



# wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 9, 2020 – 10:26 AM BST

PDB ID : 4MZE  
Title : Crystal structure of hPIV3 hemagglutinin-neuraminidase, H552Q/Q559R mutant  
Authors : Xu, R.; Wilson, I.A.  
Deposited on : 2013-09-30  
Resolution : 1.80 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](mailto: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.

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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 : 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

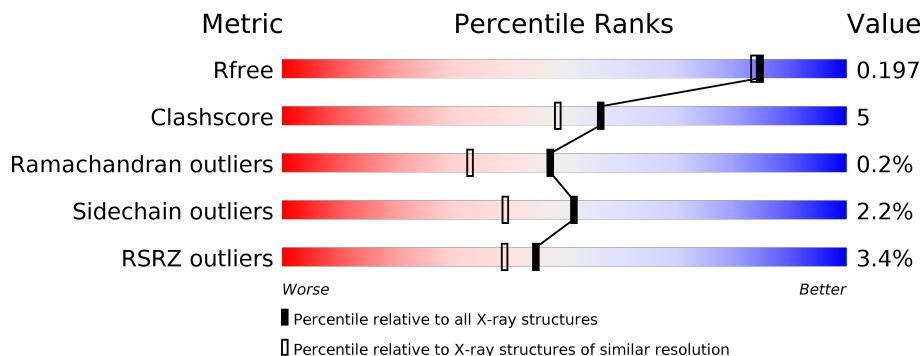
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.80 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	5950 (1.80-1.80)
Clashscore	141614	6793 (1.80-1.80)
Ramachandran outliers	138981	6697 (1.80-1.80)
Sidechain outliers	138945	6696 (1.80-1.80)
RSRZ outliers	127900	5850 (1.80-1.80)

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  $\geq 3$ , 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	437	<p>4% 89% 9%</p>
1	B	437	<p>3% 89% 9%</p>
2	C	8	<p>13% 88%</p>
3	D	2	<p>100%</p>
4	E	5	<p>40% 60%</p>
5	F	3	<p>33% 67%</p>

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:

<b>Mol</b>	<b>Type</b>	<b>Chain</b>	<b>Res</b>	<b>Chirality</b>	<b>Geometry</b>	<b>Clashes</b>	<b>Electron density</b>
10	PEG	A	622	-	X	X	-
10	PEG	A	623	-	-	X	-
10	PEG	B	621	-	X	X	-

## 2 Entry composition i

There are 12 unique types of molecules in this entry. The entry contains 7803 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.

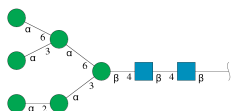
- Molecule 1 is a protein called Hemagglutinin-neuraminidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	432	Total 3409	C 2155	N 586	O 647	S 21	0	6	0
1	B	432	Total 3395	C 2145	N 586	O 644	S 20	0	2	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	552	GLN	HIS	engineered mutation	UNP P08492
A	559	ARG	GLN	engineered mutation	UNP P08492
B	552	GLN	HIS	engineered mutation	UNP P08492
B	559	ARG	GLN	engineered mutation	UNP P08492

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



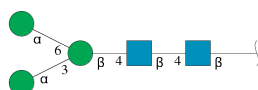
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
2	C	8	Total 94	C 52	N 2	O 40	0	0	0

- Molecule 3 is an oligosaccharide called beta-L-fucopyranose-(1-6)-2-acetamido-2-deoxy-beta-D-glucopyranose.



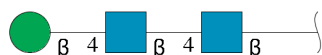
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
3	D	2	24	14	1	9	0	0	0

- Molecule 4 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			
4	E	5	61	34	2	25	0	0	0

- Molecule 5 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.



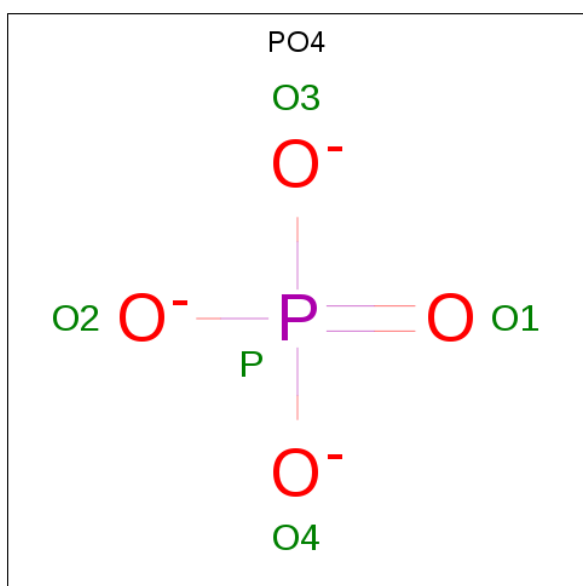
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
5	F	3	39	22	2	15	0	0	0

- Molecule 6 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: C<sub>8</sub>H<sub>15</sub>NO<sub>6</sub>).



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

- Molecule 7 is PHOSPHATE ION (three-letter code: PO4) (formula:  $O_4P$ ).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf	
			Total	O			P
7	A	1	5	4	1	0	0
7	B	1	10	8	2	0	1

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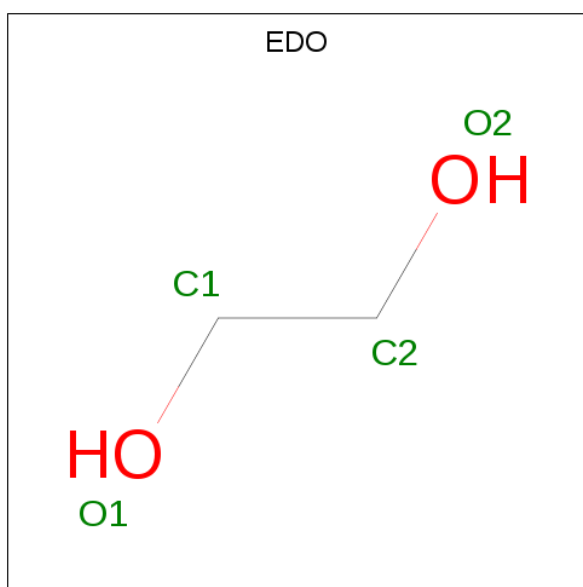
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	B	1	Total	O	P	0	0
			5	4	1		

- Molecule 8 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	B	1	Total	Ca	0	0
			1	1		
8	A	1	Total	Ca	0	0
			1	1		

- Molecule 9 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C<sub>2</sub>H<sub>6</sub>O<sub>2</sub>).



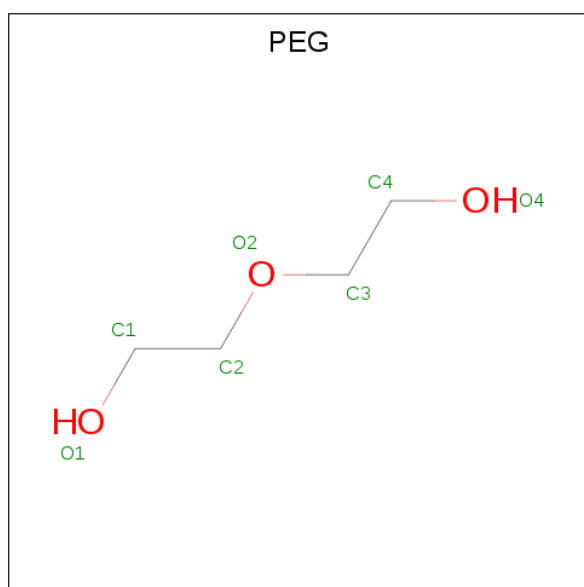
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	A	1	Total	C	O	0	0
			4	2	2		
9	A	1	Total	C	O	0	0
			4	2	2		
9	A	1	Total	C	O	0	0
			4	2	2		
9	A	1	Total	C	O	0	0
			4	2	2		
9	A	1	Total	C	O	0	0
			4	2	2		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	A	1	Total	C	O	0	0
			4	2	2		
9	A	1	Total	C	O	0	0
			4	2	2		
9	B	1	Total	C	O	0	0
			4	2	2		
9	B	1	Total	C	O	0	0
			4	2	2		
9	B	1	Total	C	O	0	0
			4	2	2		
9	B	1	Total	C	O	0	0
			4	2	2		
9	B	1	Total	C	O	0	0
			4	2	2		

- Molecule 10 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: C<sub>4</sub>H<sub>10</sub>O<sub>3</sub>).



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

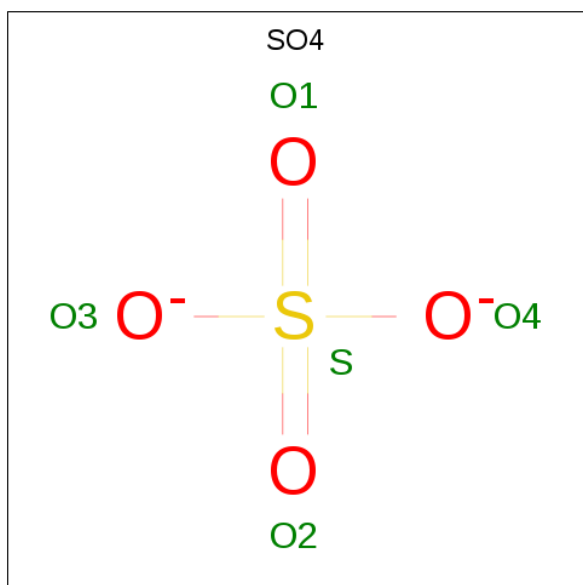
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
10	B	1	Total	C	O	0	0
			7	4	3		
10	B	1	Total	C	O	0	0
			7	4	3		

- Molecule 11 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



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

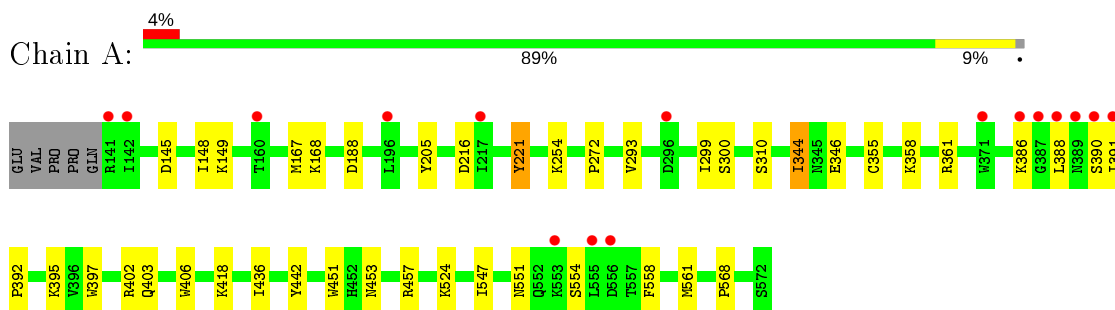
- Molecule 12 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
12	A	336	Total	O	0	0
			336	336		
12	B	302	Total	O	0	0
			302	302		

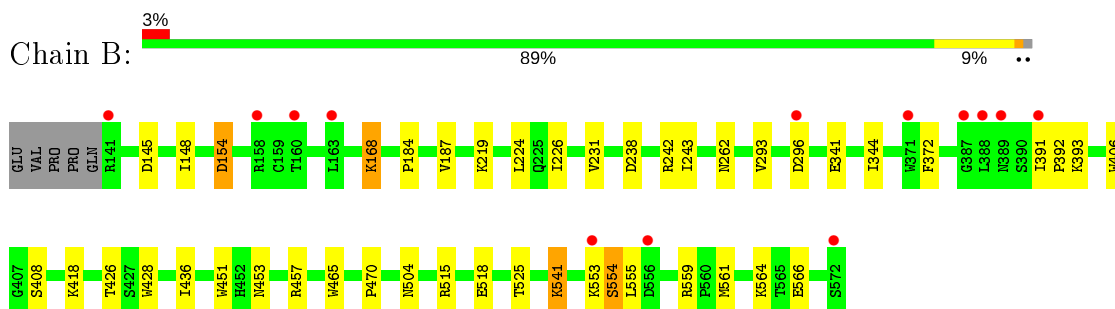
### 3 Residue-property plots [i](#)

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: Hemagglutinin-neuraminidase



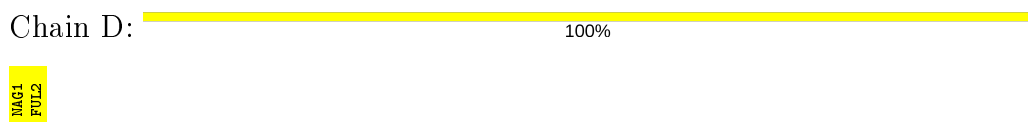
- Molecule 1: Hemagglutinin-neuraminidase



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



- Molecule 3: beta-L-fucopyranose-(1-6)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 4: 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

Chain E:  40% 60%

MAC1  
MAC2  
BMA3  
MAN4  
MAN5

- Molecule 5: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain F:  33% 67%

MAC1  
MAC2  
BMA3

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	84.03Å 96.64Å 105.34Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	28.92 – 1.80 28.92 – 1.80	Depositor EDS
% Data completeness (in resolution range)	99.8 (28.92-1.80) 99.6 (28.92-1.80)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.85 (at 1.80Å)	Xtrriage
Refinement program	PHENIX 1.8.2_1309	Depositor
R, $R_{free}$	0.161 , 0.196 0.162 , 0.197	Depositor DCC
$R_{free}$ test set	4011 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	26.8	Xtrriage
Anisotropy	0.115	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 47.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	7803	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	29.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.88% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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 [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: BMA, NAG, PO4, EDO, SO4, FUL, PEG, CA, MAN

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	0.68	0/3507	0.75	0/4775
1	B	0.67	0/3481	0.76	1/4741 (0.0%)
All	All	0.67	0/6988	0.75	1/9516 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	561	MET	CG-SD-CE	-5.63	91.19	100.20

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	3409	0	3390	33	0
1	B	3395	0	3366	30	0
2	C	94	0	79	0	0
3	D	24	0	22	0	0
4	E	61	0	52	0	0
5	F	39	0	34	0	0
6	A	14	0	13	0	0
6	B	14	0	13	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	A	5	0	0	0	0
7	B	15	0	0	2	0
8	A	1	0	0	0	0
8	B	1	0	0	0	0
9	A	32	0	48	10	0
9	B	28	0	42	3	0
10	A	14	0	20	9	0
10	B	14	0	20	8	0
11	A	5	0	0	0	0
12	A	336	0	0	5	0
12	B	302	0	0	4	0
All	All	7803	0	7099	71	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 5.

The worst 5 of 71 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:238:ASP:OD1	1:B:564:LYS:NZ	2.11	0.84
1:A:216:ASP:HB2	10:A:622:PEG:H32	1.62	0.80
1:B:148:ILE:HD11	1:B:231:VAL:HG23	1.66	0.77
7:B:610[B]:PO4:O1	12:B:963:HOH:O	2.03	0.76
1:B:541:LYS:NZ	1:B:566:GLU:OE2	2.19	0.75

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	436/437 (100%)	412 (94%)	23 (5%)	1 (0%)	47 33

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	B	432/437 (99%)	408 (94%)	23 (5%)	1 (0%)	47 33
All	All	868/874 (99%)	820 (94%)	46 (5%)	2 (0%)	47 33

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	554	SER
1	B	554	SER

### 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	397/396 (100%)	389 (98%)	8 (2%)	55 44
1	B	393/396 (99%)	384 (98%)	9 (2%)	50 37
All	All	790/792 (100%)	773 (98%)	17 (2%)	52 39

5 of 17 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	561	MET
1	B	154	ASP
1	B	296	ASP
1	A	457	ARG
1	B	344	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 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](#)

18 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	1,2	14,14,15	1.07	1 (7%)	17,19,21	0.58	0
2	NAG	C	2	2	14,14,15	0.48	0	17,19,21	0.67	0
2	BMA	C	3	2	11,11,12	1.12	1 (9%)	15,15,17	0.70	0
2	MAN	C	4	2	11,11,12	1.60	2 (18%)	15,15,17	1.61	3 (20%)
2	MAN	C	5	2	11,11,12	1.26	2 (18%)	15,15,17	1.05	1 (6%)
2	MAN	C	6	2	11,11,12	1.44	2 (18%)	15,15,17	1.15	1 (6%)
2	MAN	C	7	2	11,11,12	0.97	0	15,15,17	1.22	2 (13%)
2	MAN	C	8	2	11,11,12	1.04	0	15,15,17	1.34	3 (20%)
3	NAG	D	1	1,3	14,14,15	0.52	0	17,19,21	0.63	1 (5%)
3	FUL	D	2	3	10,10,11	1.12	1 (10%)	14,14,16	2.00	4 (28%)
4	NAG	E	1	1,4	14,14,15	0.64	0	17,19,21	0.48	0
4	NAG	E	2	4	14,14,15	0.32	0	17,19,21	0.46	0
4	BMA	E	3	4	11,11,12	0.89	0	15,15,17	1.25	2 (13%)
4	MAN	E	4	4	11,11,12	1.80	3 (27%)	15,15,17	0.94	1 (6%)
4	MAN	E	5	4	11,11,12	1.92	3 (27%)	15,15,17	1.17	1 (6%)
5	NAG	F	1	1,5	14,14,15	0.62	0	17,19,21	0.54	0
5	NAG	F	2	5	14,14,15	0.76	1 (7%)	17,19,21	0.57	0
5	BMA	F	3	5	11,11,12	1.31	1 (9%)	15,15,17	1.70	3 (20%)

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	1,2	-	0/6/23/26	0/1/1/1
2	NAG	C	2	2	-	0/6/23/26	0/1/1/1
2	BMA	C	3	2	-	0/2/19/22	0/1/1/1
2	MAN	C	4	2	-	1/2/19/22	0/1/1/1
2	MAN	C	5	2	-	0/2/19/22	0/1/1/1
2	MAN	C	6	2	-	0/2/19/22	0/1/1/1
2	MAN	C	7	2	-	2/2/19/22	0/1/1/1
2	MAN	C	8	2	-	2/2/19/22	0/1/1/1
3	NAG	D	1	1,3	-	2/6/23/26	0/1/1/1
3	FUL	D	2	3	-	-	0/1/1/1
4	NAG	E	1	1,4	-	2/6/23/26	0/1/1/1
4	NAG	E	2	4	-	0/6/23/26	0/1/1/1
4	BMA	E	3	4	-	0/2/19/22	0/1/1/1
4	MAN	E	4	4	-	1/2/19/22	0/1/1/1
4	MAN	E	5	4	-	0/2/19/22	0/1/1/1
5	NAG	F	1	1,5	-	0/6/23/26	0/1/1/1
5	NAG	F	2	5	-	0/6/23/26	0/1/1/1
5	BMA	F	3	5	-	2/2/19/22	0/1/1/1

The worst 5 of 17 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	E	5	MAN	O5-C5	4.24	1.52	1.43
4	E	4	MAN	C2-C3	4.04	1.58	1.52
2	C	1	NAG	O5-C1	-3.96	1.37	1.43
2	C	4	MAN	O5-C5	3.36	1.50	1.43
2	C	6	MAN	C2-C3	3.09	1.57	1.52

The worst 5 of 22 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	4	MAN	C1-O5-C5	4.88	118.81	112.19
5	F	3	BMA	C1-C2-C3	-4.84	103.72	109.67
3	D	2	FUL	O5-C5-C4	4.13	116.93	109.52
3	D	2	FUL	C3-C4-C5	3.94	115.91	109.77
4	E	3	BMA	C1-O5-C5	3.17	116.48	112.19

There are no chirality outliers.

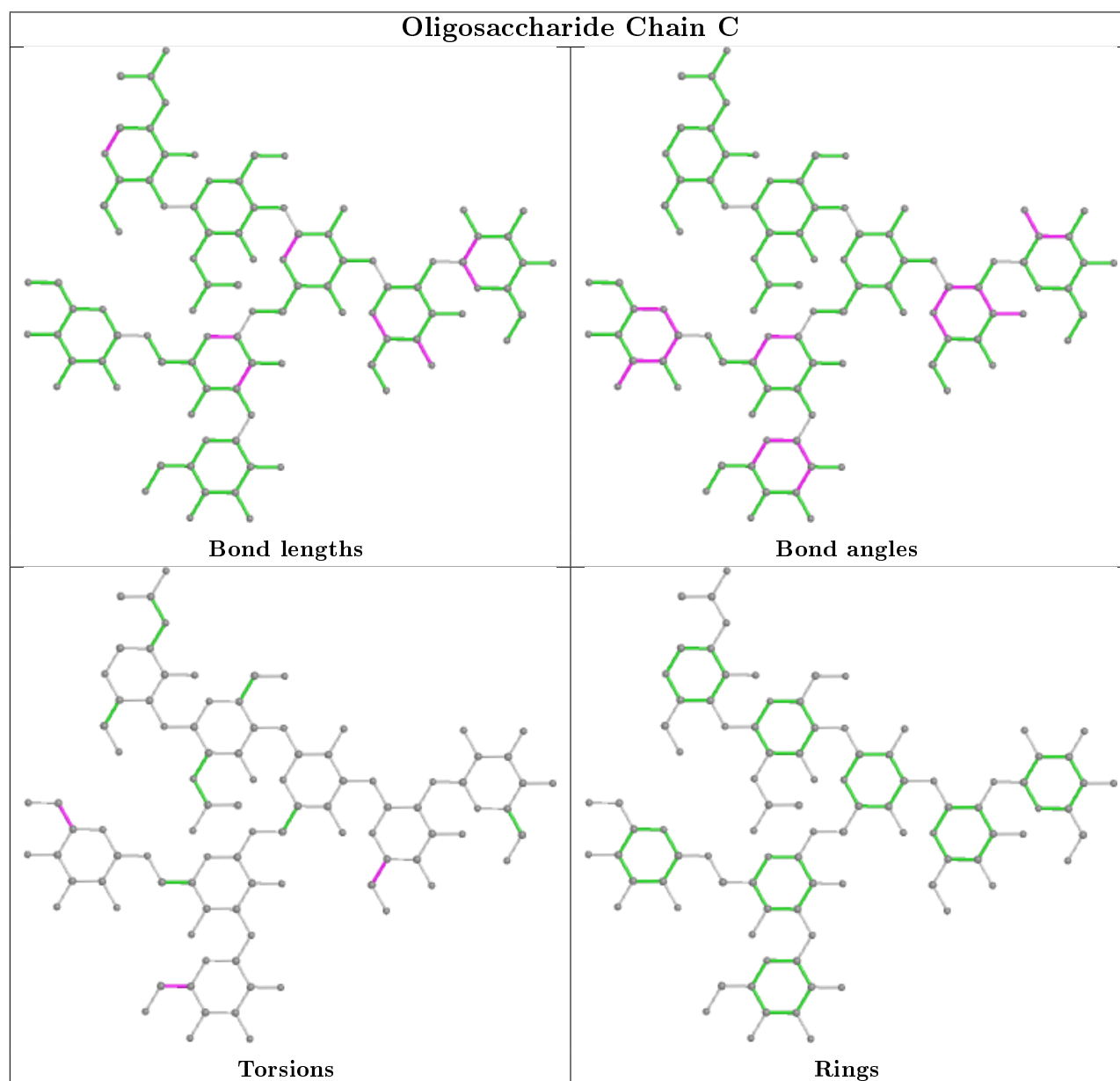
5 of 12 torsion outliers are listed below:

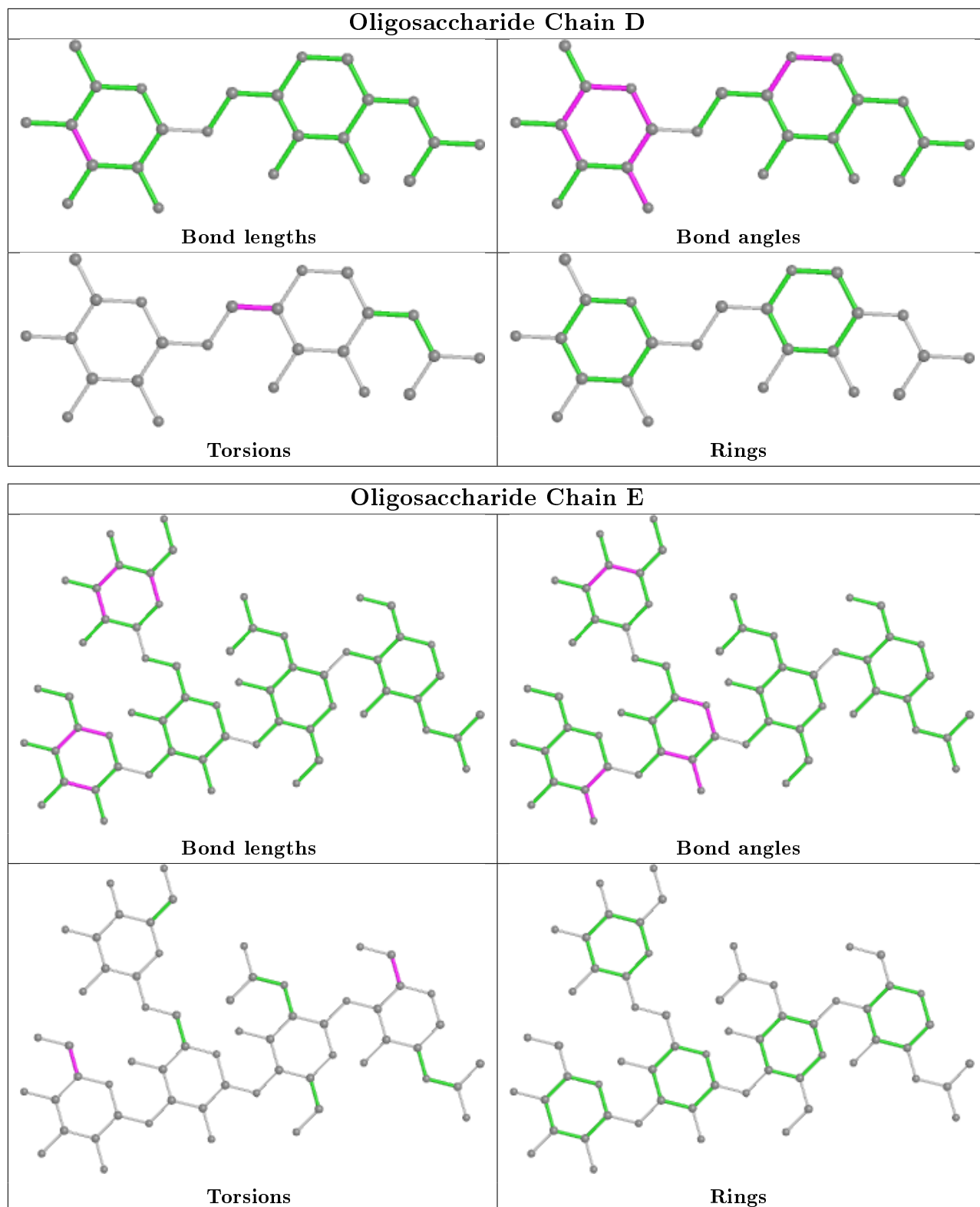
Mol	Chain	Res	Type	Atoms
3	D	1	NAG	O5-C5-C6-O6
5	F	3	BMA	O5-C5-C6-O6
2	C	8	MAN	O5-C5-C6-O6
5	F	3	BMA	C4-C5-C6-O6
2	C	8	MAN	C4-C5-C6-O6

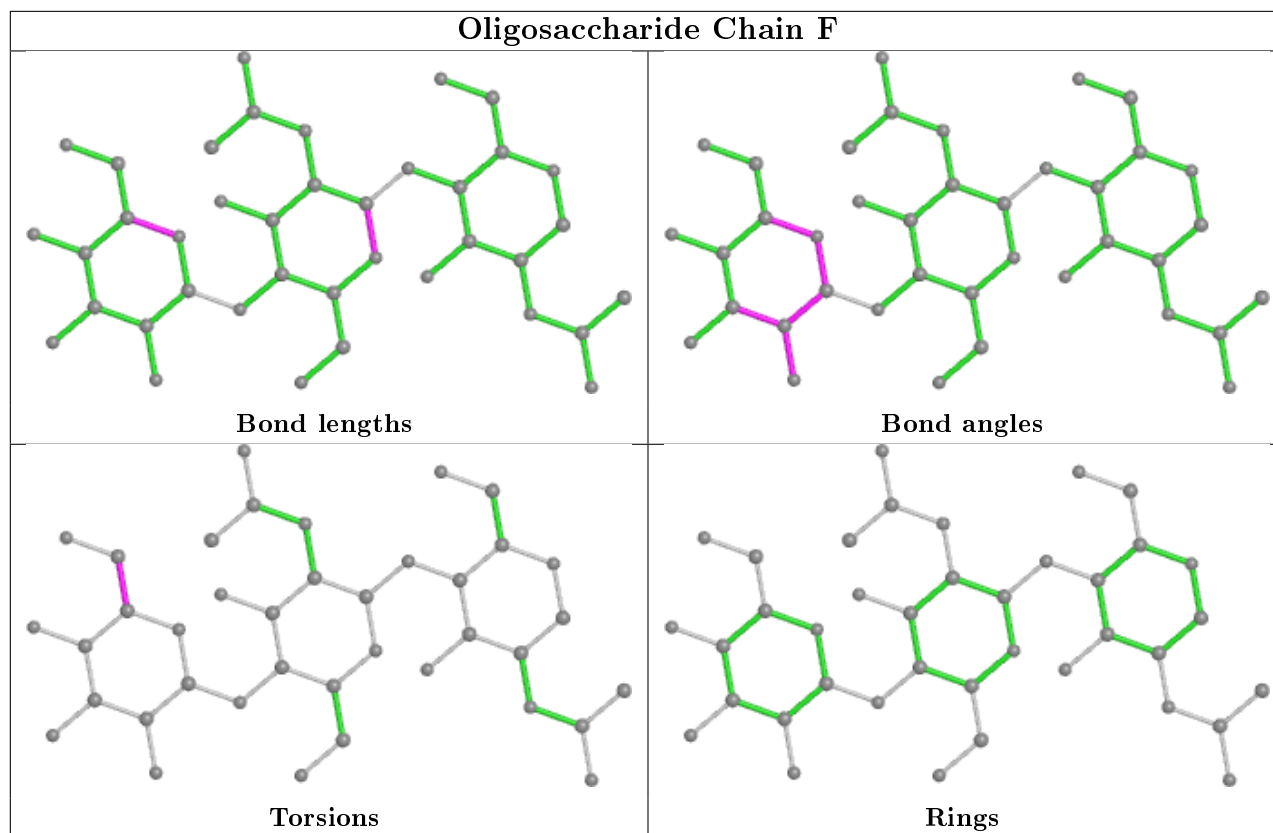
There are no ring outliers.

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.







## 5.6 Ligand geometry [i](#)

Of 28 ligands modelled in this entry, 2 are monoatomic - leaving 26 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
9	EDO	B	614	-	3,3,3	0.61	0	2,2,2	0.30	0
9	EDO	A	619	-	3,3,3	0.57	0	2,2,2	0.33	0
9	EDO	A	621	-	3,3,3	0.34	0	2,2,2	0.76	0
9	EDO	A	614	-	3,3,3	0.82	0	2,2,2	0.32	0
10	PEG	B	621	-	6,6,6	0.50	0	5,5,5	1.86	2 (40%)
9	EDO	A	618	-	3,3,3	0.50	0	2,2,2	0.70	0
6	NAG	A	601	1	14,14,15	0.62	0	17,19,21	0.95	1 (5%)
7	PO4	A	612	-	4,4,4	0.84	0	6,6,6	0.92	0
10	PEG	A	623	-	6,6,6	0.54	0	5,5,5	1.65	1 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
9	EDO	A	620	-	3,3,3	0.50	0	2,2,2	0.49	0
7	PO4	B	611	-	4,4,4	0.80	0	6,6,6	0.39	0
9	EDO	A	615	-	3,3,3	0.57	0	2,2,2	0.64	0
9	EDO	B	617	-	3,3,3	0.52	0	2,2,2	0.49	0
9	EDO	B	613	-	3,3,3	0.98	0	2,2,2	0.43	0
9	EDO	B	615	-	3,3,3	0.46	0	2,2,2	0.47	0
11	SO4	A	624	-	4,4,4	0.13	0	6,6,6	0.13	0
9	EDO	A	617	-	3,3,3	0.58	0	2,2,2	0.52	0
9	EDO	A	616	-	3,3,3	0.46	0	2,2,2	0.36	0
9	EDO	B	618	-	3,3,3	0.59	0	2,2,2	0.36	0
9	EDO	B	616	-	3,3,3	0.57	0	2,2,2	0.26	0
9	EDO	B	619	-	3,3,3	0.58	0	2,2,2	0.14	0
7	PO4	B	610[A]	-	4,4,4	0.86	0	6,6,6	0.89	0
10	PEG	B	620	-	6,6,6	0.59	0	5,5,5	1.39	1 (20%)
6	NAG	B	609	1	14,14,15	0.90	1 (7%)	17,19,21	1.06	1 (5%)
7	PO4	B	610[B]	-	4,4,4	0.97	0	6,6,6	0.47	0
10	PEG	A	622	-	6,6,6	0.45	0	5,5,5	2.06	3 (60%)

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
9	EDO	B	614	-	-	1/1/1/1	-
9	EDO	A	614	-	-	0/1/1/1	-
9	EDO	A	619	-	-	0/1/1/1	-
9	EDO	B	615	-	-	1/1/1/1	-
9	EDO	A	615	-	-	0/1/1/1	-
10	PEG	B	621	-	-	4/4/4/4	-
9	EDO	A	617	-	-	0/1/1/1	-
9	EDO	A	616	-	-	0/1/1/1	-
9	EDO	B	618	-	-	0/1/1/1	-
10	PEG	A	623	-	-	3/4/4/4	-
9	EDO	B	616	-	-	1/1/1/1	-
9	EDO	A	618	-	-	1/1/1/1	-
9	EDO	A	621	-	-	1/1/1/1	-
9	EDO	A	620	-	-	1/1/1/1	-
10	PEG	B	620	-	-	4/4/4/4	-
6	NAG	B	609	1	-	2/6/23/26	0/1/1/1
6	NAG	A	601	1	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	EDO	B	617	-	-	1/1/1/1	-
9	EDO	B	619	-	-	0/1/1/1	-
9	EDO	B	613	-	-	0/1/1/1	-
10	PEG	A	622	-	-	3/4/4/4	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	B	609	NAG	O5-C1	3.09	1.48	1.43

The worst 5 of 9 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	601	NAG	C1-O5-C5	3.45	116.87	112.19
6	B	609	NAG	C1-O5-C5	3.12	116.42	112.19
10	B	621	PEG	O2-C2-C1	2.88	122.74	110.07
10	A	622	PEG	O2-C3-C4	2.48	120.98	110.07
10	A	622	PEG	O2-C2-C1	2.37	120.46	110.07

There are no chirality outliers.

5 of 23 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
10	A	623	PEG	C1-C2-O2-C3
10	B	620	PEG	C4-C3-O2-C2
10	A	623	PEG	O1-C1-C2-O2
10	B	620	PEG	O2-C3-C4-O4
6	B	609	NAG	C4-C5-C6-O6

There are no ring outliers.

14 monomers are involved in 31 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	A	619	EDO	3	0
10	B	621	PEG	6	0
9	A	618	EDO	2	0
10	A	623	PEG	4	0
9	A	620	EDO	1	0
7	B	611	PO4	1	0
9	B	615	EDO	1	0
9	A	617	EDO	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	A	616	EDO	3	0
9	B	616	EDO	1	0
9	B	619	EDO	1	0
10	B	620	PEG	2	0
7	B	610[B]	PO4	1	0
10	A	622	PEG	5	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data [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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	432/437 (98%)	-0.15	16 (3%) 41 36	14, 25, 48, 96	0
1	B	432/437 (98%)	-0.19	13 (3%) 50 44	14, 25, 52, 75	0
All	All	864/874 (98%)	-0.17	29 (3%) 45 39	14, 25, 51, 96	0

The worst 5 of 29 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	388	LEU	12.9
1	A	389	ASN	7.2
1	A	387	GLY	7.0
1	B	388	LEU	5.6
1	B	387	GLY	4.6

### 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
5	BMA	F	3	11/12	0.76	0.26	79,89,96,99	0
2	MAN	C	5	11/12	0.78	0.33	85,94,100,113	0
2	MAN	C	6	11/12	0.78	0.18	58,68,83,84	0
2	MAN	C	8	11/12	0.81	0.25	60,72,85,87	0
3	FUL	D	2	10/11	0.81	0.29	59,82,92,102	0

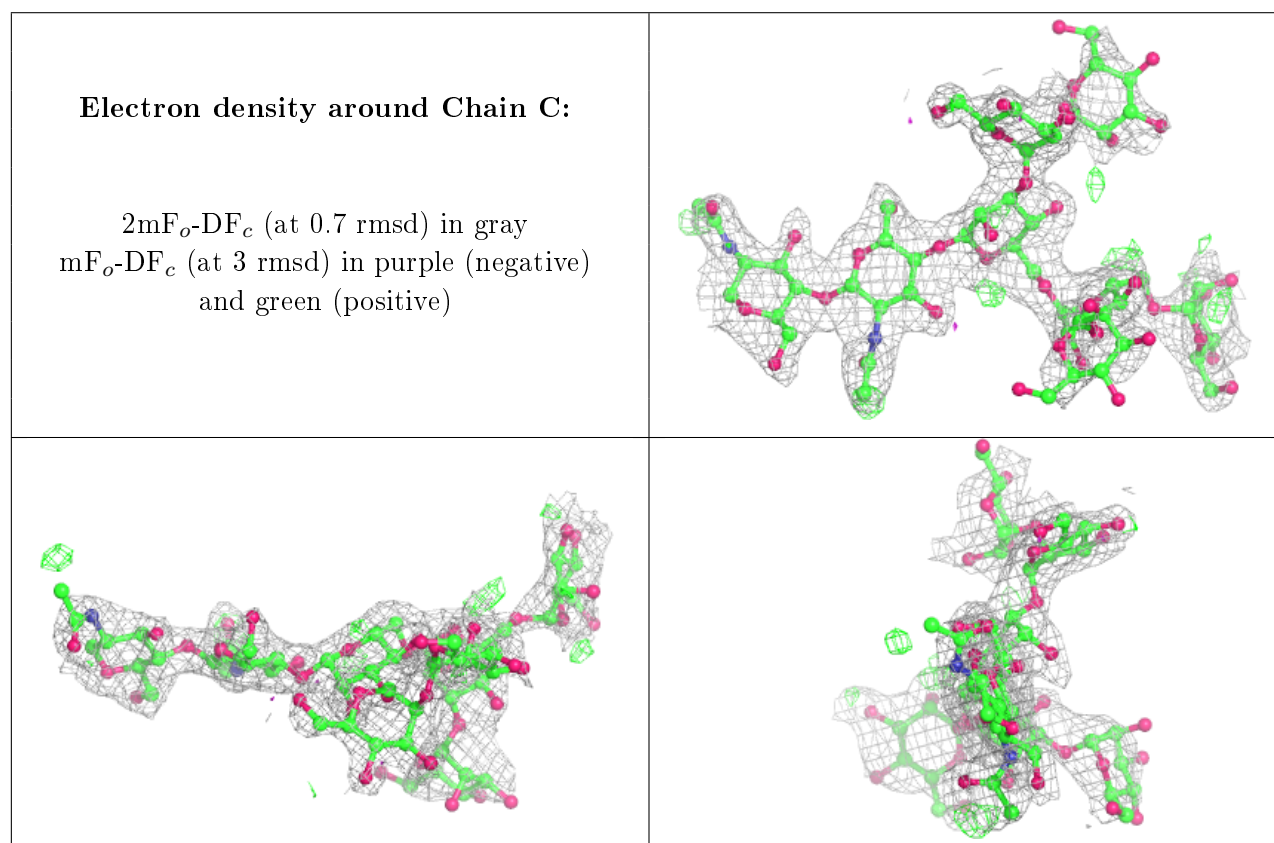
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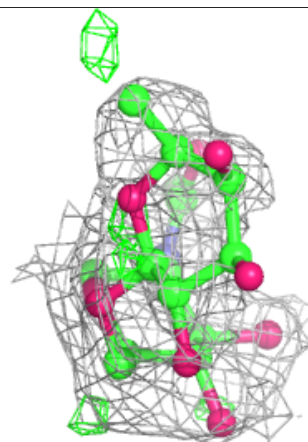
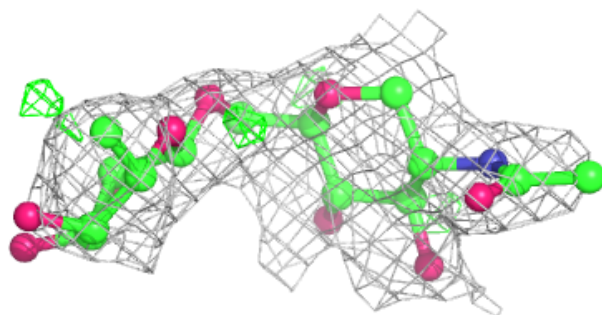
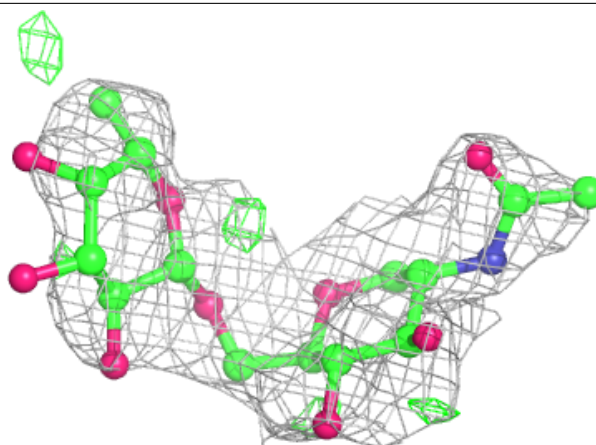
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	BMA	C	3	11/12	0.81	0.12	35,53,59,63	0
4	MAN	E	4	11/12	0.82	0.27	40,47,56,60	0
3	NAG	D	1	14/15	0.83	0.27	46,66,72,79	0
2	MAN	C	7	11/12	0.86	0.30	80,95,105,108	0
4	BMA	E	3	11/12	0.86	0.23	40,45,51,55	0
4	NAG	E	2	14/15	0.87	0.24	45,56,65,70	0
4	MAN	E	5	11/12	0.87	0.18	23,42,50,52	0
2	MAN	C	4	11/12	0.89	0.20	40,47,55,67	0
2	NAG	C	1	14/15	0.90	0.12	38,49,54,58	0
2	NAG	C	2	14/15	0.92	0.10	36,41,51,54	0
4	NAG	E	1	14/15	0.93	0.14	32,41,53,55	0
5	NAG	F	1	14/15	0.93	0.11	32,45,50,54	0
5	NAG	F	2	14/15	0.94	0.15	45,49,66,76	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.



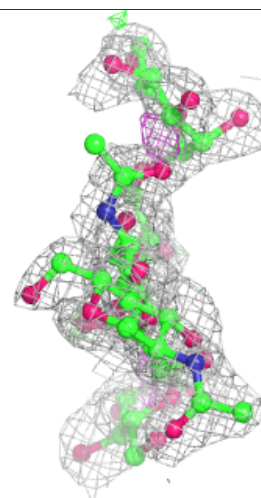
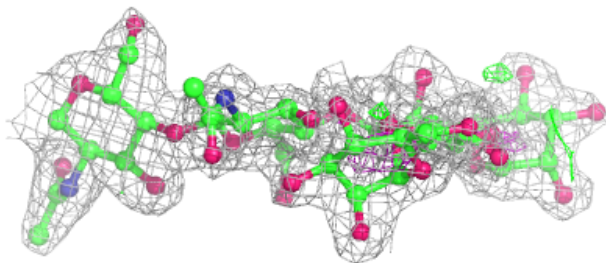
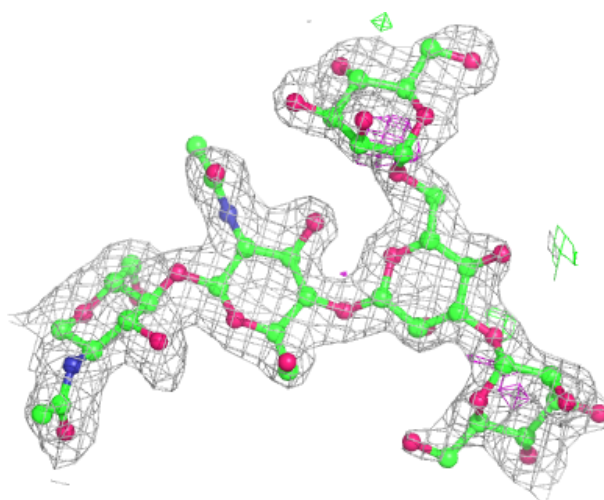
**Electron density around Chain D:**

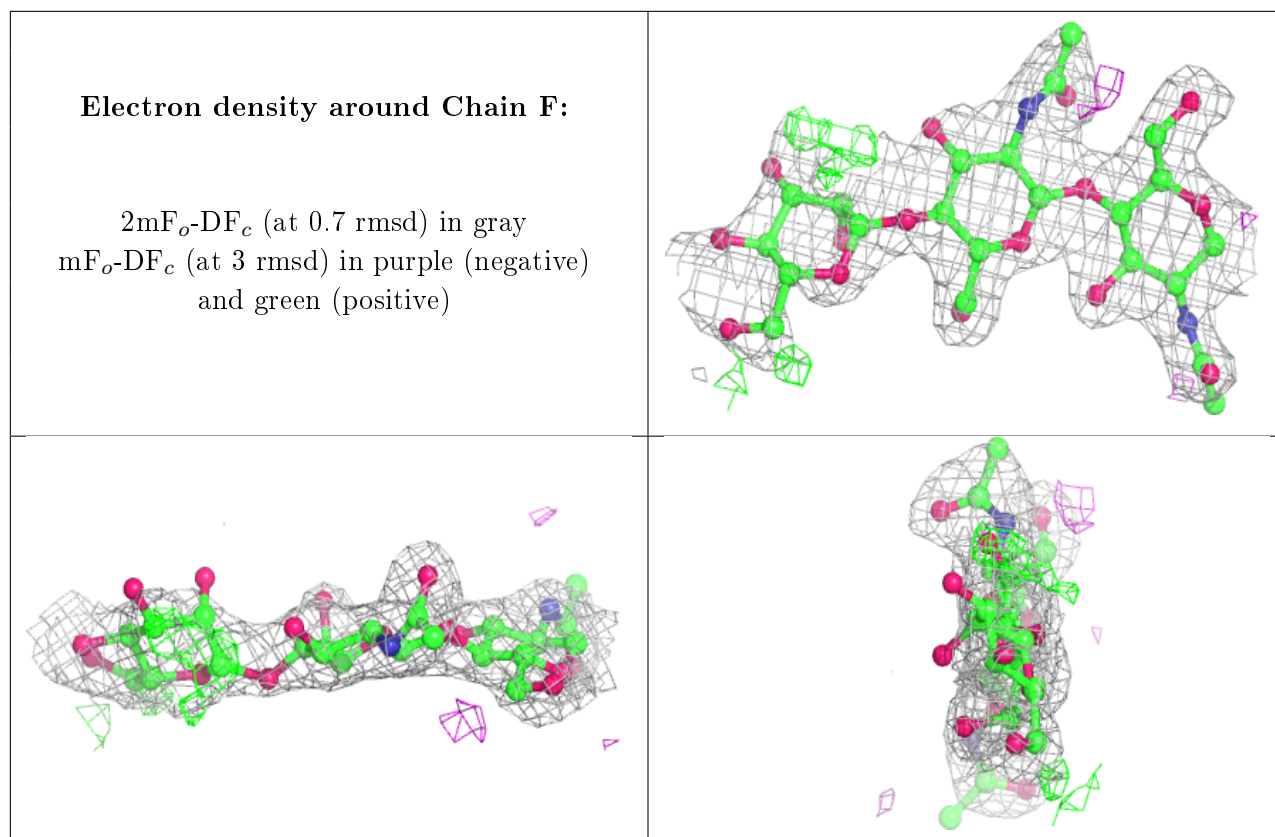
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
10	PEG	A	622	7/7	0.70	0.39	44,48,59,65	0
6	NAG	B	609	14/15	0.74	0.23	53,66,74,78	0
6	NAG	A	601	14/15	0.78	0.33	48,65,76,76	0
10	PEG	A	623	7/7	0.81	0.19	39,42,49,59	0
9	EDO	B	619	4/4	0.83	0.34	45,48,53,64	0
9	EDO	B	618	4/4	0.84	0.20	31,44,52,61	0
9	EDO	B	617	4/4	0.85	0.23	35,46,57,61	0
10	PEG	B	621	7/7	0.86	0.24	23,32,51,57	0
10	PEG	B	620	7/7	0.86	0.13	34,45,57,58	0
9	EDO	A	617	4/4	0.87	0.14	41,42,46,60	0
9	EDO	A	619	4/4	0.88	0.17	34,37,37,48	0
9	EDO	A	620	4/4	0.89	0.10	42,42,47,48	0
9	EDO	A	616	4/4	0.90	0.12	43,50,53,60	0
9	EDO	A	618	4/4	0.91	0.15	29,38,38,48	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
9	EDO	B	616	4/4	0.92	0.21	40,48,49,56	0
11	SO4	A	624	5/5	0.93	0.42	80,86,107,110	0
9	EDO	B	615	4/4	0.94	0.12	34,38,40,44	0
9	EDO	B	613	4/4	0.94	0.10	19,23,27,30	0
9	EDO	A	621	4/4	0.95	0.34	37,42,47,58	0
7	PO4	B	611	5/5	0.95	0.18	50,64,79,84	0
9	EDO	A	614	4/4	0.96	0.11	20,21,26,29	0
9	EDO	B	614	4/4	0.96	0.09	23,28,37,45	0
7	PO4	B	610[B]	5/5	0.96	0.18	26,27,32,32	5
7	PO4	B	610[A]	5/5	0.96	0.18	20,21,23,25	5
9	EDO	A	615	4/4	0.97	0.11	27,30,33,35	0
8	CA	A	613	1/1	0.99	0.05	24,24,24,24	0
7	PO4	A	612	5/5	0.99	0.05	26,27,29,33	0
8	CA	B	612	1/1	0.99	0.04	24,24,24,24	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.