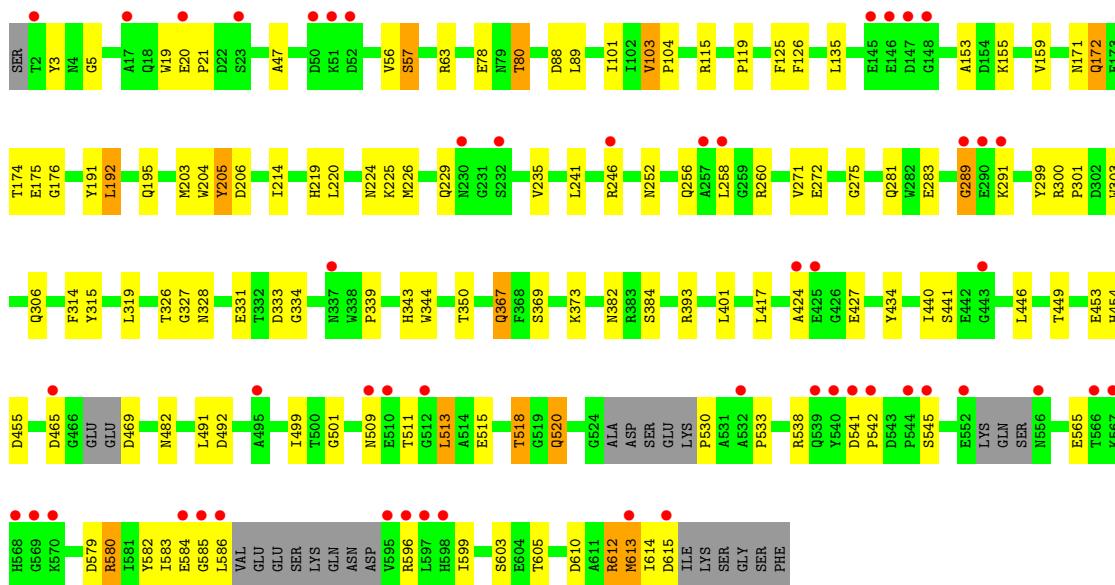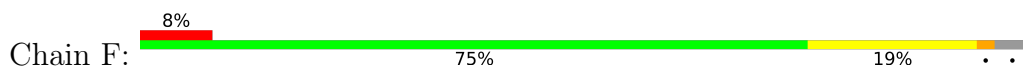
Chain F:

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

Chain C:

67%   33%

BMA1 MAN2 MAN3

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

Chain E:

33%   67%

BMA1 MAN2 MAN3

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

Chain G:

33%   67%

BMA1 MAN2 MAN3

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

Chain H:

67%   33%

BMA1 MAN2 MAN3

4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	78.33Å 79.27Å 117.04Å 80.51° 83.84° 64.33°	Depositor
Resolution (Å)	35.41 – 2.45 35.41 – 2.45	Depositor EDS
% Data completeness (in resolution range)	94.2 (35.41-2.45) 94.2 (35.41-2.45)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.46 (at 2.45Å)	Xtriage
Refinement program	PHENIX (phenix.refine)	Depositor
R, R_{free}	0.221 , 0.264 0.230 , 0.264	Depositor DCC
R_{free} test set	4331 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å^2)	36.4	Xtriage
Anisotropy	0.216	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 43.1	EDS
L-test for twinning[2]	$< |L| > = 0.51$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	20045	wwPDB-VP
Average B, all atoms (Å^2)	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.43% 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 ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: MAN, NGT, BMA

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	0.55	0/4927	0.61	0/6718
1	B	0.54	0/4902	0.60	2/6684 (0.0%)
1	D	0.56	2/4890 (0.0%)	0.61	1/6667 (0.0%)
1	F	0.51	0/4881	0.60	2/6655 (0.0%)
All	All	0.54	2/19600 (0.0%)	0.61	5/26724 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	299	TYR	CD2-CE2	-5.54	1.31	1.39
1	D	299	TYR	CD1-CE1	-5.26	1.31	1.39

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	300	ARG	N-CA-C	5.42	125.64	111.00
1	F	610	ASP	CB-CG-OD2	5.20	122.98	118.30
1	B	469	ASP	CB-CG-OD2	5.13	122.92	118.30
1	F	205	TYR	CB-CA-C	5.11	120.63	110.40
1	B	289	GLY	N-CA-C	-5.07	100.43	113.10

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	4781	0	4392	102	0
1	B	4757	0	4363	105	0
1	D	4746	0	4347	99	0
1	F	4736	0	4341	110	0
2	C	33	0	27	1	0
2	E	33	0	27	2	0
2	G	33	0	27	2	0
2	H	33	0	27	1	0
3	A	14	0	12	1	0
3	B	14	0	12	1	0
3	D	14	0	12	1	0
3	F	14	0	12	1	0
4	A	244	0	0	9	0
4	B	182	0	0	7	0
4	D	236	0	0	12	0
4	F	175	0	0	5	0
All	All	20045	0	17599	404	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 404 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:A:547:ILE:CD1	1:A:586:LEU:HD13	1.55	1.36
1:D:588:GLU:O	1:D:589:GLU:HB2	1.45	1.16
1:D:545:SER:HA	1:D:587:VAL:HB	1.28	1.13
1:A:547:ILE:HD13	1:A:586:LEU:HD13	1.23	1.10
1:A:547:ILE:HD11	1:A:586:LEU:HD13	1.30	1.05

There are no symmetry-related clashes.

5.3　Torsion angles　ⓘ

5.3.1　Protein backbone　ⓘ

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	593/621 (96%)	570 (96%)	23 (4%)	0	100	100
1	B	589/621 (95%)	566 (96%)	21 (4%)	2 (0%)	41	49
1	D	585/621 (94%)	565 (97%)	19 (3%)	1 (0%)	47	57
1	F	586/621 (94%)	562 (96%)	22 (4%)	2 (0%)	41	49
All	All	2353/2484 (95%)	2263 (96%)	85 (4%)	5 (0%)	47	57

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	290	GLU
1	B	10	HIS
1	F	206	ASP
1	D	206	ASP
1	F	289	GLY

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	498/515 (97%)	477 (96%)	21 (4%)	30	39
1	B	494/515 (96%)	477 (97%)	17 (3%)	37	48
1	D	493/515 (96%)	475 (96%)	18 (4%)	34	45
1	F	492/515 (96%)	475 (96%)	17 (4%)	36	47
All	All	1977/2060 (96%)	1904 (96%)	73 (4%)	34	45

5 of 73 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	F	80	THR
1	F	612	ARG
1	F	171	ASN

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Mol	Chain	Res	Type
1	F	469	ASP
1	B	103	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 8 such sidechains are listed below:

Mol	Chain	Res	Type
1	F	171	ASN
1	F	48	ASN
1	D	293	HIS
1	D	250	GLN
1	D	539	GLN

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 ⓘ

12 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	BMA	C	1	2,3	11,11,12	1.24	1 (9%)	15,15,17	1.93	5 (33%)
2	MAN	C	2	2	11,11,12	1.78	3 (27%)	15,15,17	2.31	7 (46%)
2	MAN	C	3	2	11,11,12	1.09	1 (9%)	15,15,17	2.34	7 (46%)
2	BMA	E	1	2,3	11,11,12	1.24	1 (9%)	15,15,17	1.93	5 (33%)
2	MAN	E	2	2	11,11,12	1.77	2 (18%)	15,15,17	2.31	7 (46%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
2	MAN	E	3	2	11,11,12	1.09	1 (9%)	15,15,17	2.35	7 (46%)
2	BMA	G	1	2,3	11,11,12	1.24	1 (9%)	15,15,17	1.92	5 (33%)
2	MAN	G	2	2	11,11,12	1.79	3 (27%)	15,15,17	2.31	7 (46%)
2	MAN	G	3	2	11,11,12	1.09	1 (9%)	15,15,17	2.35	7 (46%)
2	BMA	H	1	2,3	11,11,12	1.23	1 (9%)	15,15,17	1.94	5 (33%)
2	MAN	H	2	2	11,11,12	1.78	3 (27%)	15,15,17	2.30	7 (46%)
2	MAN	H	3	2	11,11,12	1.08	1 (9%)	15,15,17	2.34	7 (46%)

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	BMA	C	1	2,3	-	0/2/19/22	0/1/1/1
2	MAN	C	2	2	-	2/2/19/22	0/1/1/1
2	MAN	C	3	2	-	0/2/19/22	0/1/1/1
2	BMA	E	1	2,3	-	0/2/19/22	0/1/1/1
2	MAN	E	2	2	-	2/2/19/22	0/1/1/1
2	MAN	E	3	2	-	0/2/19/22	0/1/1/1
2	BMA	G	1	2,3	-	0/2/19/22	0/1/1/1
2	MAN	G	2	2	-	2/2/19/22	0/1/1/1
2	MAN	G	3	2	-	0/2/19/22	0/1/1/1
2	BMA	H	1	2,3	-	0/2/19/22	0/1/1/1
2	MAN	H	2	2	-	2/2/19/22	0/1/1/1
2	MAN	H	3	2	-	0/2/19/22	0/1/1/1

The worst 5 of 19 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	2	MAN	C2-C3	4.04	1.58	1.52
2	H	2	MAN	C2-C3	4.04	1.58	1.52
2	C	2	MAN	C2-C3	4.03	1.58	1.52
2	G	2	MAN	C2-C3	4.03	1.58	1.52
2	G	1	BMA	C1-C2	3.04	1.59	1.52

The worst 5 of 76 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	1	BMA	O2-C2-C1	4.49	118.34	109.15

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	1	BMA	O2-C2-C1	4.48	118.31	109.15
2	G	1	BMA	O2-C2-C1	4.47	118.29	109.15
2	E	1	BMA	O2-C2-C1	4.46	118.28	109.15
2	G	3	MAN	O2-C2-C3	4.34	118.83	110.14

There are no chirality outliers.

5 of 8 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	2	MAN	C4-C5-C6-O6
2	E	2	MAN	C4-C5-C6-O6
2	G	2	MAN	C4-C5-C6-O6
2	H	2	MAN	C4-C5-C6-O6
2	C	2	MAN	O5-C5-C6-O6

There are no ring outliers.

6 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	G	2	MAN	1	0
2	G	1	BMA	1	0
2	H	1	BMA	1	0
2	E	1	BMA	1	0
2	E	2	MAN	1	0
2	C	1	BMA	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 C

Bond lengths

Bond angles

Torsions

Rings

Oligosaccharide Chain E

Bond lengths

Bond angles

Torsions

Rings

Oligosaccharide Chain G

Bond lengths

Bond angles

Torsions

Rings

Oligosaccharide Chain H

Bond lengths

Bond angles

Torsions

Rings
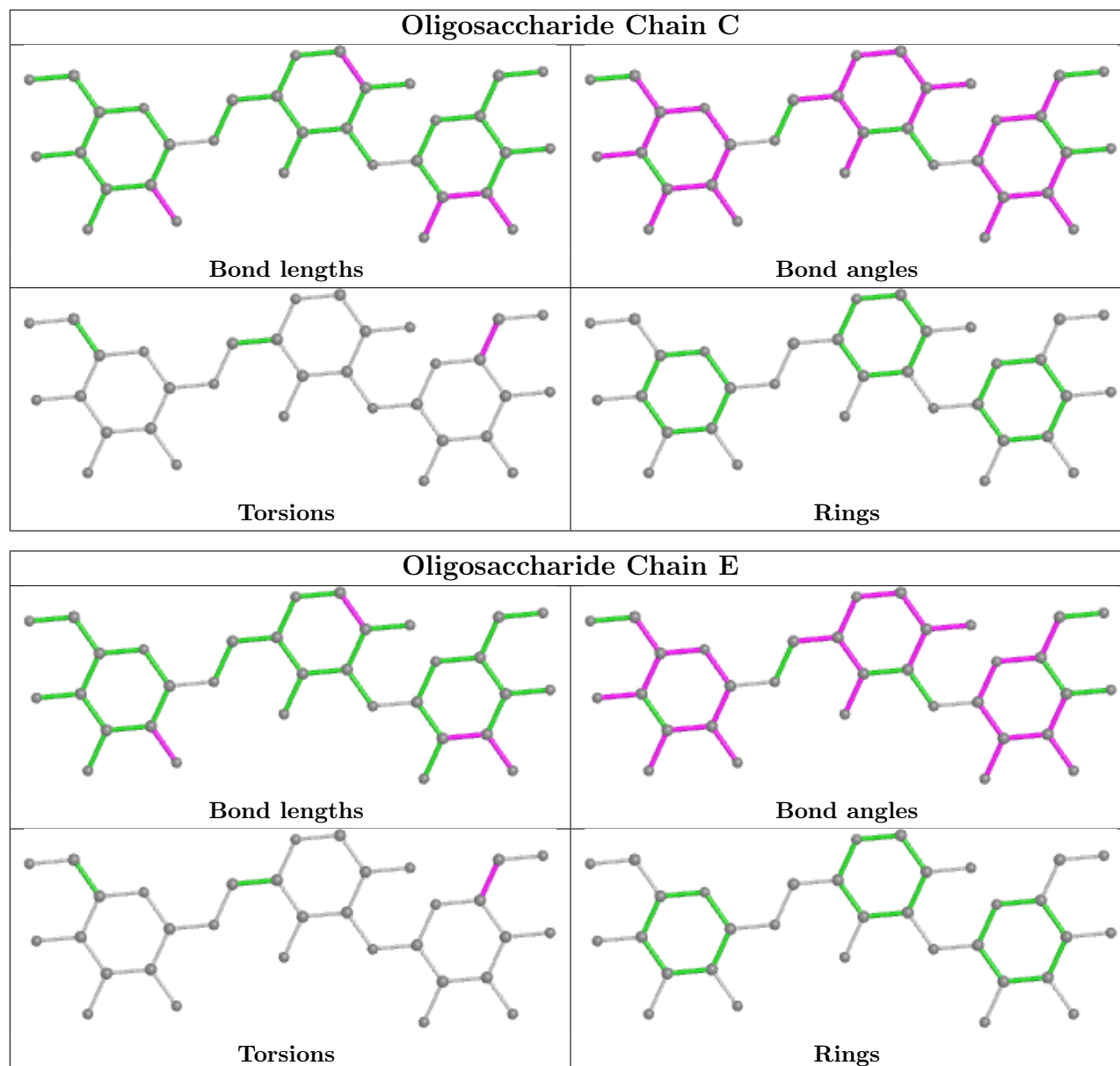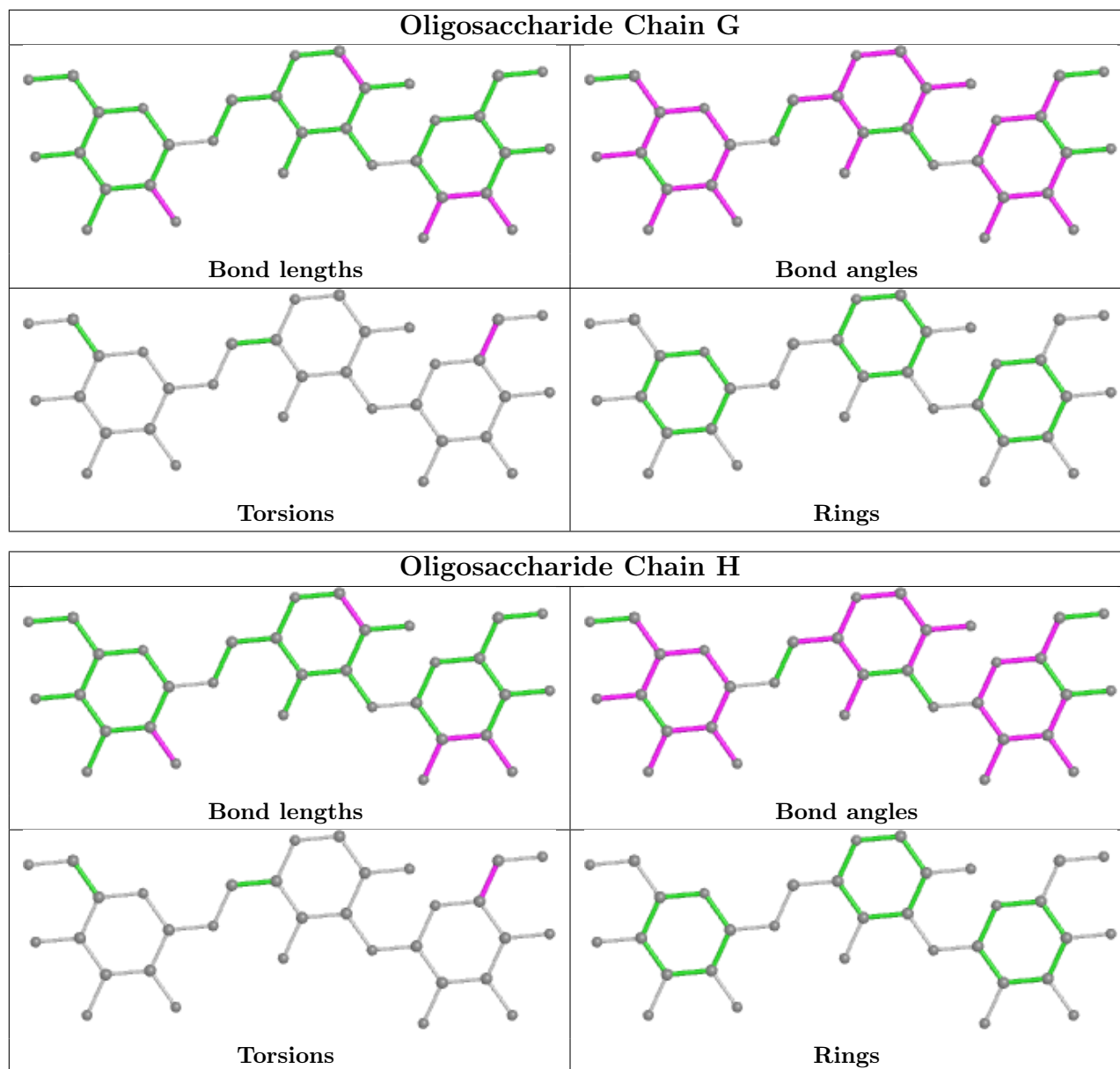
5.6   Ligand geometry ⓘ

4 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
3	NGT	D	625	2	13,15,15	2.86	1 (7%)	12,22,22	1.46	1 (8%)
3	NGT	A	625	2	13,15,15	2.84	1 (7%)	12,22,22	1.46	1 (8%)
3	NGT	B	625	2	13,15,15	2.86	1 (7%)	12,22,22	1.47	1 (8%)
3	NGT	F	625	2	13,15,15	2.82	1 (7%)	12,22,22	1.45	1 (8%)

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	NGT	D	625	2	-	0/2/30/30	0/2/2/2
3	NGT	A	625	2	-	0/2/30/30	0/2/2/2
3	NGT	B	625	2	-	0/2/30/30	0/2/2/2
3	NGT	F	625	2	-	0/2/30/30	0/2/2/2

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	625	NGT	C7-S1	-10.21	1.68	1.77
3	D	625	NGT	C7-S1	-10.21	1.68	1.77
3	A	625	NGT	C7-S1	-10.13	1.68	1.77
3	F	625	NGT	C7-S1	-10.08	1.68	1.77

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	625	NGT	C8-C7-S1	3.91	124.84	118.96
3	A	625	NGT	C8-C7-S1	3.89	124.81	118.96
3	D	625	NGT	C8-C7-S1	3.87	124.79	118.96
3	F	625	NGT	C8-C7-S1	3.85	124.76	118.96

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	625	NGT	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	625	NGT	1	0
3	B	625	NGT	1	0
3	F	625	NGT	1	0

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6   Fit of model and data ⓘ

6.1   Protein, DNA and RNA chains ⓘ

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	601/621 (96%)	0.23	22 (3%)	41	38	20, 31, 52, 75	0
1	B	599/621 (96%)	0.39	35 (5%)	23	20	20, 36, 57, 89	0
1	D	597/621 (96%)	0.21	24 (4%)	38	35	21, 33, 51, 74	0
1	F	596/621 (95%)	0.54	51 (8%)	10	7	20, 39, 60, 81	0
All	All	2393/2484 (96%)	0.34	132 (5%)	25	22	20, 34, 56, 89	0

The worst 5 of 132 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	568	HIS	6.9
1	F	510	GLU	6.7
1	F	596	ARG	6.2
1	F	257	ALA	6.1
1	A	568	HIS	5.9

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

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

6.3   Carbohydrates ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.
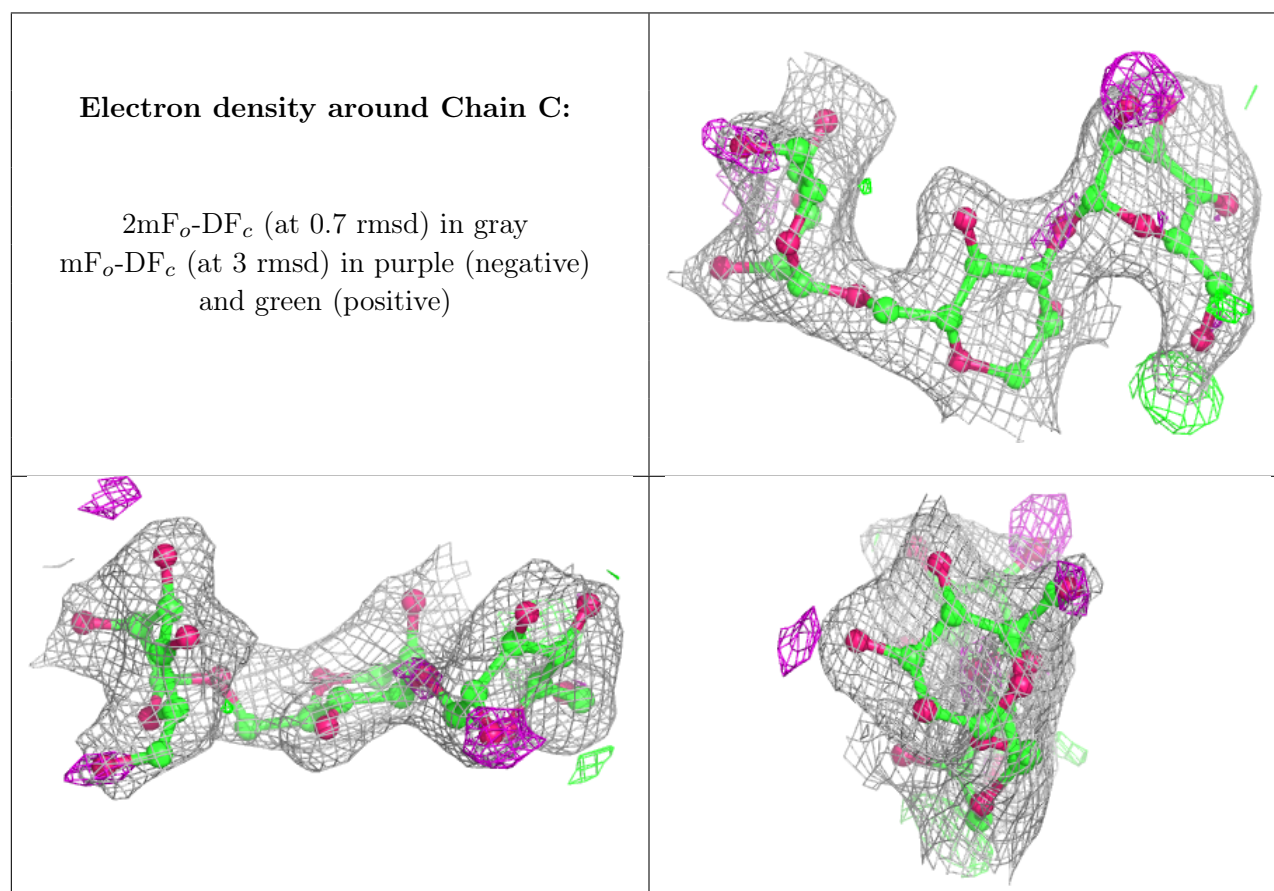
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	MAN	E	2	11/12	0.81	0.20	20,20,20,20	0
2	MAN	E	3	11/12	0.81	0.21	20,20,20,20	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($Å^2$)	Q<0.9
2	MAN	H	3	11/12	0.84	0.21	20,20,20,20	0
2	MAN	G	2	11/12	0.85	0.19	20,20,20,20	0
2	BMA	G	1	11/12	0.85	0.15	20,20,20,20	0
2	BMA	E	1	11/12	0.87	0.13	20,20,20,20	0
2	MAN	C	2	11/12	0.88	0.20	20,20,20,20	0
2	MAN	G	3	11/12	0.88	0.18	20,20,20,20	0
2	MAN	H	2	11/12	0.88	0.20	20,20,20,20	0
2	MAN	C	3	11/12	0.88	0.16	20,20,20,20	0
2	BMA	C	1	11/12	0.91	0.14	20,20,20,20	0
2	BMA	H	1	11/12	0.91	0.14	20,20,20,20	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.
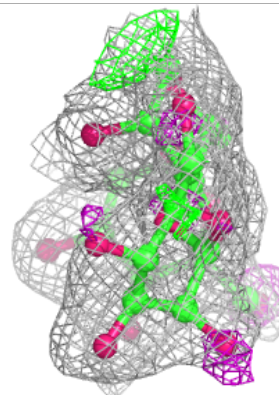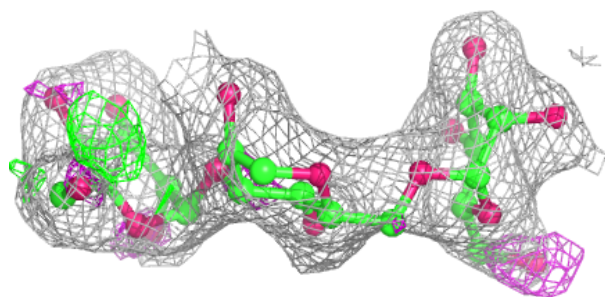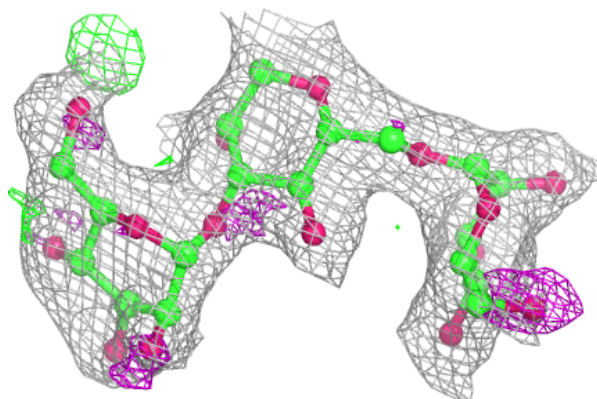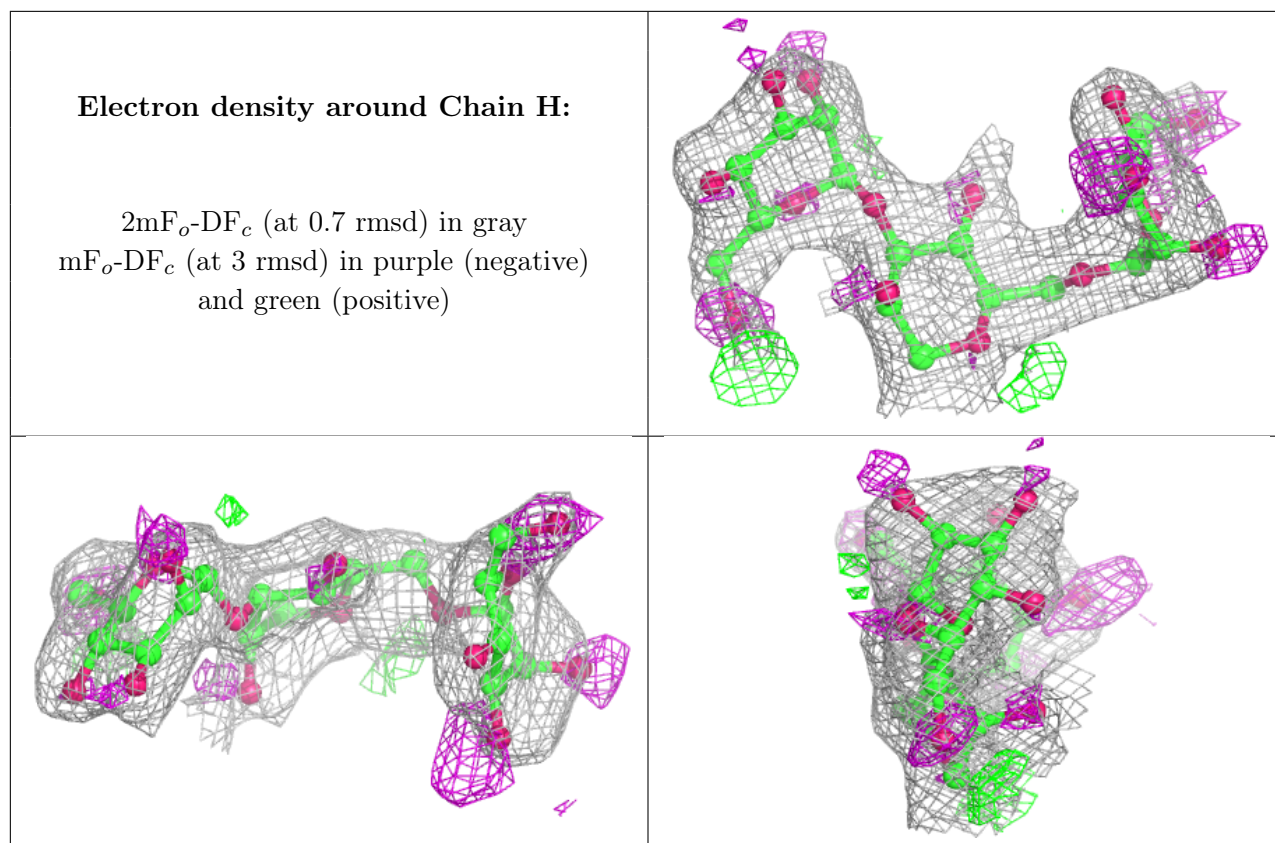

Electron density around Chain C:

$2mF_o$-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:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)
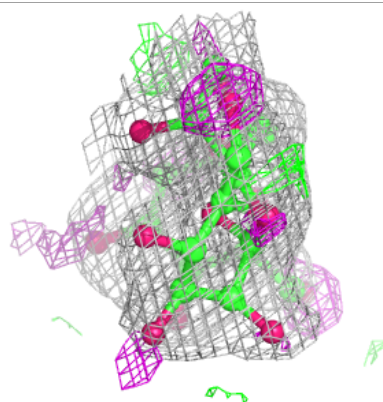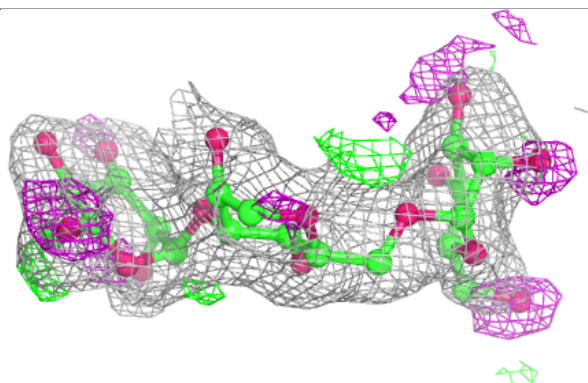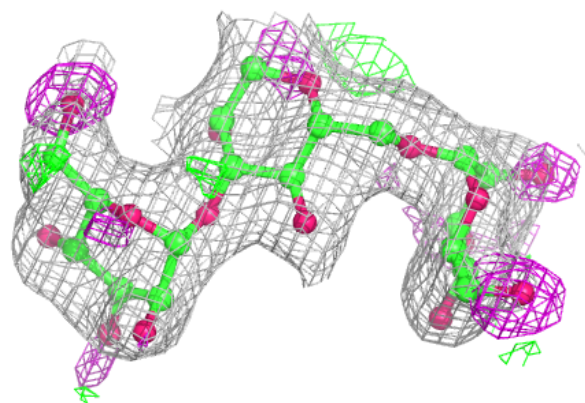
Electron density around Chain G:

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

Electron density around Chain 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 ⓘ

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	NGT	B	625	14/14	0.91	0.14	20,20,20,20	0
3	NGT	F	625	14/14	0.92	0.14	20,20,20,20	0
3	NGT	D	625	14/14	0.93	0.13	20,20,20,20	0
3	NGT	A	625	14/14	0.93	0.13	20,20,20,20	0

6.5 Other polymers ⓘ

There are no such residues in this entry.