



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 04:48 AM UTC

PDB ID : 2ASV / pdb_00002asv
Title : X-Ray studies on protein complexes: Enzymatic catalysis in Crystals of E. coli
Maltodextrin Phosphorylase (MalP)
Authors : Geremia, S.; Campagnolo, M.
Deposited on : 2005-08-24
Resolution : 1.95 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

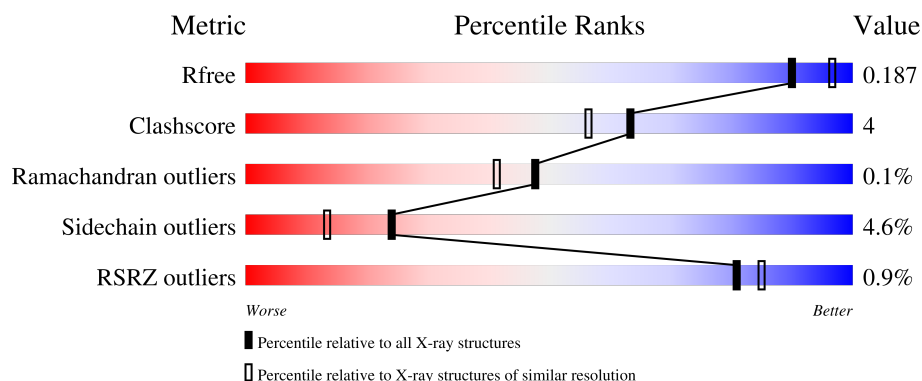
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.95 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	3494 (1.96-1.96)
Clashscore	190562	3612 (1.96-1.96)
Ramachandran outliers	187476	3587 (1.96-1.96)
Sidechain outliers	187428	3587 (1.96-1.96)
RSRZ outliers	180081	3495 (1.96-1.96)

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	87% 12%
1	B	796	87% 12%
2	C	5	40% 40% 20%
2	D	5	20% 60% 20%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	ASO	B	2998	-	-	X	-

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 14136 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.

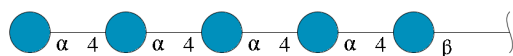
- Molecule 1 is a protein called Maltodextrin phosphorylase.

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:

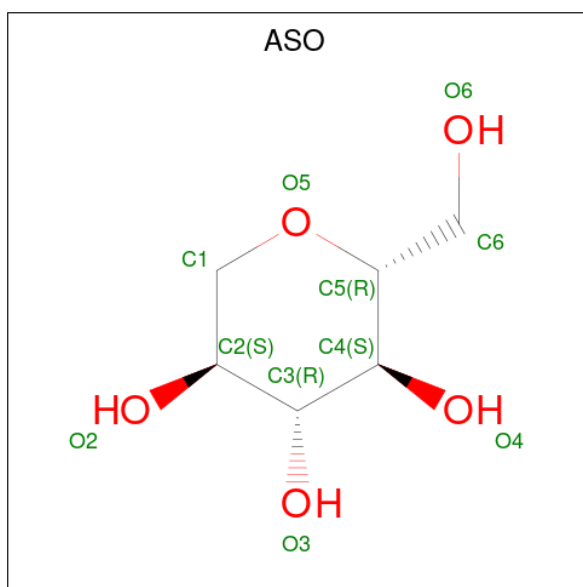
Chain	Residue	Modelled	Actual	Comment	Reference
A	261	ALA	HIS	engineered mutation	UNP P00490
A	262	PHE	THR	engineered mutation	UNP P00490
A	263	GLU	ALA	engineered mutation	UNP P00490
B	261	ALA	HIS	engineered mutation	UNP P00490
B	262	PHE	THR	engineered mutation	UNP P00490
B	263	GLU	ALA	engineered mutation	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 1,5-anhydro-D-glucitol (CCD ID: ASO) (formula: C₆H₁₂O₅).



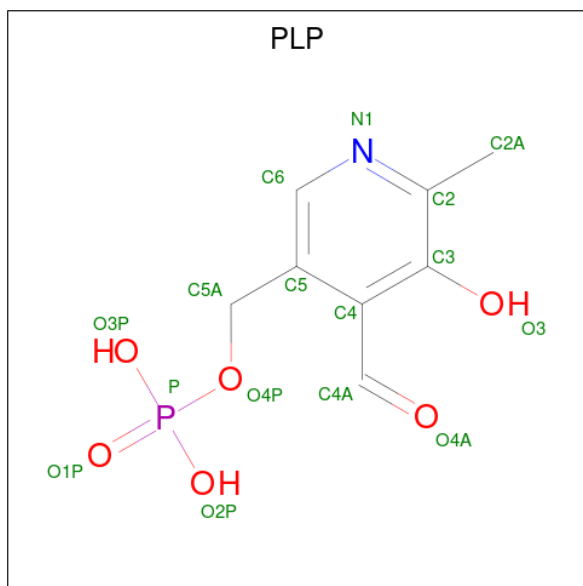
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			11	6	5		
3	B	1	Total	C	O	0	0
			11	6	5		

- Molecule 4 is PHOSPHATE ION (CCD ID: PO4) (formula: O_4P).



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

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



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

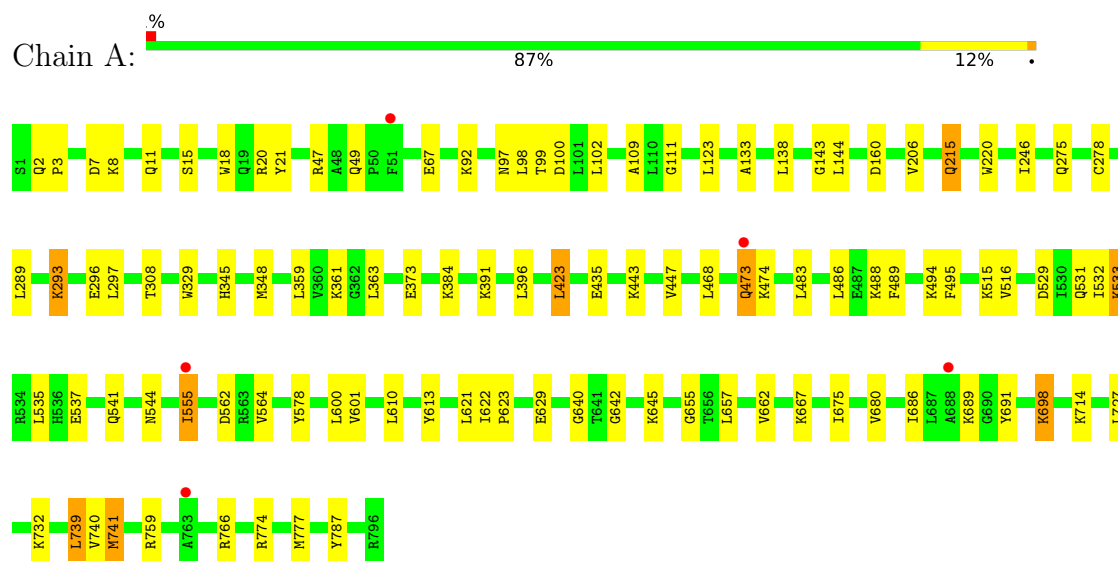
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	613	Total	O	0	0
			613	613		
6	B	571	Total	O	0	0
			571	571		

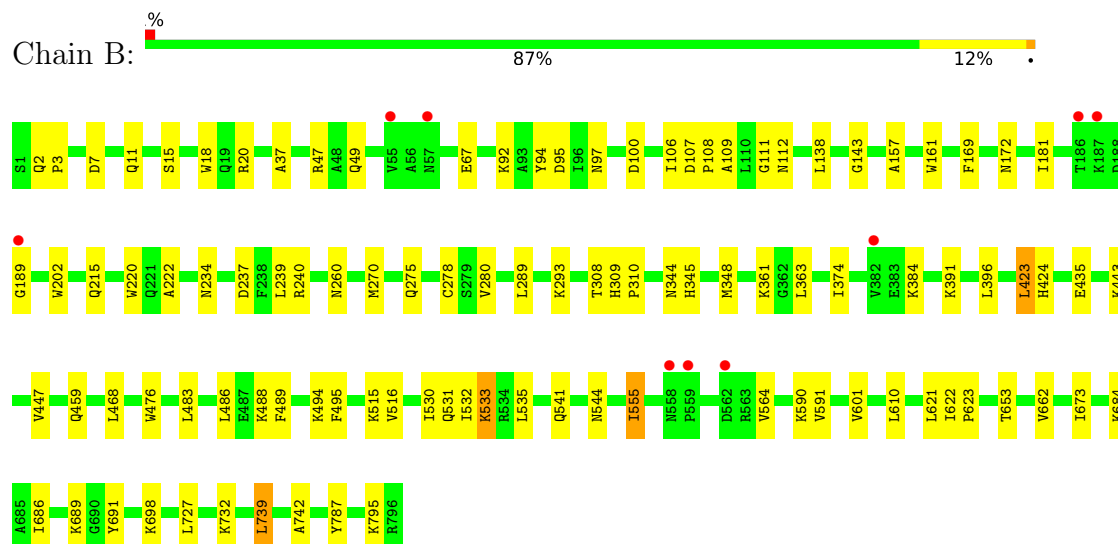
3 Residue-property plots

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.

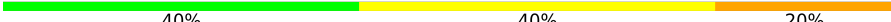
• Molecule 1: Maltodextrin phosphorylase

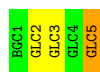


• Molecule 1: Maltodextrin phosphorylase

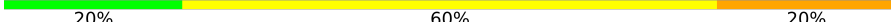


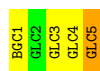
• Molecule 2: alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-beta-D-glucopyranose

Chain C:  40% 40% 20%



- 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:  20% 60% 20%



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	74.33Å 104.72Å 214.79Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	15.00 – 1.95 15.00 – 1.95	Depositor EDS
% Data completeness (in resolution range)	97.5 (15.00-1.95) 97.5 (15.00-1.95)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.42 (at 1.95Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, R_{free}	0.179 , 0.226 0.191 , 0.187	Depositor DCC
R_{free} test set	6003 reflections (4.89%)	wwPDB-VP
Wilson B-factor (Å ²)	25.8	Xtriage
Anisotropy	0.346	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.40 , 50.7	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	14136	wwPDB-VP
Average B, all atoms (Å ²)	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.99% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: BGC, ASO, PO4, GLC, 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	1.17	8/6539 (0.1%)	1.03	2/8865 (0.0%)
1	B	1.15	7/6539 (0.1%)	1.03	4/8865 (0.0%)
All	All	1.16	15/13078 (0.1%)	1.03	6/17730 (0.0%)

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	777	MET	SD-CE	8.07	1.99	1.79
1	A	215	GLN	C-O	-6.78	1.18	1.24
1	A	133	ALA	CA-CB	-6.44	1.43	1.53
1	B	37	ALA	CA-CB	-6.41	1.43	1.53
1	B	270	MET	SD-CE	-6.24	1.64	1.79
1	B	157	ALA	CA-CB	-6.08	1.46	1.54
1	B	348	MET	SD-CE	-5.91	1.64	1.79
1	B	280	VAL	CA-CB	-5.86	1.47	1.54
1	B	222	ALA	CA-CB	-5.71	1.45	1.53
1	A	308	THR	C-O	-5.66	1.16	1.24
1	A	348	MET	SD-CE	-5.54	1.65	1.79
1	A	741	MET	SD-CE	5.51	1.93	1.79
1	A	160	ASP	C-O	-5.50	1.17	1.24
1	A	144	LEU	CA-C	-5.34	1.48	1.53
1	B	308	THR	C-O	-5.26	1.17	1.24

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	680	VAL	CB-CA-C	-6.13	104.00	112.04
1	A	640	GLY	N-CA-C	-6.13	105.06	112.48
1	B	591	VAL	N-CA-C	-5.50	105.01	110.62
1	B	234	ASN	N-CA-C	-5.34	106.60	113.01

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	530	ILE	N-CA-C	5.15	115.27	107.75
1	B	374	ILE	N-CA-C	-5.01	105.61	110.42

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	6389	0	6333	56	0
1	B	6389	0	6333	46	0
2	C	56	0	48	2	0
2	D	56	0	48	3	0
3	A	11	0	11	3	0
3	B	11	0	12	6	0
4	A	5	0	0	0	0
4	B	5	0	0	0	0
5	A	15	0	6	0	0
5	B	15	0	6	0	0
6	A	613	0	0	10	0
6	B	571	0	0	6	0
All	All	14136	0	12797	104	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 (104) 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:1998:ASO:H11	2:C:5:GLC:O4	1.47	1.15
3:B:2998:ASO:H11	2:D:5:GLC:O4	1.65	0.95
1:B:345:HIS:O	3:B:2998:ASO:H12	1.74	0.86
1:A:97:ASN:HD22	1:A:100:ASP:H	1.33	0.76
3:A:1998:ASO:H11	2:C:5:GLC:HO4	1.49	0.74
1:A:3:PRO:HD2	6:A:2469:HOH:O	1.94	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:7:ASP:O	1:B:11:GLN:HG2	1.95	0.66
1:A:468:LEU:CD2	1:A:486:LEU:HD11	2.26	0.65
1:B:97:ASN:HD22	1:B:100:ASP:H	1.45	0.62
1:A:345:HIS:O	3:A:1998:ASO:H12	2.00	0.62
1:A:47:ARG:HD3	6:A:2181:HOH:O	1.99	0.62
1:B:468:LEU:CD2	1:B:486:LEU:HD11	2.30	0.61
1:A:21:TYR:O	1:B:172:ASN:HB2	2.01	0.61
1:B:3:PRO:HB3	1:B:49:GLN:OE1	2.00	0.61
3:B:2998:ASO:H11	2:D:5:GLC:C4	2.31	0.60
1:A:3:PRO:HB3	1:A:49:GLN:OE1	2.02	0.59
1:A:11:GLN:HG3	6:A:2565:HOH:O	2.03	0.58
1:A:531:GLN:HE22	1:A:541:GLN:HA	1.67	0.58
1:A:691:TYR:CE2	1:A:739:LEU:HD22	2.39	0.58
1:B:691:TYR:CE2	1:B:739:LEU:HD22	2.39	0.58
1:A:97:ASN:ND2	1:A:100:ASP:H	2.00	0.57
1:B:237:ASP:OD2	1:B:240:ARG:NH1	2.35	0.56
1:A:447:VAL:HG11	1:A:787:TYR:CD2	2.41	0.56
1:B:189:GLY:HA2	6:B:3544:HOH:O	2.06	0.55
1:A:7:ASP:O	1:A:11:GLN:HG2	2.07	0.54
1:A:610:LEU:HD12	1:A:621:LEU:HD21	1.89	0.54
1:B:544:ASN:C	1:B:544:ASN:HD22	2.15	0.54
1:B:220:TRP:CD2	1:B:278:CYS:HB3	2.42	0.54
1:B:684:LYS:NZ	6:B:3242:HOH:O	2.42	0.53
1:B:345:HIS:O	3:B:2998:ASO:C1	2.53	0.53
1:A:532:ILE:HG21	1:A:621:LEU:HD13	1.91	0.53
3:B:2998:ASO:H11	2:D:5:GLC:HO4	1.71	0.53
1:A:246:ILE:HD13	1:B:239:LEU:HD12	1.91	0.53
1:A:138:LEU:HD21	1:A:275:GLN:HB2	1.93	0.51
1:B:97:ASN:ND2	1:B:100:ASP:H	2.08	0.51
1:A:655:GLY:O	1:A:675:ILE:HA	2.11	0.50
1:B:555:ILE:HD11	1:B:601:VAL:HG22	1.93	0.50
1:A:562:ASP:O	1:A:759:ARG:NH2	2.42	0.50
1:A:473:GLN:OE1	1:A:474:LYS:HE2	2.12	0.50
1:A:396:LEU:HD21	1:A:435:GLU:HB2	1.94	0.49
1:B:344:ASN:O	1:B:424:HIS:HE1	1.96	0.49
1:A:555:ILE:HD11	1:A:601:VAL:HG22	1.95	0.48
1:A:3:PRO:HB3	1:A:49:GLN:CD	2.38	0.48
1:B:67:GLU:HB2	1:B:111:GLY:HA2	1.95	0.48
1:A:447:VAL:HG11	1:A:787:TYR:CE2	2.49	0.48
1:A:293:LYS:O	1:A:296:GLU:HG2	2.14	0.47
1:A:359:LEU:HD12	6:A:2451:HOH:O	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:67:GLU:HB2	1:A:111:GLY:HA2	1.96	0.47
1:A:423:LEU:O	1:A:423:LEU:HD23	2.15	0.47
1:A:544:ASN:C	1:A:544:ASN:HD22	2.22	0.47
1:B:610:LEU:HD12	1:B:621:LEU:HD21	1.97	0.47
1:B:653:THR:HB	1:B:673:ILE:HG13	1.96	0.47
1:B:220:TRP:CE2	1:B:278:CYS:HB3	2.50	0.46
1:A:714:LYS:NZ	6:A:2611:HOH:O	2.45	0.46
1:A:766:ARG:HD2	6:A:2218:HOH:O	2.16	0.46
1:B:447:VAL:HG11	1:B:787:TYR:CD2	2.50	0.46
1:B:109:ALA:HB1	1:B:143:GLY:HA3	1.97	0.45
1:A:489:PHE:HB3	1:A:495:PHE:CG	2.52	0.45
1:B:138:LEU:HD21	1:B:275:GLN:HB2	1.99	0.45
1:B:15:SER:HA	1:B:18:TRP:NE1	2.32	0.44
1:B:237:ASP:OD2	1:B:240:ARG:HD2	2.18	0.44
1:B:531:GLN:HE22	1:B:541:GLN:HA	1.82	0.44
1:A:473:GLN:HE21	1:A:473:GLN:HB2	1.59	0.43
1:A:740:VAL:HG12	1:A:741:MET:HE2	2.00	0.43
1:B:169:PHE:CE1	1:B:202:TRP:HB3	2.53	0.43
1:A:220:TRP:CD2	1:A:278:CYS:HB3	2.54	0.43
1:B:489:PHE:HB3	1:B:495:PHE:CG	2.53	0.43
1:B:345:HIS:O	3:B:2998:ASO:H2	2.18	0.43
1:A:691:TYR:OH	1:A:741:MET:HB2	2.19	0.43
1:A:3:PRO:CD	6:A:2469:HOH:O	2.62	0.43
1:B:47:ARG:HD3	6:B:3205:HOH:O	2.19	0.43
1:A:11:GLN:CG	6:A:2565:HOH:O	2.66	0.43
1:B:476:TRP:H	1:B:476:TRP:CD1	2.36	0.43
1:B:108:PRO:HA	1:B:161:TRP:CE3	2.54	0.42
1:A:97:ASN:HD21	1:A:99:THR:HB	1.83	0.42
1:A:246:ILE:CD1	1:B:239:LEU:HD12	2.49	0.42
1:A:544:ASN:ND2	6:A:2050:HOH:O	2.52	0.42
1:A:622:ILE:N	1:A:623:PRO:CD	2.83	0.42
1:B:532:ILE:HG21	1:B:621:LEU:HD13	2.00	0.42
1:B:396:LEU:HD21	1:B:435:GLU:HB2	2.01	0.42
1:A:98:LEU:O	1:A:102:LEU:HG	2.20	0.42
1:B:459:GLN:NE2	6:B:3263:HOH:O	2.46	0.41
1:A:109:ALA:HB1	1:A:143:GLY:HA3	2.03	0.41
1:A:529:ASP:OD1	1:A:629:GLU:OE2	2.38	0.41
1:A:123:LEU:HB3	1:A:206:VAL:HG11	2.01	0.41
1:A:532:ILE:HB	1:A:613:TYR:CZ	2.55	0.41
1:A:698:LYS:HA	1:A:698:LYS:HD2	1.93	0.41
1:A:423:LEU:HD23	1:A:423:LEU:C	2.46	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:657:LEU:HD23	1:A:657:LEU:HA	1.97	0.41
1:B:590:LYS:HA	1:B:590:LYS:HD2	1.83	0.41
1:B:260:ASN:ND2	6:B:3437:HOH:O	2.54	0.41
1:A:15:SER:HA	1:A:18:TRP:NE1	2.36	0.41
1:B:94:TYR:O	1:B:95:ASP:HB2	2.20	0.41
1:B:106:ILE:O	1:B:107:ASP:C	2.61	0.41
1:B:309:HIS:N	1:B:310:PRO:CD	2.84	0.41
1:A:329:TRP:CZ3	1:A:373:GLU:HG2	2.57	0.41
1:B:739:LEU:HB3	1:B:742:ALA:HB3	2.03	0.41
1:A:8:LYS:NZ	6:A:2473:HOH:O	2.54	0.40
1:A:642:GLY:HA2	1:A:645:LYS:HD2	2.04	0.40
1:A:537:GLU:HB2	1:A:578:TYR:OH	2.22	0.40
1:B:423:LEU:HD23	1:B:423:LEU:C	2.47	0.40
1:B:112:ASN:OD1	6:B:3563:HOH:O	2.22	0.40
1:B:622:ILE:N	1:B:623:PRO:CD	2.84	0.40
1:A:667:LYS:O	1:A:774:ARG:HD3	2.22	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%)	23 (3%)	1 (0%)	48	41
1	B	794/796 (100%)	770 (97%)	23 (3%)	1 (0%)	48	41
All	All	1588/1592 (100%)	1540 (97%)	46 (3%)	2 (0%)	48	41

All (2) Ramachandran outliers are listed below:

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

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%)	636 (95%)	31 (5%)	24	13
1	B	667/667 (100%)	637 (96%)	30 (4%)	24	14
All	All	1334/1334 (100%)	1273 (95%)	61 (5%)	24	13

All (61) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	GLN
1	A	20	ARG
1	A	92	LYS
1	A	215	GLN
1	A	289	LEU
1	A	293	LYS
1	A	297	LEU
1	A	361	LYS
1	A	363	LEU
1	A	384	LYS
1	A	391	LYS
1	A	423	LEU
1	A	443	LYS
1	A	473	GLN
1	A	483	LEU
1	A	488	LYS
1	A	494	LYS
1	A	515	LYS
1	A	516	VAL
1	A	533	LYS
1	A	535	LEU
1	A	555	ILE
1	A	564	VAL
1	A	600	LEU
1	A	662	VAL
1	A	686	ILE
1	A	689	LYS

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Mol	Chain	Res	Type
1	A	698	LYS
1	A	727	LEU
1	A	732	LYS
1	A	739	LEU
1	B	2	GLN
1	B	20	ARG
1	B	92	LYS
1	B	181	ILE
1	B	215	GLN
1	B	289	LEU
1	B	293	LYS
1	B	361	LYS
1	B	363	LEU
1	B	384	LYS
1	B	391	LYS
1	B	423	LEU
1	B	443	LYS
1	B	483	LEU
1	B	488	LYS
1	B	494	LYS
1	B	515	LYS
1	B	516	VAL
1	B	533	LYS
1	B	535	LEU
1	B	555	ILE
1	B	564	VAL
1	B	662	VAL
1	B	686	ILE
1	B	689	LYS
1	B	698	LYS
1	B	727	LEU
1	B	732	LYS
1	B	739	LEU
1	B	795	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	9	GLN
1	A	97	ASN
1	A	112	ASN
1	A	139	ASN

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Mol	Chain	Res	Type
1	A	221	GLN
1	A	260	ASN
1	A	295	HIS
1	A	306	ASN
1	A	400	HIS
1	A	446	ASN
1	A	459	GLN
1	A	523	ASN
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	112	ASN
1	B	139	ASN
1	B	221	GLN
1	B	244	GLN
1	B	260	ASN
1	B	271	GLN
1	B	295	HIS
1	B	437	HIS
1	B	446	ASN
1	B	459	GLN
1	B	531	GLN
1	B	544	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

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	0.54	0	17,17,17	0.96	0
2	GLC	C	2	2	11,11,12	0.95	0	15,15,17	1.26	1 (6%)
2	GLC	C	3	2	11,11,12	0.89	0	15,15,17	1.04	1 (6%)
2	GLC	C	4	2	11,11,12	0.89	0	15,15,17	0.73	0
2	GLC	C	5	2	11,11,12	0.93	0	15,15,17	1.34	1 (6%)
2	BGC	D	1	2	12,12,12	0.62	0	17,17,17	1.01	1 (5%)
2	GLC	D	2	2	11,11,12	0.52	0	15,15,17	1.11	0
2	GLC	D	3	2	11,11,12	0.80	0	15,15,17	1.46	1 (6%)
2	GLC	D	4	2	11,11,12	0.75	0	15,15,17	1.27	2 (13%)
2	GLC	D	5	2	11,11,12	0.83	0	15,15,17	1.68	4 (26%)

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

There are no bond length outliers.

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	3	GLC	C1-O5-C5	4.26	117.89	112.19
2	C	5	GLC	O2-C2-C3	3.41	117.22	110.15

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	5	GLC	O3-C3-C2	-3.08	103.77	110.05
2	D	5	GLC	O4-C4-C5	-2.48	103.21	109.32
2	D	4	GLC	O2-C2-C3	-2.46	105.05	110.15
2	D	5	GLC	O4-C4-C3	2.29	115.78	110.38
2	D	4	GLC	O3-C3-C2	-2.18	105.60	110.05
2	C	3	GLC	C1-C2-C3	2.15	112.77	109.64
2	C	2	GLC	C1-O5-C5	2.13	115.04	112.19
2	D	1	BGC	O3-C3-C2	-2.05	105.55	110.38
2	D	5	GLC	O2-C2-C3	2.01	114.31	110.15

There are no chirality outliers.

All (2) torsion outliers are listed below:

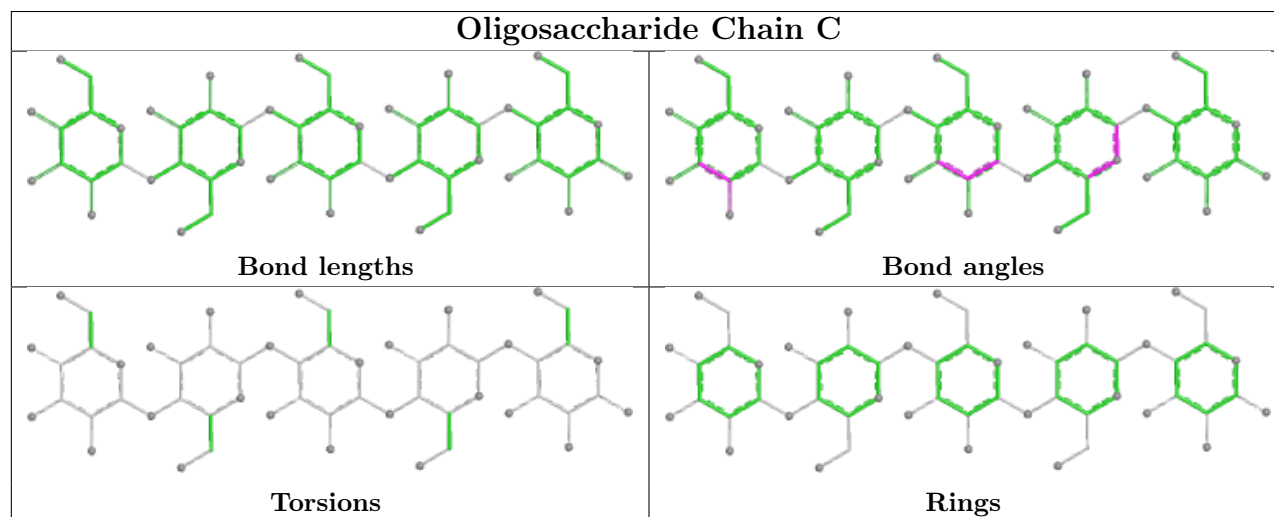
Mol	Chain	Res	Type	Atoms
2	D	5	GLC	C4-C5-C6-O6
2	D	5	GLC	O5-C5-C6-O6

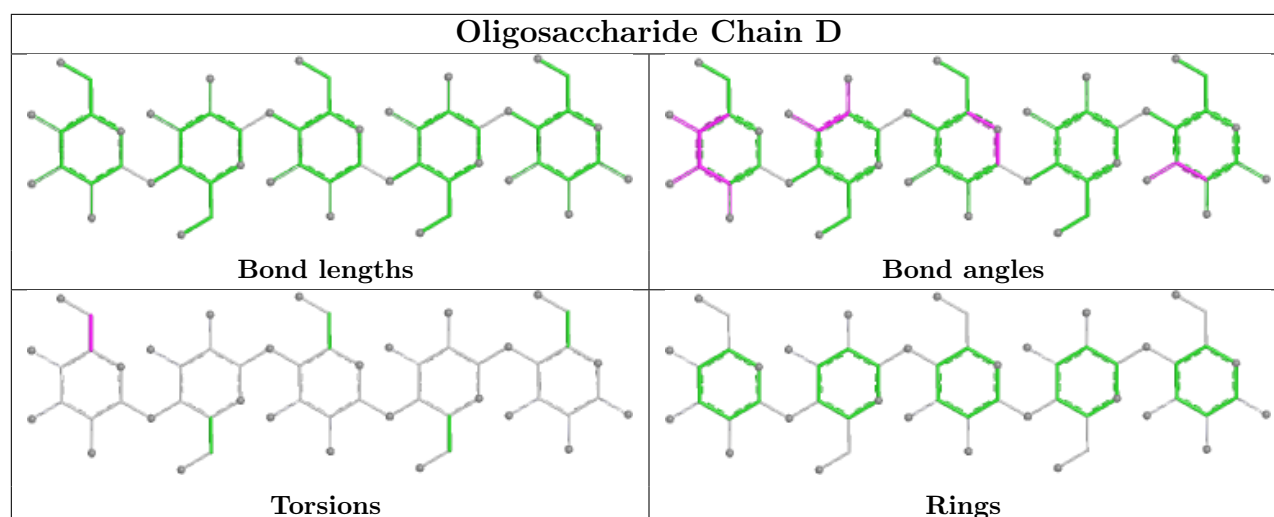
There are no ring outliers.

2 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	5	GLC	3	0
2	C	5	GLC	2	0

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





5.6 Ligand geometry [i](#)

6 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	ASO	A	1998	-	11,11,11	3.42	4 (36%)	15,15,15	3.74	6 (40%)
5	PLP	A	900	1	15,15,16	1.79	3 (20%)	21,22,23	1.79	6 (28%)
4	PO4	B	1999	-	4,4,4	1.15	1 (25%)	6,6,6	0.95	0
3	ASO	B	2998	-	11,11,11	3.32	4 (36%)	15,15,15	3.22	5 (33%)
4	PO4	A	999	-	4,4,4	0.87	0	6,6,6	1.18	0
5	PLP	B	900	1	15,15,16	1.75	4 (26%)	21,22,23	1.91	6 (28%)

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
3	ASO	A	1998	-	-	2/2/19/19	0/1/1/1
5	PLP	B	900	1	-	0/6/6/8	0/1/1/1
5	PLP	A	900	1	-	1/6/6/8	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	ASO	B	2998	-	-	0/2/19/19	0/1/1/1

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1998	ASO	O5-C1	-9.89	1.27	1.43
3	B	2998	ASO	O5-C1	-9.43	1.27	1.43
5	B	900	PLP	C3-C2	-4.80	1.36	1.41
5	A	900	PLP	C3-C2	-4.00	1.36	1.41
3	A	1998	ASO	O2-C2	-3.55	1.35	1.43
3	B	2998	ASO	O5-C5	3.55	1.50	1.43
5	A	900	PLP	C5-C4	-3.07	1.37	1.40
3	B	2998	ASO	O2-C2	-2.96	1.37	1.43
3	A	1998	ASO	C1-C2	-2.96	1.45	1.52
5	A	900	PLP	C4A-C4	-2.92	1.45	1.51
3	B	2998	ASO	C1-C2	-2.82	1.45	1.52
5	B	900	PLP	C4A-C4	-2.66	1.46	1.51
5	B	900	PLP	C6-N1	2.33	1.39	1.34
3	A	1998	ASO	O5-C5	2.18	1.47	1.43
4	B	1999	PO4	P-O1	2.10	1.55	1.50
5	B	900	PLP	C5-C4	-2.05	1.38	1.40

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1998	ASO	C1-O5-C5	11.46	127.54	112.19
3	B	2998	ASO	C1-O5-C5	9.04	124.30	112.19
3	B	2998	ASO	O5-C1-C2	5.20	123.20	110.79
3	A	1998	ASO	O5-C1-C2	4.41	121.30	110.79
3	A	1998	ASO	O2-C2-C3	4.31	119.07	110.15
5	B	900	PLP	C3-C4-C5	4.26	123.70	118.59
3	B	2998	ASO	O2-C2-C3	4.22	118.90	110.15
5	A	900	PLP	C3-C2-N1	-4.12	115.76	120.96
3	A	1998	ASO	C1-C2-C3	4.09	115.61	109.64
3	B	2998	ASO	C1-C2-C3	3.83	115.23	109.64
5	B	900	PLP	C4A-C4-C3	-3.46	114.76	120.52
5	B	900	PLP	C3-C2-N1	-3.40	116.68	120.96
5	A	900	PLP	C4A-C4-C3	-3.17	115.25	120.52
5	A	900	PLP	C3-C4-C5	3.09	122.30	118.59
5	B	900	PLP	C6-C5-C4	-3.07	115.58	118.10
5	B	900	PLP	C6-N1-C2	3.00	124.63	119.20
3	A	1998	ASO	C6-C5-C4	2.87	120.08	113.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	900	PLP	C6-N1-C2	2.83	124.34	119.20
5	A	900	PLP	C2A-C2-N1	2.58	122.50	117.64
5	B	900	PLP	C5-C6-N1	-2.49	119.78	123.83
5	A	900	PLP	C6-C5-C4	-2.28	116.23	118.10
3	A	1998	ASO	C2-C3-C4	2.27	114.84	110.86
3	B	2998	ASO	O3-C3-C2	-2.03	105.90	110.05

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1998	ASO	O5-C5-C6-O6
3	A	1998	ASO	C4-C5-C6-O6
5	A	900	PLP	C6-C5-C5A-O4P

There are no ring outliers.

2 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1998	ASO	3	0
3	B	2998	ASO	6	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, 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%)	-0.04	5 (0%) 85 89	20, 31, 50, 67	0
1	B	796/796 (100%)	-0.05	9 (1%) 78 83	20, 31, 49, 67	0
All	All	1592/1592 (100%)	-0.04	14 (0%) 81 85	20, 31, 49, 67	0

All (14) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	187	LYS	4.9
1	B	57	ASN	4.5
1	B	559	PRO	3.4
1	B	189	GLY	3.0
1	A	473	GLN	2.4
1	A	688	ALA	2.4
1	B	382	VAL	2.4
1	B	562	ASP	2.3
1	A	555	ILE	2.3
1	B	55	VAL	2.2
1	A	51	PHE	2.1
1	B	558	ASN	2.1
1	B	186	THR	2.1
1	A	763	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.

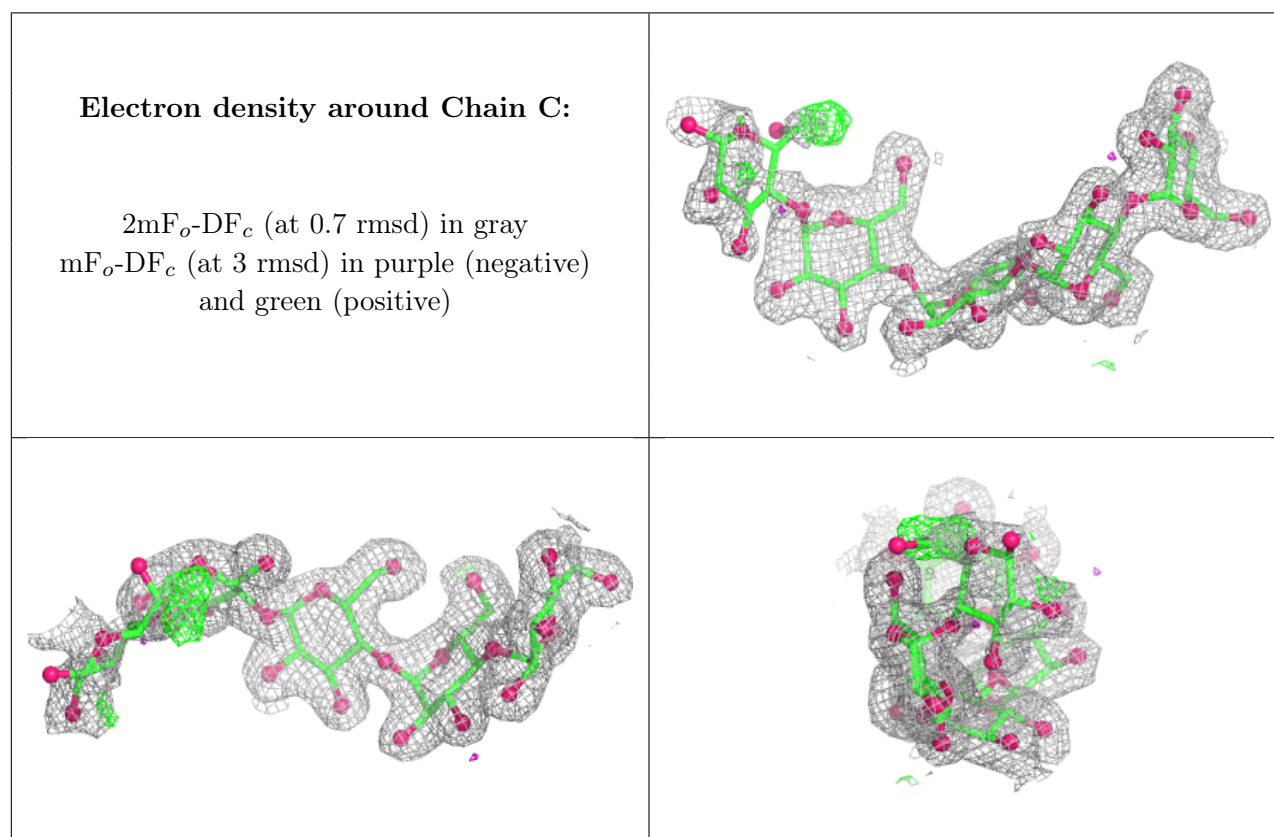
6.3 Carbohydrates [i](#)

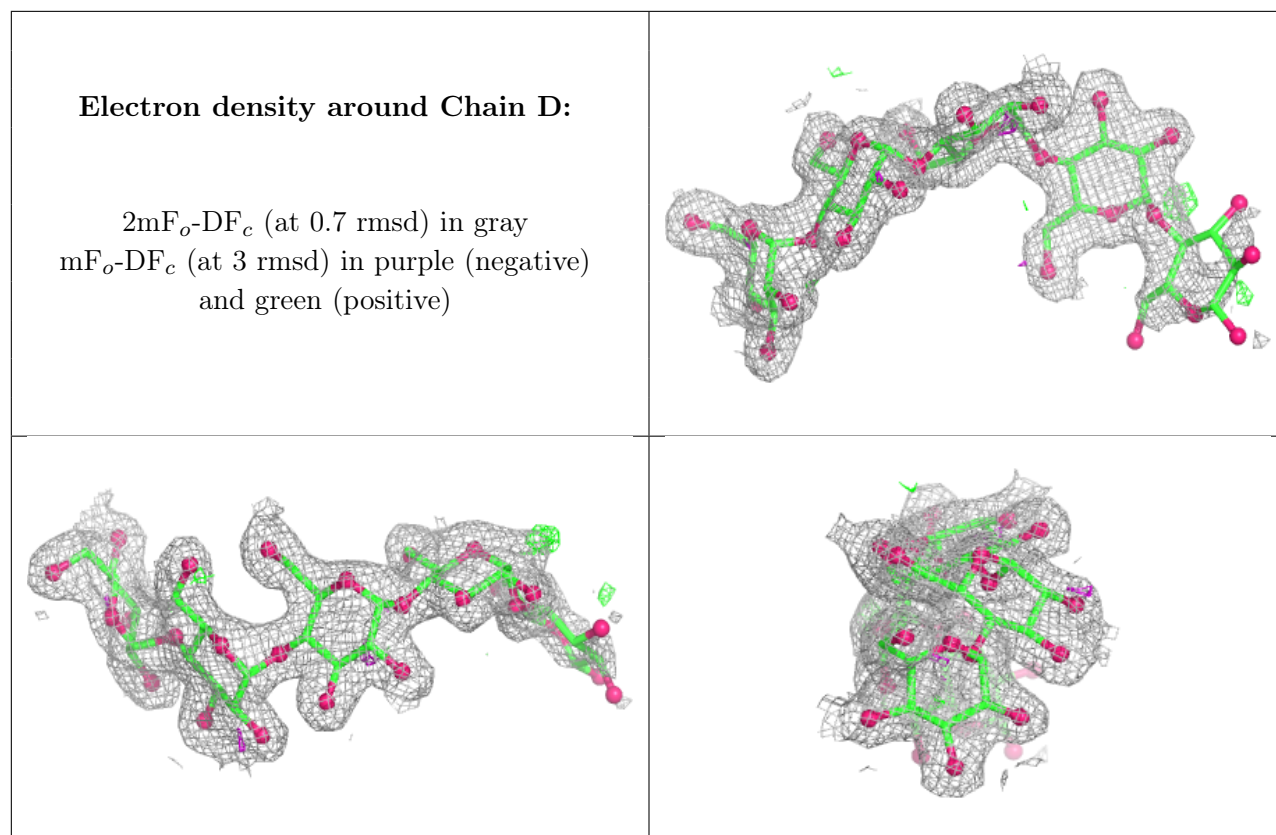
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum,

median, 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	BGC	C	1	12/12	0.43	0.22	49,53,54,54	10
2	BGC	D	1	12/12	0.67	0.19	49,53,54,55	10
2	GLC	C	3	11/12	0.92	0.08	30,32,34,35	0
2	GLC	D	2	11/12	0.92	0.07	38,40,43,44	0
2	GLC	D	4	11/12	0.92	0.07	31,32,36,36	0
2	GLC	D	3	11/12	0.93	0.07	30,34,37,39	0
2	GLC	C	5	11/12	0.94	0.07	27,28,31,35	0
2	GLC	C	2	11/12	0.95	0.06	34,37,41,42	0
2	GLC	D	5	11/12	0.95	0.06	26,30,31,34	0
2	GLC	C	4	11/12	0.96	0.06	28,30,32,35	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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	ASO	B	2998	11/11	0.88	0.11	34,41,45,47	0
3	ASO	A	1998	11/11	0.91	0.09	29,39,42,43	0
4	PO4	A	999	5/5	0.97	0.06	31,33,38,38	0
5	PLP	A	900	15/16	0.97	0.06	21,24,32,32	0
5	PLP	B	900	15/16	0.97	0.06	21,24,31,31	0
4	PO4	B	1999	5/5	0.98	0.05	30,33,36,38	0

6.5 Other polymers [i](#)

There are no such residues in this entry.