



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 5, 2026 – 08:49 PM UTC

PDB ID : 7N19 / pdb_00007n19
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

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

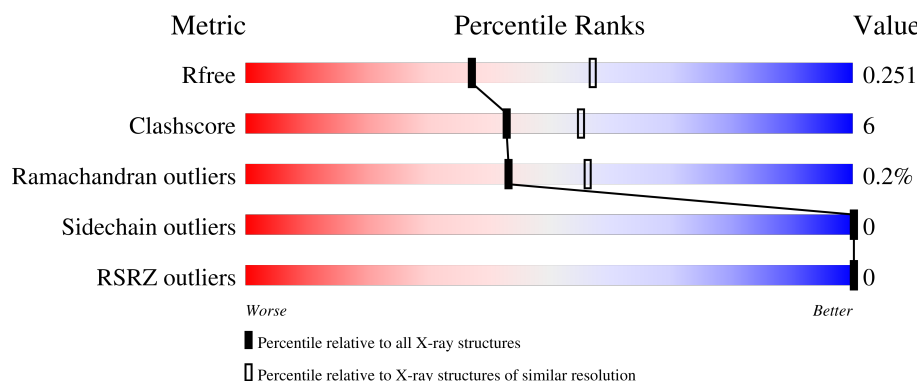
1 Overall quality at a glance

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.



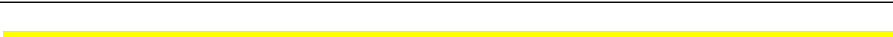
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	7164 (2.40-2.36)
Clashscore	190562	7722 (2.40-2.36)
Ramachandran outliers	187476	7626 (2.40-2.36)
Sidechain outliers	187428	7627 (2.40-2.36)
RSRZ outliers	180081	7170 (2.40-2.36)

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 ≥ 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	 84% 15% .
1	D	181	 85% 14% .
1	G	181	 83% 16% .
1	J	181	 90% 9% .
2	B	189	 83% 16% .

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	E	189	 84% 15%
2	H	189	 81% 17%
2	K	189	 85% 14%
3	C	14	 79% 14% 7%
3	F	14	 86% 7% 7%
3	I	14	 79% 14% 7%
3	L	14	 71% 14% 7% 7%
4	M	2	 50% 50%
4	N	2	 50% 50%
4	O	2	 50% 50%
4	P	2	 100%

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.

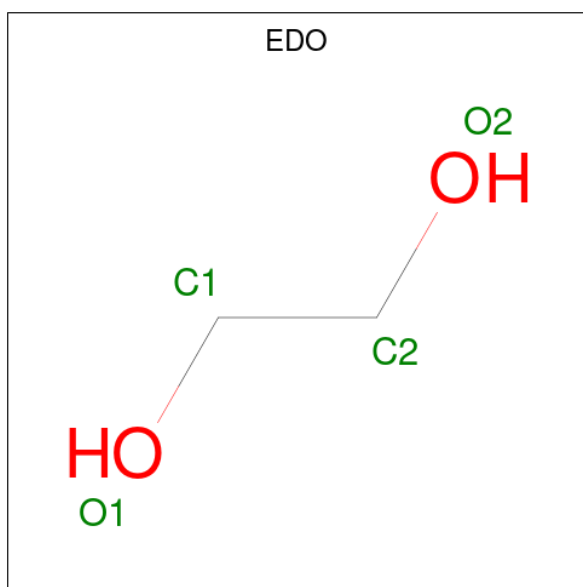
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	C	13	Total	C	N	O	0	0	0
			91	52	21	18			
3	F	13	Total	C	N	O	0	0	0
			91	52	21	18			
3	I	13	Total	C	N	O	0	0	0
			91	52	21	18			
3	L	13	Total	C	N	O	0	0	0
			91	52	21	18			

- 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 (CCD ID: EDO) (formula: C₂H₆O₂).



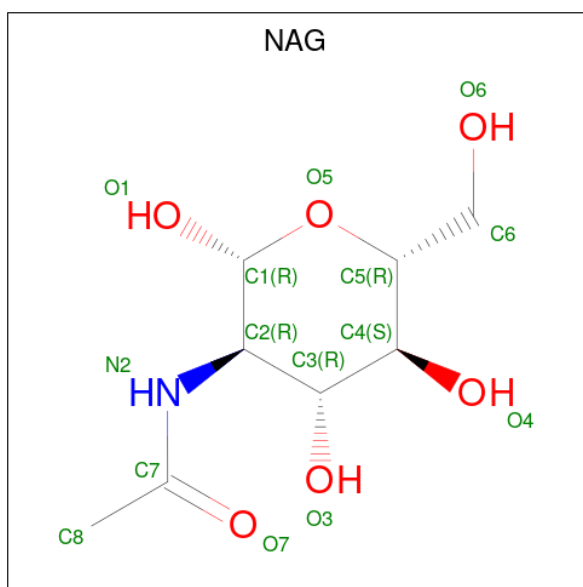
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			4	2	2		
5	B	1	Total	C	O	0	0
			4	2	2		
5	B	1	Total	C	O	0	0
			4	2	2		
5	B	1	Total	C	O	0	0
			4	2	2		
5	B	1	Total	C	O	0	0
			4	2	2		
5	B	1	Total	C	O	0	0
			4	2	2		
5	C	1	Total	C	O	0	0
			4	2	2		
5	C	1	Total	C	O	0	0
			4	2	2		
5	D	1	Total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

Continued on next page...

Continued from previous page...

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	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 (CCD ID: NAG) (formula: C₈H₁₅NO₆).



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		

Continued on next page...

Continued from previous page...

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

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: 



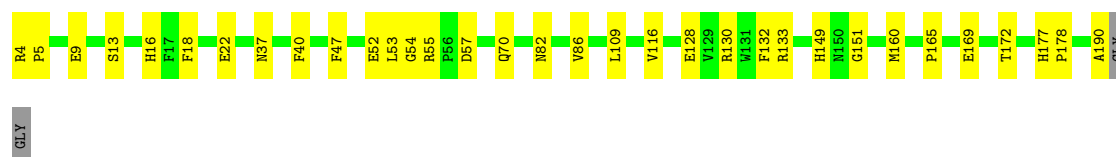
- Molecule 2: HLA class II histocompatibility antigen DR beta chain

Chain E:  84% 15%



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

Chain H:  81% 17%



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

Chain K:  85% 14%



- Molecule 3: HST4 peptide

Chain C:  79% 14% 7%



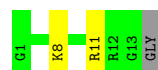
- Molecule 3: HST4 peptide

Chain F:  86% 7% 7%



- Molecule 3: HST4 peptide

Chain I:  79% 14% 7%



- Molecule 3: HST4 peptide

Chain L:  71% 14% 7% 7%



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

Chain M:  50% 50%

MAG1
MAG2

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

Chain N:  50% 50%

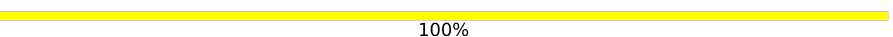
MAG1
MAG2

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

Chain O:  50% 50%

MAG1
MAG2

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

Chain P:  100%

MAG1
MAG2

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	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
$\langle I/\sigma(I) \rangle$ ¹	1.47 (at 2.37Å)	Xtriage
Refinement program	PHENIX 1.17.1_3660	Depositor
R, R_{free}	0.200 , 0.248 0.205 , 0.251	Depositor DCC
R_{free} test set	4435 reflections (4.82%)	wwPDB-VP
Wilson B-factor (Å ²)	55.4	Xtriage
Anisotropy	0.146	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 26.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	0.470 for l,-k,h	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	12988	wwPDB-VP
Average B, all atoms (Å ²)	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.*

¹Intensities estimated from amplitudes.

²Theoretical 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: EDO, 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	0.43	0/1519	0.60	0/2070
1	D	0.43	0/1519	0.61	0/2070
1	G	0.35	0/1519	0.53	0/2070
1	J	0.34	0/1519	0.54	0/2070
2	B	0.42	0/1591	0.58	0/2161
2	E	0.44	0/1591	0.63	2/2161 (0.1%)
2	H	0.36	0/1599	0.53	0/2172
2	K	0.36	0/1591	0.54	0/2161
3	C	0.48	0/90	0.76	0/117
3	F	0.54	0/90	0.86	0/117
3	I	0.39	0/90	0.77	0/117
3	L	0.34	0/90	0.69	0/117
All	All	0.39	0/12808	0.58	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

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	181	THR	CA-C-N	5.08	135.67	120.69
2	E	181	THR	C-N-CA	5.08	135.67	120.69

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

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	21	0
1	D	1474	0	1414	17	0
1	G	1474	0	1415	33	0
1	J	1474	0	1415	11	0
2	B	1548	0	1461	23	0
2	E	1548	0	1462	23	0
2	H	1556	0	1464	27	0
2	K	1548	0	1461	22	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	5	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
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

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	155	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 155 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:90:THR:HA	1:G:176:LYS:HZ2	1.06	1.05
1:G:91:VAL:H	1:G:176:LYS:NZ	1.53	1.05
1:G:91:VAL:N	1:G:176:LYS:HZ3	1.65	0.95
1:G:91:VAL:H	1:G:176:LYS:HZ3	1.01	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 [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	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%)	21	30
1	J	177/181 (98%)	175 (99%)	1 (1%)	1 (1%)	21	30
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%)	0	0
All	All	1493/1536 (97%)	1455 (98%)	35 (2%)	3 (0%)	43	56

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%)	164 (100%)	0	100	100
1	D	164/166 (99%)	164 (100%)	0	100	100
1	G	164/166 (99%)	164 (100%)	0	100	100
1	J	164/166 (99%)	164 (100%)	0	100	100
2	B	172/172 (100%)	172 (100%)	0	100	100
2	E	172/172 (100%)	172 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	H	173/172 (101%)	173 (100%)	0	100	100
2	K	172/172 (100%)	172 (100%)	0	100	100
3	C	9/9 (100%)	9 (100%)	0	100	100
3	F	9/9 (100%)	9 (100%)	0	100	100
3	I	9/9 (100%)	9 (100%)	0	100	100
3	L	9/9 (100%)	9 (100%)	0	100	100
All	All	1381/1388 (100%)	1381 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 13 such sidechains are listed below:

Mol	Chain	Res	Type
1	G	94	ASN
1	G	143	HIS
2	K	111	HIS
1	J	143	HIS
2	K	70	GLN

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	1.30	2 (14%)	17,19,21	1.53	3 (17%)
4	NAG	M	2	4	14,14,15	1.90	3 (21%)	17,19,21	1.87	5 (29%)
4	NAG	N	1	1,4	14,14,15	0.64	0	17,19,21	1.24	1 (5%)
4	NAG	N	2	4	14,14,15	0.76	1 (7%)	17,19,21	0.54	0
4	NAG	O	1	1,4	14,14,15	0.61	0	17,19,21	1.64	1 (5%)
4	NAG	O	2	4	14,14,15	0.59	0	17,19,21	0.60	0
4	NAG	P	1	1,4	14,14,15	0.87	1 (7%)	17,19,21	0.79	0
4	NAG	P	2	4	14,14,15	0.65	1 (7%)	17,19,21	0.60	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	5.12	1.59	1.52
4	M	1	NAG	O5-C1	4.21	1.50	1.43
4	M	2	NAG	O5-C1	3.50	1.49	1.43
4	P	1	NAG	O5-C1	-3.13	1.38	1.43
4	M	2	NAG	C3-C2	2.43	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	5.89	120.08	112.19
4	N	1	NAG	C1-O5-C5	4.10	117.68	112.19
4	M	1	NAG	C1-O5-C5	3.87	117.37	112.19

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
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:

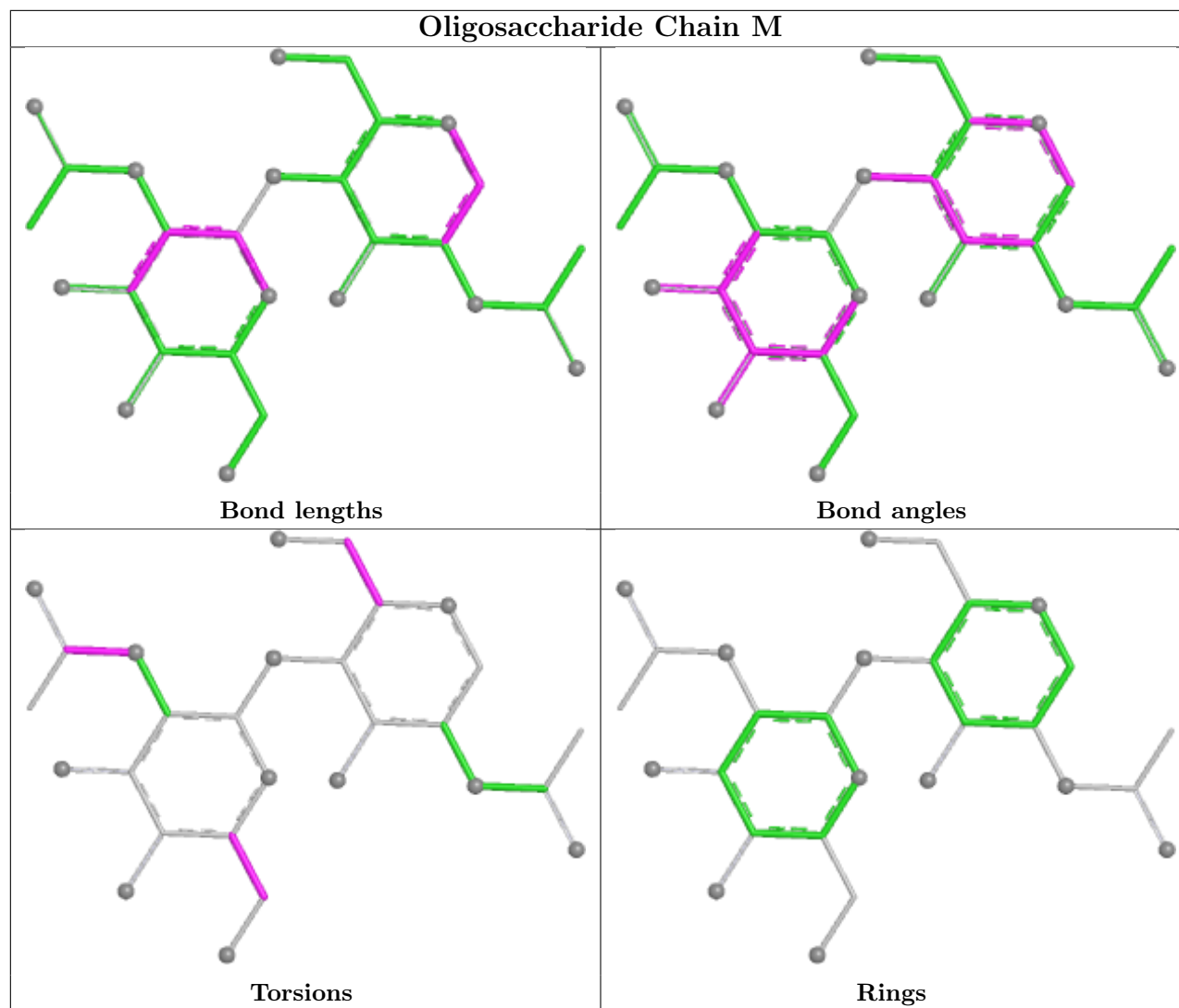
Mol	Chain	Res	Type	Atoms
4	M	2	NAG	O5-C5-C6-O6
4	M	1	NAG	C4-C5-C6-O6
4	M	1	NAG	O5-C5-C6-O6
4	M	2	NAG	C4-C5-C6-O6
4	P	2	NAG	O5-C5-C6-O6

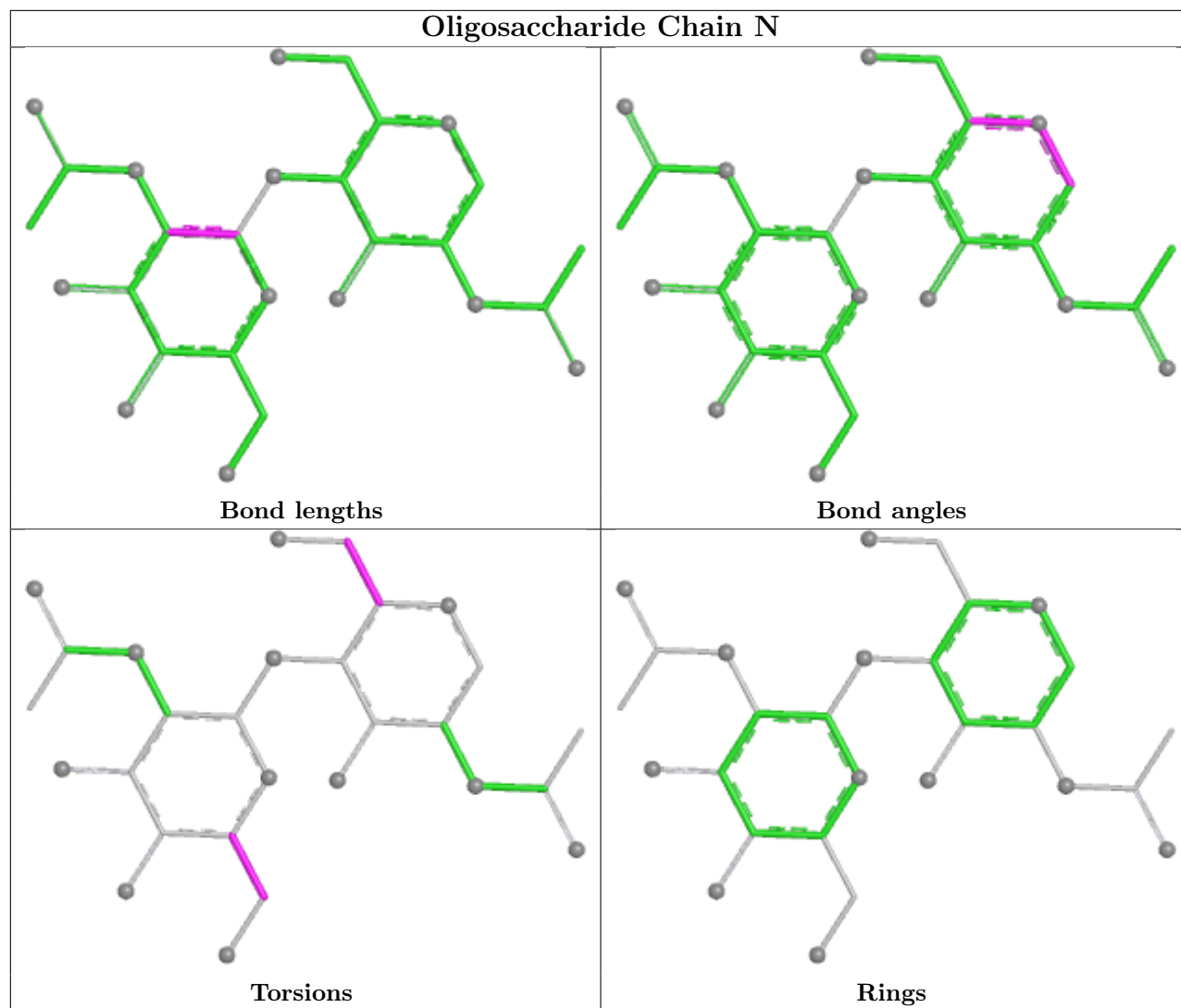
There are no ring outliers.

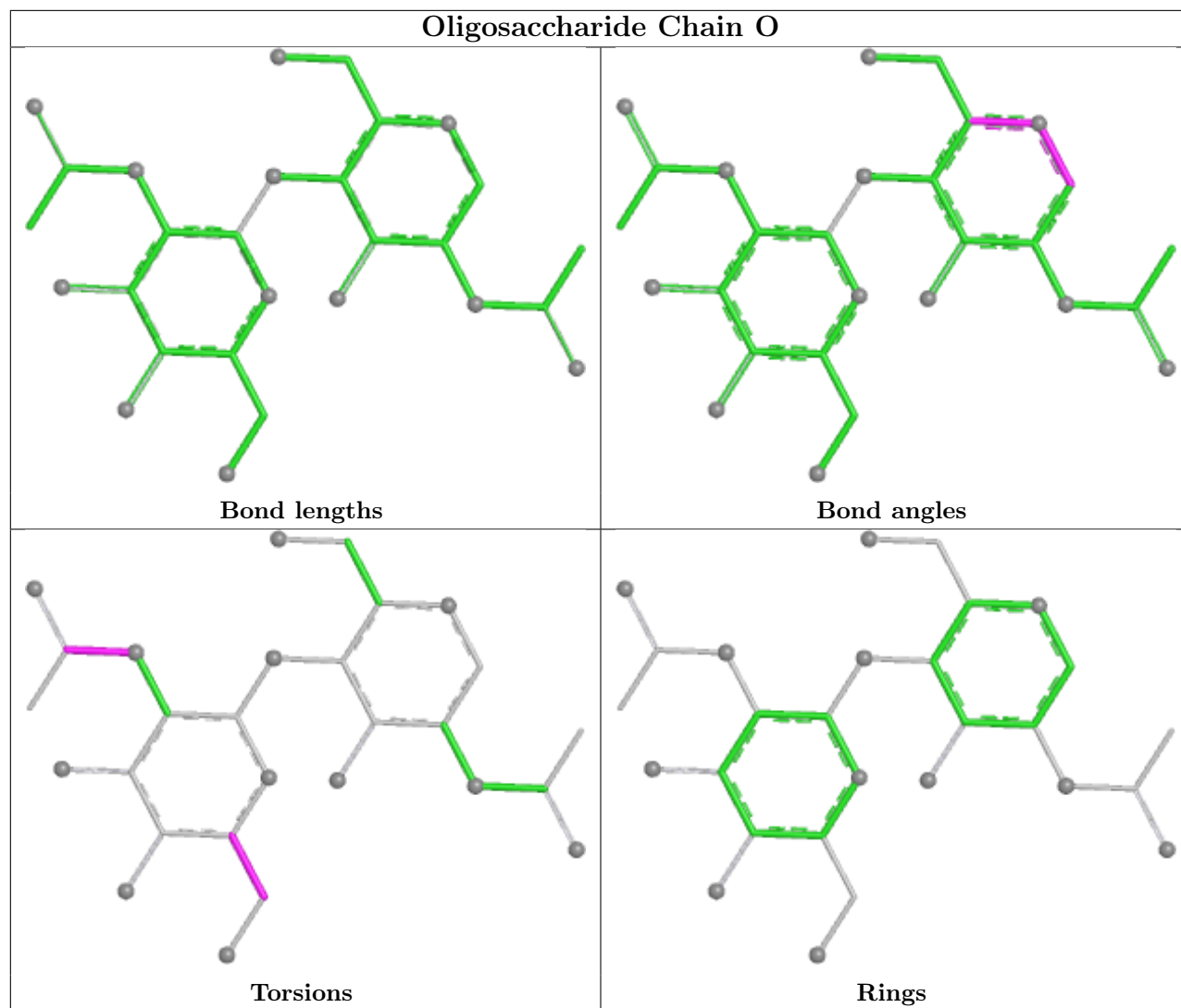
2 monomers are involved in 2 short contacts:

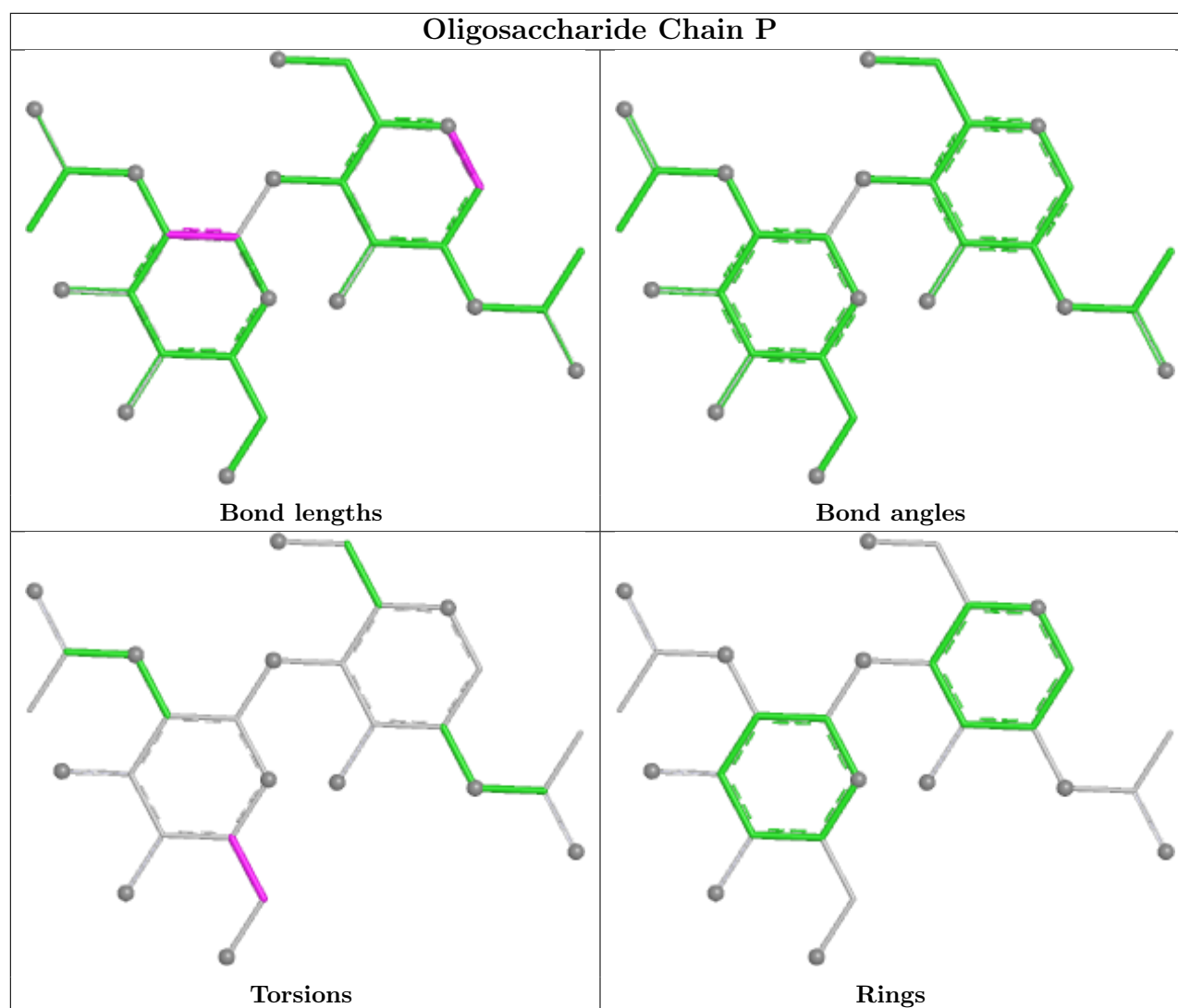
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	N	1	NAG	1	0
4	M	1	NAG	1	0

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	B	203	-	3,3,3	0.46	0	2,2,2	0.50	0
5	EDO	D	201	-	3,3,3	0.66	0	2,2,2	0.08	0
5	EDO	C	202	-	3,3,3	0.46	0	2,2,2	0.47	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	EDO	H	202	-	3,3,3	0.52	0	2,2,2	0.37	0
5	EDO	I	101	-	3,3,3	0.53	0	2,2,2	0.38	0
6	NAG	K	207	2	14,14,15	2.57	2 (14%)	17,19,21	2.50	2 (11%)
5	EDO	E	204	-	3,3,3	0.44	0	2,2,2	0.41	0
5	EDO	E	205	-	3,3,3	0.46	0	2,2,2	0.37	0
5	EDO	A	201	-	3,3,3	0.49	0	2,2,2	0.26	0
5	EDO	E	203	-	3,3,3	0.47	0	2,2,2	0.35	0
5	EDO	K	203	-	3,3,3	0.64	0	2,2,2	0.03	0
5	EDO	B	206	-	3,3,3	0.41	0	2,2,2	0.46	0
6	NAG	B	207	2	14,14,15	0.92	1 (7%)	17,19,21	0.59	0
5	EDO	L	101	-	3,3,3	0.53	0	2,2,2	0.21	0
5	EDO	B	201	-	3,3,3	0.50	0	2,2,2	0.46	0
5	EDO	K	201	-	3,3,3	0.47	0	2,2,2	0.36	0
5	EDO	H	205	-	3,3,3	0.51	0	2,2,2	0.28	0
5	EDO	J	201	-	3,3,3	0.49	0	2,2,2	0.38	0
5	EDO	C	201	-	3,3,3	0.41	0	2,2,2	0.39	0
5	EDO	B	205	-	3,3,3	0.65	0	2,2,2	0.23	0
5	EDO	B	204	-	3,3,3	0.55	0	2,2,2	0.26	0
5	EDO	K	204	-	3,3,3	0.55	0	2,2,2	0.01	0
5	EDO	B	202	-	3,3,3	0.48	0	2,2,2	0.12	0
5	EDO	K	205	-	3,3,3	0.53	0	2,2,2	0.20	0
6	NAG	H	201	2	14,14,15	1.14	1 (7%)	17,19,21	2.59	4 (23%)
5	EDO	E	202	-	3,3,3	0.48	0	2,2,2	0.32	0
5	EDO	H	204	-	3,3,3	0.35	0	2,2,2	0.63	0
5	EDO	K	206	-	3,3,3	0.44	0	2,2,2	0.47	0
5	EDO	J	202	-	3,3,3	0.49	0	2,2,2	0.28	0
5	EDO	E	201	-	3,3,3	0.57	0	2,2,2	0.24	0
5	EDO	I	102	-	3,3,3	0.38	0	2,2,2	0.57	0
6	NAG	D	202	1	14,14,15	0.81	1 (7%)	17,19,21	1.79	4 (23%)
5	EDO	K	202	-	3,3,3	0.51	0	2,2,2	0.39	0
5	EDO	H	203	-	3,3,3	0.44	0	2,2,2	0.37	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	B	203	-	-	0/1/1/1	-
5	EDO	D	201	-	-	0/1/1/1	-
5	EDO	C	202	-	-	1/1/1/1	-
5	EDO	H	202	-	-	1/1/1/1	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	EDO	I	101	-	-	0/1/1/1	-
6	NAG	K	207	2	-	1/6/23/26	0/1/1/1
5	EDO	E	204	-	-	0/1/1/1	-
5	EDO	E	205	-	-	0/1/1/1	-
5	EDO	A	201	-	-	0/1/1/1	-
5	EDO	E	203	-	-	0/1/1/1	-
5	EDO	K	203	-	-	0/1/1/1	-
5	EDO	B	206	-	-	1/1/1/1	-
6	NAG	B	207	2	-	0/6/23/26	0/1/1/1
5	EDO	L	101	-	-	1/1/1/1	-
5	EDO	B	201	-	-	0/1/1/1	-
5	EDO	K	201	-	-	1/1/1/1	-
5	EDO	H	205	-	-	1/1/1/1	-
5	EDO	J	201	-	-	0/1/1/1	-
5	EDO	C	201	-	-	0/1/1/1	-
5	EDO	B	205	-	-	0/1/1/1	-
5	EDO	B	204	-	-	1/1/1/1	-
5	EDO	K	204	-	-	0/1/1/1	-
5	EDO	B	202	-	-	1/1/1/1	-
5	EDO	K	205	-	-	1/1/1/1	-
6	NAG	H	201	2	-	5/6/23/26	0/1/1/1
5	EDO	E	202	-	-	1/1/1/1	-
5	EDO	H	204	-	-	0/1/1/1	-
5	EDO	K	206	-	-	0/1/1/1	-
5	EDO	J	202	-	-	0/1/1/1	-
5	EDO	E	201	-	-	0/1/1/1	-
5	EDO	I	102	-	-	0/1/1/1	-
6	NAG	D	202	1	-	1/6/23/26	0/1/1/1
5	EDO	K	202	-	-	1/1/1/1	-
5	EDO	H	203	-	-	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	9.02	1.58	1.43
6	H	201	NAG	O5-C1	3.69	1.49	1.43
6	B	207	NAG	C1-C2	3.03	1.56	1.52
6	K	207	NAG	C1-C2	2.96	1.56	1.52
6	D	202	NAG	C1-C2	2.40	1.55	1.52

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	K	207	NAG	C1-O5-C5	9.53	124.95	112.19
6	H	201	NAG	C2-N2-C7	7.92	133.51	122.90
6	H	201	NAG	C1-C2-N2	4.19	117.04	110.43
6	D	202	NAG	C1-O5-C5	3.79	117.26	112.19
6	H	201	NAG	C1-O5-C5	3.74	117.19	112.19

There are no chirality outliers.

5 of 18 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	A	201	EDO	1	0
5	B	201	EDO	1	0
5	H	205	EDO	1	0
5	B	204	EDO	1	0
5	K	204	EDO	1	0
5	B	202	EDO	1	0
5	K	205	EDO	1	0
6	H	201	NAG	2	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, 95th 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 ²)	Q<0.9
1	A	179/181 (98%)	-1.40	0 100 100	37, 49, 68, 75	0
1	D	179/181 (98%)	-1.38	0 100 100	37, 49, 67, 76	0
1	G	179/181 (98%)	-1.25	0 100 100	48, 64, 84, 108	0
1	J	179/181 (98%)	-1.25	0 100 100	49, 64, 85, 105	0
2	B	187/189 (98%)	-1.37	0 100 100	38, 53, 73, 88	0
2	E	187/189 (98%)	-1.38	0 100 100	37, 52, 73, 84	0
2	H	187/189 (98%)	-1.34	0 100 100	37, 62, 86, 97	1 (0%)
2	K	187/189 (98%)	-1.34	0 100 100	47, 63, 86, 95	0
3	C	13/14 (92%)	-1.03	0 100 100	41, 51, 79, 90	0
3	F	13/14 (92%)	-1.10	0 100 100	39, 49, 79, 81	0
3	I	13/14 (92%)	-1.07	0 100 100	58, 62, 89, 90	0
3	L	13/14 (92%)	-1.00	0 100 100	58, 63, 86, 92	0
All	All	1516/1536 (98%)	-1.33	0 100 100	37, 58, 81, 108	1 (0%)

There are no RSRZ outliers to report.

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

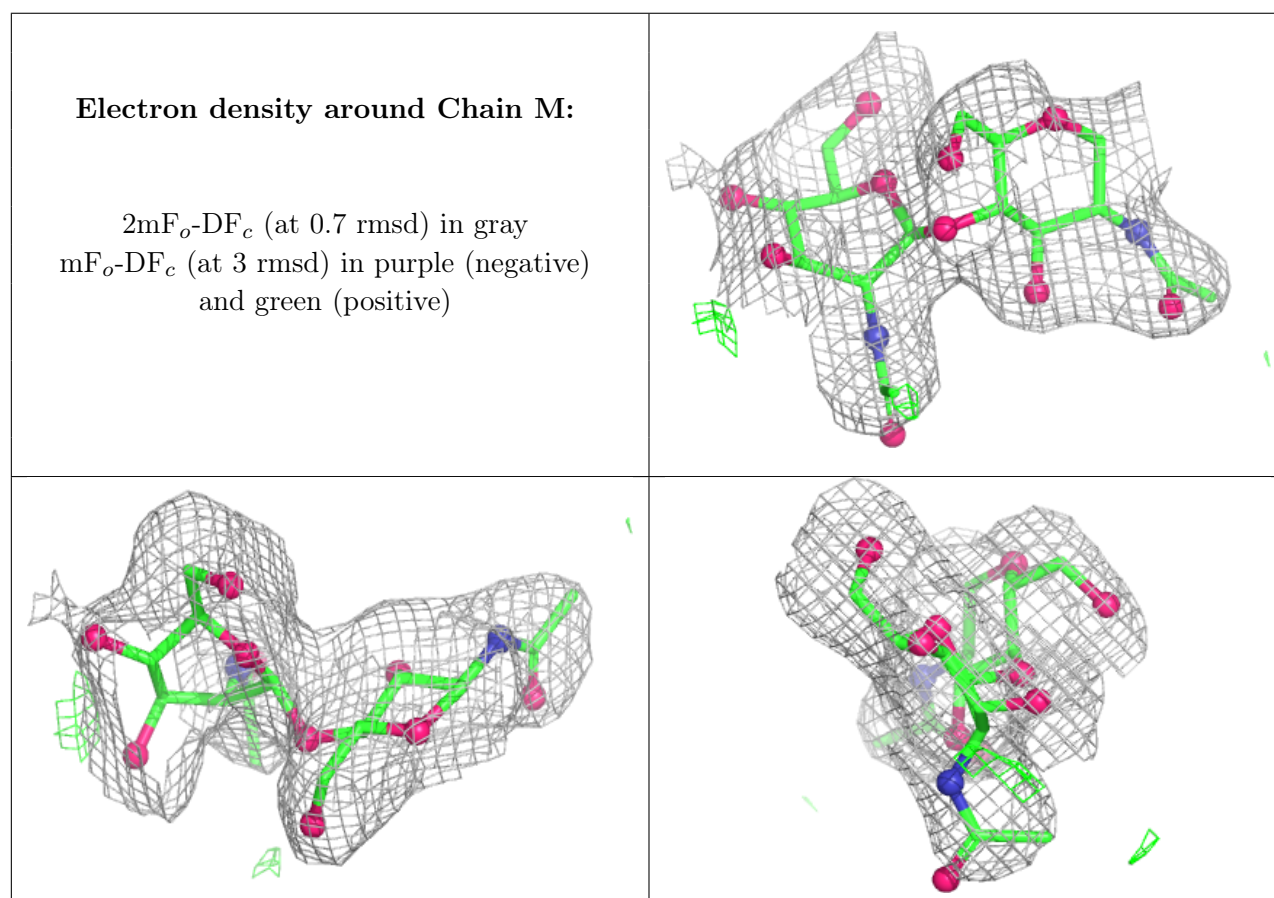
There are no non-standard protein/DNA/RNA residues in this entry.

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, 95th 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.

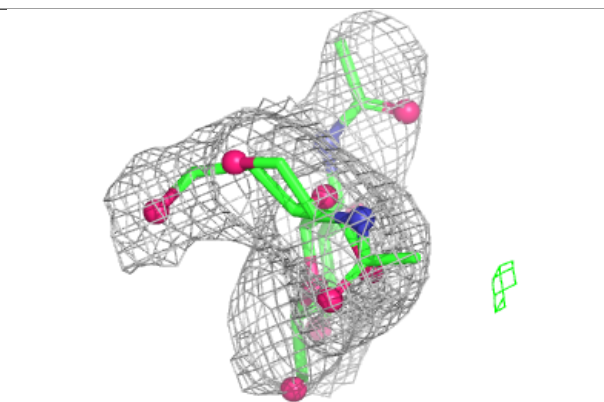
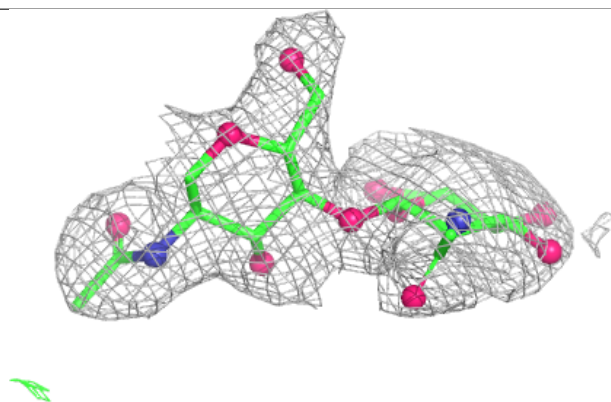
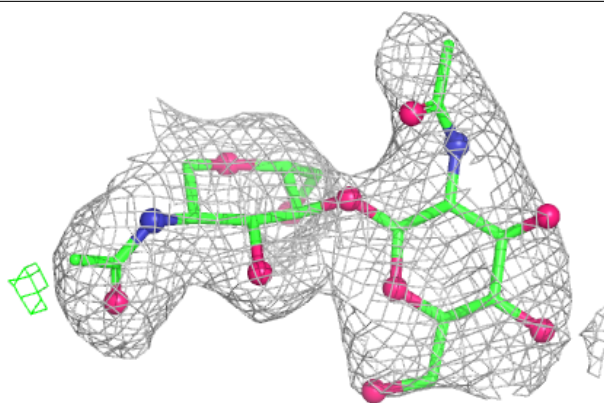
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	NAG	M	2	14/15	0.97	0.05	88,108,114,117	0
4	NAG	O	2	14/15	0.97	0.05	78,89,93,94	0
4	NAG	P	2	14/15	0.98	0.04	87,101,110,111	0
4	NAG	N	2	14/15	0.99	0.04	76,87,92,94	0
4	NAG	M	1	14/15	0.99	0.04	75,86,100,112	0
4	NAG	P	1	14/15	0.99	0.04	65,82,104,111	0
4	NAG	N	1	14/15	0.99	0.03	56,67,88,99	0
4	NAG	O	1	14/15	1.00	0.03	55,72,87,92	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.

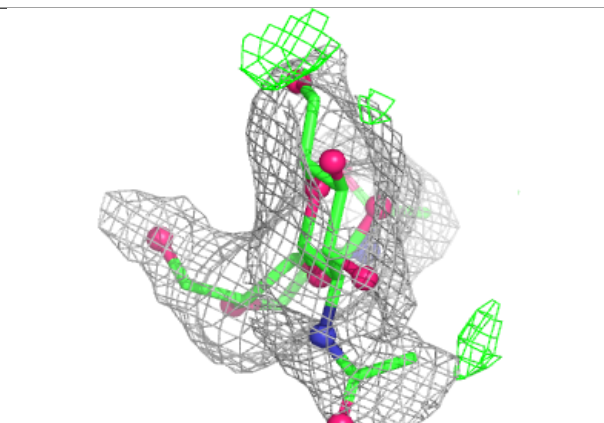
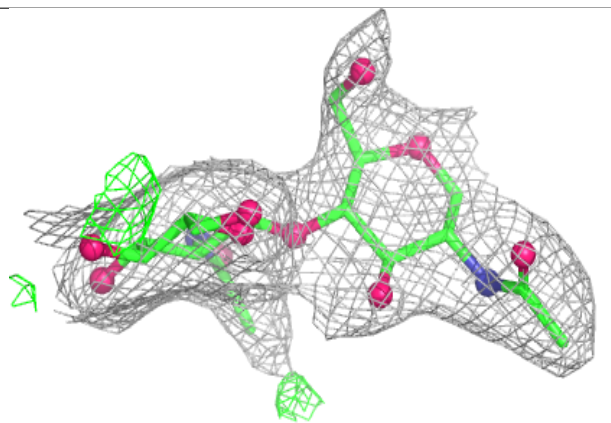
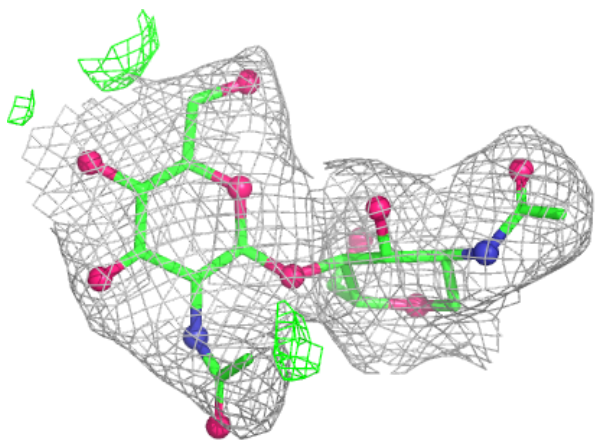


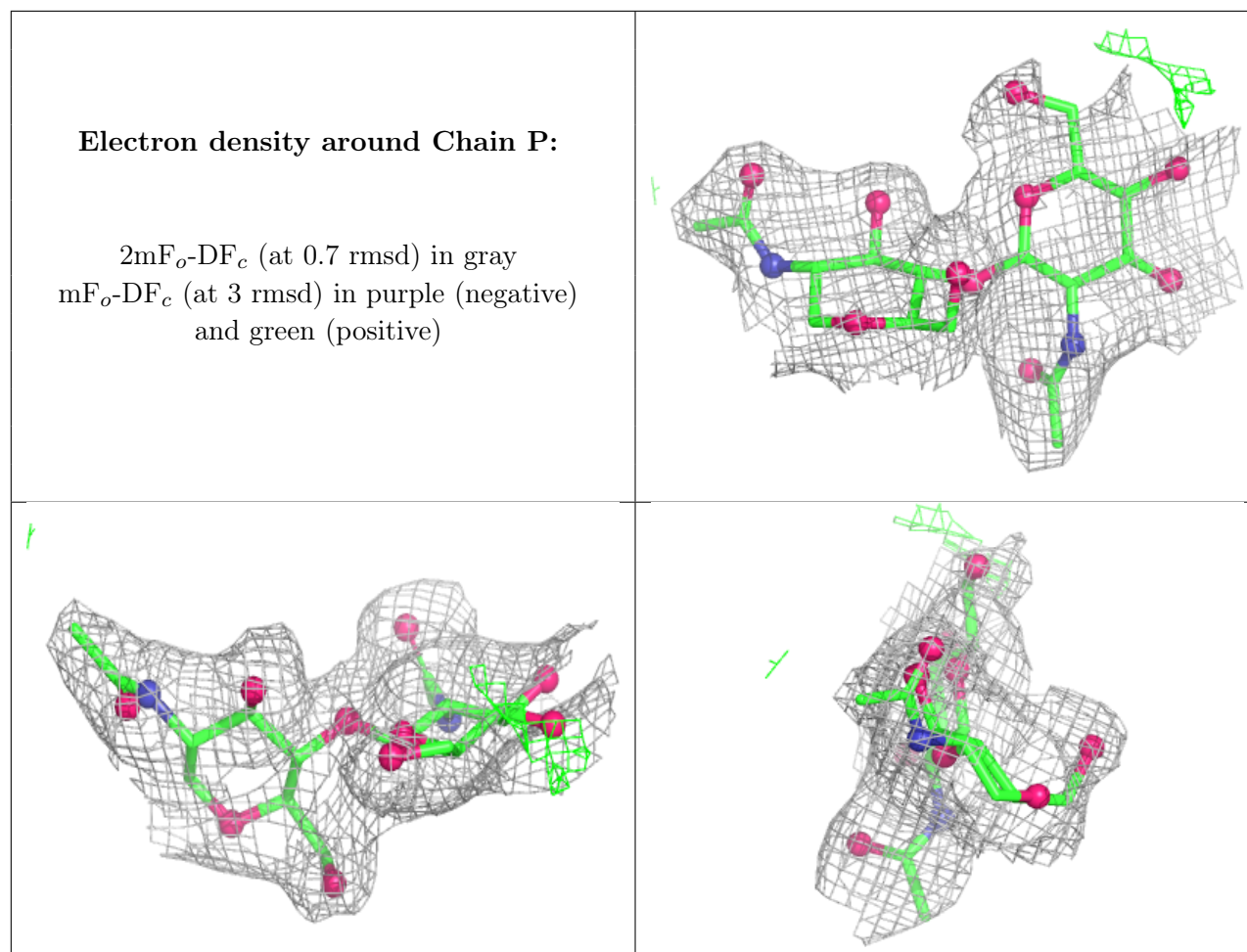
Electron density around Chain N:

$2mF_o-DF_c$ (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 [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, 95th 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 ²)	Q<0.9
5	EDO	K	206	4/4	0.94	0.11	81,89,90,94	0
6	NAG	D	202	14/15	0.95	0.05	83,104,112,117	0
5	EDO	H	203	4/4	0.96	0.08	81,86,92,97	0
5	EDO	H	205	4/4	0.96	0.10	81,82,88,90	0
6	NAG	K	207	14/15	0.96	0.07	86,110,116,118	0
5	EDO	J	202	4/4	0.97	0.07	89,94,101,106	0
5	EDO	K	204	4/4	0.97	0.09	71,75,77,81	0
5	EDO	K	205	4/4	0.97	0.07	86,93,95,97	0
5	EDO	H	204	4/4	0.97	0.06	84,91,95,95	0
6	NAG	B	207	14/15	0.97	0.04	80,90,101,104	0
5	EDO	E	205	4/4	0.97	0.10	70,70,72,72	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
6	NAG	H	201	14/15	0.97	0.05	87,104,109,112	0
5	EDO	I	101	4/4	0.97	0.11	81,81,82,87	0
5	EDO	J	201	4/4	0.98	0.05	76,80,83,86	0
5	EDO	E	203	4/4	0.98	0.07	66,69,71,73	0
5	EDO	K	201	4/4	0.98	0.08	59,63,63,68	0
5	EDO	B	205	4/4	0.98	0.08	52,55,55,62	0
5	EDO	H	202	4/4	0.98	0.08	58,64,67,72	0
5	EDO	B	206	4/4	0.98	0.07	74,74,75,76	0
5	EDO	L	101	4/4	0.98	0.11	79,83,83,85	0
5	EDO	C	201	4/4	0.98	0.07	65,70,72,73	0
5	EDO	E	201	4/4	0.98	0.06	50,53,54,62	0
5	EDO	E	202	4/4	0.98	0.05	69,69,75,79	0
5	EDO	I	102	4/4	0.98	0.06	87,90,96,98	0
5	EDO	K	202	4/4	0.99	0.09	62,70,71,74	0
5	EDO	K	203	4/4	0.99	0.07	62,71,77,82	0
5	EDO	C	202	4/4	0.99	0.05	57,65,67,68	0
5	EDO	D	201	4/4	0.99	0.05	55,65,72,76	0
5	EDO	B	203	4/4	0.99	0.05	73,77,86,93	0
5	EDO	B	204	4/4	0.99	0.05	58,60,65,67	0
5	EDO	A	201	4/4	0.99	0.05	82,86,89,89	0
5	EDO	E	204	4/4	0.99	0.07	66,68,80,84	0
5	EDO	B	201	4/4	0.99	0.06	68,69,73,73	0
5	EDO	B	202	4/4	0.99	0.05	65,68,71,76	0

6.5 Other polymers [i](#)

There are no such residues in this entry.