



# wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 8, 2020 – 06:50 PM BST

PDB ID : 5AB0  
Title : Crystal structure of aminopeptidase ERAP2 with ligand  
Authors : Mpakali, A.; Giastas, P.; Saridakis, E.; Stratikos, E.  
Deposited on : 2015-07-31  
Resolution : 2.50 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

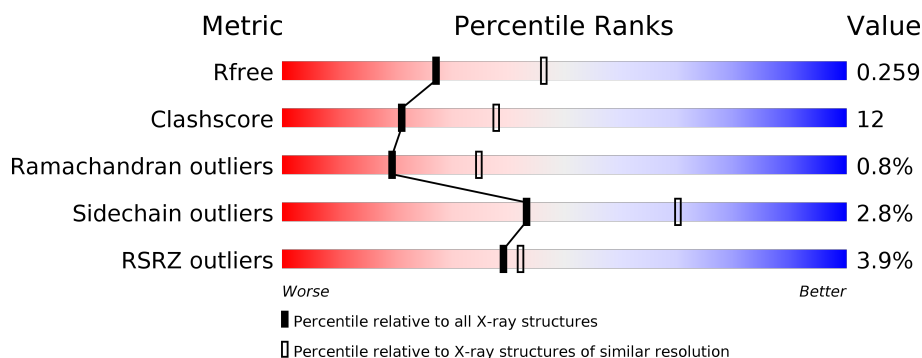
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.50 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.




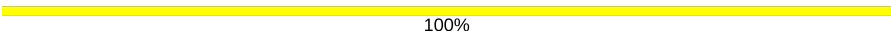


Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

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	<div> <div style="width: 100%; height: 10px; background-color: red;"></div> <div style="display: flex; justify-content: space-between; align-items: center;"> <span>%</span> <div style="width: 100%; height: 10px; background-color: green;"></div> <span>72%</span> <span>21%</span> <span>• 6%</span> </div> </div>
1	C	967	<div> <div style="width: 6%; height: 10px; background-color: red;"></div> <div style="display: flex; justify-content: space-between; align-items: center;"> <span>6%</span> <div style="width: 100%; height: 10px; background-color: green;"></div> <span>61%</span> <span>29%</span> <span>• 9%</span> </div> </div>
2	E	10	<div> <div style="width: 10%; height: 10px; background-color: green;"></div> <div style="display: flex; justify-content: space-between; align-items: center;"> <span>10%</span> <div style="width: 100%; height: 10px; background-color: yellow;"></div> <span>50%</span> <span>40%</span> </div> </div>
2	F	10	<div> <div style="width: 40%; height: 10px; background-color: red;"></div> <div style="display: flex; justify-content: space-between; align-items: center;"> <span>40%</span> <div style="width: 100%; height: 10px; background-color: yellow;"></div> <span>30%</span> <span>60%</span> <span>10%</span> </div> </div>
3	B	2	<div> <div style="width: 100%; height: 10px; background-color: green;"></div> <div style="display: flex; justify-content: space-between; align-items: center;"> <span>100%</span> </div> </div>
3	H	2	<div> <div style="width: 50%; height: 10px; background-color: green;"></div> <div style="display: flex; justify-content: space-between; align-items: center;"> <span>50%</span> <div style="width: 100%; height: 10px; background-color: yellow;"></div> <span>50%</span> </div> </div>

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Mol	Chain	Length	Quality of chain
3	J	2	 50% 50%
4	D	3	 100%
4	G	3	 33% 67%
5	I	5	 80% 20%

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
2	LYN	E	10	-	-	-	X
2	LYN	F	10	-	-	-	X

## 2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 15615 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 ENDOPLASMATIC RETICULUM AMINOPEPTIDASE 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	911	Total	C	N	O	S	0	4	1
			7425	4779	1236	1378	32			
1	C	882	Total	C	N	O	S	0	4	1
			7208	4646	1196	1338	28			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
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
A	392	ASN	LYS	variant	UNP Q6P179
C	961	ARG	-	expression tag	UNP Q6P179
C	962	HIS	-	expression tag	UNP Q6P179
C	963	HIS	-	expression tag	UNP Q6P179
C	964	HIS	-	expression tag	UNP Q6P179
C	965	HIS	-	expression tag	UNP Q6P179
C	966	HIS	-	expression tag	UNP Q6P179
C	967	HIS	-	expression tag	UNP Q6P179
C	392	ASN	LYS	variant	UNP Q6P179

- Molecule 2 is a protein called DG025.

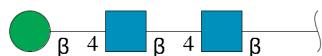
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	10	Total	C	N	O	P	0	0	0
			93	64	16	12	1			
2	F	10	Total	C	N	O	P	0	0	0
			93	64	16	12	1			

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



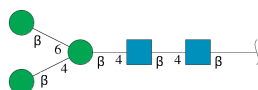
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	B	2	Total	C	N	O	0	0	0
			28	16	2	10			
3	H	2	Total	C	N	O	0	0	0
			28	16	2	10			
3	J	2	Total	C	N	O	0	0	0
			28	16	2	10			

- 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
4	D	3	Total	C	N	O	0	0	0
			39	22	2	15			
4	G	3	Total	C	N	O	0	0	0
			39	22	2	15			

- Molecule 5 is an oligosaccharide called beta-D-mannopyranose-(1-4)-[beta-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.

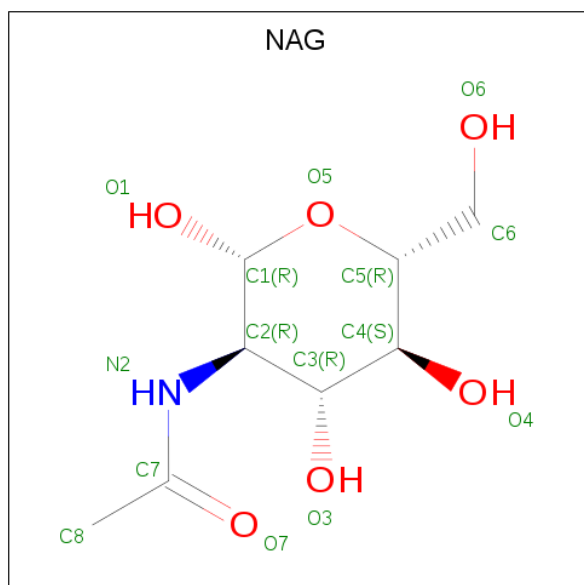


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	I	5	Total	C	N	O	0	0	0
			61	34	2	25			

- Molecule 6 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	1	Total	Zn	0	0
			1	1		
6	C	1	Total	Zn	0	0
			1	1		

- Molecule 7 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula:  $C_8H_{15}NO_6$ ).



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

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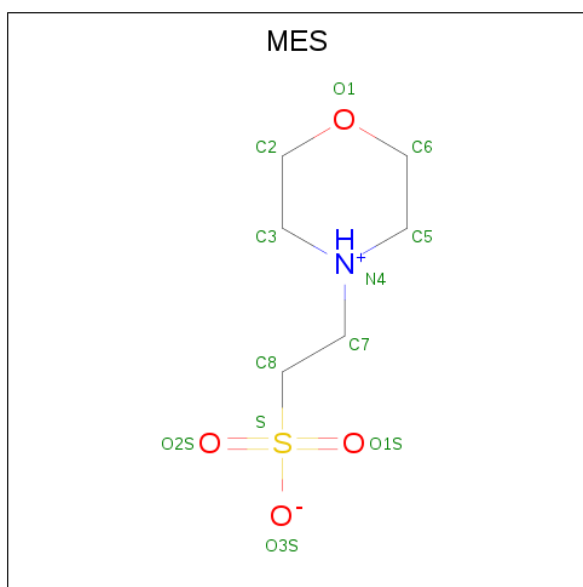
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	C	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 8 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula:  $C_2H_6O_2$ ).



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

- Molecule 9 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (three-letter code: MES) (formula:  $C_6H_{13}NO_4S$ ).



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

- Molecule 10 is water.

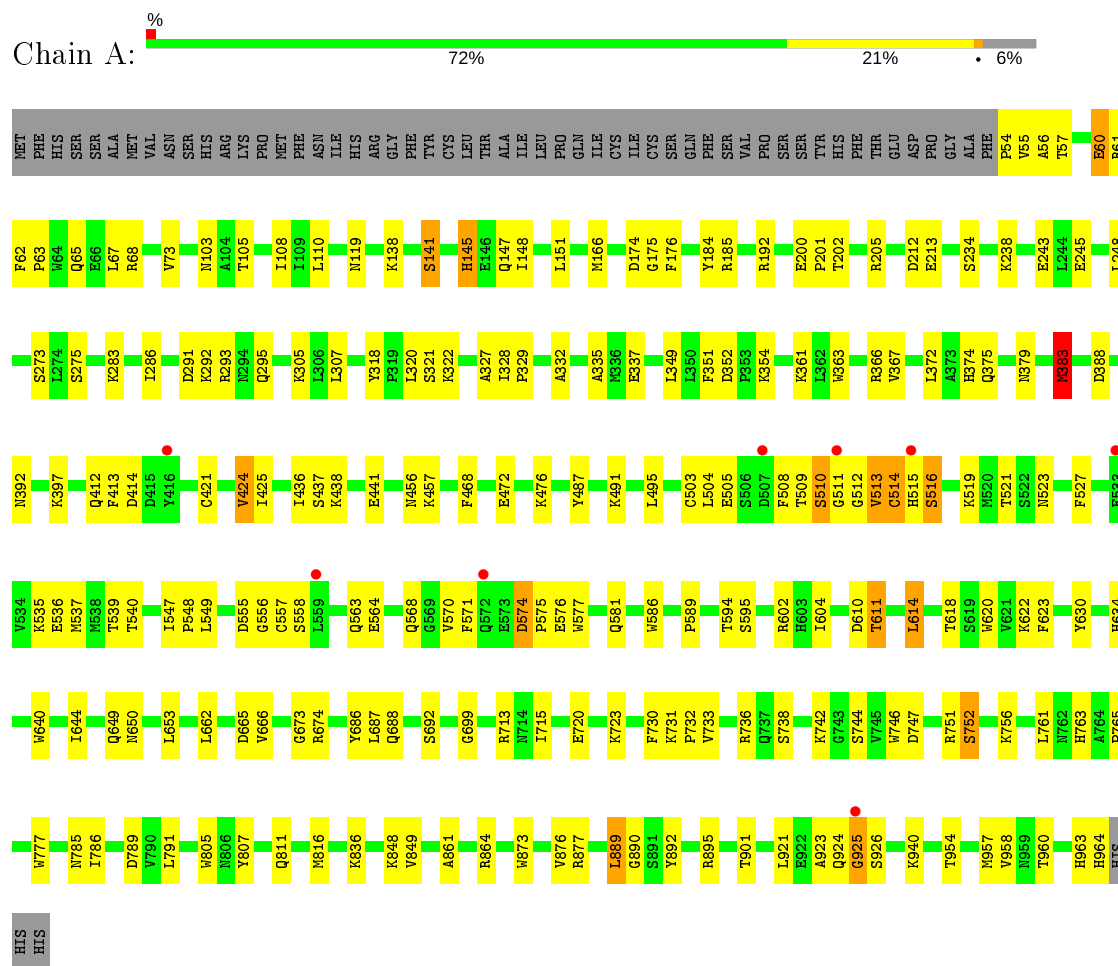
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	278	Total	O	0	0
			278	278		
10	C	125	Total	O	0	0
			125	125		



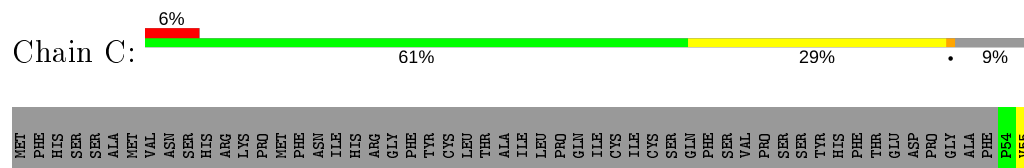
### 3 Residue-property plots

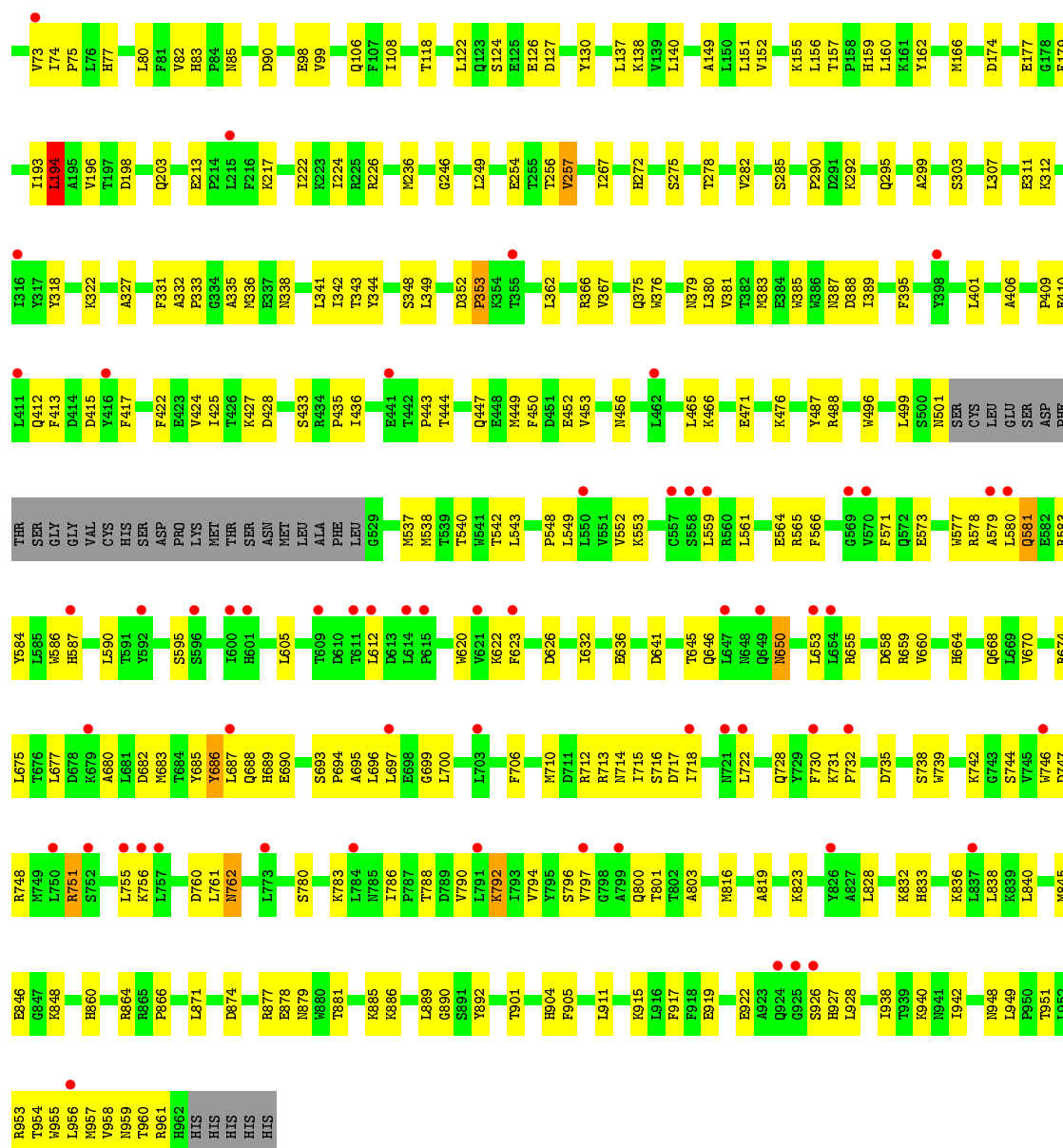
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

#### • Molecule 1: ENDOPLASMATIC RETICULUM AMINOPEPTIDASE 2



#### • Molecule 1: ENDOPLASMATIC RETICULUM AMINOPEPTIDASE 2





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

Chain B:  100%

UAG1  
UAG2

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

Chain H:  50% 50%

UAG1  
UAG2

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

Chain J:  50% 50%

UAG1  
UAG2

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

Chain D:  100%


UAG1  
UAG2  
BMA3

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

Chain G:  33% 67%

UAG1  
UAG2  
BMA3

- Molecule 5: beta-D-mannopyranose-(1-4)-[beta-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 I:  80% 20%

UAG1  
UAG2  
BMA3  
BMA4  
BMA5

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	75.35Å 134.42Å 129.00Å 90.00° 90.49° 90.00°	Depositor
Resolution (Å)	65.73 – 2.50 67.21 – 2.50	Depositor EDS
% Data completeness (in resolution range)	99.4 (65.73-2.50) 93.7 (67.21-2.50)	Depositor EDS
$R_{merge}$	0.11	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.37 (at 2.51Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, $R_{free}$	0.198 , 0.258 0.202 , 0.259	Depositor DCC
$R_{free}$ test set	4421 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	45.2	Xtriage
Anisotropy	0.410	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 51.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.017 for -h,-l,-k 0.003 for -h,l,k 0.028 for h,-k,-l	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	15615	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	59.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.80% 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, BMA, 7GA, NAG, EDO, MES, 2X0, LYN

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	0.50	0/7620	0.62	1/10327 (0.0%)
1	C	0.41	0/7395	0.57	1/10021 (0.0%)
2	E	0.73	0/65	0.85	0/85
2	F	0.39	0/65	0.65	0/85
All	All	0.46	0/15145	0.60	2/20518 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
1	A	383	MET	CG-SD-CE	-5.80	90.91	100.20
1	C	194	LEU	CA-CB-CG	5.38	127.67	115.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	889	LEU	Peptide

## 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	7425	0	7350	149	0
1	C	7208	0	7148	198	0
2	E	93	0	91	14	0
2	F	93	0	92	12	0
3	B	28	0	25	0	0
3	H	28	0	25	0	0
3	J	28	0	25	0	0
4	D	39	0	34	0	0
4	G	39	0	34	1	0
5	I	61	0	52	3	0
6	A	1	0	0	0	0
6	C	1	0	0	0	0
7	A	56	0	52	1	0
7	C	84	0	78	0	0
8	A	8	0	12	3	0
8	C	8	0	12	1	0
9	A	12	0	12	0	0
10	A	278	0	0	28	0
10	C	125	0	0	23	0
All	All	15615	0	15042	366	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 12.

The worst 5 of 366 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:C:922:GLU:HA	1:C:926:SER:HB3	1.46	0.97
1:C:424:VAL:HG22	1:C:452:GLU:HB3	1.50	0.94
1:A:720:GLU:OE2	10:A:3217:HOH:O	1.86	0.93
1:C:424:VAL:HG21	1:C:456:ASN:HB2	1.48	0.93
1:A:508:PHE:H	1:A:509:THR:HA	1.36	0.88

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	913/967 (94%)	851 (93%)	56 (6%)	6 (1%)	22	39
1	C	882/967 (91%)	815 (92%)	61 (7%)	6 (1%)	22	39
2	E	7/10 (70%)	3 (43%)	2 (29%)	2 (29%)	0	0
2	F	7/10 (70%)	3 (43%)	3 (43%)	1 (14%)	0	0
All	All	1809/1954 (93%)	1672 (92%)	122 (7%)	15 (1%)	19	35

5 of 15 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	510	SER
1	A	516	SER
2	E	4	HIS
2	F	4	HIS
1	A	730	PHE

### 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	822/870 (94%)	801 (97%)	21 (3%)	46	72
1	C	796/870 (92%)	775 (97%)	21 (3%)	46	72
2	E	6/6 (100%)	4 (67%)	2 (33%)	0	0
2	F	6/6 (100%)	5 (83%)	1 (17%)	2	4
All	All	1630/1752 (93%)	1585 (97%)	45 (3%)	43	70

5 of 45 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	963	HIS
1	C	194	LEU
1	C	961	ARG
1	C	159	HIS
1	C	257	VAL

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

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

2 non-standard protein/DNA/RNA residues 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	LYN	E	10	2	9,9,9	1.41	1 (11%)	9,10,10	0.93	1 (11%)
2	LYN	F	10	2	9,9,9	1.38	1 (11%)	9,10,10	0.77	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
2	LYN	E	10	2	-	5/9/9/9	-
2	LYN	F	10	2	-	2/9/9/9	-

All (2) bond length outliers are listed below:



Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	10	LYN	C-NT	4.05	1.43	1.32
2	F	10	LYN	C-NT	4.00	1.43	1.32

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	10	LYN	CA-C-NT	2.04	120.18	116.68

There are no chirality outliers.

5 of 7 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	E	10	LYN	O-C-CA-CB
2	E	10	LYN	NT-C-CA-CB
2	F	10	LYN	O-C-CA-N
2	F	10	LYN	NT-C-CA-N
2	E	10	LYN	CA-CB-CG-CD

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	E	10	LYN	1	0

## 5.5 Carbohydrates ⓘ

17 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	$\# Z  > 2$
3	NAG	B	1	1,3	14,14,15	0.56	0	17,19,21	0.42	0
3	NAG	B	2	3	14,14,15	0.47	0	17,19,21	0.51	0
4	NAG	D	1	1,4	14,14,15	0.61	0	17,19,21	0.65	1 (5%)
4	NAG	D	2	4	14,14,15	0.67	1 (7%)	17,19,21	0.51	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	BMA	D	3	4	11,11,12	0.80	0	15,15,17	1.38	2 (13%)
4	NAG	G	1	1,4	14,14,15	0.32	0	17,19,21	1.05	2 (11%)
4	NAG	G	2	4	14,14,15	1.15	1 (7%)	17,19,21	1.24	1 (5%)
4	BMA	G	3	4	11,11,12	1.64	2 (18%)	15,15,17	2.27	5 (33%)
3	NAG	H	1	1,3	14,14,15	1.54	1 (7%)	17,19,21	1.20	3 (17%)
3	NAG	H	2	3	14,14,15	0.26	0	17,19,21	0.35	0
5	NAG	I	1	1,5	14,14,15	0.42	0	17,19,21	0.61	0
5	NAG	I	2	5	14,14,15	1.14	1 (7%)	17,19,21	1.44	2 (11%)
5	BMA	I	3	5	11,11,12	1.97	2 (18%)	15,15,17	1.27	2 (13%)
5	BMA	I	4	5	11,11,12	1.36	2 (18%)	15,15,17	1.43	2 (13%)
5	BMA	I	5	5	11,11,12	1.18	1 (9%)	15,15,17	1.25	2 (13%)
3	NAG	J	1	1,3	14,14,15	0.70	1 (7%)	17,19,21	0.53	0
3	NAG	J	2	3	14,14,15	0.31	0	17,19,21	0.68	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
3	NAG	B	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	B	2	3	-	0/6/23/26	0/1/1/1
4	NAG	D	1	1,4	-	0/6/23/26	0/1/1/1
4	NAG	D	2	4	-	0/6/23/26	0/1/1/1
4	BMA	D	3	4	-	2/2/19/22	0/1/1/1
4	NAG	G	1	1,4	-	2/6/23/26	0/1/1/1
4	NAG	G	2	4	-	2/6/23/26	0/1/1/1
4	BMA	G	3	4	-	2/2/19/22	0/1/1/1
3	NAG	H	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	H	2	3	-	2/6/23/26	0/1/1/1
5	NAG	I	1	1,5	-	2/6/23/26	0/1/1/1
5	NAG	I	2	5	-	0/6/23/26	0/1/1/1
5	BMA	I	3	5	-	2/2/19/22	0/1/1/1
5	BMA	I	4	5	-	2/2/19/22	0/1/1/1
5	BMA	I	5	5	-	0/2/19/22	0/1/1/1
3	NAG	J	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	J	2	3	-	4/6/23/26	0/1/1/1

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	H	1	NAG	O5-C1	-5.48	1.35	1.43
5	I	3	BMA	C2-C3	-4.72	1.45	1.52
5	I	2	NAG	O5-C1	-4.21	1.37	1.43
4	G	2	NAG	O5-C1	4.10	1.50	1.43
4	G	3	BMA	C1-C2	3.98	1.61	1.52

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	G	3	BMA	C1-O5-C5	6.01	120.33	112.19
4	G	2	NAG	C1-O5-C5	4.56	118.37	112.19
5	I	2	NAG	O4-C4-C3	-3.84	101.46	110.35
4	D	3	BMA	C1-O5-C5	3.84	117.40	112.19
5	I	4	BMA	C1-O5-C5	3.78	117.31	112.19

There are no chirality outliers.

5 of 24 torsion outliers are listed below:

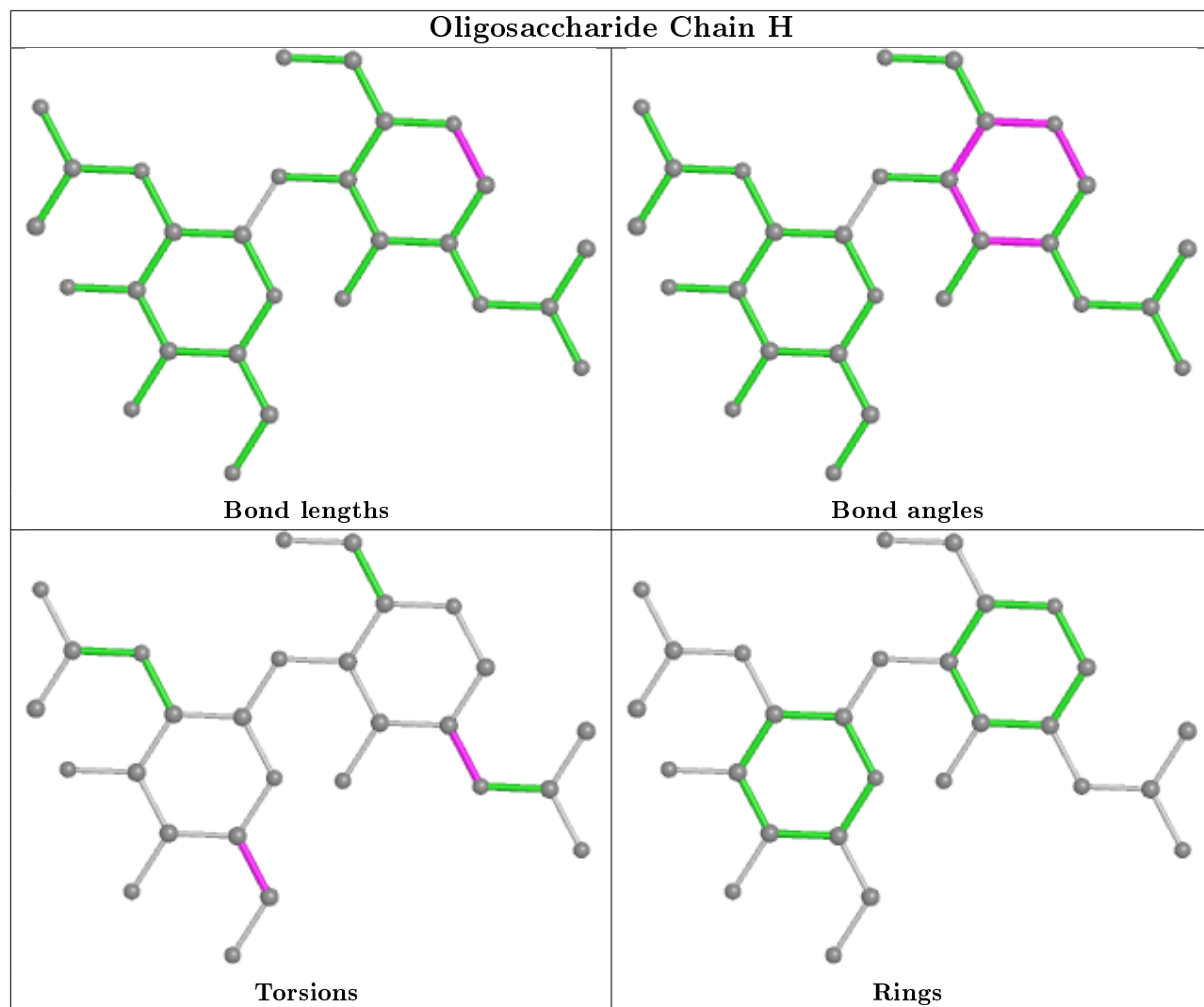
Mol	Chain	Res	Type	Atoms
3	H	1	NAG	C1-C2-N2-C7
3	B	1	NAG	O5-C5-C6-O6
4	D	3	BMA	O5-C5-C6-O6
5	I	3	BMA	O5-C5-C6-O6
3	H	2	NAG	O5-C5-C6-O6

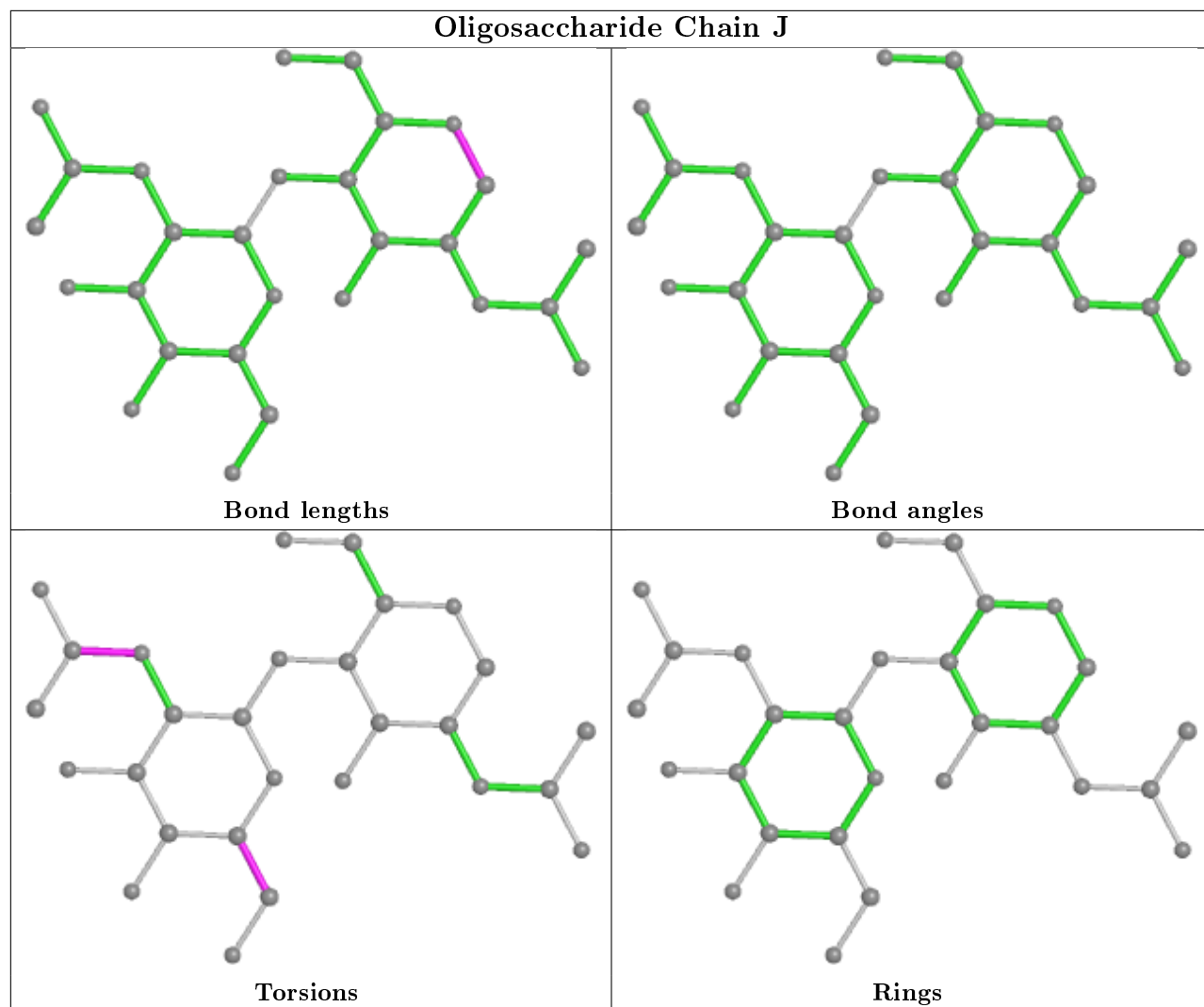
There are no ring outliers.

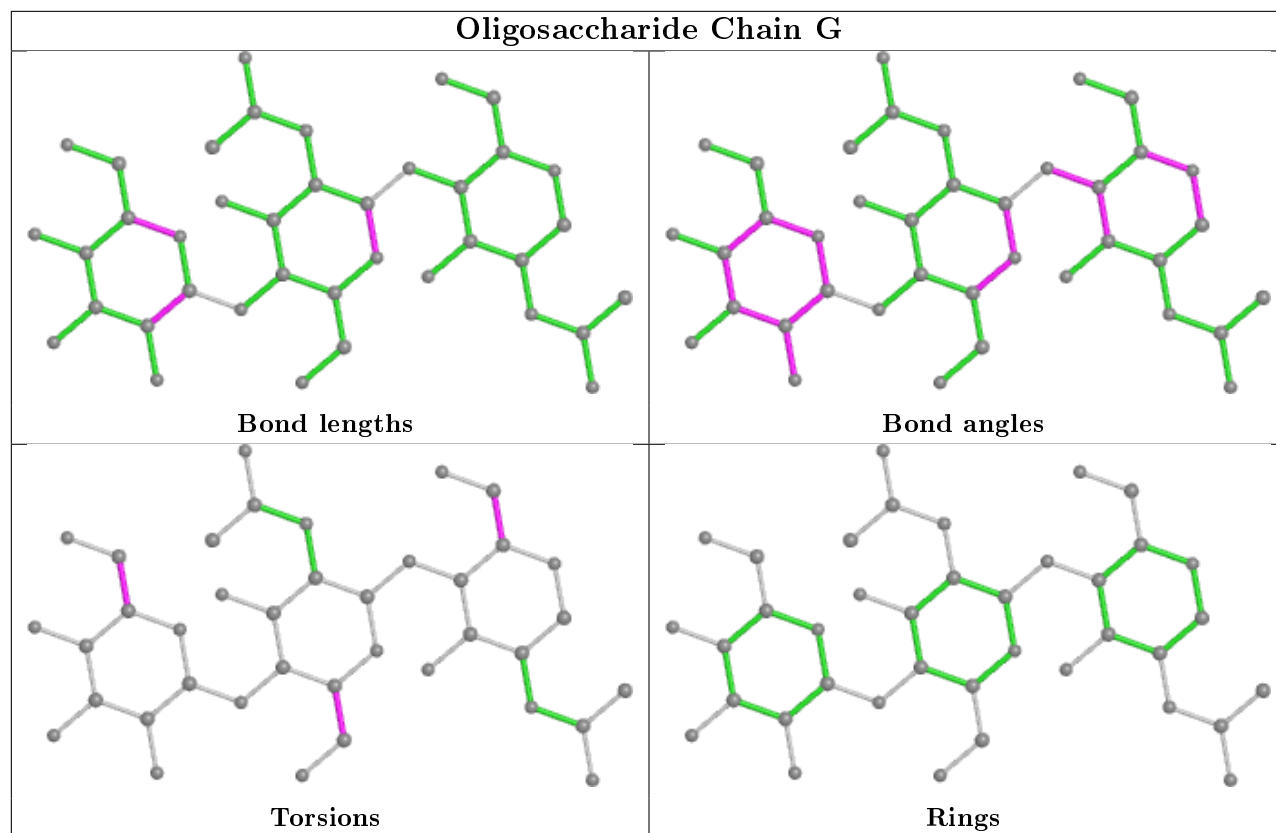
4 monomers are involved in 4 short contacts:

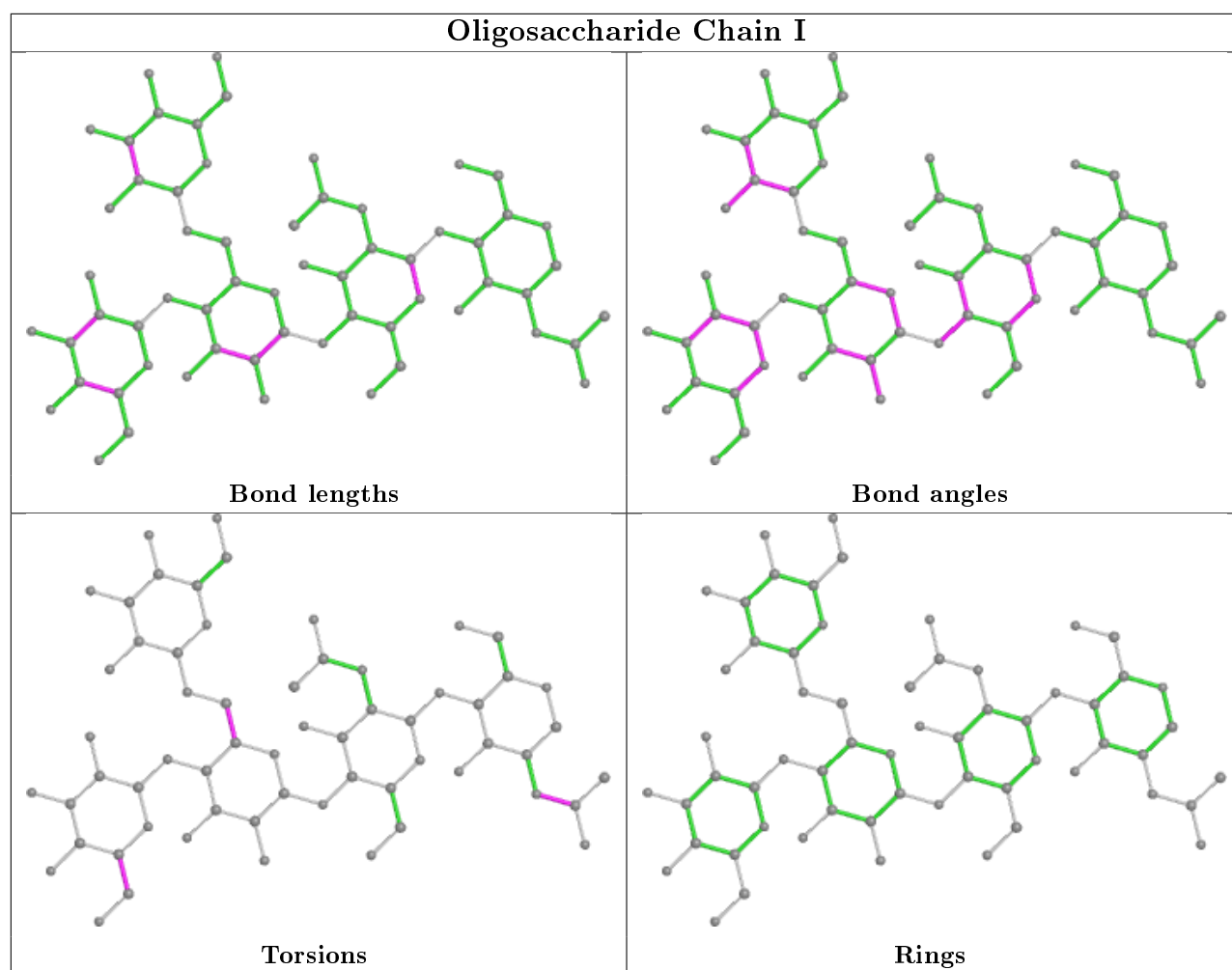
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	G	3	BMA	1	0
5	I	1	NAG	2	0
4	G	2	NAG	1	0
5	I	3	BMA	1	0

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









## 5.6 Ligand geometry [i](#)

Of 17 ligands modelled in this entry, 2 are monoatomic - leaving 15 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	$\# Z  > 2$
8	EDO	C	1963	-	3,3,3	0.53	0	2,2,2	0.61	0
7	NAG	C	1012	1	14,14,15	0.30	0	17,19,21	0.47	0
7	NAG	A	1081	1	14,14,15	0.58	0	17,19,21	0.82	1 (5%)
7	NAG	C	1006	1	14,14,15	0.68	0	17,19,21	0.64	0
7	NAG	C	1011	1	14,14,15	0.67	1 (7%)	17,19,21	0.62	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
8	EDO	C	1962	-	3,3,3	0.49	0	2,2,2	0.26	0
8	EDO	A	1965	-	3,3,3	0.33	0	2,2,2	0.44	0
7	NAG	A	1070	1	14,14,15	0.50	0	17,19,21	0.60	0
7	NAG	A	1082	1	14,14,15	0.36	0	17,19,21	0.51	0
8	EDO	A	1964	-	3,3,3	0.55	0	2,2,2	0.21	0
7	NAG	A	1069	1	14,14,15	0.92	1 (7%)	17,19,21	1.02	1 (5%)
7	NAG	C	1013	1	14,14,15	0.73	1 (7%)	17,19,21	0.76	1 (5%)
7	NAG	C	1010	1	14,14,15	0.21	0	17,19,21	0.48	0
7	NAG	C	1009	1	14,14,15	1.07	2 (14%)	17,19,21	0.88	1 (5%)
9	MES	A	2002	-	12,12,12	2.23	1 (8%)	14,16,16	2.20	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
8	EDO	C	1963	-	-	0/1/1/1	-
7	NAG	C	1012	1	-	3/6/23/26	0/1/1/1
7	NAG	A	1081	1	-	0/6/23/26	0/1/1/1
7	NAG	C	1006	1	-	0/6/23/26	0/1/1/1
7	NAG	C	1011	1	-	2/6/23/26	0/1/1/1
8	EDO	C	1962	-	-	0/1/1/1	-
8	EDO	A	1965	-	-	1/1/1/1	-
7	NAG	A	1070	1	-	2/6/23/26	0/1/1/1
7	NAG	A	1082	1	-	2/6/23/26	0/1/1/1
8	EDO	A	1964	-	-	0/1/1/1	-
7	NAG	A	1069	1	-	2/6/23/26	0/1/1/1
7	NAG	C	1013	1	-	0/6/23/26	0/1/1/1
7	NAG	C	1010	1	-	2/6/23/26	0/1/1/1
7	NAG	C	1009	1	-	2/6/23/26	0/1/1/1
9	MES	A	2002	-	-	3/6/14/14	0/1/1/1

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	A	2002	MES	C8-S	-7.36	1.67	1.77
7	A	1069	NAG	O5-C1	3.15	1.48	1.43
7	C	1009	NAG	O5-C1	-2.94	1.39	1.43
7	C	1011	NAG	O5-C1	-2.36	1.39	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	C	1009	NAG	C1-C2	2.23	1.55	1.52

The worst 5 of 11 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	A	2002	MES	C5-N4-C3	4.04	117.93	108.83
7	A	1069	NAG	C1-O5-C5	3.85	117.41	112.19
9	A	2002	MES	C7-N4-C5	3.12	119.20	111.23
7	A	1081	NAG	C1-O5-C5	3.07	116.35	112.19
9	A	2002	MES	O3S-S-C8	2.86	110.39	105.77

There are no chirality outliers.

5 of 19 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
9	A	2002	MES	N4-C7-C8-S
7	C	1009	NAG	O5-C5-C6-O6
7	C	1010	NAG	O5-C5-C6-O6
7	C	1010	NAG	C4-C5-C6-O6
7	C	1012	NAG	C8-C7-N2-C2

There are no ring outliers.

3 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	C	1962	EDO	1	0
8	A	1965	EDO	3	0
7	A	1069	NAG	1	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	911/967 (94%)	0.04	8 (0%) 84 86	22, 44, 77, 103	0
1	C	882/967 (91%)	0.37	59 (6%) 17 18	28, 68, 107, 125	0
2	E	7/10 (70%)	1.06	0 100 100	61, 66, 81, 84	0
2	F	7/10 (70%)	2.53	4 (57%) 0 0	75, 81, 95, 98	0
All	All	1807/1954 (92%)	0.22	71 (3%) 39 42	22, 54, 100, 125	0

The worst 5 of 71 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	580	LEU	5.6
2	F	9	PHE	4.5
2	F	7	PHE	4.5
1	C	746	TRP	4.4
1	C	559	LEU	4.1

### 6.2 Non-standard residues in protein, DNA, RNA chains [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	LYN	F	10	10/10	0.09	0.60	87,102,106,122	0
2	LYN	E	10	10/10	0.62	0.67	64,83,107,109	0

### 6.3 Carbohydrates ⓘ

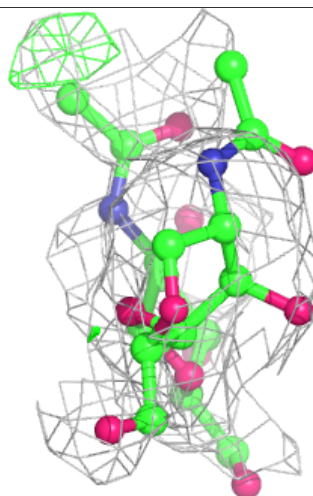
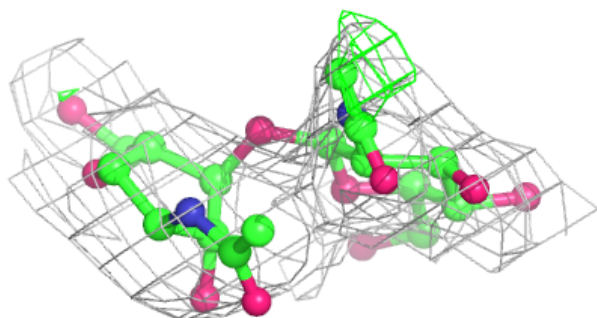
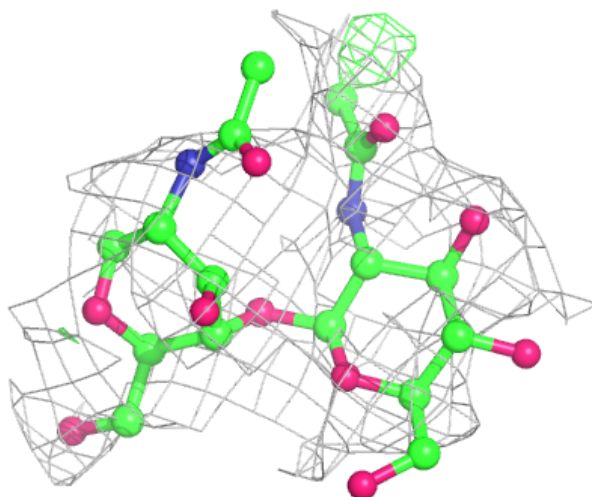
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 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
4	BMA	G	3	11/12	0.67	0.20	116,118,123,125	0
3	NAG	H	2	14/15	0.69	0.26	105,117,121,122	0
4	BMA	D	3	11/12	0.80	0.17	87,95,100,102	0
3	NAG	H	1	14/15	0.81	0.20	89,102,111,118	0
4	NAG	G	2	14/15	0.82	0.23	87,99,117,117	0
3	NAG	J	2	14/15	0.83	0.22	57,71,82,87	0
5	BMA	I	4	11/12	0.83	0.19	81,93,99,100	0
5	BMA	I	5	11/12	0.87	0.12	61,69,74,76	0
5	BMA	I	3	11/12	0.89	0.17	64,70,84,85	0
3	NAG	B	2	14/15	0.90	0.15	69,82,88,88	0
5	NAG	I	2	14/15	0.90	0.17	35,47,60,62	0
3	NAG	J	1	14/15	0.91	0.13	42,55,65,65	0
4	NAG	G	1	14/15	0.93	0.14	55,68,81,96	0
4	NAG	D	2	14/15	0.93	0.13	52,61,70,88	0
3	NAG	B	1	14/15	0.94	0.15	44,52,76,76	0
5	NAG	I	1	14/15	0.96	0.13	32,38,42,47	0
4	NAG	D	1	14/15	0.97	0.13	33,37,48,55	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.

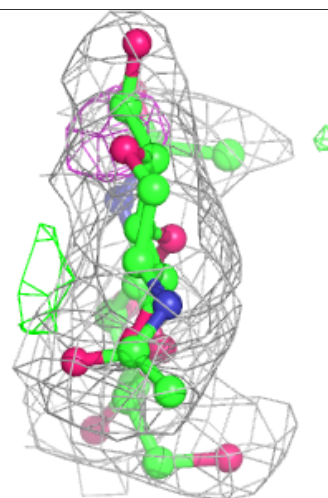
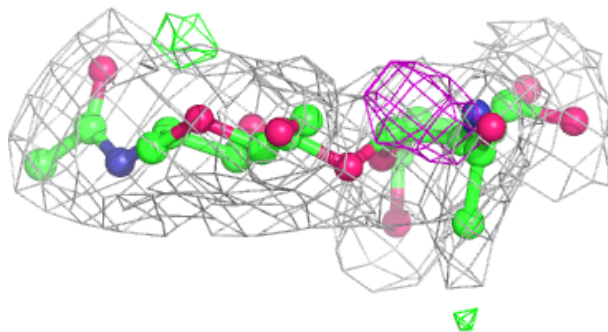
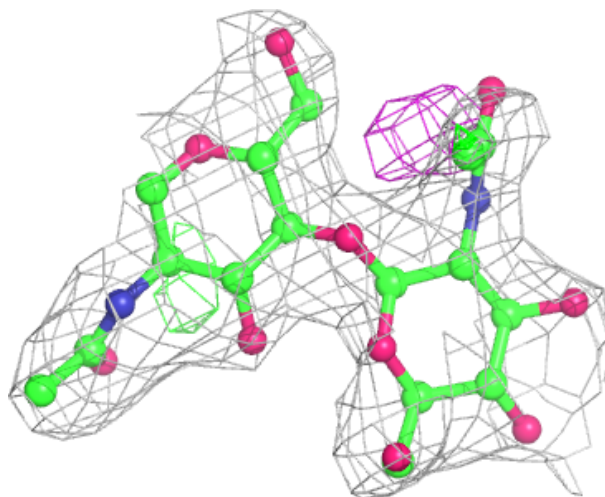
**Electron density around Chain H:**

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



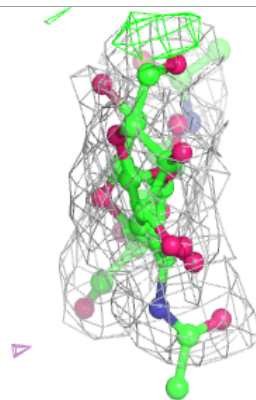
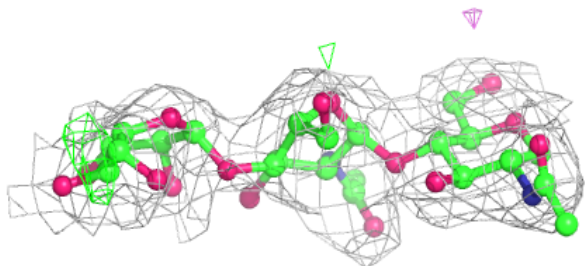
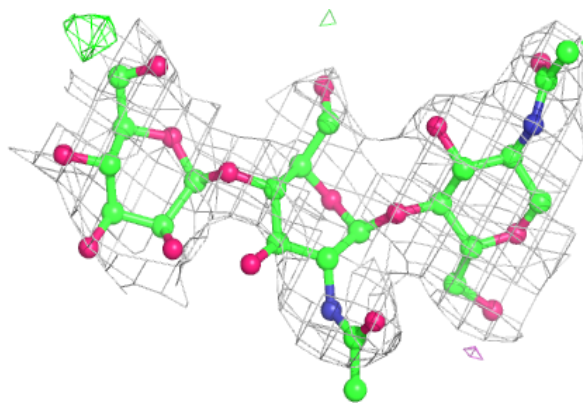
**Electron density around Chain J:**

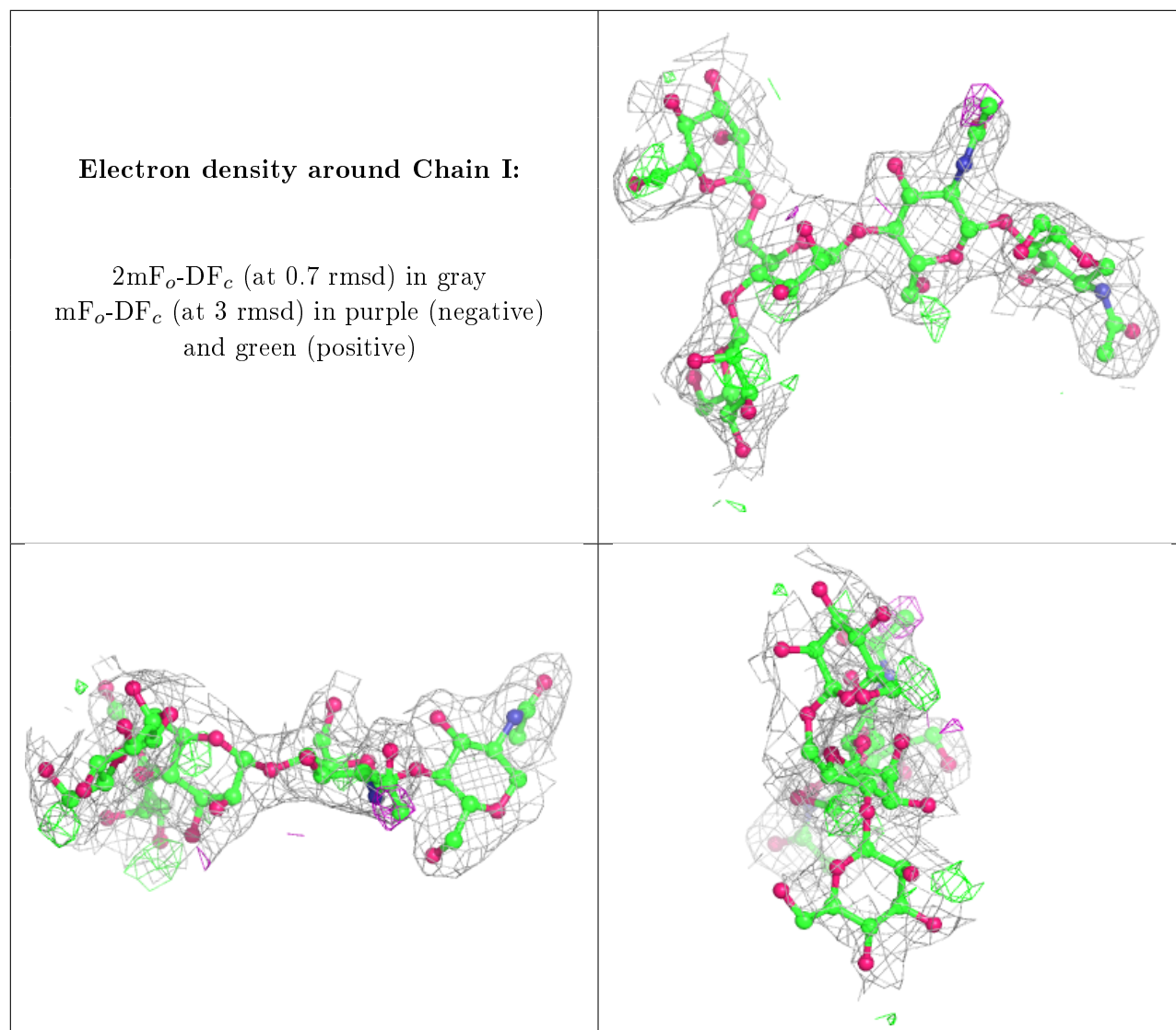
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around Chain G:**

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





## 6.4 Ligands ⓘ

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
7	NAG	A	1082	14/15	0.55	0.33	83,98,105,106	0
7	NAG	C	1013	14/15	0.56	0.32	108,122,126,127	0
7	NAG	C	1012	14/15	0.62	0.25	101,111,116,117	0
7	NAG	A	1069	14/15	0.71	0.21	84,98,99,101	0
8	EDO	A	1964	4/4	0.72	0.30	57,61,62,62	0
7	NAG	C	1006	14/15	0.74	0.20	96,107,113,123	0
7	NAG	C	1010	14/15	0.78	0.29	105,115,120,122	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
9	MES	A	2002	12/12	0.78	0.14	87,98,123,140	0
7	NAG	A	1081	14/15	0.79	0.18	88,103,108,112	0
7	NAG	C	1009	14/15	0.80	0.20	87,94,99,104	0
8	EDO	C	1963	4/4	0.81	0.20	89,91,96,99	0
7	NAG	C	1011	14/15	0.88	0.25	88,100,105,111	0
7	NAG	A	1070	14/15	0.90	0.13	72,85,96,97	0
8	EDO	C	1962	4/4	0.91	0.12	57,61,62,71	0
8	EDO	A	1965	4/4	0.91	0.17	56,59,61,74	0
6	ZN	A	1008	1/1	0.99	0.15	23,23,23,23	0
6	ZN	C	1020	1/1	0.99	0.12	39,39,39,39	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.