



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 08:41 AM UTC

PDB ID : 2D22 / pdb_00002d22
Title : Crystal structure of covalent glycosyl-enzyme intermediate of catalytic-site mutant xylanase from *Streptomyces olivaceoviridis* E-86
Authors : Suzuki, R.; Kuno, A.; Fujimoto, Z.; Ito, S.; Kawahara, S.I.; Kaneko, S.; Hasegawa, T.; Taira, K.
Deposited on : 2005-09-02
Resolution : 1.70 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)
Xtrriage (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

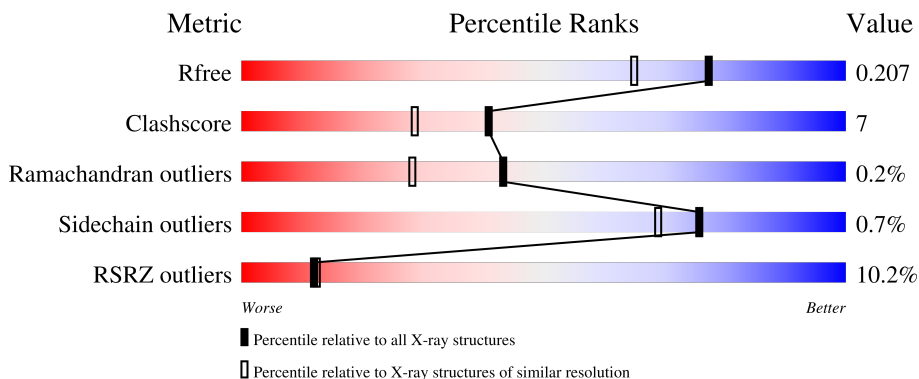
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION




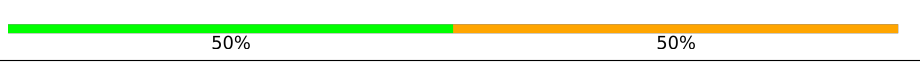
The reported resolution of this entry is 1.70 Å.

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	5551 (1.70-1.70)
Clashscore	190562	5924 (1.70-1.70)
Ramachandran outliers	187476	5846 (1.70-1.70)
Sidechain outliers	187428	5846 (1.70-1.70)
RSRZ outliers	180081	5554 (1.70-1.70)

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	436	
1	B	436	
2	C	2	
2	D	2	

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	XYS	C	2	X	-	-	-
2	XYS	D	2	X	-	-	-
4	GOL	B	966	-	-	X	-

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 7438 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-1,4-BETA-D-XYLANASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	427	3233	1988	588	641	16	0	0	0
1	B	427	3233	1988	588	641	16	0	0	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	127	SER	ASN	engineered mutation	UNP Q7SI98
A	128	HIS	GLU	engineered mutation	UNP Q7SI98
B	627	SER	ASN	engineered mutation	UNP Q7SI98
B	628	HIS	GLU	engineered mutation	UNP Q7SI98

- Molecule 2 is an oligosaccharide called alpha-D-xylopyranose-(1-4)-alpha-D-xylopyranose.



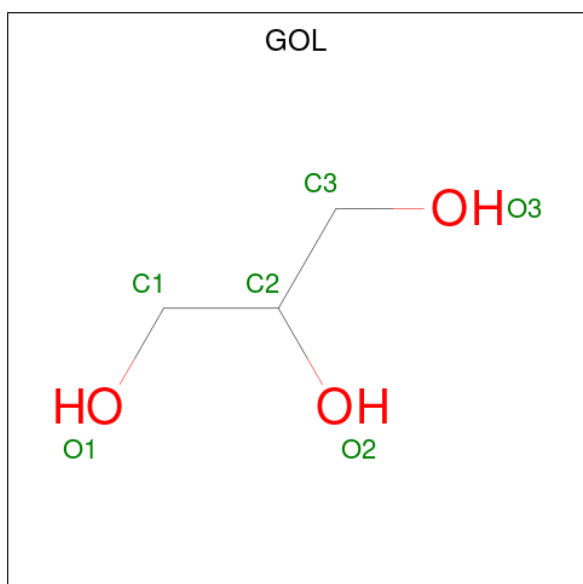
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
			Total	C	O			
2	C	2	18	10	8	0	0	0
2	D	2	18	10	8	0	0	0

- Molecule 3 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total O S 5 4 1	0	0
3	A	1	Total O S 5 4 1	0	0
3	A	1	Total O S 5 4 1	0	0
3	A	1	Total O S 5 4 1	0	0
3	B	1	Total O S 5 4 1	0	0

- Molecule 4 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



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

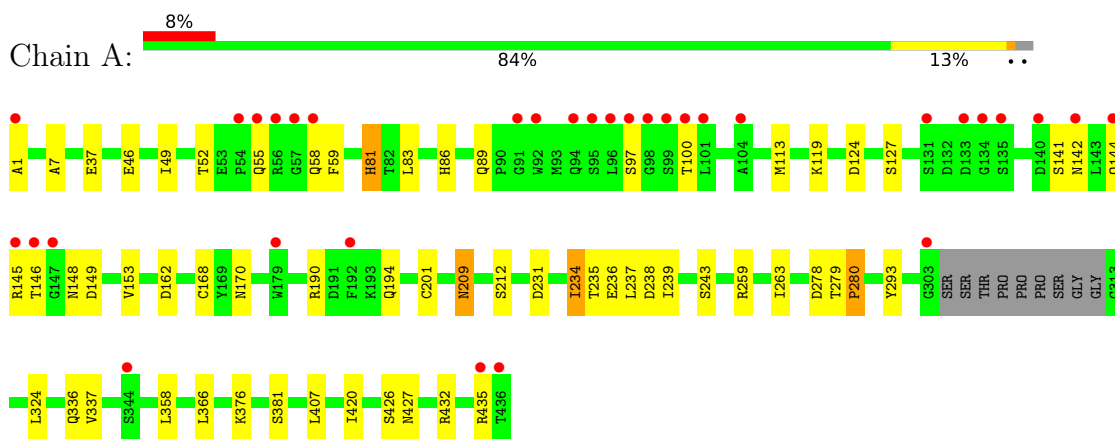
- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	389	Total O 389 389	0	0
5	B	474	Total O 474 474	0	0

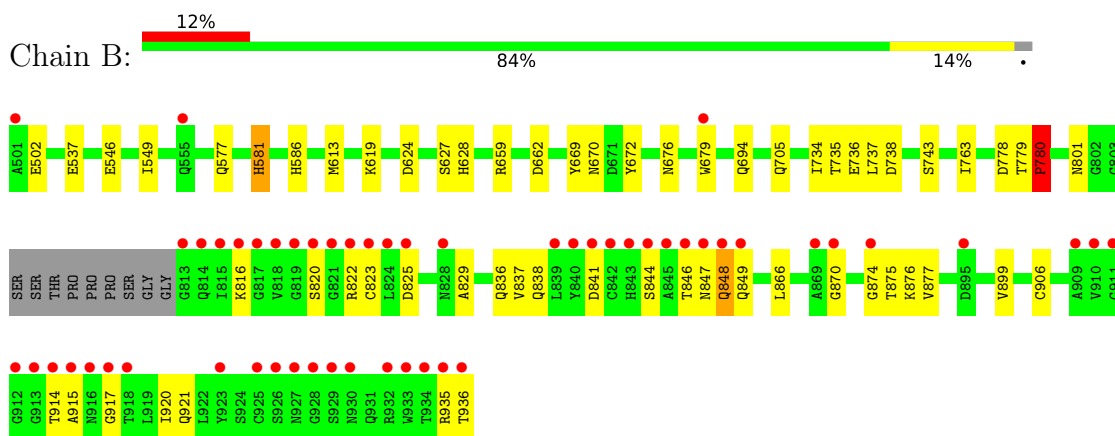
3 Residue-property plots [i](#)

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: ENDO-1,4-BETA-D-XYLANASE



- Molecule 1: ENDO-1,4-BETA-D-XYLANASE



- Molecule 2: alpha-D-xylopyranose-(1-4)-alpha-D-xylopyranose



- Molecule 2: alpha-D-xylopyranose-(1-4)-alpha-D-xylopyranose





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	78.69Å 93.96Å 139.72Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	32.21 – 1.70 32.21 – 1.70	Depositor EDS
% Data completeness (in resolution range)	(Not available) (32.21-1.70) 99.6 (32.21-1.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	8.44 (at 1.70Å)	Xtrriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.186 , 0.207 0.186 , 0.207	Depositor DCC
R_{free} test set	5727 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	14.5	Xtrriage
Anisotropy	0.011	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.40 , 44.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	7438	wwPDB-VP
Average B, all atoms (Å ²)	18.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.93% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, XYS, SO4

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	0.34	1/3298 (0.0%)	0.90	12/4473 (0.3%)
1	B	0.35	1/3298 (0.0%)	0.89	11/4473 (0.2%)
All	All	0.35	2/6596 (0.0%)	0.89	23/8946 (0.3%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	736	GLU	CD-OE2	6.91	1.38	1.25
1	A	236	GLU	CD-OE2	6.74	1.38	1.25

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	735	THR	N-CA-C	8.04	123.21	113.41
1	A	235	THR	N-CA-C	7.96	123.33	112.90
1	A	366	LEU	N-CA-C	-7.25	99.29	110.10
1	B	537	GLU	N-CA-C	7.17	122.12	113.23
1	B	546	GLU	N-CA-C	6.97	120.88	112.38
1	A	46	GLU	N-CA-C	6.58	120.77	112.87
1	B	866	LEU	N-CA-C	-6.51	100.26	109.96
1	A	37	GLU	N-CA-C	6.40	121.16	113.23
1	B	549	ILE	N-CA-C	6.38	116.55	110.42
1	A	407	LEU	N-CA-C	-5.70	101.61	110.10
1	A	49	ILE	N-CA-C	5.58	115.78	110.42
1	B	780	PRO	N-CA-C	5.57	121.55	114.92
1	A	237	LEU	N-CA-C	5.44	118.20	110.10
1	A	324	LEU	N-CA-C	-5.34	102.01	109.96
1	B	577	GLN	N-CA-C	-5.29	102.92	110.59
1	B	848	GLN	N-CA-C	-5.25	99.62	110.80
1	B	669	TYR	N-CA-C	-5.14	100.80	109.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	212	SER	CA-C-N	5.12	125.03	119.85
1	A	212	SER	C-N-CA	5.12	125.03	119.85
1	A	234	ILE	N-CA-C	-5.09	99.78	107.73
1	A	83	LEU	N-CA-C	5.08	117.93	111.69
1	B	624	ASP	N-CA-C	-5.03	99.57	108.23
1	B	737	LEU	N-CA-C	5.00	117.56	110.10

There are no chirality outliers.

There are no planarity outliers.

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	3233	0	3043	38	0
1	B	3233	0	3040	44	0
2	C	18	0	15	0	0
2	D	18	0	15	1	0
3	A	20	0	0	0	0
3	B	5	0	0	0	0
4	A	18	0	24	2	0
4	B	30	0	40	6	0
5	A	389	0	0	4	0
5	B	474	0	0	6	0
All	All	7438	0	6177	83	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 7.

All (83) 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:B:659:ARG:HH21	4:B:966:GOL:H11	1.14	1.06
1:B:935:ARG:HA	1:B:936:THR:C	2.10	0.76
1:A:336:GLN:HB2	1:A:376:LYS:HE3	1.71	0.72
1:B:836:GLN:HB2	1:B:876:LYS:HE3	1.70	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:659:ARG:HE	4:B:966:GOL:H32	1.58	0.68
1:B:816:LYS:HG2	1:B:823:CYS:SG	2.35	0.67
1:B:659:ARG:NH2	4:B:966:GOL:H11	1.99	0.66
1:A:144:GLN:HE22	1:A:148:ASN:HA	1.61	0.65
1:A:435:ARG:HB2	1:A:435:ARG:NH1	2.12	0.64
1:A:119:LYS:NZ	4:A:963:GOL:H31	2.12	0.64
1:A:234:ILE:HD12	1:A:263:ILE:HG12	1.80	0.64
1:B:822:ARG:HE	1:B:915:ALA:HA	1.63	0.63
1:A:119:LYS:HZ2	4:A:963:GOL:H31	1.64	0.63
1:A:381:SER:HB2	5:A:1164:HOH:O	2.01	0.60
1:B:837:VAL:HG23	1:B:920:ILE:HB	1.84	0.59
1:B:778:ASP:O	1:B:779:THR:C	2.47	0.58
1:B:829:ALA:HA	1:B:847:ASN:HB3	1.86	0.58
1:A:238:ASP:HB2	1:A:280:PRO:HB2	1.86	0.58
1:B:676:ASN:HB3	1:B:679:TRP:CD2	2.39	0.57
1:A:209:ASN:C	1:A:209:ASN:HD22	2.13	0.57
4:B:967:GOL:H2	5:B:1296:HOH:O	2.05	0.56
1:A:97:SER:O	1:A:100:THR:HG22	2.06	0.56
1:A:141:SER:O	1:A:145:ARG:HG3	2.05	0.56
1:A:190:ARG:O	1:A:194:GLN:HG3	2.07	0.55
1:A:86:HIS:HA	1:A:89:GLN:HE21	1.72	0.54
1:B:874:GLY:HA2	1:B:921:GLN:OE1	2.08	0.54
1:B:738:ASP:HB2	1:B:780:PRO:HB2	1.89	0.54
1:A:243:SER:HB2	5:A:1107:HOH:O	2.08	0.53
1:A:278:ASP:O	1:A:279:THR:C	2.50	0.53
1:A:231:ASP:OD1	1:A:259:ARG:HD3	2.08	0.53
1:B:846:THR:C	1:B:848:GLN:H	2.16	0.53
1:A:435:ARG:HB2	1:A:435:ARG:HH11	1.75	0.52
1:B:581:HIS:HE1	2:D:1:XYS:O3	1.92	0.52
1:A:55:GLN:HB2	1:A:58:GLN:HB2	1.91	0.52
1:A:142:ASN:HA	1:A:145:ARG:HH11	1.74	0.51
1:B:734:ILE:HD12	1:B:763:ILE:HG12	1.92	0.51
1:A:337:VAL:HG23	1:A:420:ILE:HB	1.93	0.51
1:B:659:ARG:NE	4:B:966:GOL:H32	2.26	0.50
1:A:113:MET:HE2	1:A:162:ASP:HB3	1.93	0.50
1:B:586:HIS:HD2	5:B:1003:HOH:O	1.94	0.49
1:B:694:GLN:HG3	5:B:1279:HOH:O	2.14	0.48
1:B:822:ARG:HE	1:B:915:ALA:CA	2.26	0.48
1:B:899:VAL:HG22	1:B:906:CYS:SG	2.53	0.48
1:A:149:ASP:O	1:A:153:VAL:HG23	2.13	0.48
1:B:822:ARG:NH1	1:B:841:ASP:OD1	2.47	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:81:HIS:HB2	1:A:124:ASP:HB2	1.96	0.47
1:A:1:ALA:HB3	1:A:7:ALA:HB1	1.96	0.47
1:A:432:ARG:HG3	5:A:1081:HOH:O	2.14	0.47
1:A:435:ARG:HH11	1:A:435:ARG:CB	2.28	0.47
1:B:838:GLN:OE1	1:B:917:GLY:HA2	2.14	0.47
1:B:672:TYR:HB3	1:B:705:GLN:OE1	2.15	0.47
1:B:627:SER:OG	1:B:628:HIS:ND1	2.42	0.47
1:A:426:SER:O	1:A:427:ASN:HB2	2.14	0.46
1:A:279:THR:N	1:A:280:PRO:HD3	2.30	0.46
1:B:694:GLN:HG2	5:B:1262:HOH:O	2.15	0.45
1:B:613:MET:HE2	1:B:662:ASP:HB3	1.99	0.45
1:B:825:ASP:OD2	4:B:965:GOL:H12	2.16	0.45
1:B:743:SER:HB2	5:B:1206:HOH:O	2.17	0.44
1:B:935:ARG:HA	1:B:936:THR:O	2.16	0.44
1:A:127:SER:HA	1:A:170:ASN:O	2.18	0.44
1:B:870:GLY:H	1:B:875:THR:HG21	1.82	0.44
1:A:142:ASN:O	1:A:146:THR:HG23	2.18	0.44
1:B:502:GLU:HB2	1:B:801:ASN:OD1	2.17	0.44
1:B:846:THR:C	1:B:848:GLN:N	2.75	0.44
1:B:935:ARG:CA	1:B:936:THR:C	2.87	0.43
1:B:779:THR:N	1:B:780:PRO:HD3	2.33	0.43
1:B:829:ALA:HA	1:B:847:ASN:CB	2.49	0.43
1:A:1:ALA:HB1	5:A:1032:HOH:O	2.18	0.43
1:A:144:GLN:NE2	1:A:148:ASN:HA	2.29	0.43
1:A:293:TYR:C	1:A:293:TYR:CD1	2.97	0.43
1:B:619:LYS:HE3	5:B:1349:HOH:O	2.19	0.43
1:B:822:ARG:HG2	1:B:822:ARG:HH11	1.83	0.43
1:B:820:SER:HA	1:B:914:THR:HB	2.01	0.42
1:A:86:HIS:HA	1:A:89:GLN:NE2	2.35	0.41
1:A:358:LEU:HD23	1:A:358:LEU:HA	1.96	0.41
1:A:168:CYS:HA	1:A:201:CYS:O	2.20	0.41
1:B:837:VAL:HG22	1:B:877:VAL:O	2.21	0.41
1:B:870:GLY:H	1:B:875:THR:CG2	2.33	0.41
1:B:825:ASP:OD2	1:B:847:ASN:ND2	2.55	0.40
1:B:935:ARG:HA	1:B:936:THR:OG1	2.20	0.40
1:A:52:THR:O	1:A:59:PHE:HA	2.20	0.40
1:A:239:ILE:O	1:A:280:PRO:HA	2.21	0.40
1:B:627:SER:HA	1:B:670:ASN:O	2.21	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	423/436 (97%)	411 (97%)	12 (3%)	0	100	100
1	B	423/436 (97%)	406 (96%)	15 (4%)	2 (0%)	24	12
All	All	846/872 (97%)	817 (97%)	27 (3%)	2 (0%)	43	28

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	849	GLN
1	B	844	SER

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	334/341 (98%)	331 (99%)	3 (1%)	70	62
1	B	334/341 (98%)	332 (99%)	2 (1%)	78	72
All	All	668/682 (98%)	663 (99%)	5 (1%)	76	69

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	81	HIS
1	A	209	ASN
1	A	280	PRO
1	B	581	HIS

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Mol	Chain	Res	Type
1	B	780	PRO

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	55	GLN
1	A	194	GLN
1	A	209	ASN
1	A	298	ASN
1	A	343	HIS
1	A	393	ASN
1	B	511	GLN
1	B	581	HIS
1	B	586	HIS
1	B	673	ASN
1	B	723	GLN
1	B	784	ASN
1	B	814	GLN
1	B	828	ASN
1	B	893	ASN

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	XYS	C	1	1,2	9,9,10	0.61	0	10,12,14	0.87	1 (10%)
2	XYS	C	2	2	9,9,10	0.54	0	10,12,14	0.70	0
2	XYS	D	1	1,2	9,9,10	0.61	0	10,12,14	0.91	1 (10%)
2	XYS	D	2	2	9,9,10	0.51	0	10,12,14	0.76	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
2	XYS	C	1	1,2	-	-	0/1/1/1
2	XYS	C	2	2	1/1/3/4	-	0/1/1/1
2	XYS	D	1	1,2	-	-	0/1/1/1
2	XYS	D	2	2	1/1/3/4	-	0/1/1/1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	1	XYS	C4-C3-C2	-2.20	108.31	110.92
2	C	1	XYS	C4-C3-C2	-2.03	108.51	110.92

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	C	2	XYS	C1
2	D	2	XYS	C1

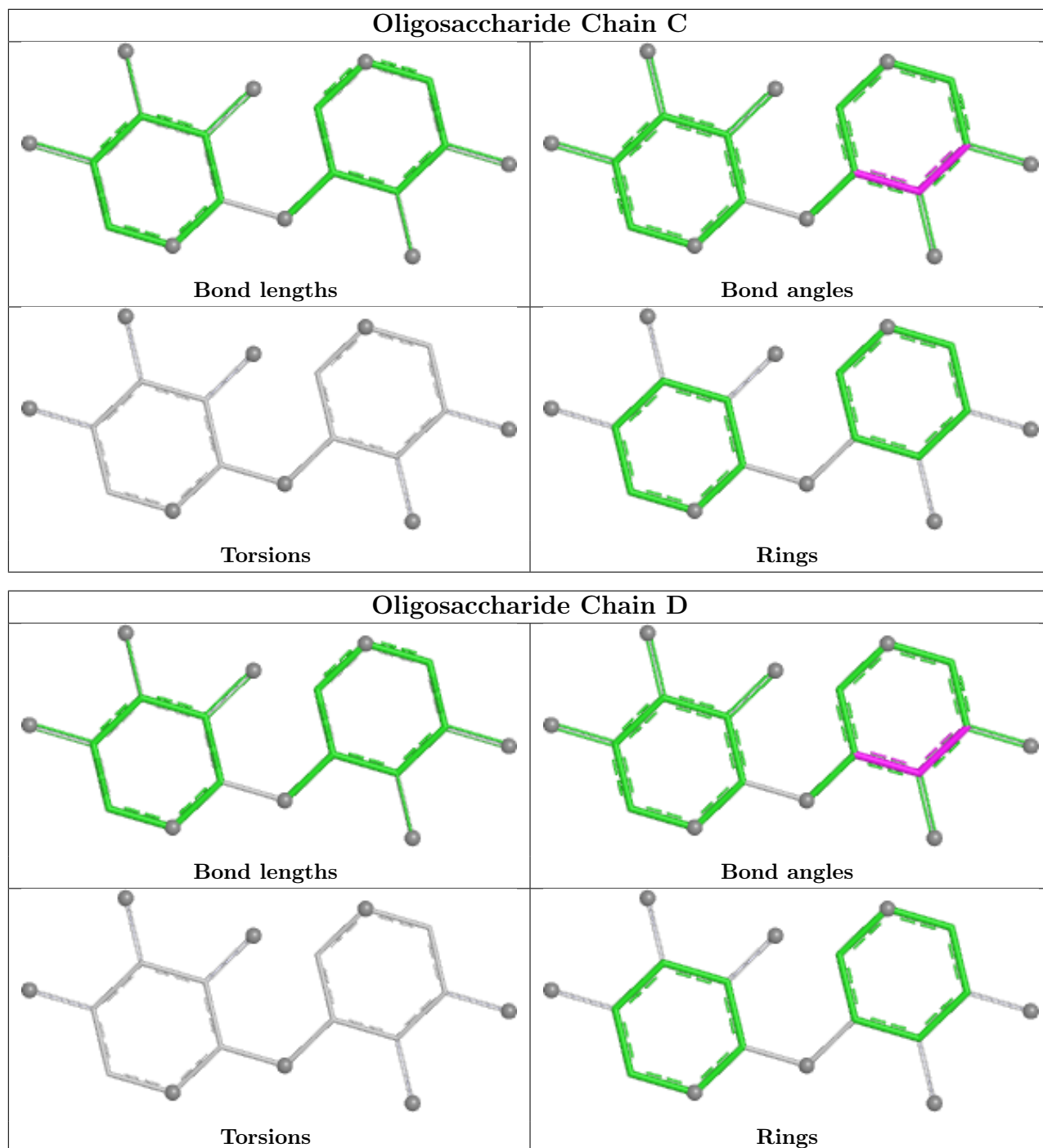
There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	1	XYS	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](#)

13 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
3	SO4	A	972	-	4,4,4	0.38	0	6,6,6	0.08	0
3	SO4	A	968	-	4,4,4	0.35	0	6,6,6	0.09	0
4	GOL	A	962	-	5,5,5	0.18	0	5,5,5	0.32	0
4	GOL	B	966	-	5,5,5	0.15	0	5,5,5	0.34	0
4	GOL	A	963	-	5,5,5	0.15	0	5,5,5	0.34	0
4	GOL	B	961	-	5,5,5	0.14	0	5,5,5	0.35	0
4	GOL	B	967	-	5,5,5	0.17	0	5,5,5	0.34	0
3	SO4	A	969	-	4,4,4	0.39	0	6,6,6	0.11	0
4	GOL	A	960	-	5,5,5	0.14	0	5,5,5	0.34	0
4	GOL	B	964	-	5,5,5	0.15	0	5,5,5	0.33	0
4	GOL	B	965	-	5,5,5	0.14	0	5,5,5	0.33	0
3	SO4	B	970	-	4,4,4	0.37	0	6,6,6	0.08	0
3	SO4	A	971	-	4,4,4	0.38	0	6,6,6	0.06	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	GOL	A	962	-	-	0/4/4/4	-
4	GOL	B	966	-	-	0/4/4/4	-
4	GOL	A	963	-	-	0/4/4/4	-
4	GOL	B	961	-	-	0/4/4/4	-
4	GOL	B	967	-	-	0/4/4/4	-
4	GOL	A	960	-	-	0/4/4/4	-
4	GOL	B	965	-	-	0/4/4/4	-
4	GOL	B	964	-	-	0/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	966	GOL	4	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	963	GOL	2	0
4	B	967	GOL	1	0
4	B	965	GOL	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

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	427/436 (97%)	0.30	33 (7%) 19 21	8, 15, 33, 47	0
1	B	427/436 (97%)	0.27	54 (12%) 8 7	7, 13, 40, 56	0
All	All	854/872 (97%)	0.29	87 (10%) 12 12	7, 14, 36, 56	0

All (87) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	819	GLY	9.1
1	B	501	ALA	8.6
1	B	936	THR	7.6
1	A	1	ALA	6.3
1	A	436	THR	5.9
1	B	818	VAL	5.4
1	B	848	GLN	4.6
1	B	849	GLN	4.3
1	B	822	ARG	4.1
1	B	911	GLY	4.1
1	B	910	VAL	4.1
1	B	846	THR	4.1
1	A	92	TRP	4.0
1	B	816	LYS	4.0
1	A	100	THR	4.0
1	A	179	TRP	4.0
1	B	813	GLY	4.0
1	B	845	ALA	3.9
1	B	843	HIS	3.8
1	B	934	THR	3.8
1	A	145	ARG	3.7
1	A	95	SER	3.7
1	B	840	TYR	3.7
1	B	869	ALA	3.7

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Mol	Chain	Res	Type	RSRZ
1	B	842	CYS	3.7
1	B	914	THR	3.6
1	A	96	LEU	3.6
1	B	915	ALA	3.5
1	B	935	ARG	3.5
1	A	344	SER	3.5
1	B	928	GLY	3.4
1	B	839	LEU	3.3
1	B	918	THR	3.3
1	B	820	SER	3.3
1	B	824	LEU	3.3
1	B	844	SER	3.2
1	A	56	ARG	3.1
1	B	817	GLY	3.1
1	B	823	CYS	3.1
1	B	925	CYS	3.0
1	B	821	GLY	3.0
1	B	923	TYR	3.0
1	A	98	GLY	3.0
1	B	916	ASN	3.0
1	A	134	GLY	3.0
1	B	909	ALA	2.9
1	B	679	TRP	2.9
1	A	147	GLY	2.9
1	B	917	GLY	2.9
1	B	927	ASN	2.9
1	A	91	GLY	2.8
1	A	435	ARG	2.8
1	A	55	GLN	2.8
1	A	97	SER	2.7
1	B	841	ASP	2.7
1	A	99	SER	2.7
1	B	929	SER	2.7
1	A	101	LEU	2.6
1	B	912	GLY	2.6
1	B	932	ARG	2.6
1	B	913	GLY	2.5
1	B	828	ASN	2.5
1	A	94	GLN	2.5
1	A	146	THR	2.5
1	B	847	ASN	2.4
1	B	874	GLY	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	815	ILE	2.4
1	B	926	SER	2.3
1	B	930	ASN	2.3
1	A	57	GLY	2.3
1	B	825	ASP	2.3
1	B	933	TRP	2.2
1	A	58	GLN	2.2
1	A	192	PHE	2.2
1	A	54	PRO	2.2
1	A	135	SER	2.2
1	A	104	ALA	2.2
1	A	133	ASP	2.1
1	A	303	GLY	2.1
1	B	870	GLY	2.1
1	B	555	GLN	2.1
1	A	142	ASN	2.1
1	B	814	GLN	2.0
1	A	140	ASP	2.0
1	B	895	ASP	2.0
1	A	131	SER	2.0
1	A	144	GLN	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](#)

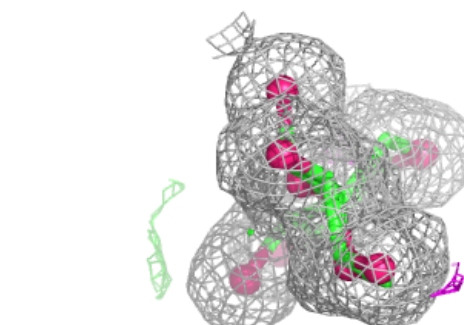
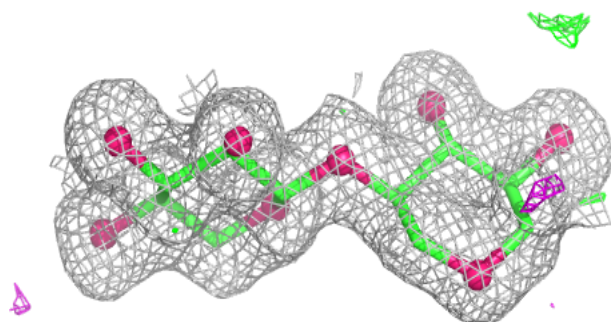
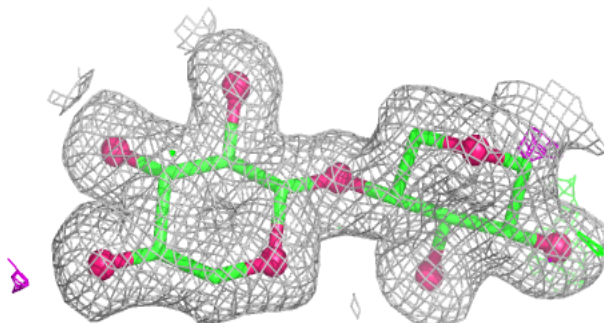
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	XYS	C	2	9/10	0.95	0.07	12,13,14,15	0
2	XYS	D	2	9/10	0.96	0.05	8,9,11,12	0
2	XYS	C	1	9/10	0.97	0.06	12,14,14,15	0
2	XYS	D	1	9/10	0.98	0.04	7,8,9,10	0

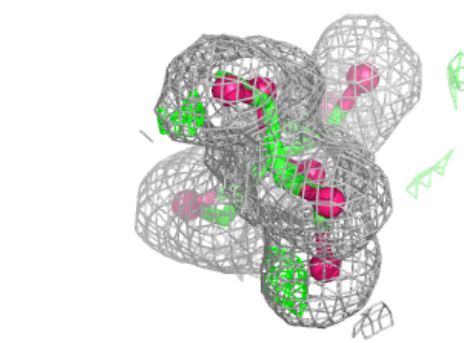
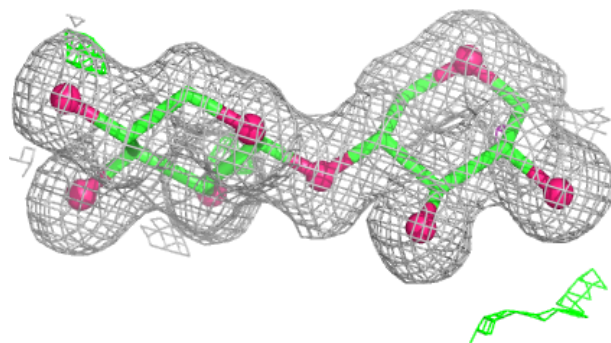
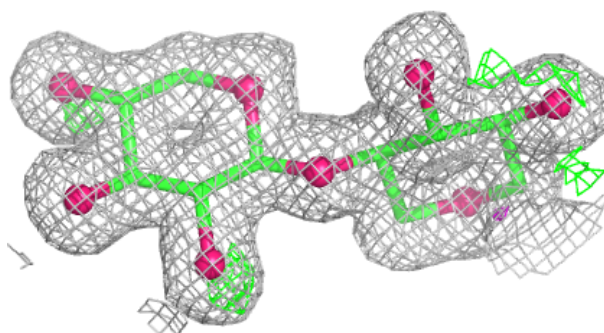
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

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 [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
4	GOL	B	965	6/6	0.55	0.34	62,63,63,63	0
4	GOL	B	967	6/6	0.63	0.24	35,40,40,41	0
3	SO4	A	972	5/5	0.74	0.13	61,61,61,62	0
4	GOL	B	966	6/6	0.75	0.20	45,45,45,46	0
4	GOL	A	963	6/6	0.75	0.26	49,50,50,51	0
3	SO4	A	969	5/5	0.77	0.17	47,49,50,50	0
3	SO4	B	970	5/5	0.83	0.15	42,42,45,45	0
4	GOL	A	962	6/6	0.84	0.17	24,28,30,34	0
4	GOL	B	964	6/6	0.86	0.15	39,40,41,42	0
3	SO4	A	971	5/5	0.86	0.14	43,44,44,44	0
4	GOL	B	961	6/6	0.89	0.12	22,23,24,26	0
3	SO4	A	968	5/5	0.90	0.15	35,35,38,39	0
4	GOL	A	960	6/6	0.95	0.07	20,20,21,24	0

6.5 Other polymers [i](#)

There are no such residues in this entry.