



# wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 9, 2021 – 12:06 PM EDT

PDB ID : 7N19  
Title : DR3 in complex with *Aspergillus nidulans* NAD-dependent histone deacetylase hst4 peptide  
Authors : Wang, Y.; Dai, S.  
Deposited on : 2021-05-27  
Resolution : 2.38 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 : 2.23.1  
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) : 2.23.1

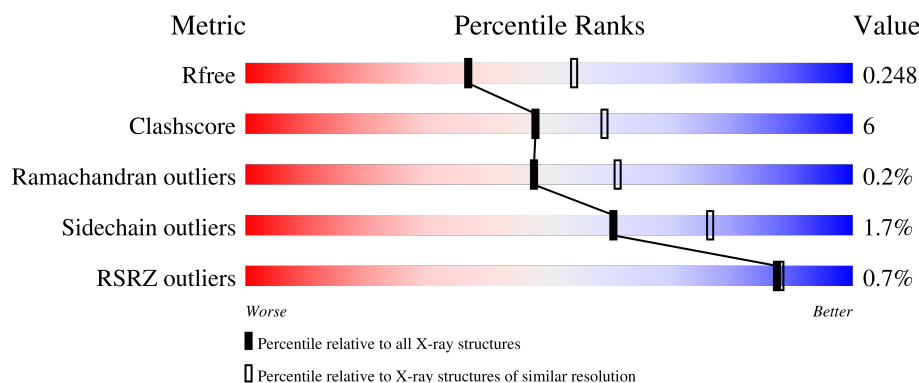
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*





The reported resolution of this entry is 2.38 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	5509 (2.40-2.36)
Clashscore	141614	6082 (2.40-2.36)
Ramachandran outliers	138981	5973 (2.40-2.36)
Sidechain outliers	138945	5975 (2.40-2.36)
RSRZ outliers	127900	5397 (2.40-2.36)

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 of 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	181	
1	D	181	
1	G	181	
1	J	181	
2	B	189	

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Mol	Chain	Length	Quality of chain
2	E	189	 84% 15% ..
2	H	189	 80% 19% .
2	K	189	 83% 14% ..
3	C	14	 14% 79% 7% 7% 7%
3	F	14	 7% 86% 7% 7%
3	I	14	 7% 79% 7% 7% 7%
3	L	14	 7% 71% 7% 14% 7%
4	M	2	 50% 50%
4	N	2	 50% 50%
4	O	2	 50% 50%
4	P	2	 50% 50%

## 2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 12988 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 HLA class II histocompatibility antigen, DR alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	179	Total	C	N	O	S	0	0	0
			1474	956	240	273	5			
1	D	179	Total	C	N	O	S	0	0	0
			1474	956	240	273	5			
1	G	179	Total	C	N	O	S	0	0	0
			1474	956	240	273	5			
1	J	179	Total	C	N	O	S	0	0	0
			1474	956	240	273	5			

- Molecule 2 is a protein called HLA class II histocompatibility antigen DR beta chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	187	Total	C	N	O	S	0	0	0
			1548	973	281	289	5			
2	E	187	Total	C	N	O	S	0	0	0
			1548	973	281	289	5			
2	H	187	Total	C	N	O	S	0	1	0
			1556	977	282	292	5			
2	K	187	Total	C	N	O	S	0	0	0
			1548	973	281	289	5			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	191	GLY	-	expression tag	UNP Q5Y7D1
B	192	GLY	-	expression tag	UNP Q5Y7D1
E	191	GLY	-	expression tag	UNP Q5Y7D1
E	192	GLY	-	expression tag	UNP Q5Y7D1
H	191	GLY	-	expression tag	UNP Q5Y7D1
H	192	GLY	-	expression tag	UNP Q5Y7D1
K	191	GLY	-	expression tag	UNP Q5Y7D1
K	192	GLY	-	expression tag	UNP Q5Y7D1

- Molecule 3 is a protein called HST4 peptide.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	C	13	Total	C	N	O	0	0	0
			91	52	21	18			
3	F	13	Total	C	N	O	0	0	0
			91	52	21	18			
3	I	13	Total	C	N	O	0	0	0
			91	52	21	18			
3	L	13	Total	C	N	O	0	0	0
			91	52	21	18			

- Molecule 4 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
4	M	2	Total	C	N	O	0	0	0
			28	16	2	10			
4	N	2	Total	C	N	O	0	0	0
			28	16	2	10			
4	O	2	Total	C	N	O	0	0	0
			28	16	2	10			
4	P	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 5 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C<sub>2</sub>H<sub>6</sub>O<sub>2</sub>).



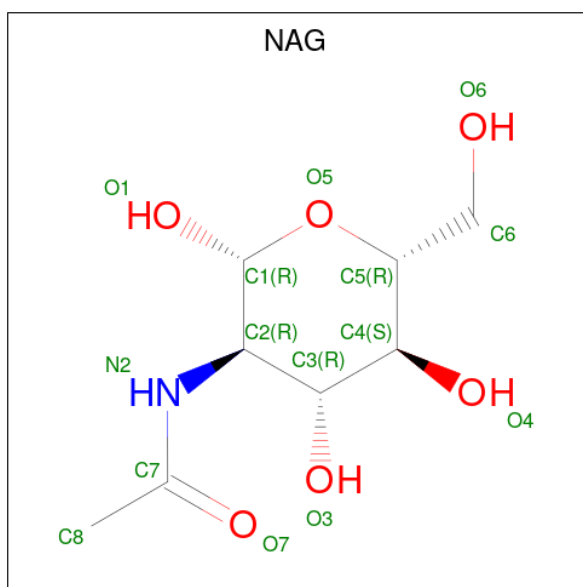
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			4	2	2		
5	B	1	Total	C	O	0	0
			4	2	2		
5	B	1	Total	C	O	0	0
			4	2	2		
5	B	1	Total	C	O	0	0
			4	2	2		
5	B	1	Total	C	O	0	0
			4	2	2		
5	B	1	Total	C	O	0	0
			4	2	2		
5	C	1	Total	C	O	0	0
			4	2	2		
5	C	1	Total	C	O	0	0
			4	2	2		
5	D	1	Total	C	O	0	0
			4	2	2		
5	E	1	Total	C	O	0	0
			4	2	2		
5	E	1	Total	C	O	0	0
			4	2	2		
5	E	1	Total	C	O	0	0
			4	2	2		
5	E	1	Total	C	O	0	0
			4	2	2		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	E	1	Total	C	O	0	0
			4	2	2		
5	H	1	Total	C	O	0	0
			4	2	2		
5	H	1	Total	C	O	0	0
			4	2	2		
5	H	1	Total	C	O	0	0
			4	2	2		
5	H	1	Total	C	O	0	0
			4	2	2		
5	I	1	Total	C	O	0	0
			4	2	2		
5	I	1	Total	C	O	0	0
			4	2	2		
5	J	1	Total	C	O	0	0
			4	2	2		
5	J	1	Total	C	O	0	0
			4	2	2		
5	K	1	Total	C	O	0	0
			4	2	2		
5	K	1	Total	C	O	0	0
			4	2	2		
5	K	1	Total	C	O	0	0
			4	2	2		
5	K	1	Total	C	O	0	0
			4	2	2		
5	K	1	Total	C	O	0	0
			4	2	2		
5	L	1	Total	C	O	0	0
			4	2	2		

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



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

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	48	Total	O	0	0
			48	48		
7	B	43	Total	O	0	0
			43	43		
7	C	4	Total	O	0	0
			4	4		
7	D	45	Total	O	0	0
			45	45		
7	E	30	Total	O	0	0
			30	30		
7	F	1	Total	O	0	0
			1	1		
7	G	21	Total	O	0	0
			21	21		
7	H	16	Total	O	0	0
			16	16		

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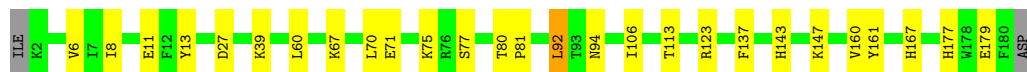
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	I	3	Total 3	O 3	0	0
7	J	14	Total 14	O 14	0	0
7	K	12	Total 12	O 12	0	0
7	L	3	Total 3	O 3	0	0

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


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

- Molecule 1: HLA class II histocompatibility antigen, DR alpha chain

Chain A: 




- Molecule 1: HLA class II histocompatibility antigen, DR alpha chain

Chain D: 




- Molecule 1: HLA class II histocompatibility antigen, DR alpha chain

Chain G: 




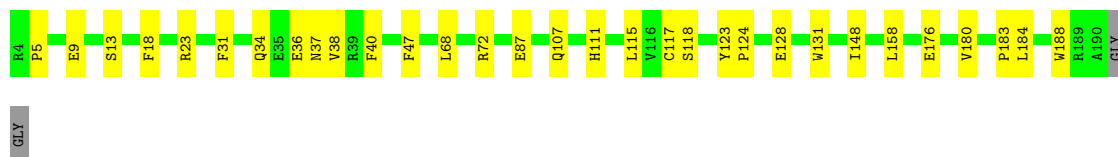
- Molecule 1: HLA class II histocompatibility antigen, DR alpha chain

Chain J: 




- Molecule 2: HLA class II histocompatibility antigen DR beta chain

Chain B: 




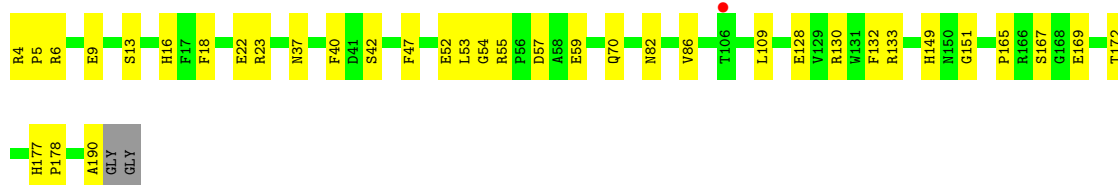
- Molecule 2: HLA class II histocompatibility antigen DR beta chain

Chain E:  84% 15% ..




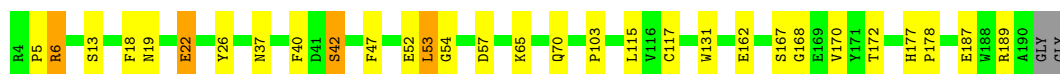
- Molecule 2: HLA class II histocompatibility antigen DR beta chain

Chain H:  80% 19% .




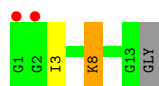
- Molecule 2: HLA class II histocompatibility antigen DR beta chain

Chain K:  83% 14% ..




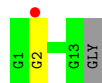
- Molecule 3: HST4 peptide

Chain C:  14% 79% 7% 7% 7%




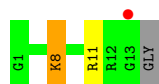
- Molecule 3: HST4 peptide

Chain F:  7% 86% 7% 7%



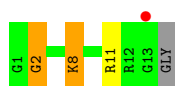
- Molecule 3: HST4 peptide

Chain I:  7% 79% 7% 7% 7%



- Molecule 3: HST4 peptide

Chain L:  7% 71% 7% 14% 7%



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



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



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



- Molecule 4: 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 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	74.46Å 214.25Å 74.55Å 90.00° 98.96° 90.00°	Depositor
Resolution (Å)	48.41 – 2.38 48.41 – 2.38	Depositor EDS
% Data completeness (in resolution range)	98.6 (48.41-2.38) 98.3 (48.41-2.38)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.47 (at 2.37Å)	Xtriage
Refinement program	PHENIX 1.17.1_3660	Depositor
R, $R_{free}$	0.200 , 0.248 0.200 , 0.248	Depositor DCC
$R_{free}$ test set	4435 reflections (4.88%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	55.4	Xtriage
Anisotropy	0.146	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 27.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	0.470 for l,-k,h	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	12988	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 3.63% 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: NAG, EDO

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	0.52	0/1519	0.64	0/2070
1	D	0.53	0/1519	0.65	1/2070 (0.0%)
1	G	0.43	0/1519	0.59	0/2070
1	J	0.43	0/1519	0.57	0/2070
2	B	0.51	0/1591	0.62	0/2161
2	E	0.56	1/1591 (0.1%)	0.64	1/2161 (0.0%)
2	H	0.43	0/1599	0.57	0/2172
2	K	0.43	0/1591	0.57	0/2161
3	C	0.38	0/90	0.77	0/117
3	F	0.44	0/90	0.88	0/117
3	I	0.36	0/90	0.65	0/117
3	L	0.38	0/90	0.63	0/117
All	All	0.48	1/12808 (0.0%)	0.61	2/17403 (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
3	F	0	1
3	L	0	1
All	All	0	2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	117	CYS	CB-SG	-5.71	1.72	1.81

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	181	THR	C-N-CA	5.59	135.67	121.70
1	D	92	LEU	CA-CB-CG	5.29	127.47	115.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	F	2	GLY	Peptide
3	L	2	GLY	Peptide

## 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	1474	0	1415	20	0
1	D	1474	0	1414	17	0
1	G	1474	0	1415	32	0
1	J	1474	0	1415	11	0
2	B	1548	0	1461	22	0
2	E	1548	0	1462	23	0
2	H	1556	0	1464	26	0
2	K	1548	0	1461	21	0
3	C	91	0	95	3	0
3	F	91	0	95	0	0
3	I	91	0	95	5	0
3	L	91	0	95	4	0
4	M	28	0	25	1	0
4	N	28	0	25	1	0
4	O	28	0	25	0	0
4	P	28	0	25	0	0
5	A	4	0	6	1	0
5	B	24	0	36	3	0
5	C	8	0	12	0	0
5	D	4	0	6	0	0
5	E	20	0	30	0	0
5	H	16	0	24	1	0
5	I	8	0	12	0	0
5	J	8	0	12	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	K	24	0	36	2	0
5	L	4	0	6	0	0
6	B	14	0	13	0	0
6	D	14	0	13	0	0
6	H	14	0	13	2	0
6	K	14	0	13	0	0
7	A	48	0	0	1	0
7	B	43	0	0	2	0
7	C	4	0	0	0	0
7	D	45	0	0	1	0
7	E	30	0	0	0	0
7	F	1	0	0	0	0
7	G	21	0	0	0	0
7	H	16	0	0	0	0
7	I	3	0	0	0	0
7	J	14	0	0	0	0
7	K	12	0	0	0	0
7	L	3	0	0	0	0
All	All	12988	0	12219	151	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 6.

The worst 5 of 151 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:G:91:VAL:H	1:G:176:LYS:NZ	1.53	1.05
1:G:91:VAL:N	1:G:176:LYS:HZ3	1.54	1.04
1:G:90:THR:HA	1:G:176:LYS:HZ2	1.18	1.03
1:G:91:VAL:H	1:G:176:LYS:HZ3	0.93	0.92
1:G:90:THR:HA	1:G:176:LYS:NZ	1.87	0.88

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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	177/181 (98%)	175 (99%)	2 (1%)	0	100	100
1	D	177/181 (98%)	174 (98%)	3 (2%)	0	100	100
1	G	177/181 (98%)	174 (98%)	2 (1%)	1 (1%)	25	34
1	J	177/181 (98%)	175 (99%)	1 (1%)	1 (1%)	25	34
2	B	185/189 (98%)	178 (96%)	7 (4%)	0	100	100
2	E	185/189 (98%)	179 (97%)	6 (3%)	0	100	100
2	H	186/189 (98%)	180 (97%)	6 (3%)	0	100	100
2	K	185/189 (98%)	179 (97%)	6 (3%)	0	100	100
3	C	11/14 (79%)	11 (100%)	0	0	100	100
3	F	11/14 (79%)	10 (91%)	1 (9%)	0	100	100
3	I	11/14 (79%)	10 (91%)	1 (9%)	0	100	100
3	L	11/14 (79%)	10 (91%)	0	1 (9%)	1	0
All	All	1493/1536 (97%)	1455 (98%)	35 (2%)	3 (0%)	47	61

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	L	2	GLY
1	G	136	VAL
1	J	136	VAL

### 5.3.2 Protein sidechains ⓘ

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	164/166 (99%)	163 (99%)	1 (1%)	86	93
1	D	164/166 (99%)	163 (99%)	1 (1%)	86	93
1	G	164/166 (99%)	162 (99%)	2 (1%)	71	84
1	J	164/166 (99%)	160 (98%)	4 (2%)	49	66

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	B	172/172 (100%)	172 (100%)	0	100	100
2	E	172/172 (100%)	171 (99%)	1 (1%)	86	93
2	H	173/172 (101%)	168 (97%)	5 (3%)	42	60
2	K	172/172 (100%)	165 (96%)	7 (4%)	30	45
3	C	9/9 (100%)	8 (89%)	1 (11%)	6	7
3	F	9/9 (100%)	9 (100%)	0	100	100
3	I	9/9 (100%)	8 (89%)	1 (11%)	6	7
3	L	9/9 (100%)	8 (89%)	1 (11%)	6	7
All	All	1381/1388 (100%)	1357 (98%)	24 (2%)	60	76

5 of 24 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	J	50	ARG
2	K	22	GLU
2	K	6	ARG
2	K	42	SER
2	H	6	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	34	GLN
2	E	19	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

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$
4	NAG	M	1	1,4	14,14,15	1.33	1 (7%)	17,19,21	1.52	3 (17%)
4	NAG	M	2	4	14,14,15	1.84	4 (28%)	17,19,21	1.87	5 (29%)
4	NAG	N	1	1,4	14,14,15	0.65	1 (7%)	17,19,21	1.23	1 (5%)
4	NAG	N	2	4	14,14,15	0.73	1 (7%)	17,19,21	0.54	0
4	NAG	O	1	1,4	14,14,15	0.61	0	17,19,21	1.63	1 (5%)
4	NAG	O	2	4	14,14,15	0.59	0	17,19,21	0.59	0
4	NAG	P	1	1,4	14,14,15	0.91	1 (7%)	17,19,21	0.78	0
4	NAG	P	2	4	14,14,15	0.62	0	17,19,21	0.59	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
4	NAG	M	1	1,4	-	2/6/23/26	0/1/1/1
4	NAG	M	2	4	-	4/6/23/26	0/1/1/1
4	NAG	N	1	1,4	-	2/6/23/26	0/1/1/1
4	NAG	N	2	4	-	2/6/23/26	0/1/1/1
4	NAG	O	1	1,4	-	0/6/23/26	0/1/1/1
4	NAG	O	2	4	-	4/6/23/26	0/1/1/1
4	NAG	P	1	1,4	-	0/6/23/26	0/1/1/1
4	NAG	P	2	4	-	2/6/23/26	0/1/1/1

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	M	2	NAG	C1-C2	4.67	1.59	1.52
4	M	1	NAG	O5-C1	4.41	1.50	1.43
4	M	2	NAG	O5-C1	3.66	1.49	1.43
4	P	1	NAG	O5-C1	-3.30	1.38	1.43
4	M	2	NAG	C3-C2	2.40	1.57	1.52

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	O	1	NAG	C1-O5-C5	5.82	120.08	112.19
4	N	1	NAG	C1-O5-C5	4.05	117.68	112.19
4	M	1	NAG	C1-O5-C5	3.82	117.37	112.19
4	M	2	NAG	C4-C3-C2	3.50	116.15	111.02
4	M	2	NAG	O5-C5-C4	-3.44	102.47	110.83

There are no chirality outliers.

5 of 16 torsion outliers are listed below:

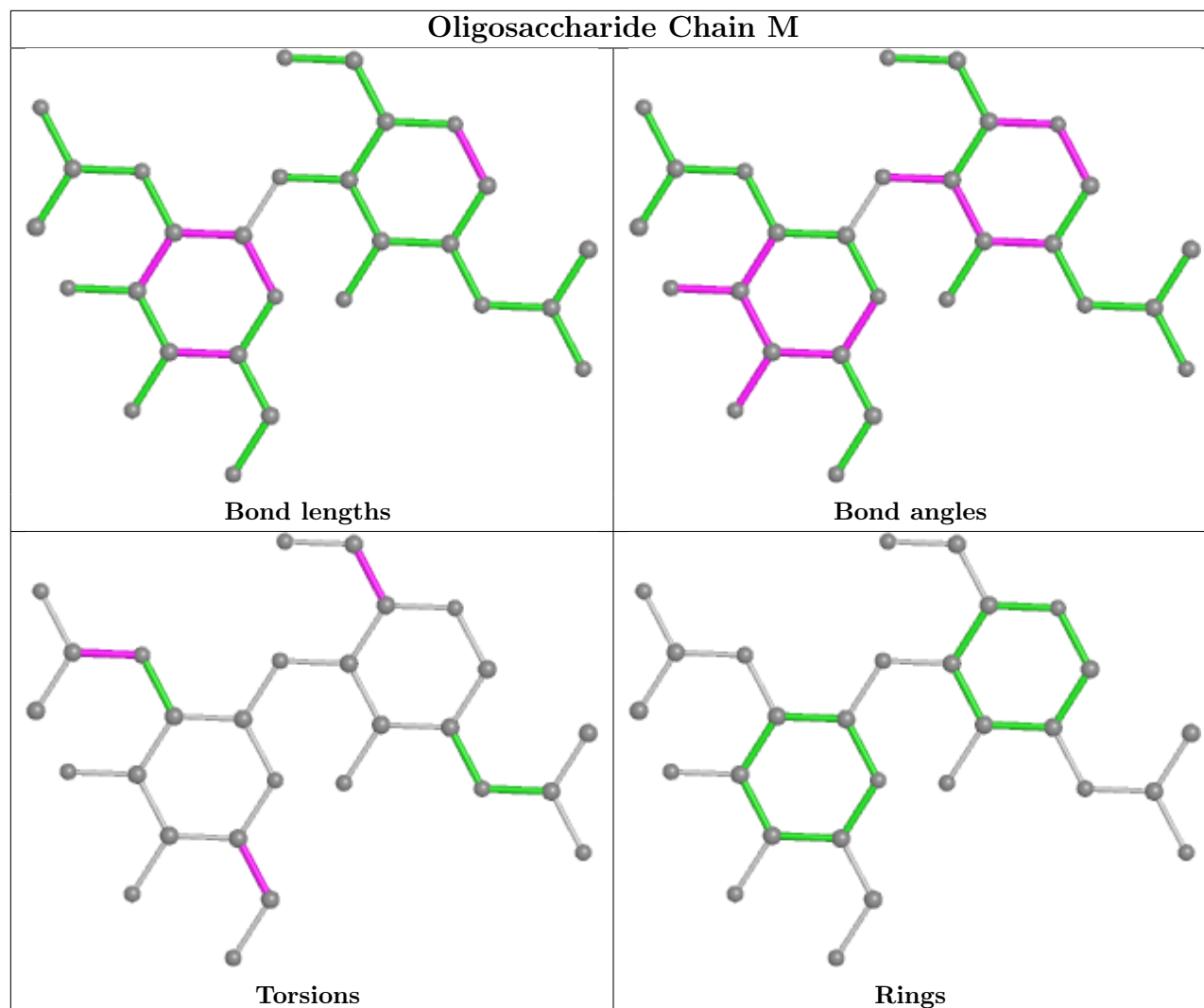
Mol	Chain	Res	Type	Atoms
4	M	2	NAG	O5-C5-C6-O6
4	M	1	NAG	C4-C5-C6-O6
4	M	1	NAG	O5-C5-C6-O6
4	M	2	NAG	C8-C7-N2-C2
4	M	2	NAG	O7-C7-N2-C2

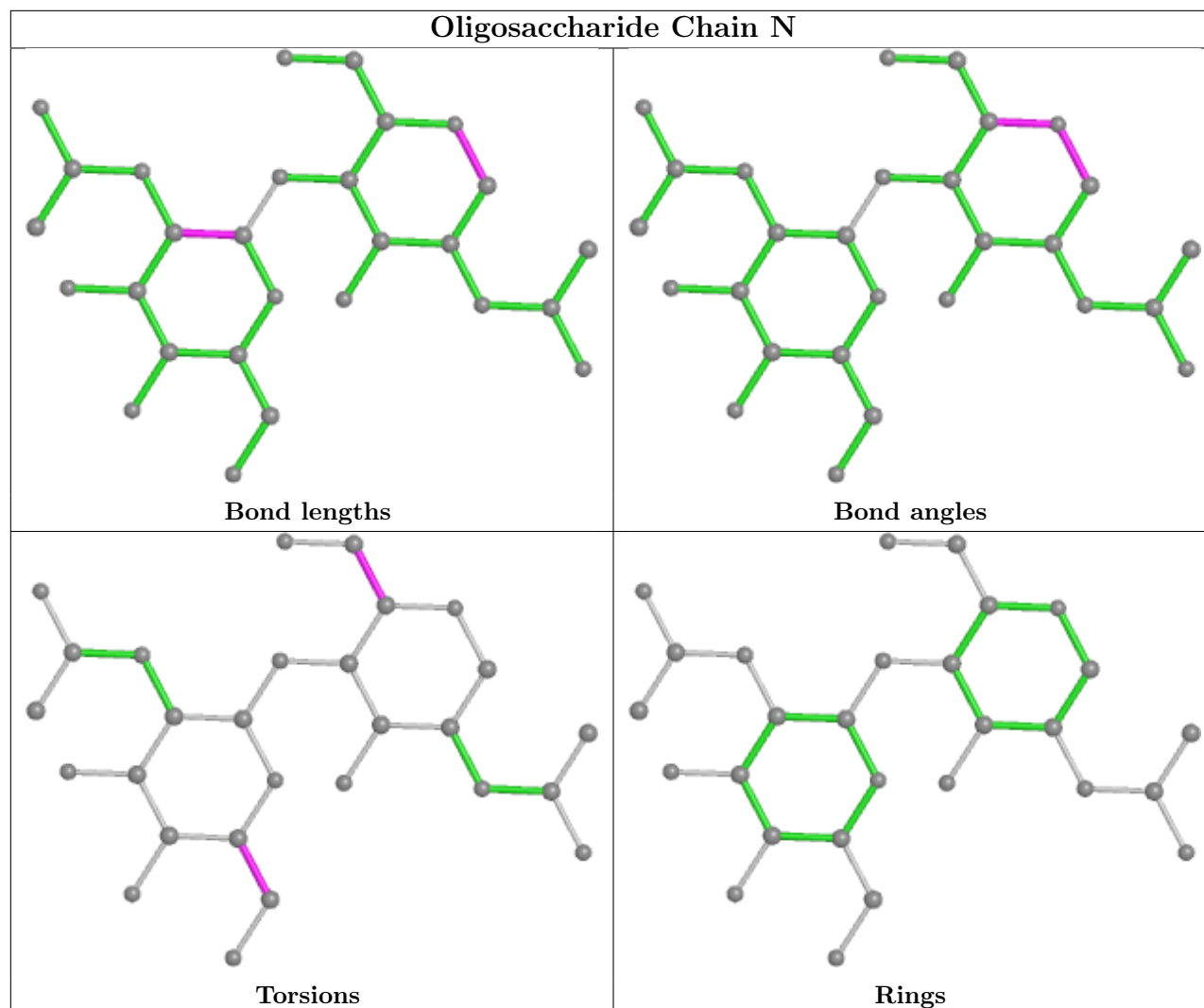
There are no ring outliers.

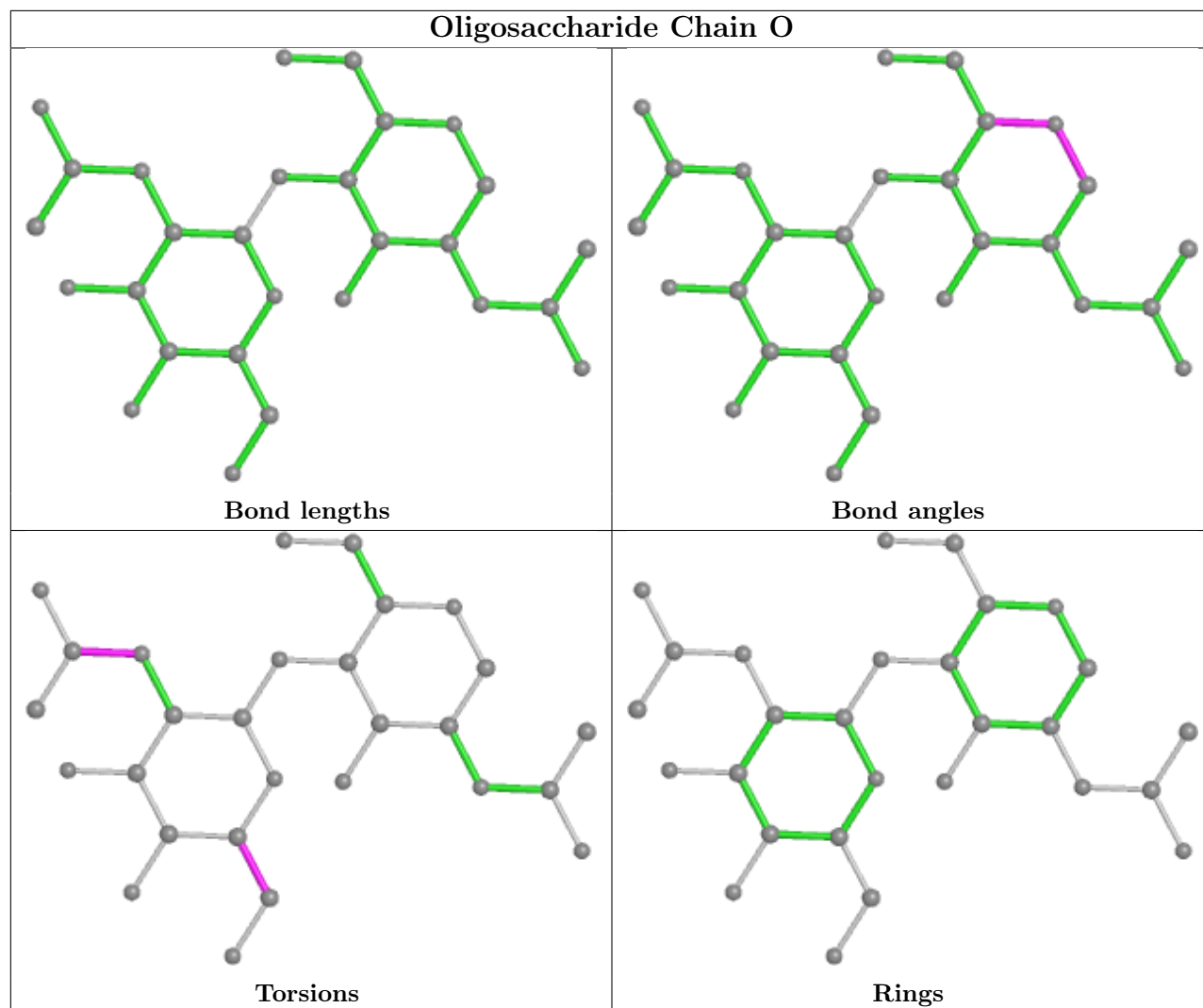
2 monomers are involved in 2 short contacts:

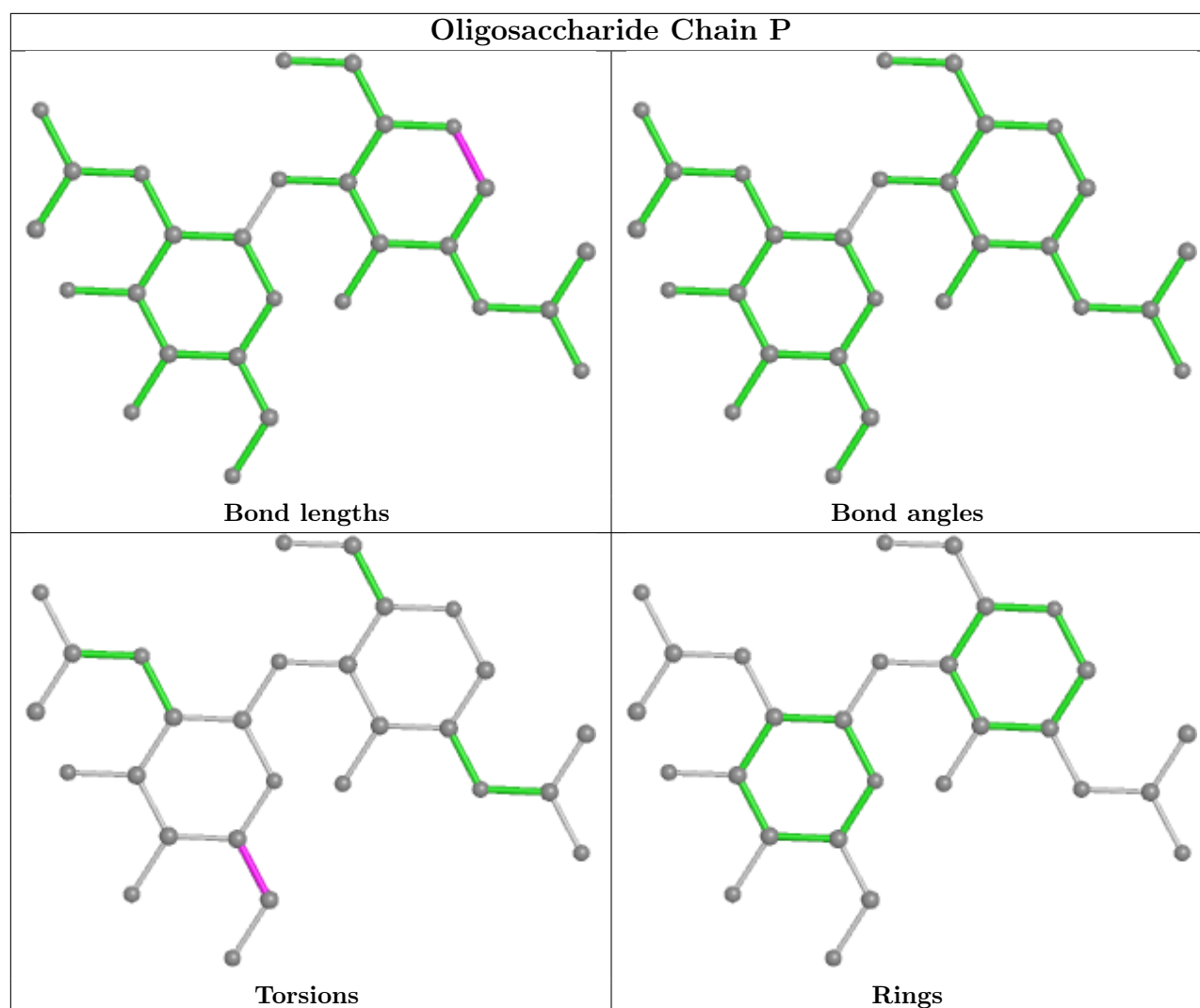
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	N	1	NAG	1	0
4	M	1	NAG	1	0

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](#)

34 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
5	EDO	E	205	-	3,3,3	0.49	0	2,2,2	0.33	0
5	EDO	K	204	-	3,3,3	0.59	0	2,2,2	0.07	0
5	EDO	C	202	-	3,3,3	0.48	0	2,2,2	0.43	0
5	EDO	I	102	-	3,3,3	0.41	0	2,2,2	0.54	0



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
5	EDO	B	204	-	3,3,3	0.59	0	2,2,2	0.22	0
6	NAG	B	207	2	14,14,15	0.86	1 (7%)	17,19,21	0.59	0
5	EDO	K	203	-	3,3,3	0.67	0	2,2,2	0.04	0
5	EDO	B	202	-	3,3,3	0.51	0	2,2,2	0.06	0
5	EDO	H	202	-	3,3,3	0.55	0	2,2,2	0.33	0
5	EDO	C	201	-	3,3,3	0.44	0	2,2,2	0.35	0
5	EDO	K	201	-	3,3,3	0.49	0	2,2,2	0.34	0
6	NAG	K	207	2	14,14,15	2.67	2 (14%)	17,19,21	2.47	2 (11%)
5	EDO	K	206	-	3,3,3	0.47	0	2,2,2	0.44	0
5	EDO	D	201	-	3,3,3	0.69	0	2,2,2	0.15	0
5	EDO	E	204	-	3,3,3	0.47	0	2,2,2	0.37	0
5	EDO	E	203	-	3,3,3	0.50	0	2,2,2	0.31	0
5	EDO	A	201	-	3,3,3	0.53	0	2,2,2	0.21	0
5	EDO	B	206	-	3,3,3	0.45	0	2,2,2	0.42	0
5	EDO	K	202	-	3,3,3	0.54	0	2,2,2	0.34	0
5	EDO	J	202	-	3,3,3	0.52	0	2,2,2	0.23	0
5	EDO	B	201	-	3,3,3	0.53	0	2,2,2	0.42	0
5	EDO	H	204	-	3,3,3	0.37	0	2,2,2	0.60	0
5	EDO	K	205	-	3,3,3	0.56	0	2,2,2	0.14	0
5	EDO	J	201	-	3,3,3	0.52	0	2,2,2	0.35	0
6	NAG	D	202	1	14,14,15	0.76	1 (7%)	17,19,21	1.78	4 (23%)
6	NAG	H	201	2	14,14,15	1.17	1 (7%)	17,19,21	2.46	4 (23%)
5	EDO	H	203	-	3,3,3	0.47	0	2,2,2	0.32	0
5	EDO	H	205	-	3,3,3	0.54	0	2,2,2	0.24	0
5	EDO	B	203	-	3,3,3	0.49	0	2,2,2	0.47	0
5	EDO	B	205	-	3,3,3	0.67	0	2,2,2	0.23	0
5	EDO	E	202	-	3,3,3	0.52	0	2,2,2	0.29	0
5	EDO	L	101	-	3,3,3	0.56	0	2,2,2	0.18	0
5	EDO	E	201	-	3,3,3	0.60	0	2,2,2	0.29	0
5	EDO	I	101	-	3,3,3	0.56	0	2,2,2	0.36	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	EDO	E	205	-	-	0/1/1/1	-
5	EDO	K	204	-	-	0/1/1/1	-
5	EDO	C	202	-	-	1/1/1/1	-
5	EDO	I	102	-	-	0/1/1/1	-
5	EDO	B	204	-	-	1/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	NAG	B	207	2	-	0/6/23/26	0/1/1/1
5	EDO	K	203	-	-	0/1/1/1	-
5	EDO	B	202	-	-	1/1/1/1	-
5	EDO	H	202	-	-	1/1/1/1	-
5	EDO	C	201	-	-	0/1/1/1	-
5	EDO	K	201	-	-	1/1/1/1	-
6	NAG	K	207	2	-	1/6/23/26	0/1/1/1
5	EDO	K	206	-	-	0/1/1/1	-
5	EDO	D	201	-	-	0/1/1/1	-
5	EDO	E	204	-	-	0/1/1/1	-
5	EDO	E	203	-	-	0/1/1/1	-
5	EDO	A	201	-	-	0/1/1/1	-
5	EDO	B	206	-	-	1/1/1/1	-
5	EDO	K	202	-	-	1/1/1/1	-
5	EDO	J	202	-	-	0/1/1/1	-
5	EDO	B	201	-	-	0/1/1/1	-
5	EDO	H	204	-	-	0/1/1/1	-
5	EDO	K	205	-	-	1/1/1/1	-
5	EDO	J	201	-	-	0/1/1/1	-
6	NAG	D	202	1	-	2/6/23/26	0/1/1/1
6	NAG	H	201	2	-	5/6/23/26	0/1/1/1
5	EDO	H	203	-	-	0/1/1/1	-
5	EDO	H	205	-	-	1/1/1/1	-
5	EDO	B	203	-	-	0/1/1/1	-
5	EDO	B	205	-	-	0/1/1/1	-
5	EDO	E	202	-	-	1/1/1/1	-
5	EDO	L	101	-	-	1/1/1/1	-
5	EDO	E	201	-	-	0/1/1/1	-
5	EDO	I	101	-	-	0/1/1/1	-

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	K	207	NAG	O5-C1	9.47	1.58	1.43
6	H	201	NAG	O5-C1	3.87	1.49	1.43
6	B	207	NAG	C1-C2	2.77	1.56	1.52
6	K	207	NAG	C1-C2	2.70	1.56	1.52
6	D	202	NAG	C1-C2	2.19	1.55	1.52

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

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
6	K	207	NAG	C1-O5-C5	9.42	124.95	112.19
6	H	201	NAG	C2-N2-C7	7.45	133.51	122.90
6	H	201	NAG	C1-C2-N2	3.84	117.05	110.49
6	D	202	NAG	C1-O5-C5	3.74	117.26	112.19
6	H	201	NAG	C1-O5-C5	3.69	117.19	112.19

There are no chirality outliers.

5 of 19 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	H	201	NAG	C3-C2-N2-C7
6	H	201	NAG	C4-C5-C6-O6
6	H	201	NAG	O5-C5-C6-O6
6	H	201	NAG	C8-C7-N2-C2
6	H	201	NAG	O7-C7-N2-C2

There are no ring outliers.

8 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	K	204	EDO	1	0
5	B	204	EDO	1	0
5	B	202	EDO	1	0
5	A	201	EDO	1	0
5	B	201	EDO	1	0
5	K	205	EDO	1	0
6	H	201	NAG	2	0
5	H	205	EDO	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	179/181 (98%)	-0.23	0 100 100	37, 49, 68, 75	0
1	D	179/181 (98%)	-0.17	0 100 100	37, 49, 67, 76	0
1	G	179/181 (98%)	-0.01	2 (1%) 80 81	48, 64, 84, 108	0
1	J	179/181 (98%)	-0.03	2 (1%) 80 81	49, 64, 85, 105	0
2	B	187/189 (98%)	-0.16	0 100 100	38, 53, 73, 88	0
2	E	187/189 (98%)	-0.20	0 100 100	37, 52, 73, 84	0
2	H	187/189 (98%)	-0.13	1 (0%) 91 91	44, 62, 86, 97	0
2	K	187/189 (98%)	-0.18	0 100 100	47, 63, 86, 95	0
3	C	13/14 (92%)	0.50	2 (15%) 2 2	41, 51, 79, 90	0
3	F	13/14 (92%)	0.09	1 (7%) 13 14	39, 49, 79, 81	0
3	I	13/14 (92%)	0.15	1 (7%) 13 14	58, 62, 89, 90	0
3	L	13/14 (92%)	0.18	1 (7%) 13 14	58, 63, 86, 92	0
All	All	1516/1536 (98%)	-0.13	10 (0%) 87 88	37, 58, 81, 108	0

The worst 5 of 10 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	C	1	GLY	3.7
3	C	2	GLY	3.3
3	L	13	GLY	3.1
1	G	128	VAL	2.8
1	J	130	THR	2.6

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

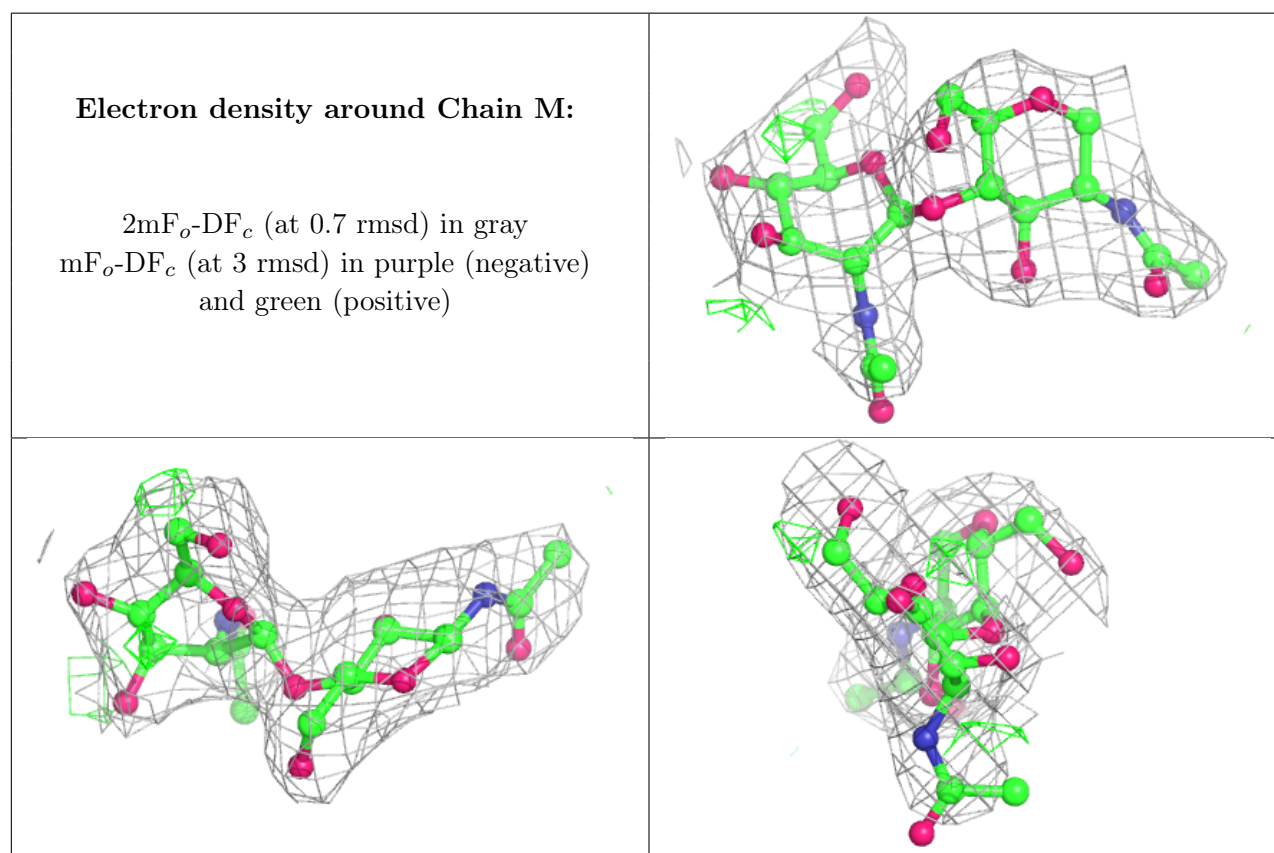
There are no non-standard protein/DNA/RNA residues in this entry.

### 6.3 Carbohydrates [i](#)

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

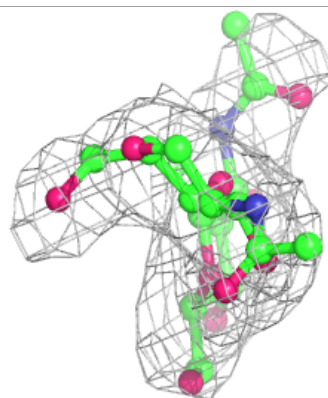
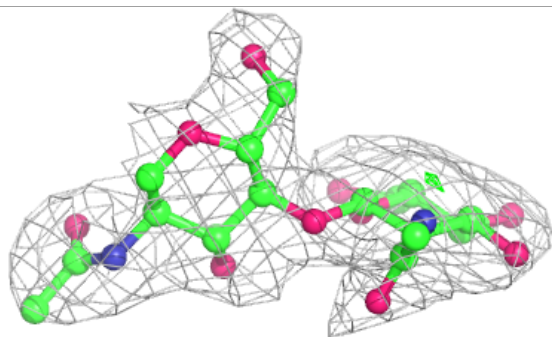
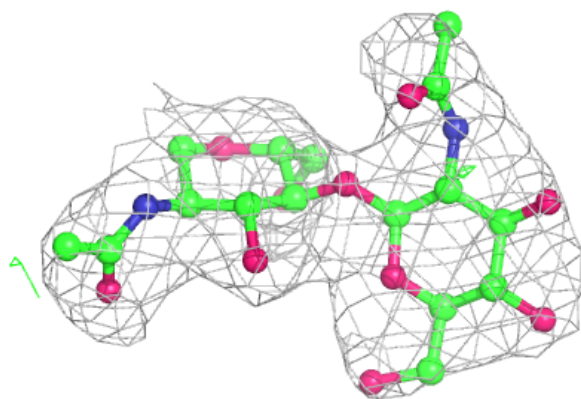
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
4	NAG	P	2	14/15	0.86	0.16	87,101,110,111	0
4	NAG	O	2	14/15	0.88	0.13	78,89,93,94	0
4	NAG	N	2	14/15	0.91	0.17	76,87,92,94	0
4	NAG	M	2	14/15	0.92	0.13	88,108,114,117	0
4	NAG	O	1	14/15	0.92	0.14	55,72,87,92	0
4	NAG	M	1	14/15	0.93	0.11	75,86,100,112	0
4	NAG	P	1	14/15	0.93	0.11	65,82,104,111	0
4	NAG	N	1	14/15	0.93	0.13	56,67,88,99	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.

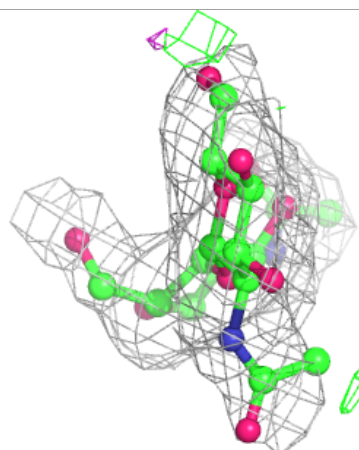
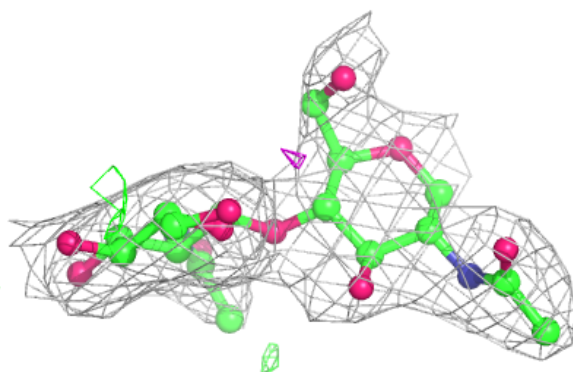
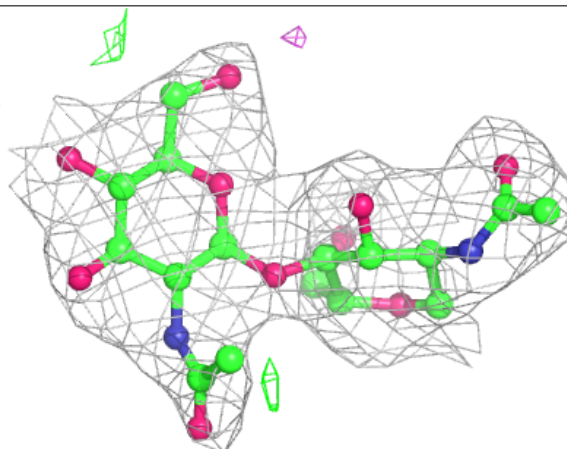


**Electron density around Chain N:**

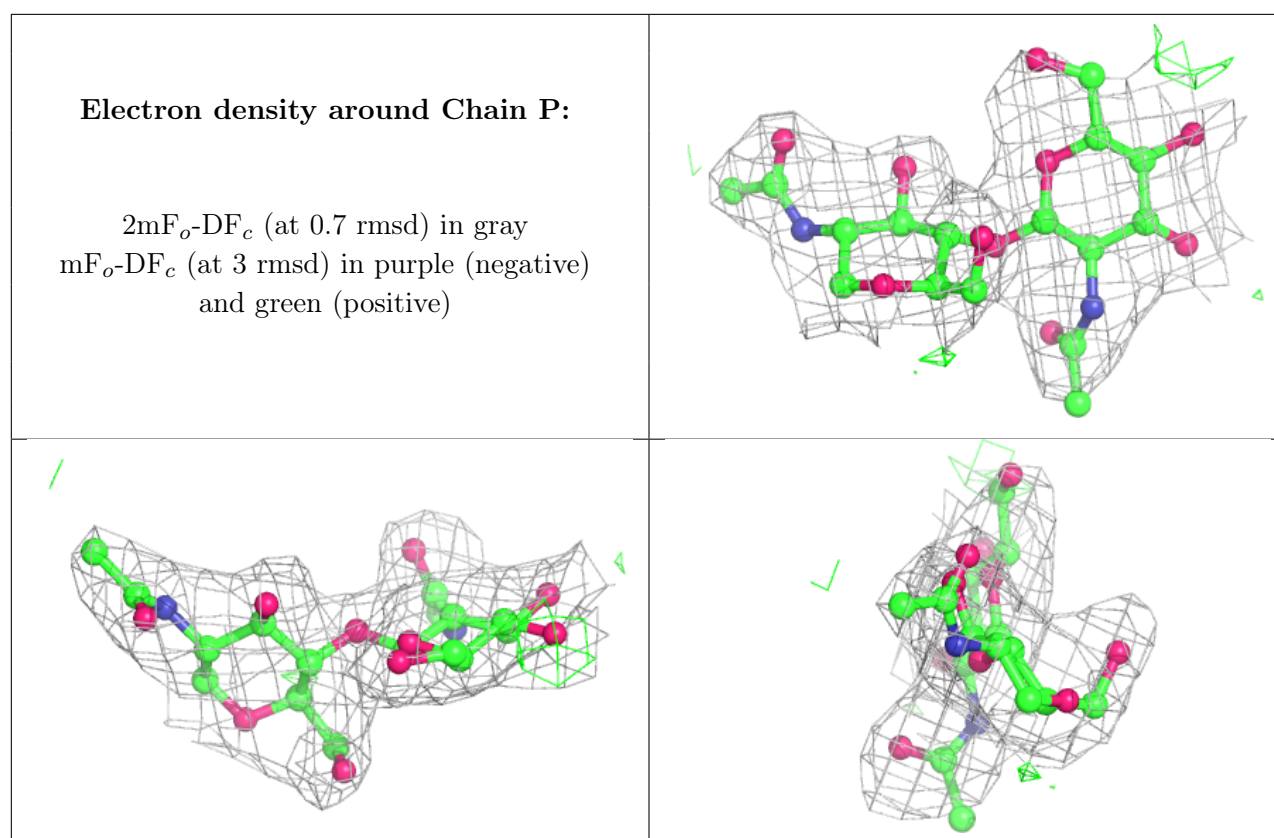
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

**Electron density around Chain O:**

$2mF_o-DF_c$  (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( $\text{\AA}^2$ )	Q<0.9
6	NAG	H	201	14/15	0.68	0.20	87,104,109,112	0
5	EDO	H	205	4/4	0.71	0.19	81,82,88,90	0
5	EDO	H	204	4/4	0.72	0.35	84,91,95,95	0
6	NAG	K	207	14/15	0.74	0.24	86,110,116,118	0
6	NAG	B	207	14/15	0.75	0.19	80,90,101,104	0
5	EDO	K	204	4/4	0.77	0.15	71,75,77,81	0
5	EDO	K	205	4/4	0.78	0.29	86,93,95,97	0
5	EDO	J	202	4/4	0.80	0.31	89,94,101,106	0
5	EDO	E	203	4/4	0.84	0.21	66,69,71,73	0
5	EDO	I	102	4/4	0.87	0.16	87,90,96,98	0
5	EDO	K	203	4/4	0.87	0.14	62,71,77,82	0
5	EDO	L	101	4/4	0.87	0.14	79,83,83,85	0
5	EDO	B	204	4/4	0.88	0.17	58,60,65,67	0
5	EDO	K	206	4/4	0.88	0.26	81,89,90,94	0

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*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
5	EDO	A	201	4/4	0.88	0.31	82,86,89,89	0
5	EDO	E	202	4/4	0.89	0.13	69,69,75,79	0
5	EDO	H	203	4/4	0.89	0.21	81,86,92,97	0
5	EDO	K	202	4/4	0.91	0.10	62,70,71,74	0
6	NAG	D	202	14/15	0.91	0.14	83,104,112,117	0
5	EDO	H	202	4/4	0.92	0.11	58,64,67,72	0
5	EDO	C	201	4/4	0.92	0.13	65,70,72,73	0
5	EDO	C	202	4/4	0.93	0.18	57,65,67,68	0
5	EDO	K	201	4/4	0.93	0.13	59,63,63,68	0
5	EDO	D	201	4/4	0.93	0.19	55,65,72,76	0
5	EDO	B	202	4/4	0.93	0.13	65,68,71,76	0
5	EDO	B	206	4/4	0.94	0.13	74,74,75,76	0
5	EDO	E	204	4/4	0.95	0.11	66,68,80,84	0
5	EDO	I	101	4/4	0.95	0.09	81,81,82,87	0
5	EDO	B	205	4/4	0.95	0.12	52,55,55,62	0
5	EDO	J	201	4/4	0.95	0.20	76,80,83,86	0
5	EDO	B	203	4/4	0.96	0.20	73,77,86,93	0
5	EDO	E	201	4/4	0.96	0.11	50,53,54,62	0
5	EDO	B	201	4/4	0.96	0.14	68,69,73,73	0
5	EDO	E	205	4/4	0.97	0.11	70,70,72,72	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.