W O R L D W I D E
wwPDB
PROTEIN DATA BANK

wwPDB X-ray Structure Validation Summary Report ⓘ

Jan 4, 2024 – 09:48 am GMT

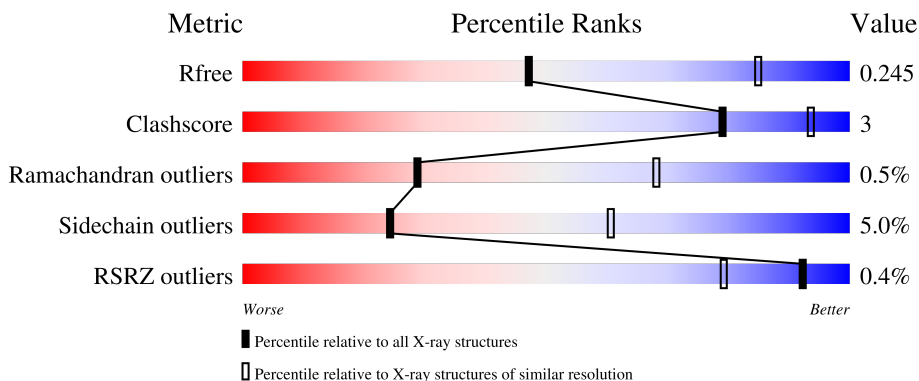|		
PDB ID	:	5LRA
Title	:	Plastidial phosphorylase PhoI from barley in complex with maltotetraose
Authors	:	Cuesta-Seijo, J.A.; Ruzanski, C.; Krucewicz, K.; Palcic, M.M.
Deposited on	:	2016-08-18
Resolution	:	3.00 Å(reported)

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	Percentile Ranks	Value
Rfree		0.245
Clashscore		3
Ramachandran outliers		0.5%
Sidechain outliers		5.0%
RSRZ outliers		0.4%

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}	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)
RSRZ outliers	127900	1990 (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 <=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	80% 9% · 10%
1	B	938	79% 11% · 10%
2	C	4	25% 75%
2	E	4	25% 75%
3	D	2	100%

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Mol	Chain	Length	Quality of chain
3	F	2	50% 50%

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 13697 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	4	1
			6740	4293	1145	1272	30			
1	B	844	Total	C	N	O	S	0	6	1
			6744	4297	1143	1273	31			

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

- Molecule 2 is an oligosaccharide called 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	4	Total 45	C 24	O 21	0	0	0
2	E	4	Total 45	C 24	O 21	0	0	0

- Molecule 3 is an oligosaccharide called alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
3	D	2	Total 23	C 12	O 11	0	0	0
3	F	2	Total 23	C 12	O 11	0	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	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	20	Total	O	0	0
			20	20		
5	B	27	Total	O	0	0
			27	27		

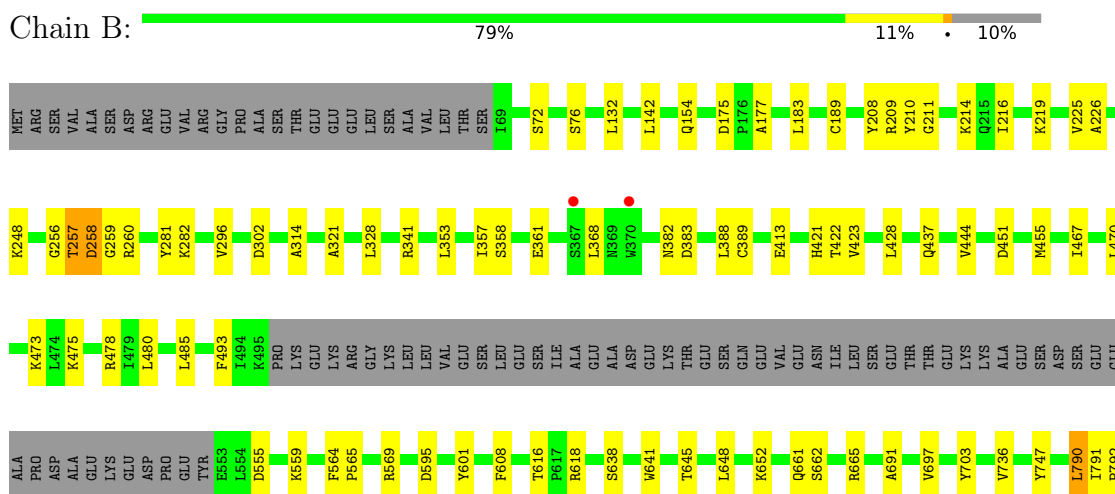# 3 Residue-property plots ⓘ

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.

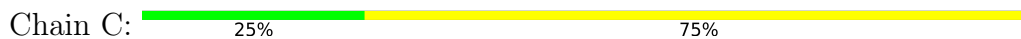- Molecule 1: Alpha-1,4 glucan phosphorylase
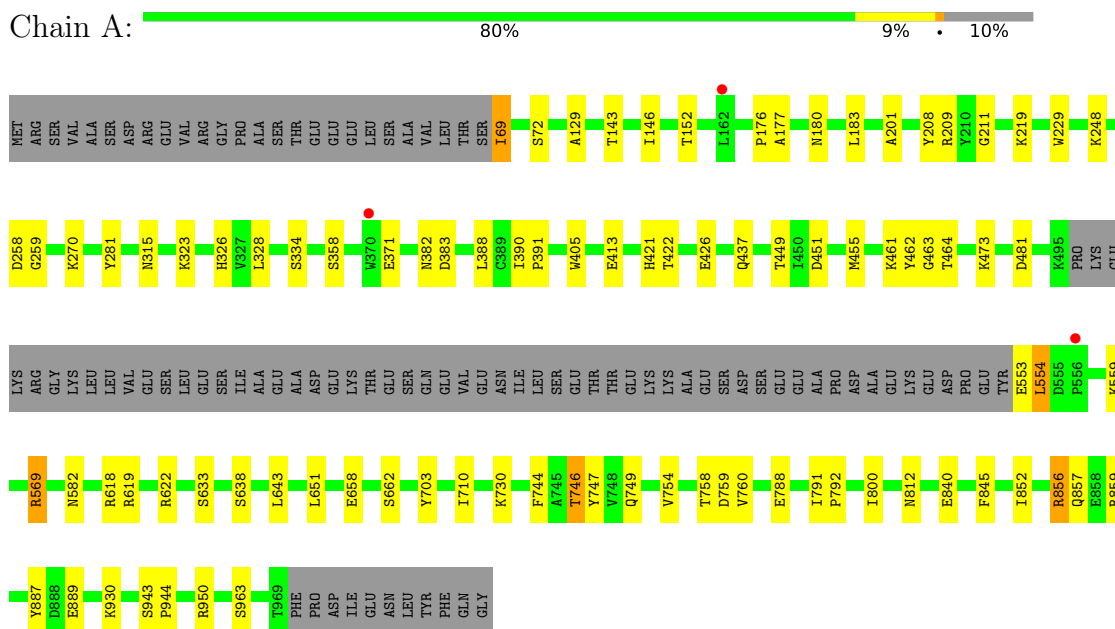
Chain A:

- Molecule 1: Alpha-1,4 glucan phosphorylase

Chain B:

T802 M805 N812 M813 K814 N830 I833 V837 G838 E839 E840 F845 H848 A849 P850 E851 R856 K863 Y905 Y915 K930 S943 P944 R950 T969 PHE PRO ASP ILE GLU ASN LEU TYR PHE GLN GLY

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

Chain C:

25% 75%

BGC1 GLC2 GLC3 GLC4
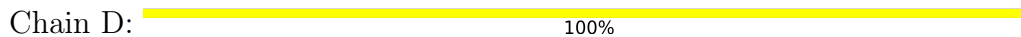
• Molecule 2: alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-beta-D-glucopyranose

Chain E:

25% 75%

BGC1 GLC2 GLC3 GLC4

• Molecule 3: alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose

Chain D:

100%

GLC1 GLC2

• Molecule 3: alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose

Chain F:

50% 50%

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	227.69Å 63.15Å 148.19Å 90.00° 114.72° 90.00°	Depositor
Resolution (Å)	49.39 – 3.00 44.87 – 3.00	Depositor EDS
% Data completeness (in resolution range)	99.8 (49.39-3.00) 99.9 (44.87-3.00)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.68 (at 3.01Å)	Xtriage
Refinement program	REFMAC 5.7.0032	Depositor
R, R_{free}	0.195 , 0.243 0.196 , 0.245	Depositor DCC
R_{free} test set	1165 reflections (3.00%)	wwPDB-VP
Wilson B-factor (Å^2)	73.7	Xtriage
Anisotropy	0.034	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 46.2	EDS
L-test for twinning[2]	$< |L| > = 0.53, < L^2 > = 0.36$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	13697	wwPDB-VP
Average B, all atoms (Å^2)	91.0	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 51.41 % 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 5.6312e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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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 (i)

5.1   Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: GLC, PLP, BGC

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	0.36	0/6907	0.57	0/9356
1	B	0.36	0/6917	0.57	0/9370
All	All	0.36	0/13824	0.57	0/18726

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 (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	6740	0	6632	30	0
1	B	6744	0	6637	45	0
2	C	45	0	39	0	0
2	E	45	0	39	0	0
3	D	23	0	21	0	0
3	F	23	0	21	1	0
4	A	15	0	6	0	0
4	B	15	0	6	1	0
5	A	20	0	0	2	0
5	B	27	0	0	0	0
All	All	13697	0	13401	76	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 3.

The worst 5 of 76 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:B:257:THR:O	1:B:258:ASP:HB2	1.89	0.71
1:B:848:HIS:N	1:B:851:GLU:OE1	2.32	0.59
1:A:759:ASP:OD2	1:A:887:TYR:OH	2.20	0.58
1:A:69:ILE:HG23	1:A:69:ILE:O	2.05	0.56
1:B:812:ASN:ND2	1:B:830:ASN:OD1	2.39	0.56

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	844/938 (90%)	803 (95%)	37 (4%)	4 (0%)	29	68
1	B	846/938 (90%)	801 (95%)	41 (5%)	4 (0%)	29	68
All	All	1690/1876 (90%)	1604 (95%)	78 (5%)	8 (0%)	29	68

5 of 8 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	259	GLY
1	B	258	ASP
1	B	259	GLY
1	A	852	ILE
1	A	258	ASP

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	729/810 (90%)	686 (94%)	43 (6%)	19	54
1	B	730/810 (90%)	699 (96%)	31 (4%)	30	66
All	All	1459/1620 (90%)	1385 (95%)	74 (5%)	24	60

5 of 74 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	428	LEU
1	B	856	ARG
1	B	559	LYS
1	B	747	TYR
1	A	633	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	138	GLN
1	A	613	ASN
1	B	138	GLN
1	B	165	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 ⓘ

10 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	#$|Z| > 2$
2	GLC	C	4	2	11,11,12	0.52	0	15,15,17	1.16	1 (6%)
2	GLC	E	2	2	11,11,12	0.74	0	15,15,17	1.58	2 (13%)
3	GLC	F	2	3	11,11,12	0.64	0	15,15,17	1.65	2 (13%)
2	GLC	E	3	2	11,11,12	0.74	0	15,15,17	1.18	2 (13%)
3	GLC	D	1	3	12,12,12	0.53	0	17,17,17	3.02	5 (29%)
3	GLC	F	1	3	12,12,12	0.50	0	17,17,17	0.79	0
2	GLC	C	3	2	11,11,12	0.61	0	15,15,17	1.74	2 (13%)
2	GLC	C	2	2	11,11,12	0.59	0	15,15,17	1.57	2 (13%)
3	GLC	D	2	3	11,11,12	0.63	0	15,15,17	2.18	3 (20%)
2	GLC	E	4	2	11,11,12	0.52	0	15,15,17	2.30	3 (20%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	GLC	C	4	2	-	2/2/19/22	0/1/1/1
2	GLC	E	2	2	-	2/2/19/22	0/1/1/1
3	GLC	F	2	3	-	2/2/19/22	0/1/1/1
2	GLC	E	3	2	-	0/2/19/22	0/1/1/1
3	GLC	D	1	3	-	0/2/22/22	0/1/1/1
3	GLC	F	1	3	-	1/2/22/22	0/1/1/1
2	GLC	C	3	2	-	0/2/19/22	0/1/1/1
2	GLC	C	2	2	-	2/2/19/22	0/1/1/1
3	GLC	D	2	3	-	2/2/19/22	0/1/1/1
2	GLC	E	4	2	-	2/2/19/22	0/1/1/1

There are no bond length outliers.

The worst 5 of 22 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	D	1	GLC	O1-C1-O5	8.92	137.16	110.38
2	E	4	GLC	C1-O5-C5	6.88	121.51	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	D	1	GLC	O5-C1-C2	-6.69	98.34	110.28
2	C	3	GLC	C1-O5-C5	5.84	120.11	112.19
3	D	2	GLC	C1-C2-C3	5.45	116.36	109.67

There are no chirality outliers.

5 of 13 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	E	2	GLC	C4-C5-C6-O6
3	F	2	GLC	C4-C5-C6-O6
3	D	2	GLC	O5-C5-C6-O6
3	D	2	GLC	C4-C5-C6-O6
2	C	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
3	F	2	GLC	1	0
3	F	1	GLC	1	0

5.5 Carbohydrates ⓘ

12 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	0.58	0	17,17,17	0.74	0
2	GLC	C	2	2	11,11,12	0.59	0	15,15,17	1.57	2 (13%)
2	GLC	C	3	2	11,11,12	0.61	0	15,15,17	1.74	2 (13%)
2	GLC	C	4	2	11,11,12	0.52	0	15,15,17	1.16	1 (6%)
3	GLC	D	1	3	12,12,12	0.53	0	17,17,17	3.02	5 (29%)
3	GLC	D	2	3	11,11,12	0.63	0	15,15,17	2.18	3 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
2	BGC	E	1	2	12,12,12	0.60	0	17,17,17	0.65	0
2	GLC	E	2	2	11,11,12	0.74	0	15,15,17	1.58	2 (13%)
2	GLC	E	3	2	11,11,12	0.74	0	15,15,17	1.18	2 (13%)
2	GLC	E	4	2	11,11,12	0.52	0	15,15,17	2.30	3 (20%)
3	GLC	F	1	3	12,12,12	0.50	0	17,17,17	0.79	0
3	GLC	F	2	3	11,11,12	0.64	0	15,15,17	1.65	2 (13%)

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	-	2/2/19/22	0/1/1/1
2	GLC	C	3	2	-	0/2/19/22	0/1/1/1
2	GLC	C	4	2	-	2/2/19/22	0/1/1/1
3	GLC	D	1	3	-	0/2/22/22	0/1/1/1
3	GLC	D	2	3	-	2/2/19/22	0/1/1/1
2	BGC	E	1	2	-	1/2/22/22	0/1/1/1
2	GLC	E	2	2	-	2/2/19/22	0/1/1/1
2	GLC	E	3	2	-	0/2/19/22	0/1/1/1
2	GLC	E	4	2	-	2/2/19/22	0/1/1/1
3	GLC	F	1	3	-	1/2/22/22	0/1/1/1
3	GLC	F	2	3	-	2/2/19/22	0/1/1/1

There are no bond length outliers.

The worst 5 of 22 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	D	1	GLC	O1-C1-O5	8.92	137.16	110.38
2	E	4	GLC	C1-O5-C5	6.88	121.51	112.19
3	D	1	GLC	O5-C1-C2	-6.69	98.34	110.28
2	C	3	GLC	C1-O5-C5	5.84	120.11	112.19
3	D	2	GLC	C1-C2-C3	5.45	116.36	109.67

There are no chirality outliers.

5 of 14 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	E	2	GLC	C4-C5-C6-O6
3	F	2	GLC	C4-C5-C6-O6
3	D	2	GLC	O5-C5-C6-O6
3	D	2	GLC	C4-C5-C6-O6
2	C	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
3	F	2	GLC	1	0
3	F	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.

Oligosaccharide Chain C

Bond lengths

Bond angles

Torsions

Rings

Oligosaccharide Chain E

Bond lengths

Bond angles

Torsions

Rings

Oligosaccharide Chain D

Bond lengths

Bond angles

Torsions

Rings

Oligosaccharide Chain F

Bond lengths

Bond angles

Torsions

Rings
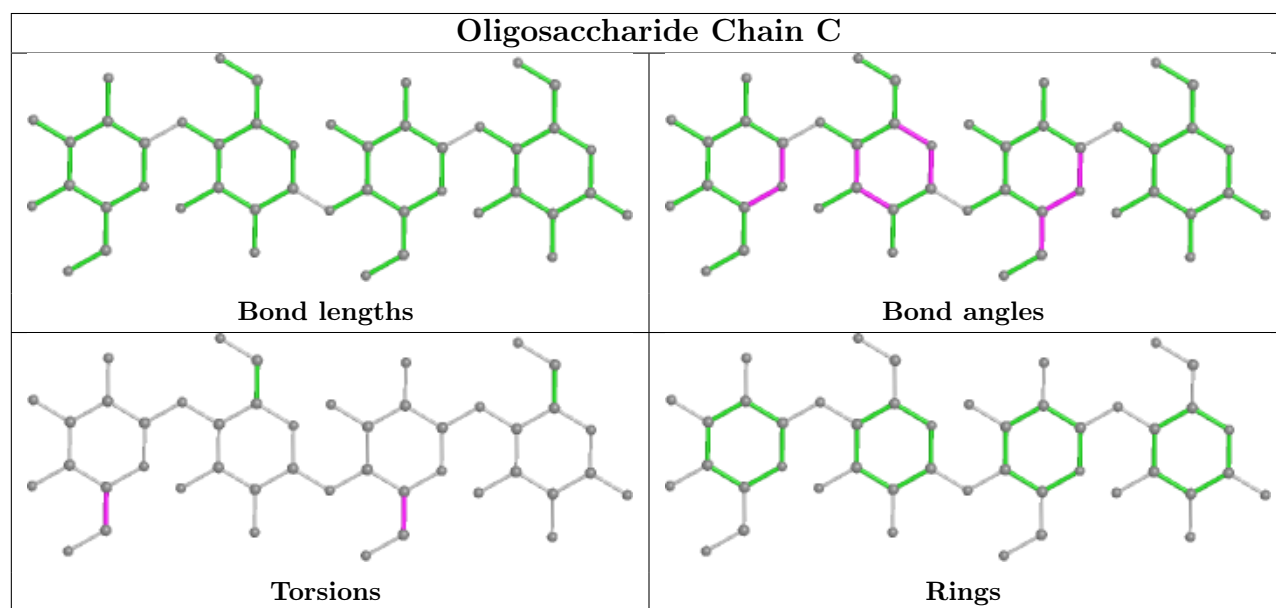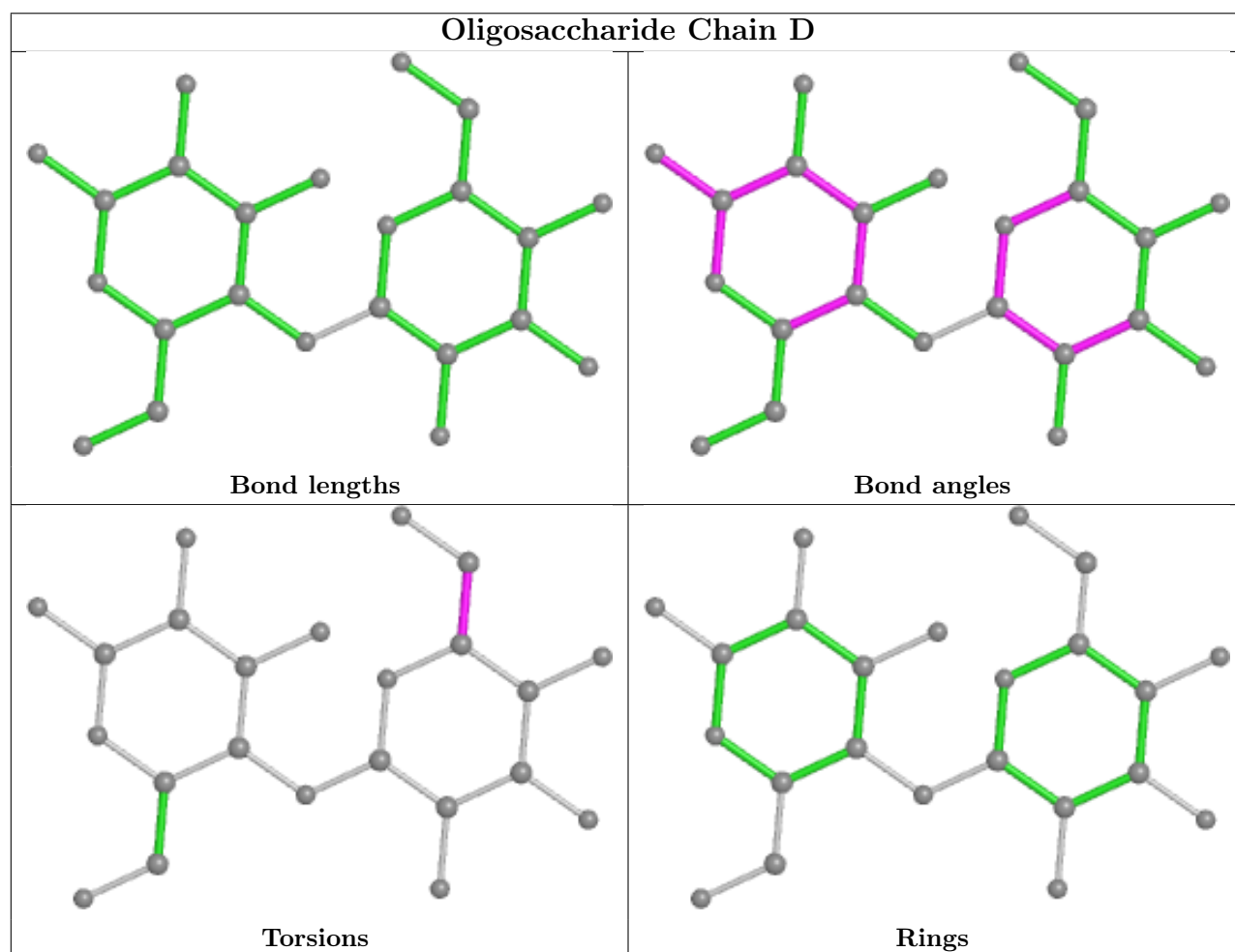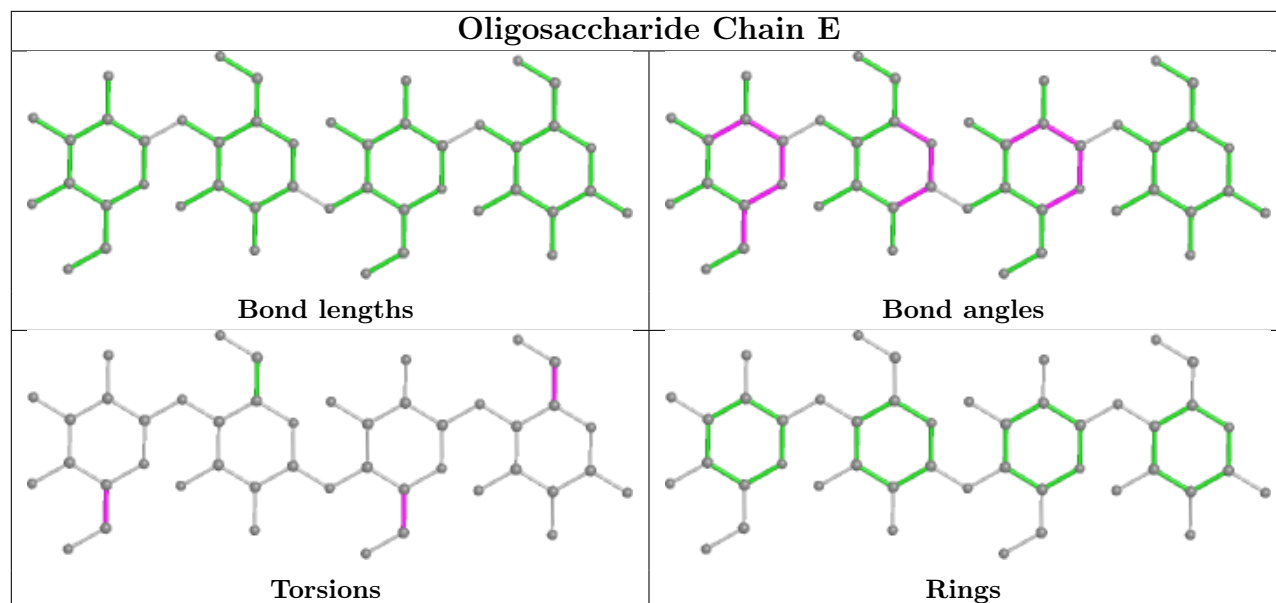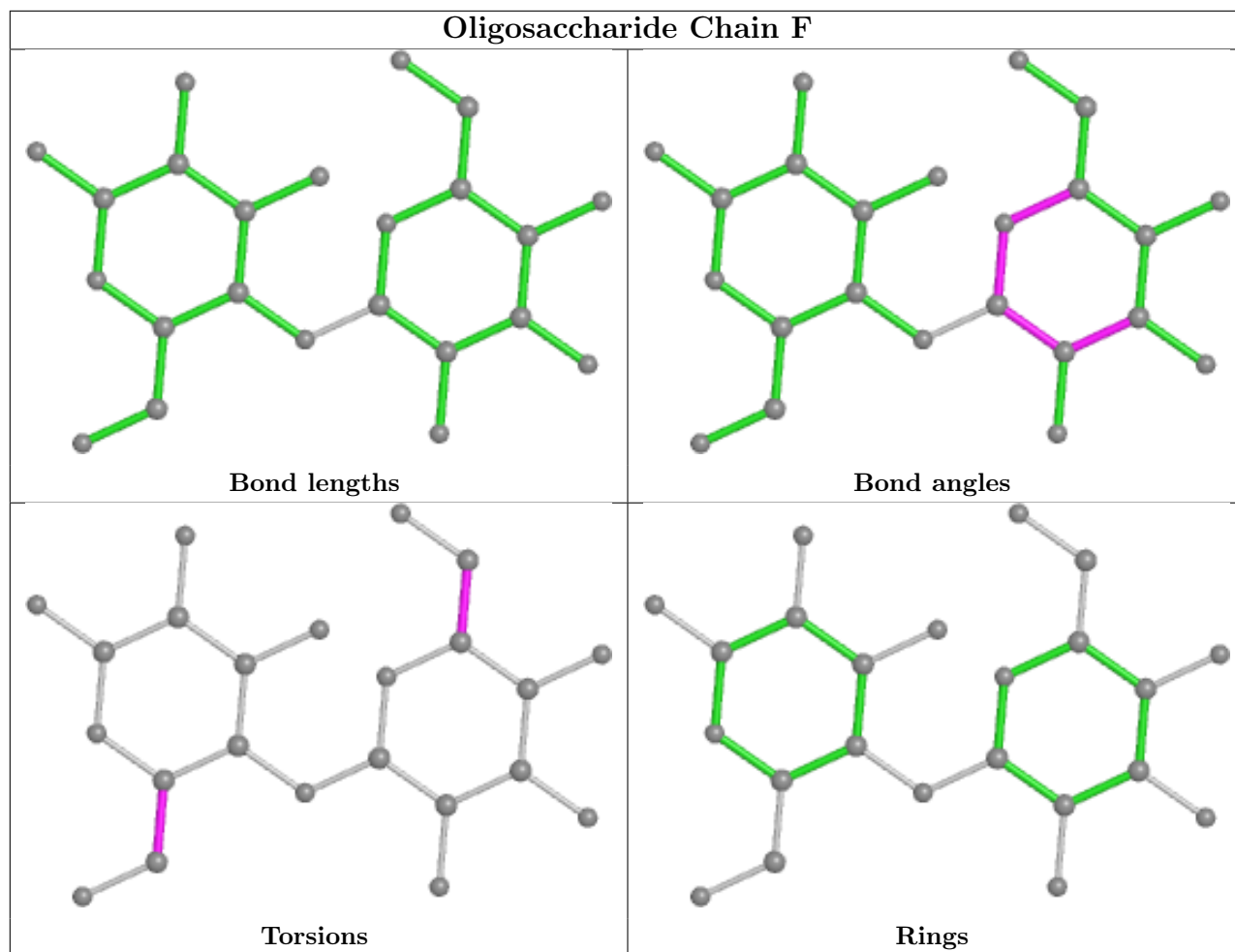
5.6 Ligand geometry ⓘ

2 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	A	1007	1	15,15,16	2.76	3 (20%)	20,22,23	1.48	4 (20%)
4	PLP	B	1007	1	15,15,16	3.01	3 (20%)	20,22,23	1.23	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	A	1007	1	-	4/6/6/8	0/1/1/1
4	PLP	B	1007	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)
4	B	1007	PLP	C3-C2	7.87	1.48	1.40
4	A	1007	PLP	C5-C4	7.79	1.49	1.40
4	B	1007	PLP	C5-C4	7.31	1.48	1.40
4	A	1007	PLP	C3-C2	5.71	1.46	1.40
4	B	1007	PLP	C3-C4	3.63	1.47	1.40

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1007	PLP	C4A-C4-C5	3.19	124.22	120.94
4	A	1007	PLP	C2A-C2-C3	-2.71	117.54	120.89
4	B	1007	PLP	O3-C3-C2	2.26	122.41	117.49
4	B	1007	PLP	C4A-C4-C5	2.25	123.25	120.94
4	A	1007	PLP	C2A-C2-N1	2.13	121.82	117.67

There are no chirality outliers.

5 of 7 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	1007	PLP	C5A-O4P-P-O2P
4	A	1007	PLP	C5A-O4P-P-O3P
4	B	1007	PLP	C5A-O4P-P-O2P
4	B	1007	PLP	C5A-O4P-P-O1P
4	B	1007	PLP	C5A-O4P-P-O3P

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	1007	PLP	1	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	844/938 (89%)	-0.37	3 (0%)	92	79	56, 88, 127, 172	0
1	B	844/938 (89%)	-0.34	3 (0%)	92	79	46, 89, 129, 170	0
All	All	1688/1876 (89%)	-0.35	6 (0%)	92	79	46, 88, 129, 172	0

The worst 5 of 6 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	370	TRP	3.7
1	A	370	TRP	2.5
1	A	556	PRO	2.3
1	B	367	SER	2.3
1	B	863	LYS	2.2

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.
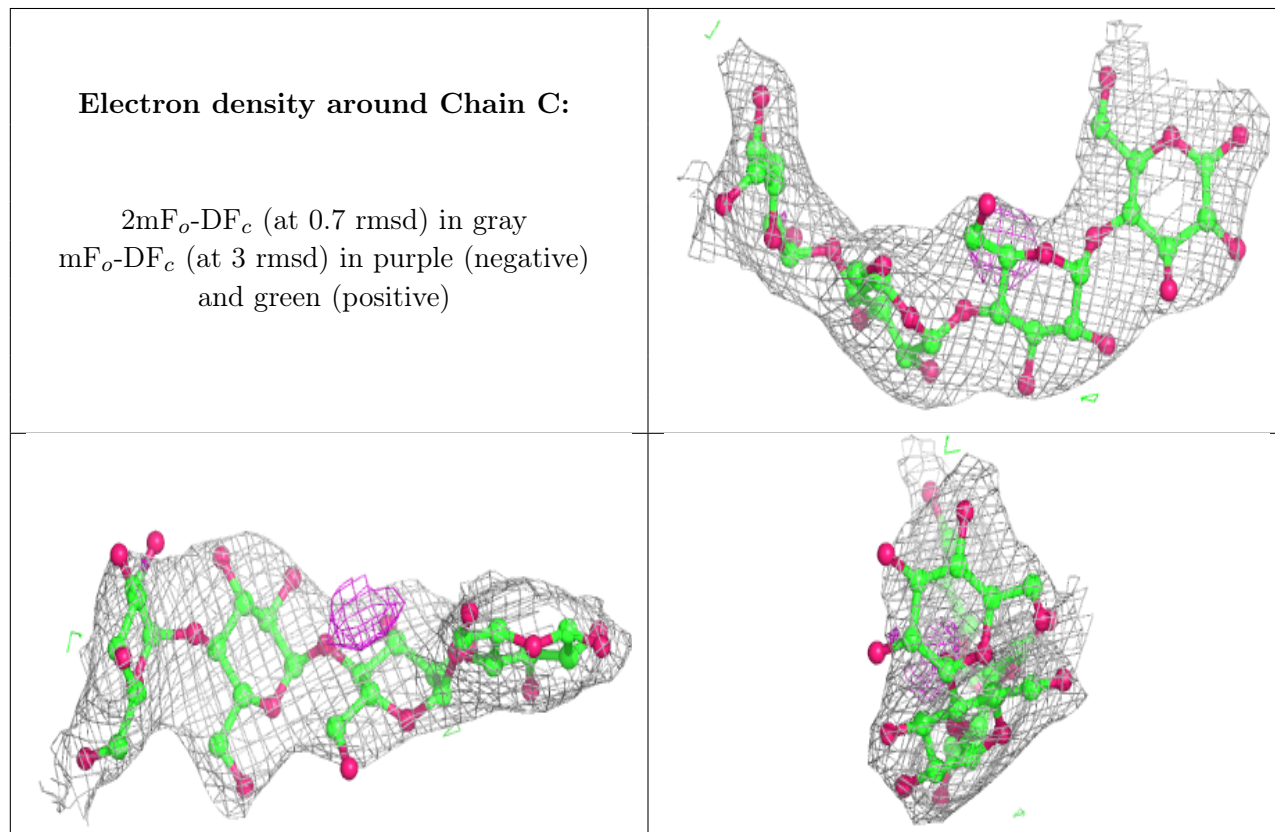
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	GLC	F	2	11/12	0.73	0.33	121,130,142,143	0
3	GLC	F	1	12/12	0.77	0.36	146,158,162,164	0
3	GLC	D	2	11/12	0.79	0.30	116,129,136,137	0
3	GLC	D	1	12/12	0.80	0.34	124,135,141,144	0
2	GLC	C	4	11/12	0.90	0.34	77,89,99,99	0
2	GLC	C	2	11/12	0.92	0.20	86,90,96,97	0
2	GLC	E	4	11/12	0.92	0.28	76,82,87,93	0
2	GLC	E	2	11/12	0.94	0.16	68,75,81,82	0
2	GLC	E	3	11/12	0.97	0.23	72,74,78,81	0
2	GLC	C	3	11/12	0.98	0.25	86,88,90,90	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
3	GLC	F	2	11/12	0.73	0.33	121,130,142,143	0
3	GLC	F	1	12/12	0.77	0.36	146,158,162,164	0
3	GLC	D	2	11/12	0.79	0.30	116,129,136,137	0
3	GLC	D	1	12/12	0.80	0.34	124,135,141,144	0
2	GLC	C	4	11/12	0.90	0.34	77,89,99,99	0
2	BGC	E	1	12/12	0.91	0.17	89,96,105,110	0
2	GLC	C	2	11/12	0.92	0.20	86,90,96,97	0
2	GLC	E	4	11/12	0.92	0.28	76,82,87,93	0
2	BGC	C	1	12/12	0.93	0.15	96,101,104,107	0
2	GLC	E	2	11/12	0.94	0.16	68,75,81,82	0
2	GLC	E	3	11/12	0.97	0.23	72,74,78,81	0
2	GLC	C	3	11/12	0.98	0.25	86,88,90,90	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.
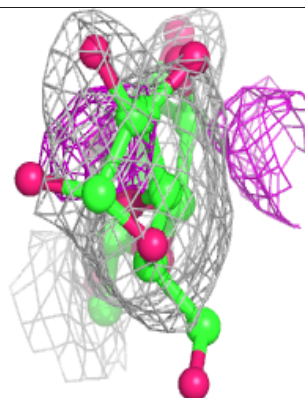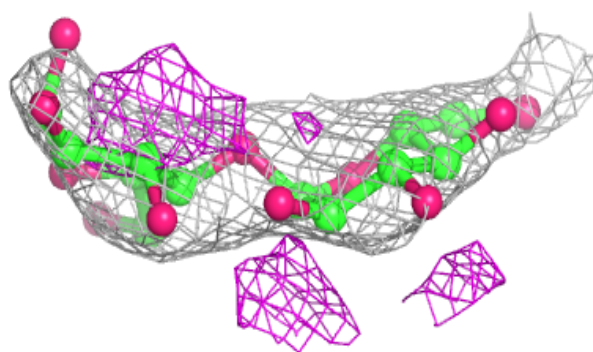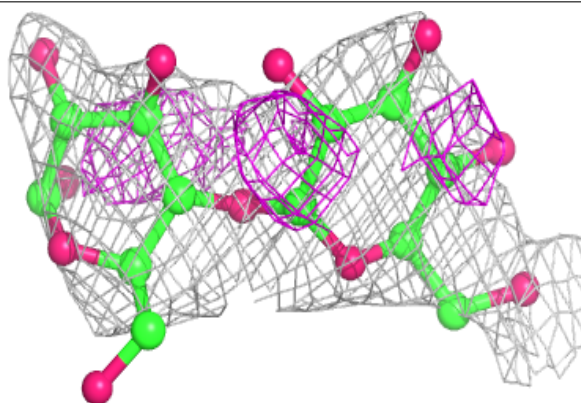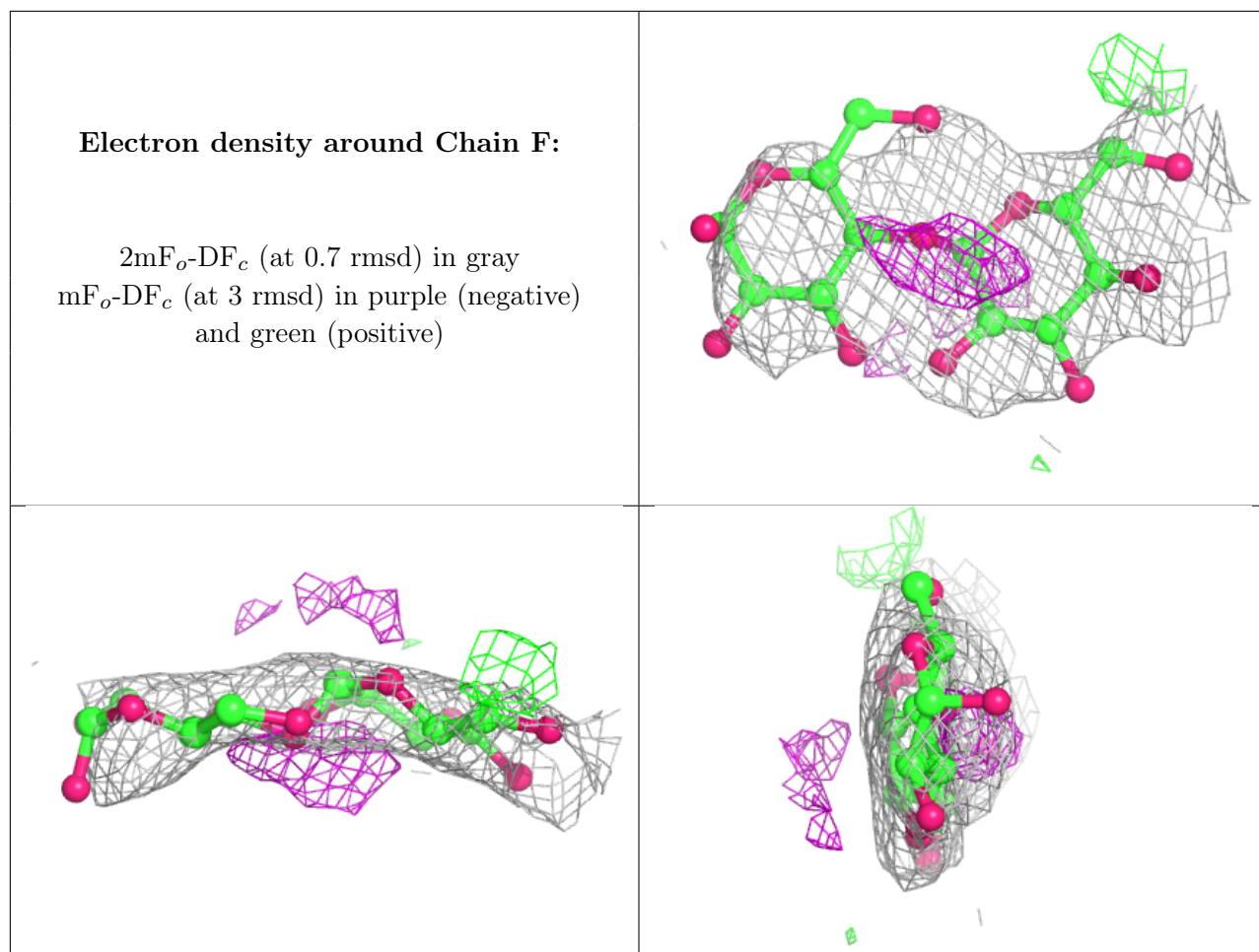

Electron density around Chain C:

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

Electron density around Chain E:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
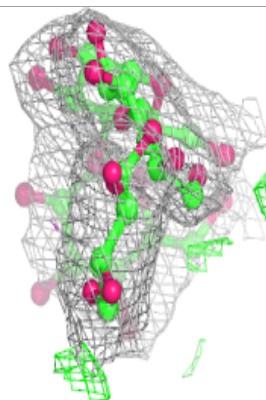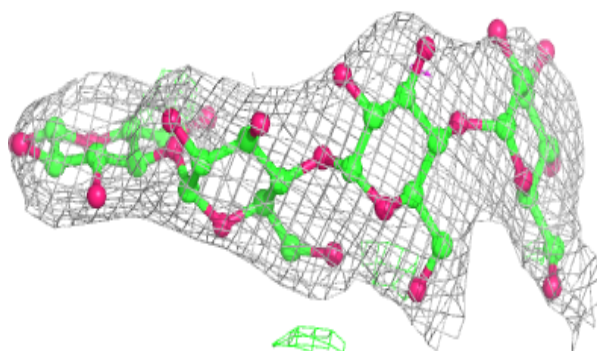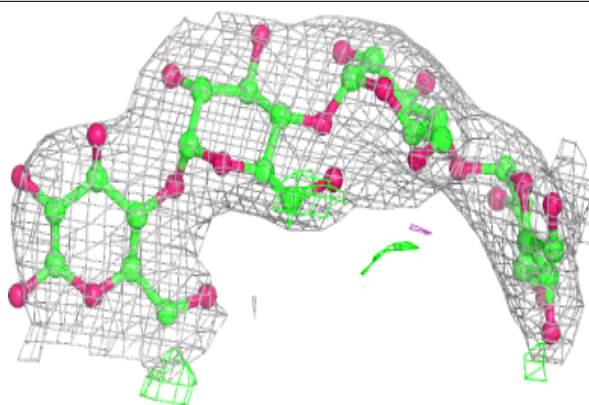
Electron density around Chain D:

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

Electron density around Chain F:

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

6.4 Ligands ⓘ

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
4	PLP	A	1007	15/16	0.96	0.26	61,67,75,76	0
4	PLP	B	1007	15/16	0.97	0.26	55,61,70,72	0

6.5 Other polymers ⓘ

There are no such residues in this entry.