W O R L D W I D E
wwPDB
P R O T E I N   D A T A   B A N K

wwPDB X-ray Structure Validation Summary Report (i)

Mar 20, 2025 – 04:39 PM EDT

PDB ID	:	2ECP
Title	:	THE CRYSTAL STRUCTURE OF THE E. COLI MALTODEXTRIN PHOS-PHORYLASE COMPLEX
Authors	:	O'Reilly, M.; Watson, K.A.; Johnson, L.N.
Deposited on	:	1998-10-27
Resolution	:	2.95 Å(reported)

The following versions of software and data (see references (i)) were used in the production of this report:

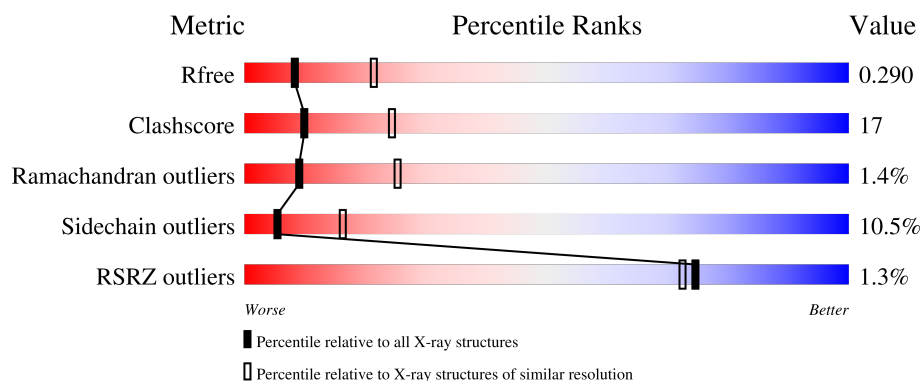|		
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.21
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.004 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.41.4

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 2.95 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	Percentile Ranks	Value
Rfree		0.290
Clashscore		17
Ramachandran outliers		1.4%
Sidechain outliers		10.5%
RSRZ outliers		1.3%

Worse   *Better*

▮ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	164625	1044 (2.98-2.94)
Clashscore	180529	1097 (2.98-2.94)
Ramachandran outliers	177936	1049 (2.98-2.94)
Sidechain outliers	177891	1049 (2.98-2.94)
RSRZ outliers	164620	1044 (2.98-2.94)

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

Mol	Chain	Length	Quality of chain
1	A	796	2% 53% 36% 10% •
1	B	796	% 51% 39% 7% •
2	C	3	33% 67%
2	D	3	33% 67%

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
2	GLC	C	1	X	-	-	-
2	GLC	D	1	X	-	-	-

2 Entry composition ⓘ

There are 5 unique types of molecules in this entry. The entry contains 12961 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
			6369	4065	1127	1157	20			
1	B	796	Total	C	N	O	S	0	0	0
			6369	4065	1127	1157	20			

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	205	ALA	LYS	conflict	UNP P00490
A	532	ASP	GLN	conflict	UNP P00490
A	582	ARG	HIS	conflict	UNP P00490
A	716	LYS	GLU	conflict	UNP P00490
A	828	ALA	LYS	conflict	UNP P00490
B	205	ALA	LYS	conflict	UNP P00490
B	532	ASP	GLN	conflict	UNP P00490
B	582	ARG	HIS	conflict	UNP P00490
B	716	LYS	GLU	conflict	UNP P00490
B	828	ALA	LYS	conflict	UNP P00490

- Molecule 2 is an oligosaccharide called 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.

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 GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).

GOL

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

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

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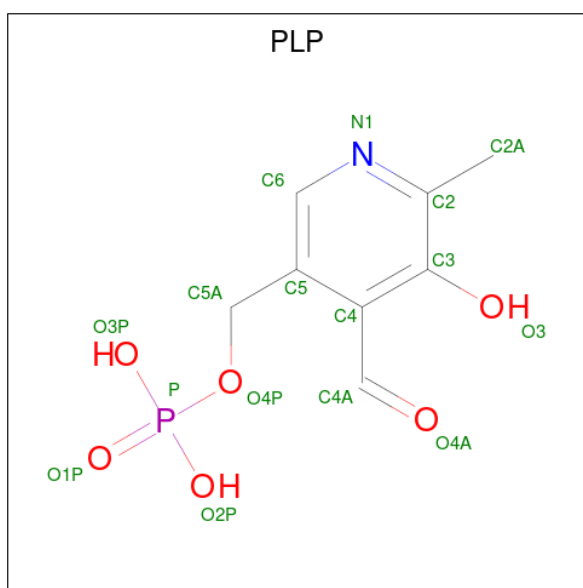
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total 15	C 8	N 1	O 5	P 1	0	0
4	B	1	Total 15	C 8	N 1	O 5	P 1	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	54	Total O 54 54	0	0
5	B	39	Total O 39 39	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

Chain B:

• 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:

• 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:
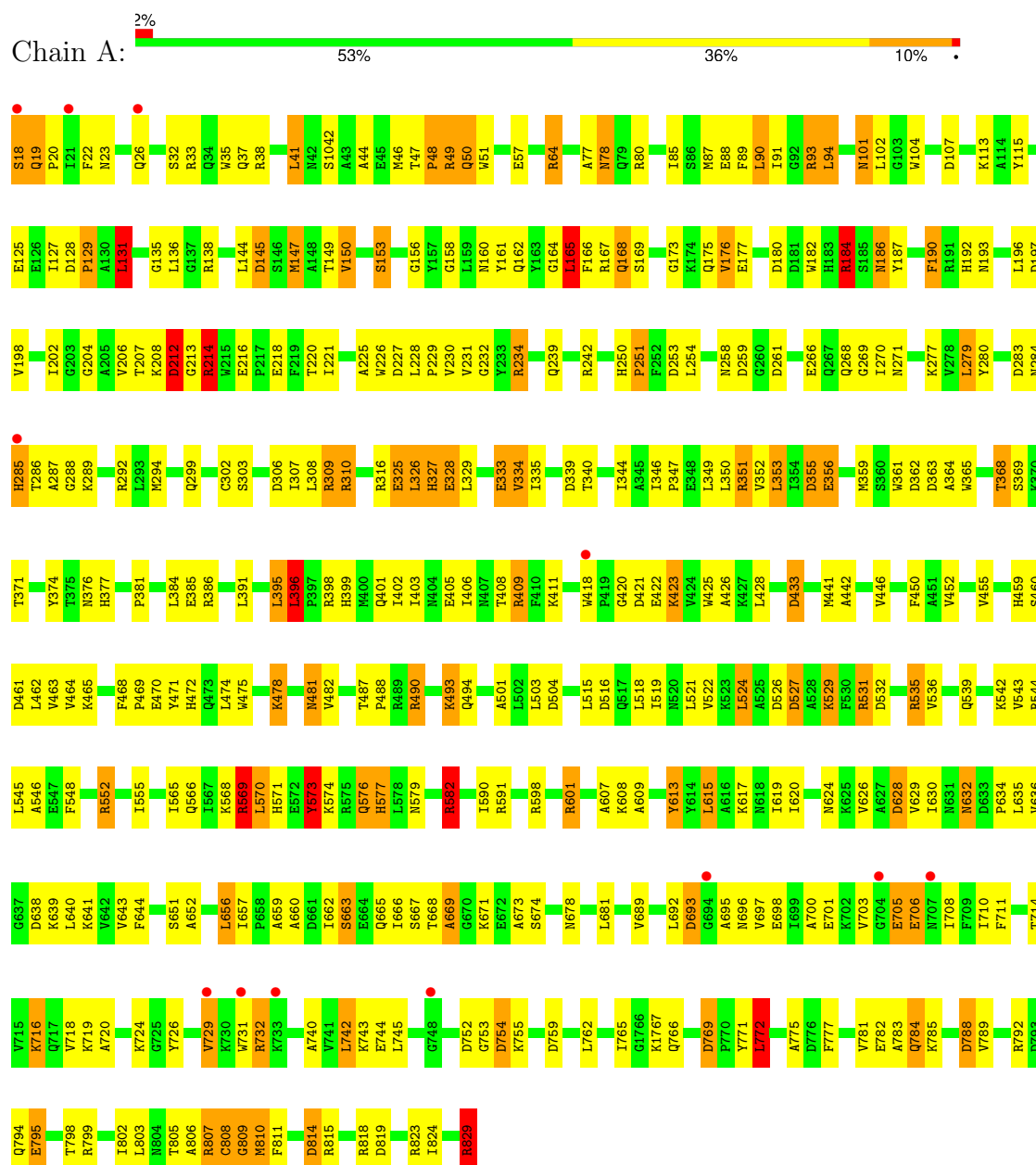
4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	76.49Å 105.84Å 217.72Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	15.00 – 2.95 15.00 – 2.95	Depositor EDS
% Data completeness (in resolution range)	88.9 (15.00-2.95) 87.7 (15.00-2.95)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.81 (at 2.96Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.241 , 0.293 0.242 , 0.290	Depositor DCC
R_{free} test set	852 reflections (2.55%)	wwPDB-VP
Wilson B-factor (Å^2)	52.5	Xtriage
Anisotropy	0.065	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 58.7	EDS
L-test for twinning[2]	$< |L| > = 0.40$, $< L^2 > = 0.23$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.88	EDS
Total number of atoms	12961	wwPDB-VP
Average B, all atoms (Å^2)	53.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.34% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.
[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: AC1, GOL, 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	0.77	1/6517 (0.0%)	1.99	165/8841 (1.9%)
1	B	0.75	1/6517 (0.0%)	2.12	163/8841 (1.8%)
All	All	0.76	2/13034 (0.0%)	2.05	328/17682 (1.9%)

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	1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	569	ARG	NE-CZ	-5.76	1.25	1.33
1	B	292	ARG	CD-NE	-5.03	1.38	1.46

The worst 5 of 328 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	292	ARG	NE-CZ-NH2	65.00	152.80	120.30
1	A	292	ARG	NE-CZ-NH2	46.98	143.79	120.30
1	B	569	ARG	NE-CZ-NH2	44.11	142.35	120.30
1	A	569	ARG	NE-CZ-NH1	32.74	136.67	120.30
1	B	292	ARG	NE-CZ-NH1	-32.15	104.22	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	516	ASP	Mainchain

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	6369	0	6324	223	0
1	B	6369	0	6324	220	0
2	C	44	0	30	2	0
2	D	44	0	30	5	0
3	A	6	0	8	2	0
3	B	6	0	8	0	0
4	A	15	0	6	1	0
4	B	15	0	6	3	0
5	A	54	0	0	11	0
5	B	39	0	0	9	0
All	All	12961	0	12736	439	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 17.

The worst 5 of 439 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:716:LYS:HE2	1:A:719:LYS:HD2	1.42	0.99
1:A:522:VAL:HG11	5:A:1777:HOH:O	1.61	0.97
1:B:310:ARG:HD2	5:B:1804:HOH:O	1.71	0.88
1:A:266:GLU:HG3	1:B:270:ILE:HD13	1.55	0.87
1:B:292:ARG:NH2	2:D:3:AC1:O2	2.09	0.85

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%)	729 (92%)	54 (7%)	11 (1%)	9	25
1	B	794/796 (100%)	725 (91%)	58 (7%)	11 (1%)	9	25
All	All	1588/1592 (100%)	1454 (92%)	112 (7%)	22 (1%)	9	25

5 of 22 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	423	LYS
1	B	423	LYS
1	A	285	HIS
1	A	421	ASP
1	B	207	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	665/665 (100%)	594 (89%)	71 (11%)	5	15
1	B	665/665 (100%)	596 (90%)	69 (10%)	5	16
All	All	1330/1330 (100%)	1190 (90%)	140 (10%)	5	16

5 of 140 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	579	ASN

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Mol	Chain	Res	Type
1	B	626	VAL
1	B	729	VAL
1	A	582	ARG
1	A	579	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 41 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	327	HIS
1	B	571	HIS
1	B	399	HIS
1	B	481	ASN
1	B	579	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 ⓘ

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	0.78	0	17,17,17	2.12	4 (23%)
2	GLC	C	2	2	11,11,12	1.43	1 (9%)	15,15,17	2.29	7 (46%)
2	AC1	C	3	2	21,22,23	1.28	2 (9%)	22,32,34	2.67	10 (45%)
2	GLC	D	1	2	12,12,12	0.76	0	17,17,17	2.07	7 (41%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#$\|Z\|>2$	Counts	RMSZ	#$\|Z\|>2$
2	GLC	D	2	2	11,11,12	1.04	1 (9%)	15,15,17	1.79	3 (20%)
2	AC1	D	3	2	21,22,23	1.76	6 (28%)	22,32,34	2.20	7 (31%)

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	1/1/5/5	1/2/22/22	0/1/1/1
2	GLC	C	2	2	-	0/2/19/22	0/1/1/1
2	AC1	C	3	2	-	3/6/43/46	0/2/2/2
2	GLC	D	1	2	1/1/5/5	1/2/22/22	0/1/1/1
2	GLC	D	2	2	-	0/2/19/22	0/1/1/1
2	AC1	D	3	2	-	3/6/43/46	0/2/2/2

The worst 5 of 10 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	3	AC1	C7B-C5B	3.80	1.38	1.32
2	D	3	AC1	C4A-C5B	3.57	1.54	1.51
2	C	2	GLC	C2-C3	3.22	1.57	1.52
2	C	3	AC1	C7B-C5B	2.99	1.37	1.32
2	D	3	AC1	O4-C4A	2.90	1.47	1.42

The worst 5 of 38 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	3	AC1	C7B-C1B-N4A	7.04	121.05	110.68
2	C	1	GLC	O3-C3-C4	5.28	122.82	110.38
2	D	1	GLC	O4-C4-C3	-5.17	98.18	110.38
2	C	2	GLC	C1-O5-C5	4.91	118.77	112.19
2	D	3	AC1	C7B-C1B-N4A	4.79	117.72	110.68

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	C	1	GLC	C1
2	D	1	GLC	C1

5 of 8 torsion outliers are listed below:

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

There are no ring outliers.

4 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	3	AC1	2	0
2	D	2	GLC	1	0
2	C	2	GLC	1	0
2	D	3	AC1	5	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.

Oligosaccharide Chain C

Bond lengths

Bond angles

Torsions

Rings

Oligosaccharide Chain D

Bond lengths

Bond angles

Torsions

Rings
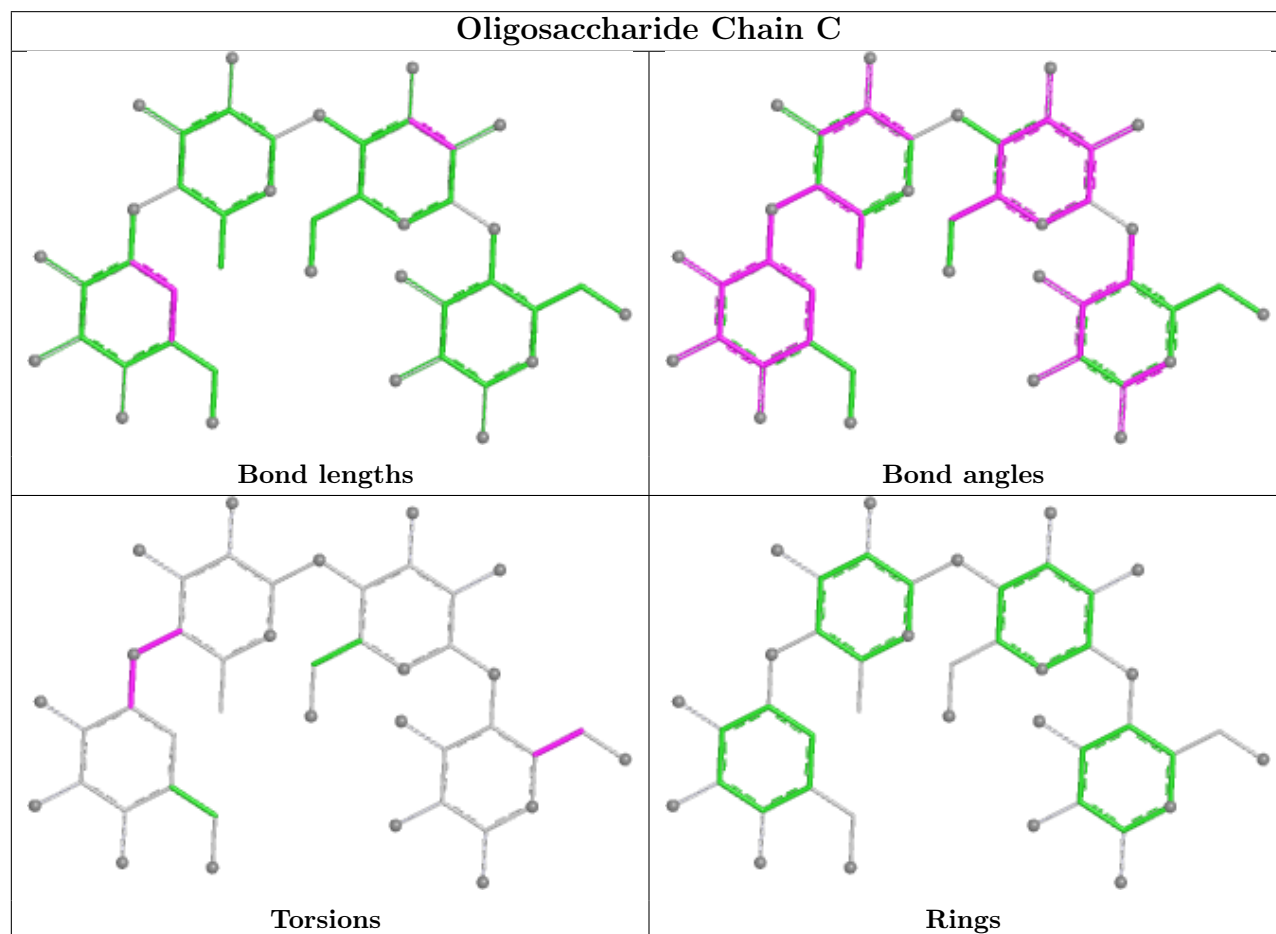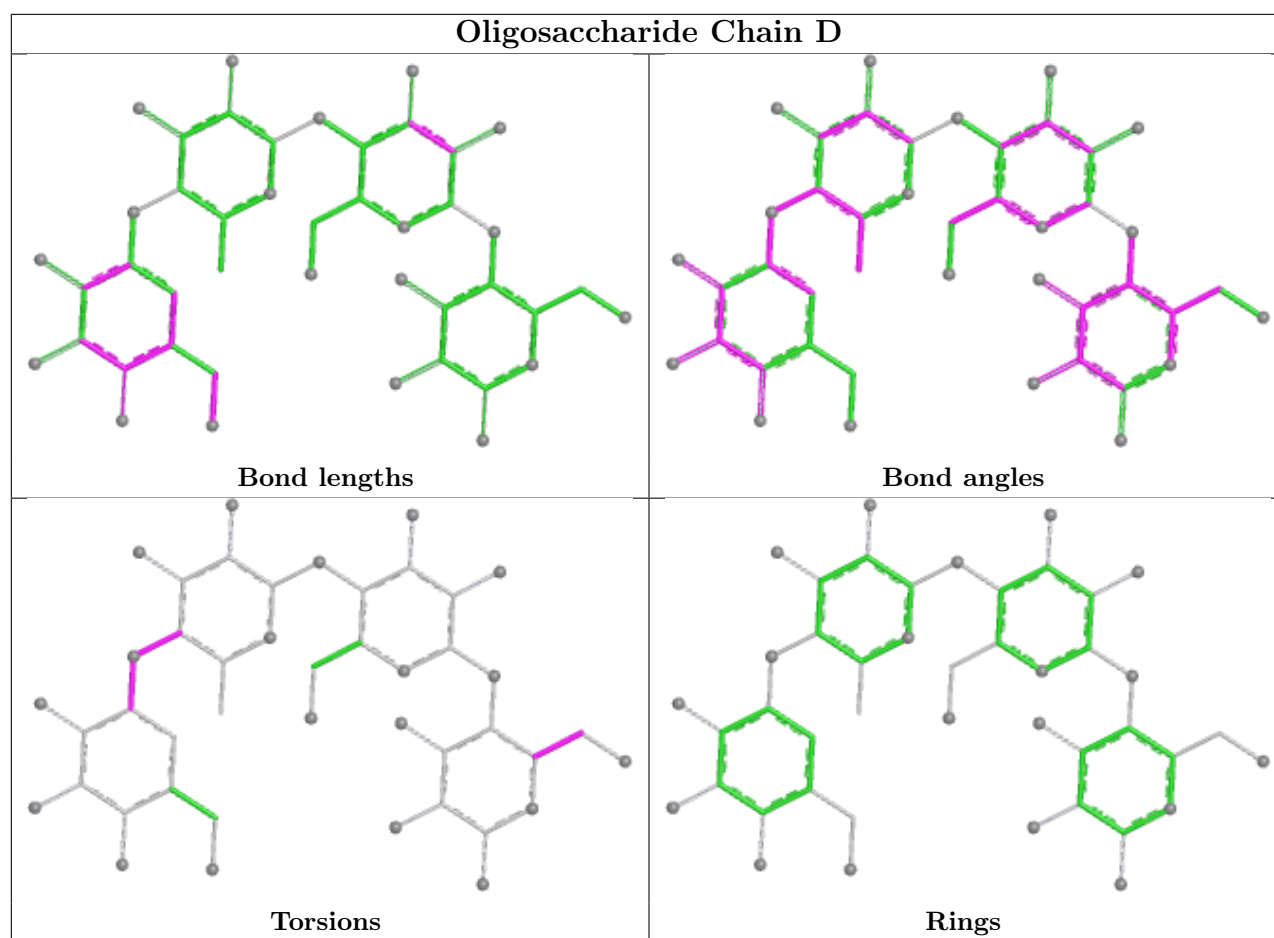
5.6   Ligand geometry ⓘ

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	GOL	B	998	-	5,5,5	0.50	0	5,5,5	0.56	0
4	PLP	A	999	1	15,15,16	1.87	3 (20%)	21,22,23	1.95	5 (23%)
3	GOL	A	998	-	5,5,5	0.78	0	5,5,5	0.88	0
4	PLP	B	999	1	15,15,16	2.61	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	GOL	B	998	-	-	2/4/4/4	-
4	PLP	A	999	1	-	3/6/6/8	0/1/1/1
3	GOL	A	998	-	-	1/4/4/4	-
4	PLP	B	999	1	-	2/6/6/8	0/1/1/1

The worst 5 of 7 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	999	PLP	C3-C2	-8.29	1.32	1.41
4	A	999	PLP	C3-C2	-4.37	1.36	1.41
4	B	999	PLP	P-O3P	-3.34	1.42	1.54
4	A	999	PLP	P-O3P	-3.25	1.42	1.54
4	B	999	PLP	C3-C4	-2.62	1.35	1.40

The worst 5 of 11 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	999	PLP	C2A-C2-C3	-5.23	114.68	120.80
4	B	999	PLP	C4A-C4-C5	4.08	125.14	120.94
4	B	999	PLP	O3P-P-O1P	3.38	124.02	110.83
4	B	999	PLP	C2A-C2-C3	-3.28	116.96	120.80
4	A	999	PLP	O2P-P-O1P	-3.02	99.05	110.83

There are no chirality outliers.

5 of 8 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	998	GOL	O1-C1-C2-C3
4	A	999	PLP	C5A-O4P-P-O1P
4	A	999	PLP	C5A-O4P-P-O2P
4	A	999	PLP	C5A-O4P-P-O3P
4	B	999	PLP	C5A-O4P-P-O3P

There are no ring outliers.

3 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	999	PLP	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	998	GOL	2	0
4	B	999	PLP	3	0

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	796/796 (100%)	0.16	12 (1%)	71	69	41, 50, 76, 114	0
1	B	796/796 (100%)	-0.07	8 (1%)	79	77	41, 50, 76, 114	0
All	All	1592/1592 (100%)	0.04	20 (1%)	74	72	41, 50, 76, 114	0

The worst 5 of 20 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	1767	LYS	5.4
1	A	18	SER	3.5
1	A	418	TRP	3.2
1	A	748	GLY	3.2
1	B	207	THR	2.9

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

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

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.
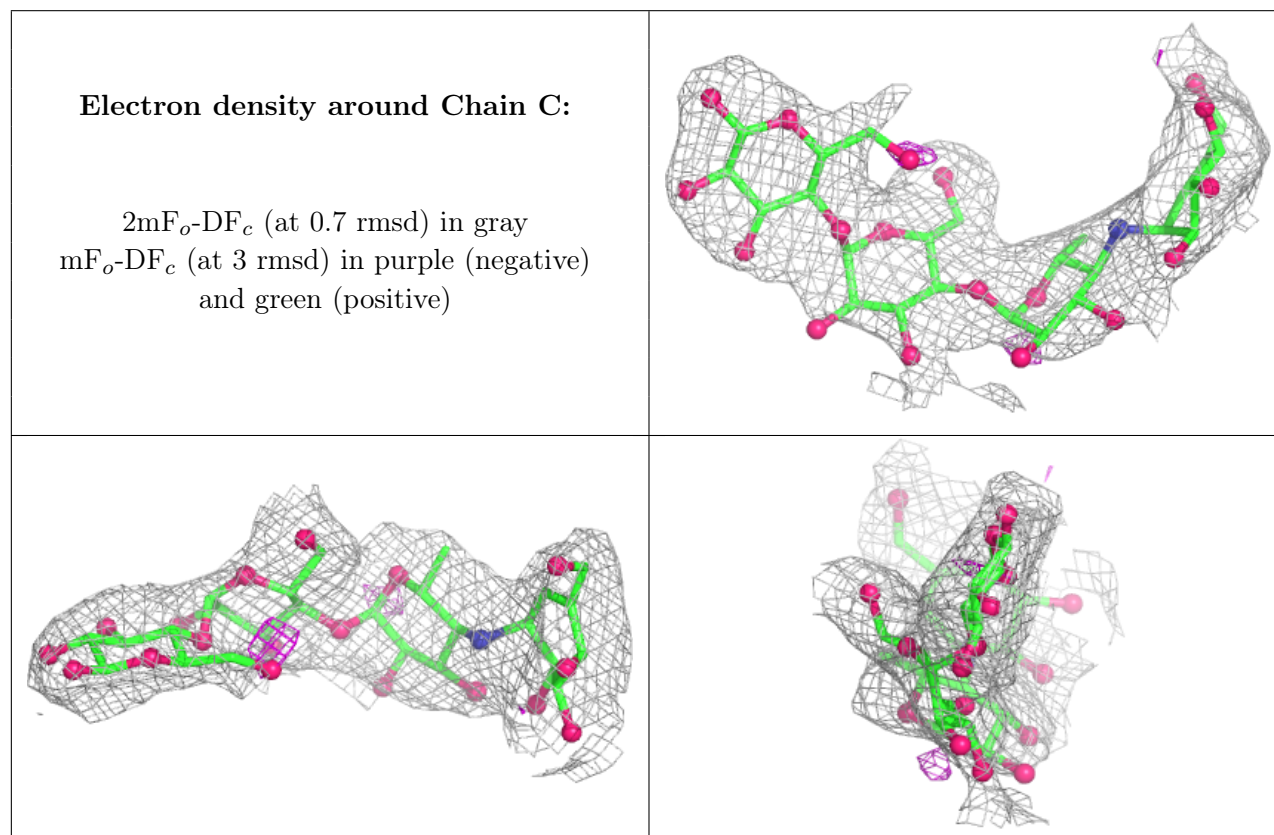
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	GLC	C	1	12/12	0.80	0.12	58,59,59,60	0
2	AC1	C	3	21/22	0.80	0.12	58,58,59,59	0
2	GLC	C	2	11/12	0.81	0.10	58,58,59,59	0
2	GLC	D	1	12/12	0.82	0.08	58,59,59,59	0
2	AC1	D	3	21/22	0.86	0.10	58,58,59,60	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	GLC	D	2	11/12	0.89	0.09	58,58,59,59	0

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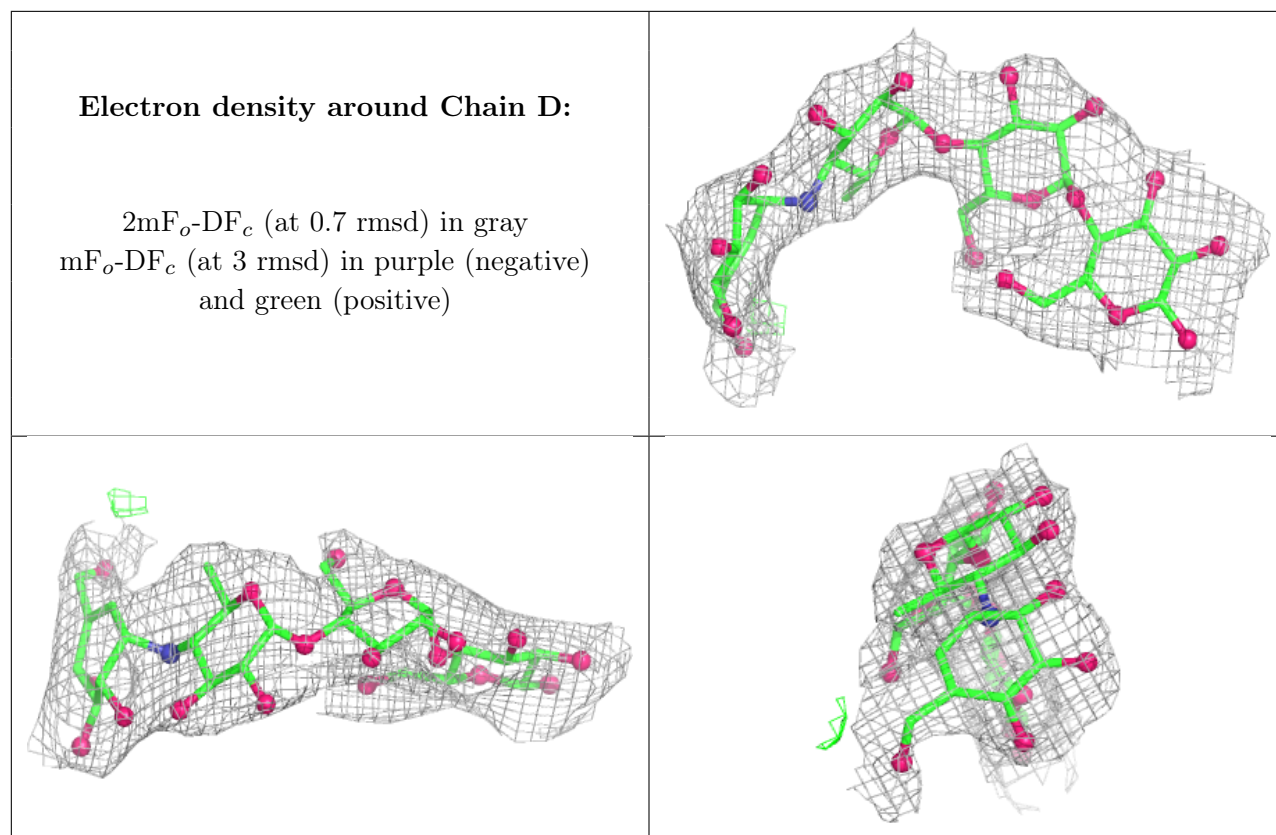
Electron density around Chain C:

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

Electron density around Chain D:

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

6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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	GOL	B	998	6/6	0.89	0.10	58,58,59,59	0
3	GOL	A	998	6/6	0.90	0.11	58,58,59,59	0
4	PLP	A	999	15/16	0.91	0.12	37,42,47,51	0
4	PLP	B	999	15/16	0.95	0.07	41,43,48,48	0

6.5 Other polymers ⓘ

There are no such residues in this entry.

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