



Full wwPDB X-ray Structure Validation Report ⓘ

Sep 21, 2020 – 05:02 PM BST

PDB ID : 5LRB
Title : Plastidial phosphorylase from Barley in complex with acarbose
Authors : Cuesta-Seijo, J.A.; Ruzanski, C.; Kruzewicz, K.; Palcic, M.M.
Deposited on : 2016-08-18
Resolution : 2.90 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The 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 : 2.14.6
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) : 2.14.6

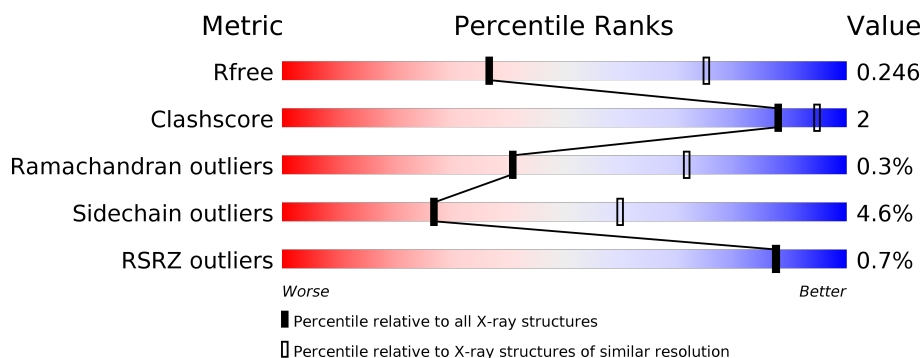
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1957 (2.90-2.90)
Clashscore	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)
RSRZ outliers	127900	1906 (2.90-2.90)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on 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	938	<div> <div style="width: 100%; height: 10px; background-color: red;"></div> <div style="display: flex; justify-content: space-between; align-items: center;"> % <div style="width: 82%; height: 10px; background-color: green;"></div> <div style="width: 8%; height: 10px; background-color: yellow;"></div> <div style="width: 10%; height: 10px; background-color: grey;"></div> </div> <div style="display: flex; justify-content: space-between; align-items: center;"> 82% 8% 10% </div> </div>
1	B	938	<div> <div style="width: 100%; height: 10px; background-color: red;"></div> <div style="display: flex; justify-content: space-between; align-items: center;"> % <div style="width: 81%; height: 10px; background-color: green;"></div> <div style="width: 8%; height: 10px; background-color: yellow;"></div> <div style="width: 10%; height: 10px; background-color: grey;"></div> </div> <div style="display: flex; justify-content: space-between; align-items: center;"> 81% 8% 10% </div> </div>
2	C	3	<div> <div style="width: 100%; height: 10px; background-color: yellow;"></div> <div style="display: flex; justify-content: space-between; align-items: center;"> 100% </div> </div>
2	D	3	<div> <div style="width: 100%; height: 10px; background-color: green;"></div> <div style="display: flex; justify-content: space-between; align-items: center;"> 33% 33% 33% </div> </div>

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
2	GLC	C	1	-	-	-	X
2	GLC	C	2	-	-	-	X
2	GLC	D	1	-	-	-	X
2	GLC	D	2	-	-	-	X
3	GLC	B	1001	X	-	-	X

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 13689 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 Alpha-1,4 glucan phosphorylase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	844	Total	C	N	O	S	0	5	1
			6744	4296	1148	1270	30			
1	B	844	Total	C	N	O	S	0	6	1
			6747	4298	1146	1273	30			

There are 26 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	43	MET	-	initiating methionine	UNP F2E0G2
A	969	THR	-	expression tag	UNP F2E0G2
A	970	PHE	-	expression tag	UNP F2E0G2
A	971	PRO	-	expression tag	UNP F2E0G2
A	972	ASP	-	expression tag	UNP F2E0G2
A	973	ILE	-	expression tag	UNP F2E0G2
A	974	GLU	-	expression tag	UNP F2E0G2
A	975	ASN	-	expression tag	UNP F2E0G2
A	976	LEU	-	expression tag	UNP F2E0G2
A	977	TYR	-	expression tag	UNP F2E0G2
A	978	PHE	-	expression tag	UNP F2E0G2
A	979	GLN	-	expression tag	UNP F2E0G2
A	980	GLY	-	expression tag	UNP F2E0G2
B	43	MET	-	initiating methionine	UNP F2E0G2
B	969	THR	-	expression tag	UNP F2E0G2
B	970	PHE	-	expression tag	UNP F2E0G2
B	971	PRO	-	expression tag	UNP F2E0G2
B	972	ASP	-	expression tag	UNP F2E0G2
B	973	ILE	-	expression tag	UNP F2E0G2
B	974	GLU	-	expression tag	UNP F2E0G2
B	975	ASN	-	expression tag	UNP F2E0G2
B	976	LEU	-	expression tag	UNP F2E0G2
B	977	TYR	-	expression tag	UNP F2E0G2
B	978	PHE	-	expression tag	UNP F2E0G2
B	979	GLN	-	expression tag	UNP F2E0G2

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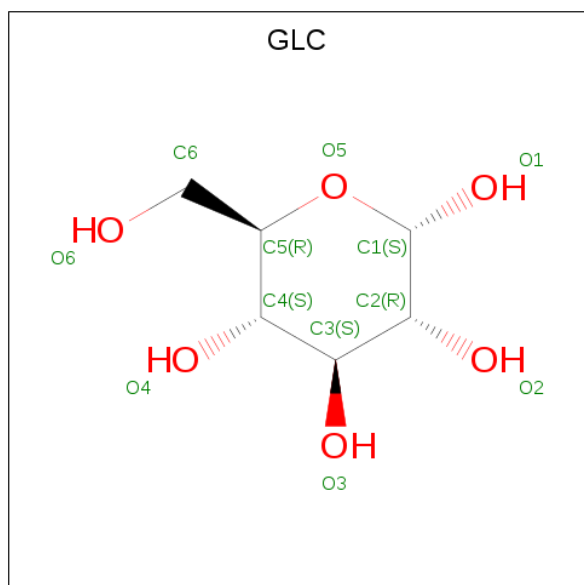
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Chain	Residue	Modelled	Actual	Comment	Reference
B	980	GLY	-	expression tag	UNP F2E0G2

- Molecule 2 is an oligosaccharide called 4,6-dideoxy-4- $\{[(1S,4R,5S,6S)-4,5,6\text{-trihydroxy-3-(hydroxymethyl)cyclohex-2-en-1-yl]amino}\}$ - α -D-glucopyranose-(1-4)- α -D-glucopyranose-(1-4)- α -D-glucopyranose.

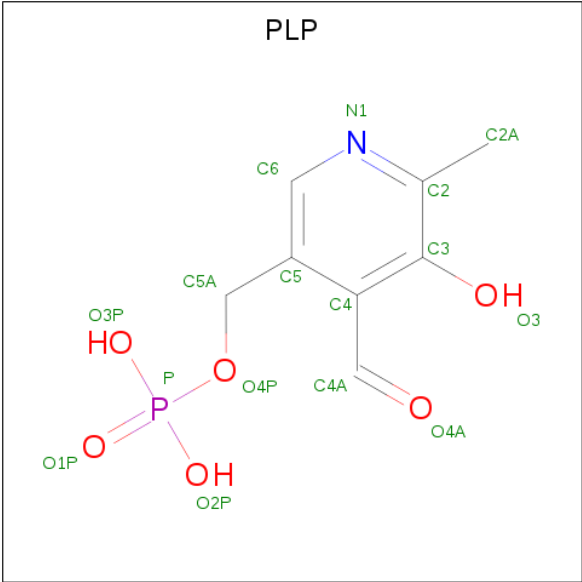
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	C	3	Total	C	N	O	0	0	0
			44	25	1	18			
2	D	3	Total	C	N	O	0	0	0
			44	25	1	18			

- Molecule 3 is α -D-glucopyranose (three-letter code: GLC) (formula: $C_6H_{12}O_6$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			12	6	6		
3	B	1	Total	C	O	0	0
			12	6	6		

- 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		

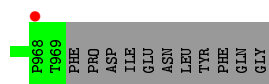
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	28	Total	O	0	0
			28	28		
5	B	28	Total	O	0	0
			28	28		

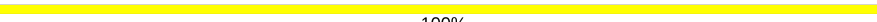
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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.

- Chain A: 

- Chain B:
-
- | Amino Acid | Percentage |
|------------|------------|
| GLU | 81% |
| SER | 8% |
| ILE | 10% |
| ALA | |
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| ALA | |
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| LYS | |
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- Molecule 2: 4,6-dideoxy-4-[(1S,4R,5S,6S)-4,5,6-trihydroxy-3-(hydroxymethyl)cyclohex-2-en-1-yl]amino}-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose

Chain C:  100%



- Molecule 2: 4,6-dideoxy-4-[(1S,4R,5S,6S)-4,5,6-trihydroxy-3-(hydroxymethyl)cyclohex-2-en-1-yl]amino}-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose

Chain D:  33% 33% 33%



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	230.33Å 63.68Å 149.33Å 90.00° 115.07° 90.00°	Depositor
Resolution (Å)	48.92 – 2.90 48.92 – 2.90	Depositor EDS
% Data completeness (in resolution range)	98.2 (48.92-2.90) 98.2 (48.92-2.90)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.16 (at 2.91Å)	Xtriage
Refinement program	REFMAC 5.7.0032	Depositor
R, R_{free}	0.213 , 0.246 0.218 , 0.246	Depositor DCC
R_{free} test set	1297 reflections (3.00%)	wwPDB-VP
Wilson B-factor (Å ²)	76.2	Xtriage
Anisotropy	0.046	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 37.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	13689	wwPDB-VP
Average B, all atoms (Å ²)	77.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 52.47 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 4.8395e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: AC1, 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	0.37	0/6914	0.57	0/9365
1	B	0.37	0/6920	0.56	0/9374
All	All	0.37	0/13834	0.56	0/18739

There are no bond length outliers.

There are no bond angle outliers.

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	6744	0	6642	25	0
1	B	6747	0	6641	28	0
2	C	44	0	30	0	0
2	D	44	0	30	1	0
3	A	12	0	12	0	0
3	B	12	0	11	0	0
4	A	15	0	6	1	0
4	B	15	0	6	0	0
5	A	28	0	0	0	0
5	B	28	0	0	1	0
All	All	13689	0	13378	54	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 2.

All (54) 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:A:422:THR:HG21	1:A:427:ALA:HB3	1.67	0.74
1:A:140:ARG:O	1:A:619:ARG:NH1	2.28	0.66
1:B:140:ARG:O	1:B:619:ARG:NH1	2.29	0.66
1:B:802:THR:HB	1:B:805:MET:HG3	1.85	0.58
1:B:146:ILE:CG2	1:B:152:THR:HA	2.38	0.53
1:B:422:THR:HG21	1:B:427:ALA:HB3	1.92	0.52
1:A:943:SER:N	1:A:944:PRO:CD	2.73	0.51
1:B:177:ALA:HB1	1:B:211:GLY:HA3	1.93	0.50
1:A:878:ARG:NH2	1:A:895:GLU:OE2	2.45	0.50
1:B:943:SER:N	1:B:944:PRO:CD	2.74	0.50
1:B:428:LEU:HA	5:B:1117:HOH:O	2.10	0.50
1:A:423:VAL:HG23	1:A:591:ILE:HG21	1.94	0.50
2:D:1:GLC:H61	2:D:2:GLC:H5	1.93	0.50
1:B:849:ALA:HB3	1:B:850:PRO:HD3	1.93	0.49
1:A:454:LEU:HD22	1:A:576:VAL:HG21	1.95	0.49
1:B:110:LEU:HD22	1:B:279:PRO:HB3	1.95	0.49
1:A:885:SER:O	1:A:886:ASN:ND2	2.44	0.49
1:B:208:TYR:CE2	1:B:328:LEU:HD13	2.47	0.49
1:A:146:ILE:CG2	1:A:152:THR:HA	2.43	0.48
1:A:733:VAL:HG11	1:A:926:TYR:CD2	2.48	0.47
1:B:454:LEU:HD22	1:B:576:VAL:HG21	1.98	0.46
1:B:805:MET:CE	1:B:856:ARG:HH22	2.29	0.46
1:B:423:VAL:HG23	1:B:591:ILE:HG21	1.97	0.46
1:B:878:ARG:NH1	1:B:895:GLU:OE2	2.48	0.46
1:A:805:MET:CE	1:A:856:ARG:HH22	2.29	0.46
1:B:697:VAL:HG13	1:B:782:TYR:CZ	2.52	0.45
1:A:177:ALA:HB1	1:A:211:GLY:HA3	1.98	0.45
1:B:422:THR:HG22	1:B:424:LEU:H	1.80	0.45
1:A:697:VAL:HG13	1:A:782:TYR:CZ	2.51	0.45
1:B:759:ASP:OD2	1:B:887:TYR:OH	2.28	0.45
1:A:759:ASP:OD2	1:A:887:TYR:OH	2.30	0.45
1:A:384:THR:OG1	1:A:429:GLU:HB2	2.18	0.44
1:B:384:THR:OG1	1:B:429:GLU:HB2	2.17	0.44
1:A:208:TYR:CE2	1:A:328:LEU:HD13	2.52	0.44
1:B:573:LEU:O	1:B:573:LEU:HD12	2.18	0.44
1:A:814:LYS:NZ	4:A:1002:PLP:O3	2.51	0.44
1:A:791:ILE:HB	1:A:792:PRO:HD3	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:433:LEU:O	1:A:437:GLN:HB2	2.18	0.43
1:B:618:ARG:O	1:B:623:PHE:CD2	2.72	0.43
1:B:791:ILE:HB	1:B:792:PRO:HD3	2.01	0.43
1:A:702:GLU:OE2	1:A:749:GLN:HG2	2.19	0.43
1:B:812:ASN:ND2	1:B:830:ASN:OD1	2.51	0.43
1:A:744:PHE:CD2	1:A:746:THR:HG22	2.54	0.42
1:A:405:TRP:CH2	1:A:449:THR:HB	2.53	0.42
1:A:802:THR:HB	1:A:805:MET:HG3	2.01	0.42
1:B:691:ALA:HB3	1:B:736:VAL:HG23	2.01	0.42
1:A:455:MET:CE	1:A:485:LEU:HD22	2.50	0.41
1:B:645:THR:O	1:B:645:THR:HG22	2.21	0.41
1:A:744:PHE:HD2	1:A:746:THR:HG22	1.85	0.41
1:B:146:ILE:HG22	1:B:152:THR:HA	2.03	0.40
1:A:176:PRO:HA	1:A:229:TRP:CE3	2.56	0.40
1:B:754:VAL:O	1:B:758:THR:HG23	2.21	0.40
1:B:478:ARG:HD2	1:B:480:LEU:O	2.22	0.40
1:B:885:SER:O	1:B:886:ASN:OD1	2.38	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	845/938 (90%)	808 (96%)	36 (4%)	1 (0%)	51	82
1	B	846/938 (90%)	807 (95%)	35 (4%)	4 (0%)	29	61
All	All	1691/1876 (90%)	1615 (96%)	71 (4%)	5 (0%)	41	71

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	258	ASP

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Mol	Chain	Res	Type
1	A	259	GLY
1	B	259	GLY
1	B	257	THR
1	B	464	THR

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	729/810 (90%)	694 (95%)	35 (5%)	25	58
1	B	730/810 (90%)	696 (95%)	34 (5%)	26	59
All	All	1459/1620 (90%)	1390 (95%)	69 (5%)	27	59

All (69) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	137	LEU
1	A	175	ASP
1	A	183	LEU
1	A	209	ARG
1	A	216	ILE
1	A	219	LYS
1	A	222	GLN
1	A	248	LYS
1	A	358	SER
1	A	371	GLU
1	A	388	LEU
1	A	413	GLU
1	A	437	GLN
1	A	473	LYS
1	A	563	GLN
1	A	569	ARG
1	A	606	THR
1	A	619	ARG
1	A	622	ARG

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Mol	Chain	Res	Type
1	A	633	SER
1	A	651	LEU
1	A	697	VAL
1	A	698	LYS
1	A	699[A]	ARG
1	A	699[B]	ARG
1	A	703	TYR
1	A	730	LYS
1	A	746	THR
1	A	747	TYR
1	A	772	ASP
1	A	812	ASN
1	A	857	GLN
1	A	886	ASN
1	A	930	LYS
1	A	950	ARG
1	B	143	THR
1	B	175	ASP
1	B	183	LEU
1	B	209	ARG
1	B	216	ILE
1	B	219	LYS
1	B	222	GLN
1	B	248	LYS
1	B	315	ASN
1	B	358	SER
1	B	371	GLU
1	B	383	ASP
1	B	388	LEU
1	B	413	GLU
1	B	437	GLN
1	B	473	LYS
1	B	491	LYS
1	B	563	GLN
1	B	569	ARG
1	B	619	ARG
1	B	622	ARG
1	B	697	VAL
1	B	698	LYS
1	B	703	TYR
1	B	730	LYS
1	B	746	THR

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Mol	Chain	Res	Type
1	B	747	TYR
1	B	812	ASN
1	B	857	GLN
1	B	886	ASN
1	B	898[A]	GLU
1	B	898[B]	GLU
1	B	930	LYS
1	B	950	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	406	ASN
1	A	437	GLN
1	A	613	ASN
1	B	613	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

2 non-standard protein/DNA/RNA residues 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	GLC	B	1001	-	12,12,12	0.59	0	17,17,17	2.36	5 (29%)
3	GLC	A	1001	-	12,12,12	0.57	0	17,17,17	0.97	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns.

'-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	GLC	B	1001	-	1/1/5/5	2/2/22/22	0/1/1/1
3	GLC	A	1001	-	-	2/2/22/22	0/1/1/1

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	1001	GLC	O5-C1-C2	7.56	123.78	110.28
3	B	1001	GLC	O1-C1-C2	2.92	117.25	109.03
3	B	1001	GLC	O1-C1-O5	2.66	118.36	110.38
3	B	1001	GLC	C3-C4-C5	-2.56	105.68	110.24
3	B	1001	GLC	O5-C5-C6	2.21	111.92	106.44

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	B	1001	GLC	C1

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	1001	GLC	O5-C5-C6-O6
3	B	1001	GLC	C4-C5-C6-O6
3	A	1001	GLC	O5-C5-C6-O6
3	A	1001	GLC	C4-C5-C6-O6

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates

6 monosaccharides are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	GLC	C	1	2	12,12,12	0.58	0	17,17,17	1.04	1 (5%)
2	GLC	C	2	2	11,11,12	0.46	0	15,15,17	1.44	3 (20%)
2	AC1	C	3	2	21,22,23	0.73	0	22,32,34	1.17	1 (4%)
2	GLC	D	1	2	12,12,12	0.56	0	17,17,17	0.55	0
2	GLC	D	2	2	11,11,12	0.54	0	15,15,17	1.20	2 (13%)
2	AC1	D	3	2	21,22,23	0.69	0	22,32,34	0.61	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	GLC	C	1	2	-	1/2/22/22	0/1/1/1
2	GLC	C	2	2	-	2/2/19/22	0/1/1/1
2	AC1	C	3	2	-	2/6/43/46	0/2/2/2
2	GLC	D	1	2	-	0/2/22/22	0/1/1/1
2	GLC	D	2	2	-	1/2/19/22	0/1/1/1
2	AC1	D	3	2	-	3/6/43/46	0/2/2/2

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	3	AC1	C1-C2-C3	4.30	114.95	109.67
2	C	2	GLC	C1-C2-C3	3.41	113.85	109.67
2	D	2	GLC	C1-O5-C5	3.15	116.46	112.19
2	D	2	GLC	C1-C2-C3	2.60	112.86	109.67
2	C	2	GLC	O5-C5-C6	2.51	111.14	107.20
2	C	2	GLC	C1-O5-C5	2.38	115.41	112.19
2	C	1	GLC	C4-C3-C2	-2.09	107.18	110.82

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	D	3	AC1	C3-C4-N4A-C1B
2	D	3	AC1	C5-C4-N4A-C1B
2	D	3	AC1	C7B-C1B-N4A-C4

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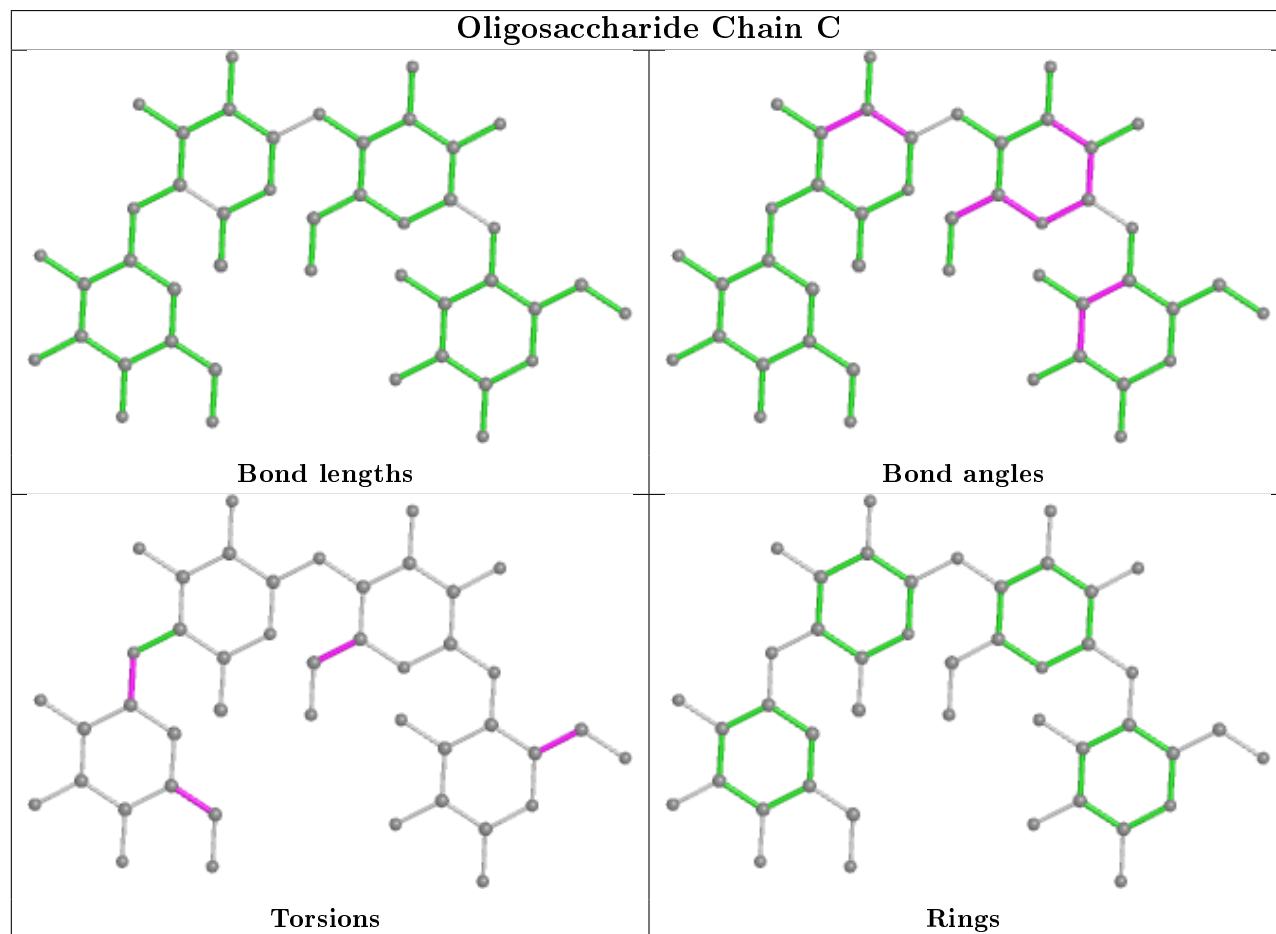
Mol	Chain	Res	Type	Atoms
2	C	3	AC1	C2B-C1B-N4A-C4
2	C	3	AC1	C7B-C5B-C6B-O6B
2	C	2	GLC	O5-C5-C6-O6
2	C	2	GLC	C4-C5-C6-O6
2	C	1	GLC	O5-C5-C6-O6
2	D	2	GLC	O5-C5-C6-O6

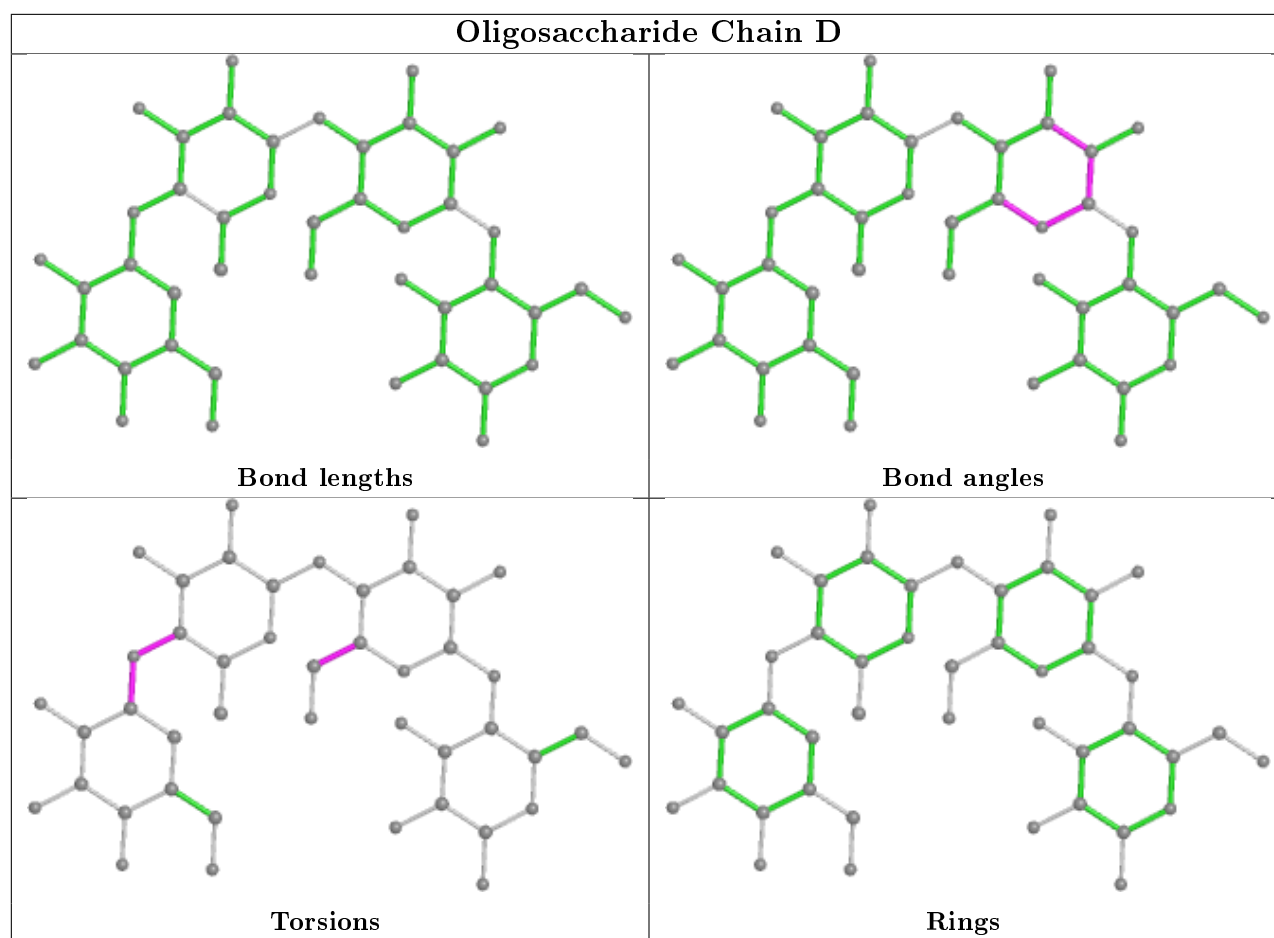
There are no ring outliers.

2 monomers are involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	1	GLC	1	0
2	D	2	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 [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	B	1002	1	15,15,16	2.89	3 (20%)	20,22,23	1.36	3 (15%)
3	GLC	B	1001	-	12,12,12	0.59	0	17,17,17	2.36	5 (29%)
3	GLC	A	1001	-	12,12,12	0.57	0	17,17,17	0.97	0
4	PLP	A	1002	1	15,15,16	2.75	3 (20%)	20,22,23	1.59	3 (15%)

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	B	1002	1	-	3/6/6/8	0/1/1/1
3	GLC	B	1001	-	1/1/5/5	2/2/22/22	0/1/1/1
3	GLC	A	1001	-	-	2/2/22/22	0/1/1/1
4	PLP	A	1002	1	-	4/6/6/8	0/1/1/1

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1002	PLP	C5-C4	7.57	1.48	1.40
4	B	1002	PLP	C3-C2	7.53	1.48	1.40
4	B	1002	PLP	C5-C4	7.06	1.48	1.40
4	A	1002	PLP	C3-C2	6.37	1.47	1.40
4	B	1002	PLP	C3-C4	3.56	1.47	1.40
4	A	1002	PLP	C3-C4	2.86	1.46	1.40

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	1001	GLC	O5-C1-C2	7.56	123.78	110.28
4	A	1002	PLP	C4A-C4-C5	3.98	125.04	120.94
3	B	1001	GLC	O1-C1-C2	2.92	117.25	109.03
3	B	1001	GLC	O1-C1-O5	2.66	118.36	110.38
3	B	1001	GLC	C3-C4-C5	-2.56	105.68	110.24
4	B	1002	PLP	C4A-C4-C5	2.34	123.34	120.94
3	B	1001	GLC	O5-C5-C6	2.21	111.92	106.44
4	A	1002	PLP	C6-N1-C2	2.17	123.18	119.17
4	B	1002	PLP	C3-C4-C5	-2.03	116.55	118.74
4	A	1002	PLP	O3-C3-C2	2.02	121.89	117.49
4	B	1002	PLP	C6-C5-C4	2.01	119.74	118.16

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	B	1001	GLC	C1

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	1002	PLP	C5A-O4P-P-O2P
4	B	1002	PLP	C5A-O4P-P-O3P
4	A	1002	PLP	C5A-O4P-P-O2P
4	A	1002	PLP	C5A-O4P-P-O3P
3	B	1001	GLC	O5-C5-C6-O6
3	B	1001	GLC	C4-C5-C6-O6
3	A	1001	GLC	O5-C5-C6-O6
4	B	1002	PLP	C5A-O4P-P-O1P
4	A	1002	PLP	C4-C5-C5A-O4P
3	A	1001	GLC	C4-C5-C6-O6
4	A	1002	PLP	C6-C5-C5A-O4P

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1002	PLP	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	844/938 (89%)	-0.09	5 (0%) 89 89	51, 74, 106, 130	0
1	B	844/938 (89%)	-0.10	7 (0%) 86 86	48, 75, 108, 134	0
All	All	1688/1876 (89%)	-0.09	12 (0%) 87 87	48, 74, 107, 134	0

All (12) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	257	THR	2.8
1	B	259	GLY	2.8
1	A	254	VAL	2.6
1	A	264	ILE	2.4
1	B	425	PRO	2.4
1	B	968	PRO	2.3
1	B	937	ILE	2.3
1	A	370	TRP	2.2
1	B	370	TRP	2.2
1	B	367	SER	2.1
1	B	467	ILE	2.1
1	A	645	THR	2.0

6.2 Non-standard residues in protein, DNA, RNA chains

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

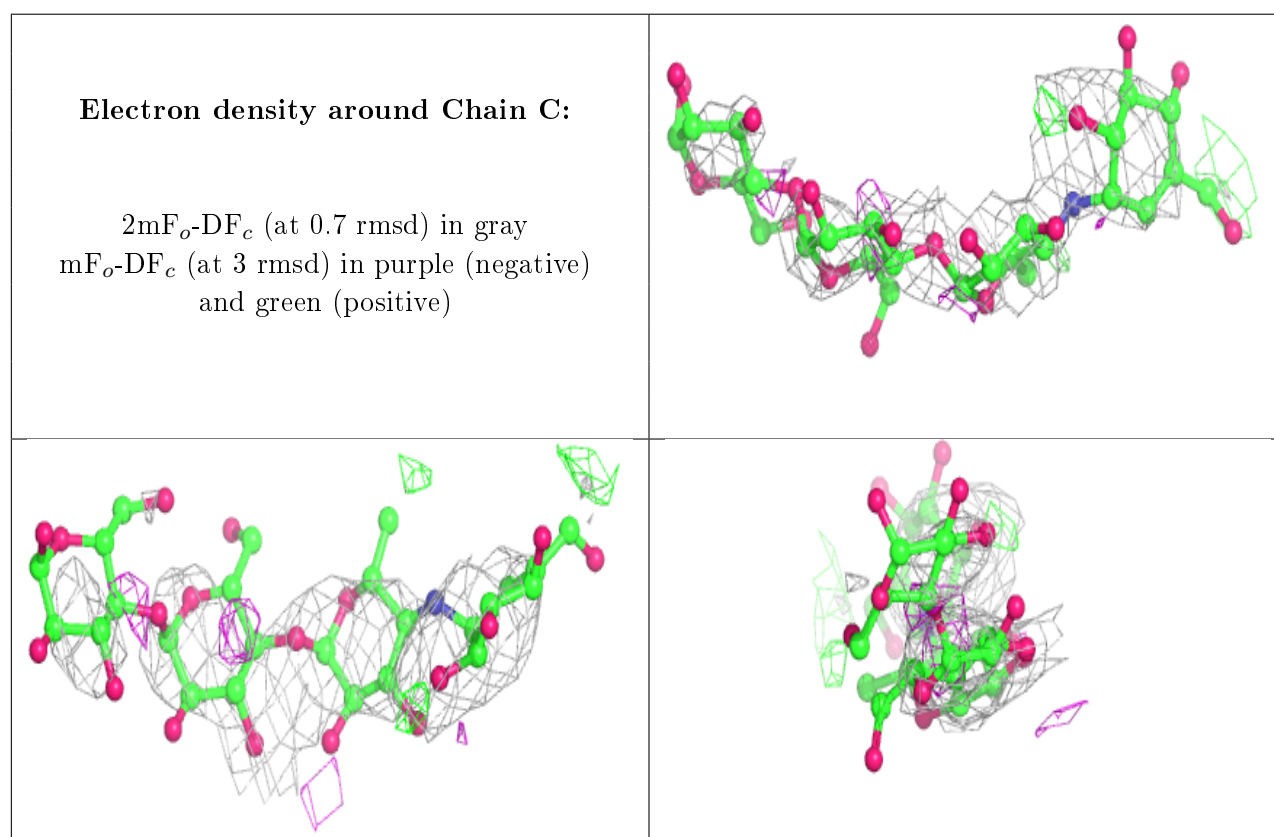
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	GLC	B	1001	12/12	0.69	0.43	106,121,127,135	0
3	GLC	A	1001	12/12	0.80	0.36	97,116,121,127	0

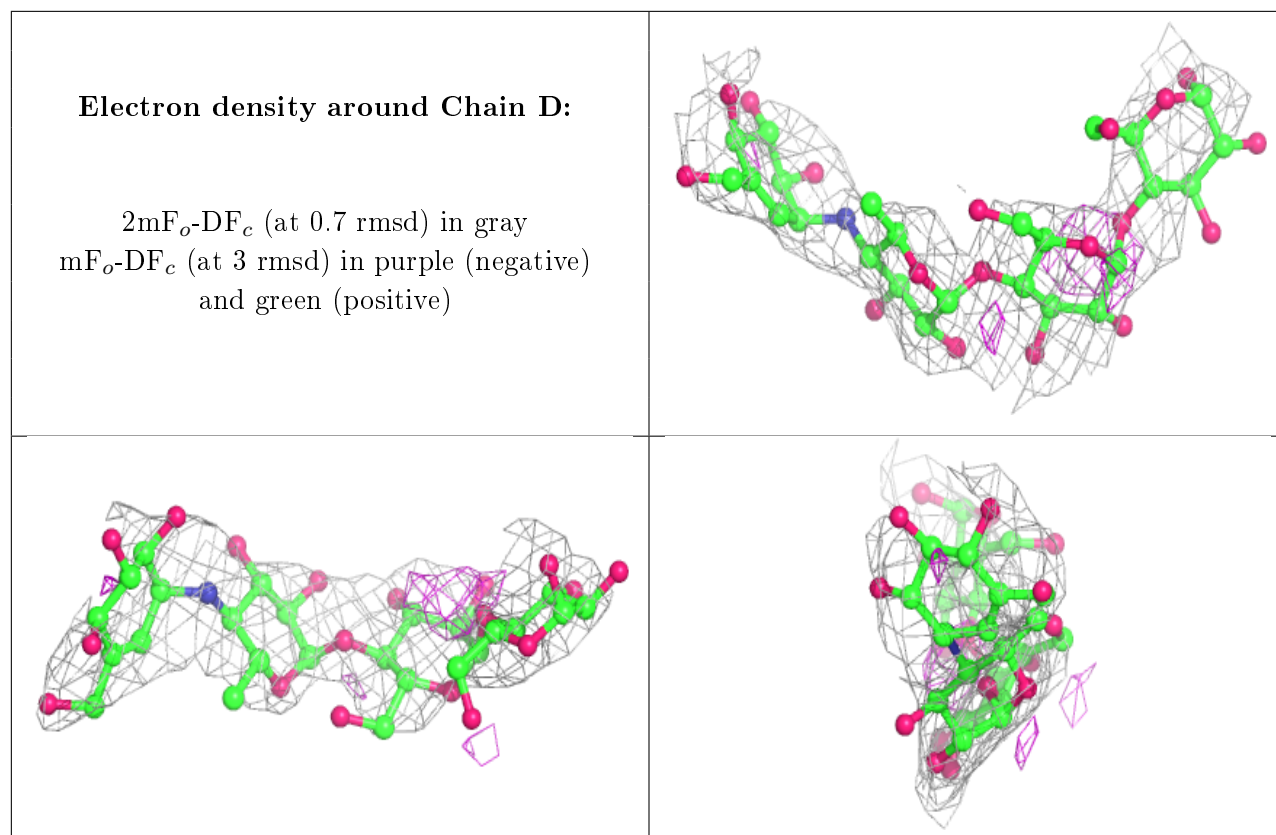
6.3 Carbohydrates ⓘ

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	GLC	D	1	12/12	0.60	0.41	150,157,165,166	0
2	GLC	C	1	12/12	0.62	0.56	159,167,172,173	0
2	GLC	C	2	11/12	0.66	0.45	148,165,168,169	0
2	AC1	D	3	21/22	0.73	0.30	121,135,145,148	0
2	GLC	D	2	11/12	0.73	0.48	146,152,157,158	0
2	AC1	C	3	21/22	0.75	0.35	127,151,168,171	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(\AA^2)	Q<0.9
3	GLC	B	1001	12/12	0.69	0.43	106,121,127,135	0
3	GLC	A	1001	12/12	0.80	0.36	97,116,121,127	0
4	PLP	B	1002	15/16	0.95	0.18	59,62,69,75	0
4	PLP	A	1002	15/16	0.96	0.20	57,62,69,72	0

6.5 Other polymers [i](#)

There are no such residues in this entry.