



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 06:35 PM UTC

PDB ID : 5A56 / pdb_00005a56
Title : The structure of GH101 from Streptococcus pneumoniae TIGR4 in complex with 1-O-methyl-T-antigen
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Deposited on : 2015-06-16
Resolution : 1.80 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

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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

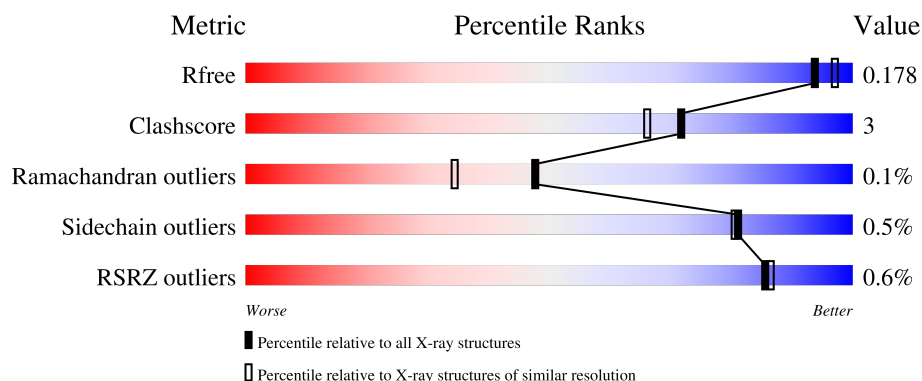
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.80 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	7662 (1.80-1.80)
Clashscore	190562	8479 (1.80-1.80)
Ramachandran outliers	187476	8391 (1.80-1.80)
Sidechain outliers	187428	8390 (1.80-1.80)
RSRZ outliers	180081	7663 (1.80-1.80)

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	1117	94% 5%
2	B	2	50% 50%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	MGC	B	1[B]	-	-	X	-
5	CIT	A	2432	-	X	-	-
6	EDO	A	2436	-	-	X	-
6	EDO	A	2447	-	-	X	-

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 10681 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 ENDO-ALPHA-N-ACETYLGALACTOSAMINIDASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	1106	8937	5637	1527	1748	25	0	32	0

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	316	MET	-	expression tag	UNP Q2MGH6
A	1426	THR	-	expression tag	UNP Q2MGH6
A	1427	HIS	-	expression tag	UNP Q2MGH6
A	1428	HIS	-	expression tag	UNP Q2MGH6
A	1429	HIS	-	expression tag	UNP Q2MGH6
A	1430	HIS	-	expression tag	UNP Q2MGH6
A	1431	HIS	-	expression tag	UNP Q2MGH6
A	1432	HIS	-	expression tag	UNP Q2MGH6
A	460	SER	ASN	conflict	UNP Q2MGH6
A	1164	ARG	ASP	conflict	UNP Q2MGH6
A	1201	ASP	GLN	conflict	UNP Q2MGH6
A	1263	HIS	ASN	conflict	UNP Q2MGH6

- Molecule 2 is an oligosaccharide called beta-D-galactopyranose-(1-3)-methyl 2-acetamido-2-deoxy-alpha-D-galactopyranoside.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
2	B	2	54	30	2	22	0	2	0

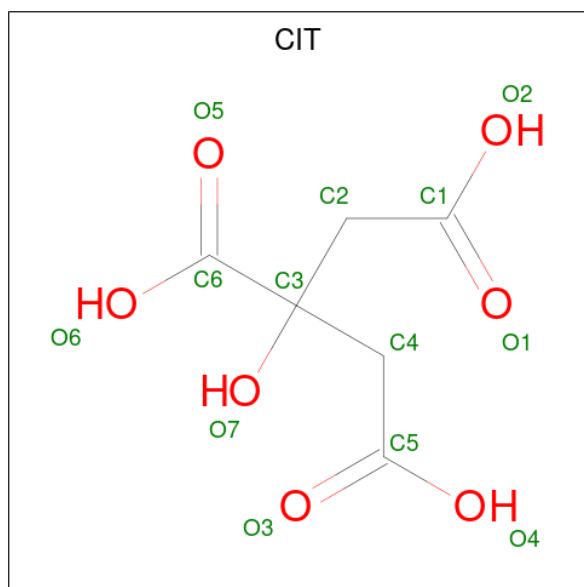
- Molecule 3 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	3	Total	Ca	0	0
			3	3		

- Molecule 4 is MANGANESE (II) ION (CCD ID: MN) (formula: Mn).

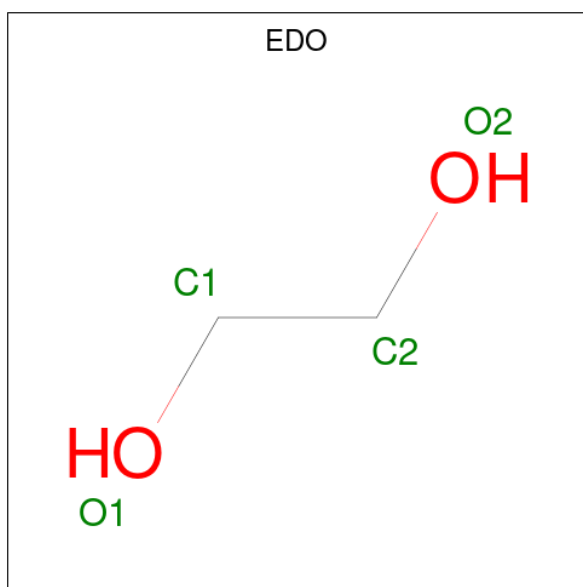
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Mn	0	0
			1	1		

- Molecule 5 is CITRIC ACID (CCD ID: CIT) (formula: C₆H₈O₇).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			13	6	7		
5	A	1	Total	C	O	0	0
			13	6	7		

- Molecule 6 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



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

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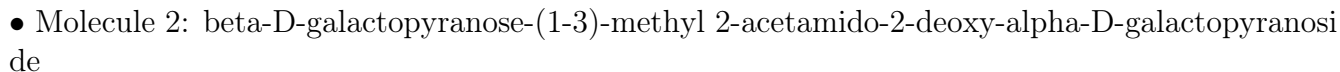
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			4	2	2		
6	A	1	Total	C	O	0	0
			4	2	2		
6	A	1	Total	C	O	0	0
			4	2	2		
6	A	1	Total	C	O	0	0
			4	2	2		
6	A	1	Total	C	O	0	0
			4	2	2		
6	A	1	Total	C	O	0	0
			4	2	2		
6	A	1	Total	C	O	0	0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

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	1536	Total	O	0	0
			1536	1536		

- Molecule 1: ENDO-ALPHA-N-ACETYL GALACTOSAMINIDASE



4 Data and refinement statistics

Property	Value	Source
Space group	P 2 21 21	Depositor
Cell constants a, b, c, α , β , γ	86.71Å 121.76Å 139.43Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	43.42 – 1.80 43.42 – 1.80	Depositor EDS
% Data completeness (in resolution range)	99.8 (43.42-1.80) 99.7 (43.42-1.80)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.05 (at 1.79Å)	Xtriage
Refinement program	REFMAC 5.8.0073	Depositor
R, R_{free}	0.152 , 0.178 0.152 , 0.178	Depositor DCC
R_{free} test set	6867 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	15.5	Xtriage
Anisotropy	0.042	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 41.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	10681	wwPDB-VP
Average B, all atoms (Å ²)	18.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.00% of the height of the origin peak. No significant pseudotranslation is detected.*

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: MN, GAL, CIT, MGC, EDO, CA

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	0.70	0/9238	0.82	0/12517

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	8937	0	8607	45	0
2	B	54	0	45	11	0
3	A	3	0	0	0	0
4	A	1	0	0	0	0
5	A	26	0	10	4	0
6	A	124	0	186	15	0
7	A	1536	0	0	13	0
All	All	10681	0	8848	59	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 3.

All (59) 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)
2:B:1[B]:MGC:HM3	2:B:1[B]:MGC:C5	1.52	1.34
2:B:1[B]:MGC:CM	2:B:1[B]:MGC:H5	1.64	1.19
2:B:1[B]:MGC:C5	2:B:1[B]:MGC:CM	2.21	1.08
2:B:1[B]:MGC:HM3	2:B:1[B]:MGC:H5	1.13	1.03
7:A:3864:HOH:O	2:B:1[B]:MGC:H83	1.57	1.03
1:A:1201:ASP:HB2	5:A:2432:CIT:H22	1.52	0.91
1:A:434:PRO:HG3	7:A:3380:HOH:O	1.77	0.85
1:A:728:ASP:HB3	6:A:2447:EDO:H22	1.57	0.84
1:A:440:ASP:HB3	1:A:443:LYS:HE2	1.63	0.78
2:B:1[B]:MGC:HM3	2:B:1[B]:MGC:C6	2.13	0.77
1:A:1391:ASN:HB3	6:A:2436:EDO:H12	1.67	0.77
2:B:1[B]:MGC:O7	2:B:1[B]:MGC:H1	1.85	0.76
1:A:728:ASP:HB3	6:A:2447:EDO:C2	2.18	0.73
2:B:1[B]:MGC:HM3	2:B:1[B]:MGC:O6	1.92	0.69
1:A:628[B]:MET:HE3	7:A:3504:HOH:O	1.94	0.67
1:A:628[A]:MET:HE2	7:A:4096:HOH:O	1.97	0.63
1:A:628[B]:MET:SD	1:A:1208[B]:GLU:OE1	2.58	0.62
1:A:628[B]:MET:HG2	7:A:3504:HOH:O	1.99	0.62
7:A:3864:HOH:O	2:B:1[B]:MGC:C8	2.30	0.62
5:A:2432:CIT:O1	5:A:2432:CIT:O4	2.22	0.56
2:B:1[A]:MGC:H83	2:B:1[A]:MGC:H3	1.88	0.56
1:A:369:GLN:OE1	1:A:376:ARG:HD3	2.06	0.54
6:A:2447:EDO:O1	7:A:4396:HOH:O	2.18	0.54
1:A:366[A]:GLN:HG3	7:A:3042:HOH:O	2.07	0.54
1:A:1391:ASN:CB	6:A:2436:EDO:H12	2.37	0.53
6:A:2436:EDO:H21	7:A:4435:HOH:O	2.07	0.53
1:A:1201:ASP:CB	5:A:2432:CIT:H22	2.30	0.52
1:A:624:ASN:HA	1:A:628[B]:MET:HE2	1.90	0.52
1:A:709:GLU:OE1	1:A:720:TYR:OH	2.24	0.50
1:A:728:ASP:CB	6:A:2447:EDO:H22	2.37	0.50
1:A:549:TRP:CD2	1:A:568:PRO:HB3	2.47	0.49
1:A:1130[A]:LYS:HG3	1:A:1145:TYR:CD2	2.47	0.49
2:B:1[A]:MGC:H3	2:B:1[A]:MGC:C8	2.43	0.49
1:A:495[A]:LYS:NZ	6:A:2439:EDO:H11	2.28	0.49
1:A:1120:TYR:OH	1:A:1208[A]:GLU:OE2	2.22	0.48
1:A:1158:TYR:CE2	1:A:1160:HIS:HB2	2.48	0.48
1:A:1312:LYS:HD3	1:A:1417:GLU:OE2	2.13	0.48
1:A:628[A]:MET:HE2	1:A:1057:MET:HE1	1.97	0.47
1:A:1016:LYS:HE3	1:A:1046:GLN:HB3	1.97	0.47
1:A:1325:ASP:H	6:A:2436:EDO:H11	1.80	0.46
1:A:675[B]:GLU:HG2	7:A:3596:HOH:O	2.15	0.46
1:A:364[B]:VAL:HG22	6:A:2445:EDO:H22	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1139[B]:GLU:HG2	7:A:4213:HOH:O	2.16	0.44
1:A:628[A]:MET:HG2	1:A:1057:MET:HE1	1.99	0.43
1:A:1412:ASN:C	6:A:2435:EDO:H11	2.44	0.43
1:A:1238:ALA:HB3	6:A:2446:EDO:H11	2.01	0.43
1:A:1201:ASP:H	5:A:2432:CIT:C1	2.32	0.42
1:A:1325:ASP:H	6:A:2436:EDO:C1	2.32	0.42
1:A:1323:GLY:HA3	1:A:1404:GLY:O	2.19	0.42
1:A:556:LYS:NZ	6:A:2440:EDO:H21	2.34	0.41
1:A:1057:MET:HB3	7:A:4090:HOH:O	2.19	0.41
1:A:1249:VAL:HA	1:A:1296:ASN:HB3	2.03	0.41
1:A:920[B]:ARG:HG2	7:A:3894:HOH:O	2.19	0.41
1:A:1054:SER:OG	1:A:1062:GLN:HG3	2.21	0.41
1:A:1013:ASP:CG	6:A:2441:EDO:O1	2.64	0.41
1:A:764:ASP:O	1:A:765[A]:VAL:HB	2.21	0.40
1:A:366[A]:GLN:HG2	1:A:368:ASN:OD1	2.21	0.40
1:A:684:ALA:HB1	1:A:689:ALA:HB3	2.03	0.40

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	1135/1117 (102%)	1098 (97%)	35 (3%)	2 (0%)	43 31

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	765[A]	VAL
1	A	765[B]	VAL

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	962/942 (102%)	956 (99%)	6 (1%)	78	77

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	795[A]	ILE
1	A	795[B]	ILE
1	A	989	GLN
1	A	1166	ASN
1	A	1193	LEU
1	A	1239	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	430	ASN
1	A	637	ASN
1	A	1014	GLN
1	A	1046	GLN
1	A	1414	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

4 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	MGC	B	1[A]	2	16,16,16	1.03	1 (6%)	22,22,22	1.89	5 (22%)
2	MGC	B	1[B]	2	16,16,16	0.76	1 (6%)	22,22,22	2.75	12 (54%)
2	GAL	B	2[A]	2	11,11,12	0.75	0	15,15,17	1.20	3 (20%)
2	GAL	B	2[B]	2	11,11,12	0.71	0	15,15,17	1.25	2 (13%)

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	MGC	B	1[A]	2	-	3/8/28/28	0/1/1/1
2	MGC	B	1[B]	2	-	3/8/28/28	0/1/1/1
2	GAL	B	2[A]	2	-	0/2/19/22	0/1/1/1
2	GAL	B	2[B]	2	-	1/2/19/22	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1[A]	MGC	O1-C1	2.65	1.44	1.40
2	B	1[B]	MGC	C7-N2	-2.47	1.26	1.34

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1[B]	MGC	C1-C2-N2	-8.18	97.20	110.92
2	B	1[A]	MGC	C2-N2-C7	5.17	135.20	123.11
2	B	1[A]	MGC	C8-C7-N2	4.17	123.03	116.12
2	B	1[B]	MGC	C1-O5-C5	-4.13	105.66	113.72
2	B	1[B]	MGC	O5-C1-O1	-3.97	101.70	110.94
2	B	1[A]	MGC	O1-C1-C2	3.67	113.70	108.13
2	B	1[B]	MGC	CM-O1-C1	-3.62	107.77	113.26
2	B	1[B]	MGC	C2-N2-C7	-3.13	115.78	123.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	2[B]	GAL	C2-C3-C4	-2.82	105.90	110.86
2	B	2[A]	GAL	C1-O5-C5	2.61	115.69	112.19
2	B	1[B]	MGC	O3-C3-C2	-2.61	104.39	109.58
2	B	1[B]	MGC	C4-C3-C2	-2.48	106.79	110.40
2	B	1[B]	MGC	O4-C4-C5	-2.43	103.34	109.32
2	B	2[A]	GAL	C1-C2-C3	2.38	113.11	109.64
2	B	1[B]	MGC	O4-C4-C3	-2.27	105.02	110.38
2	B	1[B]	MGC	C3-C2-N2	-2.18	106.60	110.62
2	B	1[B]	MGC	O5-C5-C4	-2.16	105.81	109.70
2	B	2[A]	GAL	C3-C4-C5	2.10	114.04	110.23
2	B	1[B]	MGC	O1-C1-C2	-2.08	104.98	108.13
2	B	1[A]	MGC	O7-C7-C8	-2.07	118.38	122.05
2	B	2[B]	GAL	O2-C2-C3	-2.05	105.91	110.15
2	B	1[A]	MGC	O5-C1-C2	-2.02	106.78	110.59

There are no chirality outliers.

All (7) torsion outliers are listed below:

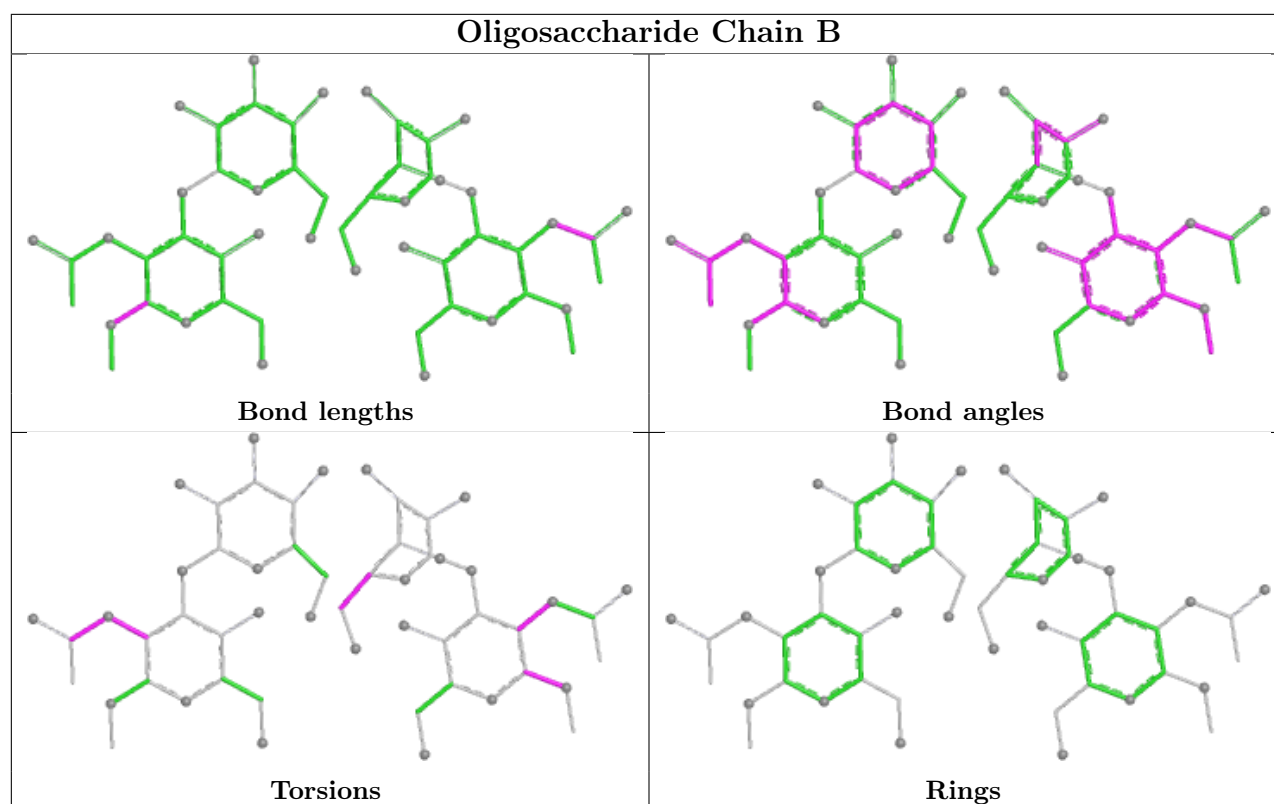
Mol	Chain	Res	Type	Atoms
2	B	1[A]	MGC	C3-C2-N2-C7
2	B	1[B]	MGC	O5-C1-O1-CM
2	B	1[A]	MGC	O7-C7-N2-C2
2	B	1[A]	MGC	C8-C7-N2-C2
2	B	1[B]	MGC	C3-C2-N2-C7
2	B	2[B]	GAL	C4-C5-C6-O6
2	B	1[B]	MGC	C1-C2-N2-C7

There are no ring outliers.

2 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	1[B]	MGC	9	0
2	B	1[A]	MGC	2	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 37 ligands modelled in this entry, 4 are monoatomic - leaving 33 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
6	EDO	A	2458	-	3,3,3	0.72	0	2,2,2	0.32	0
6	EDO	A	2438	-	3,3,3	0.50	0	2,2,2	0.37	0
6	EDO	A	2464	-	3,3,3	0.54	0	2,2,2	0.43	0
6	EDO	A	2445	-	3,3,3	0.37	0	2,2,2	0.81	0
6	EDO	A	2448	-	3,3,3	0.77	0	2,2,2	0.23	0
6	EDO	A	2443	-	3,3,3	0.40	0	2,2,2	0.20	0
6	EDO	A	2465	-	3,3,3	0.39	0	2,2,2	0.33	0
6	EDO	A	2456	-	3,3,3	0.36	0	2,2,2	0.56	0
6	EDO	A	2462	-	3,3,3	0.31	0	2,2,2	0.78	0
6	EDO	A	2435	-	3,3,3	0.55	0	2,2,2	0.45	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	EDO	A	2441	-	3,3,3	0.46	0	2,2,2	0.26	0
6	EDO	A	2454	-	3,3,3	0.64	0	2,2,2	0.63	0
6	EDO	A	2460	-	3,3,3	0.54	0	2,2,2	0.17	0
6	EDO	A	2442	-	3,3,3	0.31	0	2,2,2	0.77	0
6	EDO	A	2459	-	3,3,3	0.50	0	2,2,2	0.59	0
6	EDO	A	2451	-	3,3,3	0.52	0	2,2,2	0.47	0
6	EDO	A	2449	-	3,3,3	0.63	0	2,2,2	0.68	0
6	EDO	A	2447	-	3,3,3	0.52	0	2,2,2	0.54	0
6	EDO	A	2461	-	3,3,3	0.37	0	2,2,2	0.53	0
6	EDO	A	2455	-	3,3,3	0.25	0	2,2,2	1.00	0
5	CIT	A	2431	-	12,12,12	2.11	3 (25%)	17,17,17	3.50	7 (41%)
6	EDO	A	2440	-	3,3,3	0.30	0	2,2,2	0.63	0
5	CIT	A	2432	-	12,12,12	0.92	0	17,17,17	2.28	7 (41%)
6	EDO	A	2444	-	3,3,3	0.32	0	2,2,2	0.84	0
6	EDO	A	2436	-	3,3,3	0.65	0	2,2,2	0.19	0
6	EDO	A	2450	-	3,3,3	0.50	0	2,2,2	0.55	0
6	EDO	A	2452	-	3,3,3	0.31	0	2,2,2	0.92	0
6	EDO	A	2457	-	3,3,3	0.49	0	2,2,2	0.40	0
6	EDO	A	2437	-	3,3,3	0.43	0	2,2,2	0.57	0
6	EDO	A	2463	-	3,3,3	0.44	0	2,2,2	0.49	0
6	EDO	A	2439	-	3,3,3	0.52	0	2,2,2	0.41	0
6	EDO	A	2453	-	3,3,3	0.34	0	2,2,2	0.65	0
6	EDO	A	2446	-	3,3,3	0.39	0	2,2,2	0.42	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
6	EDO	A	2458	-	-	0/1/1/1	-
6	EDO	A	2438	-	-	0/1/1/1	-
6	EDO	A	2464	-	-	1/1/1/1	-
6	EDO	A	2445	-	-	0/1/1/1	-
6	EDO	A	2448	-	-	0/1/1/1	-
6	EDO	A	2443	-	-	0/1/1/1	-
6	EDO	A	2465	-	-	0/1/1/1	-
6	EDO	A	2456	-	-	0/1/1/1	-
6	EDO	A	2462	-	-	0/1/1/1	-
6	EDO	A	2435	-	-	0/1/1/1	-
6	EDO	A	2441	-	-	0/1/1/1	-
6	EDO	A	2454	-	-	1/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	EDO	A	2460	-	-	1/1/1/1	-
6	EDO	A	2442	-	-	0/1/1/1	-
6	EDO	A	2459	-	-	1/1/1/1	-
6	EDO	A	2451	-	-	1/1/1/1	-
6	EDO	A	2449	-	-	0/1/1/1	-
6	EDO	A	2447	-	-	1/1/1/1	-
6	EDO	A	2461	-	-	1/1/1/1	-
6	EDO	A	2455	-	-	0/1/1/1	-
5	CIT	A	2431	-	-	7/16/16/16	-
6	EDO	A	2440	-	-	1/1/1/1	-
5	CIT	A	2432	-	-	12/16/16/16	-
6	EDO	A	2444	-	-	0/1/1/1	-
6	EDO	A	2436	-	-	0/1/1/1	-
6	EDO	A	2450	-	-	0/1/1/1	-
6	EDO	A	2452	-	-	0/1/1/1	-
6	EDO	A	2457	-	-	0/1/1/1	-
6	EDO	A	2437	-	-	0/1/1/1	-
6	EDO	A	2463	-	-	0/1/1/1	-
6	EDO	A	2439	-	-	1/1/1/1	-
6	EDO	A	2453	-	-	1/1/1/1	-
6	EDO	A	2446	-	-	0/1/1/1	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	2431	CIT	C4-C3	-5.40	1.47	1.54
5	A	2431	CIT	C2-C3	-2.59	1.50	1.54
5	A	2431	CIT	O4-C5	-2.13	1.23	1.30

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	2431	CIT	O7-C3-C6	-8.76	96.53	108.96
5	A	2431	CIT	C2-C3-C6	-6.27	96.16	110.03
5	A	2431	CIT	C4-C3-C2	5.82	124.25	109.31
5	A	2432	CIT	O7-C3-C6	-4.82	102.12	108.96
5	A	2431	CIT	O7-C3-C2	4.71	120.11	109.38
5	A	2431	CIT	O6-C6-C3	4.59	121.94	113.14
5	A	2432	CIT	O6-C6-C3	3.89	120.61	113.14
5	A	2432	CIT	C4-C3-C6	3.57	117.92	110.03
5	A	2432	CIT	O4-C5-C4	3.02	123.91	114.35
5	A	2432	CIT	O3-C5-C4	-2.86	114.84	122.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	2431	CIT	C4-C3-C6	-2.71	104.05	110.03
5	A	2432	CIT	C2-C3-C6	2.29	115.11	110.03
5	A	2432	CIT	O5-C6-C3	-2.29	117.66	122.09
5	A	2431	CIT	O6-C6-O5	-2.06	117.26	123.86

There are no chirality outliers.

All (29) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	2432	CIT	O7-C3-C6-O5
5	A	2432	CIT	O7-C3-C6-O6
5	A	2432	CIT	C4-C3-C6-O5
5	A	2432	CIT	C4-C3-C6-O6
5	A	2432	CIT	C2-C3-C4-C5
5	A	2431	CIT	C2-C3-C6-O5
5	A	2431	CIT	C1-C2-C3-O7
6	A	2447	EDO	O1-C1-C2-O2
6	A	2439	EDO	O1-C1-C2-O2
6	A	2464	EDO	O1-C1-C2-O2
5	A	2432	CIT	O7-C3-C4-C5
5	A	2431	CIT	O7-C3-C6-O5
5	A	2431	CIT	O7-C3-C4-C5
6	A	2453	EDO	O1-C1-C2-O2
6	A	2460	EDO	O1-C1-C2-O2
5	A	2431	CIT	C2-C3-C6-O6
5	A	2431	CIT	C4-C3-C6-O6
5	A	2432	CIT	C1-C2-C3-O7
6	A	2440	EDO	O1-C1-C2-O2
6	A	2461	EDO	O1-C1-C2-O2
5	A	2432	CIT	C1-C2-C3-C4
5	A	2432	CIT	C2-C3-C6-O6
5	A	2432	CIT	C3-C4-C5-O4
6	A	2451	EDO	O1-C1-C2-O2
6	A	2454	EDO	O1-C1-C2-O2
6	A	2459	EDO	O1-C1-C2-O2
5	A	2431	CIT	O7-C3-C6-O6
5	A	2432	CIT	C2-C3-C6-O5
5	A	2432	CIT	C3-C4-C5-O3

There are no ring outliers.

9 monomers are involved in 19 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	2445	EDO	1	0
6	A	2435	EDO	1	0
6	A	2441	EDO	1	0
6	A	2447	EDO	4	0
6	A	2440	EDO	1	0
5	A	2432	CIT	4	0
6	A	2436	EDO	5	0
6	A	2439	EDO	1	0
6	A	2446	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, 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	1106/1117 (99%)	-0.69	7 (0%) 85 86	7, 14, 28, 47	32 (2%)

All (7) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1426	THR	3.8
1	A	1346	ALA	3.6
1	A	724[A]	TRP	3.2
1	A	317	GLU	2.5
1	A	1425	LEU	2.2
1	A	1348	ASN	2.1
1	A	439	ASP	2.1

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

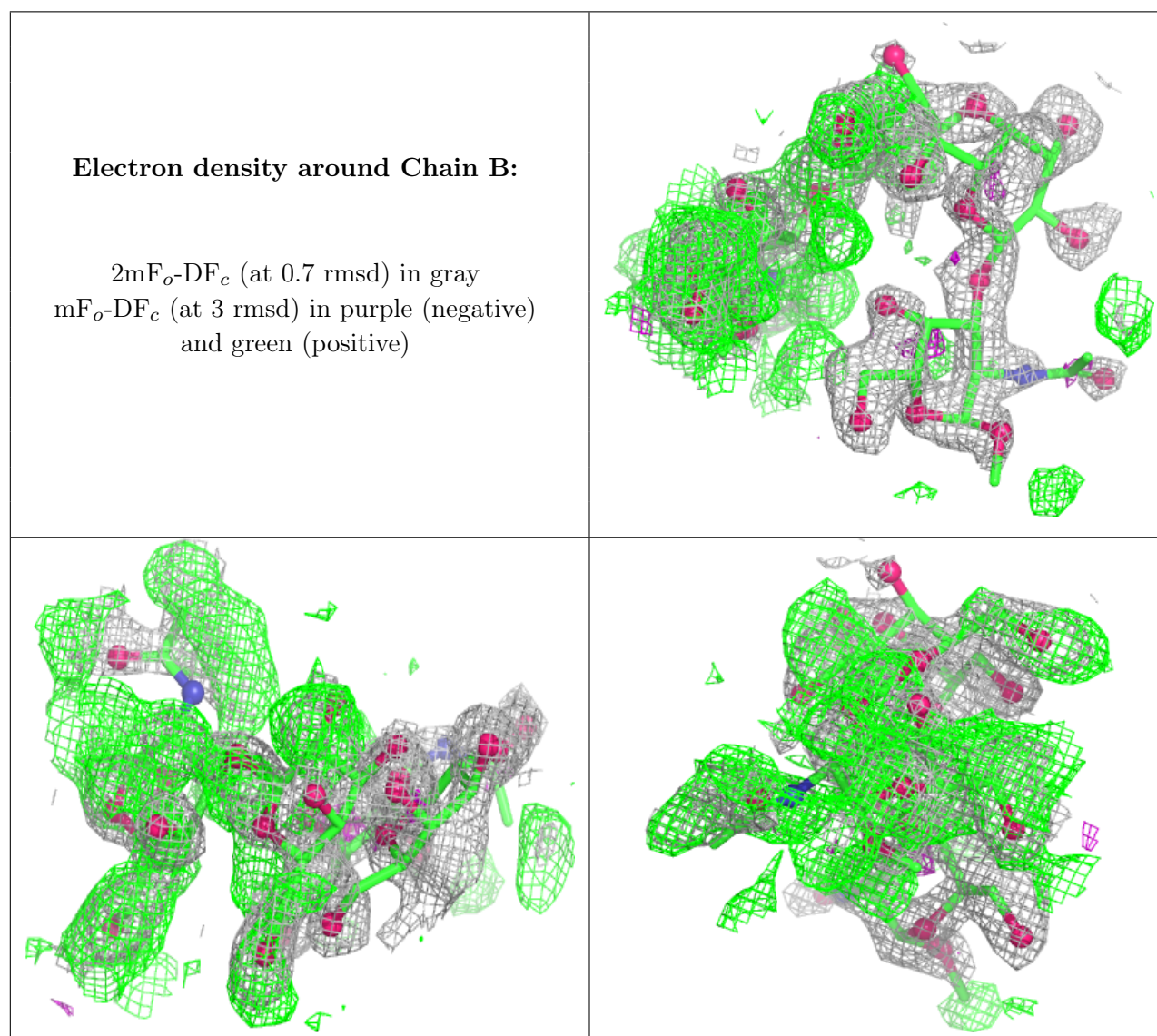
There are no non-standard protein/DNA/RNA residues in this entry.

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(Å ²)	Q<0.9
2	MGC	B	1[A]	16/16	0.78	0.20	27,31,40,41	16
2	MGC	B	1[B]	16/16	0.78	0.20	11,13,16,16	16
2	GAL	B	2[A]	11/12	0.87	0.17	22,25,27,28	11
2	GAL	B	2[B]	11/12	0.87	0.17	8,10,11,12	11

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.



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, 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
6	EDO	A	2439	4/4	0.77	0.21	45,49,49,53	0
6	EDO	A	2460	4/4	0.78	0.22	51,55,56,57	0
6	EDO	A	2463	4/4	0.80	0.20	42,43,45,47	0
6	EDO	A	2464	4/4	0.81	0.18	35,38,41,44	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
6	EDO	A	2461	4/4	0.83	0.16	38,39,44,49	0
6	EDO	A	2447	4/4	0.84	0.19	24,33,34,35	0
5	CIT	A	2432	13/13	0.85	0.14	23,38,51,52	0
6	EDO	A	2462	4/4	0.85	0.14	48,48,49,53	0
6	EDO	A	2452	4/4	0.87	0.17	22,30,35,47	0
6	EDO	A	2435	4/4	0.87	0.16	22,26,30,41	0
6	EDO	A	2436	4/4	0.87	0.21	27,28,29,32	0
6	EDO	A	2456	4/4	0.89	0.12	38,40,41,46	0
6	EDO	A	2459	4/4	0.90	0.13	32,33,33,35	0
6	EDO	A	2454	4/4	0.90	0.11	26,30,31,33	0
6	EDO	A	2441	4/4	0.91	0.13	24,25,26,28	0
6	EDO	A	2458	4/4	0.91	0.12	23,28,29,32	0
6	EDO	A	2440	4/4	0.91	0.14	33,38,39,46	0
6	EDO	A	2455	4/4	0.91	0.12	28,32,37,42	0
6	EDO	A	2444	4/4	0.92	0.11	33,33,36,41	0
6	EDO	A	2453	4/4	0.92	0.14	31,32,34,34	0
6	EDO	A	2448	4/4	0.92	0.10	23,24,25,27	0
6	EDO	A	2437	4/4	0.94	0.09	23,24,25,30	0
6	EDO	A	2451	4/4	0.94	0.10	23,28,30,36	0
6	EDO	A	2445	4/4	0.95	0.07	20,21,22,24	0
5	CIT	A	2431	13/13	0.95	0.06	18,21,24,24	0
6	EDO	A	2443	4/4	0.95	0.10	21,24,24,27	0
6	EDO	A	2438	4/4	0.95	0.09	26,28,29,33	0
6	EDO	A	2449	4/4	0.96	0.06	15,18,18,20	0
6	EDO	A	2457	4/4	0.96	0.08	22,23,24,24	0
6	EDO	A	2442	4/4	0.96	0.07	23,25,28,33	0
6	EDO	A	2446	4/4	0.97	0.09	15,16,17,17	0
6	EDO	A	2450	4/4	0.97	0.07	20,21,22,22	0
6	EDO	A	2465	4/4	0.98	0.05	22,22,23,23	0
4	MN	A	2428	1/1	0.99	0.06	21,21,21,21	0
3	CA	A	2427	1/1	0.99	0.02	15,15,15,15	0
3	CA	A	2429	1/1	1.00	0.01	12,12,12,12	0
3	CA	A	2430	1/1	1.00	0.03	13,13,13,13	0

6.5 Other polymers ⓘ

There are no such residues in this entry.