



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 20, 2026 – 06:34 PM UTC

PDB ID : 3MSG / pdb\_00003msg  
Title : Enzyme-Substrate interactions of IXT6, the intracellular xylanase of *G. stearothermophilus*.  
Authors : Solomon, V.; Zolotnitsky, G.; Alhadeff, R.; Shoham, Y.; Shoham, G.  
Deposited on : 2010-04-29  
Resolution : 1.50 Å(reported)

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<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>.

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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

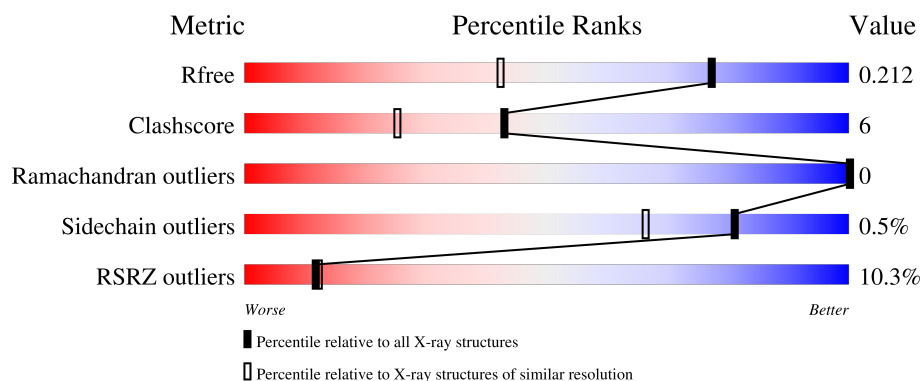
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.50 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	4037 (1.50-1.50)
Clashscore	190562	4235 (1.50-1.50)
Ramachandran outliers	187476	4153 (1.50-1.50)
Sidechain outliers	187428	4150 (1.50-1.50)
RSRZ outliers	180081	4039 (1.50-1.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	331	 9% 82% 16% .
1	B	331	 11% 84% 15% ..
2	C	2	 50% 50%
2	D	2	 50% 50%

## 2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 6256 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 Intra-cellular xylanase ixt6.

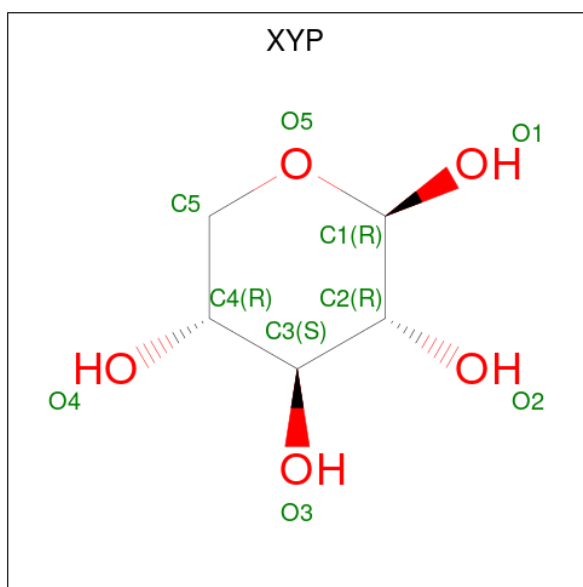
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	330	Total	C	N	O	S	0	11	0
			2789	1783	492	501	13			
1	B	328	Total	C	N	O	S	0	10	0
			2767	1768	485	501	13			

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



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
2	C	2	Total	C	O	0	0	0
			19	10	9			
2	D	2	Total	C	O	0	0	0
			19	10	9			

- Molecule 3 is beta-D-xylopyranose (CCD ID: XYP) (formula: C<sub>5</sub>H<sub>10</sub>O<sub>5</sub>).

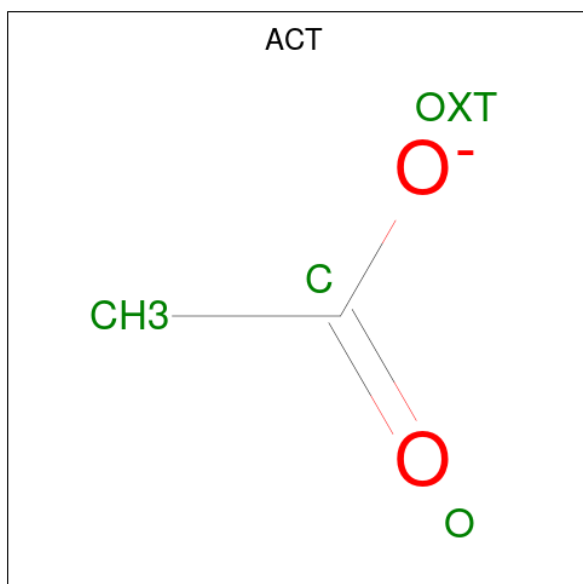


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			10	5	5		

- Molecule 4 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Na	0	0
			1	1		
4	B	1	Total	Na	0	0
			1	1		

- Molecule 5 is ACETATE ION (CCD ID: ACT) (formula: C<sub>2</sub>H<sub>3</sub>O<sub>2</sub>).



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

- Molecule 6 is GLYCEROL (CCD ID: GOL) (formula:  $C_3H_8O_3$ ).



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

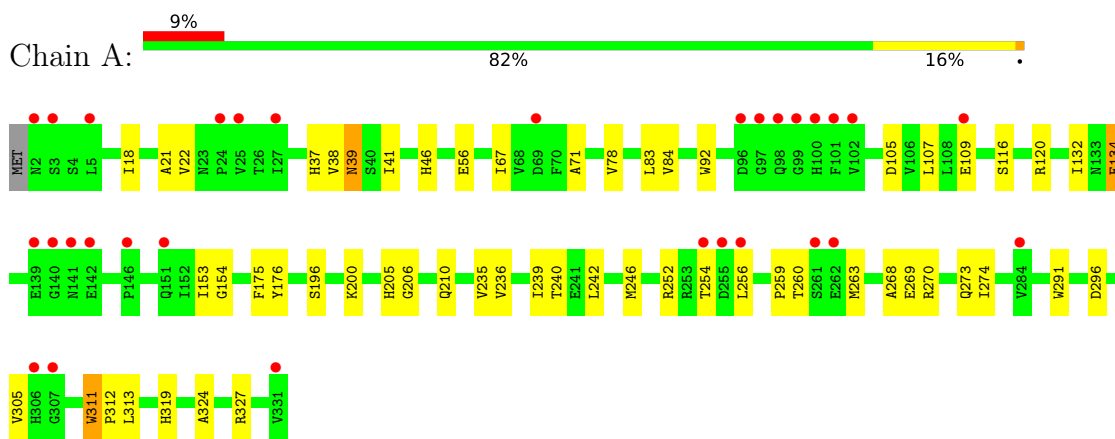
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	325	Total	O	0	0
			325	325		
7	B	293	Total	O	0	0
			293	293		

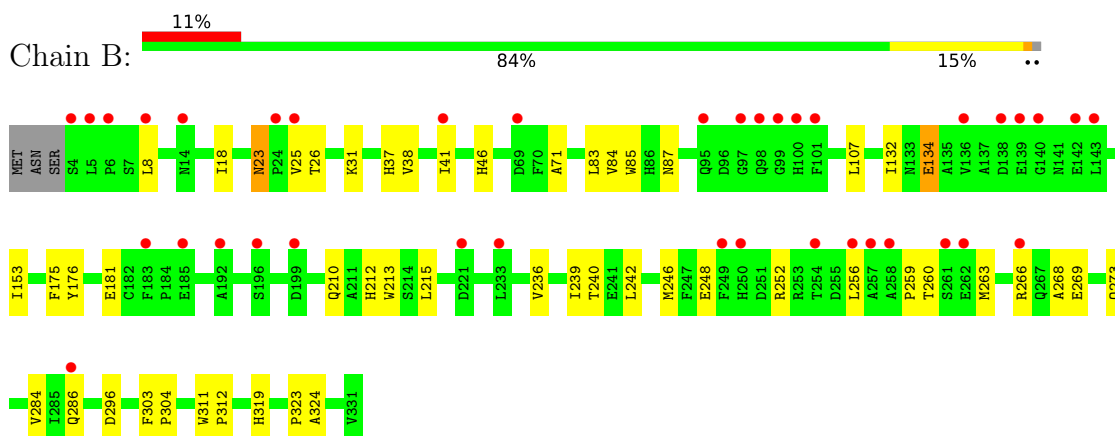
### 3 Residue-property plots

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: Intra-cellular xylanase ixt6



- Molecule 1: Intra-cellular xylanase ixt6



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



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





## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	169.23Å 80.77Å 79.06Å 90.00° 91.73° 90.00°	Depositor
Resolution (Å)	36.44 – 1.50 36.44 – 1.50	Depositor EDS
% Data completeness (in resolution range)	93.6 (36.44-1.50) 91.9 (36.44-1.50)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.07	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.09 (at 1.50Å)	Xtriage
Refinement program	CNS	Depositor
R, $R_{free}$	0.187 , 0.202 0.204 , 0.212	Depositor DCC
$R_{free}$ test set	6792 reflections (4.18%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	17.7	Xtriage
Anisotropy	0.677	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 38.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.015 for -h,-k,l	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	6256	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	23.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.36% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.



## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NA, GOL, ACT, XYP

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	0/2865	0.92	15/3880 (0.4%)
1	B	0.33	0/2843	0.90	14/3851 (0.4%)
All	All	0.34	0/5708	0.91	29/7731 (0.4%)

There are no bond length outliers.

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	240	THR	N-CA-C	9.22	124.66	113.41
1	A	239	ILE	N-CA-C	-8.46	95.29	108.23
1	B	240	THR	N-CA-C	8.42	123.68	113.41
1	B	46	HIS	N-CA-C	8.36	123.14	113.19
1	B	239	ILE	N-CA-C	-7.94	95.35	107.73
1	A	46	HIS	N-CA-C	7.89	122.58	113.19
1	B	37	HIS	N-CA-C	7.79	123.70	114.04
1	A	37	HIS	N-CA-C	7.47	123.30	114.04
1	A	176	TYR	N-CA-C	-6.85	97.35	108.52
1	B	83	LEU	N-CA-C	6.47	119.29	111.40
1	B	176	TYR	N-CA-C	-6.33	98.19	108.52
1	B	248	GLU	N-CA-C	-5.90	102.18	110.50
1	A	242	LEU	N-CA-C	5.83	118.79	110.10
1	A	83	LEU	N-CA-C	5.78	118.69	111.24
1	B	312	PRO	N-CA-C	5.71	122.91	114.80
1	B	38	VAL	N-CA-C	5.64	117.85	109.17
1	B	242	LEU	N-CA-C	5.63	118.49	110.10
1	A	175	PHE	N-CA-C	5.61	118.69	109.72
1	A	154	GLY	N-CA-C	-5.59	106.44	112.08
1	B	175	PHE	N-CA-C	5.57	118.63	109.72
1	A	134	GLU	N-CA-C	5.55	119.09	111.54
1	B	213	TRP	N-CA-C	5.50	118.23	110.14

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Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
1	B	134	GLU	N-CA-C	5.45	118.91	111.39
1	A	312	PRO	N-CA-C	5.41	123.94	114.75
1	A	38	VAL	N-CA-C	5.30	117.41	109.20
1	B	31	LYS	N-CA-C	5.27	117.43	111.11
1	A	313	LEU	N-CA-C	5.12	118.05	109.96
1	A	311	TRP	CA-C-N	5.06	125.88	120.47
1	A	311	TRP	C-N-CA	5.06	125.88	120.47

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	2789	0	2685	34	0
1	B	2767	0	2654	35	0
2	C	19	0	0	2	0
2	D	19	0	0	2	0
3	A	10	0	0	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
5	A	4	0	3	0	0
5	B	4	0	3	1	0
6	A	24	0	32	0	0
7	A	325	0	0	0	0
7	B	293	0	0	1	0
All	All	6256	0	5377	69	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.

All (69) 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:256:LEU:HD21	1:A:263[A]:MET:HE1	1.38	1.05

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:260:THR:H	1:A:263[A]:MET:HE3	1.25	1.01
1:A:41[B]:ILE:HG21	1:A:71:ALA:HB2	1.61	0.82
1:B:260:THR:H	1:B:263[B]:MET:HE3	1.44	0.81
1:B:23:ASN:ND2	1:B:26:THR:H	1.80	0.79
1:B:259:PRO:HA	1:B:263[B]:MET:HE3	1.66	0.78
1:A:22:VAL:HG21	1:A:41[B]:ILE:HD11	1.64	0.77
1:B:23:ASN:C	1:B:23:ASN:HD22	1.93	0.77
1:B:41[A]:ILE:CD1	1:B:71:ALA:HB2	2.20	0.71
1:A:18:ILE:H	1:A:39:ASN:HD21	1.39	0.70
1:B:256:LEU:HD23	1:B:263[B]:MET:HE1	1.71	0.69
1:B:236:VAL:HG13	1:B:286[A]:GLN:OE1	1.94	0.67
1:B:8[A]:LEU:HD23	1:B:18:ILE:HG21	1.77	0.66
1:A:270:ARG:O	1:A:274[A]:ILE:HG12	1.96	0.65
1:A:105:ASP:O	1:A:109:GLU:HG3	1.98	0.63
1:B:259:PRO:HA	1:B:263[B]:MET:CE	2.27	0.63
1:B:41[A]:ILE:HD13	1:B:71:ALA:HB2	1.82	0.61
1:B:260:THR:N	1:B:263[B]:MET:HE3	2.15	0.60
1:A:22:VAL:CG2	1:A:41[B]:ILE:HD11	2.30	0.60
1:B:23:ASN:HD21	1:B:26:THR:H	1.47	0.58
1:A:18:ILE:H	1:A:39:ASN:ND2	2.00	0.58
1:B:296:ASP:OD2	1:B:319:HIS:HE1	1.87	0.57
1:A:260:THR:OG1	1:A:263[B]:MET:HG3	2.04	0.57
1:B:256:LEU:HD23	1:B:263[B]:MET:CE	2.35	0.56
1:B:260:THR:H	1:B:263[B]:MET:CE	2.15	0.56
1:A:84:VAL:HB	1:A:132:ILE:HD13	1.88	0.56
1:A:252:ARG:HD2	1:A:305:VAL:CG2	2.37	0.55
1:B:23:ASN:ND2	1:B:23:ASN:C	2.64	0.55
1:B:134:GLU:OE2	2:D:1:XYP:O1	2.26	0.54
1:A:41[B]:ILE:CG2	1:A:78:VAL:HG22	2.38	0.54
1:B:259:PRO:HD3	1:B:311:TRP:CE2	2.43	0.53
1:A:254:THR:HG22	1:A:305:VAL:HG11	1.91	0.52
1:A:260:THR:HG23	1:A:263[A]:MET:CE	2.40	0.51
1:B:210:GLN:OE1	2:D:1:XYP:O1	2.30	0.50
1:A:268:ALA:C	1:A:327[A]:ARG:HD3	2.36	0.50
1:A:134:GLU:OE2	2:C:1:XYP:O1	2.31	0.49
1:B:107:LEU:HD23	1:B:153:ILE:HG13	1.95	0.49
1:A:116[B]:SER:O	1:A:120[B]:ARG:HG3	2.13	0.48
1:A:259:PRO:HD3	1:A:311:TRP:CE2	2.48	0.48
1:A:260:THR:HG23	1:A:263[A]:MET:HE3	1.96	0.48
1:B:259:PRO:CA	1:B:263[B]:MET:HE3	2.40	0.47
1:A:268:ALA:HA	1:A:324:ALA:HA	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:206:GLY:HA2	1:A:235:VAL:HB	1.96	0.47
1:B:212:HIS:HB3	5:B:338:ACT:H3	1.97	0.46
1:A:196[B]:SER:O	1:A:200[B]:LYS:HG3	2.16	0.46
1:A:21:ALA:HB2	1:A:291:TRP:CE3	2.52	0.45
1:A:210:GLN:OE1	2:C:1:XYP:O1	2.35	0.45
1:B:252:ARG:NE	7:B:1118:HOH:O	2.48	0.44
1:B:84:VAL:HB	1:B:132:ILE:HD13	2.00	0.44
1:A:107:LEU:HD23	1:A:153:ILE:HG13	1.99	0.44
1:B:41[A]:ILE:HD11	1:B:71:ALA:HB2	1.99	0.44
1:B:284:VAL:C	1:B:286[A]:GLN:HE22	2.26	0.44
1:B:303:PHE:CD1	1:B:304:PRO:HA	2.52	0.44
1:B:181:GLU:CD	1:B:181:GLU:H	2.26	0.44
1:A:205:HIS:O	1:A:236[A]:VAL:HG22	2.17	0.43
1:A:18:ILE:N	1:A:39:ASN:HD21	2.13	0.43
1:A:269:GLU:O	1:A:273:GLN:HG3	2.19	0.43
1:A:260:THR:N	1:A:263[A]:MET:HE3	2.10	0.42
1:B:269[B]:GLU:O	1:B:273:GLN:HG3	2.18	0.42
1:B:215:LEU:HD22	1:B:266[A]:ARG:HG3	2.01	0.42
1:A:246:MET:O	1:A:263[B]:MET:HE2	2.19	0.42
1:B:266[A]:ARG:O	1:B:266[A]:ARG:HD2	2.20	0.42
1:A:296:ASP:OD2	1:A:319:HIS:HE1	2.02	0.42
1:A:56:GLU:HB2	1:A:92:TRP:CE3	2.55	0.41
1:B:85:TRP:CE2	1:B:87:ASN:HB2	2.56	0.41
1:B:268:ALA:HA	1:B:324:ALA:HA	2.03	0.41
1:B:246:MET:HB3	1:B:263[A]:MET:HE3	2.02	0.41
1:B:23:ASN:HD22	1:B:25:VAL:N	2.19	0.40
1:A:41[B]:ILE:HD11	1:A:67:ILE:HG23	2.03	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	339/331 (102%)	330 (97%)	9 (3%)	0	100	100
1	B	336/331 (102%)	328 (98%)	8 (2%)	0	100	100
All	All	675/662 (102%)	658 (98%)	17 (2%)	0	100	100

There are no Ramachandran outliers to report.

### 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	296/291 (102%)	295 (100%)	1 (0%)	86	75
1	B	294/291 (101%)	292 (99%)	2 (1%)	76	57
All	All	590/582 (101%)	587 (100%)	3 (0%)	81	66

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	39	ASN
1	B	23	ASN
1	B	323	PRO

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	39	ASN
1	A	180	ASN
1	A	297	HIS
1	A	319	HIS
1	B	23	ASN
1	B	160	GLN
1	B	319	HIS

### 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	10,10,10	0.51	0	14,14,14	0.67	0
2	XYP	C	2	2	9,9,10	0.68	0	10,12,14	0.32	0
2	XYP	D	1	2	10,10,10	0.53	0	14,14,14	0.58	0
2	XYP	D	2	2	9,9,10	0.65	0	10,12,14	0.36	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	XYP	C	1	2	-	-	0/1/1/1
2	XYP	C	2	2	-	-	0/1/1/1
2	XYP	D	1	2	-	-	0/1/1/1
2	XYP	D	2	2	-	-	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

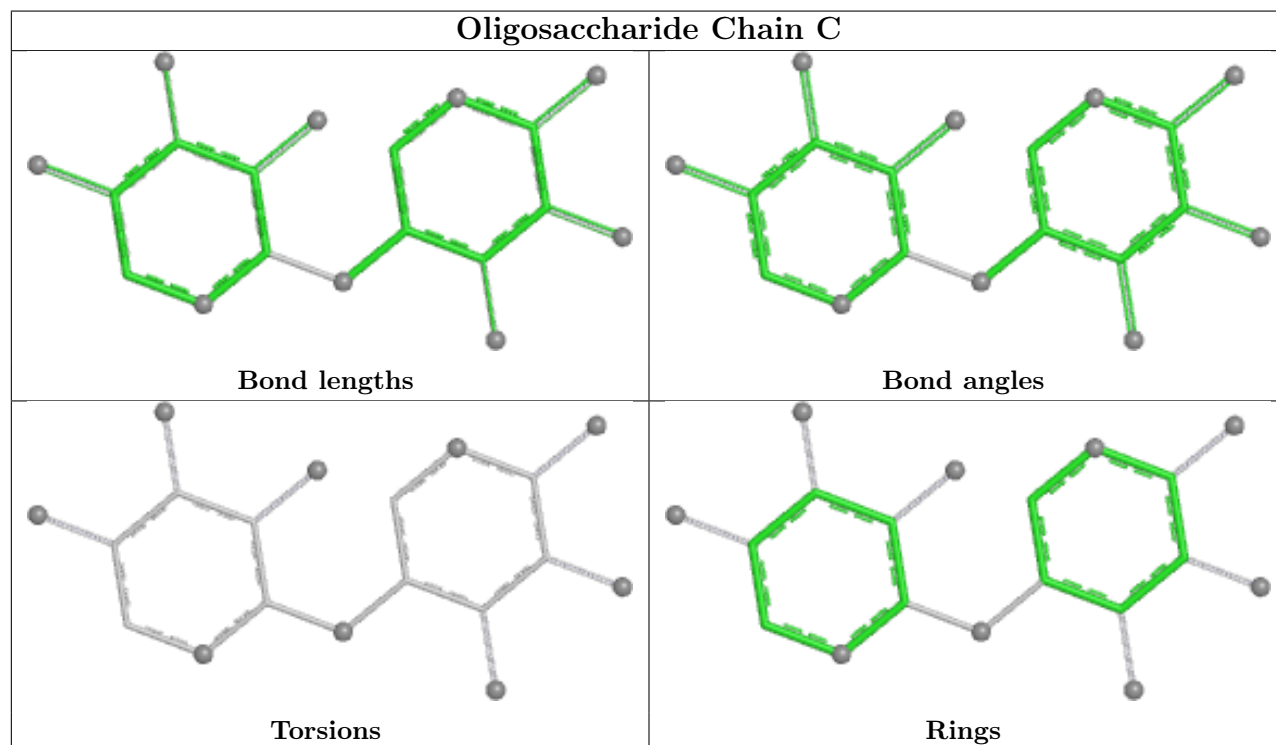
There are no torsion outliers.

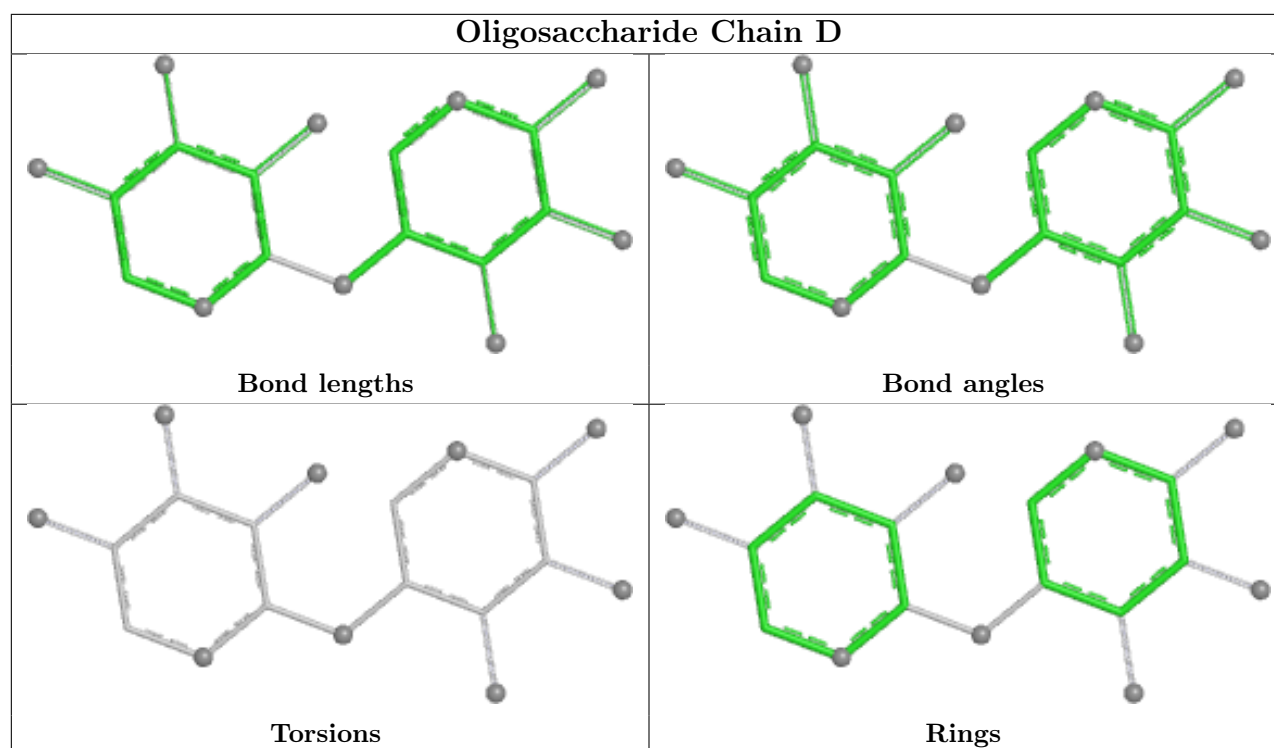
There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	1	XYP	2	0
2	C	1	XYP	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 9 ligands modelled in this entry, 2 are monoatomic - leaving 7 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$
5	ACT	A	337	-	3,3,3	1.02	0	3,3,3	0.82	0
6	GOL	A	475	-	5,5,5	0.78	0	5,5,5	0.43	0
6	GOL	A	471	-	5,5,5	0.79	0	5,5,5	0.45	0
5	ACT	B	338	-	3,3,3	1.08	0	3,3,3	0.84	0
6	GOL	A	474	-	5,5,5	0.76	0	5,5,5	0.41	0
6	GOL	A	473	-	5,5,5	0.75	0	5,5,5	0.43	0
3	XYP	A	449	-	10,10,10	0.48	0	14,14,14	0.27	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	GOL	A	475	-	-	4/4/4/4	-
6	GOL	A	471	-	-	3/4/4/4	-
6	GOL	A	474	-	-	2/4/4/4	-
6	GOL	A	473	-	-	0/4/4/4	-
3	XYP	A	449	-	-	-	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	471	GOL	C1-C2-C3-O3
6	A	474	GOL	C1-C2-C3-O3
6	A	474	GOL	O2-C2-C3-O3
6	A	471	GOL	O2-C2-C3-O3
6	A	471	GOL	O1-C1-C2-C3
6	A	475	GOL	O1-C1-C2-C3
6	A	475	GOL	O1-C1-C2-O2
6	A	475	GOL	O2-C2-C3-O3
6	A	475	GOL	C1-C2-C3-O3

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	338	ACT	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, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	330/331 (99%)	0.55	30 (9%) 15 15	8, 19, 34, 49	11 (3%)
1	B	328/331 (99%)	0.77	38 (11%) 9 9	8, 22, 35, 45	10 (3%)
All	All	658/662 (99%)	0.66	68 (10%) 12 12	8, 20, 35, 49	21 (3%)

All (68) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	99	GLY	5.8
1	A	99	GLY	4.7
1	B	100	HIS	4.5
1	A	24	PRO	4.5
1	A	97	GLY	4.5
1	B	249	PHE	4.3
1	B	4	SER	3.9
1	A	3	SER	3.8
1	A	2	ASN	3.6
1	B	256	LEU	3.6
1	A	100	HIS	3.6
1	B	140	GLY	3.6
1	A	101	PHE	3.4
1	B	266[A]	ARG	3.3
1	B	183	PHE	3.3
1	B	97	GLY	3.3
1	B	24	PRO	3.2
1	B	5	LEU	3.1
1	A	146	PRO	3.0
1	B	41[A]	ILE	3.0
1	A	307	GLY	3.0
1	B	261[A]	SER	3.0
1	A	255	ASP	3.0
1	A	141	ASN	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	25	VAL	2.9
1	B	139	GLU	2.9
1	A	5	LEU	2.8
1	A	284[A]	VAL	2.8
1	A	98	GLN	2.8
1	A	256	LEU	2.8
1	A	69	ASP	2.7
1	B	250	HIS	2.7
1	B	98	GLN	2.7
1	B	254	THR	2.6
1	A	140	GLY	2.6
1	B	262	GLU	2.6
1	A	96	ASP	2.6
1	B	142	GLU	2.5
1	B	258	ALA	2.4
1	A	109	GLU	2.4
1	B	8[A]	LEU	2.4
1	B	69	ASP	2.4
1	A	262	GLU	2.4
1	B	286[A]	GLN	2.3
1	A	27	ILE	2.3
1	B	185	GLU	2.3
1	A	331	VAL	2.3
1	B	143	LEU	2.3
1	B	257	ALA	2.3
1	B	101	PHE	2.3
1	B	196	SER	2.3
1	A	142	GLU	2.2
1	A	151	GLN	2.2
1	B	6	PRO	2.2
1	B	95	GLN	2.2
1	B	138	ASP	2.2
1	B	221	ASP	2.2
1	A	261[A]	SER	2.1
1	A	139	GLU	2.1
1	B	199	ASP	2.1
1	B	192	ALA	2.1
1	B	14	ASN	2.1
1	B	25	VAL	2.0
1	B	136	VAL	2.0
1	A	254	THR	2.0
1	A	306	HIS	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	102	VAL	2.0
1	B	233	LEU	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](#)

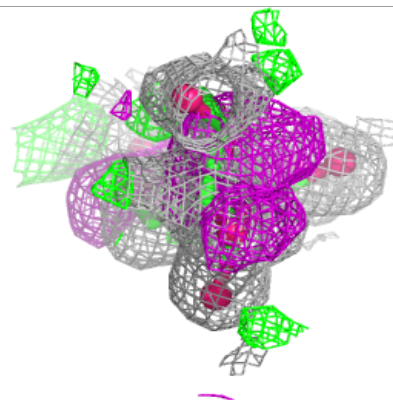
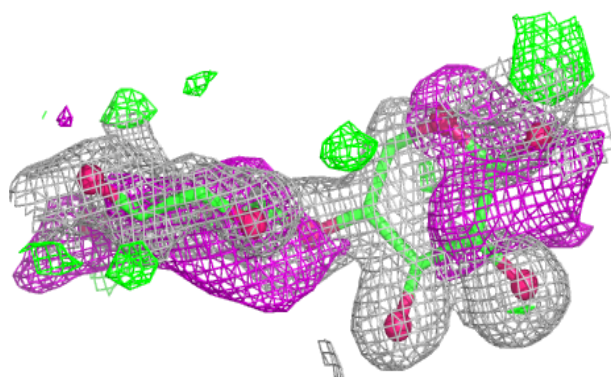
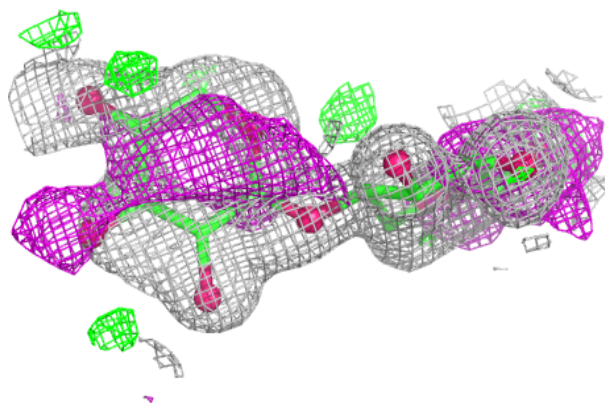
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
2	XYP	C	2	9/10	0.72	0.18	38,39,42,43	0
2	XYP	D	1	10/10	0.82	0.19	20,31,37,40	0
2	XYP	D	2	9/10	0.82	0.14	26,31,33,35	0
2	XYP	C	1	10/10	0.84	0.17	21,32,35,37	0

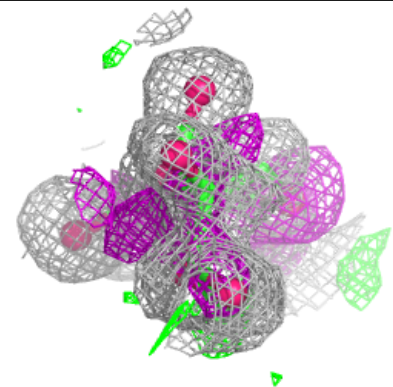
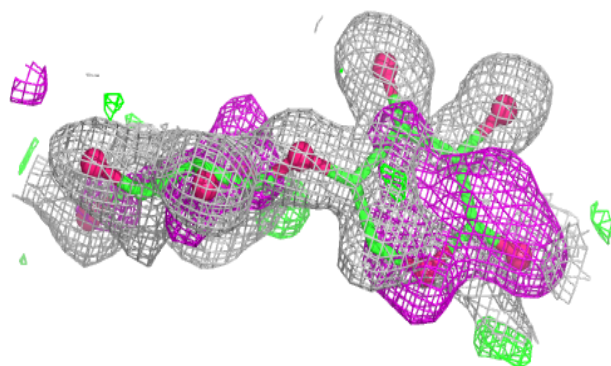
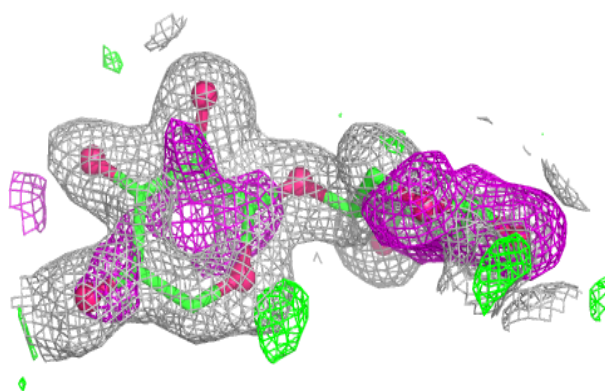
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

**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, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
3	XYP	A	449	10/10	0.46	0.25	59,60,61,61	0
6	GOL	A	473	6/6	0.70	0.23	45,48,48,50	0
6	GOL	A	475	6/6	0.70	0.21	52,56,56,58	0
6	GOL	A	474	6/6	0.74	0.22	56,57,57,59	0
6	GOL	A	471	6/6	0.80	0.20	50,51,52,52	0
5	ACT	B	338	4/4	0.82	0.20	50,51,51,51	0
5	ACT	A	337	4/4	0.89	0.15	29,31,31,32	0
4	NA	B	402	1/1	0.97	0.06	24,24,24,24	0
4	NA	A	401	1/1	1.00	0.05	20,20,20,20	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.