Full wwPDB X-ray Structure Validation Report (i)

Aug 6, 2023 – 06:07 PM EDT

PDB ID	:	1L5W
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 (i) 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 (i)) were used in the production of this report:

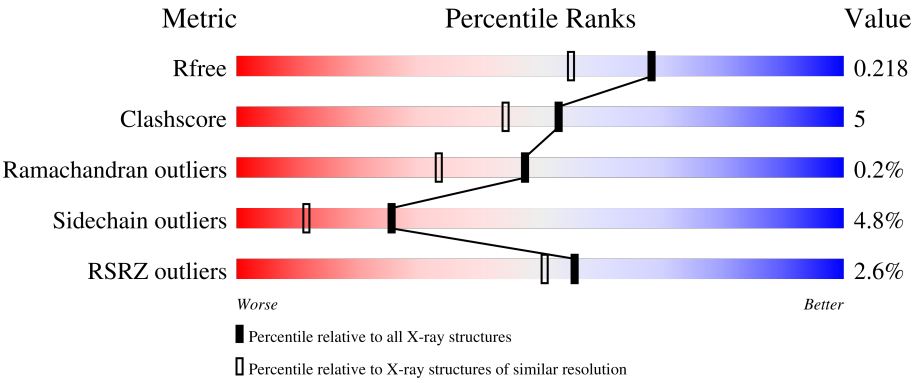
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

1 Overall quality at a glance (i)

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}	130704	5950 (1.80-1.80)
Clashscore	141614	6793 (1.80-1.80)
Ramachandran outliers	138981	6697 (1.80-1.80)
Sidechain outliers	138945	6696 (1.80-1.80)
RSRZ outliers	127900	5850 (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 <=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% 84% 14%
1	B	796	3% 84% 14%
2	C	4	100%
2	D	4	100%

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			

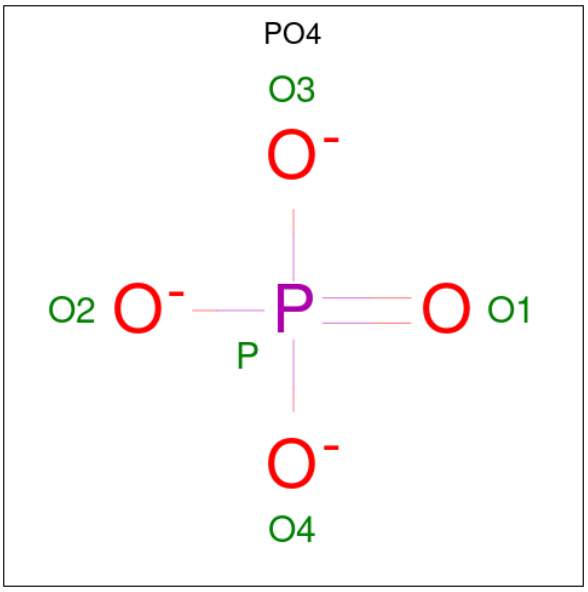
There are 6 discrepancies between the modelled and reference sequences:

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.

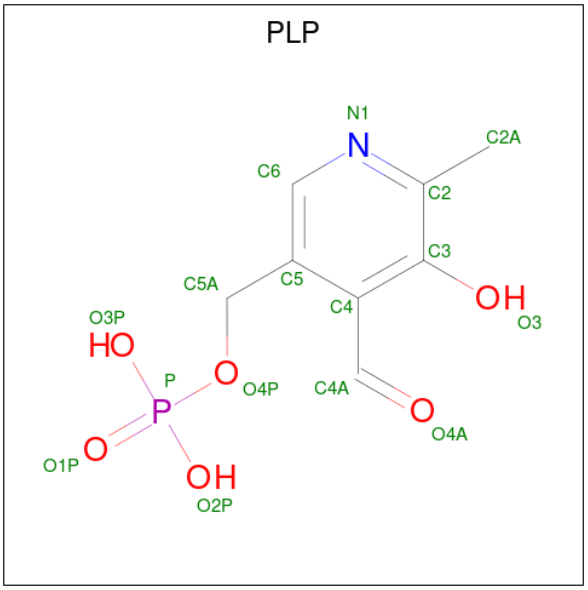
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	C	4	Total	C	O		0	0	0
			45	24	21				
2	D	4	Total	C	O		0	0	0
			45	24	21				

- Molecule 3 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).



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

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



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

- Molecule 5 is water.

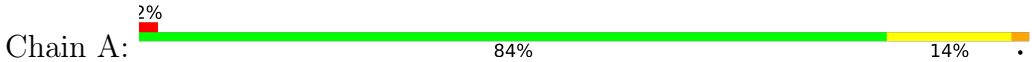
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	565	Total O 565 565	0	0
5	B	520	Total O 520 520	0	0

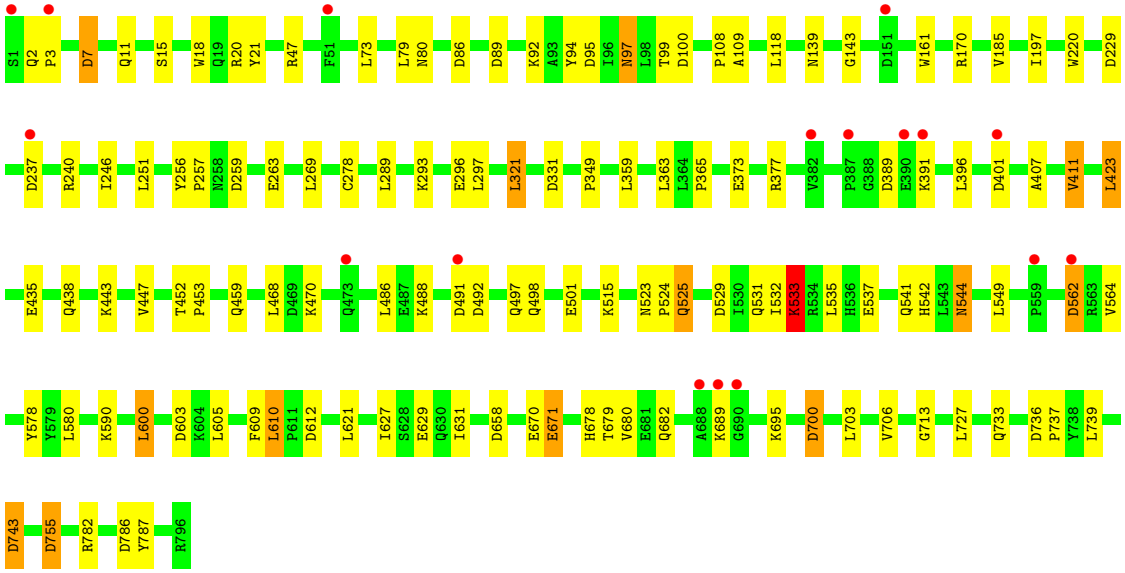
3 Residue-property plots (i)

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: MALTODEXTRIN PHOSPHORYLASE

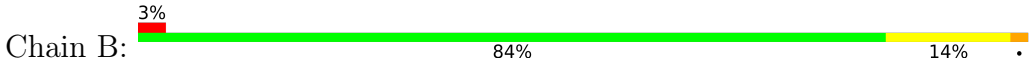
Chain A:

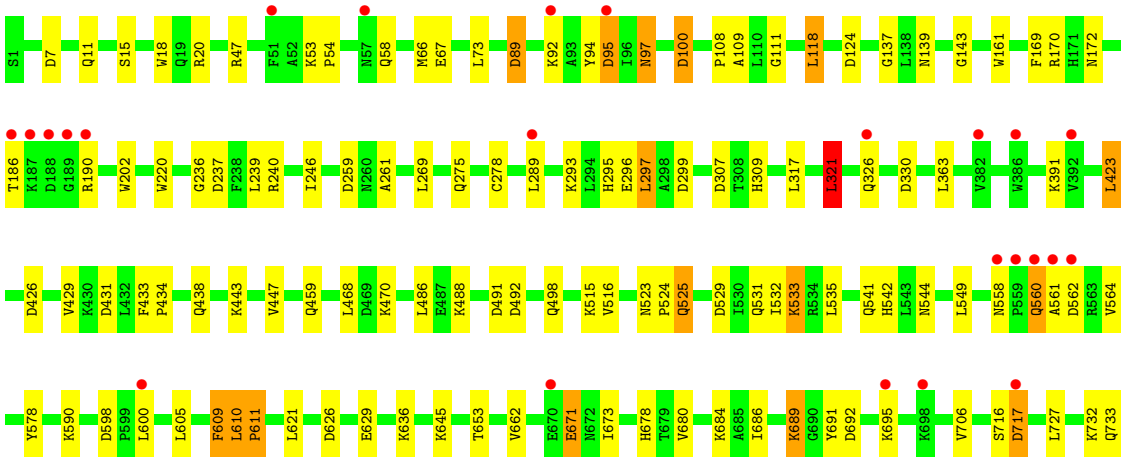




• Molecule 1: MALTODEXTRIN PHOSPHORYLASE

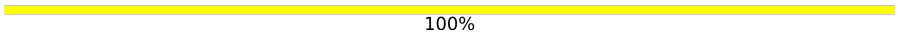
Chain B:





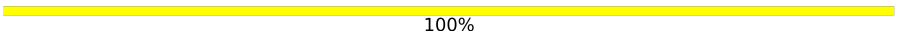
• Molecule 2: alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose

Chain C:



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

Chain D:



4 Data and refinement statistics (i)

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 16.68 – 1.80	Depositor EDS
% Data completeness (in resolution range)	85.0 (20.00-1.80) 85.1 (16.68-1.80)	Depositor EDS
R_{merge}	0.18	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [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)	0.38 , 46.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.44$, $< L^2 > = 0.26$	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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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	0.84	0/6540	0.95	19/8865 (0.2%)
1	B	0.82	0/6540	0.94	17/8865 (0.2%)
All	All	0.83	0/13080	0.95	36/17730 (0.2%)

There are no bond length outliers.

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	492	ASP	CB-CG-OD2	8.22	125.70	118.30
1	A	562	ASP	CB-CG-OD2	7.54	125.09	118.30
1	B	95	ASP	CB-CG-OD2	7.29	124.87	118.30
1	B	307	ASP	CB-CG-OD2	6.83	124.45	118.30
1	A	401	ASP	CB-CG-OD2	6.83	124.44	118.30
1	B	492	ASP	CB-CG-OD2	6.74	124.36	118.30
1	B	717	ASP	CB-CG-OD2	6.59	124.23	118.30
1	A	603	ASP	CB-CG-OD2	6.49	124.14	118.30
1	A	755	ASP	CB-CG-OD2	6.30	123.97	118.30
1	A	700	ASP	CB-CG-OD2	6.27	123.94	118.30
1	A	229	ASP	CB-CG-OD1	6.13	123.81	118.30
1	B	259	ASP	CB-CG-OD2	6.10	123.79	118.30
1	A	86	ASP	CB-CG-OD2	6.02	123.72	118.30
1	B	89	ASP	CB-CG-OD2	5.97	123.67	118.30
1	B	598	ASP	CB-CG-OD2	5.85	123.56	118.30
1	A	786	ASP	CB-CG-OD2	5.81	123.53	118.30
1	A	389	ASP	CB-CG-OD2	5.78	123.50	118.30
1	B	100	ASP	CB-CG-OD2	5.76	123.49	118.30
1	A	782	ARG	NE-CZ-NH2	-5.69	117.45	120.30
1	A	612	ASP	CB-CG-OD2	5.52	123.27	118.30
1	A	331	ASP	CB-CG-OD2	5.52	123.27	118.30
1	A	321	LEU	CB-CG-CD2	5.44	120.24	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	491	ASP	CB-CG-OD2	5.39	123.15	118.30
1	A	259	ASP	CB-CG-OD2	5.37	123.13	118.30
1	B	321	LEU	CB-CG-CD1	5.34	120.08	111.00
1	B	299	ASP	CB-CG-OD2	5.34	123.11	118.30
1	B	431	ASP	CB-CG-OD2	5.33	123.09	118.30
1	B	426	ASP	CB-CG-OD2	5.31	123.08	118.30
1	B	626	ASP	CB-CG-OD2	5.31	123.08	118.30
1	B	297	LEU	CB-CG-CD2	5.23	119.89	111.00
1	B	692	ASP	CB-CG-OD2	5.18	122.96	118.30
1	B	124	ASP	CB-CG-OD2	5.17	122.96	118.30
1	A	743	ASP	CB-CG-OD2	5.16	122.94	118.30
1	A	658	ASP	CB-CG-OD2	5.15	122.94	118.30
1	B	330	ASP	CB-CG-OD2	5.12	122.91	118.30
1	A	7	ASP	CB-CG-OD2	5.07	122.86	118.30

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	6390	0	6333	68	0
1	B	6390	0	6333	76	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	9	0
5	B	520	0	0	11	0
All	All	13995	0	12756	138	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 5.

All (138) 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:B:47:ARG:HD3	5:B:1062:HOH:O	1.89	0.73
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
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:671:GLU:H	1:A:671:GLU:CD	1.96	0.69
1:B:237:ASP:OD2	1:B:240:ARG:NH1	2.25	0.68
1:A:733:GLN:H	1:A:733:GLN:CD	1.97	0.67
1:A:269:LEU:HD23	1:A:363:LEU:HD12	1.75	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:671:GLU:H	1:B:671:GLU:CD	2.01	0.63
1:B:468:LEU:CD2	1:B:486:LEU:HD11	2.28	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:B:733:GLN:H	1:B:733:GLN:CD	2.04	0.58
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:20:ARG:O	1:B:170:ARG:HB2	2.09	0.53
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:97:ASN:HD22	1:A:97:ASN:C	2.15	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:A:544:ASN:C	1:A:544:ASN:HD22	2.16	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: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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:293:LYS:O	1:A:296:GLU:HG2	2.17	0.45
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: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:A:447:VAL:HG11	1:A:787:TYR:CD2	2.52	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: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:A:97:ASN:ND2	1:A:97:ASN:C	2.72	0.42
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:256:TYR:N	1:A:257:PRO:CD	2.82	0.42
1:B:58:GLN:C	5:B:1313:HOH:O	2.58	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
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:A:452:THR:HA	1:A:453:PRO:HD3	1.96	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:671:GLU:CD	1:B:671:GLU:N	2.72	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: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:B:636:LYS:NZ	5:B:1468:HOH:O	2.50	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%)	41	27
1	B	794/796 (100%)	770 (97%)	23 (3%)	1 (0%)	51	36
All	All	1588/1592 (100%)	1540 (97%)	45 (3%)	3 (0%)	47	33

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%)	635 (95%)	32 (5%)	25	11
1	B	667/667 (100%)	635 (95%)	32 (5%)	25	11
All	All	1334/1334 (100%)	1270 (95%)	64 (5%)	25	11

All (64) 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	139	ASN
1	A	289	LEU
1	A	297	LEU
1	A	321	LEU
1	A	349	PRO
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	515	LYS
1	A	525	GLN
1	A	533	LYS
1	A	535	LEU
1	A	542	HIS
1	A	544	ASN
1	A	564	VAL
1	A	578	TYR
1	A	600	LEU
1	A	605	LEU
1	A	609	PHE
1	A	610	LEU
1	A	671	GLU

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Mol	Chain	Res	Type
1	A	689	LYS
1	A	695	LYS
1	A	727	LEU
1	A	739	LEU
1	A	755	ASP
1	B	73	LEU
1	B	97	ASN
1	B	118	LEU
1	B	139	ASN
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	443	LYS
1	B	488	LYS
1	B	515	LYS
1	B	516	VAL
1	B	525	GLN
1	B	535	LEU
1	B	542	HIS
1	B	544	ASN
1	B	560	GLN
1	B	564	VAL
1	B	578	TYR
1	B	600	LEU
1	B	605	LEU
1	B	609	PHE
1	B	610	LEU
1	B	611	PRO
1	B	662	VAL
1	B	671	GLU
1	B	689	LYS
1	B	695	LYS
1	B	727	LEU
1	B	732	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (30) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	2	GLN

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Mol	Chain	Res	Type
1	A	9	GLN
1	A	57	ASN
1	A	97	ASN
1	A	112	ASN
1	A	139	ASN
1	A	260	ASN
1	A	446	ASN
1	A	459	GLN
1	A	498	GLN
1	A	525	GLN
1	A	531	GLN
1	A	544	ASN
1	A	678	HIS
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	260	ASN
1	B	446	ASN
1	B	459	GLN
1	B	498	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	0.50	0	17,17,17	1.42	3 (17%)
2	GLC	C	2	2	11,11,12	0.68	0	15,15,17	1.73	3 (20%)
2	GLC	C	3	2	11,11,12	1.38	2 (18%)	15,15,17	1.58	1 (6%)
2	GLC	C	4	2	11,11,12	1.24	2 (18%)	15,15,17	0.92	0
2	GLC	D	1	2	12,12,12	0.55	0	17,17,17	1.02	1 (5%)
2	GLC	D	2	2	11,11,12	0.64	0	15,15,17	1.03	1 (6%)
2	GLC	D	3	2	11,11,12	0.79	0	15,15,17	1.44	1 (6%)
2	GLC	D	4	2	11,11,12	0.84	0	15,15,17	1.14	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	-3.08	1.38	1.43
2	C	4	GLC	O5-C1	-2.82	1.39	1.43
2	C	4	GLC	C2-C3	2.19	1.55	1.52
2	C	3	GLC	O4-C4	-2.13	1.38	1.43

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	3	GLC	C1-O5-C5	4.58	118.39	112.19
2	C	2	GLC	C1-C2-C3	3.50	113.97	109.67
2	C	1	GLC	O5-C1-C2	3.08	115.78	110.28
2	C	2	GLC	C1-O5-C5	3.06	116.34	112.19
2	D	3	GLC	C1-O5-C5	2.90	116.12	112.19
2	C	1	GLC	O2-C2-C3	-2.59	104.36	110.35
2	D	2	GLC	C1-O5-C5	2.26	115.25	112.19
2	C	2	GLC	O5-C1-C2	-2.23	107.33	110.77
2	C	1	GLC	C6-C5-C4	-2.06	108.17	113.00
2	D	4	GLC	C1-O5-C5	2.03	114.94	112.19
2	D	1	GLC	O3-C3-C2	-2.01	105.71	110.35

There are no chirality outliers.

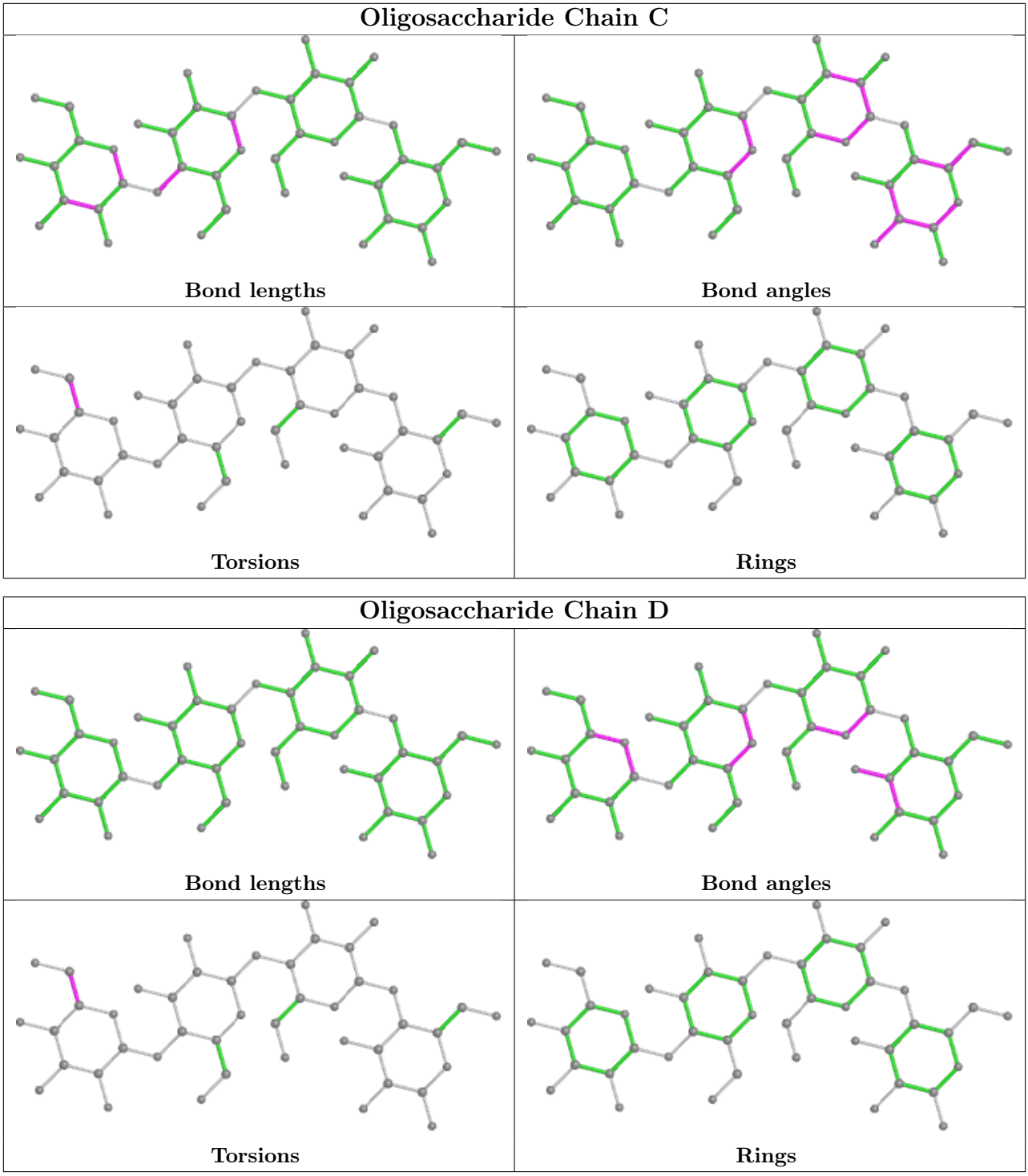
All (4) torsion outliers are listed below:

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	$\#\|Z\| > 2$
4	PLP	A	900	1	15,15,16	1.44	3 (20%)	20,22,23	1.39	3 (15%)
3	PO4	A	998	-	4,4,4	1.35	1 (25%)	6,6,6	0.69	0
3	PO4	B	999	-	4,4,4	1.31	0	6,6,6	0.87	0
4	PLP	B	900	1	15,15,16	1.27	2 (13%)	20,22,23	1.26	1 (5%)

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	-3.09	1.37	1.40
4	B	900	PLP	C3-C2	-2.62	1.38	1.40
4	A	900	PLP	C6-N1	2.43	1.39	1.34
4	A	900	PLP	C5-C4	-2.43	1.37	1.40
3	A	998	PO4	P-O3	-2.12	1.48	1.54
4	B	900	PLP	C2-N1	2.04	1.37	1.33

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
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	2.71	121.67	118.74
4	A	900	PLP	C5-C6-N1	-2.36	119.89	123.82

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, 95^{th} 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%)	-0.08	17 (2%)	63	59	11, 20, 41, 84	0
1	B	796/796 (100%)	-0.06	24 (3%)	50	44	11, 20, 41, 83	0
All	All	1592/1592 (100%)	-0.07	41 (2%)	56	51	11, 20, 41, 84	0

All (41) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	562	ASP	6.8
1	A	51	PHE	6.1
1	B	187	LYS	5.9
1	B	559	PRO	5.7
1	B	560	GLN	5.3
1	B	57	ASN	5.3
1	B	188	ASP	5.1
1	B	382	VAL	4.7
1	B	189	GLY	4.6
1	B	561	ALA	4.2
1	B	190	ARG	3.9
1	B	186	THR	3.9
1	B	717	ASP	3.6
1	B	386	TRP	3.5
1	A	237	ASP	3.3
1	A	391	LYS	3.2
1	B	95	ASP	3.0
1	A	689	LYS	3.0
1	A	1	SER	3.0
1	A	151	ASP	2.9
1	B	392	VAL	2.9
1	B	92	LYS	2.9
1	B	51	PHE	2.7
1	A	491	ASP	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	562	ASP	2.6
1	B	558	ASN	2.6
1	B	600	LEU	2.6
1	A	387	PRO	2.6
1	A	390	GLU	2.5
1	A	473	GLN	2.4
1	B	289	LEU	2.4
1	A	3	PRO	2.4
1	B	670	GLU	2.4
1	B	695	LYS	2.3
1	B	698	LYS	2.3
1	A	401	ASP	2.3
1	B	326	GLN	2.2
1	A	690	GLY	2.1
1	A	559	PRO	2.1
1	A	382	VAL	2.1
1	A	688	ALA	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)

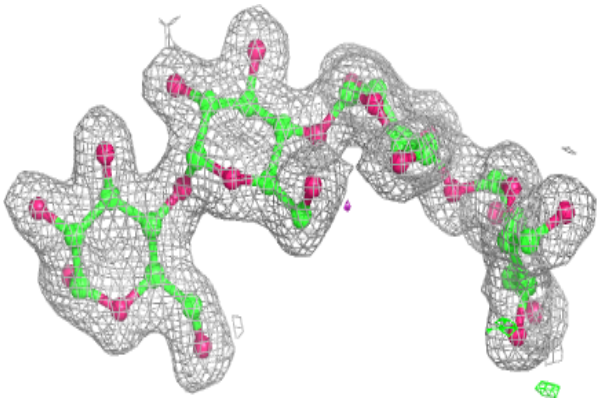
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

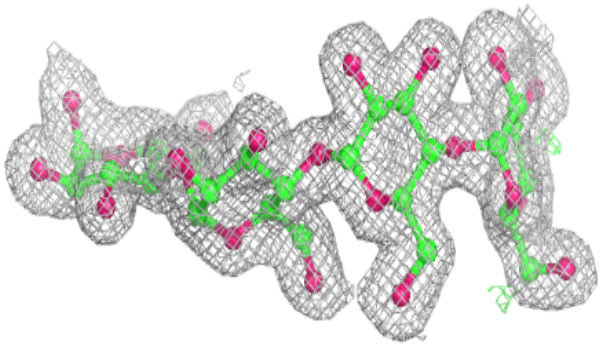
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	GLC	D	1	12/12	0.94	0.16	21,23,29,35	0
2	GLC	C	2	11/12	0.95	0.08	15,19,21,21	0
2	GLC	C	1	12/12	0.95	0.13	21,23,28,35	0
2	GLC	D	2	11/12	0.95	0.09	15,19,21,22	0
2	GLC	C	3	11/12	0.97	0.09	16,18,19,19	0
2	GLC	C	4	11/12	0.97	0.08	16,17,19,19	0
2	GLC	D	3	11/12	0.97	0.07	16,18,19,19	0
2	GLC	D	4	11/12	0.97	0.07	15,18,19,19	0

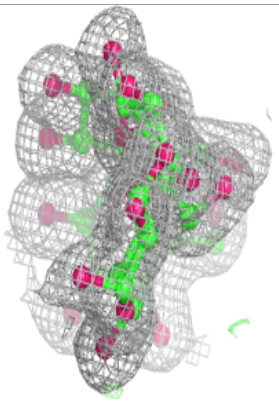
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

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)

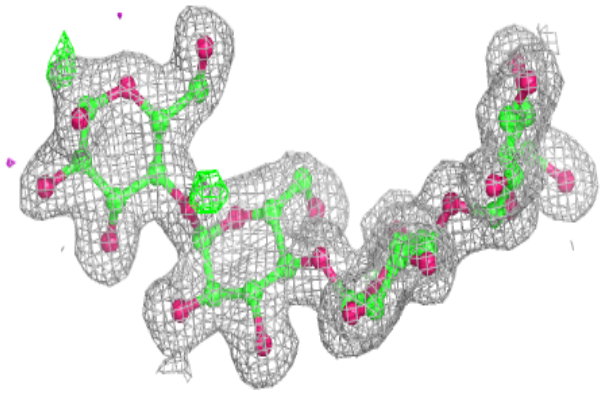


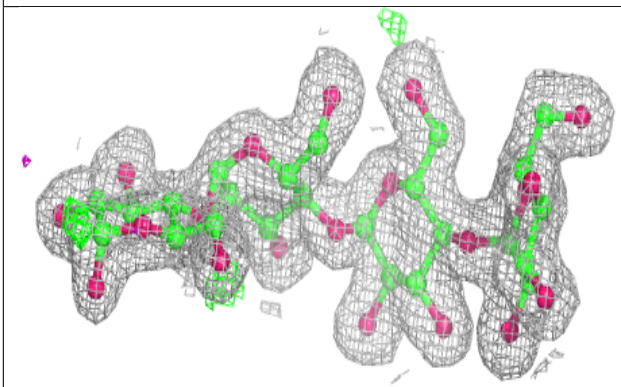


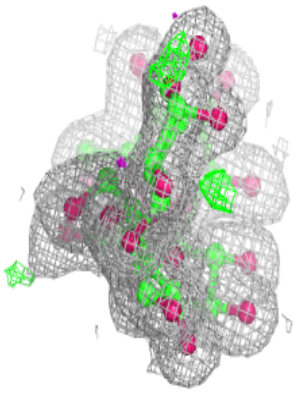


Electron density around Chain D:

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







6.4 Ligands

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^{th} 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	0.95	0.09	14,17,25,26	0
4	PLP	B	900	15/16	0.97	0.08	14,17,25,25	0
3	PO4	B	999	5/5	0.98	0.06	17,19,22,22	0
3	PO4	A	998	5/5	0.99	0.05	17,17,21,22	0

6.5 Other polymers

There are no such residues in this entry.