



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 20, 2026 – 06:46 PM UTC

PDB ID : 2W5F / pdb_00002w5f
Title : High resolution crystallographic structure of the Clostridium thermocellum N-terminal endo-1,4-beta-D-xylanase 10B (Xyn10B) CBM22-1- GH10 modules complexed with xylohexaose
Authors : Najmudin, S.; Pinheiro, B.A.; Romao, M.J.; Prates, J.A.M.; Fontes, C.M.G.A.
Deposited on : 2008-12-10
Resolution : 1.90 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

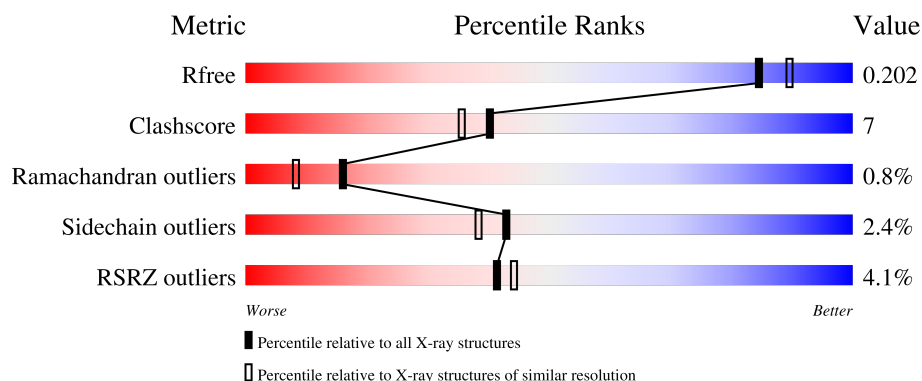
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 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	7789 (1.90-1.90)
Clashscore	190562	8410 (1.90-1.90)
Ramachandran outliers	187476	8333 (1.90-1.90)
Sidechain outliers	187428	8333 (1.90-1.90)
RSRZ outliers	180081	7790 (1.90-1.90)

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	540	5% 84% 8% • 5%
1	B	540	3% 84% 10% • 5%
2	C	3	33% 67%
2	D	3	67% 33%

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
3	ACT	B	1553	-	-	X	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 9818 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-XYLANASE Y.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	511	Total	C	N	O	S	0	5	0
			4046	2539	694	797	16			
1	B	513	Total	C	N	O	S	0	9	0
			4069	2559	689	804	17			

There are 42 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	12	MET	-	expression tag	UNP P51584
A	13	GLY	-	expression tag	UNP P51584
A	14	SER	-	expression tag	UNP P51584
A	15	SER	-	expression tag	UNP P51584
A	16	HIS	-	expression tag	UNP P51584
A	17	HIS	-	expression tag	UNP P51584
A	18	HIS	-	expression tag	UNP P51584
A	19	HIS	-	expression tag	UNP P51584
A	20	HIS	-	expression tag	UNP P51584
A	21	HIS	-	expression tag	UNP P51584
A	22	SER	-	expression tag	UNP P51584
A	23	SER	-	expression tag	UNP P51584
A	24	GLY	-	expression tag	UNP P51584
A	25	LEU	-	expression tag	UNP P51584
A	26	VAL	-	expression tag	UNP P51584
A	27	PRO	-	expression tag	UNP P51584
A	28	ARG	-	expression tag	UNP P51584
A	29	GLY	-	expression tag	UNP P51584
A	30	SER	-	expression tag	UNP P51584
A	31	HIS	-	expression tag	UNP P51584
B	12	MET	-	expression tag	UNP P51584
B	13	GLY	-	expression tag	UNP P51584
B	14	SER	-	expression tag	UNP P51584
B	15	SER	-	expression tag	UNP P51584
B	16	HIS	-	expression tag	UNP P51584

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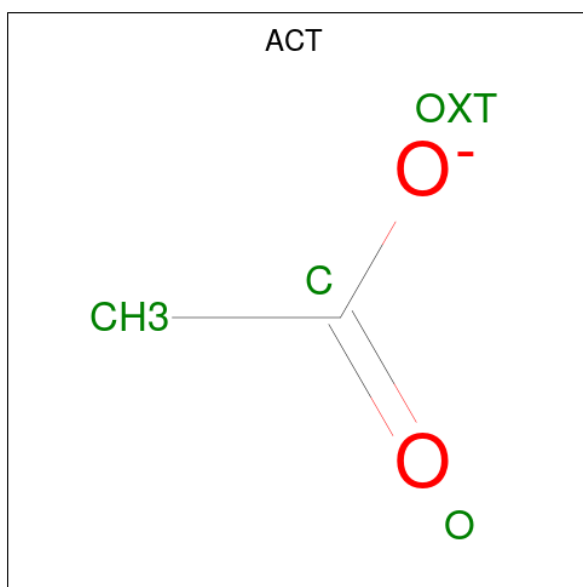
Chain	Residue	Modelled	Actual	Comment	Reference
B	17	HIS	-	expression tag	UNP P51584
B	18	HIS	-	expression tag	UNP P51584
B	19	HIS	-	expression tag	UNP P51584
B	20	HIS	-	expression tag	UNP P51584
B	21	HIS	-	expression tag	UNP P51584
B	22	SER	-	expression tag	UNP P51584
B	23	SER	-	expression tag	UNP P51584
B	24	GLY	-	expression tag	UNP P51584
B	25	LEU	-	expression tag	UNP P51584
B	26	VAL	-	expression tag	UNP P51584
B	27	PRO	-	expression tag	UNP P51584
B	28	ARG	-	expression tag	UNP P51584
B	29	GLY	-	expression tag	UNP P51584
B	30	SER	-	expression tag	UNP P51584
B	31	HIS	-	expression tag	UNP P51584
A	337	ALA	GLU	engineered mutation	UNP P51584
B	337	ALA	GLU	engineered mutation	UNP P51584

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



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
2	C	3	Total	C	O	0	0	0
			28	15	13			
2	D	3	Total	C	O	0	0	0
			28	15	13			

- Molecule 3 is ACETATE ION (CCD ID: ACT) (formula: C₂H₃O₂).



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

- Molecule 4 is CADMIUM ION (CCD ID: CD) (formula: Cd).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	8	Total Cd 8 8	0	0
4	B	5	Total Cd 5 5	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	745	Total 745	O 745	0	0
5	B	853	Total 853	O 853	0	0



4 Data and refinement statistics

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α , β , γ	173.18Å 173.18Å 131.71Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	150.76 – 1.90 149.98 – 1.90	Depositor EDS
% Data completeness (in resolution range)	98.9 (150.76-1.90) 92.5 (149.98-1.90)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.46 (at 1.86Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.164 , 0.194 (Not available) , 0.202	Depositor DCC
R_{free} test set	8839 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å ²)	32.2	Xtriage
Anisotropy	0.059	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 86.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.017 for -h,-k,l	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	9818	wwPDB-VP
Average B, all atoms (Å ²)	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.67% 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: ACT, CD, 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	0.67	1/4144 (0.0%)	0.83	5/5627 (0.1%)
1	B	0.72	1/4187 (0.0%)	0.80	3/5687 (0.1%)
All	All	0.69	2/8331 (0.0%)	0.82	8/11314 (0.1%)

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	2
1	B	0	1
All	All	0	3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	494	SER	C-N	-16.39	1.10	1.33
1	A	495	LYS	C-N	-7.30	1.27	1.33

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	40	THR	CB-CA-C	-7.39	100.90	111.76
1	B	494	SER	O-C-N	6.79	133.87	123.00
1	B	33	ASP	N-CA-C	6.32	121.16	113.38
1	A	495	LYS	N-CA-C	-5.92	98.18	110.80
1	A	370	ASP	N-CA-CB	-5.46	103.25	111.56
1	A	190	ALA	CA-C-N	5.16	130.99	121.70
1	A	190	ALA	C-N-CA	5.16	130.99	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	58	THR	CB-CA-C	-5.11	100.45	109.70

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	369	GLY	Peptide
1	A	494	SER	Peptide
1	B	494	SER	Peptide

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4046	0	3865	49	0
1	B	4069	0	3887	51	0
2	C	28	0	0	0	0
2	D	28	0	0	0	0
3	A	24	0	18	1	0
3	B	12	0	9	5	0
4	A	8	0	0	1	0
4	B	5	0	0	1	0
5	A	745	0	0	20	0
5	B	853	0	0	21	0
All	All	9818	0	7779	105	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 (105) 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:493:SER:CA	1:B:494:SER:HB3	1.56	1.32
1:B:493:SER:HA	1:B:494:SER:CB	1.60	1.25
1:A:40:THR:C	5:A:2014:HOH:O	1.93	1.11

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:425:MET:SD	5:A:2577:HOH:O	2.09	1.09
1:B:157:ASN:HB3	5:B:2273:HOH:O	1.58	1.01
1:B:35:GLU:OE1	5:B:2002:HOH:O	1.79	0.97
1:B:300:VAL:HG21	1:B:305[A]:MET:HE2	1.45	0.97
4:A:1560:CD:CD	5:A:2004:HOH:O	1.31	0.97
1:A:429:ILE:HD12	1:A:478:LYS:HE3	1.57	0.86
1:A:40:THR:O	1:A:40:THR:OG1	1.86	0.83
4:B:1557:CD:CD	5:B:2002:HOH:O	1.46	0.83
1:B:300:VAL:CG2	1:B:305[A]:MET:HE2	2.07	0.82
1:A:40:THR:O	1:A:42:GLU:N	2.13	0.82
1:A:41:PHE:N	5:A:2014:HOH:O	2.05	0.81
1:B:289:PHE:HA	1:B:305[A]:MET:HE1	1.64	0.78
3:B:1553:ACT:CH3	5:B:2566:HOH:O	2.35	0.74
1:B:350:GLY:HA2	3:B:1553:ACT:O	1.88	0.73
1:B:469:LYS:HD2	5:B:2738:HOH:O	1.88	0.72
1:B:493:SER:HA	1:B:494:SER:HB3	0.77	0.71
1:B:480:LYS:HG3	1:B:538[A]:ILE:HD11	1.73	0.71
1:B:413:ASN:HB2	5:B:2663:HOH:O	1.91	0.70
1:B:493:SER:CB	1:B:494:SER:HB3	2.20	0.70
1:A:493:SER:N	1:A:494:SER:HB3	2.07	0.69
1:A:35:GLU:OE2	5:A:2004:HOH:O	2.09	0.69
1:A:87:LYS:HB2	1:A:91:LEU:HD22	1.75	0.68
1:B:410[A]:ILE:HD11	5:B:2602:HOH:O	1.93	0.68
1:B:388[B]:ASN:ND2	5:B:2629:HOH:O	2.26	0.67
1:A:493:SER:HA	1:A:494:SER:OG	1.95	0.67
1:A:72:MET:HE3	5:A:2291:HOH:O	1.95	0.67
1:A:190:ALA:HA	1:A:191:ALA:HB2	1.76	0.66
1:A:493:SER:HA	1:A:494:SER:CB	2.26	0.66
1:B:110:THR:HG22	5:B:2158:HOH:O	1.96	0.65
1:A:40:THR:CA	5:A:2014:HOH:O	2.36	0.64
1:B:58:THR:CG2	5:B:2534:HOH:O	2.47	0.62
1:A:176:THR:HG22	5:A:2137:HOH:O	2.01	0.61
1:A:430:ASN:O	1:A:478:LYS:HE2	2.01	0.60
1:A:493:SER:CA	1:A:494:SER:CB	2.79	0.60
1:B:493:SER:CA	1:B:494:SER:CB	2.43	0.60
1:B:300:VAL:CG2	1:B:305[A]:MET:CE	2.79	0.57
1:A:493:SER:HA	1:A:494:SER:HG	1.70	0.56
1:A:493:SER:CA	1:A:494:SER:HB3	2.35	0.56
1:B:346:THR:O	3:B:1553:ACT:C	2.54	0.56
1:B:58:THR:HG22	5:B:2534:HOH:O	2.07	0.54
1:B:289:PHE:HA	1:B:305[A]:MET:CE	2.34	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:495:LYS:NZ	5:B:2665:HOH:O	2.33	0.53
1:A:527:GLN:NE2	5:A:2710:HOH:O	2.42	0.53
1:A:537:SER:HB3	5:A:2715:HOH:O	2.08	0.52
1:B:388[B]:ASN:CG	5:B:2629:HOH:O	2.52	0.52
1:A:425:MET:HE2	1:A:456:VAL:HG11	1.93	0.50
1:B:32:ALA:N	5:B:2001:HOH:O	2.45	0.50
1:A:87:LYS:CB	1:A:91:LEU:HD22	2.42	0.49
1:A:437:SER:O	1:A:478:LYS:NZ	2.42	0.49
3:B:1552:ACT:O	3:B:1553:ACT:OXT	2.30	0.49
1:A:463:ILE:HD13	1:A:478:LYS:HB3	1.93	0.49
1:A:527:GLN:HG3	5:A:2709:HOH:O	2.12	0.49
1:B:535:VAL:HA	1:B:538[A]:ILE:HD13	1.95	0.49
3:B:1553:ACT:H1	5:B:2562:HOH:O	2.13	0.48
1:B:361:ARG:NH1	5:B:2590:HOH:O	2.46	0.47
1:B:401[A]:ASP:OD2	5:B:2649:HOH:O	2.20	0.47
1:A:190:ALA:CA	1:A:191:ALA:HB2	2.44	0.47
1:B:219:ILE:O	1:B:223:ILE:HG12	2.15	0.47
1:B:213:THR:C	1:B:215:ASN:H	2.23	0.47
1:B:534:ALA:O	1:B:538[A]:ILE:CD1	2.63	0.47
1:A:219:ILE:O	1:A:223:ILE:HG12	2.15	0.47
1:A:38:HIS:ND1	5:A:2004:HOH:O	2.35	0.46
1:A:396:TYR:HB3	1:A:426:GLN:OE1	2.15	0.46
1:A:347:ARG:HD3	5:A:2524:HOH:O	2.15	0.46
1:B:189:TYR:CE2	1:B:191:ALA:HA	2.51	0.46
1:B:72:MET:HE2	5:B:2300:HOH:O	2.16	0.46
1:B:463:ILE:HD12	1:B:479:TYR:CD1	2.51	0.46
1:B:38:HIS:HA	1:B:175:VAL:O	2.17	0.45
1:B:494:SER:HA	1:B:497:LYS:NZ	2.31	0.45
1:A:76:ARG:NH2	1:A:164:THR:OG1	2.45	0.45
1:A:33:ASP:HB3	1:A:180:LYS:HA	2.00	0.44
1:A:89:PHE:CE2	1:A:214:VAL:HG22	2.53	0.44
1:A:370:ASP:OD1	1:A:372:LYS:N	2.50	0.44
1:B:258:ARG:HD3	5:B:2449:HOH:O	2.17	0.44
1:B:396:TYR:HB3	1:B:426:GLN:OE1	2.17	0.44
1:B:493:SER:OG	1:B:494:SER:CB	2.66	0.44
1:A:126:GLU:OE2	3:A:1556:ACT:OXT	2.35	0.43
1:A:72:MET:CE	5:A:2291:HOH:O	2.61	0.43
1:B:115:LEU:HB2	1:B:133:ALA:HB3	2.01	0.43
1:B:296:ASN:HB3	5:B:2194:HOH:O	2.17	0.43
1:A:141:GLU:HG2	5:A:2104:HOH:O	2.18	0.42
1:A:544:TRP:HZ2	5:A:2718:HOH:O	2.03	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:361:ARG:HD2	5:A:2540:HOH:O	2.18	0.42
1:A:35:GLU:HA	1:A:178:THR:HG22	2.02	0.42
1:A:480:LYS:NZ	1:A:537:SER:OG	2.53	0.42
1:A:119:TYR:CZ	1:A:128:ASN:HB3	2.55	0.41
1:B:534:ALA:O	1:B:538[A]:ILE:HD12	2.20	0.41
1:B:119:TYR:CZ	1:B:128:ASN:HB3	2.56	0.41
1:B:493:SER:OG	1:B:494:SER:HB3	2.20	0.41
1:B:60:VAL:HG23	1:B:63:GLU:HB2	2.03	0.41
1:B:272:ALA:HB1	1:B:330:TYR:CD2	2.55	0.41
1:A:382:ARG:HD3	1:A:382:ARG:HA	1.90	0.41
1:B:195:LEU:HA	1:B:198:MET:HE3	2.01	0.41
1:B:399:TYR:HA	1:B:445:ALA:HB2	2.02	0.41
1:A:541:GLN:HA	1:A:544:TRP:CE2	2.56	0.40
1:B:167:THR:O	5:B:2295:HOH:O	2.22	0.40
1:A:129:LYS:NZ	5:A:2196:HOH:O	2.54	0.40
1:A:157:ASN:HB3	5:A:2267:HOH:O	2.20	0.40
1:B:89:PHE:HD1	1:B:89:PHE:HA	1.72	0.40
1:A:278:LEU:HG	1:A:332:TYR:CE2	2.57	0.40
1:A:495:LYS:N	5:A:2683:HOH:O	2.55	0.40
1:B:300:VAL:HG21	1:B:305[A]:MET:CE	2.32	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	512/540 (95%)	489 (96%)	17 (3%)	6 (1%)	10	4
1	B	518/540 (96%)	494 (95%)	22 (4%)	2 (0%)	30	22
All	All	1030/1080 (95%)	983 (95%)	39 (4%)	8 (1%)	16	8

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	41	PHE
1	A	495	LYS
1	B	494	SER
1	A	33	ASP
1	A	191	ALA
1	B	214	VAL
1	A	359	ASN
1	A	494	SER

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	435/453 (96%)	425 (98%)	10 (2%)	44	40
1	B	440/453 (97%)	429 (98%)	11 (2%)	42	37
All	All	875/906 (97%)	854 (98%)	21 (2%)	43	38

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	51	LEU
1	A	91	LEU
1	A	176	THR
1	A	214	VAL
1	A	218	SER
1	A	294	GLN
1	A	382	ARG
1	A	471	SER
1	A	478	LYS
1	A	494	SER
1	B	58	THR
1	B	72	MET
1	B	89	PHE
1	B	110	THR
1	B	115	LEU
1	B	138	VAL

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Mol	Chain	Res	Type
1	B	165	ASP
1	B	294	GLN
1	B	382	ARG
1	B	473	GLN
1	B	494	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	286	GLN
1	A	307	GLN
1	A	413	ASN
1	A	447	GLN
1	B	298	ASN
1	B	307	GLN
1	B	447	GLN
1	B	484	GLN
1	B	510	ASN

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 ⓘ

6 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	0.55	0	14,14,14	1.00	1 (7%)
2	XYP	C	2	2	9,9,10	0.51	0	10,12,14	1.40	2 (20%)
2	XYP	C	3	2	9,9,10	0.30	0	10,12,14	0.76	0
2	XYP	D	1	2	10,10,10	0.64	0	14,14,14	0.97	0
2	XYP	D	2	2	9,9,10	0.38	0	10,12,14	0.66	0
2	XYP	D	3	2	9,9,10	0.34	0	10,12,14	0.97	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	1	2	-	-	0/1/1/1
2	XYP	C	2	2	-	-	0/1/1/1
2	XYP	C	3	2	-	-	0/1/1/1
2	XYP	D	1	2	-	-	0/1/1/1
2	XYP	D	2	2	-	-	0/1/1/1
2	XYP	D	3	2	-	-	0/1/1/1

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	2	XYP	C1-C2-C3	-2.71	105.69	109.64
2	C	1	XYP	O5-C5-C4	-2.55	104.71	110.79
2	C	2	XYP	C5-C4-C3	2.35	113.06	109.64
2	D	3	XYP	C1-C2-C3	-2.04	106.67	109.64

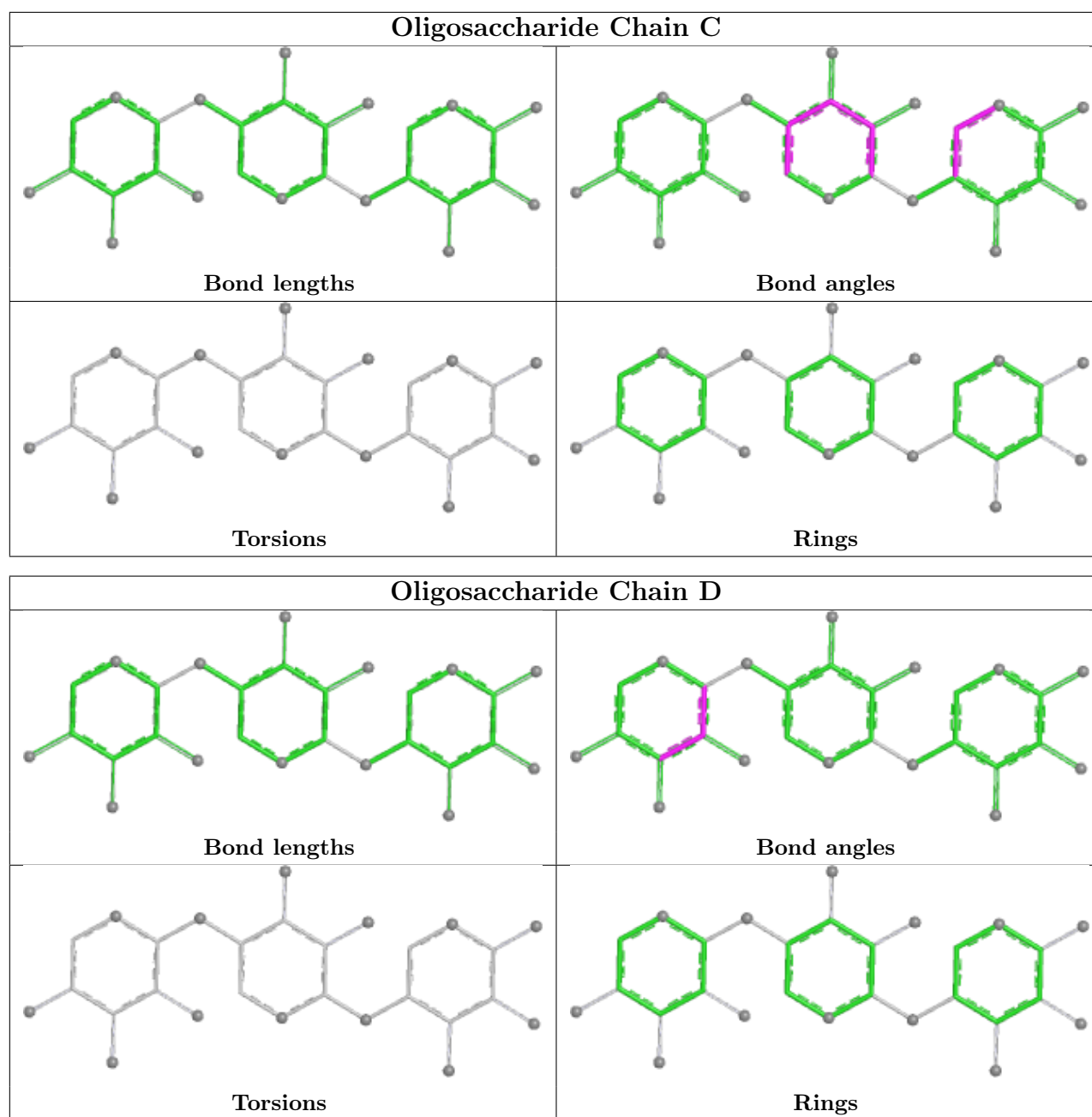
There are no chirality outliers.

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 22 ligands modelled in this entry, 13 are monoatomic - leaving 9 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
3	ACT	A	1554	4	3,3,3	0.94	0	3,3,3	1.72	1 (33%)
3	ACT	B	1554	4	3,3,3	0.92	0	3,3,3	1.71	2 (66%)
3	ACT	A	1553	4	3,3,3	0.75	0	3,3,3	1.44	0
3	ACT	A	1557	4	3,3,3	0.75	0	3,3,3	1.31	0
3	ACT	A	1552	4	3,3,3	0.95	0	3,3,3	1.18	0
3	ACT	B	1552	4	3,3,3	0.87	0	3,3,3	1.16	0
3	ACT	B	1553	4	3,3,3	0.74	0	3,3,3	1.82	1 (33%)
3	ACT	A	1555	-	3,3,3	0.82	0	3,3,3	0.94	0
3	ACT	A	1556	4	3,3,3	0.97	0	3,3,3	1.71	1 (33%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	1553	ACT	OXT-C-CH3	2.52	125.63	115.05
3	A	1556	ACT	OXT-C-O	-2.34	113.34	122.03
3	A	1554	ACT	OXT-C-O	-2.23	113.75	122.03
3	B	1554	ACT	OXT-C-O	-2.09	114.27	122.03
3	B	1554	ACT	OXT-C-CH3	2.09	123.82	115.05

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	1552	ACT	1	0
3	B	1553	ACT	5	0
3	A	1556	ACT	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	B	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	494:SER	C	495:LYS	N	1.10

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	511/540 (94%)	0.21	27 (5%) 32 34	11, 23, 33, 41	5 (0%)
1	B	513/540 (95%)	-0.08	15 (2%) 53 57	9, 21, 36, 53	9 (1%)
All	All	1024/1080 (94%)	0.06	42 (4%) 41 44	9, 22, 35, 53	14 (1%)

All (42) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	551	ALA	6.0
1	A	493	SER	5.6
1	A	504	TRP	4.7
1	B	32	ALA	4.6
1	A	512	TRP	4.0
1	B	181	GLY	3.8
1	B	33	ASP	3.7
1	B	524	ALA	3.6
1	B	494	SER	3.4
1	B	493	SER	3.4
1	B	168	VAL	3.3
1	A	40	THR	3.2
1	A	500	ALA	3.2
1	A	214	VAL	3.0
1	A	498	VAL	3.0
1	A	32	ALA	3.0
1	B	495	LYS	3.0
1	A	190	ALA	3.0
1	A	369	GLY	2.8
1	A	473	GLN	2.7
1	A	501	VAL	2.7
1	A	496	GLY	2.6
1	A	33	ASP	2.6
1	A	34	TYR	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	494	SER	2.6
1	B	34	TYR	2.5
1	A	513	LEU	2.4
1	B	347	ARG	2.3
1	B	169	ASP	2.3
1	A	533[A]	ASN	2.3
1	B	167	THR	2.3
1	A	347	ARG	2.3
1	B	164	THR	2.3
1	A	157	ASN	2.2
1	A	502	CYS	2.2
1	A	547	GLY	2.1
1	A	361	ARG	2.1
1	A	370	ASP	2.1
1	A	462	ASP	2.1
1	B	218	SER	2.0
1	B	170	PHE	2.0
1	A	550	PRO	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](#)

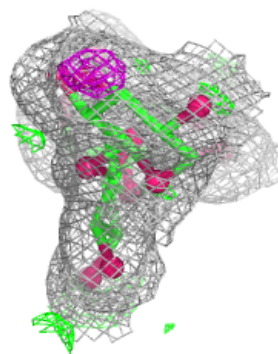
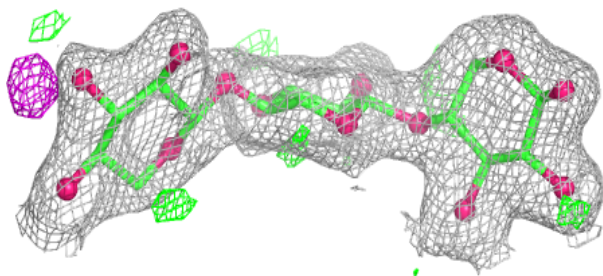
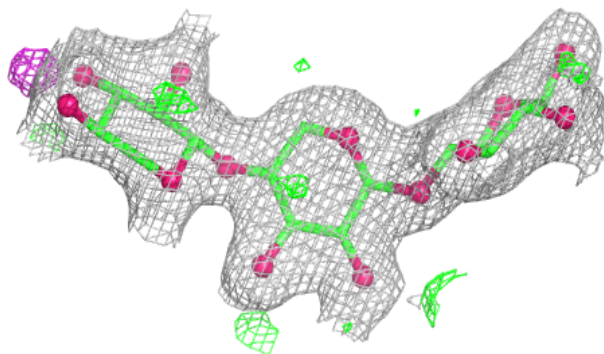
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	XYP	C	3	9/10	0.94	0.08	41,43,48,52	0
2	XYP	D	3	9/10	0.96	0.07	38,42,48,49	0
2	XYP	C	1	10/10	0.98	0.05	25,28,29,30	0
2	XYP	C	2	9/10	0.98	0.05	27,29,31,34	0
2	XYP	D	2	9/10	0.99	0.03	24,25,27,30	0
2	XYP	D	1	10/10	0.99	0.04	25,27,28,29	0

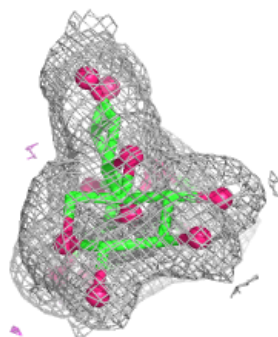
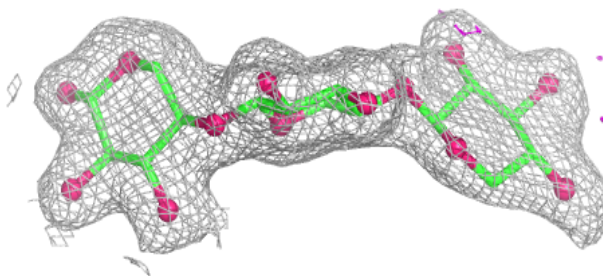
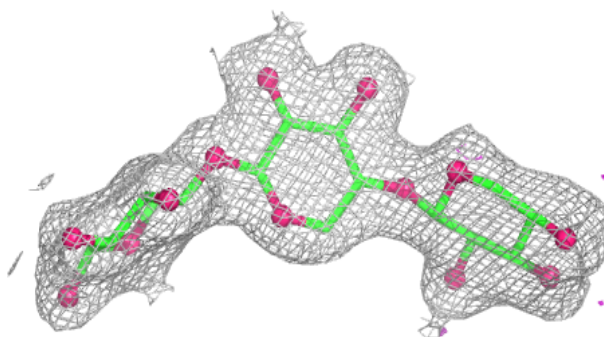
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

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
3	ACT	A	1555	4/4	0.79	0.23	67,67,68,68	0
3	ACT	A	1557	4/4	0.92	0.13	68,68,68,68	0
3	ACT	B	1553	4/4	0.92	0.24	43,45,45,46	0
3	ACT	A	1554	4/4	0.93	0.13	59,60,60,60	0
4	CD	A	1563	1/1	0.93	0.18	68,68,68,68	1
3	ACT	A	1556	4/4	0.94	0.11	63,64,64,64	0
4	CD	B	1559	1/1	0.94	0.10	72,72,72,72	1
3	ACT	B	1552	4/4	0.95	0.11	45,45,46,46	0
3	ACT	B	1554	4/4	0.95	0.11	55,56,56,56	0
4	CD	A	1565	1/1	0.97	0.06	58,58,58,58	1
3	ACT	A	1552	4/4	0.98	0.07	32,34,34,34	0
3	ACT	A	1553	4/4	0.99	0.07	34,36,36,36	0
4	CD	A	1564	1/1	0.99	0.04	74,74,74,74	1
4	CD	A	1561	1/1	0.99	0.03	57,57,57,57	1
4	CD	B	1556	1/1	0.99	0.03	39,39,39,39	1
4	CD	B	1557	1/1	0.99	0.03	46,46,46,46	1
4	CD	B	1558	1/1	0.99	0.03	48,48,48,48	1
4	CD	A	1562	1/1	0.99	0.03	61,61,61,61	1
4	CD	A	1560	1/1	1.00	0.03	47,47,47,47	1
4	CD	A	1558	1/1	1.00	0.02	34,34,34,34	0
4	CD	A	1559	1/1	1.00	0.03	40,40,40,40	1
4	CD	B	1555	1/1	1.00	0.02	36,36,36,36	1

6.5 Other polymers [i](#)

There are no such residues in this entry.