



# wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 9, 2020 – 01:43 PM BST

PDB ID : 3SE6  
Title : Crystal structure of the human Endoplasmic Reticulum Aminopeptidase 2  
Authors : Birtley, J.R.; Saridakis, E.; Stratikos, E.; Mavridis, I.M.  
Deposited on : 2011-06-10  
Resolution : 3.08 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

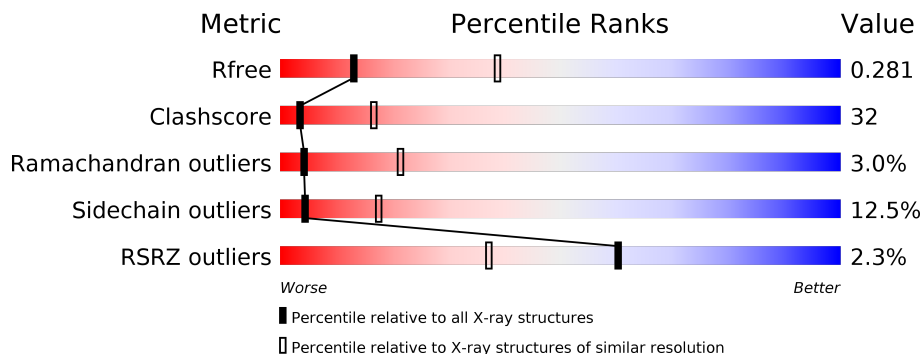
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.08 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	1447 (3.10-3.06)
Clashscore	141614	1546 (3.10-3.06)
Ramachandran outliers	138981	1487 (3.10-3.06)
Sidechain outliers	138945	1486 (3.10-3.06)
RSRZ outliers	127900	1416 (3.10-3.06)

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	967	
1	B	967	
2	C	2	
2	D	2	
3	E	4	

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>
2	NAG	D	2	-	-	-	X
3	MAN	E	3	X	-	-	-
3	MAN	E	4	X	-	-	-

## 2 Entry composition [i](#)

There are 8 unique types of molecules in this entry. The entry contains 14348 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 Endoplasmic reticulum aminopeptidase 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	869	7050	4548	1173	1302	27	2	2	0
1	B	859	6978	4504	1160	1287	27	0	0	0

There are 18 discrepancies between the modelled and reference sequences:

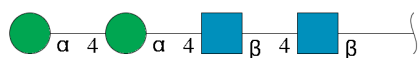
Chain	Residue	Modelled	Actual	Comment	Reference
A	2	VAL	PHE	engineered mutation	UNP Q6P179
A	392	ASN	LYS	SEE REMARK 999	UNP Q6P179
A	961	ARG	-	expression tag	UNP Q6P179
A	962	HIS	-	expression tag	UNP Q6P179
A	963	HIS	-	expression tag	UNP Q6P179
A	964	HIS	-	expression tag	UNP Q6P179
A	965	HIS	-	expression tag	UNP Q6P179
A	966	HIS	-	expression tag	UNP Q6P179
A	967	HIS	-	expression tag	UNP Q6P179
B	2	VAL	PHE	engineered mutation	UNP Q6P179
B	392	ASN	LYS	SEE REMARK 999	UNP Q6P179
B	961	ARG	-	expression tag	UNP Q6P179
B	962	HIS	-	expression tag	UNP Q6P179
B	963	HIS	-	expression tag	UNP Q6P179
B	964	HIS	-	expression tag	UNP Q6P179
B	965	HIS	-	expression tag	UNP Q6P179
B	966	HIS	-	expression tag	UNP Q6P179
B	967	HIS	-	expression tag	UNP Q6P179

- 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
2	C	2	Total	C	N	O	0	0	0
			28	16	2	10			
2	D	2	Total	C	N	O	0	0	0
			28	16	2	10			

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

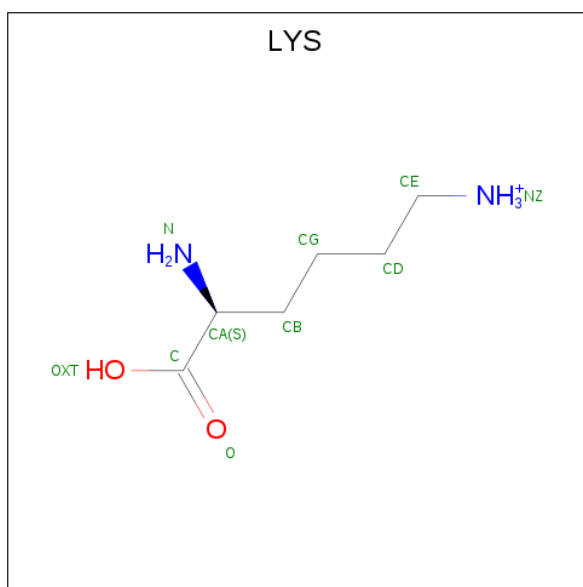


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	E	4	Total	C	N	O	0	0	0
			50	28	2	20			

- Molecule 4 is ZINC ION (three-letter code: ZN) (formula: Zn).

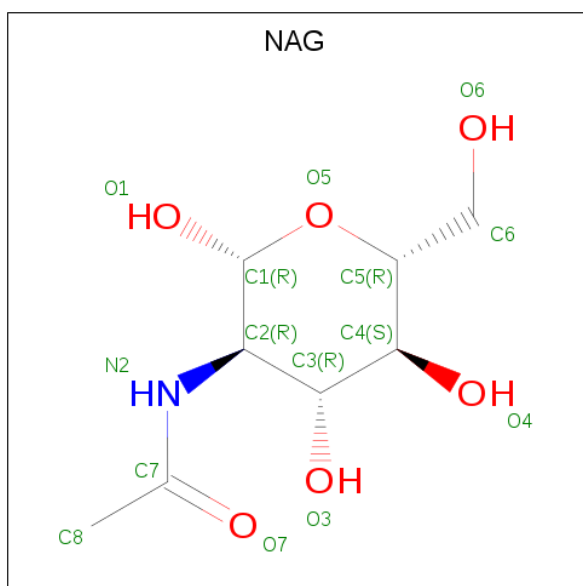
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	1	Total	Zn	0	0
			1	1		
4	A	1	Total	Zn	0	0
			1	1		

- Molecule 5 is LYSINE (three-letter code: LYS) (formula: C<sub>6</sub>H<sub>15</sub>N<sub>2</sub>O<sub>2</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
5	A	1	10	6	2	2	0	0
5	B	1	10	6	2	2	0	0

- Molecule 6 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula:  $C_8H_{15}NO_6$ ).



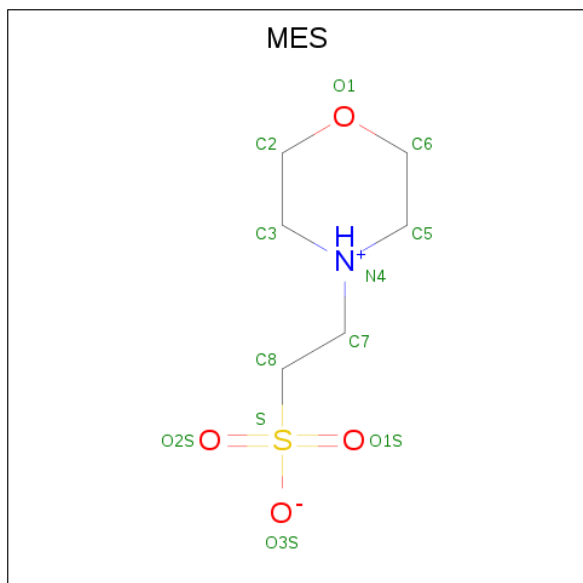
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
6	A	1	14	8	1	5	0	0

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

- Molecule 7 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (three-letter code: MES) (formula: C<sub>6</sub>H<sub>13</sub>NO<sub>4</sub>S).



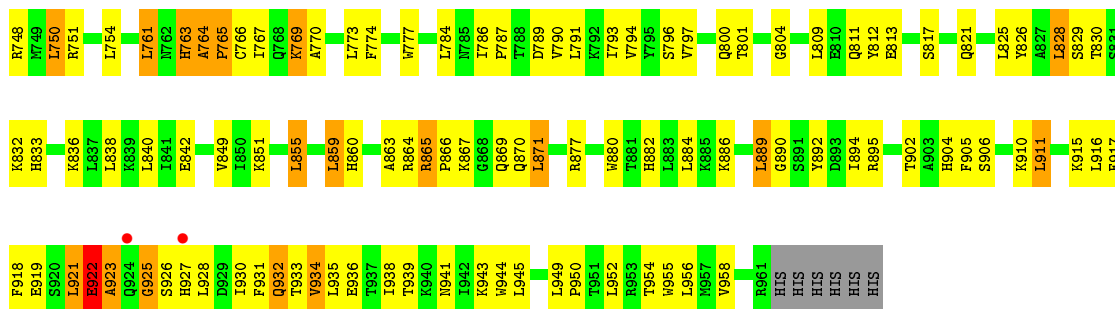
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
7	A	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
7	B	1	Total	C	N	O	S	0	0
			12	6	1	4	1		

- Molecule 8 is water.

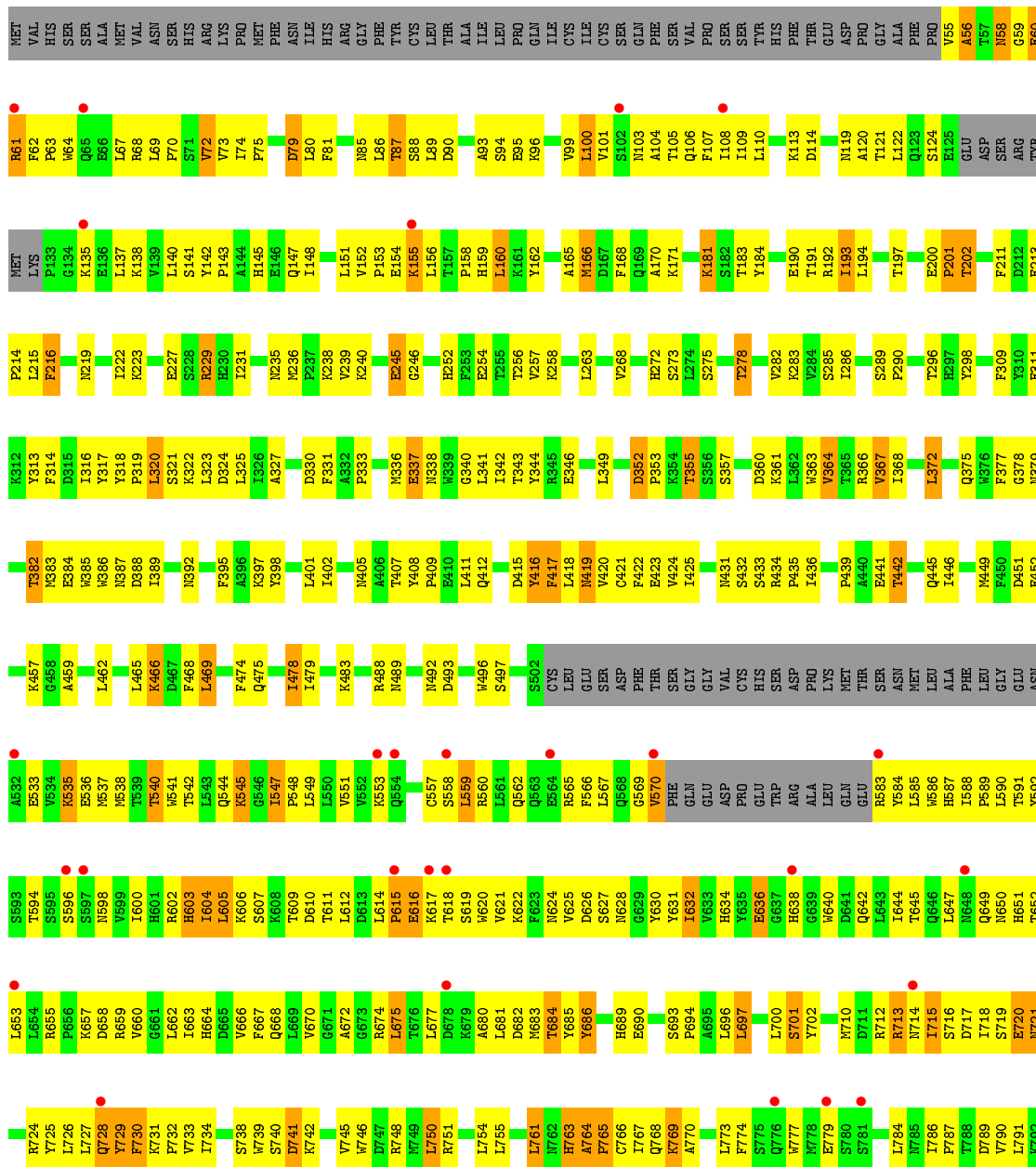
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	73	Total	O	0	0
			73	73		
8	B	53	Total	O	0	0
			53	53		

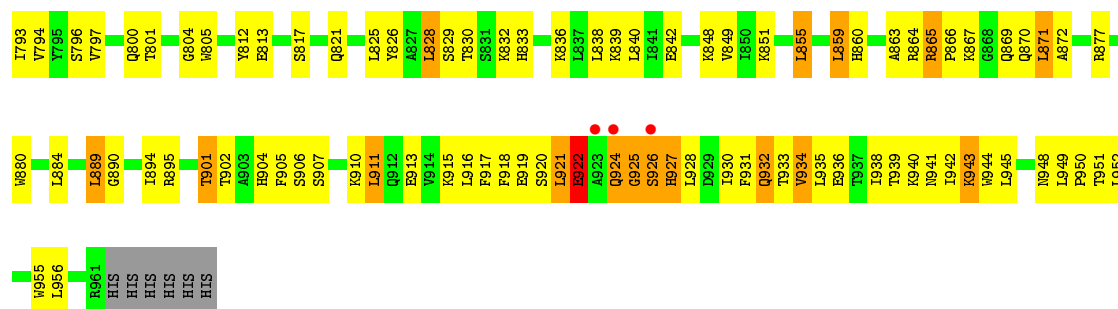






● Molecule 1: Endoplasmic reticulum aminopeptidase 2





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

Chain C: 100%

MAG1  
MAG2

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

Chain D: 50% 50%

MAG1  
MAG2

- Molecule 3: alpha-D-mannopyranose-(1-4)-alpha-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain E: 100%

MAG1  
MAG2  
MAN3  
MAN4

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	74.58Å 134.36Å 128.01Å 90.00° 90.71° 90.00°	Depositor
Resolution (Å)	11.00 – 3.08 20.03 – 3.08	Depositor EDS
% Data completeness (in resolution range)	94.3 (11.00-3.08) 93.3 (20.03-3.08)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.21 (at 3.09Å)	Xtriage
Refinement program	PHENIX (phenix.refine)	Depositor
R, $R_{free}$	0.212 , 0.277 0.215 , 0.281	Depositor DCC
$R_{free}$ test set	2330 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	60.6	Xtriage
Anisotropy	0.260	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 70.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.018 for -h,-l,-k 0.005 for -h,l,k 0.034 for h,-k,-l	Xtriage
$F_o, F_c$ correlation	0.90	EDS
Total number of atoms	14348	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	65.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.00% 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: ZN, NAG, MES, 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	0.40	0/7227	0.58	1/9794 (0.0%)
1	B	0.41	0/7148	0.58	0/9686
All	All	0.41	0/14375	0.58	1/19480 (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	A	923	ALA	N-CA-C	-5.60	95.88	111.00

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	7050	0	6987	431	0
1	B	6978	0	6946	474	0
2	C	28	0	25	3	0
2	D	28	0	25	2	0
3	E	50	0	43	1	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
5	A	10	0	12	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	B	10	0	12	2	0
6	A	28	0	26	0	0
6	B	14	0	13	3	0
7	A	12	0	12	2	0
7	B	12	0	12	4	0
8	A	73	0	0	4	0
8	B	53	0	0	12	0
All	All	14348	0	14113	904	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 32.

The worst 5 of 904 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:56:ALA:HB1	1:B:61:ARG:HA	1.23	1.09
1:A:56:ALA:HB1	1:A:57:THR:HA	1.34	1.06
1:B:245:GLU:HG2	1:B:246:GLY:H	1.27	0.98
1:A:245:GLU:HG2	1:A:246:GLY:H	1.23	0.98
1:A:544:GLN:HE21	1:A:584:TYR:HD1	1.16	0.93

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	863/967 (89%)	746 (86%)	95 (11%)	22 (2%)	5	25
1	B	851/967 (88%)	732 (86%)	89 (10%)	30 (4%)	3	18
All	All	1714/1934 (89%)	1478 (86%)	184 (11%)	52 (3%)	4	21

5 of 52 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	55	VAL
1	A	245	GLU
1	A	417	PHE
1	A	596	SER
1	A	616	GLU

### 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	773/870 (89%)	677 (88%)	96 (12%)	4	18
1	B	770/870 (88%)	672 (87%)	98 (13%)	4	17
All	All	1543/1740 (89%)	1349 (87%)	194 (13%)	4	17

5 of 194 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	871	LEU
1	B	181	LYS
1	B	855	LEU
1	A	911	LEU
1	B	72	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 53 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	870	GLN
1	B	58	ASN
1	B	870	GLN
1	A	882	HIS
1	A	927	HIS

### 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](#)

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	NAG	C	1	1,2	14,14,15	0.69	0	17,19,21	1.17	3 (17%)
2	NAG	C	2	2	14,14,15	0.50	0	17,19,21	1.45	2 (11%)
2	NAG	D	1	1,2	14,14,15	0.61	0	17,19,21	1.80	2 (11%)
2	NAG	D	2	2	14,14,15	0.54	0	17,19,21	0.68	0
3	NAG	E	1	1,3	14,14,15	0.47	0	17,19,21	1.43	2 (11%)
3	NAG	E	2	3	14,14,15	0.58	0	17,19,21	1.35	2 (11%)
3	MAN	E	3	3	11,11,12	0.72	0	15,15,17	0.97	0
3	MAN	E	4	3	11,11,12	0.60	0	15,15,17	0.76	1 (6%)

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	-	4/6/23/26	0/1/1/1
2	NAG	C	2	2	-	2/6/23/26	0/1/1/1
2	NAG	D	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	D	2	2	-	0/6/23/26	0/1/1/1
3	NAG	E	1	1,3	-	3/6/23/26	0/1/1/1
3	NAG	E	2	3	-	2/6/23/26	0/1/1/1
3	MAN	E	3	3	1/1/4/5	2/2/19/22	0/1/1/1
3	MAN	E	4	3	1/1/4/5	0/2/19/22	0/1/1/1

There are no bond length outliers.

The worst 5 of 12 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	1	NAG	C1-O5-C5	6.19	120.58	112.19
2	C	2	NAG	C1-O5-C5	4.45	118.22	112.19
3	E	2	NAG	C1-O5-C5	3.90	117.48	112.19
3	E	1	NAG	C1-O5-C5	3.51	116.95	112.19
3	E	1	NAG	C4-C3-C2	-2.93	106.72	111.02

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	E	3	MAN	C1
3	E	4	MAN	C1

5 of 15 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	D	1	NAG	C8-C7-N2-C2
2	C	1	NAG	C8-C7-N2-C2
2	D	1	NAG	O7-C7-N2-C2
2	C	1	NAG	O5-C5-C6-O6
2	C	1	NAG	O7-C7-N2-C2

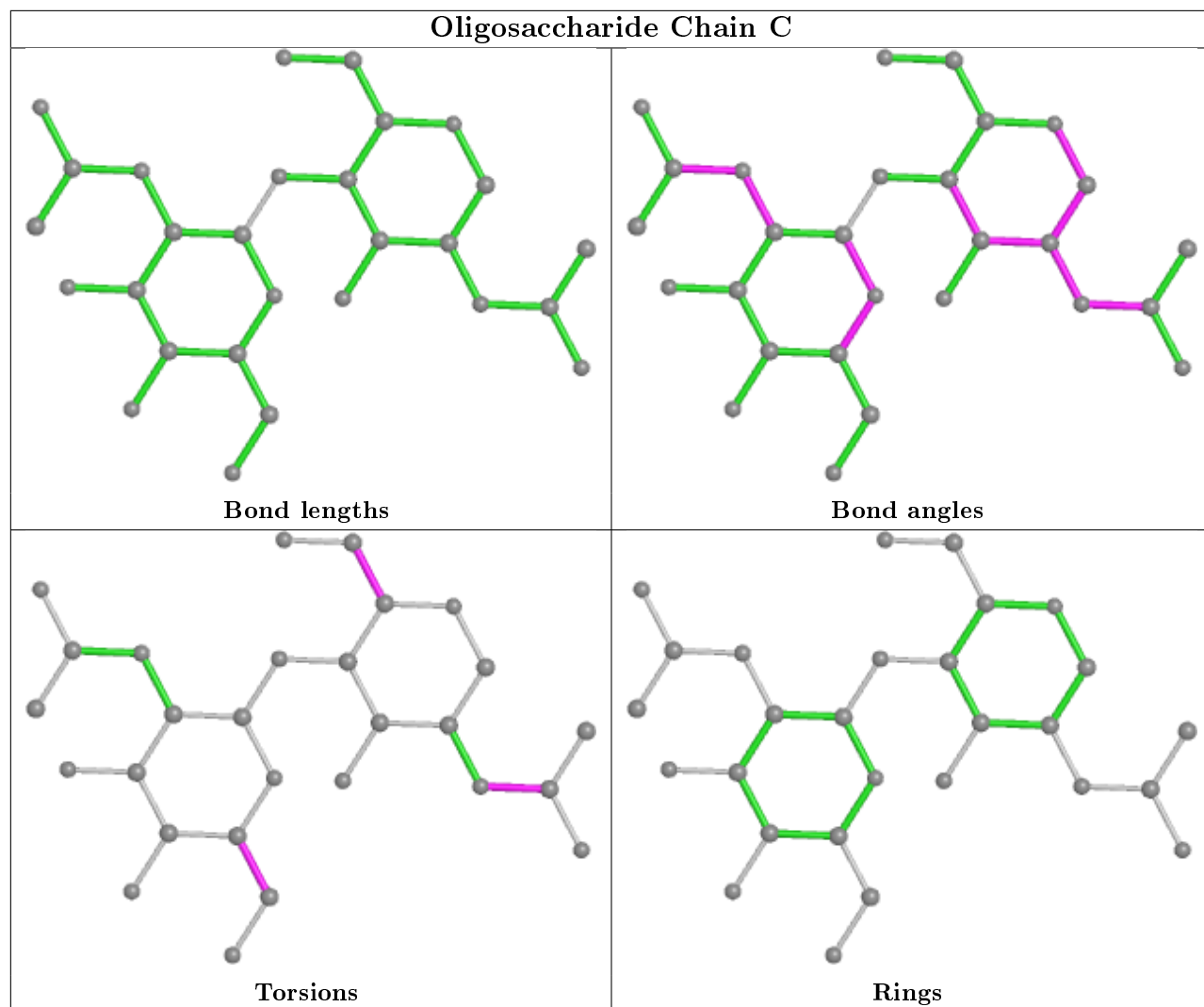
There are no ring outliers.

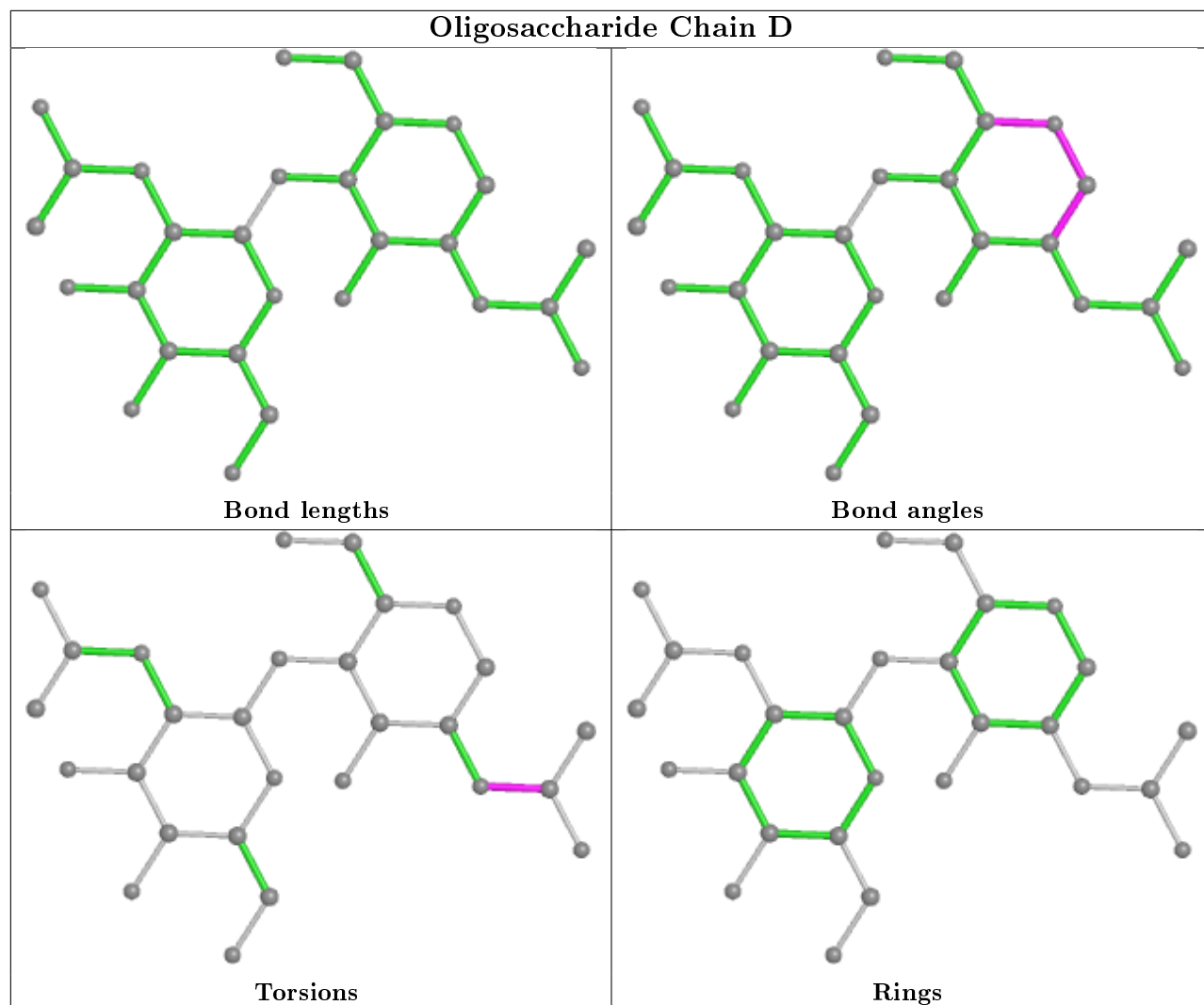
5 monomers are involved in 6 short contacts:

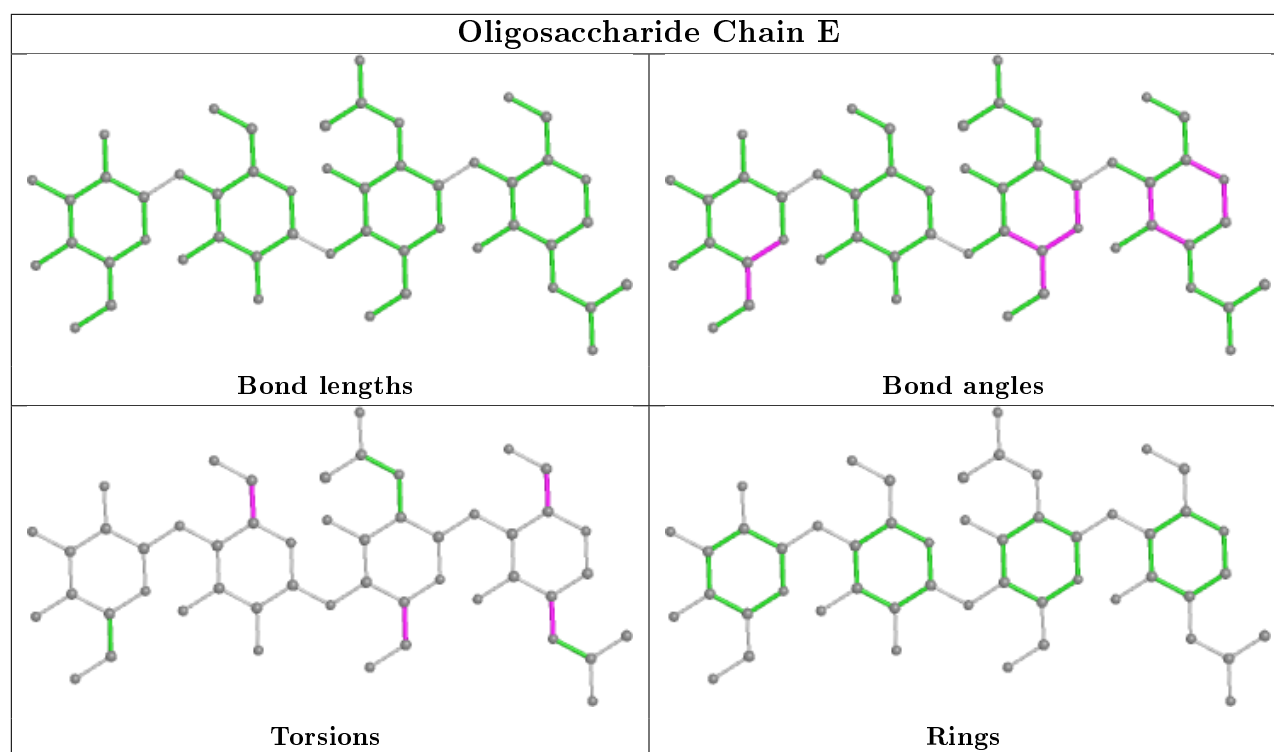
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	1	NAG	3	0
2	D	1	NAG	2	0
2	C	2	NAG	1	0
2	D	2	NAG	1	0
3	E	3	MAN	1	0

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









## 5.6 Ligand geometry [i](#)

Of 9 ligands modelled in this entry, 2 are monoatomic - leaving 7 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$
6	NAG	A	1076	1	14,14,15	0.69	0	17,19,21	1.65	3 (17%)
6	NAG	A	1075	1	14,14,15	0.51	0	17,19,21	1.05	1 (5%)
7	MES	A	1083	-	12,12,12	2.29	2 (16%)	14,16,16	2.47	6 (42%)
6	NAG	B	1081	1	14,14,15	0.71	0	17,19,21	0.97	0
7	MES	B	1084	-	12,12,12	2.11	1 (8%)	14,16,16	2.67	7 (50%)

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	NAG	A	1076	1	-	2/6/23/26	0/1/1/1
6	NAG	A	1075	1	-	2/6/23/26	0/1/1/1
7	MES	A	1083	-	-	3/6/14/14	0/1/1/1
6	NAG	B	1081	1	-	0/6/23/26	0/1/1/1
7	MES	B	1084	-	-	4/6/14/14	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	A	1083	MES	C8-S	-7.44	1.66	1.77
7	B	1084	MES	C8-S	-6.90	1.67	1.77
7	A	1083	MES	O2S-S	2.01	1.51	1.45

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A	1083	MES	C5-N4-C3	4.75	119.53	108.83
7	B	1084	MES	C5-N4-C3	4.54	119.04	108.83
7	B	1084	MES	C6-C5-N4	-4.43	103.39	110.10
7	A	1083	MES	C6-C5-N4	-3.74	104.43	110.10
7	B	1084	MES	C7-N4-C5	3.74	120.79	111.23

There are no chirality outliers.

5 of 11 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	A	1083	MES	C8-C7-N4-C3
7	A	1083	MES	N4-C7-C8-S
7	B	1084	MES	C8-C7-N4-C3
6	A	1076	NAG	C8-C7-N2-C2
6	A	1076	NAG	O7-C7-N2-C2

There are no ring outliers.

3 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	A	1083	MES	2	0
6	B	1081	NAG	3	0
7	B	1084	MES	4	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	869/967 (89%)	-0.26	9 (1%) 82 66	26, 61, 108, 138	2 (0%)
1	B	859/967 (88%)	-0.12	30 (3%) 44 22	27, 63, 111, 139	0
All	All	1728/1934 (89%)	-0.19	39 (2%) 60 37	26, 62, 109, 139	2 (0%)

The worst 5 of 39 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	570	VAL	4.1
1	B	617	LYS	4.0
1	B	596	SER	3.5
1	A	102	SER	3.5
1	B	638	HIS	3.2

### 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.

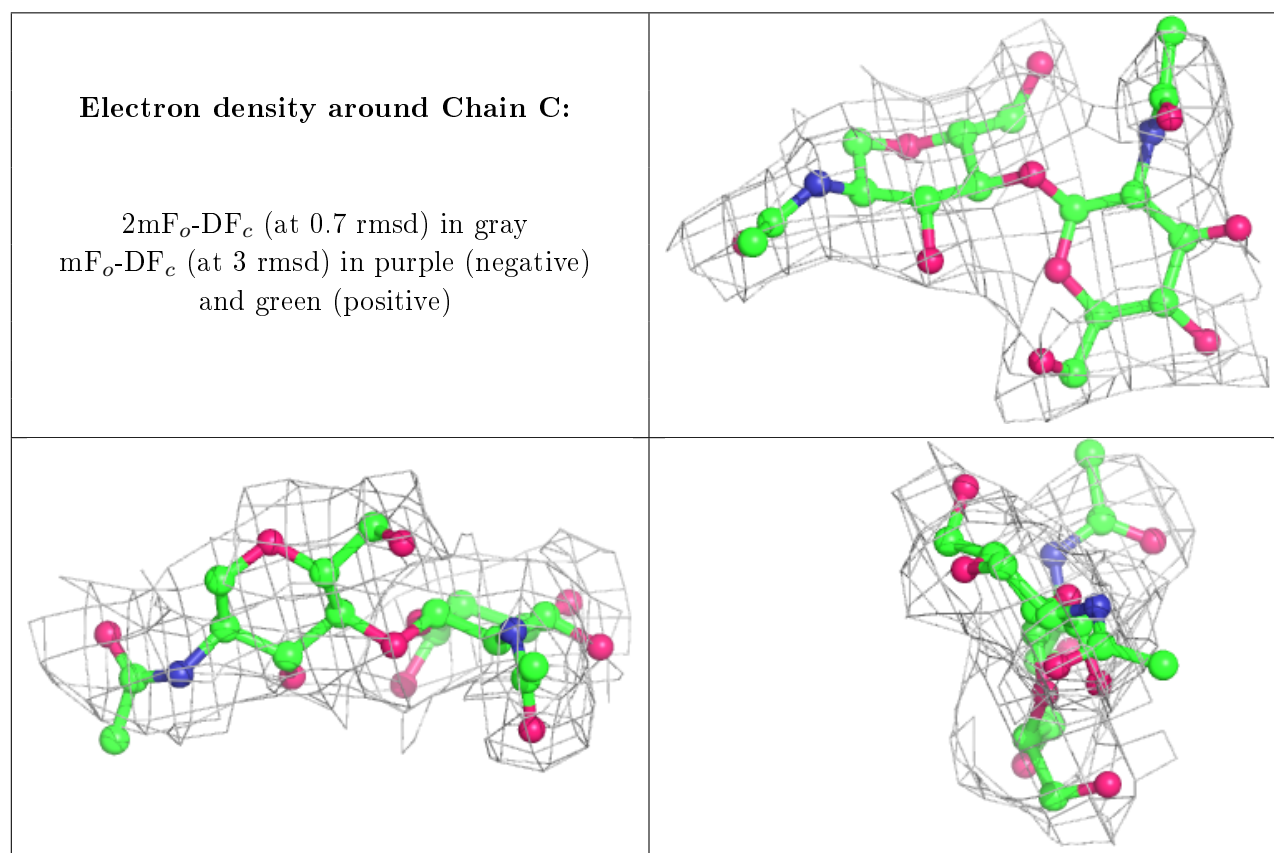
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q < 0.9
2	NAG	D	2	14/15	0.63	0.63	78,88,106,128	0
3	MAN	E	3	11/12	0.82	0.34	94,102,111,115	0
3	MAN	E	4	11/12	0.86	0.35	98,112,120,124	0
2	NAG	D	1	14/15	0.89	0.33	44,63,69,71	0
3	NAG	E	2	14/15	0.89	0.23	57,74,91,95	0

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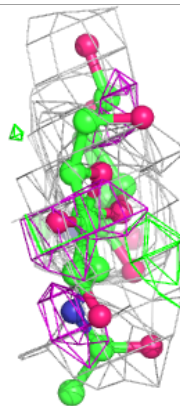
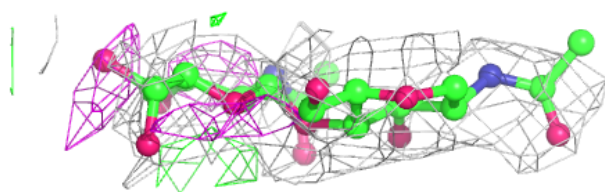
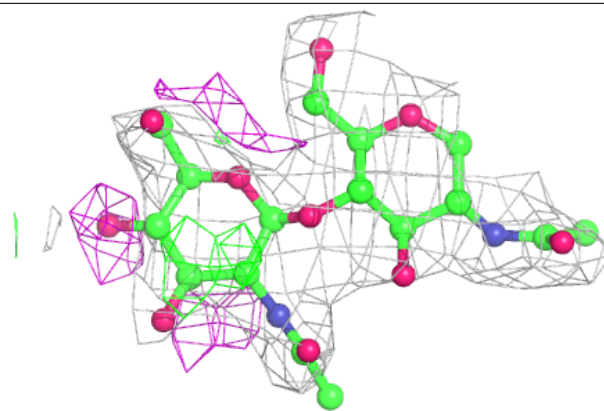
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	NAG	C	2	14/15	0.91	0.22	62,77,82,90	0
3	NAG	E	1	14/15	0.93	0.21	45,65,74,75	0
2	NAG	C	1	14/15	0.94	0.20	43,58,70,72	0

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.

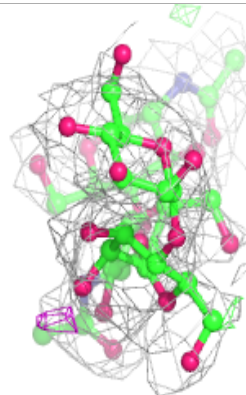
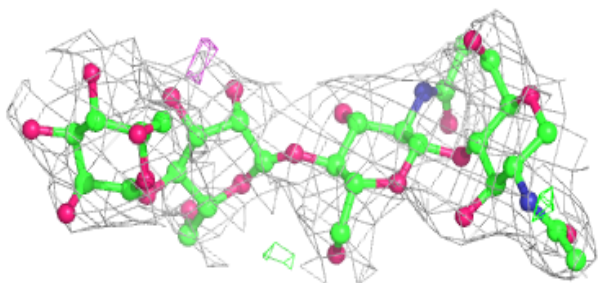
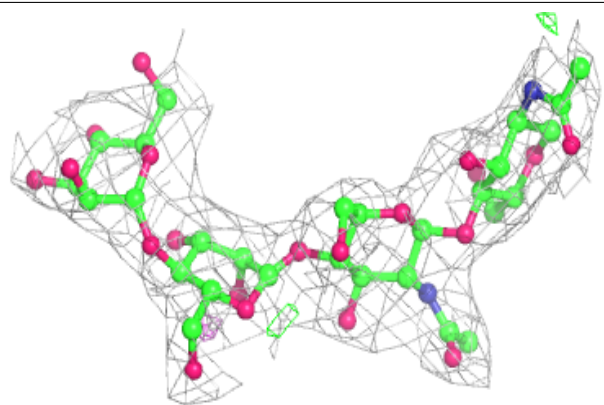


**Electron density around Chain D:**

$2mF_o-DF_c$  (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( $\text{\AA}^2$ )	Q<0.9
6	NAG	A	1076	14/15	0.84	0.31	59,91,103,108	0
7	MES	B	1084	12/12	0.88	0.27	53,71,88,100	0
6	NAG	B	1081	14/15	0.88	0.37	53,72,97,99	0
7	MES	A	1083	12/12	0.91	0.22	46,68,81,96	0
6	NAG	A	1075	14/15	0.91	0.30	58,81,86,93	0
5	LYS	B	968	10/10	0.95	0.20	36,51,71,71	0
5	LYS	A	968	10/10	0.99	0.12	32,39,51,51	0
4	ZN	B	6000	1/1	0.99	0.07	36,36,36,36	0
4	ZN	A	5000	1/1	1.00	0.09	31,31,31,31	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.