



wwPDB X-ray Structure Validation Summary Report ⓘ

Dec 4, 2023 – 10:30 am GMT

PDB ID : 2J25
Title : Partially deglycosylated glucoceramidase
Authors : Brumshtein, B.; Wormald, M.R.; Silman, I.; Futerman, A.H.; Sussman, J.L.
Deposited on : 2006-08-16
Resolution : 2.90 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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 : **FAILED**
Mogul : 1.8.4, CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.36
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) : 2.36

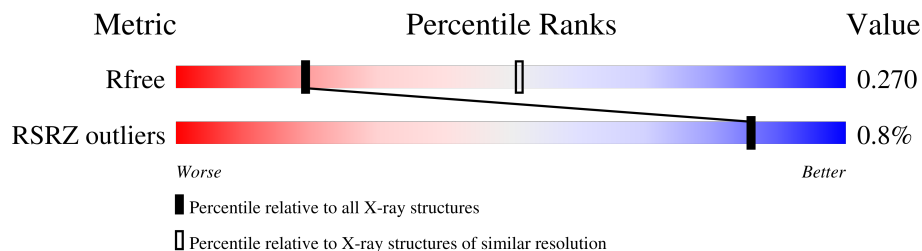
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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	1957 (2.90-2.90)
RSRZ outliers	127900	1906 (2.90-2.90)

MolProbity failed to run properly - the sequence quality summary graphics cannot be shown.

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	MAN	D	4	-	-	-	X
3	MAN	D	5	X	-	-	X
5	NAG	A	1500	X	-	-	-

2 Entry composition i

There are 7 unique types of molecules in this entry. The entry contains 8124 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 GLUCOSYLCERAMIDASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	497	3903	2512	669	706	16	0	0	0
1	B	497	3898	2509	669	704	16	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

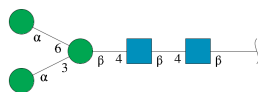
Chain	Residue	Modelled	Actual	Comment	Reference
A	495	HIS	ARG	conflict	UNP P04062
B	495	HIS	ARG	conflict	UNP P04062

- Molecule 2 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
			Total	C	N	O			
2	C	2	28	16	2	10	0	0	0
2	F	2	28	16	2	10	0	0	0

- Molecule 3 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



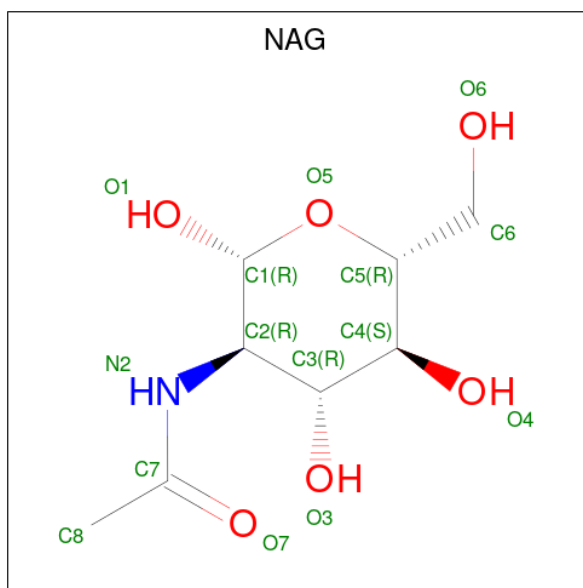
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
3	D	5	61	34	2	25	0	0	0

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



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
4	E	3	39	22	2	15	0	0	0

- Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



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

- Molecule 6 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	O	S	0	0
			5	4	1		
6	A	1	Total	O	S	0	0
			5	4	1		
6	A	1	Total	O	S	0	0
			5	4	1		
6	A	1	Total	O	S	0	0
			5	4	1		
6	A	1	Total	O	S	0	0
			5	4	1		
6	A	1	Total	O	S	0	0
			5	4	1		
6	A	1	Total	O	S	0	0
			5	4	1		
6	A	1	Total	O	S	0	0
			5	4	1		
6	B	1	Total	O	S	0	0
			5	4	1		
6	B	1	Total	O	S	0	0
			5	4	1		
6	B	1	Total	O	S	0	0
			5	4	1		
6	B	1	Total	O	S	0	0
			5	4	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	B	1	Total	O	S	0	0
			5	4	1		
6	B	1	Total	O	S	0	0
			5	4	1		
6	B	1	Total	O	S	0	0
			5	4	1		

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	37	Total	O	0	0
			37	37		
7	B	31	Total	O	0	0
			31	31		

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3 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	108.63Å 280.82Å 91.06Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.67 – 2.90 29.67 – 2.90	Depositor EDS
% Data completeness (in resolution range)	100.0 (29.67-2.90) 100.0 (29.67-2.90)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.37 (at 2.90Å)	Xtrriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.215 , 0.273 0.215 , 0.270	Depositor DCC
R_{free} test set	1539 reflections (4.91%)	wwPDB-VP
Wilson B-factor (Å ²)	37.0	Xtrriage
Anisotropy	0.218	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 28.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	8124	wwPDB-VP
Average B, all atoms (Å ²)	33.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.79% 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.

4 Model quality [i](#)

4.1 Standard geometry [i](#)

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4.2 Too-close contacts [i](#)

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4.3 Torsion angles [i](#)

4.3.1 Protein backbone [i](#)

MolProbity failed to run properly - this section is therefore empty.

4.3.2 Protein sidechains [i](#)

MolProbity failed to run properly - this section is therefore empty.

4.3.3 RNA [i](#)

MolProbity failed to run properly - this section is therefore empty.

4.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

4.5 Carbohydrates [i](#)

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	NAG	C	1	2,1	14,14,15	0.60	0	17,19,21	1.55	3 (17%)
2	NAG	C	2	2	14,14,15	0.61	0	17,19,21	1.35	2 (11%)
3	NAG	D	1	3,1	14,14,15	0.62	0	17,19,21	1.14	2 (11%)
3	NAG	D	2	3	14,14,15	0.65	0	17,19,21	2.65	6 (35%)
3	BMA	D	3	3	11,11,12	1.63	1 (9%)	15,15,17	1.79	1 (6%)
3	MAN	D	4	3	11,11,12	1.42	1 (9%)	15,15,17	1.14	1 (6%)
3	MAN	D	5	3	11,11,12	7.00	3 (27%)	15,15,17	1.85	4 (26%)
4	NAG	E	1	1,4	14,14,15	0.62	0	17,19,21	1.58	5 (29%)
4	NAG	E	2	4	14,14,15	0.77	0	17,19,21	2.27	5 (29%)
4	BMA	E	3	4	11,11,12	2.91	3 (27%)	15,15,17	2.63	3 (20%)
2	NAG	F	1	2,1	14,14,15	0.49	0	17,19,21	1.44	2 (11%)
2	NAG	F	2	2	14,14,15	0.57	0	17,19,21	1.76	4 (23%)

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

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

The worst 5 of 8 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	5	MAN	O2-C2	19.15	1.83	1.43
3	D	5	MAN	C1-C2	12.29	1.80	1.52
4	E	3	BMA	O2-C2	6.11	1.56	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	E	3	BMA	O5-C1	5.31	1.52	1.43
3	D	3	BMA	O6-C6	4.92	1.63	1.42

The worst 5 of 38 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	2	NAG	C1-O5-C5	8.11	123.19	112.19
4	E	3	BMA	C1-C2-C3	6.75	117.97	109.67
4	E	3	BMA	C1-O5-C5	6.44	120.91	112.19
3	D	3	BMA	C1-O5-C5	-6.29	103.67	112.19
4	E	2	NAG	O5-C1-C2	-5.83	102.08	111.29

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	D	5	MAN	C1

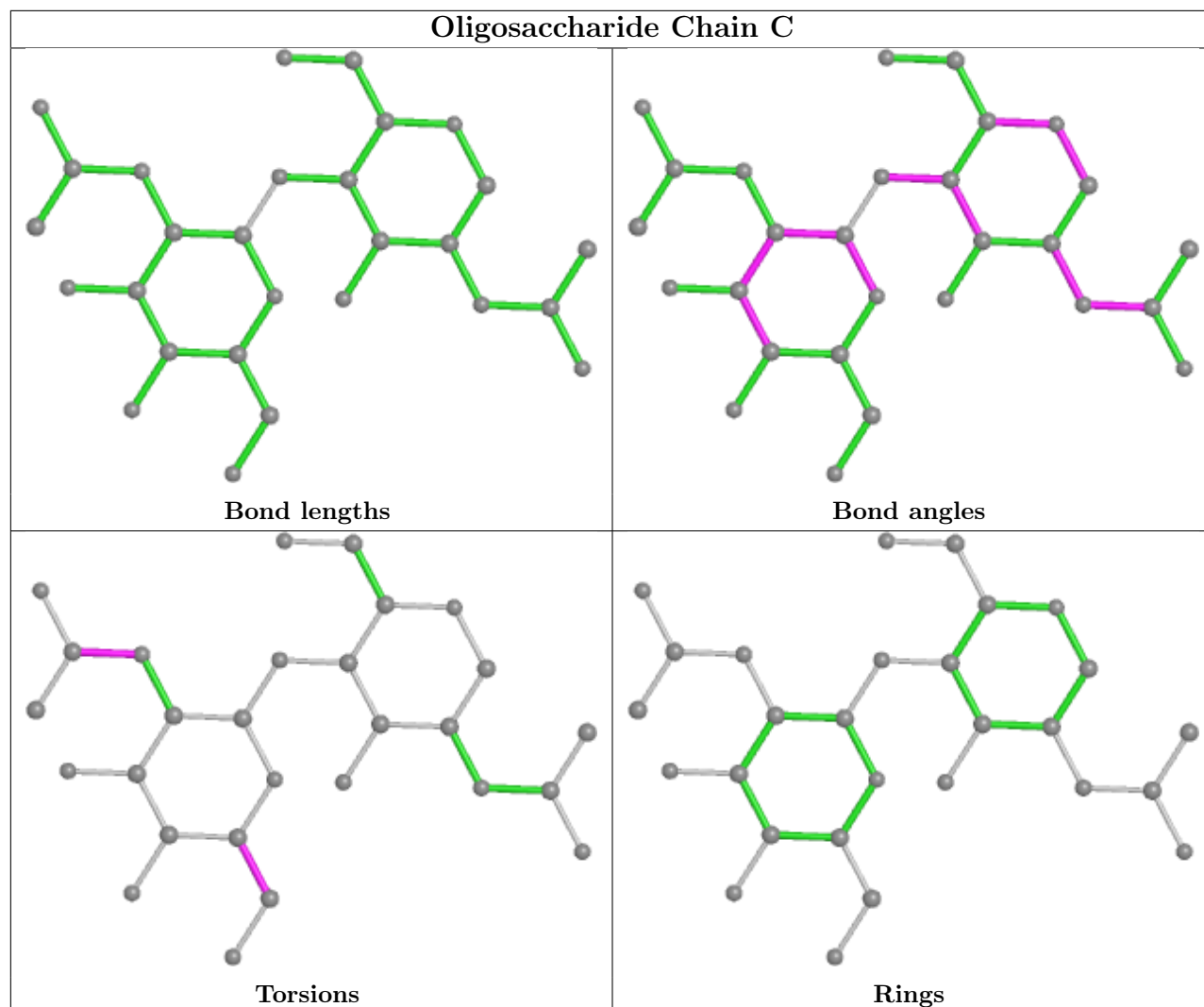
5 of 16 torsion outliers are listed below:

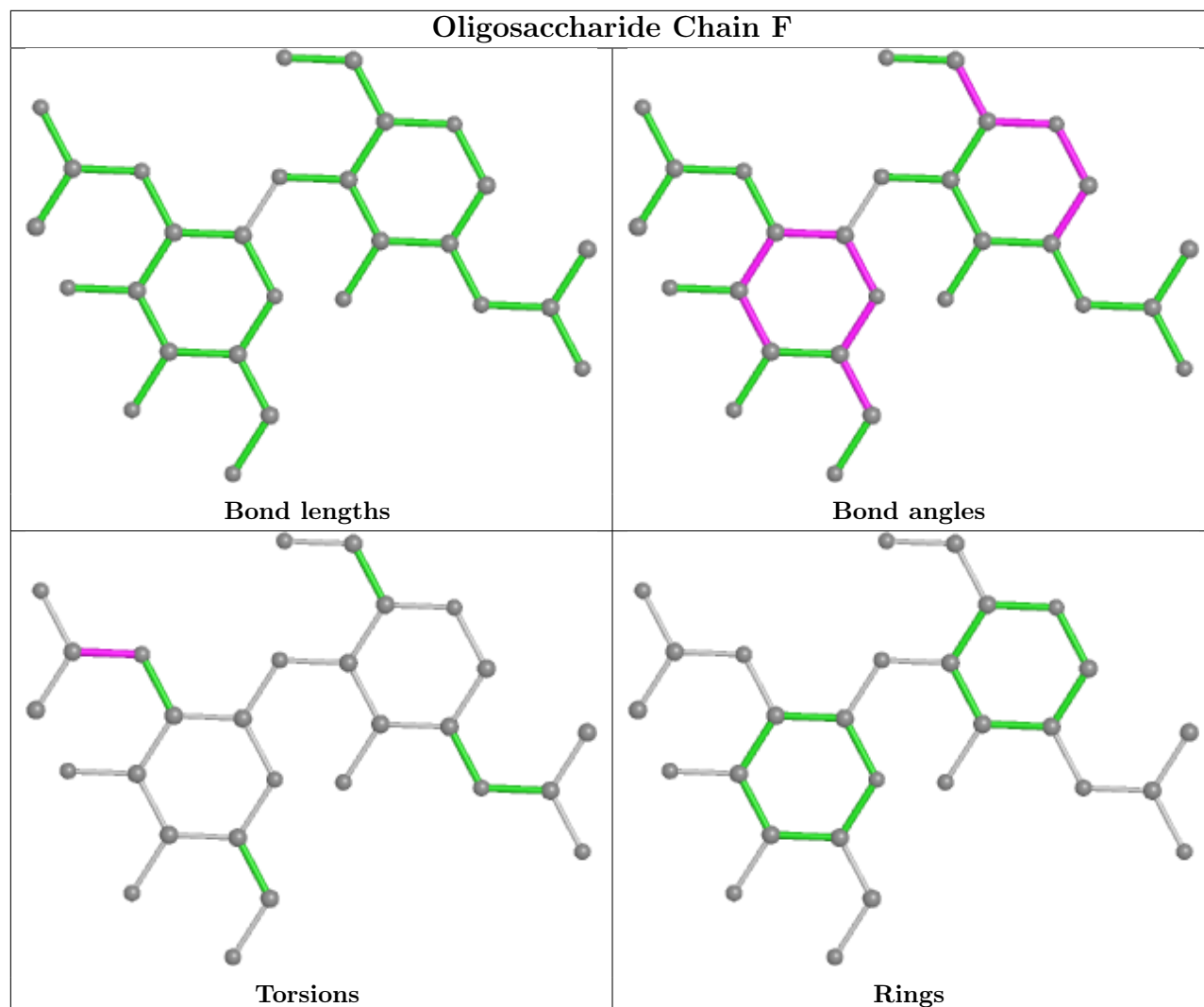
Mol	Chain	Res	Type	Atoms
4	E	2	NAG	C8-C7-N2-C2
4	E	2	NAG	O7-C7-N2-C2
2	C	2	NAG	C8-C7-N2-C2
3	D	5	MAN	O5-C5-C6-O6
2	C	2	NAG	O7-C7-N2-C2

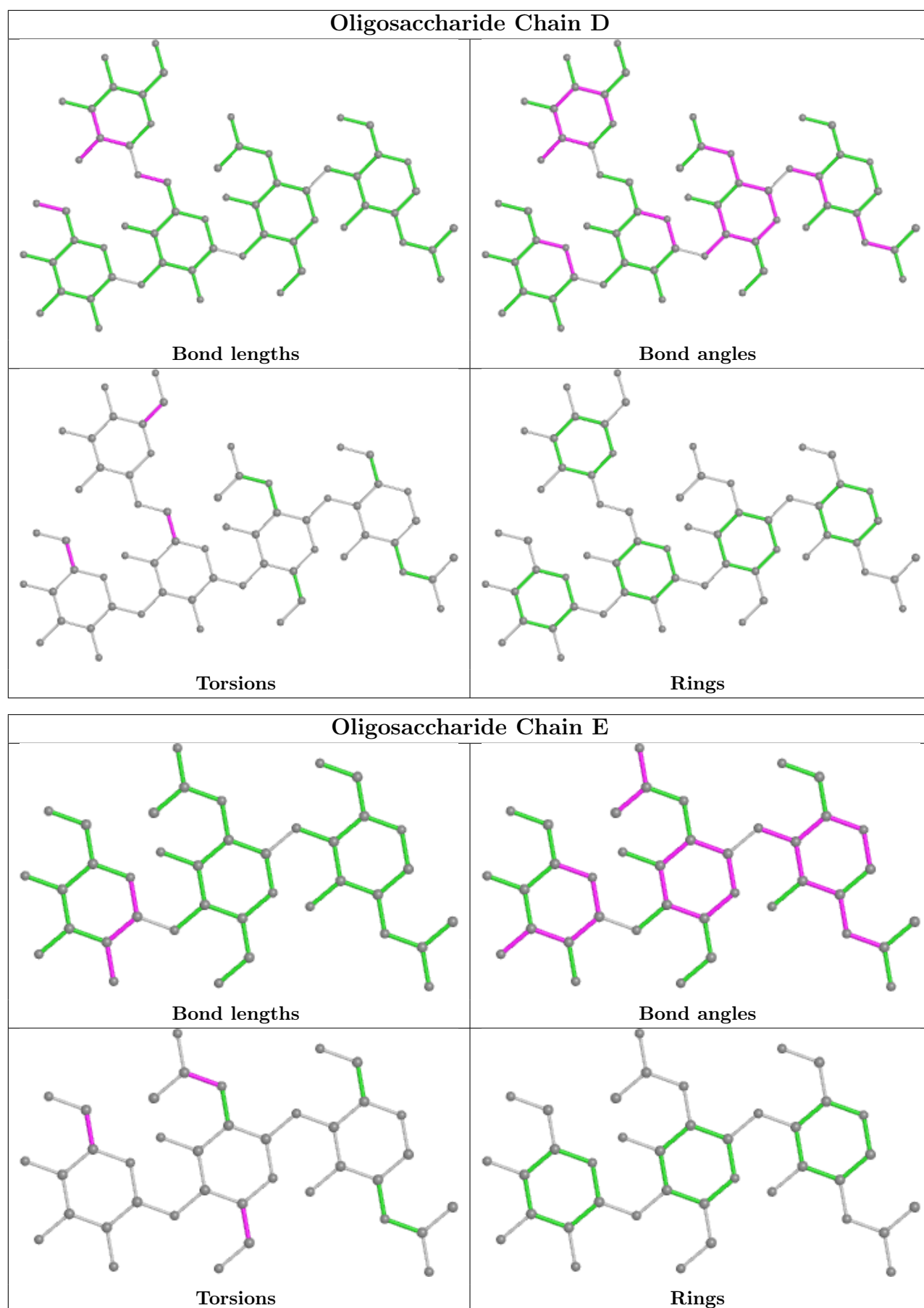
There are no ring outliers.

No monomer is involved in short contacts.

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







4.6 Ligand geometry

18 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	SO4	A	1501	-	4,4,4	0.12	0	6,6,6	0.47	0
6	SO4	A	1502	-	4,4,4	0.18	0	6,6,6	0.38	0
6	SO4	B	1510	-	4,4,4	0.17	0	6,6,6	0.26	0
6	SO4	B	1509	-	4,4,4	0.15	0	6,6,6	0.19	0
6	SO4	B	1512	-	4,4,4	0.24	0	6,6,6	0.44	0
6	SO4	A	1509	-	4,4,4	0.20	0	6,6,6	0.33	0
6	SO4	A	1503	-	4,4,4	0.20	0	6,6,6	0.33	0
6	SO4	B	1511	-	4,4,4	0.10	0	6,6,6	0.61	0
6	SO4	A	1505	-	4,4,4	0.09	0	6,6,6	0.60	0
6	SO4	A	1506	-	4,4,4	0.19	0	6,6,6	0.44	0
6	SO4	A	1507	-	4,4,4	0.11	0	6,6,6	0.31	0
6	SO4	B	1514	-	4,4,4	0.19	0	6,6,6	0.19	0
6	SO4	B	1515	-	4,4,4	0.18	0	6,6,6	0.17	0
6	SO4	B	1513	-	4,4,4	0.21	0	6,6,6	0.38	0
5	NAG	A	1500	1	14,14,15	2.10	3 (21%)	17,19,21	3.13	8 (47%)
6	SO4	A	1508	-	4,4,4	0.24	0	6,6,6	0.34	0
6	SO4	B	1508	-	4,4,4	0.22	0	6,6,6	0.43	0
6	SO4	A	1504	-	4,4,4	0.21	0	6,6,6	0.55	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	NAG	A	1500	1	1/1/5/7	3/6/23/26	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	1500	NAG	C1-C2	4.74	1.59	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	1500	NAG	O4-C4	3.68	1.51	1.43
5	A	1500	NAG	C4-C3	3.36	1.60	1.52

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	1500	NAG	C1-O5-C5	6.70	121.27	112.19
5	A	1500	NAG	C4-C3-C2	-6.00	102.23	111.02
5	A	1500	NAG	C2-N2-C7	5.07	130.12	122.90
5	A	1500	NAG	C3-C4-C5	-4.13	102.86	110.24
5	A	1500	NAG	O4-C4-C5	3.66	118.39	109.30

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
5	A	1500	NAG	C1

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	1500	NAG	C3-C2-N2-C7
5	A	1500	NAG	C4-C5-C6-O6
5	A	1500	NAG	O5-C5-C6-O6

There are no ring outliers.

No monomer is involved in short contacts.

4.7 Other polymers [i](#)

There are no such residues in this entry.

4.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

5 Fit of model and data [i](#)

5.1 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	497/497 (100%)	-0.14	2 (0%) 92 93	19, 32, 48, 61	0
1	B	497/497 (100%)	-0.21	6 (1%) 79 79	19, 32, 49, 63	0
All	All	994/994 (100%)	-0.17	8 (0%) 86 86	19, 32, 49, 63	0

The worst 5 of 8 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	140	ASP	3.9
1	B	274	HIS	2.4
1	B	63	THR	2.4
1	B	329	ARG	2.3
1	B	318	ALA	2.3

5.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.3 Carbohydrates [i](#)

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

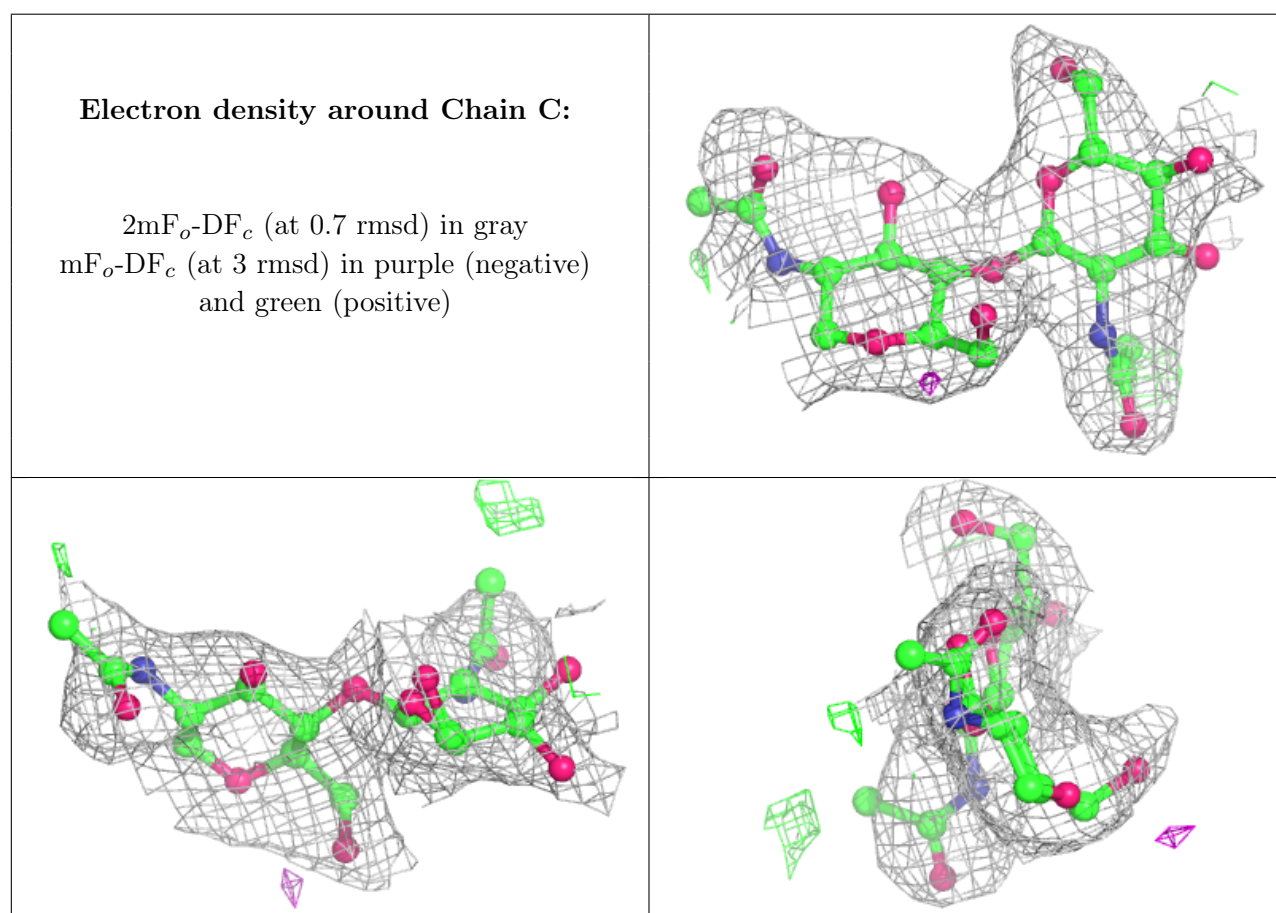
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	MAN	D	4	11/12	0.55	0.43	89,90,90,90	0
3	MAN	D	5	11/12	0.67	0.49	90,90,91,91	0
4	BMA	E	3	11/12	0.70	0.24	65,68,68,69	0
2	NAG	F	2	14/15	0.81	0.29	62,64,65,65	0
3	NAG	D	2	14/15	0.83	0.27	67,68,72,77	0

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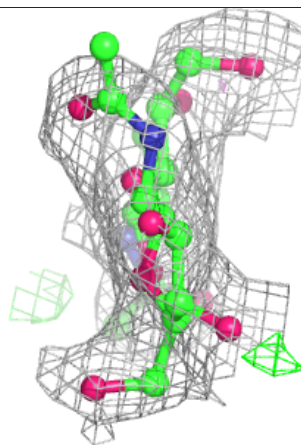
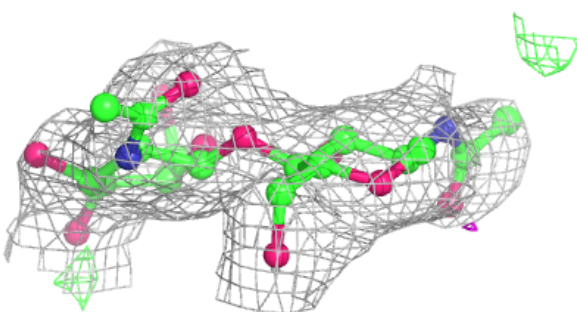
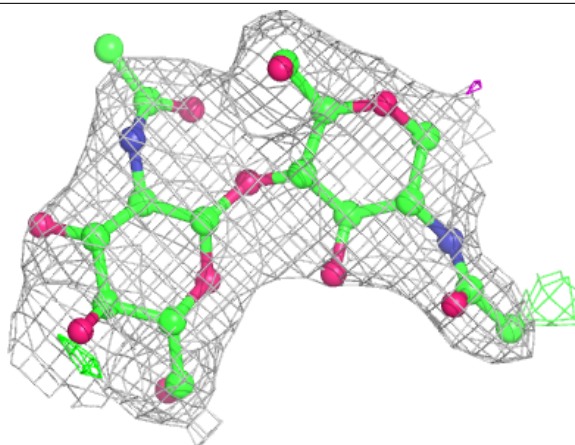
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	NAG	C	2	14/15	0.84	0.28	59,62,64,64	0
3	BMA	D	3	11/12	0.85	0.33	82,85,87,88	0
2	NAG	F	1	14/15	0.86	0.22	55,58,60,62	0
2	NAG	C	1	14/15	0.87	0.19	54,58,60,62	0
4	NAG	E	2	14/15	0.88	0.38	66,68,69,69	0
3	NAG	D	1	14/15	0.91	0.22	54,58,60,63	0
4	NAG	E	1	14/15	0.91	0.29	55,58,60,63	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.



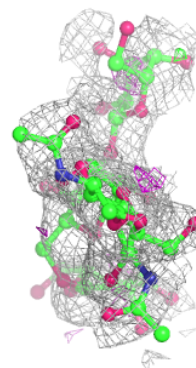
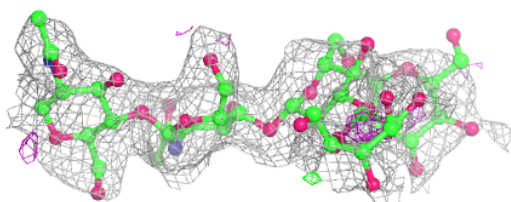
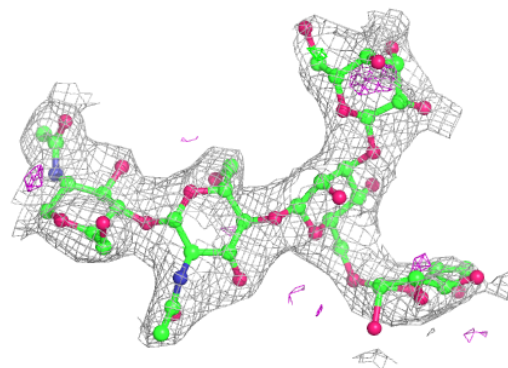
Electron density around Chain F:

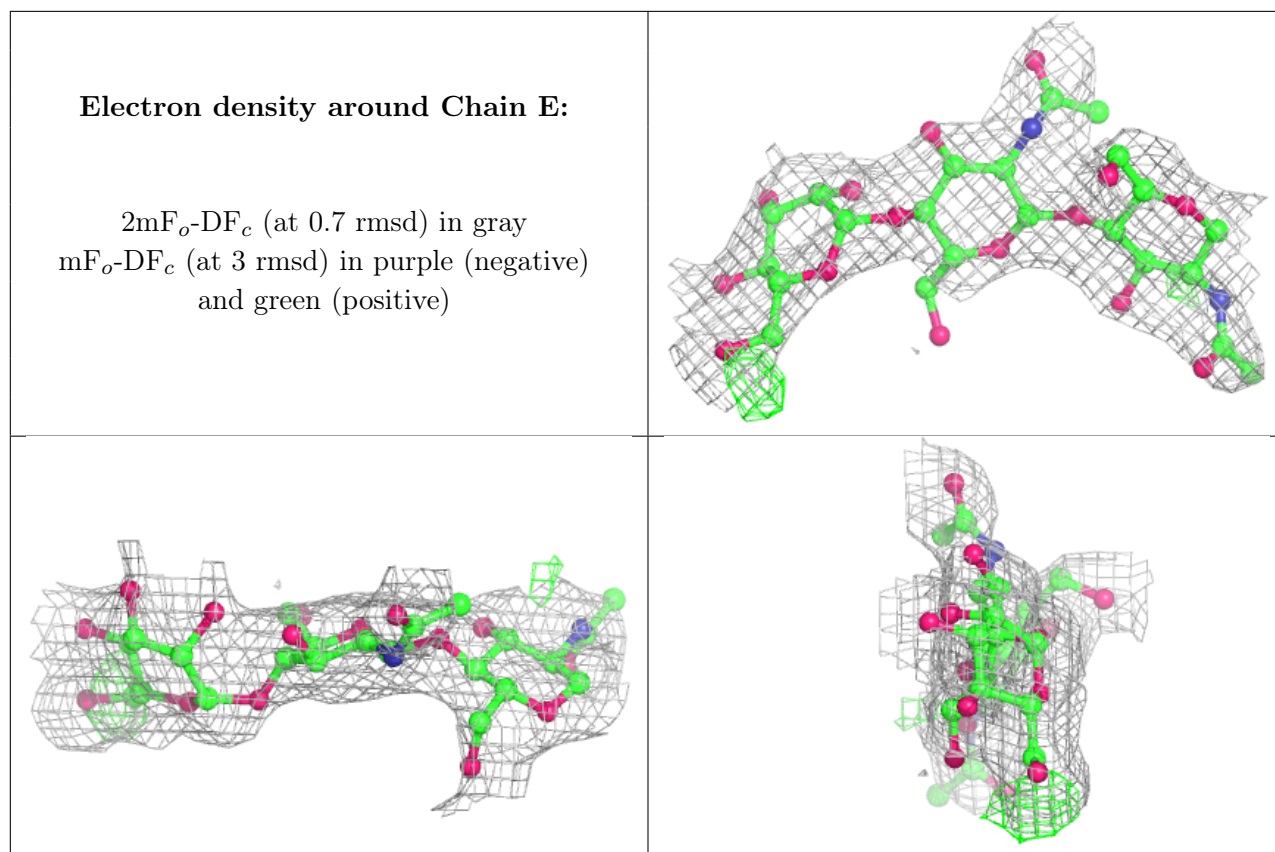
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around Chain D:

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





5.4 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
5	NAG	A	1500	14/15	0.59	0.38	55,58,60,62	0
6	SO4	A	1509	5/5	0.84	0.24	88,88,88,88	0
6	SO4	A	1508	5/5	0.85	0.17	89,89,90,90	0
6	SO4	A	1507	5/5	0.89	0.36	76,76,77,77	0
6	SO4	B	1513	5/5	0.93	0.42	55,55,55,55	0
6	SO4	B	1514	5/5	0.93	0.27	69,69,69,69	0
6	SO4	A	1506	5/5	0.94	0.20	57,57,58,58	0
6	SO4	B	1510	5/5	0.94	0.18	60,60,61,61	0
6	SO4	A	1505	5/5	0.95	0.22	64,65,65,65	0
6	SO4	B	1509	5/5	0.96	0.20	63,64,64,64	0
6	SO4	A	1503	5/5	0.96	0.28	55,56,56,56	0
6	SO4	B	1515	5/5	0.96	0.34	75,75,75,75	0
6	SO4	A	1504	5/5	0.97	0.22	51,51,52,53	0
6	SO4	B	1508	5/5	0.97	0.12	48,49,49,49	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
6	SO4	B	1512	5/5	0.97	0.15	44,44,44,45	0
6	SO4	A	1501	5/5	0.98	0.14	35,36,36,36	0
6	SO4	A	1502	5/5	0.98	0.10	47,47,48,49	0
6	SO4	B	1511	5/5	0.99	0.07	36,37,38,38	0

5.5 Other polymers [i](#)

There are no such residues in this entry.