



# wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 7, 2020 – 11:29 PM BST

PDB ID : 2Y74  
Title : THE CRYSTAL STRUCTURE OF HUMAN SOLUBLE PRIMARY AMINE  
OXIDASE AOC3 IN THE OFF-COPPER CONFORMATION  
Authors : Elovaara, H.; Kidron, H.; Parkash, V.; Nymalm, Y.; Bligt, E.; Ollikka, P.;  
Smith, D.J.; Pihlavisto, M.; Salmi, M.; Jalkanen, S.; Salminen, T.A.  
Deposited on : 2011-01-28  
Resolution : 2.95 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

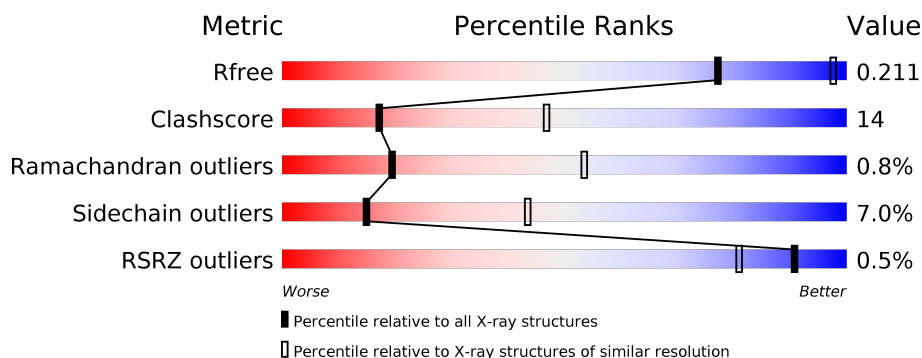
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.95 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	3104 (3.00-2.92)
Clashscore	141614	3462 (3.00-2.92)
Ramachandran outliers	138981	3340 (3.00-2.92)
Sidechain outliers	138945	3343 (3.00-2.92)
RSRZ outliers	127900	2986 (3.00-2.92)

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	763	<div> <div style="width: 67%;"></div> <div style="width: 21%;"></div> <div style="width: 9%;"></div> </div>
1	B	763	<div> <div style="width: 66%;"></div> <div style="width: 22%;"></div> <div style="width: 8%;"></div> </div>
2	C	3	<div> <div style="width: 67%;"></div> <div style="width: 33%;"></div> </div>
3	D	2	<div> <div style="width: 100%;"></div> </div>
3	E	2	<div> <div style="width: 100%;"></div> </div>
3	F	2	<div> <div style="width: 100%;"></div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	NAG	D	2	-	-	-	X
7	NAG	A	812	-	-	-	X
7	NAG	A	813	-	-	-	X
8	MAN	B	809	-	-	-	X

## 2 Entry composition [i](#)

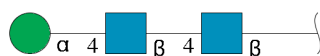
There are 9 unique types of molecules in this entry. The entry contains 11371 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 MEMBRANE PRIMARY AMINE OXIDASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	695	Total	C	N	O	S	0	0	0
			5490	3532	942	997	19			
1	B	699	Total	C	N	O	S	0	0	0
			5526	3551	950	1005	20			

- Molecule 2 is an oligosaccharide called 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
2	C	3	Total	C	N	O	0	0	0
			39	22	2	15			

- 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	D	2	Total	C	N	O	0	0	0
			28	16	2	10			
3	E	2	Total	C	N	O	0	0	0
			28	16	2	10			
3	F	2	Total	C	N	O	0	0	0
			28	16	2	10			

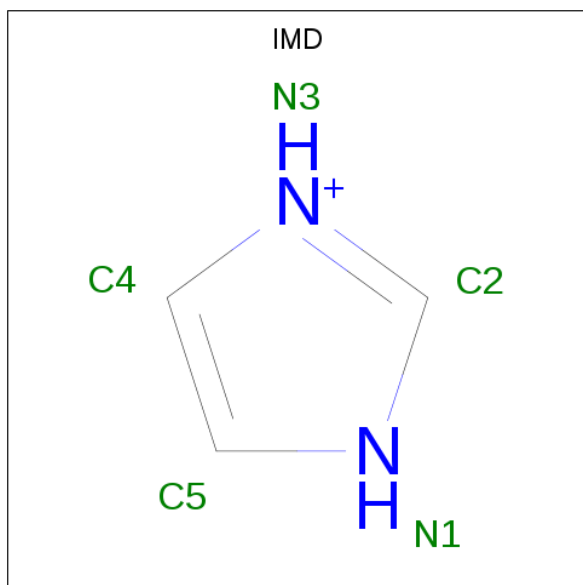
- Molecule 4 is COPPER (II) ION (three-letter code: CU) (formula: Cu).

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

- Molecule 5 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	B	2	Total Ca 2 2	0	0
5	A	2	Total Ca 2 2	0	0

- Molecule 6 is IMIDAZOLE (three-letter code: IMD) (formula: C<sub>3</sub>H<sub>5</sub>N<sub>2</sub>).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total C N 5 3 2	0	0
6	A	1	Total C N 5 3 2	0	0
6	A	1	Total C N 5 3 2	0	0
6	B	1	Total C N 5 3 2	0	0
6	B	1	Total C N 5 3 2	0	0
6	B	1	Total C N 5 3 2	0	0

- 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	B	1	Total	C	N	O	0	0
			14	8	1	5		
7	B	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 8 is alpha-D-mannopyranose (three-letter code: MAN) (formula:  $C_6H_{12}O_6$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	B	1	Total	C	O	0	0
			11	6	5		

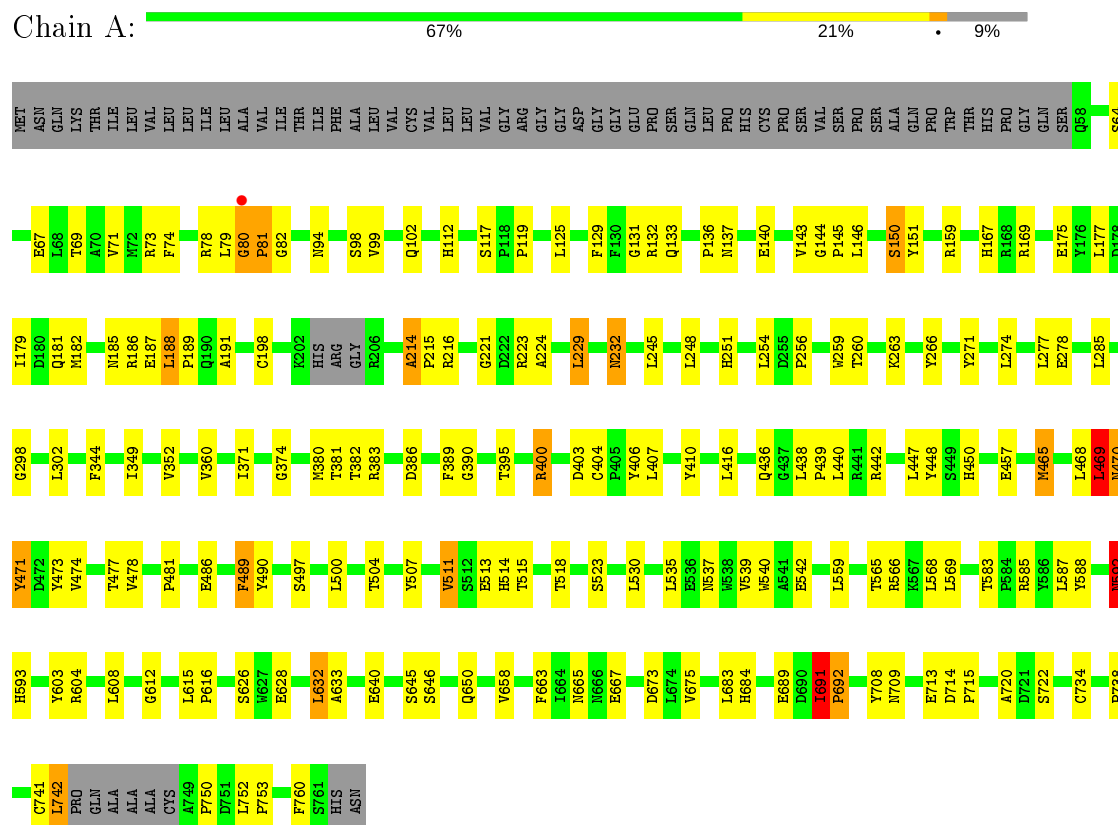
- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	60	Total	O	0	0
			60	60		
9	B	69	Total	O	0	0
			69	69		

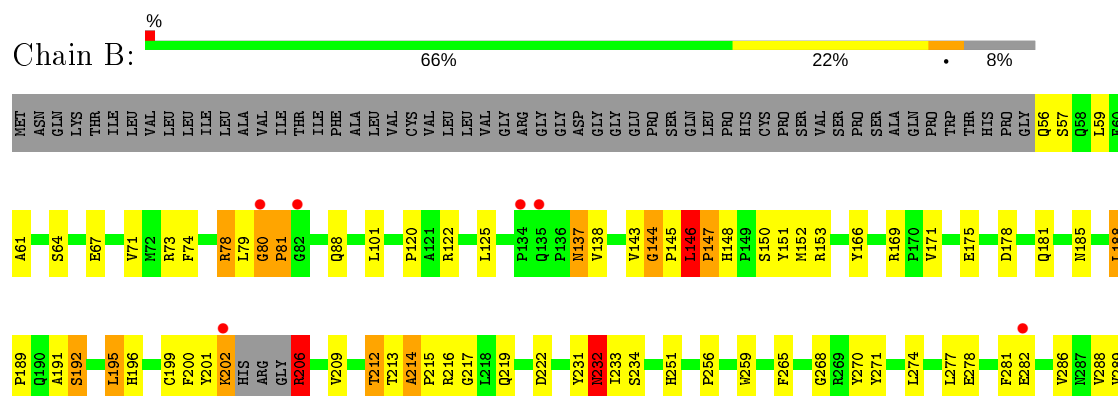
### 3 Residue-property plots

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.

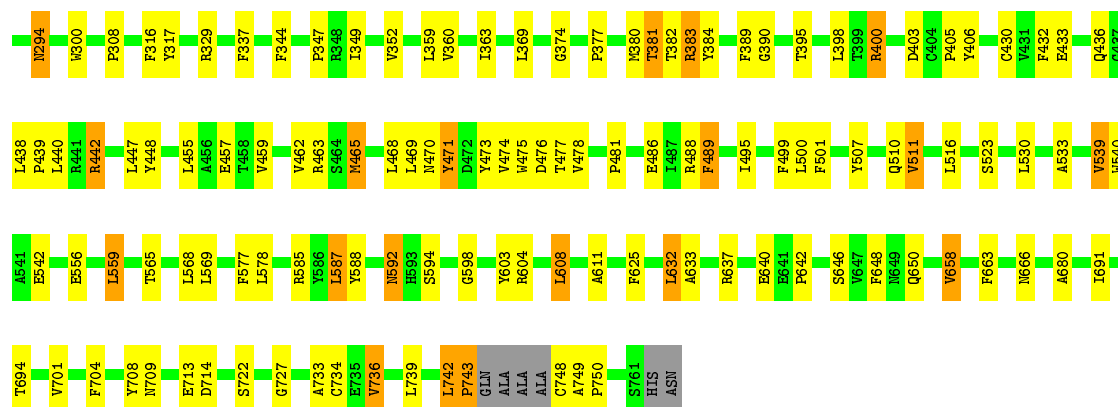
#### • Molecule 1: MEMBRANE PRIMARY AMINE OXIDASE



#### • Molecule 1: MEMBRANE PRIMARY AMINE OXIDASE







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



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



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



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



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 65 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	225.80 Å   225.80 Å   218.70 Å 90.00°   90.00°   120.00°	Depositor
Resolution (Å)	38.21 – 2.95 38.50 – 2.95	Depositor EDS
% Data completeness (in resolution range)	99.8 (38.21-2.95) 99.9 (38.50-2.95)	Depositor EDS
$R_{merge}$	0.14	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.09 (at 2.95 Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, $R_{free}$	0.179   ,   0.214 0.178   ,   0.211	Depositor DCC
$R_{free}$ test set	3503 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	35.6	Xtriage
Anisotropy	0.767	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 40.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	11371	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.68% 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

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: IMD, CA, T0I, MAN, CU, NAG

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	0.60	5/5644 (0.1%)	0.55	3/7694 (0.0%)
1	B	0.59	3/5681 (0.1%)	0.55	4/7744 (0.1%)
All	All	0.59	8/11325 (0.1%)	0.55	7/15438 (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	3
1	B	0	3
All	All	0	6

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	469	LEU	C-N	11.74	1.61	1.34
1	B	137	ASN	CG-ND2	6.99	1.50	1.32
1	B	232	ASN	CG-ND2	5.89	1.47	1.32
1	A	266	TYR	CD2-CE2	-5.41	1.31	1.39
1	A	232	ASN	CG-ND2	5.40	1.46	1.32

The worst 5 of 7 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	469	LEU	C-N-CA	-9.68	97.50	121.70
1	A	691	ILE	C-N-CD	-7.93	103.16	120.60
1	B	743	PRO	CB-CA-C	-6.88	94.80	112.00
1	A	592	ASN	N-CA-CB	6.36	122.04	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	592	ASN	CA-CB-CG	6.23	127.10	113.40

There are no chirality outliers.

5 of 6 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	146	LEU	Peptide
1	A	592	ASN	Sidechain
1	A	691	ILE	Peptide
1	B	137	ASN	Sidechain
1	B	146	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	5490	0	5243	143	0
1	B	5526	0	5280	167	0
2	C	39	0	34	5	0
3	D	28	0	25	3	0
3	E	28	0	22	0	0
3	F	28	0	25	4	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
5	A	2	0	0	0	0
5	B	2	0	0	0	0
6	A	15	0	15	0	0
6	B	15	0	15	0	0
7	A	28	0	26	2	0
7	B	28	0	26	2	0
8	B	11	0	10	0	0
9	A	60	0	0	1	0
9	B	69	0	0	3	0
All	All	11371	0	10721	305	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 14.

The worst 5 of 305 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:A:137:ASN:HD21	2:C:1:NAG:C1	1.25	1.45
1:B:214:ALA:HB1	1:B:215:PRO:CD	1.61	1.30
1:A:137:ASN:ND2	2:C:1:NAG:C1	2.01	1.24
1:B:206:ARG:HH11	1:B:206:ARG:HG2	0.95	1.09
1:B:214:ALA:HB1	1:B:215:PRO:HD2	1.31	1.07

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	688/763 (90%)	645 (94%)	38 (6%)	5 (1%)	22	56
1	B	692/763 (91%)	650 (94%)	36 (5%)	6 (1%)	17	51
All	All	1380/1526 (90%)	1295 (94%)	74 (5%)	11 (1%)	19	53

5 of 11 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	81	PRO
1	A	214	ALA
1	A	692	PRO
1	B	81	PRO
1	B	147	PRO

### 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	577/634 (91%)	543 (94%)	34 (6%)	19	50
1	B	583/634 (92%)	536 (92%)	47 (8%)	11	36
All	All	1160/1268 (92%)	1079 (93%)	81 (7%)	15	43

5 of 81 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	73	ARG
1	B	199	CYS
1	B	694	THR
1	B	78	ARG
1	B	153	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 6 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	470	ASN
1	A	699	ASN
1	A	537	ASN
1	A	267	GLN
1	A	650	GLN

### 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
1	T0I	A	471	1	17,19,20	1.27	1 (5%)	20,26,28	1.40	2 (10%)
1	T0I	B	471	1	17,19,20	1.27	2 (11%)	20,26,28	1.46	4 (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
1	T0I	A	471	1	-	4/9/10/12	0/2/2/2
1	T0I	B	471	1	-	4/9/10/12	0/2/2/2

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	471	T0I	C14-N13	-3.33	1.34	1.39
1	B	471	T0I	C14-N13	-3.29	1.34	1.39
1	B	471	T0I	CB-C1	-2.08	1.48	1.51

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	471	T0I	C1-CB-CA	3.86	120.49	114.53
1	B	471	T0I	C1-CB-CA	3.38	119.76	114.53
1	B	471	T0I	C3-C4-C5	3.11	120.06	117.91
1	A	471	T0I	C3-C4-C5	2.90	119.92	117.91
1	B	471	T0I	CB-CA-C	-2.55	106.69	111.47

There are no chirality outliers.

5 of 8 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	471	T0I	C-CA-CB-C1
1	A	471	T0I	N-CA-CB-C1
1	B	471	T0I	C-CA-CB-C1
1	B	471	T0I	N-CA-CB-C1
1	B	471	T0I	C6-C5-N13-C14

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	471	T0I	1	0
1	B	471	T0I	2	0

## 5.5 Carbohydrates ⓘ

9 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	NAG	C	1	2	14,14,15	2.62	6 (42%)	17,19,21	1.38	3 (17%)
2	NAG	C	2	2	14,14,15	2.17	6 (42%)	17,19,21	1.39	2 (11%)
2	MAN	C	3	2	11,11,12	2.09	4 (36%)	15,15,17	1.26	1 (6%)
3	NAG	D	1	1,3	14,14,15	2.30	6 (42%)	17,19,21	1.25	2 (11%)
3	NAG	D	2	3	14,14,15	2.30	6 (42%)	17,19,21	1.25	2 (11%)
3	NAG	E	1	1,3	14,14,15	2.66	6 (42%)	17,19,21	1.94	6 (35%)
3	NAG	E	2	3	14,14,15	2.66	9 (64%)	17,19,21	2.17	7 (41%)
3	NAG	F	1	1,3	14,14,15	2.53	6 (42%)	17,19,21	1.83	5 (29%)
3	NAG	F	2	3	14,14,15	2.23	8 (57%)	17,19,21	1.44	2 (11%)

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

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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	F	1	1,3	-	4/6/23/26	0/1/1/1
3	NAG	F	2	3	-	0/6/23/26	0/1/1/1

The worst 5 of 57 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	1	NAG	C3-C2	-5.73	1.40	1.52
2	C	1	NAG	C3-C2	-5.68	1.40	1.52
3	E	1	NAG	C3-C2	-5.55	1.40	1.52
2	C	2	NAG	O5-C5	5.01	1.53	1.43
2	C	1	NAG	C1-C2	-4.51	1.45	1.52

The worst 5 of 30 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	2	NAG	C2-N2-C7	-4.15	117.00	122.90
3	E	2	NAG	O5-C5-C6	-3.82	101.21	107.20
3	E	1	NAG	O5-C1-C2	-3.58	105.64	111.29
3	F	1	NAG	O4-C4-C3	-3.51	102.23	110.35
3	F	1	NAG	C1-C2-N2	-3.21	105.01	110.49

There are no chirality outliers.

5 of 17 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	D	2	NAG	C4-C5-C6-O6
3	D	1	NAG	C4-C5-C6-O6
2	C	2	NAG	O5-C5-C6-O6
3	D	2	NAG	O7-C7-N2-C2
3	D	1	NAG	O7-C7-N2-C2

All (1) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	3	MAN	C1-C2-C3-C4-C5-O5

5 monomers are involved in 12 short contacts:

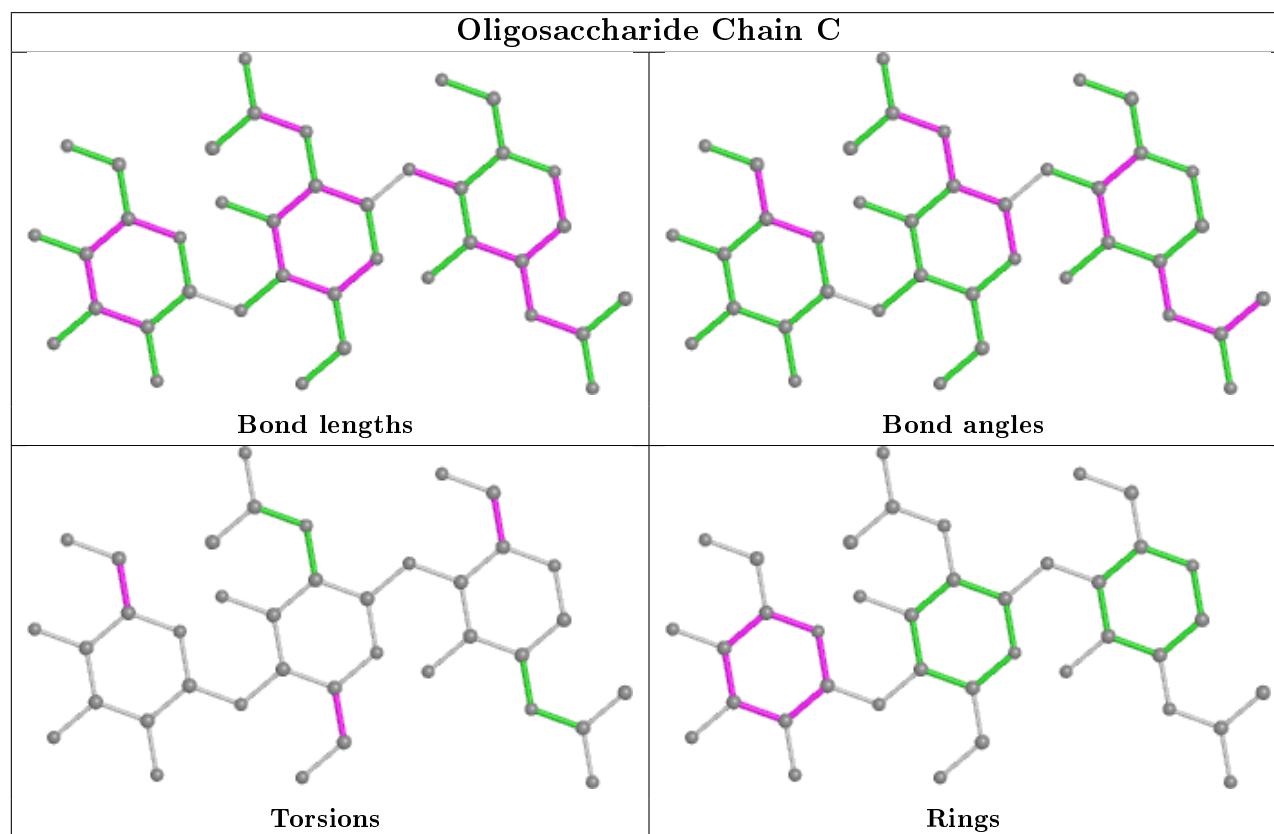
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	F	2	NAG	2	0
3	D	2	NAG	2	0

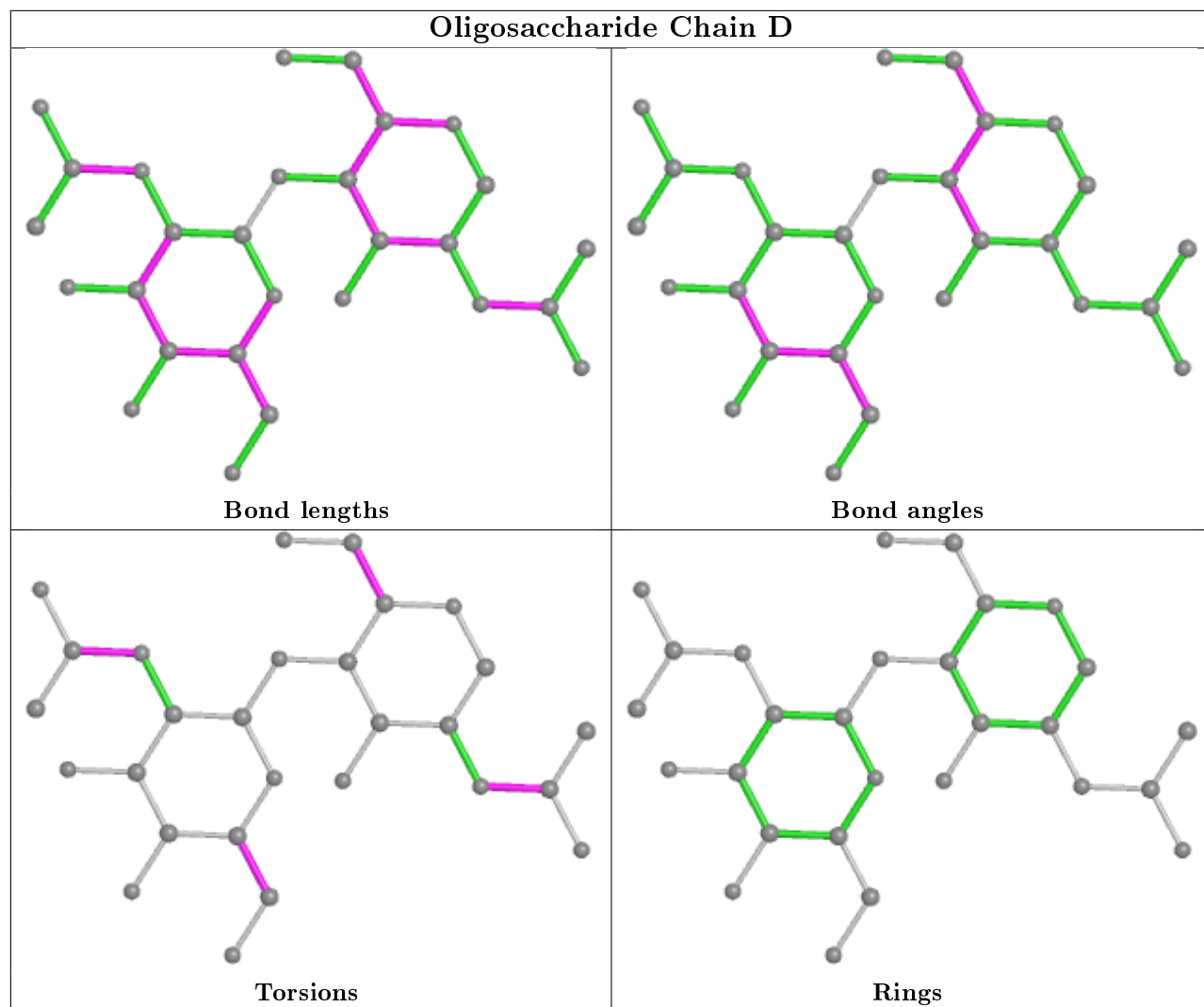
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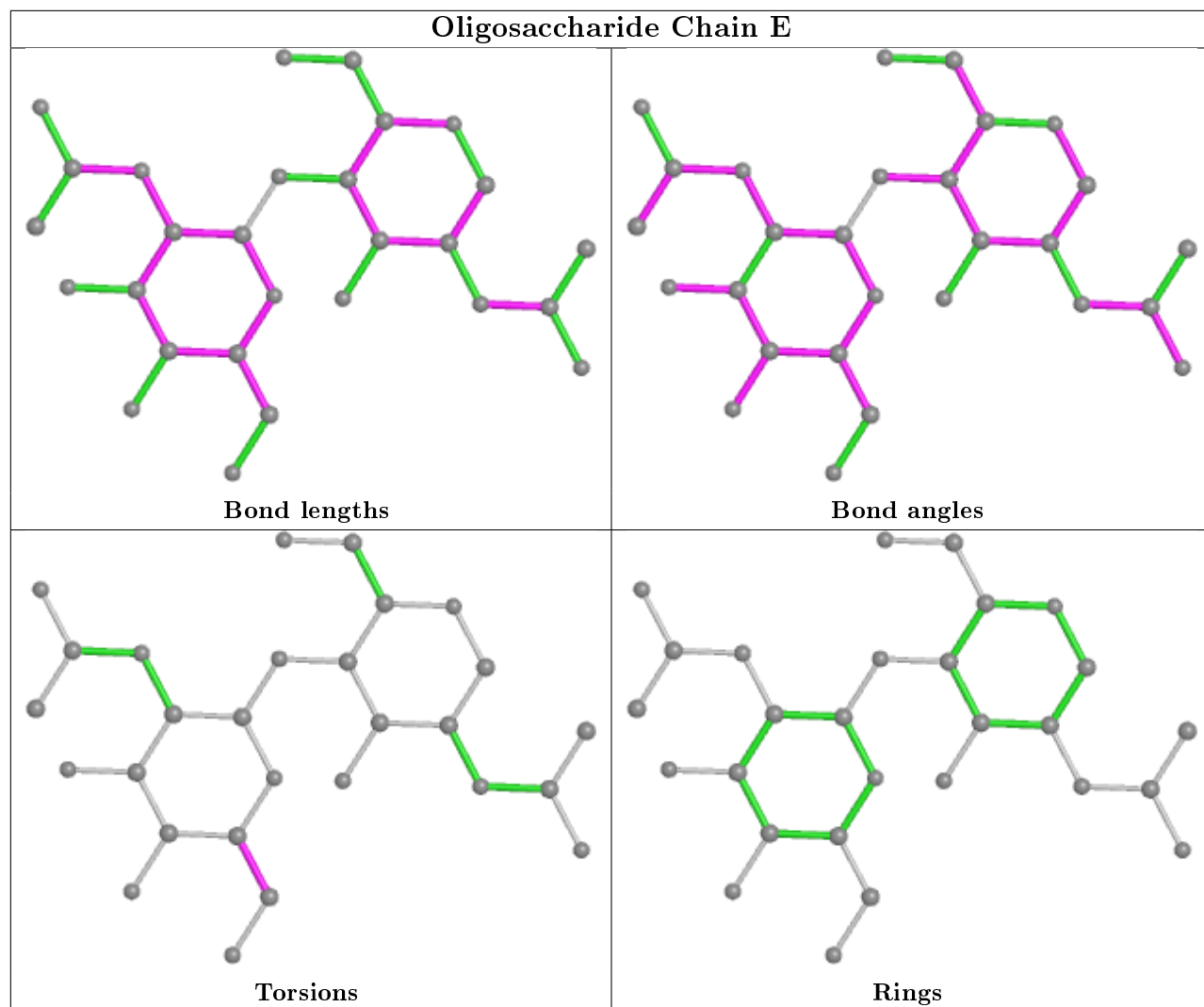
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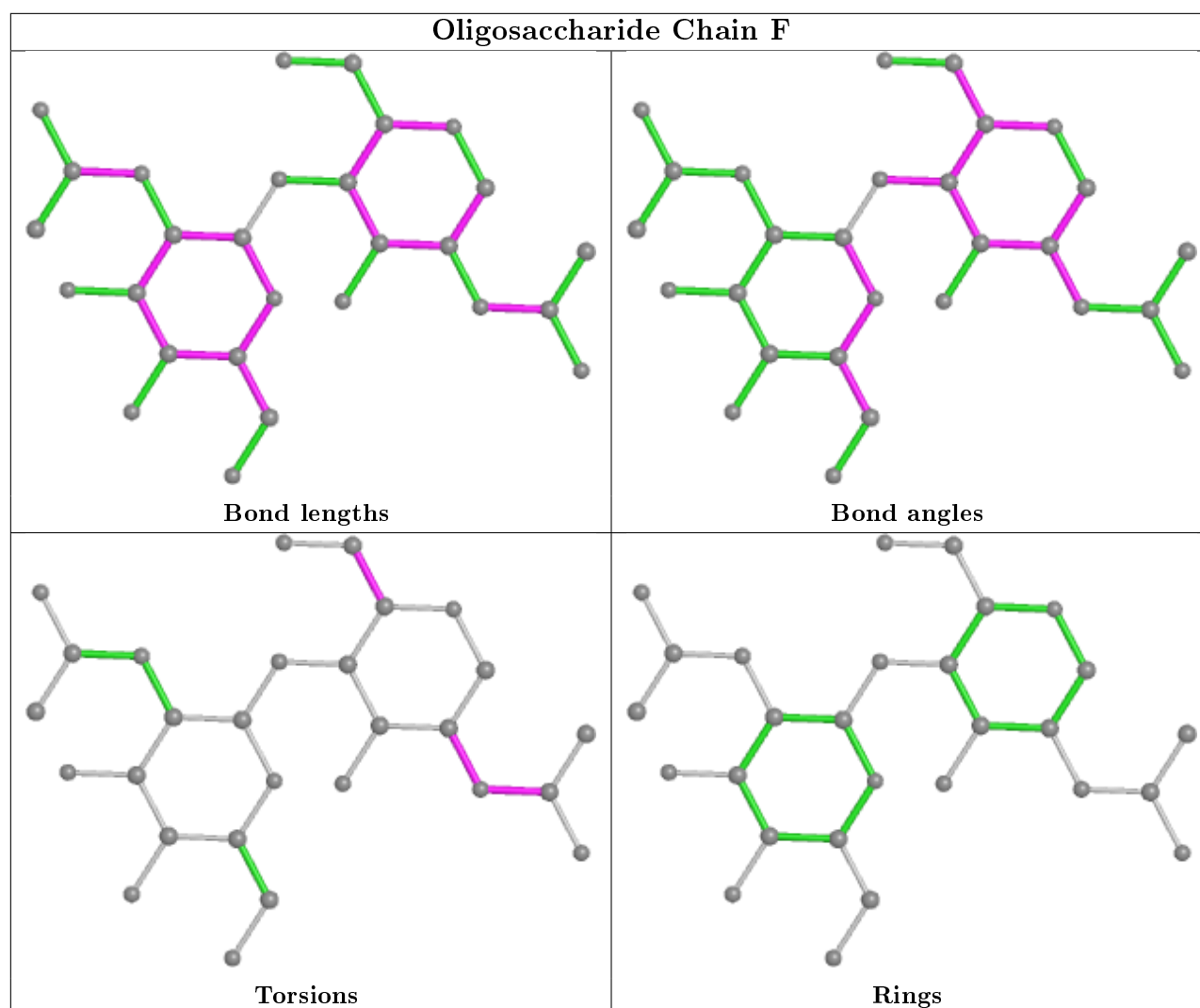
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	1	NAG	5	0
3	F	1	NAG	3	0
3	D	1	NAG	3	0

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, 6 are monoatomic - leaving 11 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	$\# Z  > 2$
7	NAG	B	811	1	14,14,15	0.70	0	17,19,21	0.92	0
6	IMD	A	806	-	3,5,5	1.02	0	4,5,5	0.84	0
6	IMD	B	806	-	3,5,5	1.02	0	4,5,5	0.88	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
8	MAN	B	809	-	11,11,12	2.08	4 (36%)	15,15,17	1.25	1 (6%)
6	IMD	B	805	-	3,5,5	1.52	0	4,5,5	0.82	0
7	NAG	A	813	1	14,14,15	0.52	0	17,19,21	0.82	0
6	IMD	B	804	-	3,5,5	0.79	0	4,5,5	0.65	0
6	IMD	A	804	-	3,5,5	0.41	0	4,5,5	0.55	0
7	NAG	B	810	1	14,14,15	2.18	5 (35%)	17,19,21	2.23	9 (52%)
7	NAG	A	812	1	14,14,15	1.02	1 (7%)	17,19,21	1.48	3 (17%)
6	IMD	A	805	-	3,5,5	1.08	0	4,5,5	1.04	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
7	NAG	B	811	1	-	2/6/23/26	0/1/1/1
6	IMD	A	806	-	-	-	0/1/1/1
6	IMD	B	806	-	-	-	0/1/1/1
8	MAN	B	809	-	-	2/2/19/22	1/1/1/1
6	IMD	B	805	-	-	-	0/1/1/1
7	NAG	A	813	1	-	2/6/23/26	0/1/1/1
6	IMD	B	804	-	-	-	0/1/1/1
6	IMD	A	804	-	-	-	0/1/1/1
7	NAG	B	810	1	-	4/6/23/26	0/1/1/1
7	NAG	A	812	1	-	4/6/23/26	0/1/1/1
6	IMD	A	805	-	-	-	0/1/1/1

The worst 5 of 10 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	B	810	NAG	C4-C3	-4.50	1.40	1.52
8	B	809	MAN	C4-C3	-4.17	1.41	1.52
7	B	810	NAG	C3-C2	-3.83	1.44	1.52
7	B	810	NAG	C7-N2	3.42	1.46	1.34
8	B	809	MAN	O5-C5	3.34	1.50	1.43

The worst 5 of 13 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	B	810	NAG	O5-C5-C6	4.35	114.02	107.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A	812	NAG	C1-O5-C5	-3.30	107.72	112.19
7	B	810	NAG	O6-C6-C5	3.16	122.12	111.29
8	B	809	MAN	O5-C5-C6	3.07	112.01	107.20
7	B	810	NAG	O5-C1-C2	-2.93	106.67	111.29

There are no chirality outliers.

5 of 14 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	B	810	NAG	C8-C7-N2-C2
7	B	810	NAG	O5-C5-C6-O6
7	B	810	NAG	O7-C7-N2-C2
7	A	812	NAG	C8-C7-N2-C2
7	A	812	NAG	O7-C7-N2-C2

All (1) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	B	809	MAN	C1-C2-C3-C4-C5-O5

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	B	810	NAG	2	0
7	A	812	NAG	2	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	469:LEU	C	470:ASN	N	1.61



## 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	694/763 (90%)	-0.49	1 (0%) 95 92	17, 31, 55, 87	0
1	B	698/763 (91%)	-0.55	6 (0%) 84 71	12, 30, 54, 90	0
All	All	1392/1526 (91%)	-0.52	7 (0%) 91 81	12, 31, 54, 90	0

The worst 5 of 7 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	134	PRO	2.9
1	B	135	GLN	2.7
1	B	80	GLY	2.7
1	A	80	GLY	2.6
1	B	82	GLY	2.4

### 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.

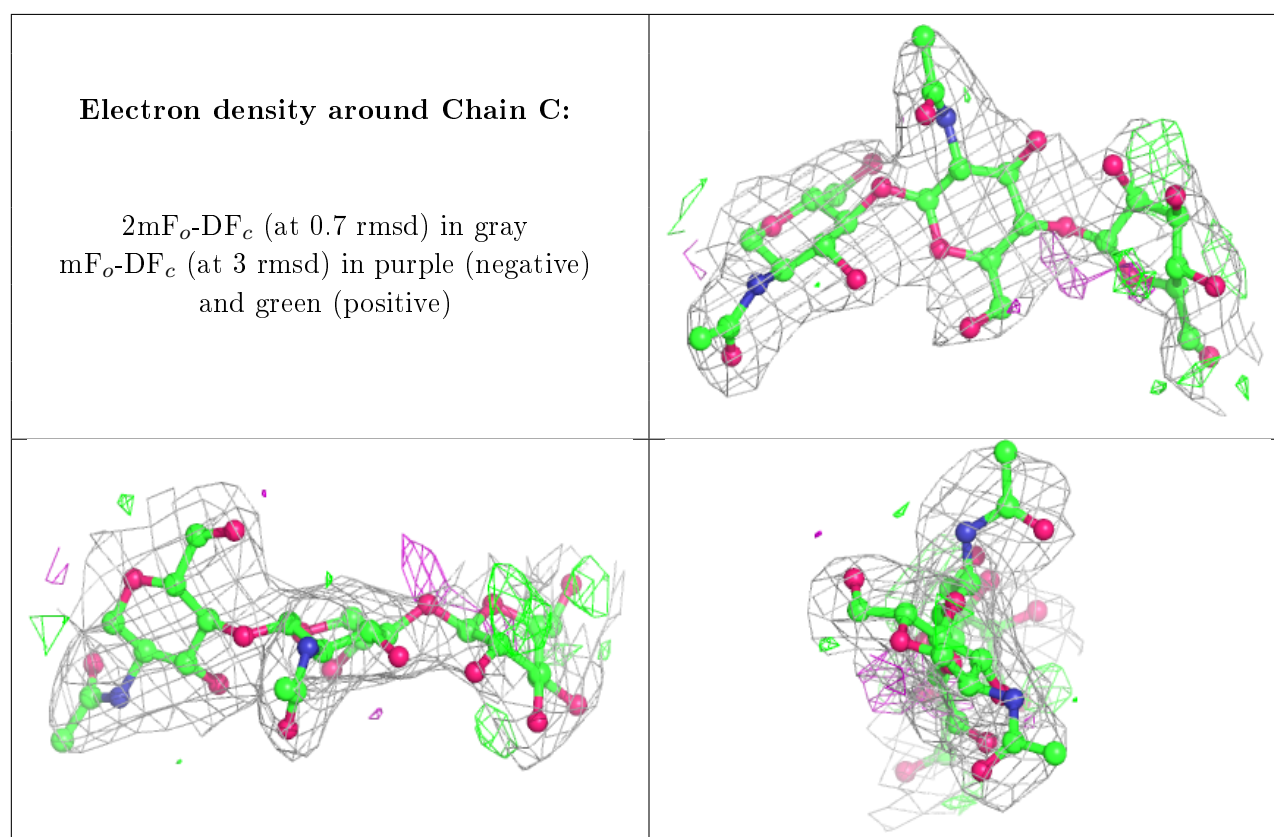
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
1	T0I	B	471	18/19	0.94	0.20	23,47,61,63	0
1	T0I	A	471	18/19	0.96	0.17	24,43,54,54	0

### 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.

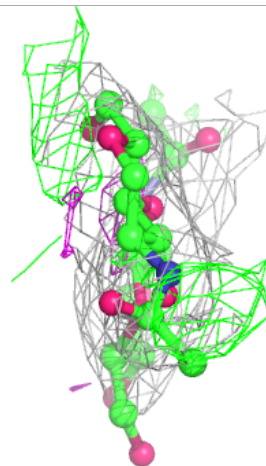
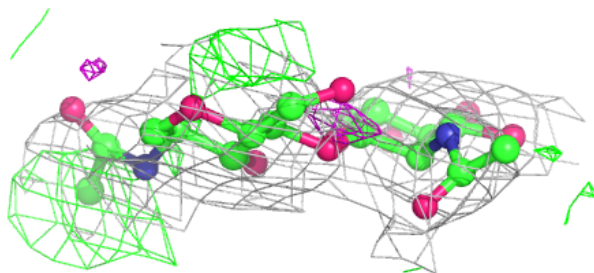
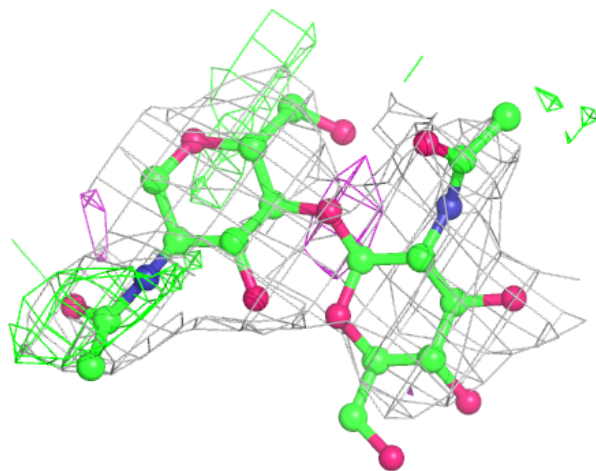
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	MAN	C	3	11/12	0.71	0.34	59,84,96,98	0
3	NAG	D	1	14/15	0.74	0.29	70,99,111,112	0
3	NAG	D	2	14/15	0.77	0.48	70,99,111,112	0
3	NAG	F	2	14/15	0.86	0.31	63,94,105,111	0
2	NAG	C	2	14/15	0.89	0.27	46,55,78,83	0
3	NAG	F	1	14/15	0.92	0.17	44,68,83,94	0
3	NAG	E	2	14/15	0.95	0.21	37,55,72,86	0
2	NAG	C	1	14/15	0.97	0.15	28,36,46,50	0
3	NAG	E	1	14/15	0.97	0.18	24,43,54,59	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.



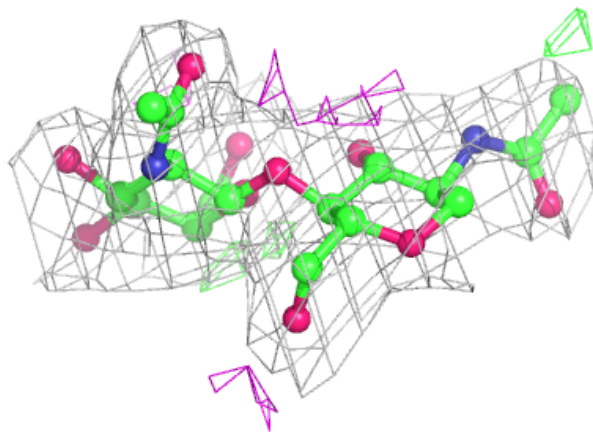
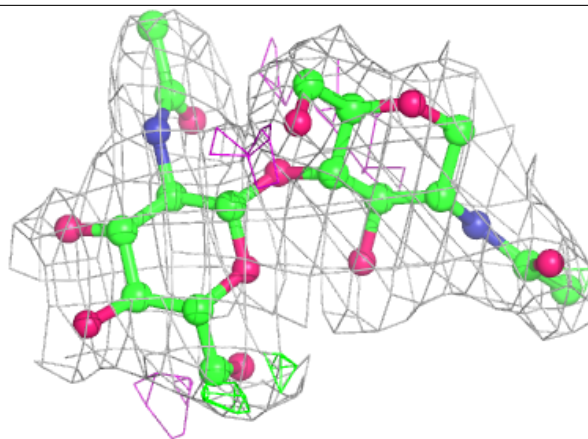
**Electron density around Chain D:**

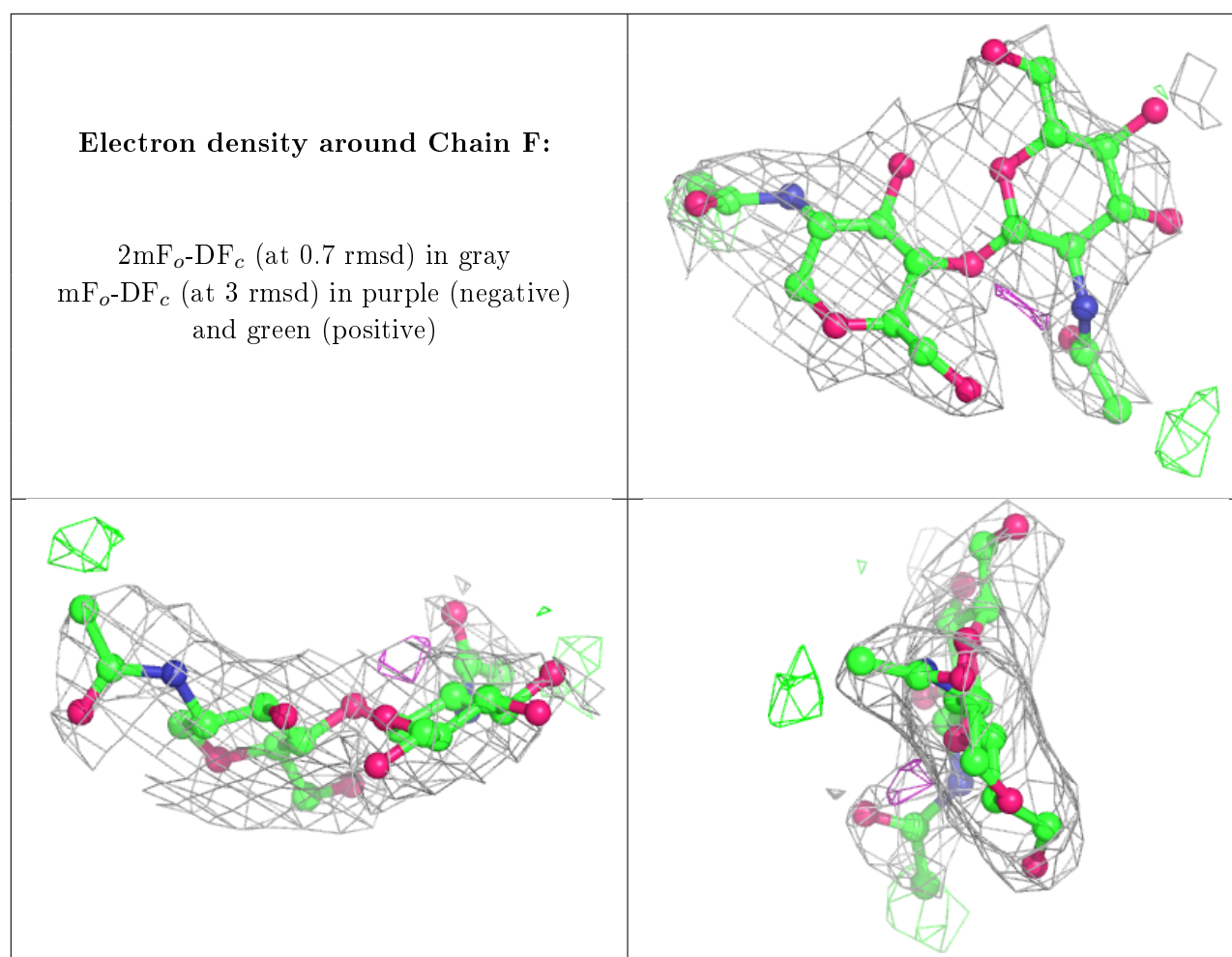
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**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 ⓘ

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
8	MAN	B	809	11/12	0.65	0.48	59,84,96,98	0
7	NAG	B	810	14/15	0.75	0.37	44,75,101,104	0
7	NAG	A	813	14/15	0.76	0.50	0,4,9,9	0
7	NAG	A	812	14/15	0.79	0.41	44,75,101,104	0
5	CA	B	803	1/1	0.81	0.10	33,33,33,33	0
7	NAG	B	811	14/15	0.87	0.51	0,4,9,9	0
5	CA	A	803	1/1	0.92	0.07	22,22,22,22	0
6	IMD	B	805	5/5	0.93	0.30	41,46,48,49	0
6	IMD	A	806	5/5	0.97	0.23	41,46,48,49	0
6	IMD	B	804	5/5	0.97	0.14	44,48,54,59	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
6	IMD	B	806	5/5	0.97	0.24	41,46,48,49	0
6	IMD	A	804	5/5	0.97	0.14	41,46,48,49	0
5	CA	A	802	1/1	0.97	0.07	30,30,30,30	0
4	CU	A	801	1/1	0.98	0.05	22,22,22,22	0
4	CU	B	801	1/1	0.98	0.14	31,31,31,31	0
6	IMD	A	805	5/5	0.98	0.24	41,46,48,49	0
5	CA	B	802	1/1	0.99	0.09	23,23,23,23	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.