



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 22, 2024 – 01:28 AM JST

PDB ID : 6JE0
Title : Ligand complex structure of GH10 family xylanase XynAF1, soaking for 30 minutes
Authors : Li, G.; Miao, Y.; Zhang, R.
Deposited on : 2019-02-02
Resolution : 1.43 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

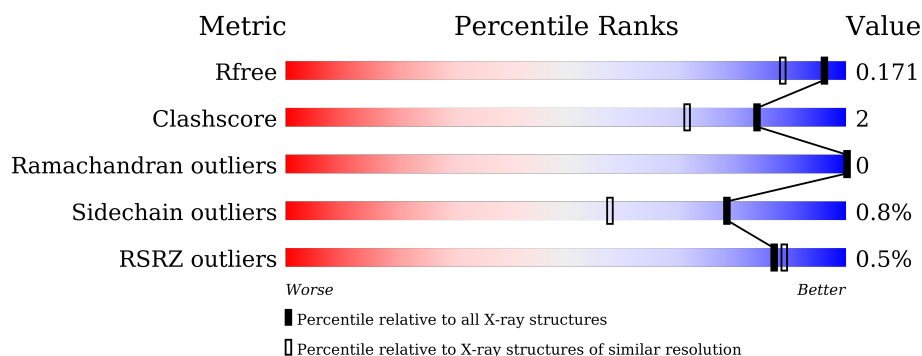
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.43 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}	164625	2809 (1.46-1.42)
Clashscore	180529	3008 (1.46-1.42)
Ramachandran outliers	177936	2971 (1.46-1.42)
Sidechain outliers	177891	2971 (1.46-1.42)
RSRZ outliers	164620	2809 (1.46-1.42)

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 $\leq 5\%$. 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	319	<div> <div>92%</div> <div>7%</div> </div>
1	B	319	<div> <div>%</div> <div>97%</div> </div>
2	C	2	<div> <div>50%</div> <div>50%</div> </div>
2	D	2	<div> <div>50%</div> <div>50%</div> </div>
2	E	2	<div> <div>50%</div> <div>50%</div> </div>
2	F	2	<div> <div>50%</div> <div>50%</div> </div>

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 5749 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 Beta-xylanase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	319	Total	C	N	O	S	0	10	0
			2500	1588	412	490	10			
1	B	319	Total	C	N	O	S	0	13	0
			2524	1601	416	496	11			

- Molecule 2 is an oligosaccharide called beta-D-xylopyranose-(1-4)-beta-D-xylopyranose.



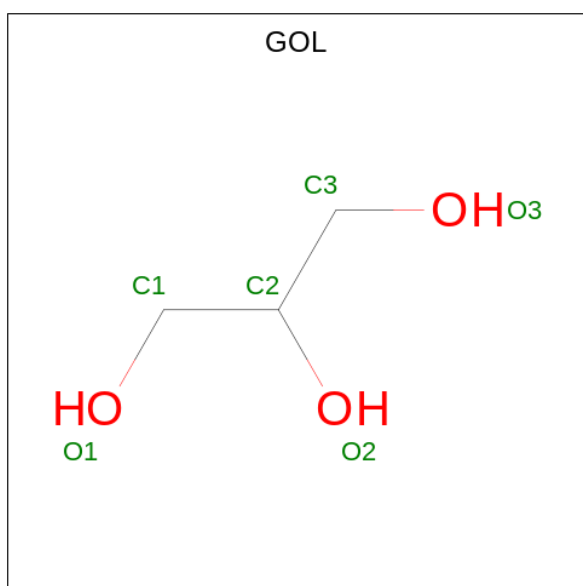
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
2	C	2	Total	C	O	0	0	0
			18	10	8			
2	D	2	Total	C	O	0	0	0
			19	10	9			
2	E	2	Total	C	O	0	0	0
			18	10	8			
2	F	2	Total	C	O	0	0	0
			19	10	9			

- Molecule 3 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: C₈H₁₅NO₆).



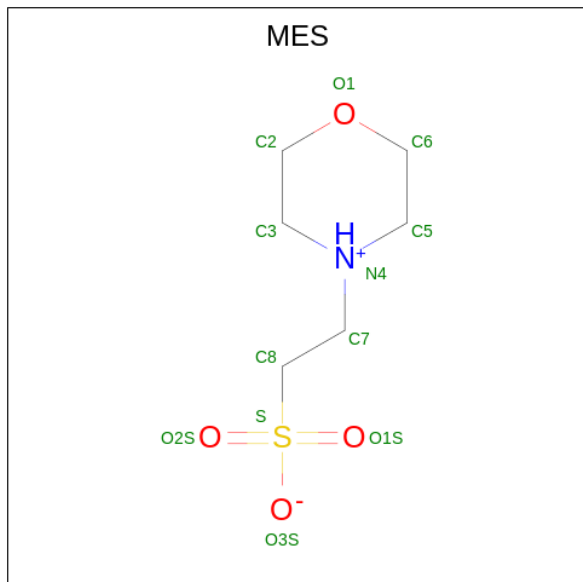
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	B	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



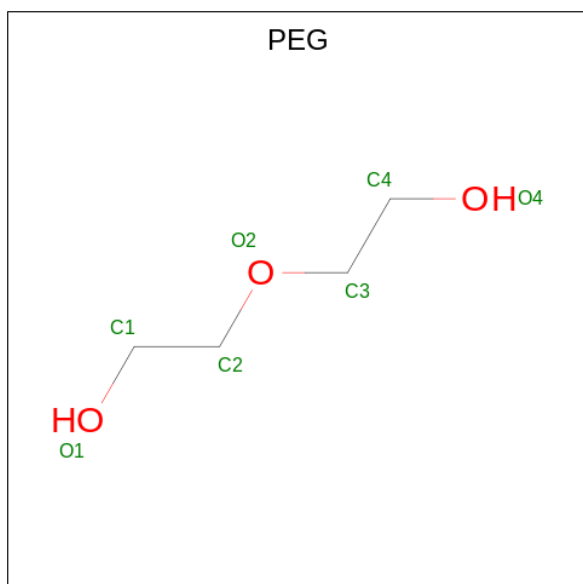
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			6	3	3		
4	B	1	Total	C	O	0	0
			6	3	3		

- Molecule 5 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (three-letter code: MES) (formula: $C_6H_{13}NO_4S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	N	O	S	0	0
			12	6	1	4	1		

- Molecule 6 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: $C_4H_{10}O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			7	4	3		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			7	4	3		
6	B	1	Total	C	O	0	0
			7	4	3		

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	304	Total	O	0	0
			304	304		
7	B	274	Total	O	0	0
			274	274		

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.

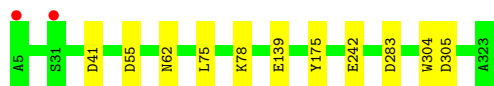
- Molecule 1: Beta-xylanase

Chain A: 



- Molecule 1: Beta-xylanase

Chain B: 



- Molecule 2: beta-D-xylopyranose-(1-4)-beta-D-xylopyranose

Chain C: 



- Molecule 2: beta-D-xylopyranose-(1-4)-beta-D-xylopyranose

Chain D: 



- Molecule 2: beta-D-xylopyranose-(1-4)-beta-D-xylopyranose

Chain E: 



- Molecule 2: beta-D-xylopyranose-(1-4)-beta-D-xylopyranose

Chain F: 



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	44.43Å 57.36Å 64.91Å 73.97° 80.80° 68.77°	Depositor
Resolution (Å)	62.25 – 1.43 62.25 – 1.43	Depositor EDS
% Data completeness (in resolution range)	91.6 (62.25-1.43) 91.6 (62.25-1.43)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.62 (at 1.43Å)	Xtriage
Refinement program	REFMAC 5.8.0135	Depositor
R, R_{free}	0.139 , 0.170 0.140 , 0.171	Depositor DCC
R_{free} test set	5220 reflections (4.90%)	wwPDB-VP
Wilson B-factor (Å ²)	12.3	Xtriage
Anisotropy	0.124	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 37.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	5749	wwPDB-VP
Average B, all atoms (Å ²)	14.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.24% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ 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: NAG, XYP, PEG, GOL, MES

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	1.21	2/2563 (0.1%)	1.14	11/3500 (0.3%)
1	B	1.20	3/2587 (0.1%)	1.10	7/3531 (0.2%)
All	All	1.21	5/5150 (0.1%)	1.12	18/7031 (0.3%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	175	TYR	CE1-CZ	-7.22	1.29	1.38
1	B	242	GLU	CD-OE1	6.79	1.33	1.25
1	B	175	TYR	CG-CD2	-6.29	1.30	1.39
1	A	33	TYR	CG-CD2	-5.58	1.31	1.39
1	A	149	TYR	CE1-CZ	-5.04	1.31	1.38

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	305	ASP	CB-CG-OD2	-7.76	111.32	118.30
1	B	139	GLU	OE1-CD-OE2	7.66	132.49	123.30
1	B	55	ASP	CB-CG-OD1	7.58	125.12	118.30
1	B	41	ASP	CB-CG-OD2	-7.04	111.97	118.30
1	A	84	ARG	NE-CZ-NH1	6.95	123.78	120.30
1	A	84	ARG	NE-CZ-NH2	-6.61	117.00	120.30
1	B	175	TYR	CB-CG-CD1	-6.23	117.26	121.00
1	B	305	ASP	CB-CG-OD2	-6.07	112.84	118.30
1	A	41	ASP	CB-CG-OD2	-5.92	112.97	118.30
1	A	263	PHE	CB-CG-CD1	5.67	124.77	120.80
1	A	70	ASP	CB-CG-OD1	5.62	123.36	118.30
1	B	304	TRP	CA-CB-CG	5.53	124.21	113.70
1	A	24	ASP	CB-CG-OD1	5.49	123.24	118.30
1	A	55	ASP	CB-CG-OD1	5.44	123.19	118.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	54	TRP	CD1-NE1-CE2	5.28	113.75	109.00
1	A	174	TYR	CB-CG-CD1	5.19	124.11	121.00
1	B	175	TYR	CZ-CE2-CD2	-5.18	115.14	119.80
1	A	30	ASP	CB-CG-OD1	5.07	122.86	118.30

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	2500	0	2389	12	0
1	B	2524	0	2408	4	0
2	C	18	0	0	2	0
2	D	19	0	0	2	0
2	E	18	0	0	3	0
2	F	19	0	0	3	0
3	A	14	0	13	0	0
3	B	14	0	13	0	0
4	A	6	0	8	3	0
4	B	6	0	8	0	0
5	A	12	0	13	1	0
6	A	14	0	20	3	0
6	B	7	0	10	0	0
7	A	304	0	0	3	1
7	B	274	0	0	3	1
All	All	5749	0	4882	22	1

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 2.

All (22) 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:62:ASN:HB2	7:B:611:HOH:O	1.46	1.15

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:62:ASN:CB	7:B:611:HOH:O	2.05	0.99
2:E:1:XYP:O5	2:F:2:XYP:O4	1.84	0.96
2:C:1:XYP:O5	2:D:2:XYP:O4	2.06	0.73
1:A:8:ASN:HD21	6:A:508:PEG:H32	1.56	0.70
1:B:62:ASN:CG	7:B:611:HOH:O	2.31	0.62
2:E:1:XYP:C1	2:F:2:XYP:O4	2.54	0.55
1:A:56:ALA:O	1:A:65[B]:SER:OG	2.25	0.54
1:A:24:ASP:HB2	4:A:506:GOL:C1	2.38	0.54
1:A:8:ASN:HD21	6:A:508:PEG:C3	2.22	0.52
1:A:75[A]:LEU:C	1:A:75[A]:LEU:HD13	2.30	0.52
1:A:124:LYS:NZ	7:A:604:HOH:O	2.36	0.51
1:A:44:GLY:HA3	6:A:508:PEG:H32	1.92	0.51
1:A:24:ASP:HB2	4:A:506:GOL:H12	1.93	0.49
2:E:1:XYP:O5	2:F:2:XYP:C4	2.61	0.49
1:A:90:TRP:CE2	1:A:92[B]:SER:HB2	2.51	0.45
1:A:24:ASP:HB2	4:A:506:GOL:H11	2.00	0.44
1:B:75:LEU:HD12	1:B:78:LYS:HE3	1.98	0.44
1:A:300:ALA:N	1:A:301:PRO:HD3	2.33	0.43
5:A:507:MES:H61	7:A:877:HOH:O	2.20	0.41
1:A:100:SER:O	7:A:602:HOH:O	2.21	0.41
2:C:1:XYP:O5	2:D:2:XYP:C4	2.69	0.41

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:A:815:HOH:O	7:B:652:HOH:O[1_654]	2.17	0.03

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	328/319 (103%)	323 (98%)	5 (2%)	0	100	100
1	B	331/319 (104%)	325 (98%)	6 (2%)	0	100	100
All	All	659/638 (103%)	648 (98%)	11 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	262/251 (104%)	258 (98%)	4 (2%)	60	30
1	B	265/251 (106%)	264 (100%)	1 (0%)	89	78
All	All	527/502 (105%)	522 (99%)	5 (1%)	79	51

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	75[A]	LEU
1	A	75[B]	LEU
1	A	283	ASP
1	A	296	GLN
1	B	283	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	114	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$
2	XYP	C	1	2	9,9,10	1.91	2 (22%)	10,12,14	2.10	3 (30%)
2	XYP	C	2	2	9,9,10	1.01	0	10,12,14	1.57	1 (10%)
2	XYP	D	1	2	10,10,10	1.07	1 (10%)	14,14,14	2.20	7 (50%)
2	XYP	D	2	2	9,9,10	1.12	1 (11%)	10,12,14	1.96	3 (30%)
2	XYP	E	1	2	9,9,10	1.31	1 (11%)	10,12,14	3.86	7 (70%)
2	XYP	E	2	2	9,9,10	1.34	1 (11%)	10,12,14	1.72	3 (30%)
2	XYP	F	1	2	10,10,10	0.82	0	14,14,14	1.85	4 (28%)
2	XYP	F	2	2	9,9,10	1.41	2 (22%)	10,12,14	1.68	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	XYP	C	1	2	-	-	0/1/1/1
2	XYP	C	2	2	-	-	0/1/1/1
2	XYP	D	1	2	-	-	0/1/1/1
2	XYP	D	2	2	-	-	0/1/1/1
2	XYP	E	1	2	-	-	0/1/1/1
2	XYP	E	2	2	-	-	0/1/1/1
2	XYP	F	1	2	-	-	0/1/1/1
2	XYP	F	2	2	-	-	0/1/1/1

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	1	XYP	C4-C3	-3.95	1.46	1.52
2	C	1	XYP	C2-C3	-2.77	1.48	1.52
2	F	2	XYP	O4-C4	-2.72	1.37	1.43
2	F	2	XYP	O5-C1	-2.59	1.37	1.42
2	E	1	XYP	O5-C1	2.52	1.47	1.42
2	E	2	XYP	C4-C3	2.27	1.55	1.52
2	D	1	XYP	O2-C2	-2.05	1.38	1.43
2	D	2	XYP	O5-C1	-2.04	1.39	1.42

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	1	XYP	C5-C4-C3	6.13	117.20	109.67
2	E	1	XYP	O4-C4-C5	5.63	120.66	109.15
2	E	1	XYP	O3-C3-C4	-5.58	99.30	109.99
2	E	1	XYP	C1-C2-C3	4.50	115.20	109.67
2	C	1	XYP	O2-C2-C3	4.03	118.21	110.14
2	F	1	XYP	O5-C1-C2	-3.63	104.04	109.43
2	E	1	XYP	C4-C3-C2	-3.61	106.64	110.92
2	E	2	XYP	O2-C2-C1	-3.58	101.82	109.15
2	D	2	XYP	C4-C3-C2	-3.55	106.71	110.92
2	D	1	XYP	O3-C3-C4	-3.49	103.32	109.99
2	D	1	XYP	C5-O5-C1	-3.48	106.86	112.71
2	D	2	XYP	O4-C4-C5	3.42	116.15	109.15
2	C	1	XYP	O3-C3-C4	-3.34	103.60	109.99
2	D	2	XYP	C5-C4-C3	3.23	113.64	109.67
2	F	2	XYP	O3-C3-C2	-2.99	104.26	109.99
2	D	1	XYP	C4-C3-C2	-2.94	105.80	110.89
2	F	1	XYP	C1-C2-C3	-2.86	104.38	110.31
2	C	2	XYP	C4-C3-C2	-2.77	107.63	110.92
2	E	1	XYP	O3-C3-C2	-2.71	104.80	109.99
2	D	1	XYP	O2-C2-C3	-2.55	104.46	110.35
2	D	1	XYP	O2-C2-C1	-2.40	103.60	109.16
2	F	2	XYP	O4-C4-C3	-2.38	105.37	110.14
2	C	1	XYP	C4-C3-C2	2.28	113.62	110.92
2	D	1	XYP	O3-C3-C2	2.27	115.61	110.35
2	F	1	XYP	O2-C2-C1	-2.20	104.06	109.16
2	F	2	XYP	O2-C2-C3	-2.19	105.75	110.14
2	F	2	XYP	O2-C2-C1	-2.15	104.75	109.15
2	D	1	XYP	O4-C4-C5	2.15	113.54	109.15
2	E	1	XYP	C5-O5-C1	2.13	114.79	111.52
2	E	2	XYP	C1-C2-C3	-2.12	107.06	109.67
2	E	2	XYP	C4-C3-C2	-2.07	108.46	110.92

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	1	XYP	O5-C5-C4	-2.05	107.61	110.77

There are no chirality outliers.

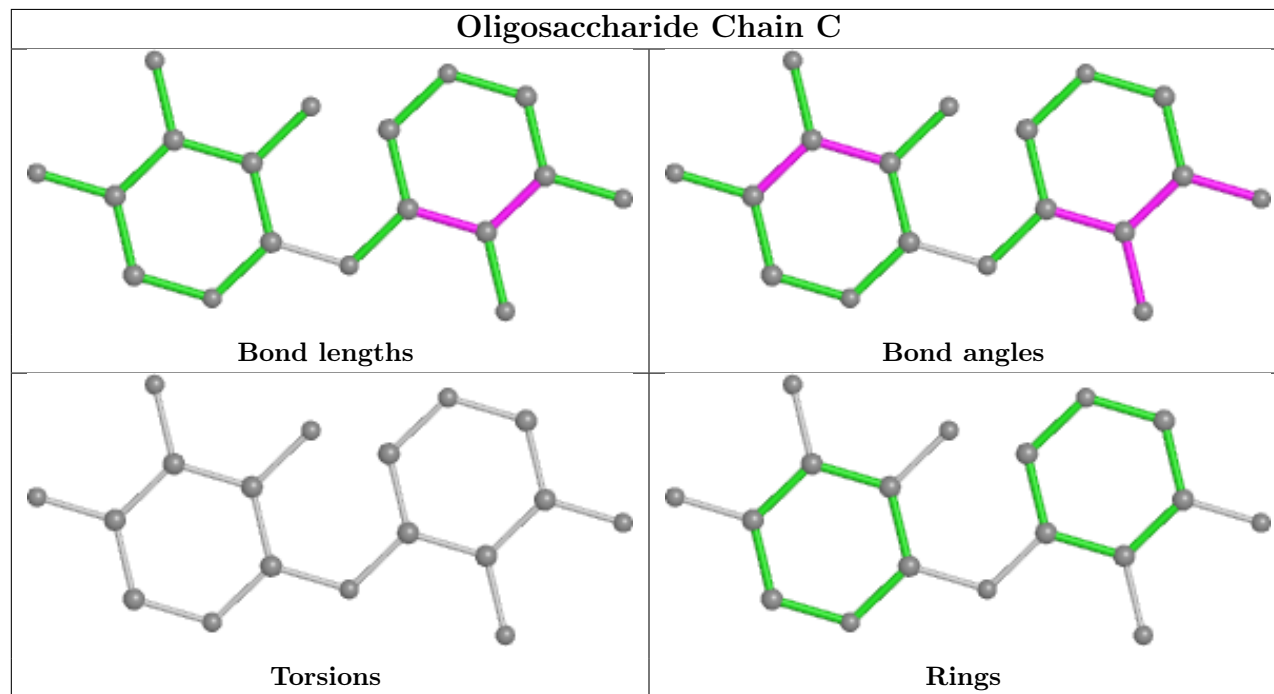
There are no torsion outliers.

There are no ring outliers.

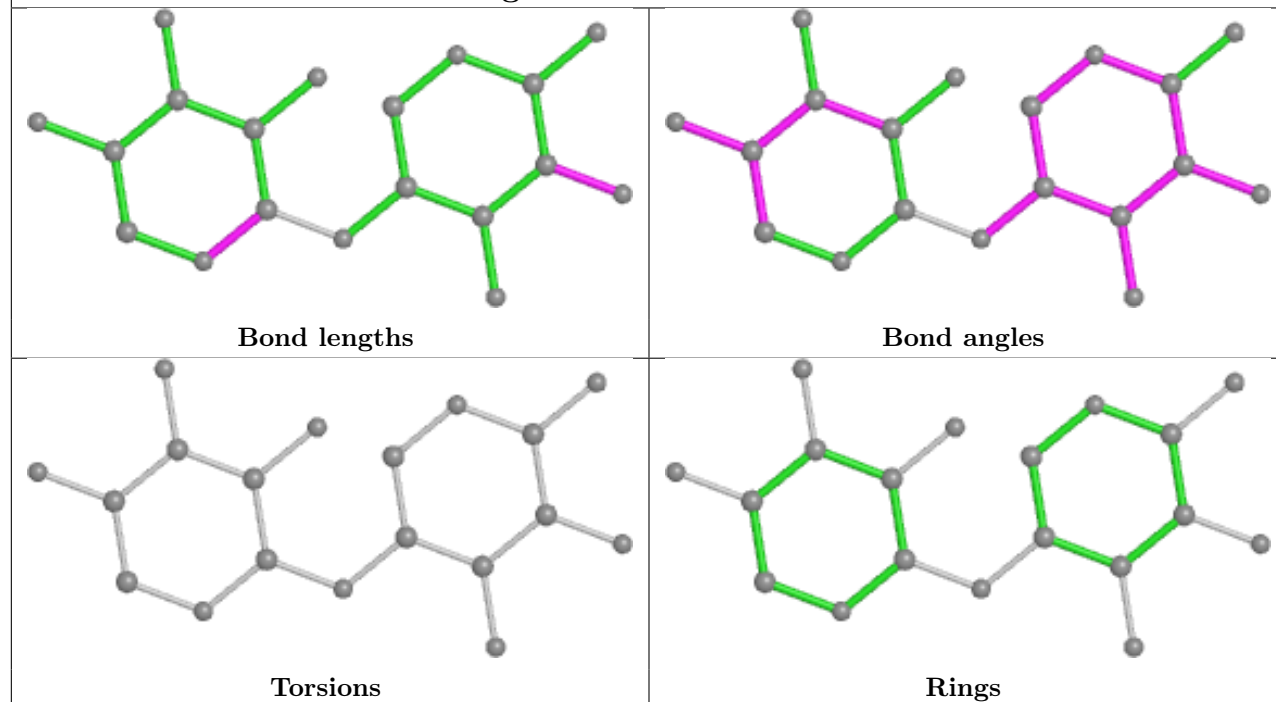
4 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	1	XYP	2	0
2	E	1	XYP	3	0
2	F	2	XYP	3	0
2	D	2	XYP	2	0

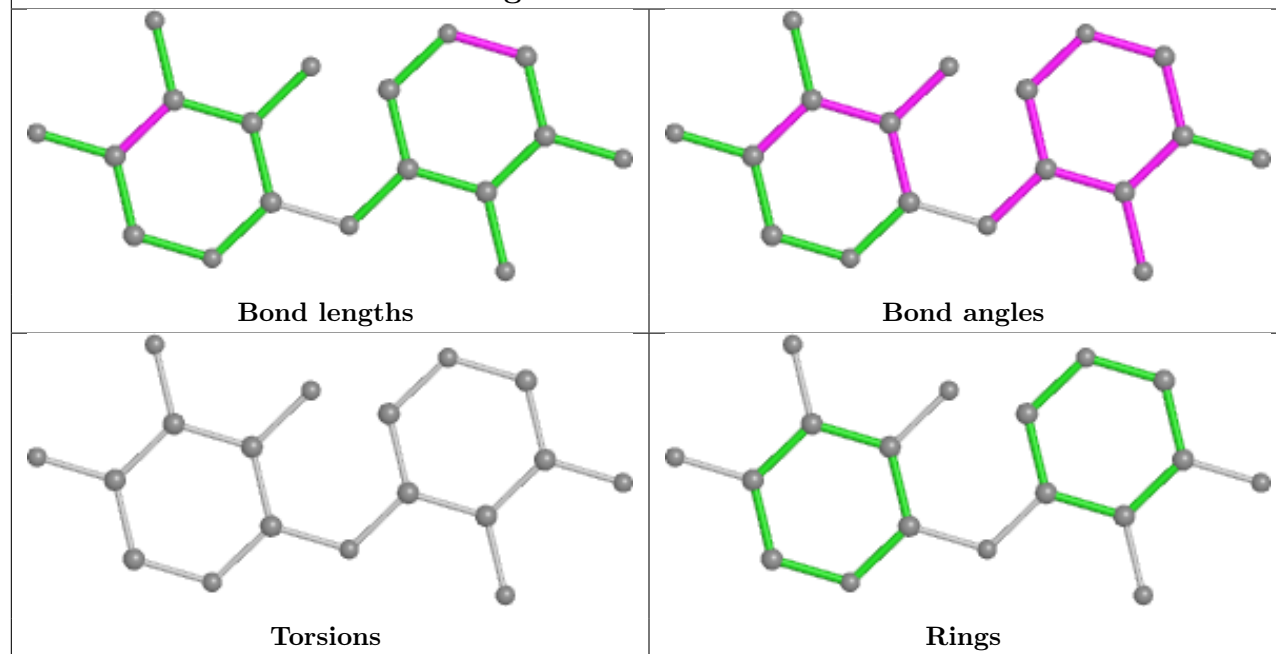
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

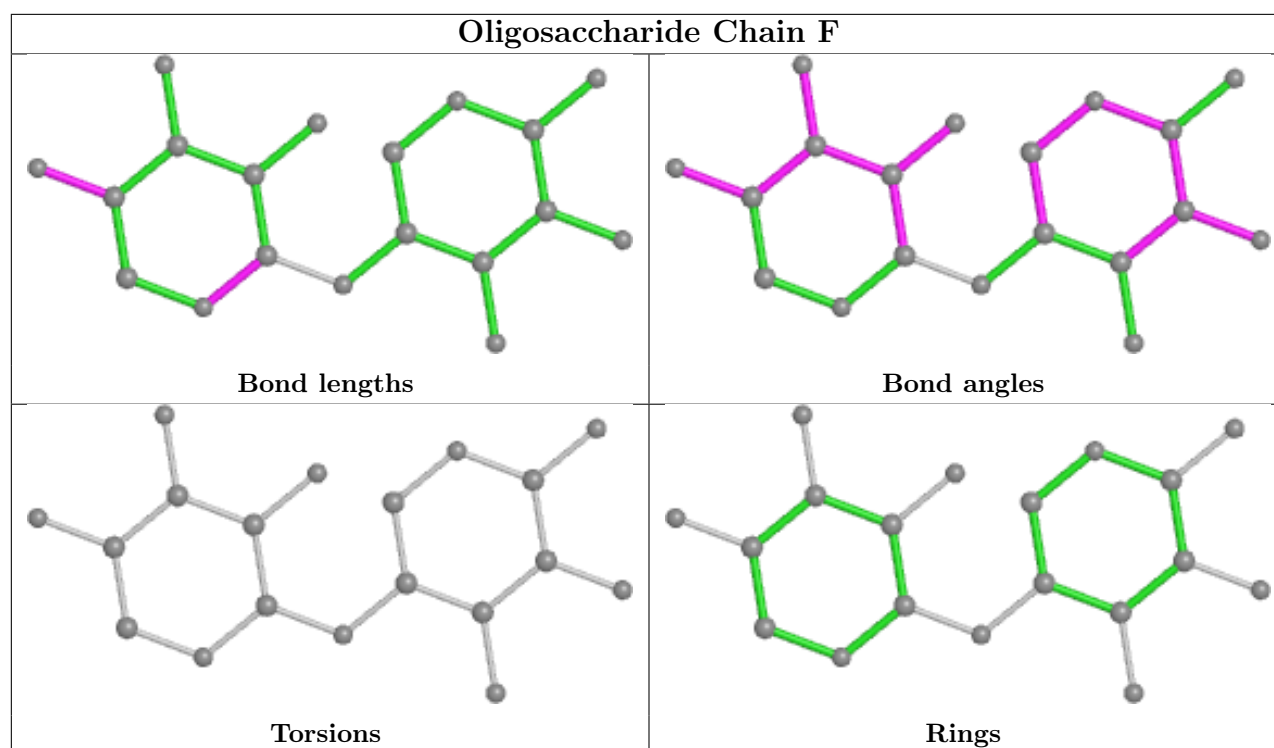


Oligosaccharide Chain D



Oligosaccharide Chain E





5.6 Ligand geometry [i](#)

8 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	PEG	A	509	-	6,6,6	0.65	0	5,5,5	1.24	1 (20%)
3	NAG	B	505	1	14,14,15	0.97	0	17,19,21	2.40	7 (41%)
4	GOL	A	506	-	5,5,5	0.45	0	5,5,5	1.20	0
6	PEG	B	507	-	6,6,6	0.46	0	5,5,5	1.16	0
6	PEG	A	508	-	6,6,6	1.64	1 (16%)	5,5,5	1.78	1 (20%)
3	NAG	A	505	1	14,14,15	2.27	3 (21%)	17,19,21	3.50	9 (52%)
4	GOL	B	506	-	5,5,5	0.82	0	5,5,5	2.55	2 (40%)
5	MES	A	507	-	12,12,12	1.28	2 (16%)	14,16,16	3.09	5 (35%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	PEG	A	509	-	-	3/4/4/4	-
3	NAG	B	505	1	-	0/6/23/26	0/1/1/1
4	GOL	A	506	-	-	2/4/4/4	-
6	PEG	B	507	-	-	2/4/4/4	-
6	PEG	A	508	-	-	1/4/4/4	-
3	NAG	A	505	1	-	0/6/23/26	0/1/1/1
4	GOL	B	506	-	-	2/4/4/4	-
5	MES	A	507	-	-	3/6/14/14	0/1/1/1

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	505	NAG	O5-C1	-6.91	1.32	1.43
6	A	508	PEG	O2-C3	2.96	1.54	1.42
5	A	507	MES	O2S-S	2.67	1.52	1.45
3	A	505	NAG	C1-C2	2.67	1.56	1.52
3	A	505	NAG	O5-C5	2.52	1.48	1.43
5	A	507	MES	O1S-S	2.13	1.51	1.45

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	507	MES	O1S-S-C8	-8.92	96.18	106.92
3	A	505	NAG	C1-O5-C5	7.20	121.95	112.19
3	B	505	NAG	C2-N2-C7	6.71	132.46	122.90
3	A	505	NAG	C2-N2-C7	5.69	131.01	122.90
3	A	505	NAG	O3-C3-C4	4.90	121.68	110.35
3	A	505	NAG	C8-C7-N2	4.75	124.15	116.10
4	B	506	GOL	O2-C2-C1	-4.66	88.59	109.12
5	A	507	MES	O1-C2-C3	-4.25	102.43	111.80
3	A	505	NAG	O7-C7-C8	-4.25	114.17	122.06
3	A	505	NAG	O3-C3-C2	-4.15	100.88	109.47
3	A	505	NAG	C3-C4-C5	4.08	117.51	110.24
5	A	507	MES	O2S-S-C8	3.39	111.00	106.92
6	A	508	PEG	O2-C3-C4	3.19	124.08	110.07
5	A	507	MES	O3S-S-C8	2.99	110.60	105.77
3	A	505	NAG	O6-C6-C5	-2.97	101.09	111.29
3	B	505	NAG	O7-C7-N2	-2.92	116.59	121.95

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	505	NAG	O5-C5-C6	-2.88	102.68	107.20
3	B	505	NAG	C6-C5-C4	2.84	119.66	113.00
5	A	507	MES	O3S-S-O1S	-2.74	104.57	111.27
6	A	509	PEG	O2-C3-C4	2.67	121.79	110.07
3	B	505	NAG	C3-C4-C5	-2.65	105.52	110.24
3	B	505	NAG	C1-C2-N2	2.48	114.73	110.49
3	A	505	NAG	C1-C2-N2	2.30	114.41	110.49
4	B	506	GOL	O2-C2-C3	-2.06	100.04	109.12
3	B	505	NAG	O4-C4-C5	-2.03	104.25	109.30

There are no chirality outliers.

All (13) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	506	GOL	C1-C2-C3-O3
5	A	507	MES	C7-C8-S-O3S
6	A	509	PEG	O2-C3-C4-O4
4	B	506	GOL	O1-C1-C2-C3
4	A	506	GOL	O2-C2-C3-O3
4	B	506	GOL	O1-C1-C2-O2
6	A	509	PEG	O1-C1-C2-O2
6	A	509	PEG	C1-C2-O2-C3
5	A	507	MES	C7-C8-S-O1S
5	A	507	MES	C7-C8-S-O2S
6	A	508	PEG	C4-C3-O2-C2
6	B	507	PEG	O1-C1-C2-O2
6	B	507	PEG	C1-C2-O2-C3

There are no ring outliers.

3 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	506	GOL	3	0
6	A	508	PEG	3	0
5	A	507	MES	1	0

5.7 Other polymers [i](#)

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 [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	319/319 (100%)	-0.46	1 (0%) 90 92	6, 11, 19, 37	10 (3%)
1	B	319/319 (100%)	-0.31	2 (0%) 85 88	5, 13, 21, 34	13 (4%)
All	All	638/638 (100%)	-0.38	3 (0%) 87 89	5, 12, 20, 37	23 (3%)

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	31[A]	SER	5.1
1	B	5	ALA	4.0
1	A	5	ALA	3.6

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.

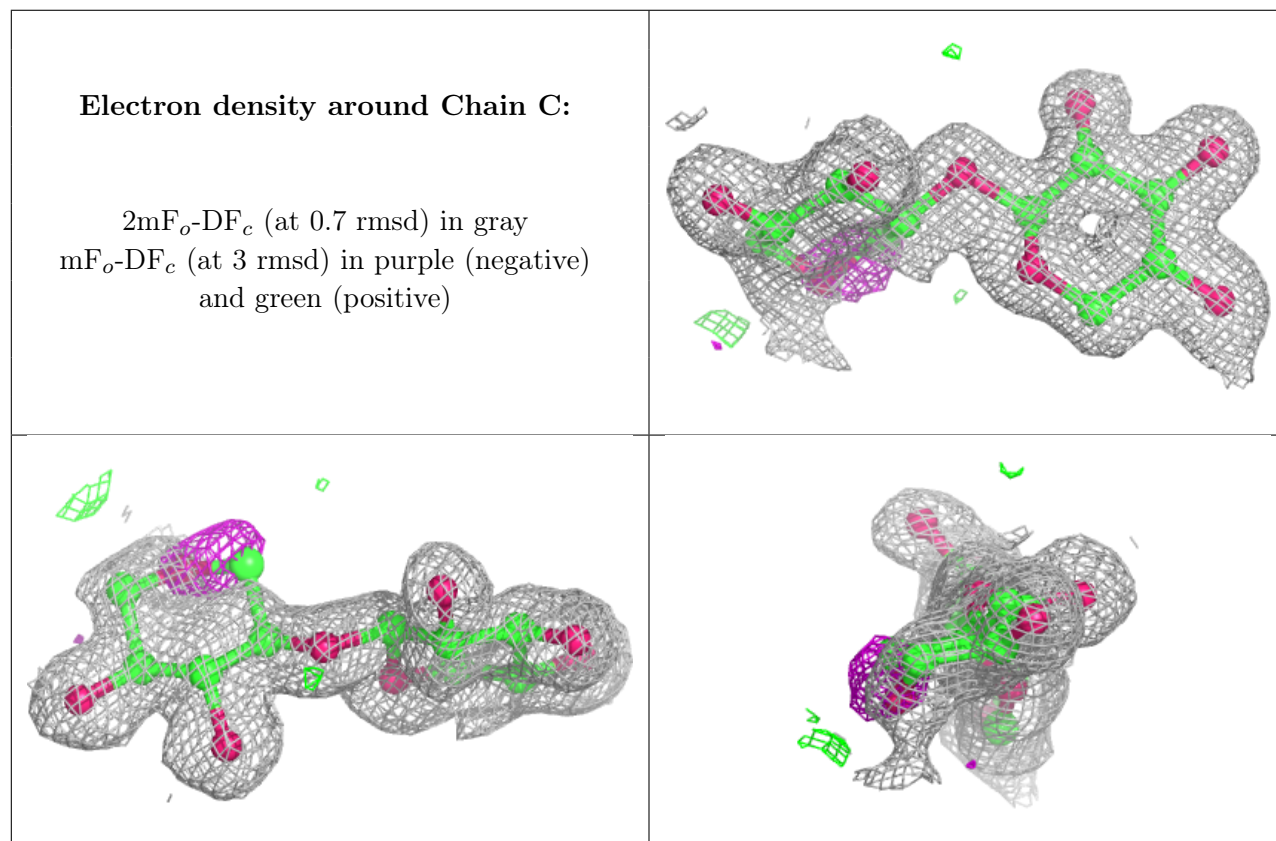
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	XYP	F	1	10/10	0.76	0.14	50,56,58,66	0
2	XYP	F	2	9/10	0.82	0.12	27,34,41,42	0
2	XYP	D	1	10/10	0.84	0.11	35,36,41,47	0
2	XYP	D	2	9/10	0.87	0.10	27,29,32,34	0
2	XYP	E	2	9/10	0.95	0.06	15,16,17,20	0
2	XYP	C	1	9/10	0.95	0.09	12,16,29,36	0

Continued on next page...

Continued from previous page...

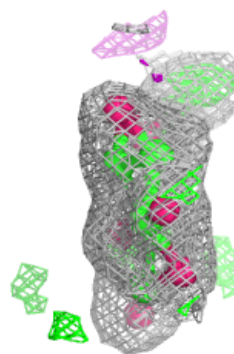
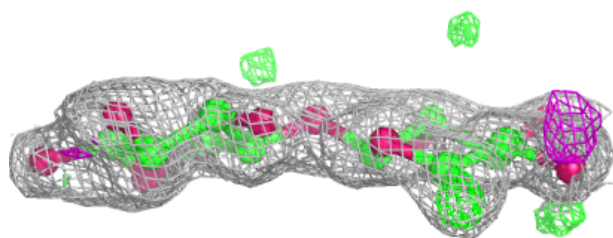
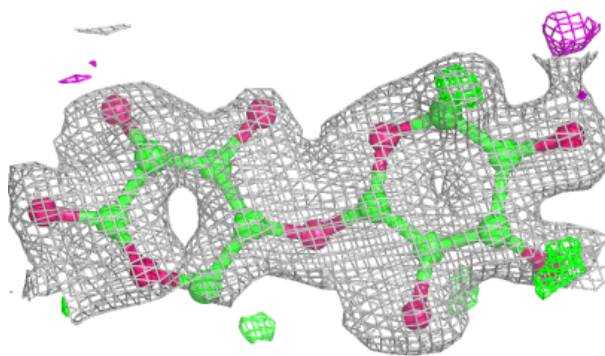
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	XYP	E	1	9/10	0.95	0.09	11,15,28,35	0
2	XYP	C	2	9/10	0.96	0.06	16,19,20,21	0

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.

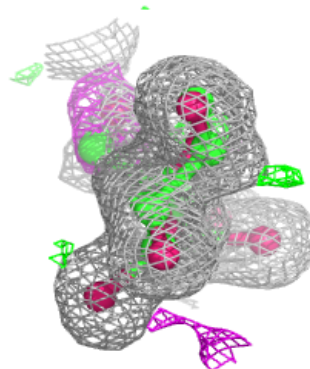
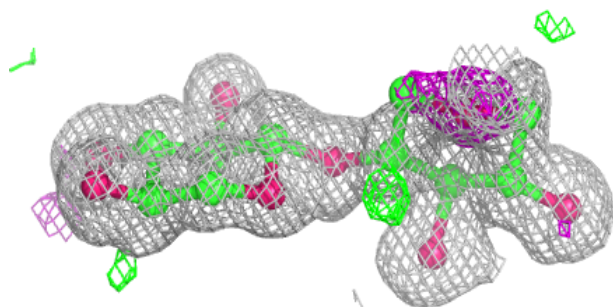
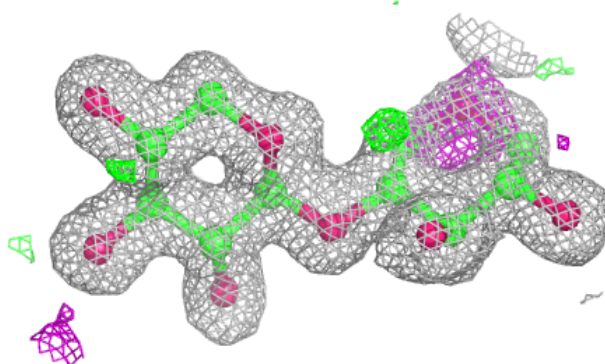


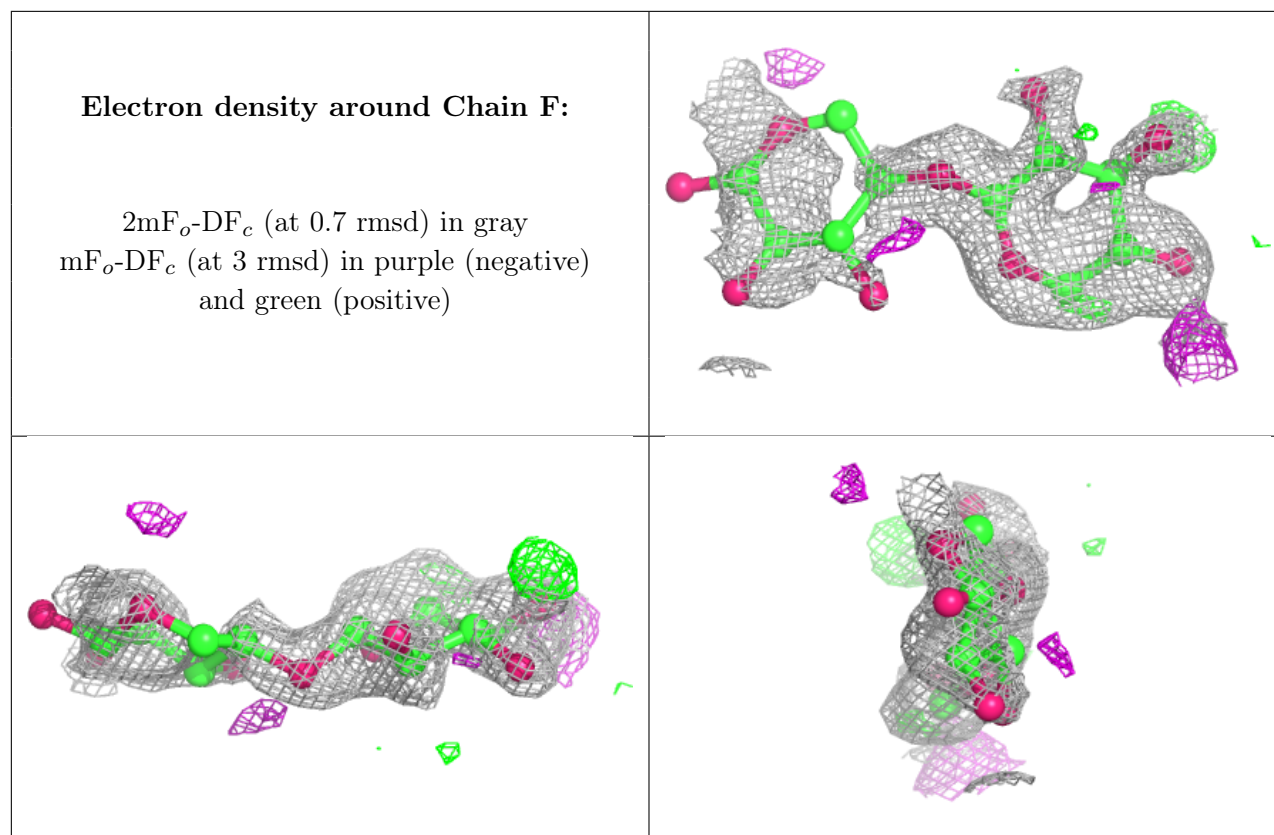
Electron density around Chain D:

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

**Electron density around Chain E:**

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





6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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(\AA^2)	Q<0.9
6	PEG	B	507	7/7	0.81	0.14	36,38,41,48	0
6	PEG	A	509	7/7	0.82	0.15	34,38,41,42	0
6	PEG	A	508	7/7	0.82	0.14	20,32,38,43	0
4	GOL	B	506	6/6	0.89	0.11	16,25,28,35	0
5	MES	A	507	12/12	0.90	0.12	20,26,29,30	0
4	GOL	A	506	6/6	0.91	0.12	20,33,35,38	0
3	NAG	B	505	14/15	0.91	0.10	18,22,30,33	0
3	NAG	A	505	14/15	0.92	0.09	16,21,30,37	0

6.5 Other polymers [i](#)

There are no such residues in this entry.