



wwPDB X-ray Structure Validation Summary Report ⓘ

Oct 23, 2021 – 11:57 AM EDT

PDB ID : 1AHP
Title : OLIGOSACCHARIDE SUBSTRATE BINDING IN ESCHERICHIA COLI
MALTODEXTRIN PHSPHORYLASE
Authors : O'Reilly, M.; Watson, K.A.; Schinzel, R.; Palm, D.; Johnson, L.N.
Deposited on : 1997-04-10
Resolution : 3.00 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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 : 2.23.2
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) : 2.23.2

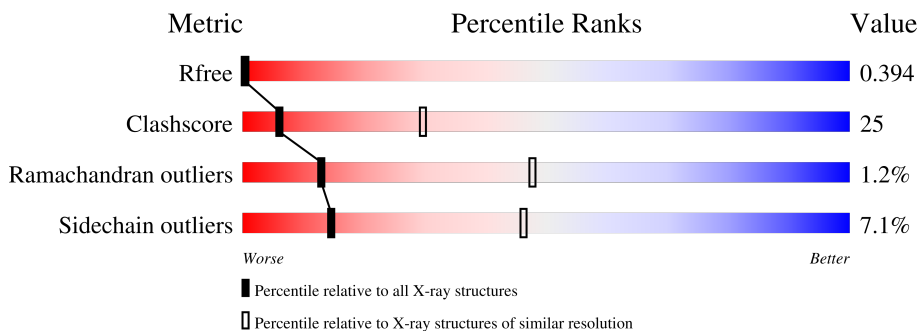
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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	2092 (3.00-3.00)
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)

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 $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	A	797	56% 39% .
1	B	797	57% 39% .
2	C	2	100%
2	D	2	100%

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 12830 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 E.COLI MALTODEXTRIN PHOSPHORYLASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	796	6366	4064	1126	1156	20	0	0	0
1	B	796	6366	4064	1126	1156	20	0	0	0

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	112	ALA	ASN	engineered mutation	UNP P00490
A	184	ALA	LYS	conflict	UNP P00490
A	497	ASP	GLN	conflict	UNP P00490
A	547	ARG	HIS	conflict	UNP P00490
A	681	LYS	GLU	conflict	UNP P00490
A	795	ALA	LYS	conflict	UNP P00490
B	112	ALA	ASN	engineered mutation	UNP P00490
B	184	ALA	LYS	conflict	UNP P00490
B	497	ASP	GLN	conflict	UNP P00490
B	547	ARG	HIS	conflict	UNP P00490
B	681	LYS	GLU	conflict	UNP P00490
B	795	ALA	LYS	conflict	UNP P00490

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



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
			Total	C	O			
2	C	2	23	12	11	0	0	0
2	D	2	23	12	11	0	0	0

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



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 GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



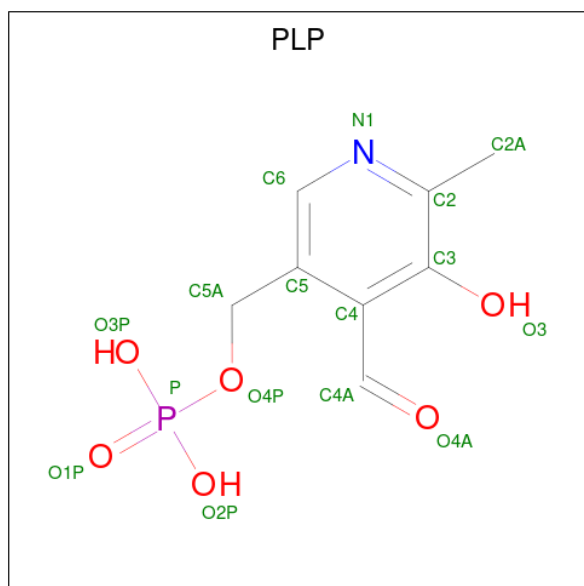
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			6	3	3		

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

- Molecule 5 is PYRIDOXAL-5'-PHOSPHATE (three-letter code: PLP) (formula: C₈H₁₀NO₆P).



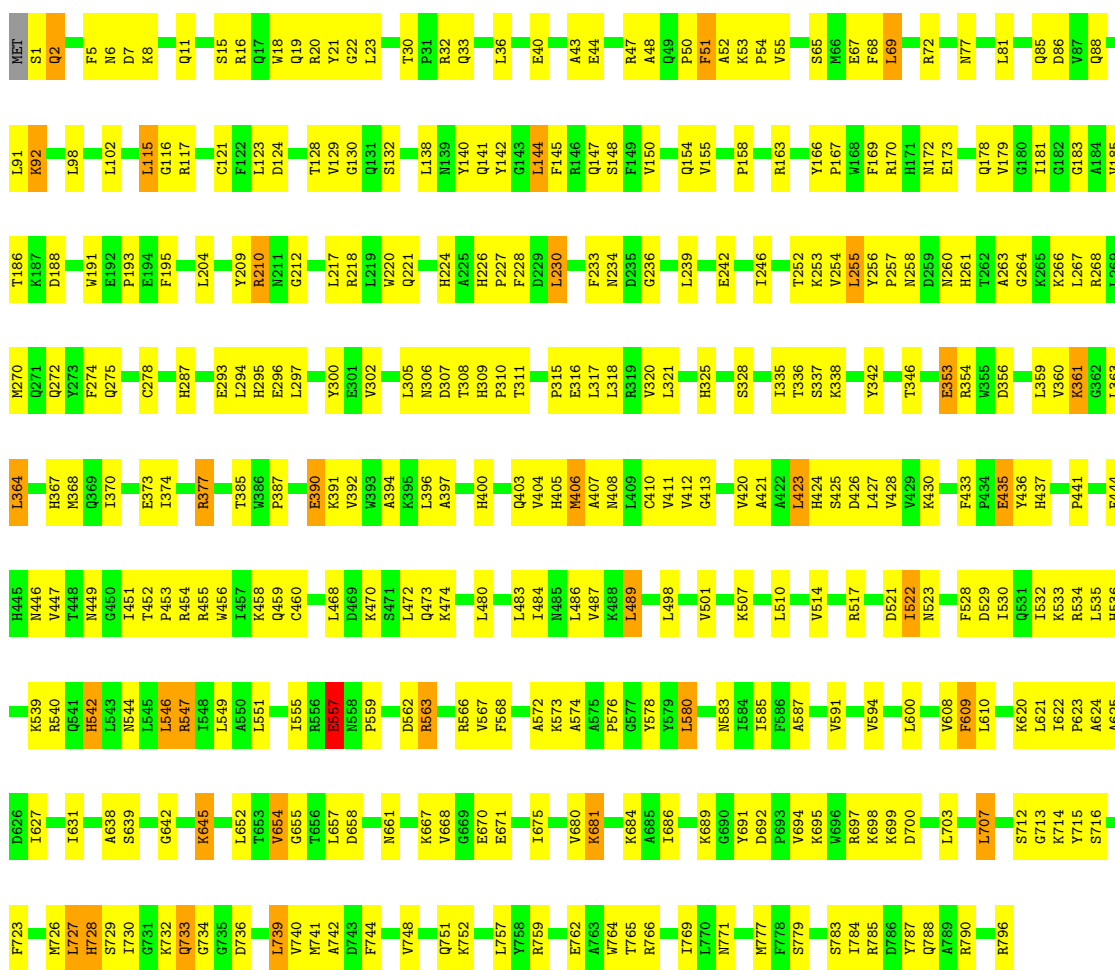
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	N	O	P	0	0
			15	8	1	5	1		
5	B	1	Total	C	N	O	P	0	0
			15	8	1	5	1		

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. 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. 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: E.COLI MALTODEXTRIN PHOSPHORYLASE

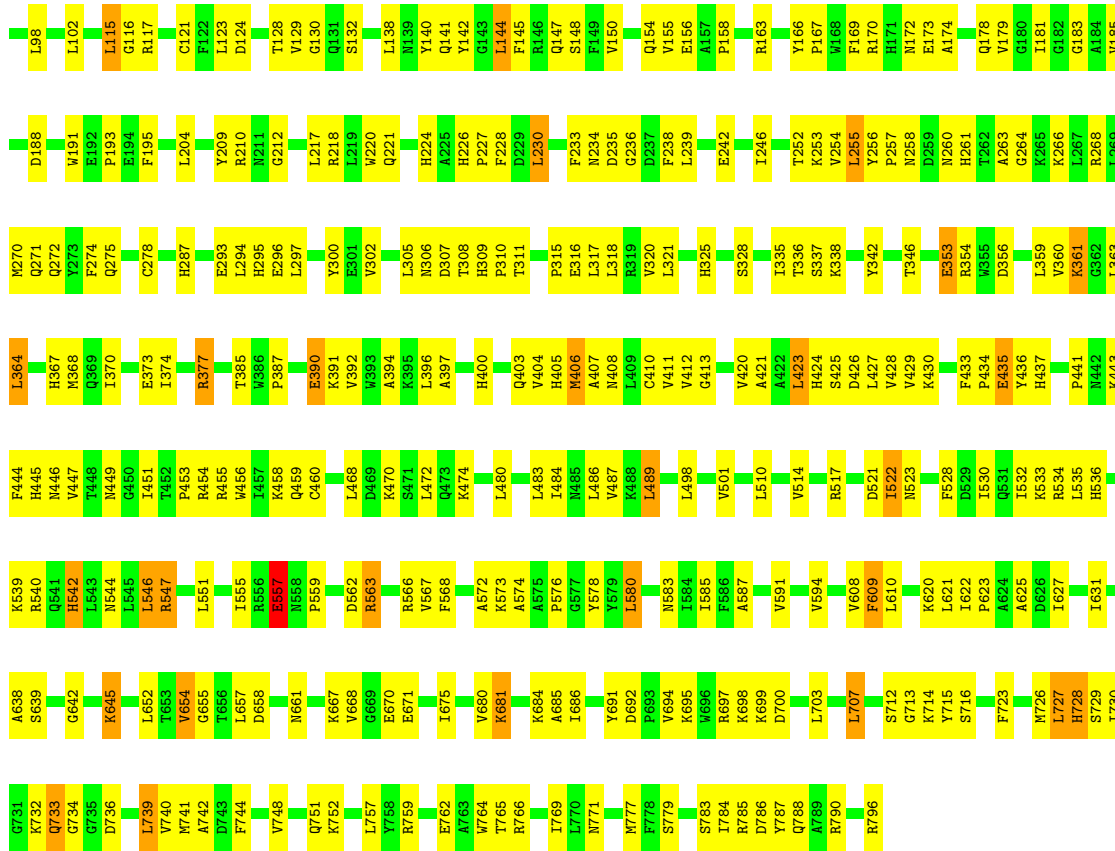
Chain A: 



- Molecule 1: E.COLI MALTODEXTRIN PHOSPHORYLASE

Chain B: 





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

Chain C: 100%

GLC1
GLC2

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

Chain D: 100%

GLC1
GLC2

4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	173.20Å 112.40Å 121.70Å 90.00° 119.70° 90.00°	Depositor
Resolution (Å)	10.00 – 3.00 9.99 – 3.00	Depositor EDS
% Data completeness (in resolution range)	73.0 (10.00-3.00) 73.6 (9.99-3.00)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.39 (at 2.99Å)	Xtrriage
Refinement program	X-PLOR 3.1	Depositor
R, R_{free}	0.232 , 0.278 0.390 , 0.394	Depositor DCC
R_{free} test set	608 reflections (2.09%)	wwPDB-VP
Wilson B-factor (Å ²)	34.3	Xtrriage
Anisotropy	0.277	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 55.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.57	EDS
Total number of atoms	12830	wwPDB-VP
Average B, all atoms (Å ²)	25.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.97% 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: PLP, GOL, SO4, GLC

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	0.40	1/6514 (0.0%)	0.64	1/8837 (0.0%)
1	B	0.40	1/6514 (0.0%)	0.64	1/8837 (0.0%)
All	All	0.40	2/13028 (0.0%)	0.64	2/17674 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	645	LYS	CE-NZ	-5.32	1.35	1.49
1	A	645	LYS	CE-NZ	-5.31	1.35	1.49

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	654	VAL	N-CA-C	-5.21	96.92	111.00
1	B	654	VAL	N-CA-C	-5.20	96.95	111.00

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	6366	0	6326	398	11
1	B	6366	0	6326	394	9

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	23	0	20	5	0
2	D	23	0	20	4	0
3	A	5	0	0	1	0
3	B	5	0	0	0	0
4	A	6	0	8	0	0
4	B	6	0	8	0	0
5	A	15	0	7	2	0
5	B	15	0	7	2	0
All	All	12830	0	12722	630	12

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 25.

The worst 5 of 630 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:170:ARG:CG	1:B:20:ARG:O	1.67	1.40
1:A:158:PRO:HG2	1:B:228:PHE:O	1.49	1.11
1:A:253:LYS:HE3	1:B:242:GLU:OE2	1.54	1.07
1:A:20:ARG:HG3	1:B:47:ARG:CZ	1.84	1.07
1:A:20:ARG:NH1	1:B:40:GLU:OE1	1.91	1.01

The worst 5 of 12 symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:600:LEU:CD2	1:A:714:LYS:CE[2_555]	0.84	1.36
1:A:600:LEU:CD2	1:A:714:LYS:NZ[2_555]	1.14	1.06
1:A:85:GLN:OE1	1:B:474:LYS:NZ[4_546]	1.22	0.98
1:A:85:GLN:CD	1:B:474:LYS:NZ[4_546]	1.50	0.70
1:A:689:LYS:NZ	1:B:685:ALA:CA[1_545]	1.61	0.59

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	794/797 (100%)	716 (90%)	68 (9%)	10 (1%)	12	45
1	B	794/797 (100%)	717 (90%)	68 (9%)	9 (1%)	14	50
All	All	1588/1594 (100%)	1433 (90%)	136 (9%)	19 (1%)	13	48

5 of 19 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	2	GLN
1	B	2	GLN
1	A	210	ARG
1	A	390	GLU
1	A	391	LYS

5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	664/665 (100%)	617 (93%)	47 (7%)	14	46
1	B	664/665 (100%)	617 (93%)	47 (7%)	14	46
All	All	1328/1330 (100%)	1234 (93%)	94 (7%)	14	46

5 of 94 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	260	ASN
1	B	468	LEU
1	B	302	VAL
1	B	364	LEU
1	B	522	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 36 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	445	HIS
1	B	728	HIS
1	B	446	ASN
1	B	542	HIS
1	A	446	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

4 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	1.77	3 (25%)	17,17,17	2.40	7 (41%)
2	GLC	C	2	2	11,11,12	2.04	4 (36%)	15,15,17	3.45	9 (60%)
2	GLC	D	1	2	12,12,12	1.77	4 (33%)	17,17,17	2.40	7 (41%)
2	GLC	D	2	2	11,11,12	2.05	4 (36%)	15,15,17	3.45	9 (60%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	GLC	C	1	2	-	0/2/22/22	0/1/1/1
2	GLC	C	2	2	-	2/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	GLC	D	1	2	-	0/2/22/22	0/1/1/1
2	GLC	D	2	2	-	2/2/19/22	0/1/1/1

The worst 5 of 15 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	1	GLC	O2-C2	-3.68	1.34	1.43
2	C	1	GLC	O2-C2	-3.66	1.34	1.43
2	D	2	GLC	C4-C5	3.65	1.60	1.53
2	C	2	GLC	C4-C5	3.62	1.60	1.53
2	C	2	GLC	C1-C2	3.08	1.59	1.52

The worst 5 of 32 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	2	GLC	C1-C2-C3	6.96	118.22	109.67
2	D	2	GLC	C1-C2-C3	6.92	118.17	109.67
2	D	2	GLC	C6-C5-C4	-6.45	97.91	113.00
2	C	2	GLC	C6-C5-C4	-6.43	97.94	113.00
2	C	1	GLC	O5-C1-C2	-5.25	100.92	110.28

There are no chirality outliers.

All (4) torsion outliers are listed below:

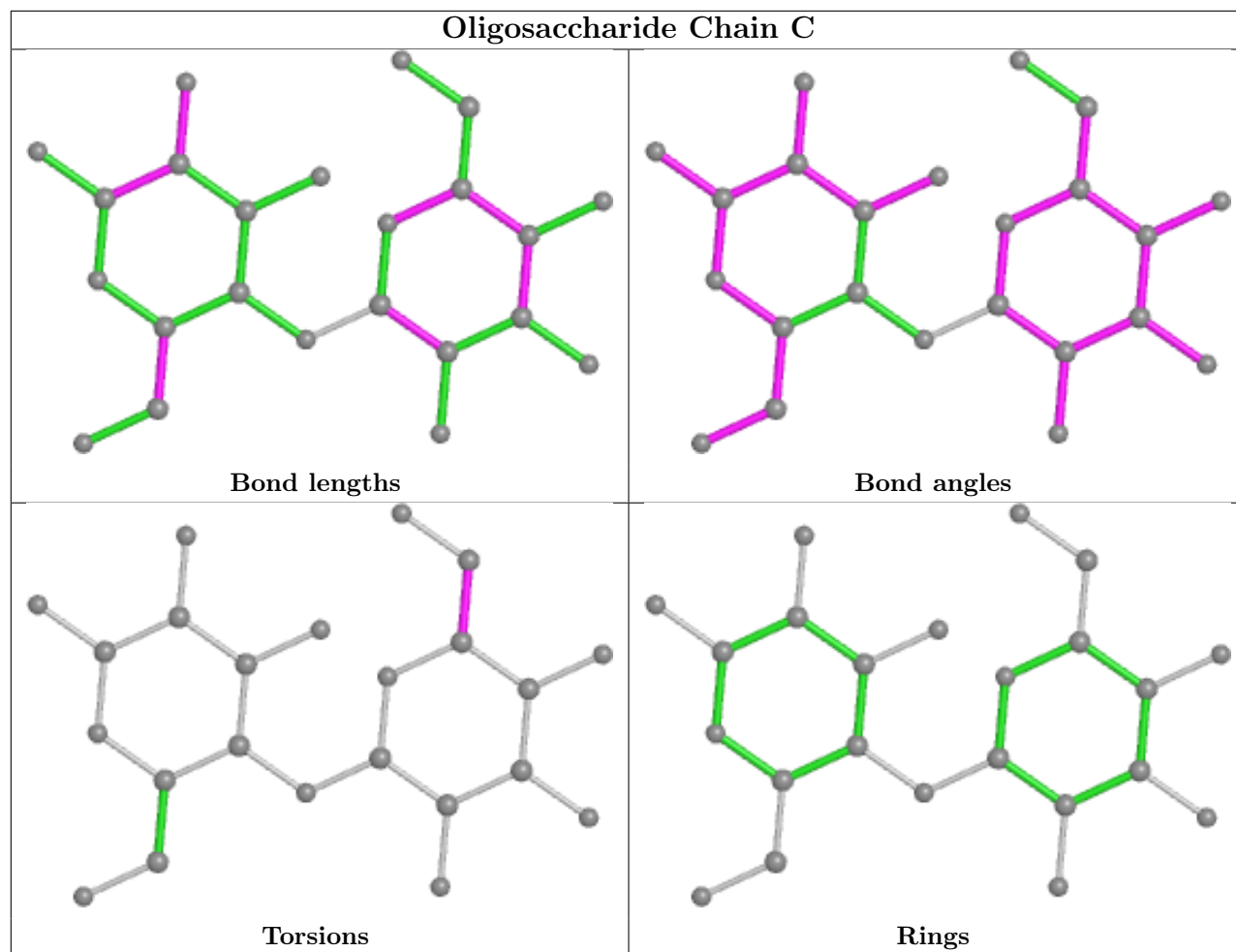
Mol	Chain	Res	Type	Atoms
2	C	2	GLC	O5-C5-C6-O6
2	D	2	GLC	O5-C5-C6-O6
2	C	2	GLC	C4-C5-C6-O6
2	D	2	GLC	C4-C5-C6-O6

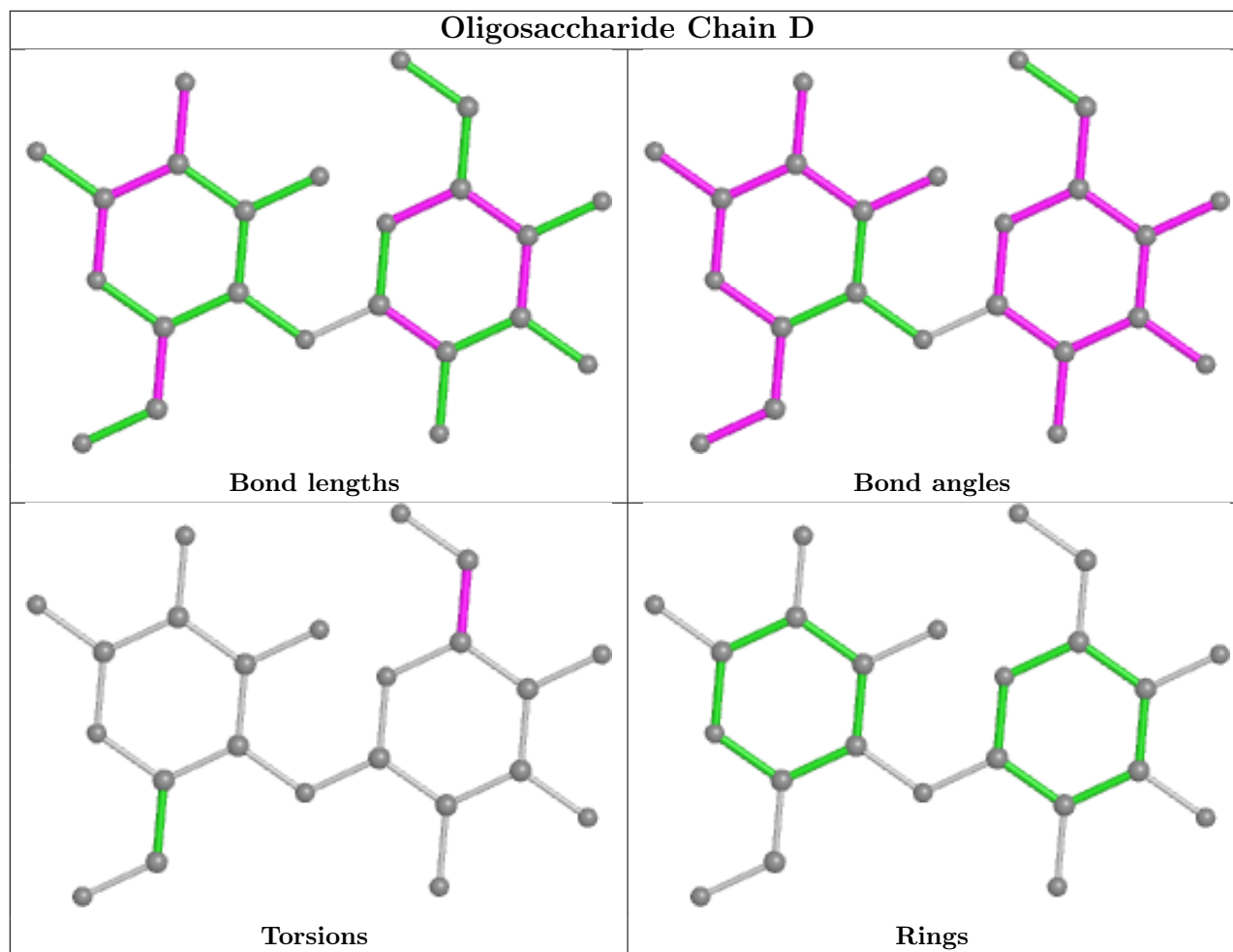
There are no ring outliers.

4 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	2	GLC	4	0
2	D	1	GLC	1	0
2	D	2	GLC	3	0
2	C	1	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](#)

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	SO4	B	997	-	4,4,4	0.60	0	6,6,6	1.06	0
3	SO4	A	997	-	4,4,4	0.61	0	6,6,6	1.06	0
5	PLP	B	999	1	15,15,16	2.02	3 (20%)	20,22,23	1.57	5 (25%)
5	PLP	A	999	1	15,15,16	2.02	3 (20%)	20,22,23	1.56	5 (25%)
4	GOL	A	998	-	5,5,5	0.31	0	5,5,5	0.72	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	GOL	B	998	-	5,5,5	0.31	0	5,5,5	0.73	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
4	GOL	B	998	-	-	0/4/4/4	-
5	PLP	B	999	1	-	3/6/6/8	0/1/1/1
4	GOL	A	998	-	-	0/4/4/4	-
5	PLP	A	999	1	-	3/6/6/8	0/1/1/1

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	999	PLP	C3-C2	-6.56	1.34	1.40
5	A	999	PLP	C3-C2	-6.53	1.34	1.40
5	A	999	PLP	C5-C4	-2.16	1.38	1.40
5	B	999	PLP	C5-C4	-2.13	1.38	1.40
5	A	999	PLP	P-O2P	2.04	1.62	1.54

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	999	PLP	C4A-C4-C5	-3.30	117.54	120.94
5	A	999	PLP	C4A-C4-C5	-3.26	117.57	120.94
5	B	999	PLP	O3P-P-O1P	2.93	122.14	110.68
5	A	999	PLP	O3P-P-O1P	2.93	122.14	110.68
5	A	999	PLP	C5-C6-N1	-2.57	119.53	123.82

There are no chirality outliers.

5 of 6 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	999	PLP	C5A-O4P-P-O1P
5	A	999	PLP	C5A-O4P-P-O2P
5	A	999	PLP	C5A-O4P-P-O3P
5	B	999	PLP	C5A-O4P-P-O1P
5	B	999	PLP	C5A-O4P-P-O2P

There are no ring outliers.

3 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	997	SO4	1	0
5	B	999	PLP	2	0
5	A	999	PLP	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

6.1 Protein, DNA and RNA chains

Unable to reproduce the depositors R factor - this section is therefore empty.

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

Unable to reproduce the depositors R factor - this section is therefore empty.

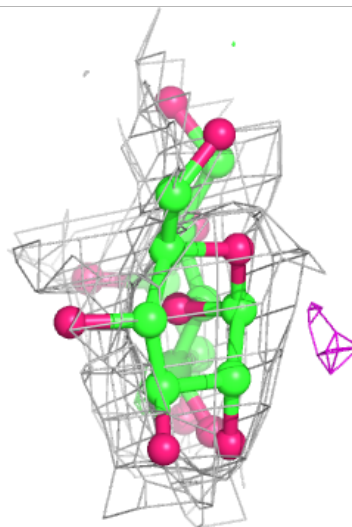
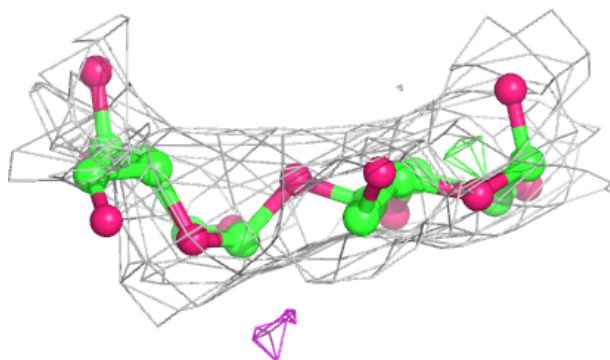
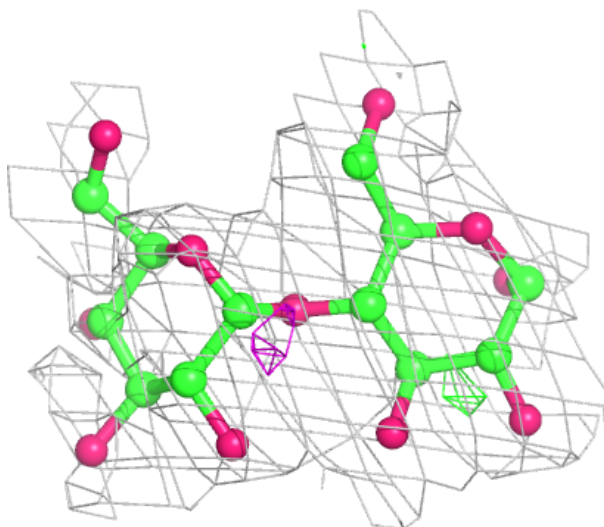
6.3 Carbohydrates

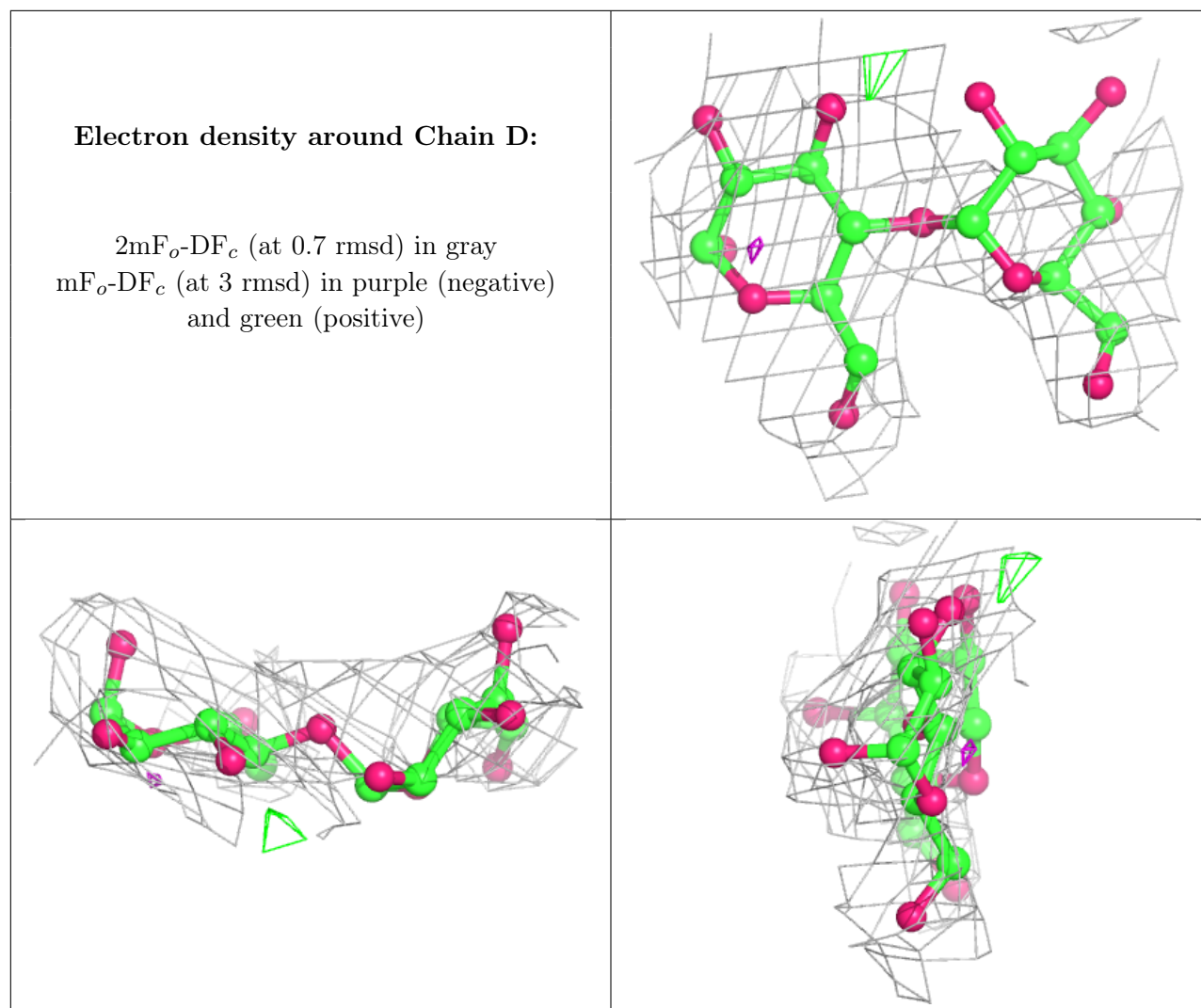
Unable to reproduce the depositors R factor - this section is therefore empty.

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

Electron density around Chain C:

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





6.4 Ligands [i](#)

Unable to reproduce the depositor's R factor - this section is therefore empty.

6.5 Other polymers [i](#)

Unable to reproduce the depositor's R factor - this section is therefore empty.