



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 12:26 PM UTC

PDB ID : 1GQL / pdb_00001gql
Title : Structure of Pseudomonas cellulosa alpha-D-glucuronidase complexed with glucuronic acid and xylotriose
Authors : Nurizzo, D.; Nagy, T.; Gilbert, H.J.; Davies, G.J.
Deposited on : 2001-11-26
Resolution : 1.67 Å(reported)

This is a Full wwPDB X-ray Structure Validation 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

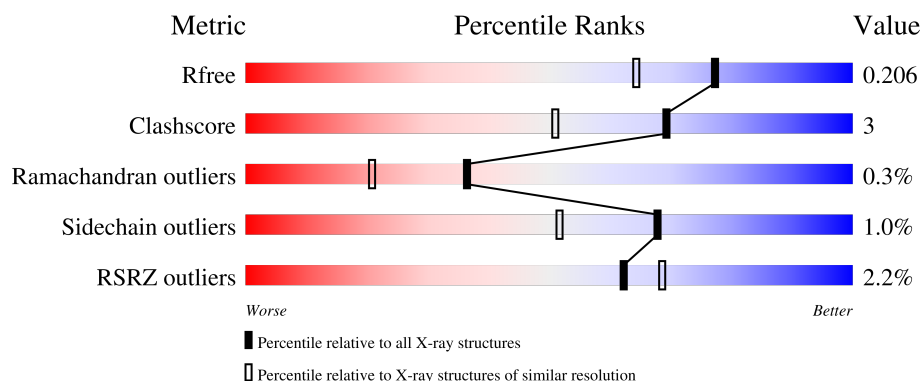
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.67 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	1054 (1.68-1.68)
Clashscore	190562	1078 (1.68-1.68)
Ramachandran outliers	187476	1068 (1.68-1.68)
Sidechain outliers	187428	1067 (1.68-1.68)
RSRZ outliers	180081	1055 (1.68-1.68)

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	708	2% 92% 7%
1	B	708	2% 92% 7%
2	C	2	50% 50%
2	D	2	50% 50%

2 Entry composition

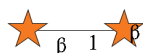
There are 6 unique types of molecules in this entry. The entry contains 12936 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 ALPHA-D-GLUCURONIDASE.

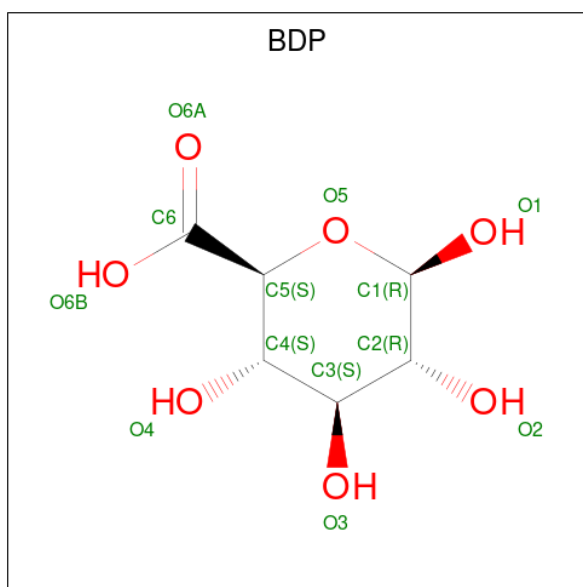
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	701	Total	C	N	O	S	0	17	0
			5714	3648	1013	1035	18			
1	B	700	Total	C	N	O	S	0	20	0
			5700	3642	1007	1033	18			

- Molecule 2 is an oligosaccharide called beta-D-xylopyranose-(1-1)-beta-D-xylopyranose.



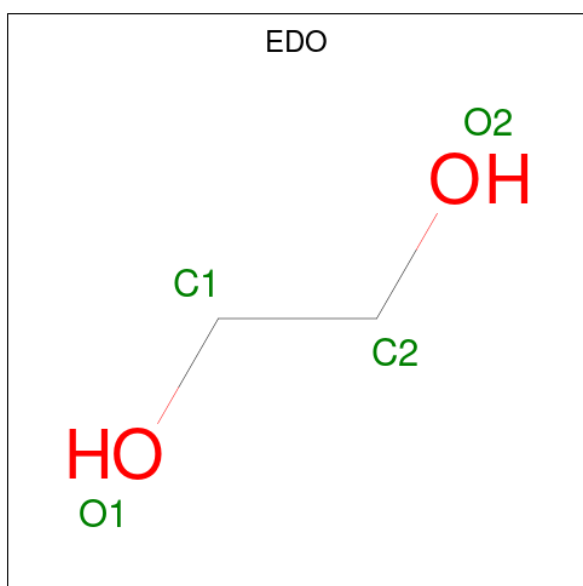
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
2	C	2	Total	C	O	0	0	1
			11	6	5			
2	D	2	Total	C	O	0	0	1
			11	6	5			

- Molecule 3 is beta-D-glucopyranuronic acid (CCD ID: BDP) (formula: C₆H₁₀O₇).



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

- Molecule 4 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: $C_2H_6O_2$).



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

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

- Molecule 5 is COBALT (II) ION (CCD ID: CO) (formula: Co).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	4	Total Co 4 4	0	4
5	B	4	Total Co 4 4	0	0

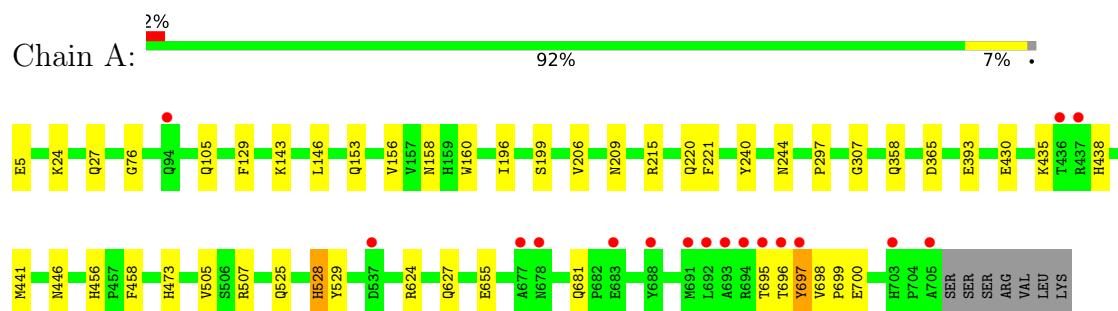
- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	705	Total O 705 705	0	0
6	B	717	Total O 717 717	0	0

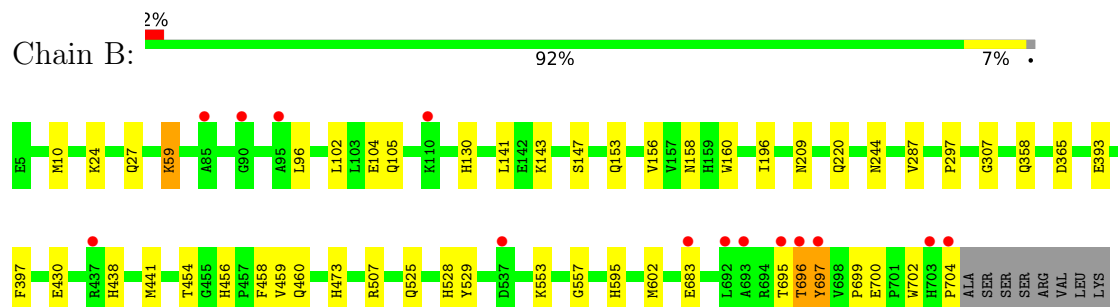
3 Residue-property plots

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: ALPHA-D-GLUCURONIDASE



- Molecule 1: ALPHA-D-GLUCURONIDASE



- Molecule 2: beta-D-xylopyranose-(1-1)-beta-D-xylopyranose



- Molecule 2: beta-D-xylopyranose-(1-1)-beta-D-xylopyranose



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	69.26Å 74.32Å 87.27Å 115.15° 92.94° 109.24°	Depositor
Resolution (Å)	20.00 – 1.67 20.00 – 1.67	Depositor EDS
% Data completeness (in resolution range)	94.1 (20.00-1.67) 94.0 (20.00-1.67)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.35 (at 1.67Å)	Xtriage
Refinement program	REFMAC 5.0	Depositor
R, R_{free}	0.146 , 0.172 (Not available) , 0.206	Depositor DCC
R_{free} test set	1256 reflections (0.79%)	wwPDB-VP
Wilson B-factor (Å ²)	15.2	Xtriage
Anisotropy	0.359	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 49.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	12936	wwPDB-VP
Average B, all atoms (Å ²)	17.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.39% 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: XYP, EDO, BDP, CO

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	0.86	1/5946 (0.0%)	0.96	2/8088 (0.0%)
1	B	0.89	2/5957 (0.0%)	0.96	1/8103 (0.0%)
All	All	0.88	3/11903 (0.0%)	0.96	3/16191 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	1
All	All	0	2

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	441	MET	SD-CE	-7.81	1.60	1.79
1	A	441	MET	SD-CE	-7.22	1.61	1.79
1	B	602	MET	SD-CE	-5.14	1.66	1.79

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	287	VAL	N-CA-C	5.70	116.21	107.77
1	A	528	HIS	N-CA-C	5.24	119.25	112.86
1	A	76	GLY	N-CA-C	5.06	117.45	110.56

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	697	TYR	Mainchain
1	B	695	THR	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	5714	0	5537	43	0
1	B	5700	0	5530	38	0
2	C	11	0	0	0	0
2	D	11	0	0	0	0
3	A	13	0	9	0	0
3	B	13	0	9	0	0
4	A	20	0	30	2	0
4	B	24	0	36	4	0
5	A	4	0	0	0	0
5	B	4	0	0	0	0
6	A	705	0	0	6	0
6	B	717	0	0	9	0
All	All	12936	0	11151	79	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 (79) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:529[B]:TYR:OH	1:A:655[B]:GLU:CD	2.00	1.04
1:A:529[B]:TYR:OH	1:A:655[B]:GLU:OE2	1.75	1.03
1:A:529[B]:TYR:OH	1:A:655[B]:GLU:OE1	1.82	0.97
1:A:696:THR:HG23	6:B:2265:HOH:O	1.64	0.96
1:A:525:GLN:HE22	1:A:528:HIS:HE1	1.15	0.93
1:B:525:GLN:HE22	1:B:528:HIS:HE1	1.18	0.91
1:A:529[B]:TYR:CZ	1:A:655[B]:GLU:OE1	2.31	0.84
1:A:456:HIS:HD2	1:A:458:PHE:H	1.36	0.73
1:A:529[B]:TYR:CZ	1:A:655[B]:GLU:CD	2.69	0.71
1:A:699:PRO:HG2	6:A:2540:HOH:O	1.93	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:525:GLN:NE2	1:B:528:HIS:HE1	1.90	0.69
1:A:525:GLN:HE22	1:A:528:HIS:CE1	2.06	0.68
1:A:697:TYR:O	6:A:2690:HOH:O	2.09	0.68
1:A:525:GLN:NE2	1:A:528:HIS:HE1	1.89	0.68
1:B:456:HIS:HD2	1:B:458:PHE:H	1.42	0.67
1:A:5:GLU:N	6:A:2001:HOH:O	2.28	0.66
1:B:153:GLN:HE22	1:B:438:HIS:HD2	1.43	0.64
1:B:696[B]:THR:O	1:B:697:TYR:C	2.40	0.64
1:B:525:GLN:HE22	1:B:528:HIS:CE1	2.10	0.63
1:A:529[B]:TYR:CZ	1:A:655[B]:GLU:OE2	2.51	0.63
1:B:196:ILE:HD11	4:B:1709:EDO:H22	1.84	0.60
1:A:698:VAL:HG12	1:A:700[B]:GLU:HG2	1.86	0.57
1:A:215[B]:ARG:NH1	1:B:696[B]:THR:HG22	2.19	0.57
1:B:196:ILE:HG13	4:B:1709:EDO:H11	1.87	0.56
1:A:529[B]:TYR:CE2	1:A:655[B]:GLU:OE2	2.59	0.56
1:A:196:ILE:HG13	4:A:1710:EDO:H11	1.87	0.55
1:A:220:GLN:NE2	6:A:2280:HOH:O	2.40	0.55
1:A:393:GLU:OE2	1:A:528:HIS:HD2	1.91	0.54
1:A:160:TRP:H	1:A:446:ASN:ND2	2.05	0.54
1:B:105:GLN:NE2	1:B:143:LYS:H	2.06	0.54
1:A:696:THR:HA	6:B:2265:HOH:O	2.08	0.54
1:B:557:GLY:O	1:B:595:HIS:HD2	1.91	0.54
1:A:105:GLN:NE2	1:A:143:LYS:H	2.05	0.54
1:B:700[B]:GLU:HG3	1:B:702:TRP:O	2.08	0.53
1:A:430:GLU:OE1	1:A:473:HIS:HE1	1.91	0.53
1:A:525:GLN:NE2	1:A:528:HIS:CE1	2.73	0.53
1:B:393:GLU:OE2	1:B:528:HIS:HD2	1.92	0.53
1:A:158:ASN:HD21	1:A:358:GLN:HE22	1.57	0.53
1:B:158:ASN:HD21	1:B:358:GLN:HE22	1.57	0.52
1:B:525:GLN:NE2	1:B:528:HIS:CE1	2.74	0.52
1:A:196:ILE:HD11	4:A:1710:EDO:H22	1.93	0.51
1:B:430:GLU:OE1	1:B:473:HIS:HE1	1.95	0.49
1:B:153:GLN:HE22	1:B:438:HIS:CD2	2.28	0.49
1:A:695:THR:HG21	6:B:2053:HOH:O	2.12	0.48
1:A:297:PRO:HG3	1:A:307:GLY:HA3	1.94	0.48
1:A:456:HIS:HE1	6:A:2447:HOH:O	1.97	0.48
1:A:160:TRP:H	1:A:446:ASN:HD21	1.60	0.47
1:B:456:HIS:HE1	6:B:2434:HOH:O	1.96	0.47
1:A:215[B]:ARG:NH1	1:B:696[B]:THR:CG2	2.77	0.47
1:B:397:PHE:CZ	1:B:529[B]:TYR:HB2	2.50	0.47
1:B:473:HIS:HD2	6:B:2487:HOH:O	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:196:ILE:CD1	4:B:1709:EDO:H22	2.45	0.46
1:B:96:LEU:HD21	1:B:147:SER:HB2	1.97	0.46
1:B:24:LYS:NZ	1:B:27:GLN:HE22	2.14	0.46
1:B:699:PRO:HG3	6:B:2535:HOH:O	2.17	0.45
1:B:702:TRP:CH2	1:B:704:PRO:HA	2.52	0.45
1:A:160:TRP:HA	1:A:209:ASN:HA	1.99	0.45
1:A:153[B]:GLN:OE1	1:A:438:HIS:HA	2.16	0.45
1:B:220:GLN:NE2	6:B:2268:HOH:O	2.45	0.44
1:A:24:LYS:NZ	1:A:27:GLN:HE22	2.14	0.44
1:B:507:ARG:HD3	1:B:507:ARG:C	2.42	0.44
1:B:59:LYS:HE2	6:B:2051:HOH:O	2.17	0.44
1:B:10[B]:MET:SD	1:B:460:GLN:HG2	2.57	0.44
1:A:129:PHE:CG	1:A:199:SER:HA	2.53	0.43
1:A:206:VAL:HG22	1:A:240:TYR:HB2	2.00	0.43
1:A:215[B]:ARG:HD3	1:A:221:PHE:CE2	2.53	0.43
1:B:699:PRO:CG	6:B:2535:HOH:O	2.65	0.43
1:B:102[B]:LEU:HD21	1:B:104:GLU:HB2	2.00	0.43
1:A:507:ARG:C	1:A:507:ARG:HD3	2.44	0.43
1:B:393:GLU:OE2	1:B:528:HIS:CD2	2.72	0.43
1:B:153:GLN:NE2	1:B:438:HIS:HA	2.35	0.42
1:A:473:HIS:HD2	6:A:2459:HOH:O	2.02	0.42
1:A:393:GLU:OE2	1:A:528:HIS:CD2	2.71	0.42
1:B:160:TRP:HA	1:B:209:ASN:HA	2.02	0.42
1:A:696:THR:O	1:A:697:TYR:C	2.62	0.42
1:B:130:HIS:CE1	4:B:1711:EDO:H12	2.55	0.42
1:B:297:PRO:HG3	1:B:307:GLY:HA3	2.03	0.41
1:B:454:THR:HB	1:B:459:VAL:HB	2.02	0.41
1:A:624:ARG:HA	1:A:627:GLN:HE21	1.86	0.41

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	716/708 (101%)	699 (98%)	16 (2%)	1 (0%)	48	31
1	B	718/708 (101%)	697 (97%)	17 (2%)	4 (1%)	21	7
All	All	1434/1416 (101%)	1396 (97%)	33 (2%)	5 (0%)	36	21

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	696[A]	THR
1	B	696[B]	THR
1	B	365	ASP
1	B	697	TYR
1	A	365	ASP

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	597/588 (102%)	589 (99%)	8 (1%)	61	39
1	B	600/588 (102%)	593 (99%)	7 (1%)	63	43
All	All	1197/1176 (102%)	1182 (99%)	15 (1%)	68	39

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	146	LEU
1	A	156[A]	VAL
1	A	156[B]	VAL
1	A	244	ASN
1	A	435	LYS
1	A	505[A]	VAL
1	A	505[B]	VAL
1	A	681	GLN
1	B	59	LYS
1	B	141	LEU
1	B	156[A]	VAL

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Mol	Chain	Res	Type
1	B	156[B]	VAL
1	B	244	ASN
1	B	553	LYS
1	B	683	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (34) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	27	GLN
1	A	32	HIS
1	A	105	GLN
1	A	136	GLN
1	A	158	ASN
1	A	244	ASN
1	A	446	ASN
1	A	456	HIS
1	A	473	HIS
1	A	512	ASN
1	A	525	GLN
1	A	528	HIS
1	A	600	HIS
1	A	627	GLN
1	B	27	GLN
1	B	105	GLN
1	B	109	ASN
1	B	119	ASN
1	B	136	GLN
1	B	153	GLN
1	B	154	HIS
1	B	158	ASN
1	B	244	ASN
1	B	438	HIS
1	B	456	HIS
1	B	473	HIS
1	B	512	ASN
1	B	525	GLN
1	B	528	HIS
1	B	595	HIS
1	B	618	GLN
1	B	627	GLN
1	B	633	GLN
1	B	681	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 ⓘ

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	XYP	C	1	2	1,1,10	0.10	0	-		
2	XYP	C	2	2	9,9,10	1.48	1 (11%)	10,12,14	1.35	1 (10%)
2	XYP	D	1	2	1,1,10	0.20	0	-		
2	XYP	D	2	2	9,9,10	1.62	1 (11%)	10,12,14	1.20	1 (10%)

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	XYP	C	2	2	-	-	0/1/1/1
2	XYP	D	2	2	-	-	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	2	XYP	O5-C1	-4.54	1.34	1.43
2	C	2	XYP	O5-C1	-3.95	1.35	1.43

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	2	XYP	C4-C3-C2	-2.85	107.54	110.92
2	D	2	XYP	C5-O5-C1	2.72	115.81	111.42

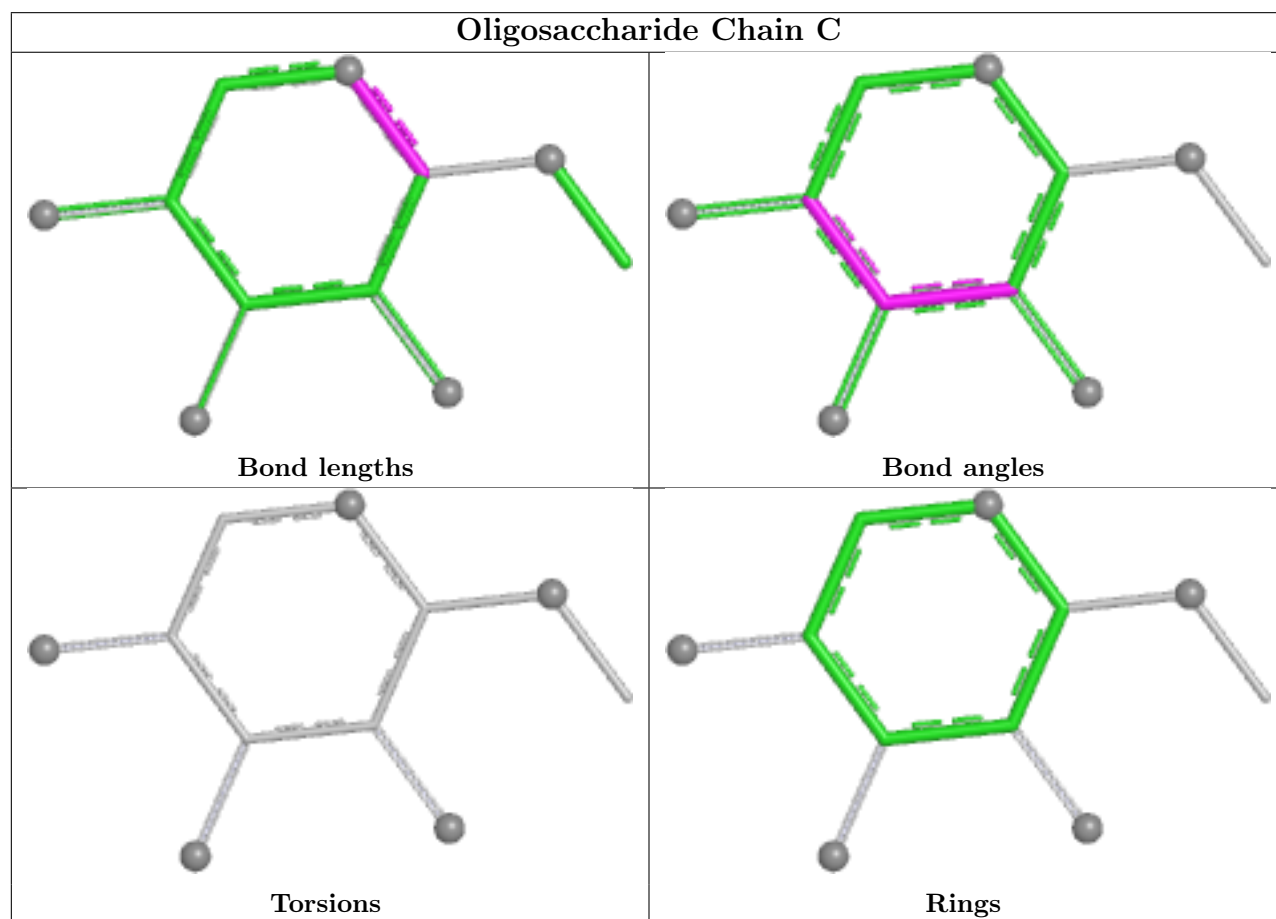
There are no chirality outliers.

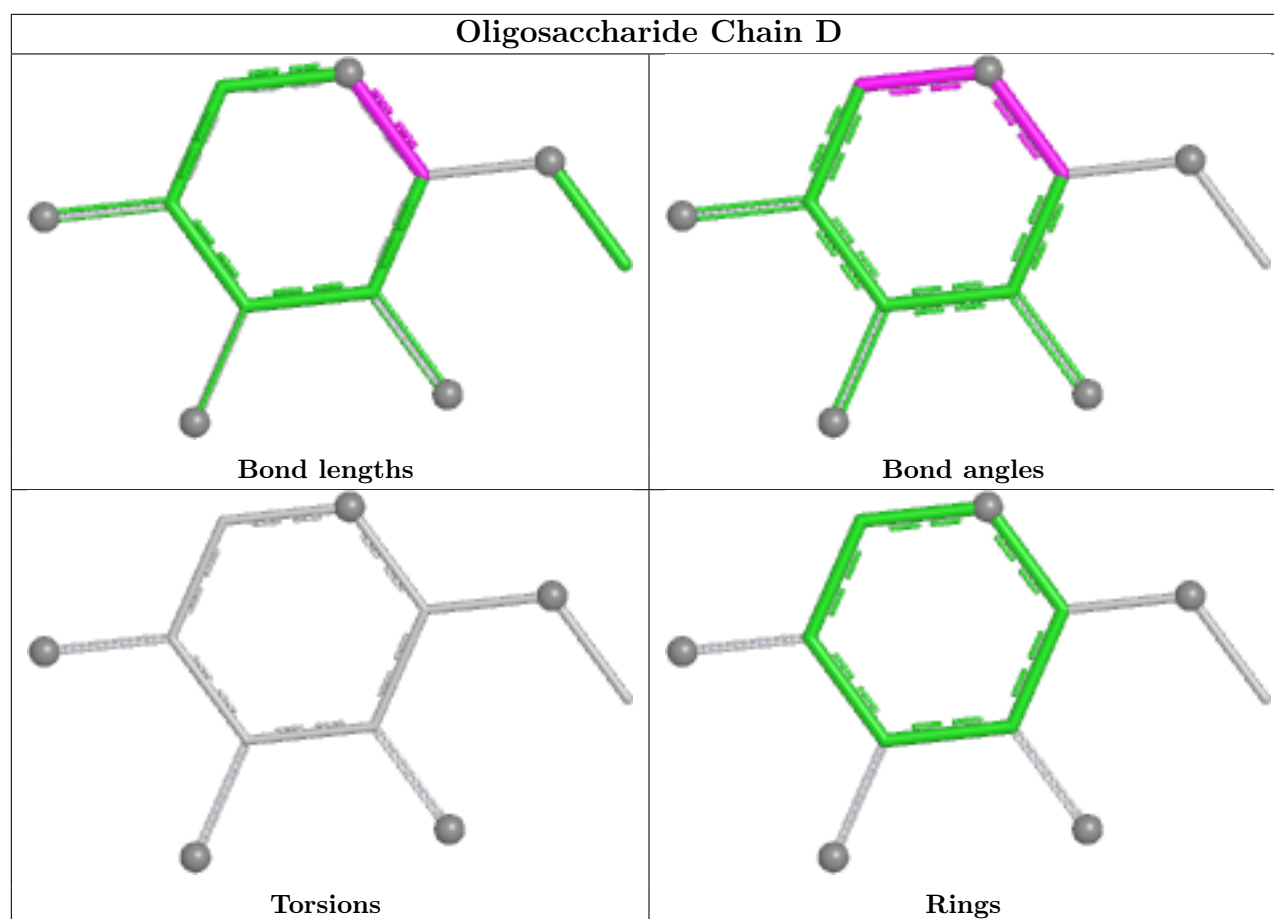
There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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 21 ligands modelled in this entry, 8 are monoatomic - leaving 13 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	$\# Z > 2$
4	EDO	B	1707	-	3,3,3	0.39	0	2,2,2	1.08	0
4	EDO	A	1708	-	3,3,3	0.34	0	2,2,2	0.67	0
4	EDO	A	1709	-	3,3,3	0.23	0	2,2,2	0.55	0
4	EDO	B	1708	-	3,3,3	0.16	0	2,2,2	0.57	0
4	EDO	B	1711	-	3,3,3	0.41	0	2,2,2	0.36	0
4	EDO	A	1707	-	3,3,3	0.45	0	2,2,2	0.74	0
3	BDP	B	1705	-	13,13,13	0.71	0	18,19,19	1.28	2 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	EDO	A	1711	-	3,3,3	0.32	0	2,2,2	0.45	0
4	EDO	A	1710	-	3,3,3	0.42	0	2,2,2	0.48	0
3	BDP	A	1706	-	13,13,13	0.70	0	18,19,19	1.47	4 (22%)
4	EDO	B	1710	-	3,3,3	0.36	0	2,2,2	0.55	0
4	EDO	B	1706	-	3,3,3	0.35	0	2,2,2	0.52	0
4	EDO	B	1709	-	3,3,3	0.37	0	2,2,2	0.65	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	EDO	B	1707	-	-	1/1/1/1	-
4	EDO	A	1708	-	-	0/1/1/1	-
4	EDO	A	1709	-	-	0/1/1/1	-
4	EDO	B	1708	-	-	1/1/1/1	-
4	EDO	B	1711	-	-	0/1/1/1	-
4	EDO	A	1707	-	-	0/1/1/1	-
3	BDP	B	1705	-	-	0/4/24/24	0/1/1/1
4	EDO	A	1711	-	-	0/1/1/1	-
4	EDO	A	1710	-	-	0/1/1/1	-
3	BDP	A	1706	-	-	0/4/24/24	0/1/1/1
4	EDO	B	1710	-	-	1/1/1/1	-
4	EDO	B	1706	-	-	0/1/1/1	-
4	EDO	B	1709	-	-	0/1/1/1	-

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1706	BDP	C1-C2-C3	3.02	116.51	110.36
3	B	1705	BDP	O1-C1-O5	-2.69	102.43	110.41
3	A	1706	BDP	C1-O5-C5	2.46	115.84	112.22
3	B	1705	BDP	C1-C2-C3	2.42	115.29	110.36
3	A	1706	BDP	O1-C1-O5	-2.30	103.57	110.41
3	A	1706	BDP	O6B-C6-C5	2.04	121.02	113.64

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	1710	EDO	O1-C1-C2-O2
4	B	1708	EDO	O1-C1-C2-O2
4	B	1707	EDO	O1-C1-C2-O2

There are no ring outliers.

3 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	1711	EDO	1	0
4	A	1710	EDO	2	0
4	B	1709	EDO	3	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

6.1 Protein, DNA and RNA chains

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	701/708 (99%)	-0.33	17 (2%) 59 67	7, 14, 28, 45	18 (2%)
1	B	700/708 (98%)	-0.37	14 (2%) 65 73	7, 14, 29, 45	20 (2%)
All	All	1401/1416 (98%)	-0.35	31 (2%) 62 68	7, 14, 29, 45	38 (2%)

All (31) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	695	THR	8.3
1	A	696	THR	7.9
1	B	695	THR	5.0
1	A	693[A]	ALA	4.8
1	A	692	LEU	4.3
1	B	693[A]	ALA	3.9
1	B	696[A]	THR	3.9
1	B	683	GLU	3.8
1	A	697	TYR	3.7
1	B	437	ARG	3.6
1	A	94	GLN	3.3
1	A	437	ARG	3.3
1	A	537	ASP	3.3
1	A	705	ALA	3.1
1	B	537	ASP	2.9
1	A	694	ARG	2.7
1	B	95	ALA	2.6
1	B	704	PRO	2.5
1	A	683	GLU	2.5
1	B	703	HIS	2.4
1	B	692	LEU	2.3
1	B	697	TYR	2.3
1	B	90	GLY	2.3
1	B	110	LYS	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	703	HIS	2.2
1	A	677	ALA	2.2
1	A	688	TYR	2.2
1	A	436	THR	2.2
1	B	85	ALA	2.1
1	A	678	ASN	2.0
1	A	691	MET	2.0

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](#)

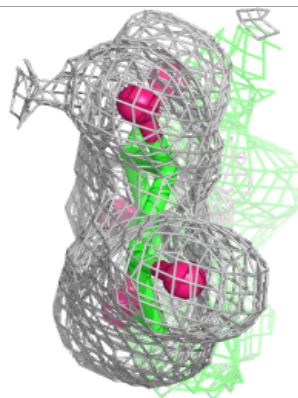
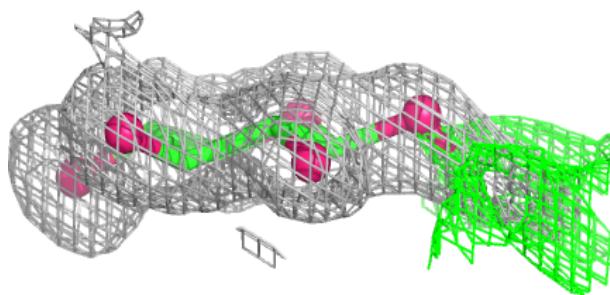
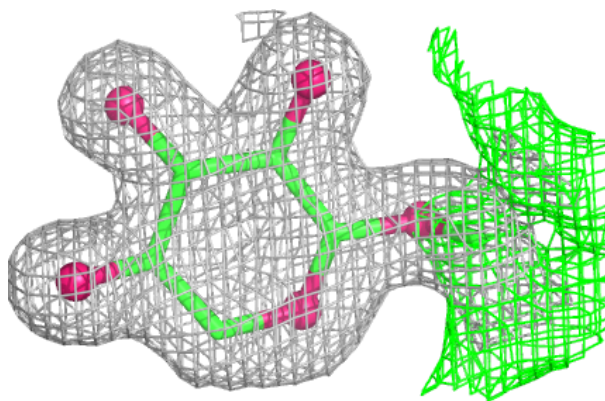
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	XYP	D	1	2/10	0.73	0.37	17,17,17,23	2
2	XYP	C	1	2/10	0.76	0.35	18,18,18,25	2
2	XYP	C	2	9/10	0.97	0.05	17,18,20,21	0
2	XYP	D	2	9/10	0.97	0.06	15,17,19,22	0

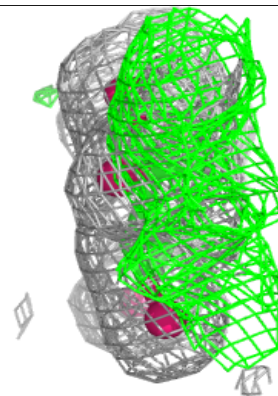
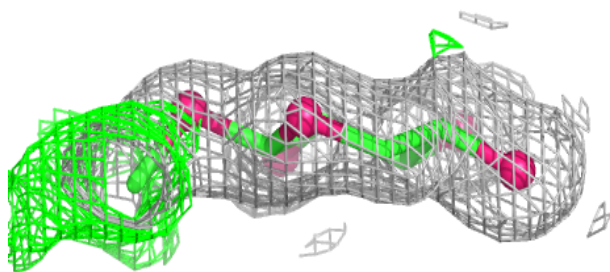
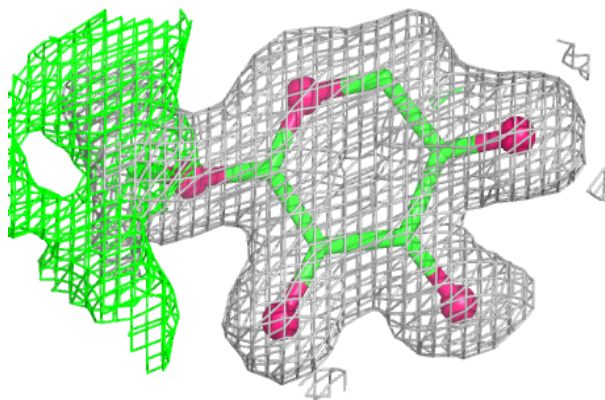
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around Chain C:

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

**Electron density around Chain D:**

$2mF_o-DF_c$ (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, 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
4	EDO	B	1710	4/4	0.86	0.14	36,42,42,45	0
4	EDO	B	1707	4/4	0.89	0.12	16,21,26,38	0
3	BDP	A	1706	13/13	0.96	0.05	8,12,14,16	0
4	EDO	B	1708	4/4	0.96	0.06	19,26,26,26	0
4	EDO	A	1711	4/4	0.96	0.09	16,24,27,30	0
4	EDO	B	1711	4/4	0.96	0.07	16,18,19,20	0
4	EDO	A	1710	4/4	0.97	0.06	13,14,17,17	0
3	BDP	B	1705	13/13	0.97	0.04	7,11,12,13	0
4	EDO	A	1709	4/4	0.98	0.04	17,17,18,19	0
4	EDO	A	1707	4/4	0.98	0.04	11,12,14,14	0
4	EDO	A	1708	4/4	0.98	0.04	17,17,21,25	0
4	EDO	B	1706	4/4	0.98	0.04	12,12,13,13	0
4	EDO	B	1709	4/4	0.99	0.07	12,13,18,18	0
5	CO	A	1715[A]	1/1	0.99	0.04	13,13,13,13	1
5	CO	A	1716[A]	1/1	0.99	0.11	20,20,20,20	1
5	CO	B	1717	1/1	0.99	0.11	21,21,21,21	1
5	CO	A	1717[A]	1/1	1.00	0.11	16,16,16,16	1
5	CO	B	1714	1/1	1.00	0.04	16,16,16,16	1
5	CO	B	1715	1/1	1.00	0.05	14,14,14,14	1
5	CO	B	1716	1/1	1.00	0.09	17,17,17,17	1
5	CO	A	1714[A]	1/1	1.00	0.04	17,17,17,17	1

6.5 Other polymers ⓘ

There are no such residues in this entry.