



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 7, 2020 – 12:43 AM BST

PDB ID : 2AW3  
Title : X-Ray studies on maltodextrin phosphorylase complexes: recognition of substrates and catalytic mechanism of phosphorylase family  
Authors : Geremia, S.; Campagnolo, M.  
Deposited on : 2005-08-31  
Resolution : 2.20 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](mailto: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 following versions of software and data (see [references ⓘ](#)) 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 : 2.13.1  
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) : 2.13.1

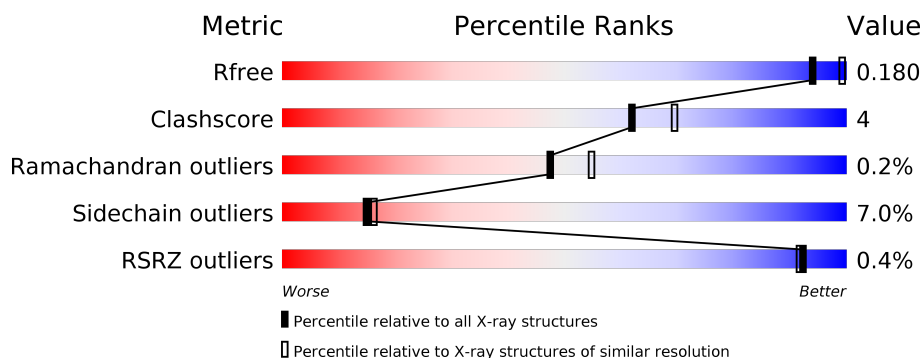
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.20 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	4898 (2.20-2.20)
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)
RSRZ outliers	127900	4800 (2.20-2.20)

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 on 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	796	
1	B	796	
2	C	5	
2	D	5	

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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	SO4	A	1999	-	-	X	-

## 2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 14092 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
			6389	4079	1128	1162	20			
1	B	796	Total	C	N	O	S	0	0	0
			6389	4079	1128	1162	20			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	261	ALA	HIS	SEE REMARK 999	UNP P00490
A	262	PHE	THR	SEE REMARK 999	UNP P00490
A	263	GLU	ALA	SEE REMARK 999	UNP P00490
B	261	ALA	HIS	SEE REMARK 999	UNP P00490
B	262	PHE	THR	SEE REMARK 999	UNP P00490
B	263	GLU	ALA	SEE REMARK 999	UNP P00490

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



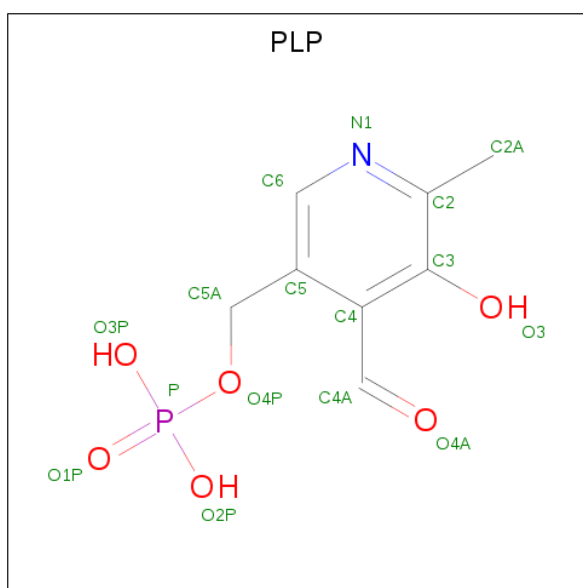
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
2	C	5	Total	C	O	0	0	0
			56	30	26			
2	D	5	Total	C	O	0	0	0
			56	30	26			

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



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

- 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	0	0
			15	8	1	5	1		
4	B	1	Total	C	N	O	P	0	0
			15	8	1	5	1		

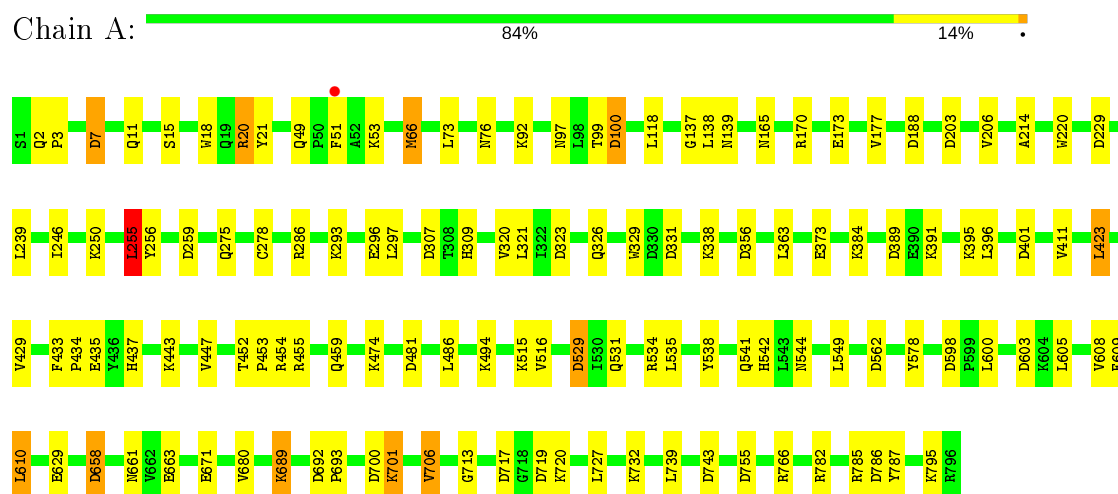
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	592	Total 592	O 592	0	0
5	B	570	Total 570	O 570	0	0

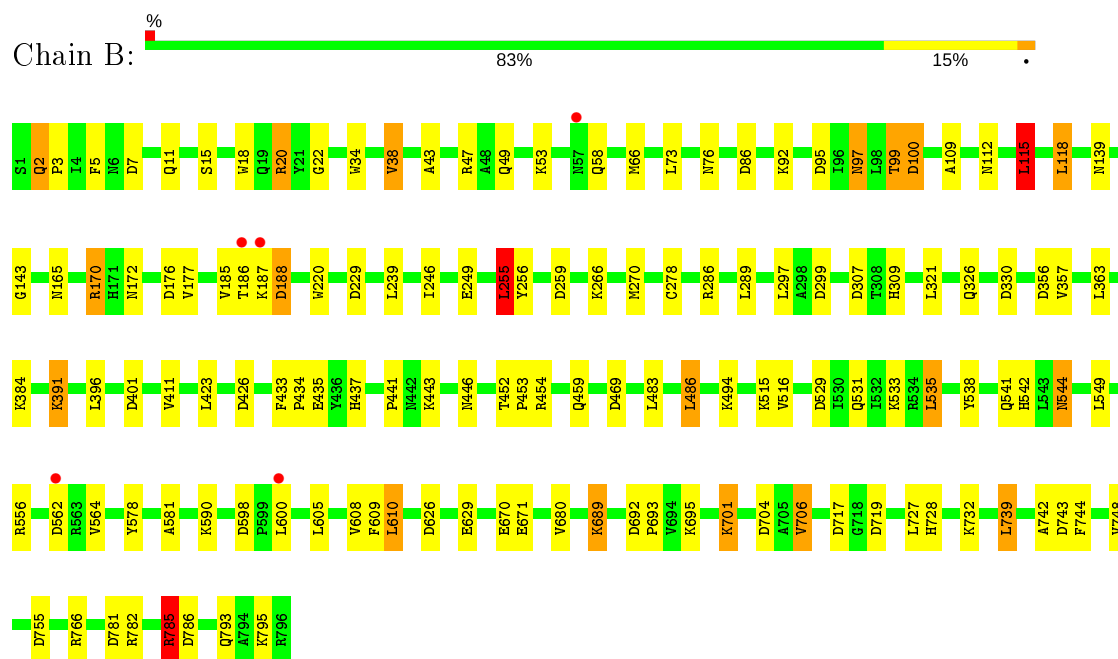
### 3 Residue-property plots

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-(1-4)-beta-D-glucopyranose

Chain C:  80% 20%

BGC1
GLC2
GLC3
GLC4
GLC5

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

Chain D:  60% 40%

BGC1
GLC2
GLC3
GLC4
GLC5



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	75.30Å 105.89Å 219.52Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	15.00 – 2.20 109.76 – 2.20	Depositor EDS
% Data completeness (in resolution range)	98.0 (15.00-2.20) 98.0 (109.76-2.20)	Depositor EDS
$R_{merge}$	0.25	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.07 (at 2.20Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, $R_{free}$	0.175 , 0.236 0.186 , 0.180	Depositor DCC
$R_{free}$ test set	4426 reflections (4.92%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	26.9	Xtriage
Anisotropy	0.038	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 48.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	14092	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.14% 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: GLC, BGC, SO4, PLP

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	1.03	2/6539 (0.0%)	0.99	27/8865 (0.3%)
1	B	1.04	2/6539 (0.0%)	1.00	29/8865 (0.3%)
All	All	1.03	4/13078 (0.0%)	0.99	56/17730 (0.3%)

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	B	0	3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	173	GLU	CD-OE2	8.13	1.34	1.25
1	B	38	VAL	CB-CG2	-5.70	1.40	1.52
1	B	357	VAL	CB-CG2	-5.42	1.41	1.52
1	A	320	VAL	CB-CG2	-5.36	1.41	1.52

All (56) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	743	ASP	CB-CG-OD2	8.94	126.35	118.30
1	B	598	ASP	CB-CG-OD2	8.47	125.92	118.30
1	A	229	ASP	CB-CG-OD2	8.21	125.69	118.30
1	B	782	ARG	NE-CZ-NH2	-8.00	116.30	120.30
1	B	259	ASP	CB-CG-OD2	7.89	125.40	118.30
1	B	401	ASP	CB-CG-OD2	7.66	125.20	118.30
1	A	100	ASP	CB-CG-OD2	7.65	125.19	118.30

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	562	ASP	CB-CG-OD2	7.44	124.99	118.30
1	B	95	ASP	CB-CG-OD2	7.36	124.92	118.30
1	A	786	ASP	CB-CG-OD2	7.32	124.89	118.30
1	B	719	ASP	CB-CG-OD2	7.23	124.81	118.30
1	A	356	ASP	CB-CG-OD2	7.11	124.69	118.30
1	B	786	ASP	CB-CG-OD2	7.11	124.70	118.30
1	A	603	ASP	CB-CG-OD2	7.10	124.69	118.30
1	A	401	ASP	CB-CG-OD2	6.95	124.56	118.30
1	A	782	ARG	NE-CZ-NH2	-6.93	116.83	120.30
1	A	743	ASP	CB-CG-OD2	6.59	124.23	118.30
1	A	658	ASP	CB-CG-OD2	6.55	124.20	118.30
1	B	330	ASP	CB-CG-OD2	6.52	124.17	118.30
1	B	781	ASP	CB-CG-OD1	6.50	124.15	118.30
1	A	7	ASP	CB-CG-OD2	6.43	124.09	118.30
1	B	426	ASP	CB-CG-OD2	6.42	124.08	118.30
1	B	299	ASP	CB-CG-OD2	6.18	123.86	118.30
1	A	203	ASP	CB-CG-OD1	6.13	123.82	118.30
1	B	626	ASP	CB-CG-OD2	6.05	123.74	118.30
1	A	259	ASP	CB-CG-OD2	6.04	123.73	118.30
1	B	229	ASP	CB-CG-OD2	6.04	123.73	118.30
1	A	782	ARG	NE-CZ-NH1	6.00	123.30	120.30
1	B	356	ASP	CB-CG-OD1	5.99	123.69	118.30
1	B	176	ASP	CB-CG-OD1	5.98	123.68	118.30
1	A	719	ASP	CB-CG-OD2	5.96	123.66	118.30
1	B	170	ARG	NE-CZ-NH1	5.92	123.26	120.30
1	B	115	LEU	CB-CG-CD1	-5.86	101.04	111.00
1	A	389	ASP	CB-CG-OD2	5.85	123.57	118.30
1	B	100	ASP	CB-CG-OD2	5.79	123.51	118.30
1	A	717	ASP	CB-CG-OD1	5.70	123.43	118.30
1	A	598	ASP	CB-CG-OD2	5.67	123.40	118.30
1	B	704	ASP	CB-CG-OD2	5.57	123.31	118.30
1	B	562	ASP	CB-CG-OD2	5.56	123.30	118.30
1	B	469	ASP	CB-CG-OD2	5.47	123.22	118.30
1	B	717	ASP	CB-CG-OD1	5.44	123.19	118.30
1	B	286	ARG	NE-CZ-NH2	-5.33	117.64	120.30
1	A	481	ASP	CB-CG-OD2	5.32	123.09	118.30
1	A	331	ASP	CB-CG-OD2	5.30	123.07	118.30
1	A	255	LEU	CB-CG-CD2	5.30	120.00	111.00
1	B	286	ARG	NE-CZ-NH1	5.28	122.94	120.30
1	A	323	ASP	CB-CG-OD1	5.15	122.94	118.30
1	B	229	ASP	OD1-CG-OD2	-5.14	113.54	123.30
1	B	255	LEU	CB-CG-CD2	5.14	119.73	111.00

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	700	ASP	CB-CG-OD2	5.10	122.89	118.30
1	A	455	ARG	NE-CZ-NH2	-5.10	117.75	120.30
1	B	185	VAL	CB-CA-C	-5.08	101.74	111.40
1	A	286	ARG	NE-CZ-NH1	5.08	122.84	120.30
1	A	529	ASP	CB-CG-OD2	5.05	122.85	118.30
1	B	785	ARG	NE-CZ-NH2	-5.05	117.77	120.30
1	A	188	ASP	CB-CG-OD2	5.00	122.80	118.30

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	186	THR	Peptide
1	B	188	ASP	Peptide
1	B	446	ASN	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	6389	0	6333	54	0
1	B	6389	0	6333	64	0
2	C	56	0	48	1	0
2	D	56	0	48	4	0
3	A	5	0	0	2	0
3	B	5	0	0	1	0
4	A	15	0	6	0	0
4	B	15	0	6	0	0
5	A	592	0	0	11	0
5	B	570	0	0	11	0
All	All	14092	0	12774	112	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 4.

All (112) 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)
3:A:1999:SO4:O4	2:C:4:GLC:H61	1.86	0.75
1:A:474:LYS:HE2	5:A:2470:HOH:O	1.87	0.73
1:B:97:ASN:HD22	1:B:100:ASP:H	1.38	0.72
1:B:97:ASN:HD21	1:B:99:THR:HB	1.58	0.68
1:A:395:LYS:NZ	5:A:2445:HOH:O	2.23	0.65
1:A:97:ASN:HD22	1:A:100:ASP:H	1.43	0.64
1:B:670:GLU:HB3	5:B:3447:HOH:O	1.98	0.64
1:A:671:GLU:H	1:A:671:GLU:CD	2.06	0.58
1:A:396:LEU:HD21	1:A:435:GLU:HB2	1.84	0.58
1:A:97:ASN:HD21	1:A:99:THR:HB	1.67	0.58
1:A:51:PHE:HA	5:A:2418:HOH:O	2.04	0.58
1:B:396:LEU:HD21	1:B:435:GLU:HB2	1.85	0.57
1:B:610:LEU:HD23	1:B:610:LEU:N	2.20	0.57
1:B:608:VAL:HG12	1:B:610:LEU:HD23	1.87	0.57
1:A:720:LYS:HD2	5:A:2428:HOH:O	2.05	0.56
1:B:459:GLN:NE2	5:B:3266:HOH:O	2.37	0.56
1:B:255:LEU:HD22	1:B:256:TYR:CG	2.41	0.55
1:B:97:ASN:ND2	1:B:99:THR:HB	2.22	0.54
1:B:7:ASP:O	1:B:11:GLN:HG2	2.07	0.54
1:A:7:ASP:O	1:A:11:GLN:HG2	2.08	0.54
1:A:474:LYS:CE	5:A:2470:HOH:O	2.52	0.54
1:A:529:ASP:OD1	1:A:629:GLU:OE2	2.26	0.53
1:B:109:ALA:HB1	1:B:143:GLY:HA3	1.89	0.53
1:B:165:ASN:HB2	5:B:3027:HOH:O	2.07	0.53
1:B:249:GLU:HG2	5:B:3323:HOH:O	2.09	0.53
1:A:20:ARG:O	1:B:170:ARG:HB2	2.09	0.53
1:B:220:TRP:CE2	1:B:278:CYS:HB3	2.45	0.52
1:A:255:LEU:HD22	1:A:256:TYR:CG	2.45	0.52
1:A:549:LEU:HB3	1:A:706:VAL:HG22	1.92	0.51
1:A:447:VAL:HG11	1:A:787:TYR:CD2	2.45	0.51
1:A:608:VAL:HG12	1:A:610:LEU:HD23	1.93	0.51
1:A:610:LEU:N	1:A:610:LEU:HD23	2.26	0.51
1:B:608:VAL:HG12	1:B:610:LEU:CD2	2.40	0.50
1:A:713:GLY:HA2	5:A:2180:HOH:O	2.11	0.50
1:B:544:ASN:HD22	1:B:544:ASN:C	2.15	0.49
1:B:118:LEU:HA	5:B:3046:HOH:O	2.13	0.49
1:A:76:ASN:HB2	1:A:459:GLN:HE22	1.76	0.49
1:B:66:MET:HG3	1:B:309:HIS:CB	2.43	0.49
1:B:671:GLU:H	1:B:671:GLU:CD	2.16	0.49
1:B:744:PHE:O	1:B:748:VAL:HG23	2.12	0.49
1:B:115:LEU:HB2	2:D:4:GLC:H4	1.95	0.49
1:B:115:LEU:HD13	2:D:4:GLC:H2	1.93	0.49

Continued on next page...

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:58:GLN:C	5:B:3325:HOH:O	2.51	0.48
1:A:220:TRP:CE2	1:A:278:CYS:HB3	2.48	0.48
1:B:220:TRP:CD2	1:B:278:CYS:HB3	2.48	0.48
1:B:66:MET:HG3	1:B:309:HIS:HB3	1.94	0.48
1:B:34:TRP:O	1:B:38:VAL:HG13	2.14	0.48
1:A:239:LEU:HD11	1:B:239:LEU:CD1	2.44	0.48
1:A:293:LYS:O	1:A:296:GLU:HG2	2.14	0.47
1:A:689:LYS:O	1:A:689:LYS:HG2	2.15	0.47
1:A:329:TRP:CH2	1:A:373:GLU:HG2	2.48	0.47
1:B:165:ASN:CB	5:B:3027:HOH:O	2.62	0.47
3:B:2999:SO4:O4	2:D:4:GLC:H61	2.14	0.47
1:B:433:PHE:N	1:B:434:PRO:CD	2.78	0.47
1:B:531:GLN:HE22	1:B:541:GLN:HA	1.79	0.47
1:B:739:LEU:HB3	1:B:742:ALA:HB3	1.96	0.47
1:A:165:ASN:CB	5:A:2531:HOH:O	2.63	0.47
1:A:239:LEU:CD1	1:B:239:LEU:HD11	2.45	0.47
1:A:433:PHE:N	1:A:434:PRO:CD	2.78	0.46
1:B:43:ALA:O	1:B:47:ARG:HG3	2.16	0.46
1:B:11:GLN:NE2	5:B:3552:HOH:O	2.47	0.46
1:A:531:GLN:HE22	1:A:541:GLN:HA	1.81	0.45
1:A:338:LYS:HE2	5:A:2301:HOH:O	2.15	0.45
1:A:21:TYR:O	1:B:172:ASN:HB2	2.17	0.45
1:A:246:ILE:HD13	1:B:239:LEU:CD1	2.46	0.45
1:A:663:GLU:HG2	5:A:2573:HOH:O	2.15	0.45
1:B:549:LEU:HB3	1:B:706:VAL:HG22	1.97	0.45
1:B:112:ASN:HD22	2:D:3:GLC:H61	1.82	0.45
1:A:429:VAL:HG13	1:A:437:HIS:CG	2.52	0.45
1:A:138:LEU:HD21	1:A:275:GLN:HB2	1.99	0.45
1:A:608:VAL:HG12	1:A:610:LEU:CD2	2.47	0.45
1:A:170:ARG:HB2	1:B:20:ARG:O	2.16	0.44
1:A:66:MET:HG3	1:A:309:HIS:HB3	1.99	0.44
1:B:452:THR:HA	1:B:453:PRO:HD3	1.79	0.44
1:A:447:VAL:HG11	1:A:787:TYR:CE2	2.53	0.44
1:A:658:ASP:O	1:A:661:ASN:HB2	2.18	0.44
1:A:3:PRO:HB3	1:A:49:GLN:OE1	2.18	0.44
1:B:785:ARG:NE	5:B:3345:HOH:O	2.38	0.44
1:B:97:ASN:ND2	1:B:100:ASP:H	2.11	0.43
1:A:15:SER:HA	1:A:18:TRP:NE1	2.33	0.43
1:A:701:LYS:HD3	1:A:701:LYS:HA	1.68	0.43
1:A:452:THR:HA	1:A:453:PRO:HD3	1.78	0.43
1:B:58:GLN:HB3	1:B:793:GLN:CD	2.39	0.43

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:188:ASP:O	1:B:188:ASP:OD2	2.36	0.43
1:B:76:ASN:HB2	1:B:459:GLN:HE22	1.84	0.43
1:B:3:PRO:HB3	1:B:49:GLN:OE1	2.19	0.43
1:B:692:ASP:HA	1:B:693:PRO:HD2	1.90	0.43
1:A:423:LEU:HD21	1:A:680:VAL:HG21	2.01	0.42
1:B:266:LYS:O	1:B:270:MET:HG3	2.19	0.42
1:B:391:LYS:HG3	5:B:3478:HOH:O	2.20	0.42
1:B:689:LYS:O	1:B:689:LYS:HG2	2.18	0.42
1:A:474:LYS:NZ	5:A:2470:HOH:O	2.53	0.42
1:A:170:ARG:HH11	1:B:22:GLY:HA2	1.84	0.42
1:B:590:LYS:HD2	1:B:590:LYS:HA	1.83	0.42
1:A:206:VAL:O	1:A:214:ALA:HA	2.19	0.42
1:A:66:MET:HG3	1:A:309:HIS:CB	2.50	0.42
1:A:534:ARG:NE	3:A:1999:SO4:O2	2.38	0.42
1:B:2:GLN:HA	1:B:3:PRO:HD3	1.95	0.41
1:B:437:HIS:CD2	1:B:441:PRO:HA	2.55	0.41
1:B:483:LEU:O	1:B:486:LEU:HB2	2.21	0.41
1:B:423:LEU:HD21	1:B:680:VAL:HG21	2.02	0.41
1:A:459:GLN:NE2	5:A:2237:HOH:O	2.28	0.41
1:A:692:ASP:HA	1:A:693:PRO:HD2	1.91	0.41
1:A:246:ILE:HD11	1:B:246:ILE:HD11	2.03	0.41
1:B:529:ASP:OD1	1:B:629:GLU:OE2	2.39	0.41
1:A:137:GLY:HA2	1:A:275:GLN:NE2	2.36	0.41
1:B:535:LEU:HD12	1:B:581:ALA:HB1	2.03	0.41
1:A:97:ASN:ND2	1:A:99:THR:HB	2.35	0.40
1:B:5:PHE:CD2	1:B:86:ASP:HB3	2.56	0.40
1:B:701:LYS:HD3	1:B:701:LYS:HA	1.79	0.40
1:B:170:ARG:NH2	5:B:3132:HOH:O	2.55	0.40
1:B:15:SER:HA	1:B:18:TRP:NE1	2.36	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	794/796 (100%)	769 (97%)	24 (3%)	1 (0%)	51	60
1	B	794/796 (100%)	767 (97%)	25 (3%)	2 (0%)	41	46
All	All	1588/1592 (100%)	1536 (97%)	49 (3%)	3 (0%)	47	55

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	307	ASP
1	B	533	LYS
1	B	307	ASP

### 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	667/667 (100%)	623 (93%)	44 (7%)	16	19
1	B	667/667 (100%)	617 (92%)	50 (8%)	13	14
All	All	1334/1334 (100%)	1240 (93%)	94 (7%)	15	16

All (94) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	GLN
1	A	20	ARG
1	A	53	LYS
1	A	66	MET
1	A	73	LEU
1	A	92	LYS
1	A	118	LEU
1	A	139	ASN
1	A	177	VAL
1	A	250	LYS
1	A	255	LEU
1	A	297	LEU
1	A	321	LEU

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type
1	A	326	GLN
1	A	363	LEU
1	A	384	LYS
1	A	391	LYS
1	A	411	VAL
1	A	423	LEU
1	A	443	LYS
1	A	454	ARG
1	A	486	LEU
1	A	494	LYS
1	A	515	LYS
1	A	516	VAL
1	A	535	LEU
1	A	538	TYR
1	A	542	HIS
1	A	544	ASN
1	A	578	TYR
1	A	600	LEU
1	A	605	LEU
1	A	609	PHE
1	A	610	LEU
1	A	689	LYS
1	A	701	LYS
1	A	706	VAL
1	A	727	LEU
1	A	732	LYS
1	A	739	LEU
1	A	755	ASP
1	A	766	ARG
1	A	785	ARG
1	A	795	LYS
1	B	2	GLN
1	B	20	ARG
1	B	53	LYS
1	B	73	LEU
1	B	92	LYS
1	B	97	ASN
1	B	99	THR
1	B	115	LEU
1	B	118	LEU
1	B	139	ASN
1	B	177	VAL

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	B	187	LYS
1	B	255	LEU
1	B	289	LEU
1	B	297	LEU
1	B	321	LEU
1	B	326	GLN
1	B	363	LEU
1	B	384	LYS
1	B	391	LYS
1	B	411	VAL
1	B	443	LYS
1	B	454	ARG
1	B	486	LEU
1	B	494	LYS
1	B	515	LYS
1	B	516	VAL
1	B	535	LEU
1	B	538	TYR
1	B	542	HIS
1	B	544	ASN
1	B	556	ARG
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	689	LYS
1	B	695	LYS
1	B	701	LYS
1	B	706	VAL
1	B	727	LEU
1	B	728	HIS
1	B	732	LYS
1	B	739	LEU
1	B	755	ASP
1	B	766	ARG
1	B	785	ARG
1	B	795	LYS

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

Mol	Chain	Res	Type
1	A	57	ASN
1	A	97	ASN
1	A	112	ASN
1	A	139	ASN
1	A	162	HIS
1	A	178	GLN
1	A	221	GLN
1	A	260	ASN
1	A	288	HIS
1	A	446	ASN
1	A	459	GLN
1	A	525	GLN
1	A	531	GLN
1	A	544	ASN
1	A	678	HIS
1	B	9	GLN
1	B	57	ASN
1	B	97	ASN
1	B	139	ASN
1	B	178	GLN
1	B	221	GLN
1	B	244	GLN
1	B	260	ASN
1	B	437	HIS
1	B	446	ASN
1	B	459	GLN
1	B	498	GLN
1	B	531	GLN
1	B	544	ASN
1	B	560	GLN

### 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 ⓘ

10 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	BGC	C	1	2	12,12,12	0.76	0	17,17,17	1.46	3 (17%)
2	GLC	C	2	2	11,11,12	1.22	2 (18%)	15,15,17	0.99	0
2	GLC	C	3	2	11,11,12	0.98	0	15,15,17	1.51	4 (26%)
2	GLC	C	4	2	11,11,12	0.81	0	15,15,17	1.53	3 (20%)
2	GLC	C	5	2	11,11,12	1.29	2 (18%)	15,15,17	2.52	3 (20%)
2	BGC	D	1	2	12,12,12	0.60	0	17,17,17	1.18	2 (11%)
2	GLC	D	2	2	11,11,12	0.85	0	15,15,17	1.53	4 (26%)
2	GLC	D	3	2	11,11,12	0.98	0	15,15,17	1.65	3 (20%)
2	GLC	D	4	2	11,11,12	0.84	0	15,15,17	1.69	3 (20%)
2	GLC	D	5	2	11,11,12	1.16	2 (18%)	15,15,17	2.51	3 (20%)

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	BGC	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	C	5	2	-	0/2/19/22	0/1/1/1
2	BGC	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
2	GLC	D	5	2	-	0/2/19/22	0/1/1/1

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	5	GLC	C1-C2	3.09	1.59	1.52

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	2	GLC	C2-C3	2.59	1.56	1.52
2	D	5	GLC	C2-C3	2.51	1.56	1.52
2	D	5	GLC	C1-C2	2.46	1.57	1.52
2	C	5	GLC	C2-C3	2.02	1.55	1.52
2	C	2	GLC	O5-C1	-2.01	1.40	1.43

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	5	GLC	C1-O5-C5	7.29	122.07	112.19
2	C	5	GLC	C1-C2-C3	6.37	117.49	109.67
2	C	5	GLC	C1-O5-C5	6.08	120.43	112.19
2	D	5	GLC	C1-C2-C3	4.87	115.66	109.67
2	D	4	GLC	C1-O5-C5	4.56	118.36	112.19
2	D	3	GLC	O2-C2-C1	4.21	117.76	109.15
2	C	1	BGC	O2-C2-C1	3.31	116.83	109.16
2	C	4	GLC	C1-O5-C5	3.24	116.59	112.19
2	D	4	GLC	O4-C4-C3	3.07	117.44	110.35
2	C	5	GLC	O3-C3-C2	3.03	115.80	109.99
2	D	3	GLC	O2-C2-C3	-2.91	104.31	110.14
2	D	2	GLC	C1-C2-C3	2.90	113.23	109.67
2	C	1	BGC	O3-C3-C2	-2.86	103.75	110.35
2	C	3	GLC	C1-C2-C3	2.61	112.88	109.67
2	D	1	BGC	O5-C1-C2	-2.47	105.87	110.28
2	D	2	GLC	O3-C3-C4	2.43	115.98	110.35
2	D	2	GLC	O2-C2-C3	-2.41	105.31	110.14
2	C	3	GLC	O4-C4-C3	-2.39	104.82	110.35
2	C	3	GLC	O2-C2-C3	-2.33	105.46	110.14
2	D	5	GLC	O3-C3-C2	2.32	114.44	109.99
2	D	4	GLC	C1-C2-C3	2.30	112.49	109.67
2	C	4	GLC	O5-C1-C2	2.29	114.31	110.77
2	D	1	BGC	O4-C4-C3	-2.22	105.22	110.35
2	C	4	GLC	O2-C2-C3	2.17	114.49	110.14
2	C	3	GLC	O3-C3-C4	2.11	115.22	110.35
2	C	1	BGC	C1-C2-C3	-2.09	105.97	110.31
2	D	2	GLC	C1-O5-C5	2.07	115.00	112.19
2	D	3	GLC	O4-C4-C3	-2.02	105.68	110.35

There are no chirality outliers.

All (4) torsion outliers are listed below:

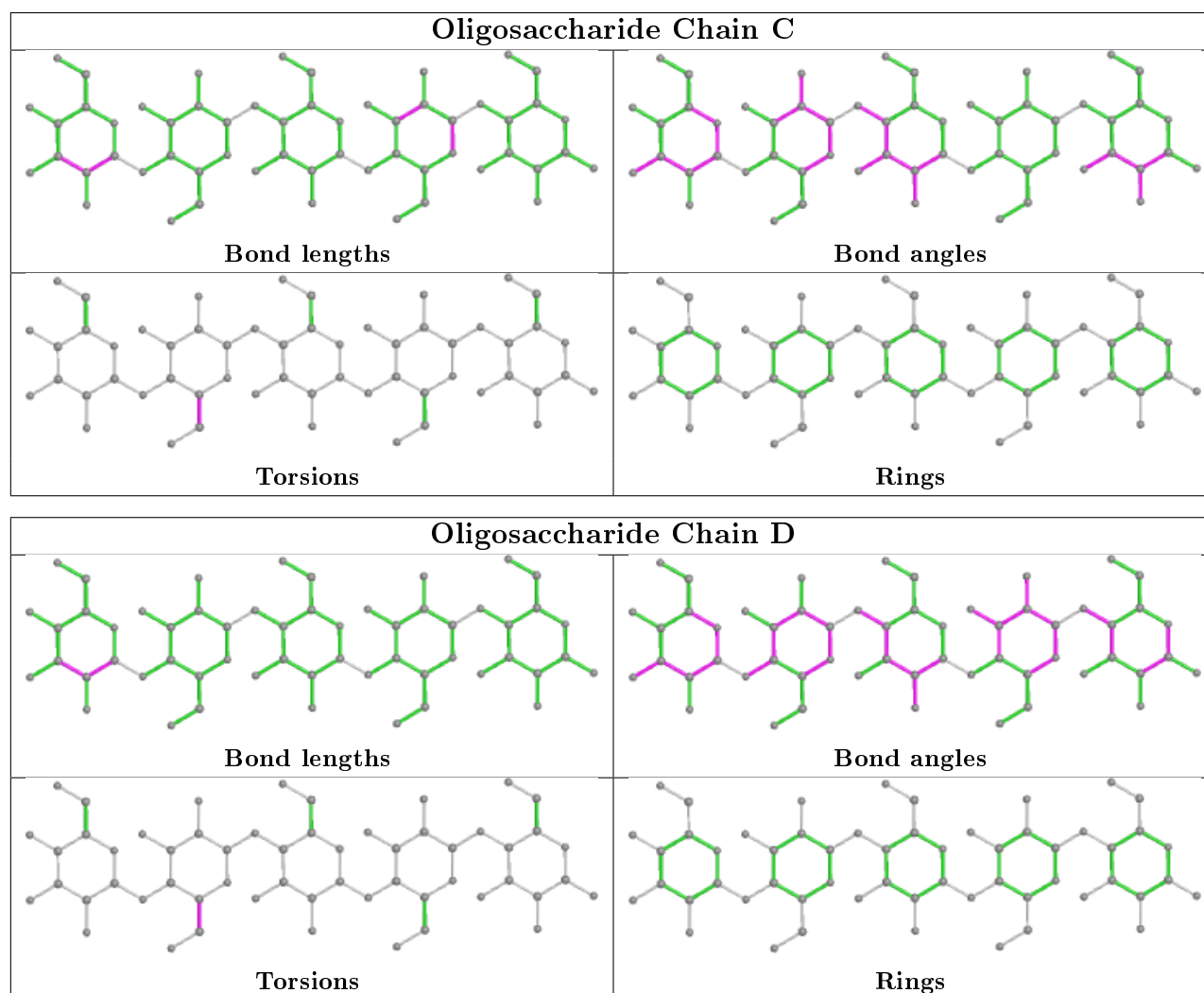
Mol	Chain	Res	Type	Atoms
2	C	4	GLC	C4-C5-C6-O6
2	D	4	GLC	C4-C5-C6-O6
2	D	4	GLC	O5-C5-C6-O6
2	C	4	GLC	O5-C5-C6-O6

There are no ring outliers.

3 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	4	GLC	3	0
2	C	4	GLC	1	0
2	D	3	GLC	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.



## 5.6 Ligand geometry

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	SO4	B	2999	-	4,4,4	0.31	0	6,6,6	0.42	0
4	PLP	A	900	1	15,15,16	1.51	3 (20%)	20,22,23	1.39	5 (25%)
3	SO4	A	1999	-	4,4,4	0.30	0	6,6,6	1.08	0
4	PLP	B	900	1	15,15,16	1.08	2 (13%)	20,22,23	1.16	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	-	3/6/6/8	0/1/1/1
4	PLP	B	900	1	-	3/6/6/8	0/1/1/1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	900	PLP	C3-C2	-3.57	1.37	1.40
4	A	900	PLP	C6-N1	3.29	1.41	1.34
4	B	900	PLP	C2-N1	2.47	1.38	1.33
4	A	900	PLP	C2-N1	2.43	1.38	1.33
4	B	900	PLP	C3-C2	-2.08	1.38	1.40

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	900	PLP	O4P-P-O1P	2.52	113.55	106.47
4	A	900	PLP	O3P-P-O4P	2.43	113.21	106.73
4	A	900	PLP	C5-C6-N1	-2.23	120.11	123.82
4	A	900	PLP	C3-C4-C5	2.10	121.01	118.74

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	900	PLP	C5-C6-N1	-2.09	120.33	123.82
4	A	900	PLP	C2A-C2-N1	2.05	121.67	117.67

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	900	PLP	C5A-O4P-P-O1P
4	A	900	PLP	C5A-O4P-P-O3P
4	B	900	PLP	C5A-O4P-P-O1P
4	B	900	PLP	C5A-O4P-P-O3P
4	B	900	PLP	C5A-O4P-P-O2P
4	A	900	PLP	C4-C5-C5A-O4P

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	2999	SO4	1	0
3	A	1999	SO4	2	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 [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

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	796/796 (100%)	-0.60	1 (0%) 95 95	17, 29, 48, 74	0
1	B	796/796 (100%)	-0.58	5 (0%) 89 88	17, 29, 48, 74	0
All	All	1592/1592 (100%)	-0.59	6 (0%) 92 91	17, 29, 48, 74	0

All (6) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	57	ASN	3.4
1	B	562	ASP	3.3
1	A	51	PHE	3.2
1	B	187	LYS	2.9
1	B	186	THR	2.5
1	B	600	LEU	2.5

### 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.

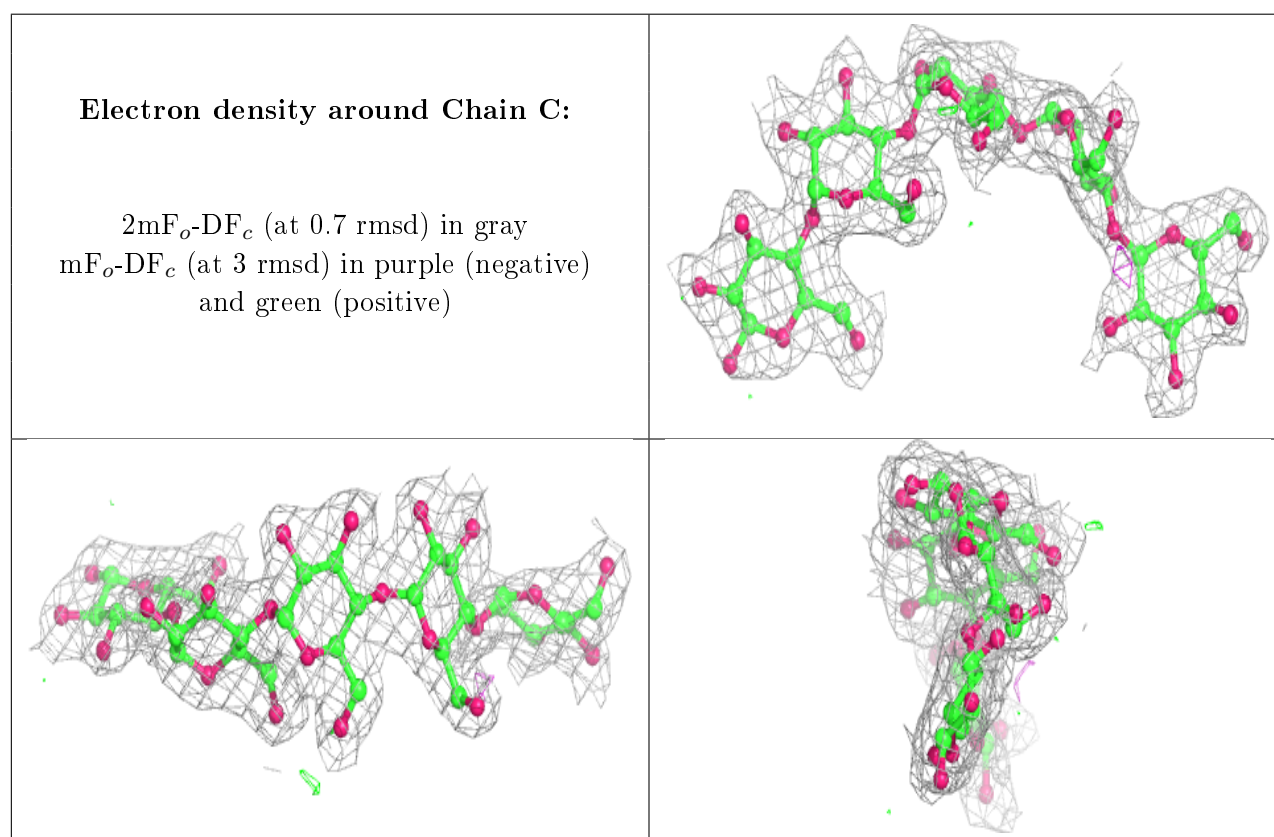
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
2	GLC	D	5	11/12	0.90	0.18	39,41,45,45	0
2	GLC	D	4	11/12	0.91	0.13	30,36,38,42	0
2	GLC	C	5	11/12	0.93	0.17	37,38,42,43	0

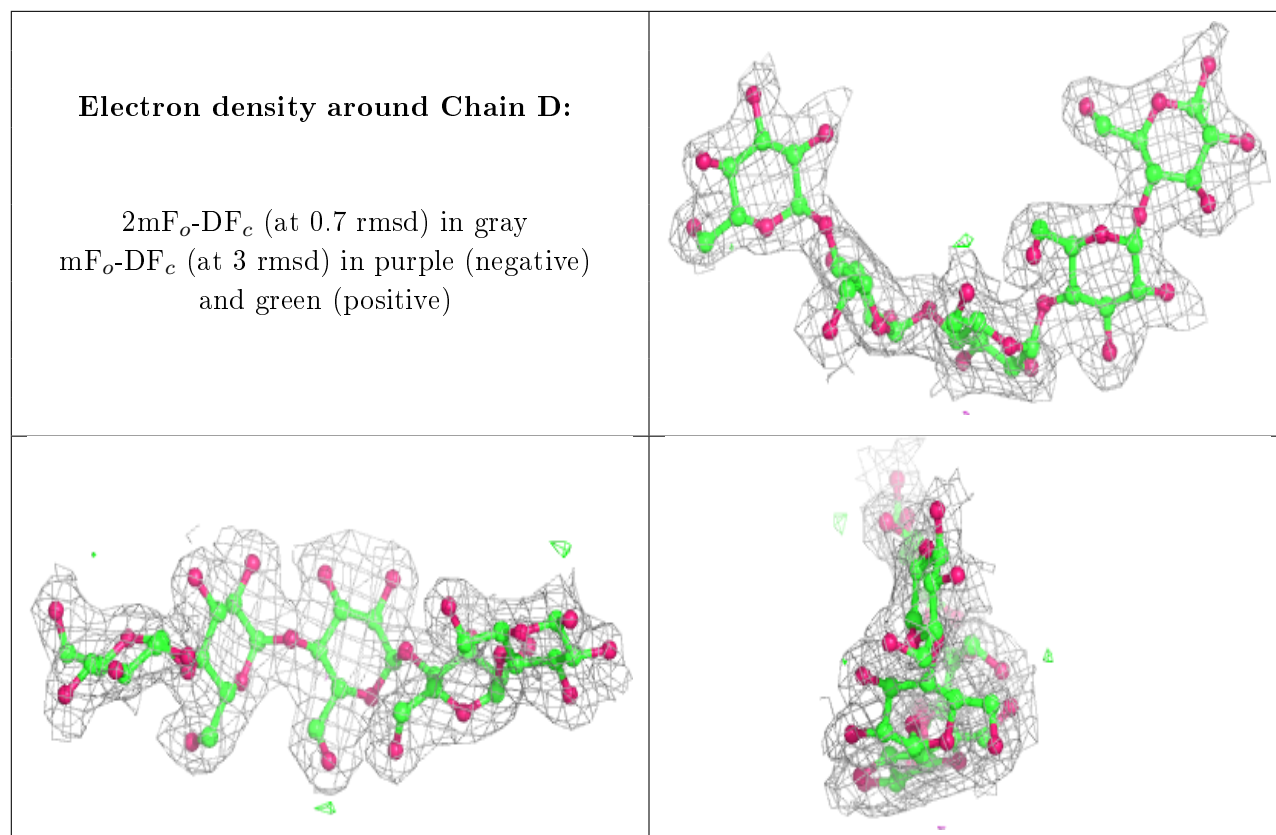
*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	BGC	D	1	12/12	0.94	0.16	34,38,41,45	0
2	BGC	C	1	12/12	0.94	0.11	33,37,39,46	0
2	GLC	D	2	11/12	0.94	0.11	27,31,35,35	0
2	GLC	C	4	11/12	0.96	0.11	29,35,37,42	0
2	GLC	D	3	11/12	0.96	0.07	28,31,33,35	0
2	GLC	C	3	11/12	0.97	0.08	27,29,31,33	0
2	GLC	C	2	11/12	0.98	0.07	28,30,32,33	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.





## 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	SO4	B	2999	5/5	0.92	0.26	78,78,81,82	0
4	PLP	A	900	15/16	0.96	0.10	22,26,38,38	0
3	SO4	A	1999	5/5	0.96	0.25	51,52,58,60	0
4	PLP	B	900	15/16	0.96	0.08	23,26,38,39	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.