



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 07:39 AM UTC

PDB ID : 1L5W / pdb_00001l5w
Title : Crystal Structure of the Maltodextrin Phosphorylase Complexed with the Products of the Enzymatic Reaction between Glucose-1-phosphate and Maltotetraose
Authors : Geremia, S.; Campagnolo, M.; Schinzel, R.; Johnson, L.N.
Deposited on : 2002-03-08
Resolution : 1.80 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

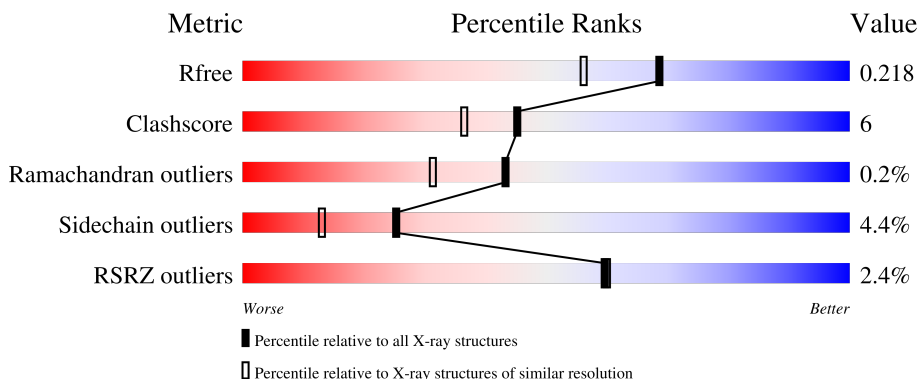
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.80 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	7662 (1.80-1.80)
Clashscore	190562	8479 (1.80-1.80)
Ramachandran outliers	187476	8391 (1.80-1.80)
Sidechain outliers	187428	8390 (1.80-1.80)
RSRZ outliers	180081	7663 (1.80-1.80)

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

Mol	Chain	Length	Quality of chain
1	A	796	2% 83% 15% .
1	B	796	3% 84% 14% .
2	C	4	100%
2	D	4	25% 75%

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 13995 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 MALTODEXTRIN PHOSPHORYLASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	796	Total	C	N	O	S	0	0	0
			6390	4079	1128	1163	20			
1	B	796	Total	C	N	O	S	0	0	0
			6390	4079	1128	1163	20			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	261	ALA	HIS	SEE REMARK 999	GB 606352
A	262	PHE	THR	SEE REMARK 999	GB 606352
A	263	GLU	ALA	SEE REMARK 999	GB 606352
B	261	ALA	HIS	SEE REMARK 999	GB 606352
B	262	PHE	THR	SEE REMARK 999	GB 606352
B	263	GLU	ALA	SEE REMARK 999	GB 606352

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



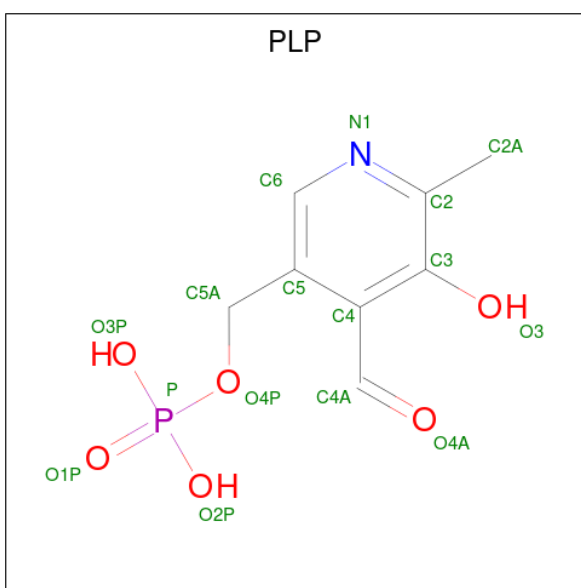
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
2	C	4	Total	C	O	0	0	0
			45	24	21			
2	D	4	Total	C	O	0	0	0
			45	24	21			

- Molecule 3 is PHOSPHATE ION (CCD ID: PO4) (formula: O₄P).



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

- Molecule 4 is PYRIDOXAL-5'-PHOSPHATE (CCD ID: PLP) (formula: $C_8H_{10}NO_6P$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			15	8	1	5	1		
4	B	1	Total	C	N	O	P	0	0
			15	8	1	5	1		

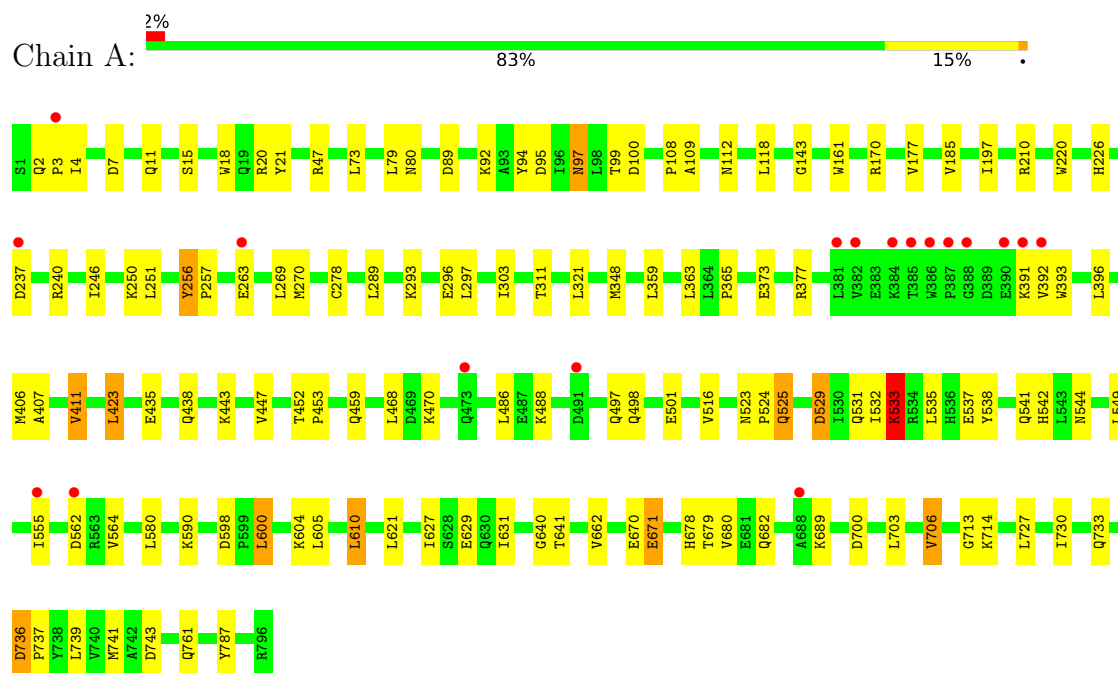
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	565	Total 565	O 565	0	0
5	B	520	Total 520	O 520	0	0

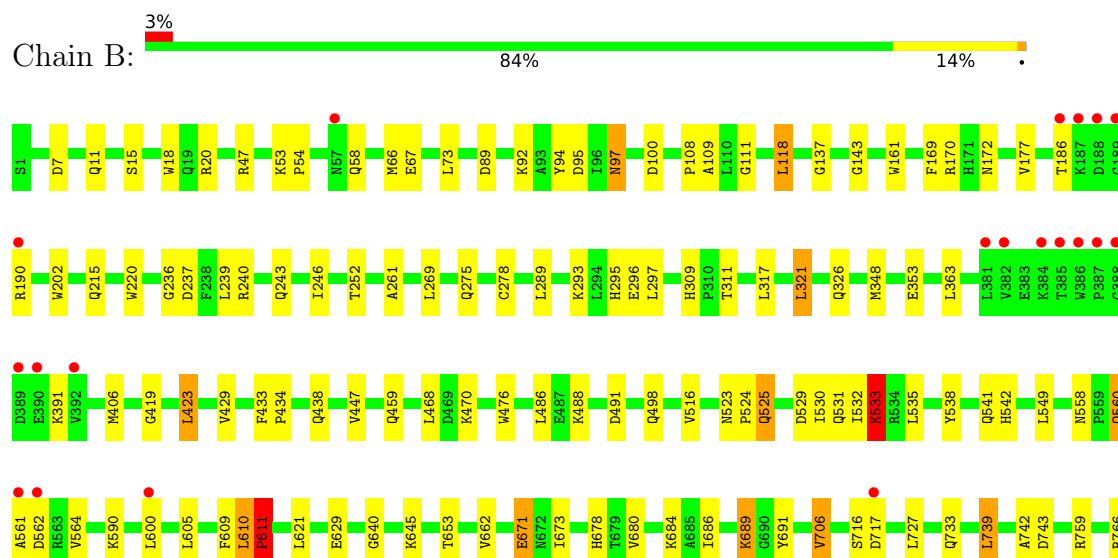
3 Residue-property plots

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: MALTODEXTRIN PHOSPHORYLASE

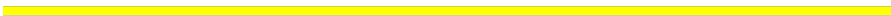


• Molecule 1: MALTODEXTRIN PHOSPHORYLASE





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

Chain C:  100%



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

Chain D:  25% 75%



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	74.51Å 105.24Å 217.36Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 1.80 20.00 – 1.80	Depositor EDS
% Data completeness (in resolution range)	85.0 (20.00-1.80) 84.9 (20.00-1.80)	Depositor EDS
R_{merge}	0.18	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.70 (at 1.80Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.186 , 0.216 0.189 , 0.218	Depositor DCC
R_{free} test set	6782 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	21.4	Xtriage
Anisotropy	0.279	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.40 , 43.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	13995	wwPDB-VP
Average B, all atoms (Å ²)	24.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.02% 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: GLC, PLP, PO4

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	1.06	4/6540 (0.1%)	1.13	11/8865 (0.1%)
1	B	1.03	1/6540 (0.0%)	1.10	5/8865 (0.1%)
All	All	1.05	5/13080 (0.0%)	1.12	16/17730 (0.1%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	252	THR	CA-CB	6.41	1.61	1.53
1	A	736	ASP	C-O	-6.23	1.21	1.23
1	A	303	ILE	CA-CB	-6.03	1.46	1.54
1	A	256	TYR	CA-C	-5.39	1.50	1.53
1	A	256	TYR	C-O	-5.04	1.21	1.23

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	419	GLY	N-CA-C	-6.41	103.79	112.57
1	A	226	HIS	CA-C-N	6.24	125.81	119.19
1	A	226	HIS	C-N-CA	6.24	125.81	119.19
1	A	761	GLN	N-CA-C	6.18	118.82	111.71
1	A	210	ARG	N-CA-C	5.89	119.67	111.90
1	B	243	GLN	N-CA-C	5.80	117.28	111.07
1	A	641	THR	N-CA-C	-5.60	108.23	114.62
1	B	640	GLY	N-CA-C	-5.58	105.73	112.48
1	A	640	GLY	N-CA-C	-5.47	105.86	112.48
1	A	529	ASP	CA-C-N	-5.46	115.99	123.14
1	A	529	ASP	C-N-CA	-5.46	115.99	123.14
1	A	4	ILE	N-CA-C	5.19	115.57	107.99
1	B	353	GLU	N-CA-C	5.16	117.70	110.23
1	A	112	ASN	CA-C-N	-5.06	115.81	121.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	112	ASN	C-N-CA	-5.06	115.81	121.83
1	B	611	PRO	CA-N-CD	-5.05	104.93	112.00

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	6390	0	6333	79	0
1	B	6390	0	6333	78	0
2	C	45	0	39	0	0
2	D	45	0	39	0	0
3	A	5	0	0	0	0
3	B	5	0	0	0	0
4	A	15	0	6	0	0
4	B	15	0	6	1	0
5	A	565	0	0	11	0
5	B	520	0	0	10	0
All	All	13995	0	12756	151	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 (151) 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:558:ASN:OD1	1:B:560:GLN:HB2	1.77	0.84
1:B:261:ALA:HB2	5:B:1023:HOH:O	1.85	0.75
1:A:468:LEU:CD2	1:A:486:LEU:HD11	2.17	0.75
1:A:671:GLU:H	1:A:671:GLU:CD	1.96	0.74
1:B:47:ARG:HD3	5:B:1062:HOH:O	1.89	0.73
1:A:733:GLN:H	1:A:733:GLN:CD	1.97	0.72
1:B:89:ASP:O	1:B:92:LYS:HG2	1.89	0.71
1:B:97:ASN:HD22	1:B:100:ASP:H	1.38	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:678:HIS:HE1	5:A:1487:HOH:O	1.73	0.70
1:A:47:ARG:HD3	5:A:1034:HOH:O	1.90	0.70
1:A:470:LYS:NZ	1:A:498:GLN:HE22	1.90	0.70
1:A:311:THR:HB	1:A:406:MET:HE3	1.74	0.69
1:B:671:GLU:H	1:B:671:GLU:CD	2.01	0.69
1:B:237:ASP:OD2	1:B:240:ARG:NH1	2.25	0.68
1:A:269:LEU:HD23	1:A:363:LEU:HD12	1.75	0.66
1:B:348:MET:HE3	1:B:538:TYR:CD2	2.31	0.66
1:B:97:ASN:ND2	1:B:100:ASP:H	1.93	0.65
1:B:609:PHE:O	1:B:611:PRO:HD3	1.95	0.65
1:B:733:GLN:OE1	1:B:733:GLN:N	2.20	0.64
1:B:468:LEU:CD2	1:B:486:LEU:HD11	2.28	0.63
1:B:733:GLN:H	1:B:733:GLN:CD	2.04	0.63
1:A:470:LYS:HZ3	1:A:498:GLN:HE22	1.46	0.62
1:B:423:LEU:HD11	1:B:680:VAL:HG21	1.81	0.62
1:A:733:GLN:OE1	1:A:733:GLN:N	2.21	0.62
1:B:560:GLN:HA	1:B:560:GLN:OE1	1.99	0.62
1:B:684:LYS:NZ	5:B:1240:HOH:O	2.33	0.61
1:A:237:ASP:OD2	1:A:240:ARG:NH1	2.33	0.61
1:A:97:ASN:HD22	1:A:100:ASP:H	1.48	0.61
1:A:532:ILE:O	1:A:533:LYS:HB3	2.01	0.60
1:A:21:TYR:O	1:B:172:ASN:HB2	2.01	0.59
1:A:97:ASN:ND2	1:A:100:ASP:H	2.00	0.59
1:A:89:ASP:O	1:A:92:LYS:HG2	2.02	0.59
1:B:326:GLN:NE2	5:B:1478:HOH:O	2.35	0.59
1:A:525:GLN:HE21	1:A:525:GLN:HA	1.68	0.58
1:A:348:MET:HE3	1:A:538:TYR:CD2	2.39	0.57
1:A:459:GLN:NE2	5:A:1232:HOH:O	2.36	0.57
1:B:7:ASP:O	1:B:11:GLN:HG2	2.05	0.56
1:B:186:THR:OG1	1:B:190:ARG:HB2	2.04	0.56
1:A:549:LEU:HB3	1:A:706:VAL:HG22	1.88	0.56
1:B:459:GLN:NE2	5:B:1261:HOH:O	2.39	0.56
1:B:491:ASP:OD2	1:B:766:ARG:NH1	2.38	0.55
1:B:686:ILE:HG13	5:B:1424:HOH:O	2.07	0.55
1:A:97:ASN:HD22	1:A:97:ASN:C	2.15	0.55
1:B:558:ASN:ND2	1:B:561:ALA:HB2	2.22	0.55
1:A:246:ILE:HD13	1:B:239:LEU:HD12	1.89	0.54
1:A:423:LEU:HD11	1:A:680:VAL:HG21	1.89	0.54
1:A:468:LEU:HD21	1:A:486:LEU:HD11	1.90	0.54
1:A:544:ASN:C	1:A:544:ASN:HD22	2.16	0.53
1:A:20:ARG:O	1:B:170:ARG:HB2	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:531:GLN:HE22	1:A:541:GLN:HA	1.74	0.52
1:A:713:GLY:HA2	5:A:1177:HOH:O	2.11	0.50
1:A:3:PRO:HD2	5:A:1439:HOH:O	2.11	0.50
1:B:447:VAL:HG11	1:B:787:TYR:CD2	2.46	0.50
1:A:373:GLU:OE2	1:A:377:ARG:NE	2.37	0.50
1:B:739:LEU:HB3	1:B:742:ALA:HB3	1.93	0.50
1:A:246:ILE:HD11	1:B:246:ILE:HD11	1.94	0.49
1:A:680:VAL:HG23	5:A:1278:HOH:O	2.11	0.49
1:B:680:VAL:HG23	5:B:1302:HOH:O	2.12	0.49
1:B:109:ALA:HB1	1:B:143:GLY:HA3	1.95	0.49
1:A:670:GLU:HG3	1:A:671:GLU:OE1	2.13	0.48
1:B:67:GLU:HB2	1:B:111:GLY:HA2	1.95	0.48
1:A:529:ASP:OD1	1:A:629:GLU:OE2	2.31	0.48
1:A:537:GLU:OE1	1:A:580:LEU:HD23	2.14	0.48
1:A:170:ARG:HB2	1:B:20:ARG:O	2.14	0.48
1:A:269:LEU:HD23	1:A:359:LEU:CD2	2.44	0.48
1:B:610:LEU:CD1	1:B:621:LEU:HD21	2.43	0.47
1:B:549:LEU:HB3	1:B:706:VAL:HG22	1.95	0.47
1:B:311:THR:HB	1:B:406:MET:HE3	1.95	0.47
1:B:11:GLN:NE2	5:B:1294:HOH:O	2.42	0.47
1:B:66:MET:HG3	1:B:309:HIS:CB	2.45	0.47
1:A:497:GLN:NE2	1:A:501:GLU:OE2	2.36	0.47
1:A:713:GLY:CA	5:A:1177:HOH:O	2.63	0.46
1:B:560:GLN:OE1	1:B:560:GLN:CA	2.61	0.46
1:B:562:ASP:O	1:B:759:ARG:NH2	2.48	0.46
1:A:407:ALA:O	1:A:411:VAL:HG12	2.16	0.46
1:A:590:LYS:HA	1:A:590:LYS:HD2	1.74	0.46
1:B:58:GLN:C	5:B:1313:HOH:O	2.58	0.46
1:A:94:TYR:O	1:A:95:ASP:HB2	2.16	0.46
1:B:531:GLN:HE22	1:B:541:GLN:HA	1.80	0.46
1:B:678:HIS:HD2	1:B:743:ASP:OD1	1.98	0.46
1:A:263:GLU:OE2	1:B:236:GLY:O	2.34	0.46
1:A:714:LYS:NZ	5:A:1337:HOH:O	2.49	0.45
1:B:429:VAL:O	1:B:434:PRO:HA	2.17	0.45
1:B:523:ASN:HA	1:B:524:PRO:HD3	1.81	0.45
1:B:15:SER:HA	1:B:18:TRP:NE1	2.31	0.45
1:A:7:ASP:O	1:A:11:GLN:HG2	2.17	0.45
1:A:447:VAL:HG11	1:A:787:TYR:CE2	2.52	0.45
1:A:713:GLY:N	5:A:1177:HOH:O	2.47	0.45
1:A:97:ASN:ND2	1:A:97:ASN:C	2.72	0.45
1:A:293:LYS:O	1:A:296:GLU:HG2	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:220:TRP:CD2	1:B:278:CYS:HB3	2.51	0.45
1:A:15:SER:HA	1:A:18:TRP:NE1	2.32	0.45
1:A:97:ASN:HD21	1:A:99:THR:HB	1.82	0.45
1:A:348:MET:HE3	1:A:538:TYR:CG	2.52	0.45
1:B:94:TYR:O	1:B:95:ASP:HB2	2.17	0.45
1:B:610:LEU:HD13	1:B:621:LEU:HD21	1.98	0.45
1:B:671:GLU:CD	1:B:671:GLU:N	2.72	0.45
1:A:447:VAL:HG11	1:A:787:TYR:CD2	2.52	0.44
1:A:604:LYS:NZ	5:A:1512:HOH:O	2.47	0.44
1:B:525:GLN:HE21	1:B:525:GLN:HA	1.81	0.44
1:A:678:HIS:HD2	1:A:743:ASP:OD1	2.01	0.44
1:A:109:ALA:HB1	1:A:143:GLY:HA3	1.99	0.44
1:A:679:THR:OG1	1:A:682:GLN:HG3	2.18	0.44
1:B:66:MET:HG3	1:B:309:HIS:HB3	2.00	0.44
1:B:689:LYS:O	1:B:689:LYS:HG2	2.16	0.44
1:B:529:ASP:OD1	1:B:629:GLU:OE2	2.36	0.44
1:B:609:PHE:O	1:B:611:PRO:CD	2.62	0.44
1:A:736:ASP:N	1:A:737:PRO:HD3	2.33	0.44
1:B:220:TRP:CE2	1:B:278:CYS:HB3	2.53	0.44
1:B:645:LYS:NZ	4:B:900:PLP:O3	2.50	0.44
1:B:691:TYR:CE2	1:B:739:LEU:HD22	2.52	0.43
1:B:716:SER:O	1:B:717:ASP:HB3	2.17	0.43
1:A:598:ASP:OD1	1:A:598:ASP:C	2.61	0.43
1:B:108:PRO:HA	1:B:161:TRP:CE3	2.54	0.43
1:B:433:PHE:N	1:B:434:PRO:CD	2.81	0.43
1:B:532:ILE:O	1:B:533:LYS:HB3	2.19	0.43
1:A:627:ILE:HD13	1:A:627:ILE:HA	1.76	0.43
1:B:137:GLY:HA2	1:B:275:GLN:NE2	2.33	0.43
1:B:317:LEU:HG	1:B:321:LEU:HD22	2.01	0.43
1:B:295:HIS:CD2	1:B:296:GLU:HG3	2.54	0.42
1:B:269:LEU:HD23	1:B:363:LEU:HD12	2.00	0.42
1:B:293:LYS:HA	1:B:293:LYS:HD3	1.75	0.42
1:A:250:LYS:HE3	1:A:270:MET:HE1	2.02	0.42
1:A:256:TYR:N	1:A:257:PRO:CD	2.82	0.42
1:A:392:VAL:O	1:A:393:TRP:C	2.63	0.42
1:B:590:LYS:HD2	1:B:590:LYS:HA	1.77	0.42
1:A:2:GLN:HG3	5:A:1439:HOH:O	2.18	0.42
1:A:610:LEU:HD13	1:A:621:LEU:HD21	2.01	0.42
1:B:470:LYS:NZ	1:B:498:GLN:HE22	2.16	0.42
1:A:185:VAL:HG23	1:A:365:PRO:HB2	2.01	0.42
1:A:631:ILE:HG21	1:A:631:ILE:HD13	1.82	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:108:PRO:HA	1:A:161:TRP:CE3	2.55	0.41
1:A:396:LEU:HD21	1:A:435:GLU:HB2	2.01	0.41
1:B:476:TRP:H	1:B:476:TRP:CD1	2.36	0.41
1:A:452:THR:HA	1:A:453:PRO:HD3	1.96	0.41
1:A:671:GLU:CD	1:A:671:GLU:N	2.71	0.41
1:B:53:LYS:HA	1:B:54:PRO:HD3	1.91	0.41
1:A:197:ILE:HD13	1:A:251:LEU:CD1	2.50	0.41
1:A:700:ASP:HB3	1:A:703:LEU:HB3	2.01	0.41
1:B:423:LEU:HD11	1:B:680:VAL:CG2	2.49	0.41
1:B:716:SER:O	1:B:717:ASP:CB	2.66	0.41
1:A:537:GLU:CD	1:A:580:LEU:CD2	2.94	0.41
1:B:433:PHE:N	1:B:434:PRO:HD3	2.36	0.41
1:A:220:TRP:CE2	1:A:278:CYS:HB3	2.56	0.41
1:B:653:THR:HB	1:B:673:ILE:HG13	2.02	0.41
1:B:118:LEU:HA	5:B:1041:HOH:O	2.21	0.41
1:A:79:LEU:HD23	1:A:80:ASN:OD1	2.22	0.40
1:A:523:ASN:HA	1:A:524:PRO:HD3	1.96	0.40
1:A:600:LEU:HD13	1:A:600:LEU:HA	1.85	0.40
1:A:730:ILE:HD12	1:A:741:MET:HE3	2.02	0.40
1:B:169:PHE:CE1	1:B:202:TRP:HB3	2.56	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	794/796 (100%)	770 (97%)	22 (3%)	2 (0%)	36	25
1	B	794/796 (100%)	770 (97%)	23 (3%)	1 (0%)	48	34
All	All	1588/1592 (100%)	1540 (97%)	45 (3%)	3 (0%)	43	31

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	533	LYS
1	B	533	LYS
1	A	562	ASP

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	667/667 (100%)	638 (96%)	29 (4%)	26	13
1	B	667/667 (100%)	637 (96%)	30 (4%)	24	12
All	All	1334/1334 (100%)	1275 (96%)	59 (4%)	25	13

All (59) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	73	LEU
1	A	97	ASN
1	A	118	LEU
1	A	177	VAL
1	A	289	LEU
1	A	297	LEU
1	A	321	LEU
1	A	391	LYS
1	A	411	VAL
1	A	423	LEU
1	A	438	GLN
1	A	443	LYS
1	A	488	LYS
1	A	516	VAL
1	A	525	GLN
1	A	533	LYS
1	A	535	LEU
1	A	542	HIS
1	A	555	ILE
1	A	564	VAL
1	A	600	LEU

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Mol	Chain	Res	Type
1	A	605	LEU
1	A	610	LEU
1	A	662	VAL
1	A	671	GLU
1	A	689	LYS
1	A	706	VAL
1	A	727	LEU
1	A	739	LEU
1	B	73	LEU
1	B	97	ASN
1	B	118	LEU
1	B	177	VAL
1	B	215	GLN
1	B	289	LEU
1	B	297	LEU
1	B	321	LEU
1	B	391	LYS
1	B	423	LEU
1	B	438	GLN
1	B	488	LYS
1	B	516	VAL
1	B	525	GLN
1	B	530	ILE
1	B	533	LYS
1	B	535	LEU
1	B	542	HIS
1	B	560	GLN
1	B	564	VAL
1	B	600	LEU
1	B	605	LEU
1	B	610	LEU
1	B	611	PRO
1	B	662	VAL
1	B	671	GLU
1	B	689	LYS
1	B	706	VAL
1	B	727	LEU
1	B	739	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (38) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	2	GLN
1	A	57	ASN
1	A	85	GLN
1	A	88	GLN
1	A	97	ASN
1	A	112	ASN
1	A	244	GLN
1	A	260	ASN
1	A	271	GLN
1	A	288	HIS
1	A	400	HIS
1	A	446	ASN
1	A	498	GLN
1	A	525	GLN
1	A	531	GLN
1	A	544	ASN
1	A	560	GLN
1	A	678	HIS
1	A	725	GLN
1	B	2	GLN
1	B	9	GLN
1	B	57	ASN
1	B	97	ASN
1	B	112	ASN
1	B	139	ASN
1	B	162	HIS
1	B	178	GLN
1	B	244	GLN
1	B	260	ASN
1	B	271	GLN
1	B	326	GLN
1	B	459	GLN
1	B	498	GLN
1	B	504	GLN
1	B	525	GLN
1	B	531	GLN
1	B	544	ASN
1	B	678	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 ⓘ

8 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	GLC	C	1	2	12,12,12	0.48	0	17,17,17	1.41	2 (11%)
2	GLC	C	2	2	11,11,12	0.65	0	15,15,17	1.56	2 (13%)
2	GLC	C	3	2	11,11,12	1.32	2 (18%)	15,15,17	1.49	1 (6%)
2	GLC	C	4	2	11,11,12	1.20	2 (18%)	15,15,17	0.87	0
2	GLC	D	1	2	12,12,12	0.55	0	17,17,17	1.01	0
2	GLC	D	2	2	11,11,12	0.63	0	15,15,17	0.98	1 (6%)
2	GLC	D	3	2	11,11,12	0.76	0	15,15,17	1.39	1 (6%)
2	GLC	D	4	2	11,11,12	0.80	0	15,15,17	1.06	1 (6%)

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	GLC	C	1	2	-	0/2/22/22	0/1/1/1
2	GLC	C	2	2	-	0/2/19/22	0/1/1/1
2	GLC	C	3	2	-	0/2/19/22	0/1/1/1
2	GLC	C	4	2	-	2/2/19/22	0/1/1/1
2	GLC	D	1	2	-	0/2/22/22	0/1/1/1
2	GLC	D	2	2	-	0/2/19/22	0/1/1/1
2	GLC	D	3	2	-	0/2/19/22	0/1/1/1
2	GLC	D	4	2	-	2/2/19/22	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	3	GLC	O5-C1	-2.91	1.38	1.43
2	C	4	GLC	O5-C1	-2.67	1.39	1.43
2	C	4	GLC	C2-C3	2.12	1.55	1.52
2	C	3	GLC	O4-C4	-2.01	1.38	1.43

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	3	GLC	C1-O5-C5	4.63	118.39	112.19
2	C	1	GLC	O5-C1-C2	3.12	115.78	110.30
2	C	2	GLC	C1-O5-C5	3.10	116.34	112.19
2	C	2	GLC	C1-C2-C3	2.97	113.97	109.64
2	D	3	GLC	C1-O5-C5	2.94	116.12	112.19
2	C	1	GLC	O2-C2-C3	-2.55	104.36	110.38
2	D	2	GLC	C1-O5-C5	2.29	115.25	112.19
2	D	4	GLC	C1-O5-C5	2.05	114.94	112.19

There are no chirality outliers.

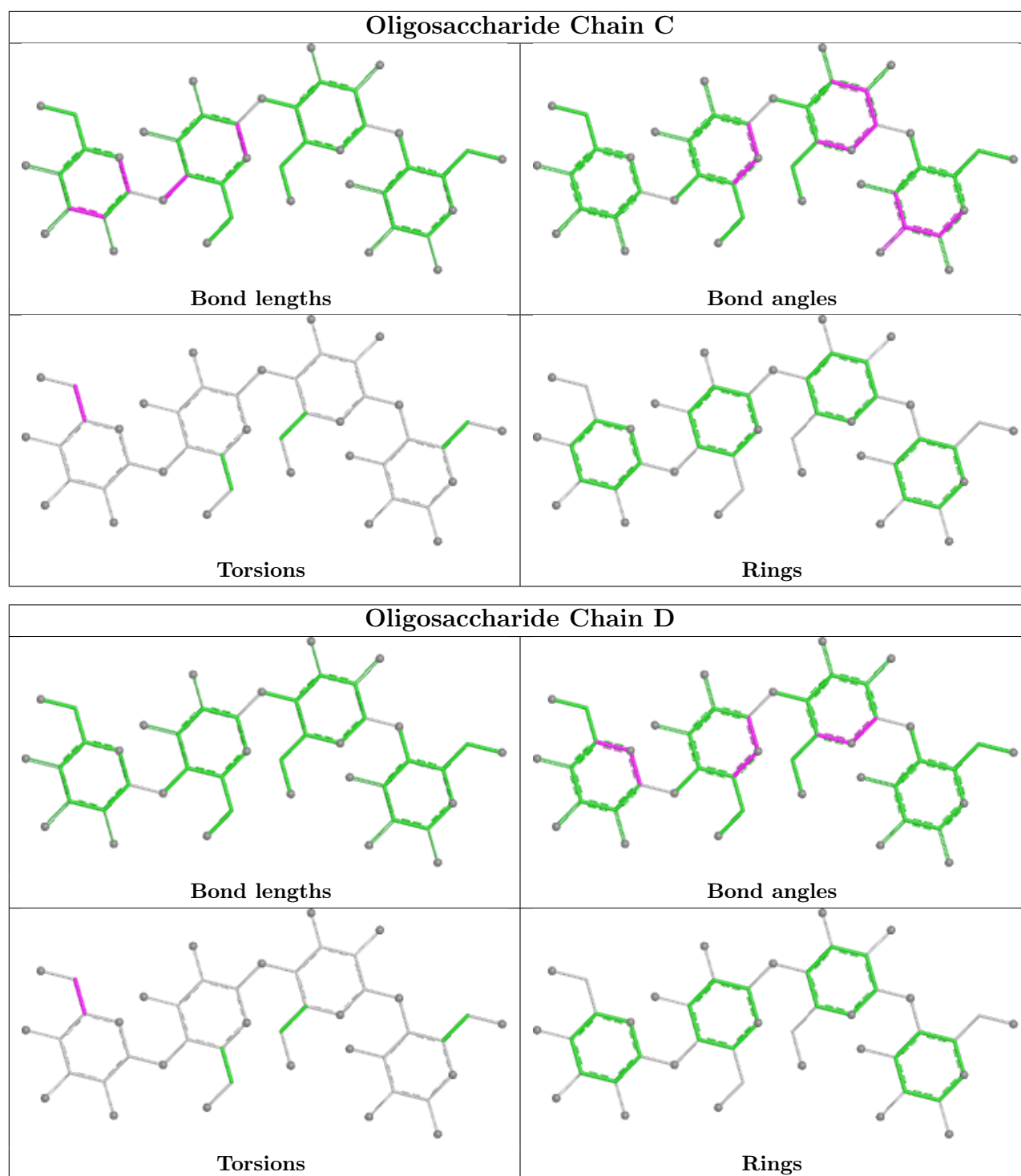
All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	4	GLC	C4-C5-C6-O6
2	D	4	GLC	C4-C5-C6-O6
2	C	4	GLC	O5-C5-C6-O6
2	D	4	GLC	O5-C5-C6-O6

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](#)

4 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	PO4	B	999	-	4,4,4	1.38	0	6,6,6	0.90	0
4	PLP	A	900	1	15,15,16	1.45	3 (20%)	21,22,23	1.38	3 (14%)
4	PLP	B	900	1	15,15,16	1.30	2 (13%)	21,22,23	1.30	2 (9%)
3	PO4	A	998	-	4,4,4	1.41	1 (25%)	6,6,6	0.72	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	PLP	A	900	1	-	1/6/6/8	0/1/1/1
4	PLP	B	900	1	-	0/6/6/8	0/1/1/1

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	900	PLP	C3-C2	-3.04	1.37	1.41
4	B	900	PLP	C3-C2	-2.59	1.38	1.41
4	A	900	PLP	C6-N1	2.52	1.39	1.34
4	A	900	PLP	C5-C4	-2.42	1.37	1.40
3	A	998	PO4	P-O3	-2.20	1.48	1.54
4	B	900	PLP	C2-N1	2.16	1.37	1.33

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	900	PLP	C4A-C4-C5	-3.47	117.36	120.94
4	B	900	PLP	C4A-C4-C5	-3.20	117.64	120.94
4	A	900	PLP	C3-C4-C5	2.57	121.67	118.59
4	A	900	PLP	C5-C6-N1	-2.42	119.89	123.83
4	B	900	PLP	O3P-P-O4P	2.01	111.92	106.67

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	900	PLP	C5A-O4P-P-O1P

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	900	PLP	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	796/796 (100%)	-0.33	18 (2%) 61 61	11, 20, 41, 84	0
1	B	796/796 (100%)	-0.31	20 (2%) 58 58	11, 20, 41, 83	0
All	All	1592/1592 (100%)	-0.32	38 (2%) 59 60	11, 20, 41, 84	0

All (38) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	386	TRP	5.3
1	B	562	ASP	4.5
1	B	382	VAL	4.3
1	B	187	LYS	4.1
1	A	386	TRP	4.0
1	B	188	ASP	3.7
1	B	385	THR	3.4
1	B	57	ASN	3.4
1	B	392	VAL	3.3
1	B	388	GLY	3.3
1	B	389	ASP	3.2
1	B	387	PRO	3.2
1	A	237	ASP	3.2
1	A	387	PRO	3.1
1	A	388	GLY	3.0
1	B	600	LEU	2.9
1	B	189	GLY	2.9
1	B	561	ALA	2.6
1	B	717	ASP	2.6
1	A	384	LYS	2.5
1	A	562	ASP	2.5
1	A	392	VAL	2.4
1	A	491	ASP	2.3
1	A	381	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	263	GLU	2.3
1	A	385	THR	2.3
1	B	384	LYS	2.3
1	A	3	PRO	2.2
1	A	382	VAL	2.2
1	B	390	GLU	2.2
1	B	190	ARG	2.2
1	A	688	ALA	2.2
1	A	391	LYS	2.1
1	A	390	GLU	2.1
1	B	186	THR	2.1
1	A	555	ILE	2.1
1	A	473	GLN	2.1
1	B	381	LEU	2.1

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

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

6.3 Carbohydrates [i](#)

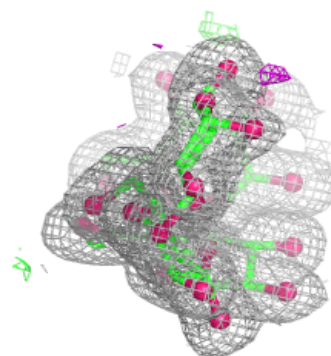
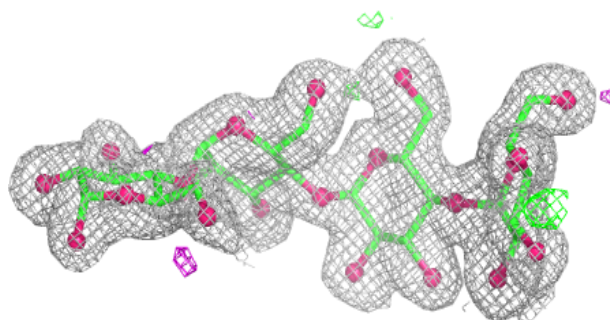
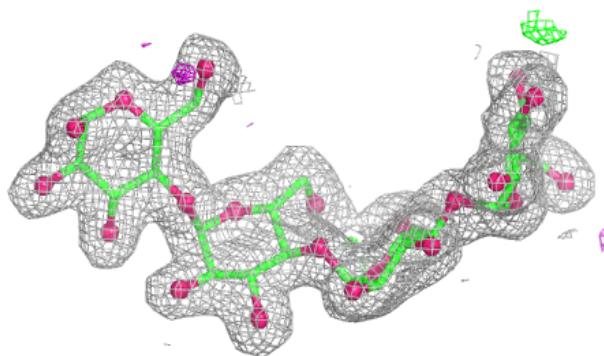
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	GLC	D	1	12/12	0.93	0.06	21,23,29,35	0
2	GLC	C	1	12/12	0.95	0.06	21,23,28,35	0
2	GLC	C	2	11/12	0.96	0.05	15,19,21,21	0
2	GLC	D	3	11/12	0.96	0.05	16,18,19,19	0
2	GLC	D	2	11/12	0.97	0.05	15,19,21,22	0
2	GLC	C	4	11/12	0.97	0.05	16,17,19,19	0
2	GLC	C	3	11/12	0.98	0.04	16,18,19,19	0
2	GLC	D	4	11/12	0.98	0.03	15,18,19,19	0

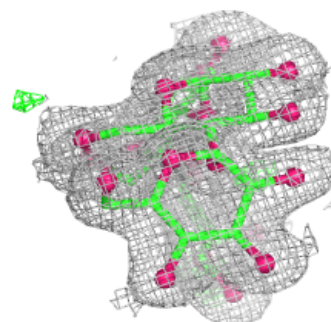
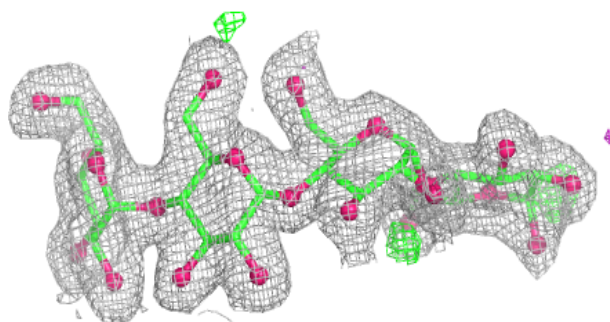
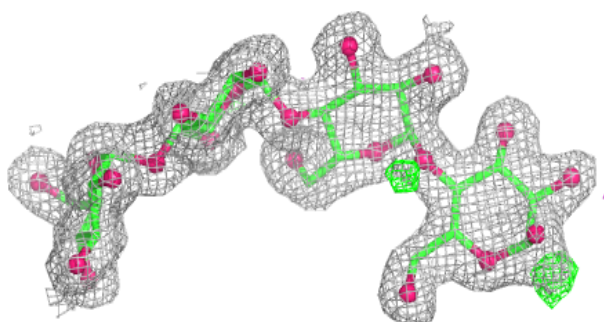
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

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	PLP	A	900	15/16	0.97	0.05	14,17,25,26	0
4	PLP	B	900	15/16	0.98	0.04	14,17,25,25	0
3	PO4	A	998	5/5	0.99	0.05	17,17,21,22	0
3	PO4	B	999	5/5	0.99	0.05	17,19,22,22	0

6.5 Other polymers [i](#)

There are no such residues in this entry.