



wwPDB X-ray Structure Validation Summary Report ⓘ

Dec 15, 2024 – 03:16 PM EST

PDB ID : 3FU9
Title : Melanocarpus albomyces laccase crystal soaked (20 min) with 2,6-dimethoxyphenol
Authors : Kallio, J.P.; Hakulinen, N.; Rouvinen, J.
Deposited on : 2009-01-14
Resolution : 2.00 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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4.02b-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)	:	2.40

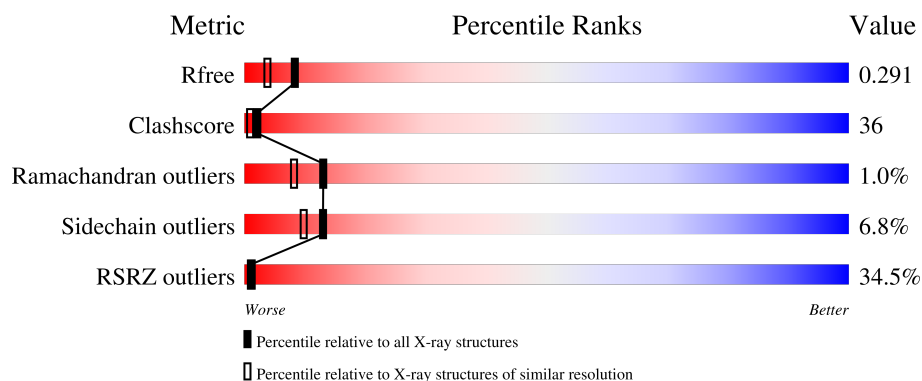
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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}	164625	9409 (2.00-2.00)
Clashscore	180529	10737 (2.00-2.00)
Ramachandran outliers	177936	10628 (2.00-2.00)
Sidechain outliers	177891	10627 (2.00-2.00)
RSRZ outliers	164620	9409 (2.00-2.00)

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	559	<div> <div>31%</div> <div>52%</div> <div>40%</div> <div>7%</div> </div>
1	B	559	<div> <div>38%</div> <div>48%</div> <div>42%</div> <div>9%</div> </div>
2	C	2	<div> <div>100%</div> </div>
2	D	2	<div> <div>50%</div> <div>50%</div> </div>
2	E	2	<div> <div>100%</div> </div>
2	F	2	<div> <div>50%</div> <div>50%</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 criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	CL	A	605	-	-	X	-
7	KIB	B	611	-	-	X	-

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 9692 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 Laccase-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	559	Total	C	N	O	S	0	0	0
			4369	2764	759	831	15			
1	B	559	Total	C	N	O	S	0	0	0
			4369	2764	759	831	15			

- Molecule 2 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	C	2	Total	C	N	O	0	0	0
			28	16	2	10			
2	D	2	Total	C	N	O	0	0	0
			28	16	2	10			
2	E	2	Total	C	N	O	0	0	0
			28	16	2	10			
2	F	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 3 is COPPER (II) ION (three-letter code: CU) (formula: Cu).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	4	Total	Cu	0	0
			4	4		
3	B	4	Total	Cu	0	0
			4	4		

- Molecule 4 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total Cl 1 1	0	0
4	B	1	Total Cl 1 1	0	0

- Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



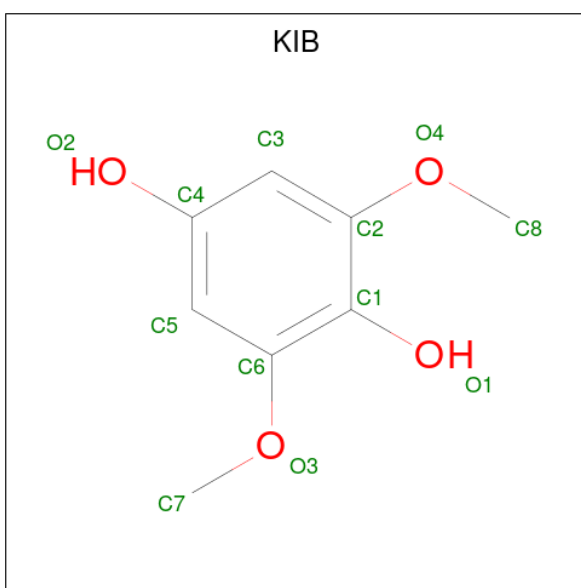
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C N O 14 8 1 5	0	0
5	A	1	Total C N O 14 8 1 5	0	0
5	A	1	Total C N O 14 8 1 5	0	0
5	B	1	Total C N O 14 8 1 5	0	0
5	B	1	Total C N O 14 8 1 5	0	0
5	B	1	Total C N O 14 8 1 5	0	0
5	B	1	Total C N O 14 8 1 5	0	0

- Molecule 6 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



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

- Molecule 7 is 2,6-dimethoxybenzene-1,4-diol (three-letter code: KIB) (formula: $C_8H_{10}O_4$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	C	O	0	0
			12	8	4		
7	B	1	Total	C	O	0	0
			12	8	4		

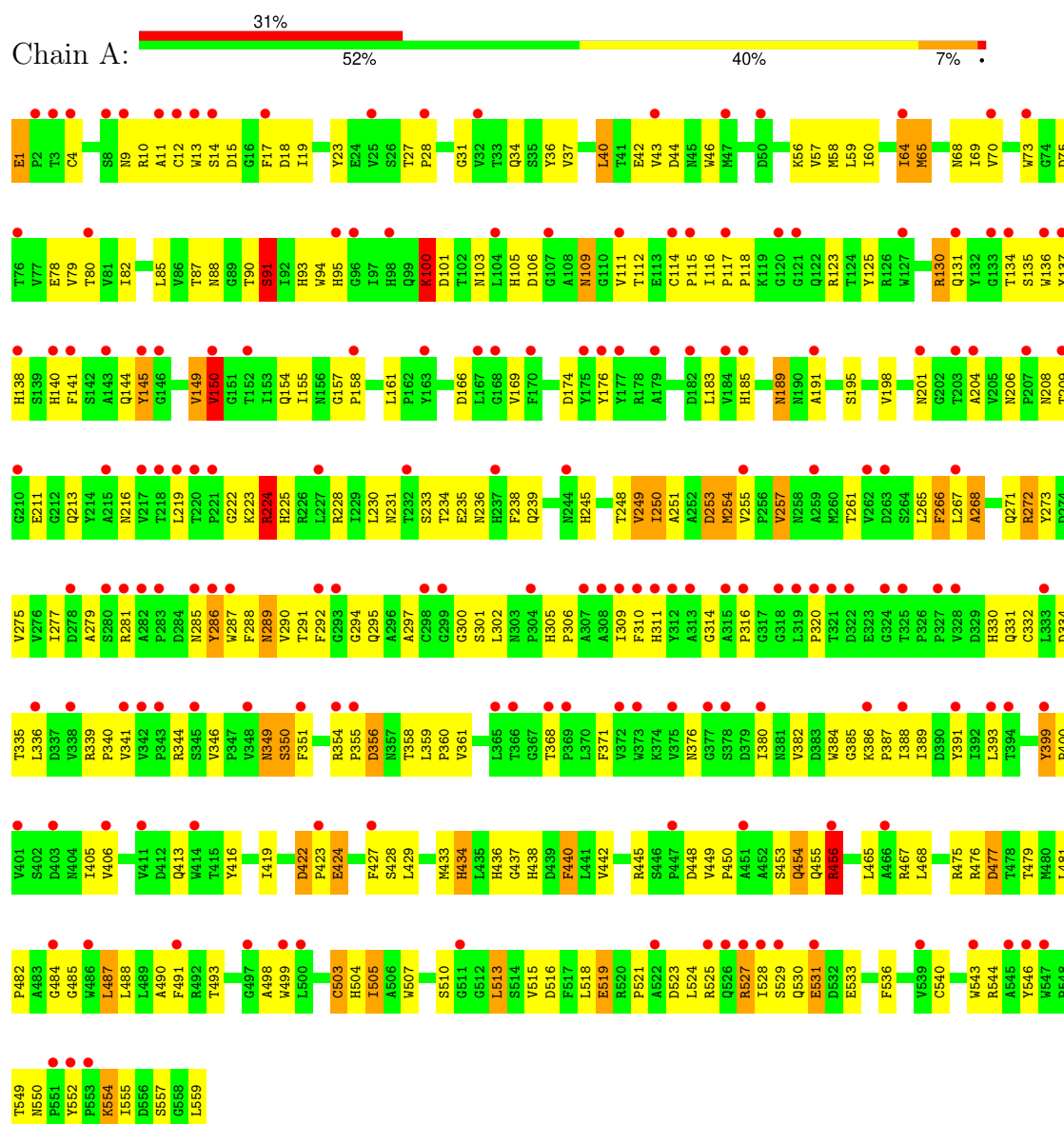
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	340	Total 340	O 340	0	0
8	B	360	Total 360	O 360	0	0

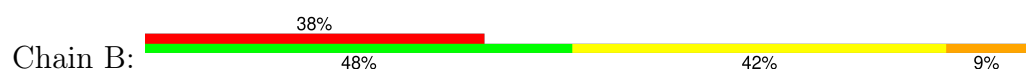
3 Residue-property plots

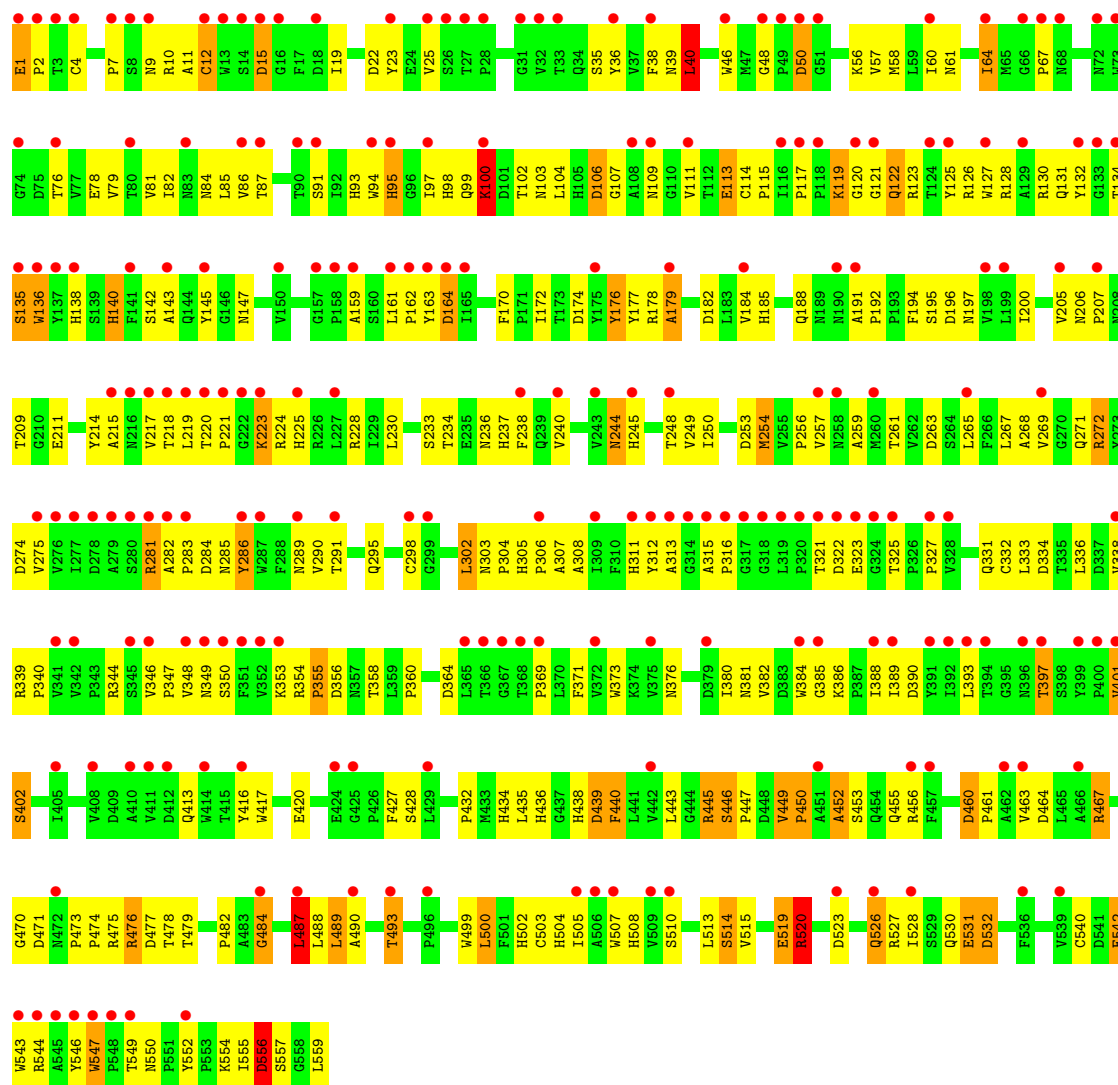
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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: Laccase-1



• Molecule 1: Laccase-1





- Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain C: 100%

MAG1
MAG2

- Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain D: 50%

MAG1
MAG2

- Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain E:  100%

MAG1
MAG2

- Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain F:  50% 50%

MAG1
MAG2

4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	174.12Å 60.23Å 117.13Å 90.00° 98.36° 90.00°	Depositor
Resolution (Å)	19.61 – 2.00 19.61 – 2.00	Depositor EDS
% Data completeness (in resolution range)	100.0 (19.61-2.00) 97.4 (19.61-2.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.09	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.03 (at 1.90Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.230 , 0.330 0.291 , 0.291	Depositor DCC
R_{free} test set	3972 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	10.1	Xtriage
Anisotropy	1.421	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.41 , 49.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.39$, $\langle L^2 \rangle = 0.22$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.75	EDS
Total number of atoms	9692	wwPDB-VP
Average B, all atoms (Å ²)	13.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.57% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: KIB, CL, SO4, CU, NAG

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	1.44	29/4506 (0.6%)	1.26	22/6191 (0.4%)
1	B	1.40	20/4506 (0.4%)	1.33	37/6191 (0.6%)
All	All	1.42	49/9012 (0.5%)	1.30	59/12382 (0.5%)

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	A	0	1
1	B	0	1
All	All	0	2

The worst 5 of 49 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	286	TYR	CD2-CE2	11.69	1.56	1.39
1	B	286	TYR	CD1-CE1	9.74	1.53	1.39
1	B	286	TYR	CD2-CE2	8.73	1.52	1.39
1	A	531	GLU	CG-CD	8.67	1.65	1.51
1	A	255	VAL	CB-CG2	8.35	1.70	1.52

The worst 5 of 59 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	130	ARG	NE-CZ-NH2	-10.41	115.09	120.30
1	A	40	LEU	CA-CB-CG	10.27	138.93	115.30
1	B	130	ARG	NE-CZ-NH1	9.37	124.98	120.30
1	B	520	ARG	NE-CZ-NH2	-8.65	115.97	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	554	LYS	CD-CE-NZ	-8.64	91.82	111.70

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	437	GLY	Peptide
1	B	514	SER	Peptide

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	4369	0	4114	253	0
1	B	4369	0	4114	365	1
2	C	28	0	24	5	0
2	D	28	0	24	3	0
2	E	28	0	25	8	0
2	F	28	0	25	4	0
3	A	4	0	0	0	0
3	B	4	0	0	0	0
4	A	1	0	0	3	0
4	B	1	0	0	0	0
5	A	42	0	39	5	1
5	B	56	0	52	0	0
6	A	5	0	0	0	0
6	B	5	0	0	0	0
7	A	12	0	8	1	0
7	B	12	0	8	7	0
8	A	340	0	0	109	0
8	B	360	0	0	182	0
All	All	9692	0	8433	631	1

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 36.

The worst 5 of 631 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:261:THR:HG22	8:B:854:HOH:O	1.28	1.28
1:B:211:GLU:HB2	8:B:717:HOH:O	1.26	1.28
1:B:143:ALA:HA	8:B:877:HOH:O	1.29	1.27
1:B:230:LEU:HB3	8:B:824:HOH:O	1.34	1.27
1:A:510:SER:HB2	8:A:702:HOH:O	1.29	1.25

All (1) 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:B:78:GLU:OE2	5:A:606:NAG:O7[3_545]	2.04	0.16

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	557/559 (100%)	504 (90%)	47 (8%)	6 (1%)	12	7
1	B	557/559 (100%)	502 (90%)	50 (9%)	5 (1%)	14	10
All	All	1114/1118 (100%)	1006 (90%)	97 (9%)	11 (1%)	13	8

5 of 11 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	350	SER
1	B	402	SER
1	A	91	SER
1	A	493	THR
1	B	15	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	478/478 (100%)	444 (93%)	34 (7%)	12	9
1	B	478/478 (100%)	447 (94%)	31 (6%)	14	11
All	All	956/956 (100%)	891 (93%)	65 (7%)	13	10

5 of 65 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	487	LEU
1	B	507	TRP
1	A	424	GLU
1	A	422	ASP
1	B	510	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 20 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	244	ASN
1	B	455	GLN
1	B	550	ASN
1	B	526	GLN
1	A	236	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 ⓘ

8 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	NAG	C	1	1,2	14,14,15	1.23	1 (7%)	17,19,21	3.08	5 (29%)
2	NAG	C	2	2	14,14,15	0.98	1 (7%)	17,19,21	2.17	5 (29%)
2	NAG	D	1	1,2	14,14,15	1.41	2 (14%)	17,19,21	3.74	10 (58%)
2	NAG	D	2	2	14,14,15	1.65	5 (35%)	17,19,21	2.75	7 (41%)
2	NAG	E	1	1,2	14,14,15	1.13	1 (7%)	17,19,21	2.37	7 (41%)
2	NAG	E	2	2	14,14,15	0.88	0	17,19,21	1.35	2 (11%)
2	NAG	F	1	1,2	14,14,15	1.71	3 (21%)	17,19,21	4.75	13 (76%)
2	NAG	F	2	2	14,14,15	1.53	2 (14%)	17,19,21	3.91	12 (70%)

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	NAG	C	1	1,2	-	4/6/23/26	0/1/1/1
2	NAG	C	2	2	-	0/6/23/26	0/1/1/1
2	NAG	D	1	1,2	-	1/6/23/26	0/1/1/1
2	NAG	D	2	2	-	2/6/23/26	0/1/1/1
2	NAG	E	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	E	2	2	-	0/6/23/26	0/1/1/1
2	NAG	F	1	1,2	-	4/6/23/26	0/1/1/1
2	NAG	F	2	2	-	6/6/23/26	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	F	1	NAG	O5-C5	-4.05	1.35	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	1	NAG	C2-N2	3.92	1.52	1.46
2	F	2	NAG	O5-C5	-3.55	1.36	1.43
2	D	2	NAG	C1-C2	-3.36	1.47	1.52
2	F	1	NAG	C3-C2	-3.11	1.46	1.52

The worst 5 of 61 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	1	NAG	C1-O5-C5	11.20	127.20	112.19
2	D	1	NAG	C1-C2-N2	9.73	125.77	110.43
2	F	2	NAG	C1-O5-C5	-9.42	99.56	112.19
2	C	1	NAG	C1-O5-C5	9.29	124.64	112.19
2	F	1	NAG	C2-N2-C7	7.87	133.44	122.90

There are no chirality outliers.

5 of 19 torsion outliers are listed below:

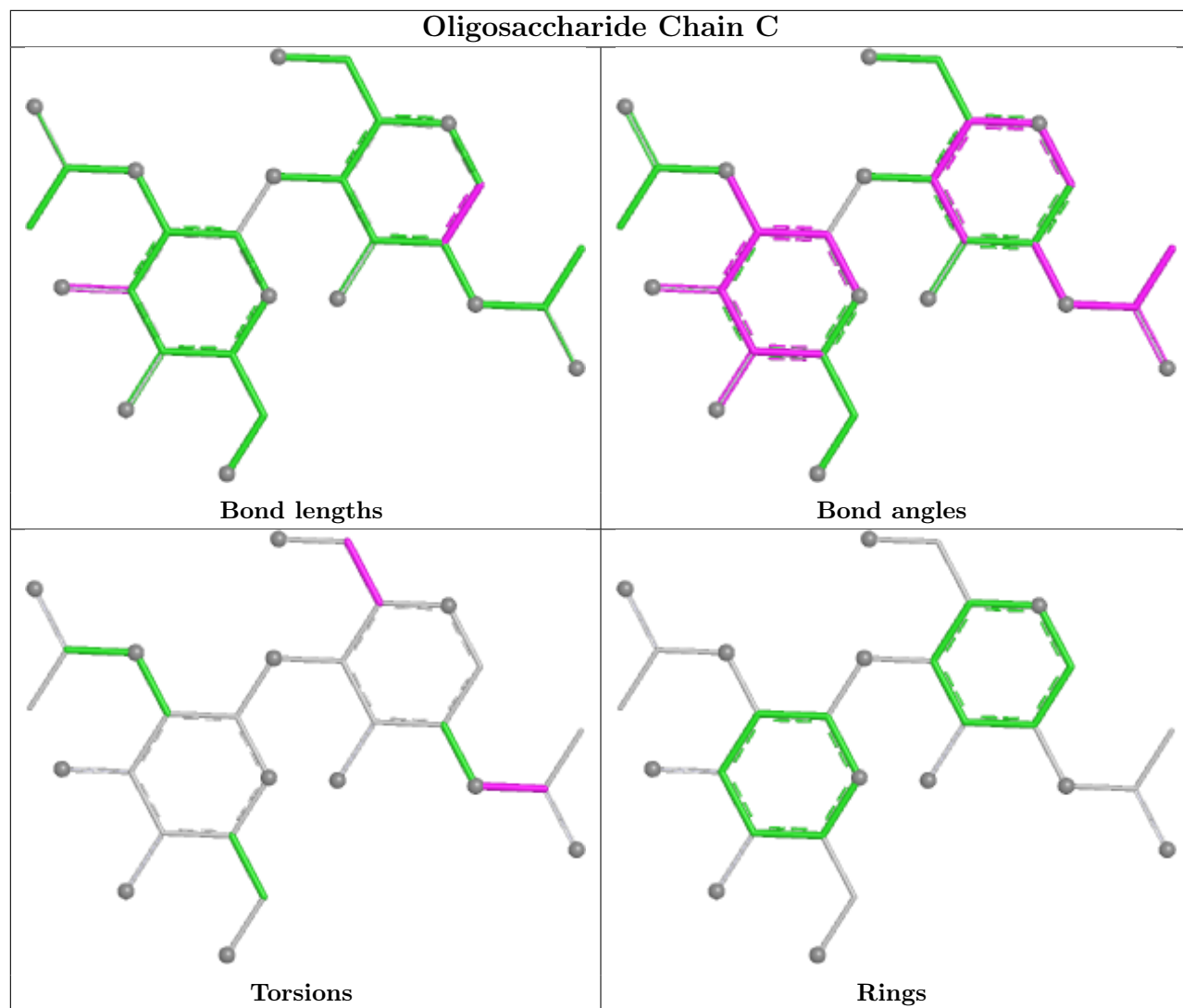
Mol	Chain	Res	Type	Atoms
2	F	1	NAG	C8-C7-N2-C2
2	F	1	NAG	O7-C7-N2-C2
2	F	2	NAG	C8-C7-N2-C2
2	F	2	NAG	O7-C7-N2-C2
2	F	2	NAG	O5-C5-C6-O6

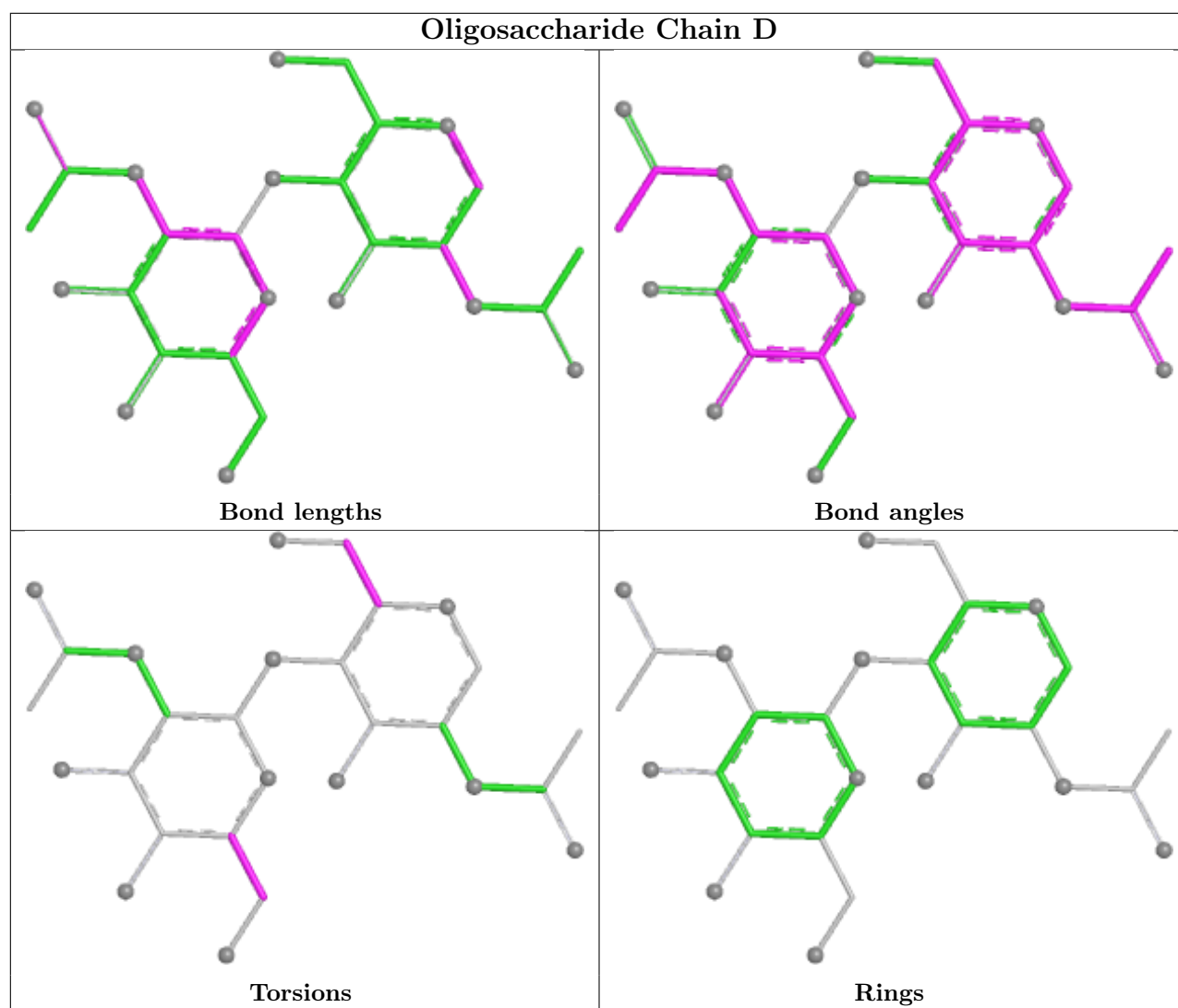
There are no ring outliers.

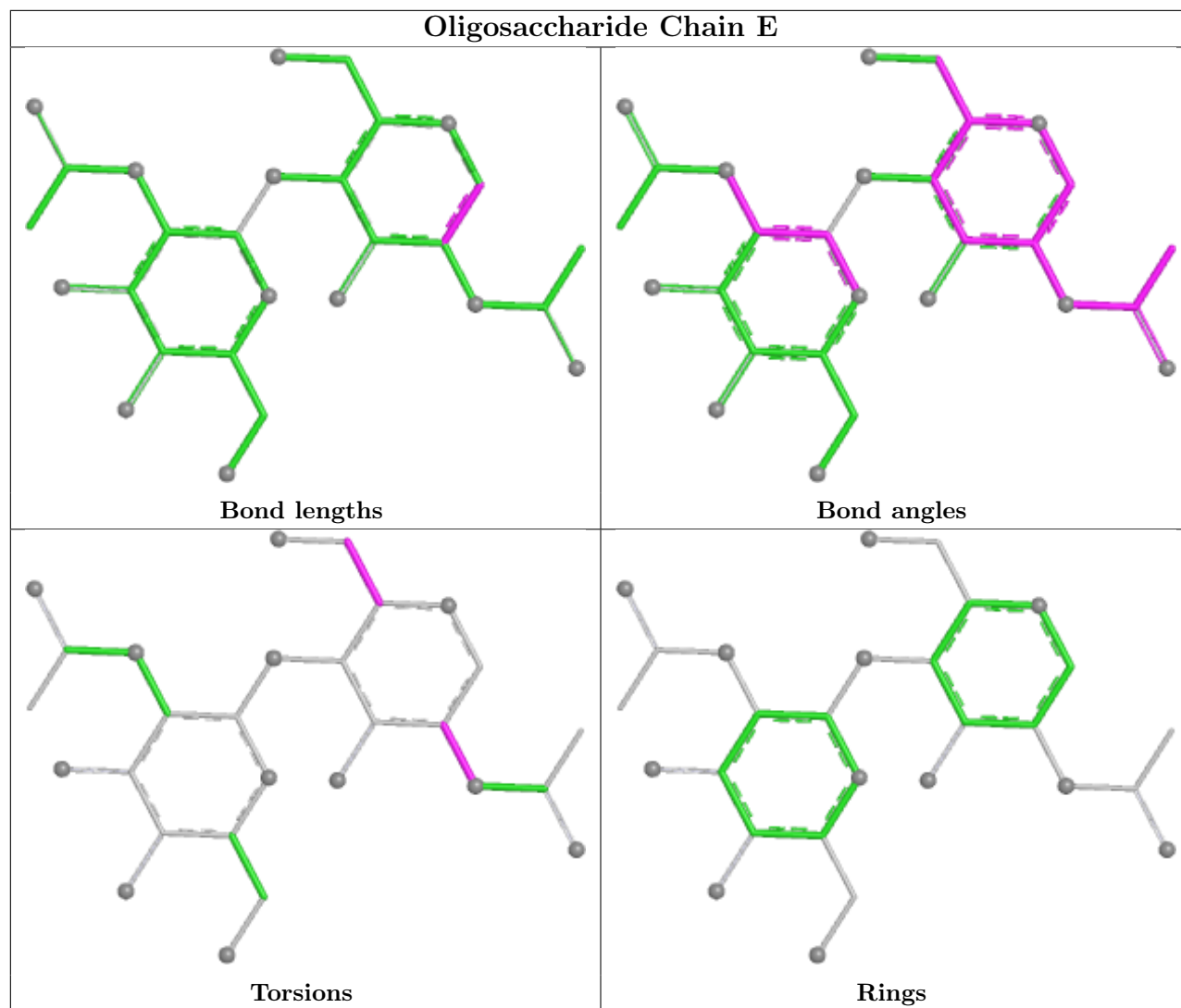
6 monomers are involved in 20 short contacts:

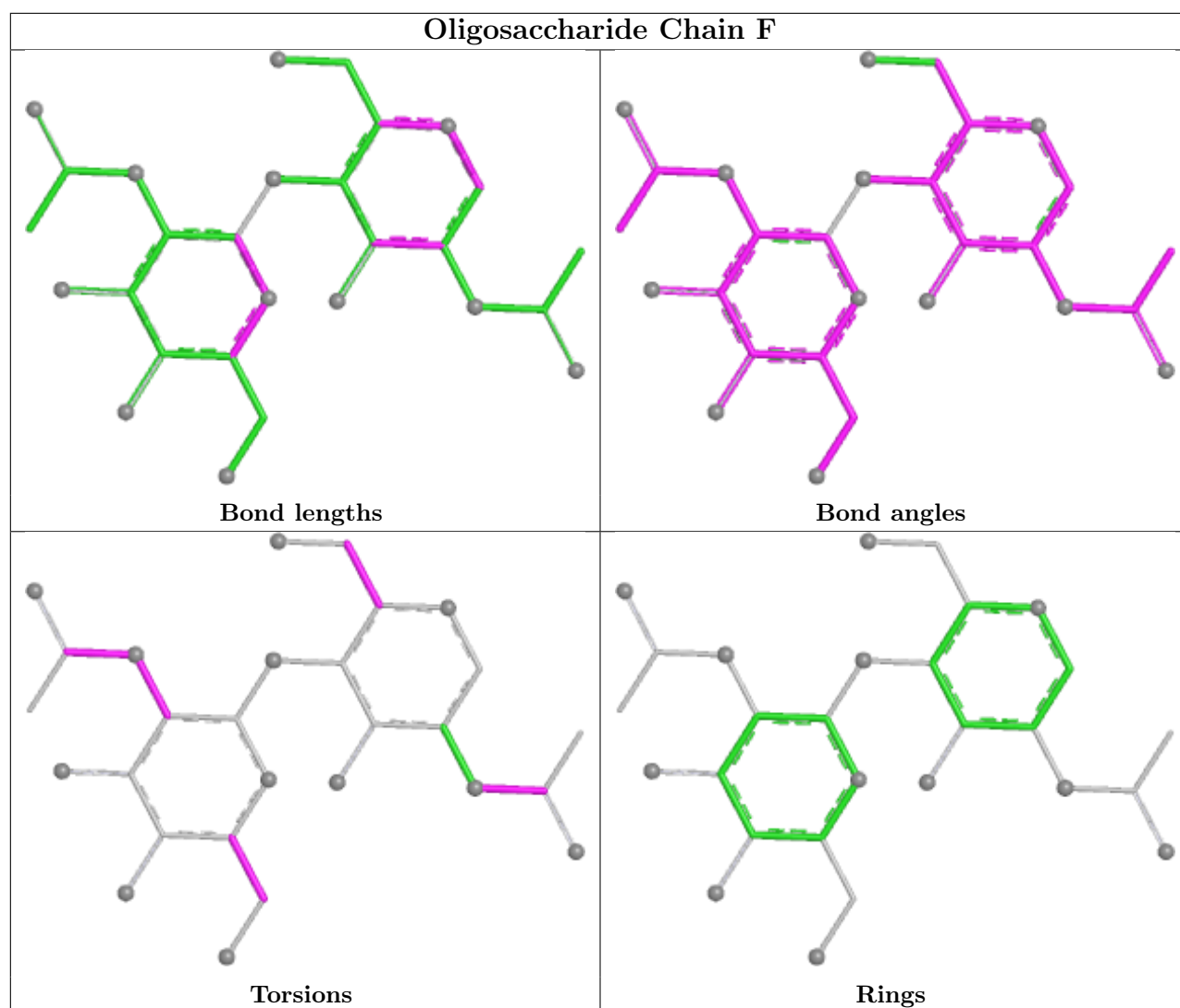
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	1	NAG	2	0
2	E	1	NAG	3	0
2	C	2	NAG	3	0
2	D	1	NAG	3	0
2	F	1	NAG	4	0
2	E	2	NAG	5	0

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









5.6 Ligand geometry [i](#)

Of 21 ligands modelled in this entry, 10 are monoatomic - leaving 11 for Mogul analysis.

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	$\# Z > 2$
5	NAG	A	606	1	14,14,15	1.07	1 (7%)	17,19,21	1.48	3 (17%)
5	NAG	B	609	1	14,14,15	0.95	1 (7%)	17,19,21	2.03	6 (35%)
6	SO4	B	610	-	4,4,4	0.36	0	6,6,6	1.08	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	NAG	A	607	1	14,14,15	1.08	0	17,19,21	2.62	8 (47%)
5	NAG	B	606	1	14,14,15	1.00	1 (7%)	17,19,21	2.54	6 (35%)
6	SO4	A	609	-	4,4,4	0.37	0	6,6,6	0.53	0
5	NAG	B	607	1	14,14,15	0.74	0	17,19,21	1.45	2 (11%)
5	NAG	A	608	1	14,14,15	0.78	0	17,19,21	2.48	6 (35%)
5	NAG	B	608	1	14,14,15	0.85	1 (7%)	17,19,21	2.26	5 (29%)
7	KIB	A	610	-	12,12,12	3.08	4 (33%)	16,16,16	2.12	7 (43%)
7	KIB	B	611	-	12,12,12	3.64	6 (50%)	16,16,16	2.07	5 (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
5	NAG	A	606	1	-	4/6/23/26	0/1/1/1
5	NAG	B	609	1	-	2/6/23/26	0/1/1/1
5	NAG	A	607	1	-	2/6/23/26	0/1/1/1
5	NAG	B	606	1	-	0/6/23/26	0/1/1/1
5	NAG	B	607	1	-	0/6/23/26	0/1/1/1
5	NAG	A	608	1	-	0/6/23/26	0/1/1/1
5	NAG	B	608	1	-	2/6/23/26	0/1/1/1
7	KIB	A	610	-	-	0/4/4/4	0/1/1/1
7	KIB	B	611	-	-	2/4/4/4	0/1/1/1

The worst 5 of 14 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	B	611	KIB	C6-C1	8.18	1.51	1.40
7	A	610	KIB	C2-C1	7.48	1.50	1.40
7	B	611	KIB	C2-C1	5.80	1.48	1.40
7	A	610	KIB	O1-C1	-4.41	1.26	1.36
7	B	611	KIB	C5-C4	4.17	1.45	1.39

The worst 5 of 48 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	606	NAG	O4-C4-C3	-6.66	94.67	110.38
5	A	608	NAG	C3-C4-C5	-5.71	99.88	110.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	608	NAG	C2-N2-C7	-5.41	115.65	122.90
5	B	609	NAG	O5-C1-C2	-4.93	103.66	111.29
7	B	611	KIB	C3-C2-C1	-4.69	116.13	120.59

There are no chirality outliers.

5 of 12 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	607	NAG	C8-C7-N2-C2
5	A	607	NAG	O7-C7-N2-C2
7	B	611	KIB	C1-C6-O3-C7
7	B	611	KIB	C5-C6-O3-C7
5	A	606	NAG	C8-C7-N2-C2

There are no ring outliers.

5 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	606	NAG	0	1
5	A	607	NAG	4	0
5	A	608	NAG	1	0
7	A	610	KIB	1	0
7	B	611	KIB	7	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

Warning: The R factor obtained from EDS is 0.3418, which does not match the depositor's R factor of 0.23047. Please interpret the results in this section carefully.

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	559/559 (100%)	1.71	171 (30%) 1 1	2, 12, 24, 31	0
1	B	559/559 (100%)	1.85	215 (38%) 1 1	3, 13, 23, 32	0
All	All	1118/1118 (100%)	1.78	386 (34%) 1 1	2, 13, 24, 32	0

The worst 5 of 386 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	315	ALA	4.8
1	A	11	ALA	4.6
1	B	12	CYS	4.6
1	B	401	VAL	4.5
1	A	12	CYS	4.5

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

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

6.3 Carbohydrates [i](#)

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

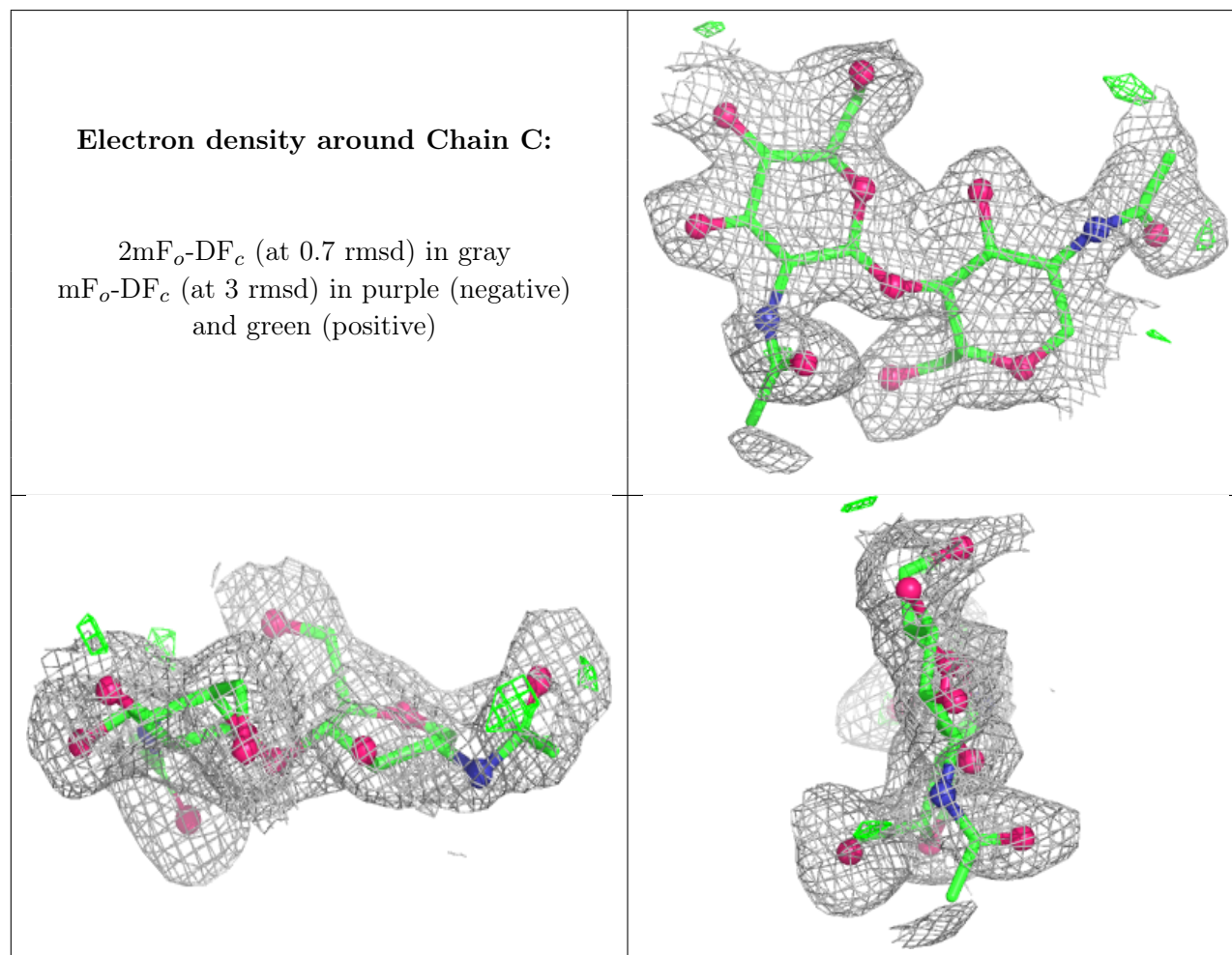
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	NAG	F	2	14/15	0.61	0.17	7,18,24,25	0
2	NAG	D	2	14/15	0.64	0.16	16,22,28,28	0

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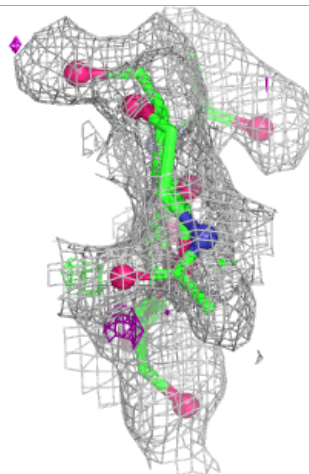
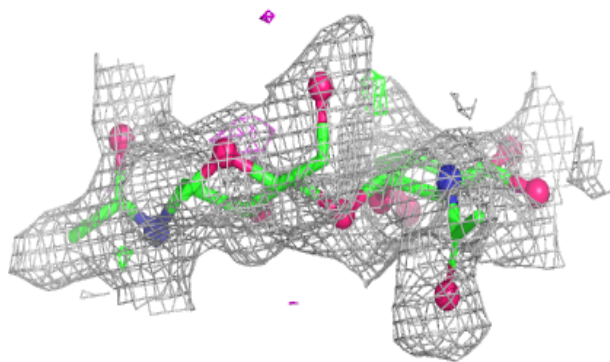
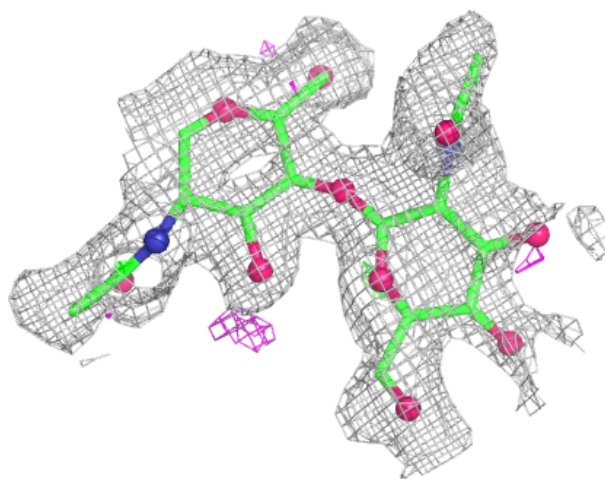
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	NAG	D	1	14/15	0.72	0.15	10,13,19,20	0
2	NAG	F	1	14/15	0.78	0.16	5,12,23,23	0
2	NAG	C	1	14/15	0.81	0.14	8,16,18,18	0
2	NAG	E	1	14/15	0.81	0.14	8,15,16,17	0
2	NAG	E	2	14/15	0.82	0.12	9,14,18,22	0
2	NAG	C	2	14/15	0.86	0.12	9,15,19,19	0

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.



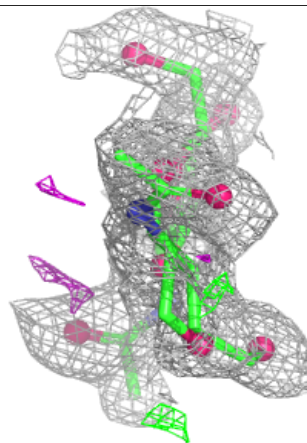
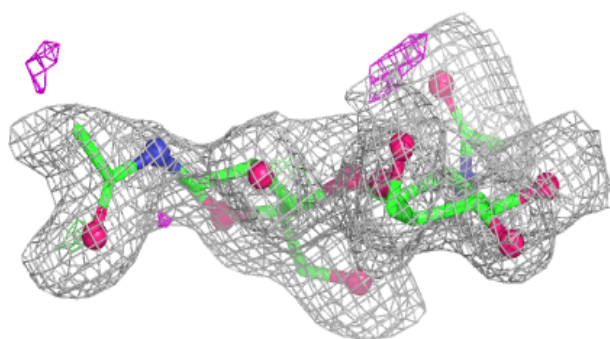
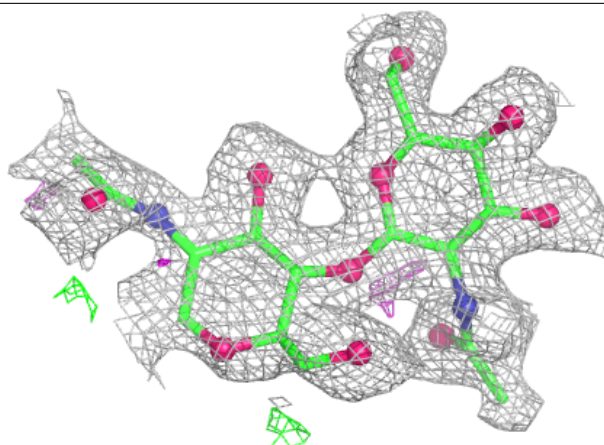
Electron density around Chain D:

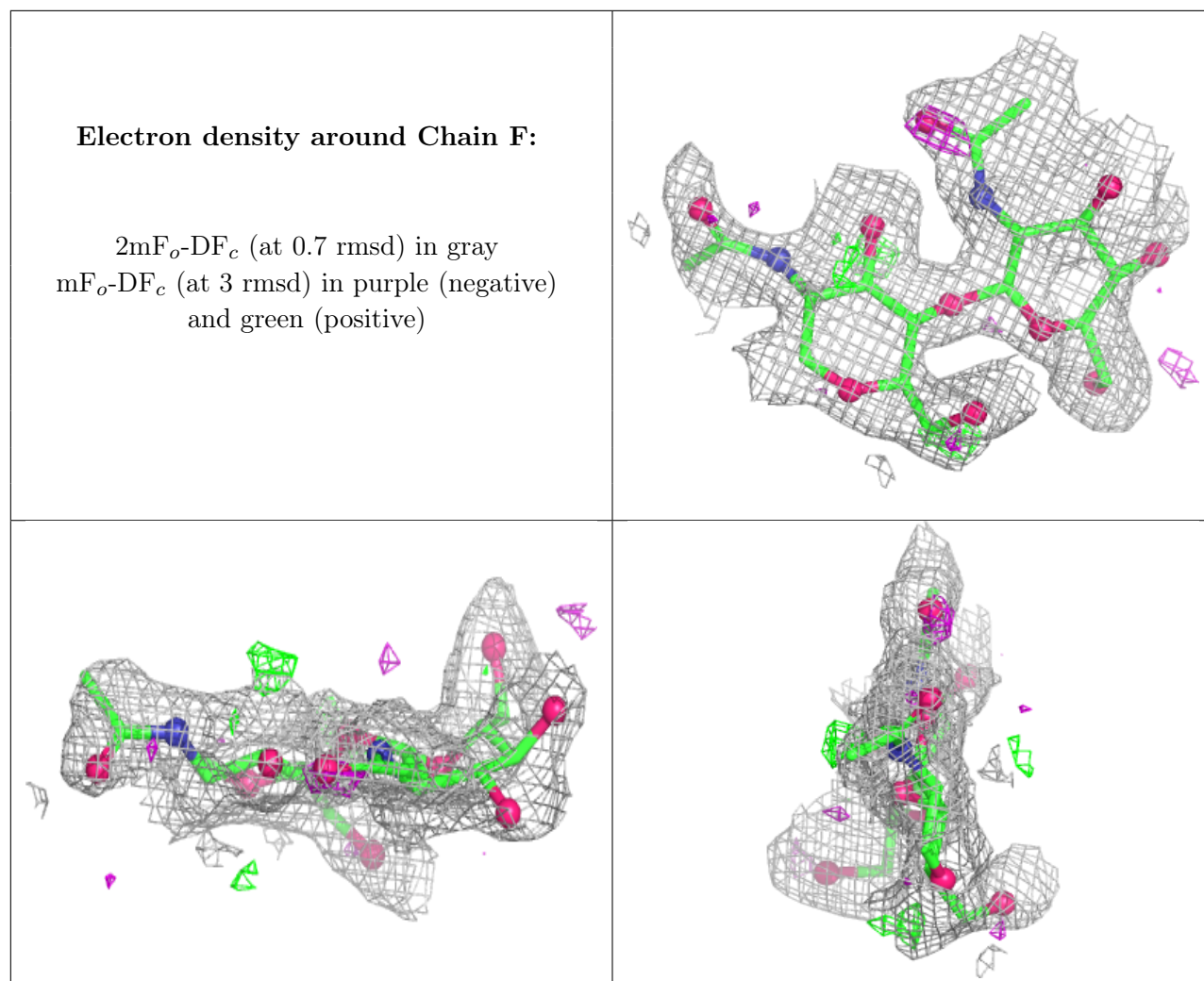
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around Chain E:

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





6.4 Ligands [i](#)

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
5	NAG	A	606	14/15	0.60	0.19	26,29,32,34	0
5	NAG	B	607	14/15	0.60	0.19	13,19,24,24	0
5	NAG	A	608	14/15	0.63	0.17	8,23,27,28	0
7	KIB	A	610	12/12	0.68	0.18	7,17,20,23	0
5	NAG	B	608	14/15	0.69	0.16	17,20,25,26	0
5	NAG	B	609	14/15	0.71	0.18	8,15,27,28	0
5	NAG	A	607	14/15	0.71	0.17	16,22,33,33	0
4	CL	A	605	1/1	0.75	0.20	41,41,41,41	0
5	NAG	B	606	14/15	0.77	0.13	9,17,19,24	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
6	SO4	B	610	5/5	0.83	0.12	17,25,25,29	0
7	KIB	B	611	12/12	0.85	0.13	2,7,15,16	0
4	CL	B	605	1/1	0.92	0.11	26,26,26,26	0
3	CU	A	603	1/1	0.92	0.07	11,11,11,11	0
6	SO4	A	609	5/5	0.92	0.09	22,23,26,29	0
3	CU	B	604	1/1	0.94	0.05	15,15,15,15	0
3	CU	B	601	1/1	0.94	0.04	12,12,12,12	0
3	CU	A	602	1/1	0.96	0.04	22,22,22,22	0
3	CU	A	601	1/1	0.97	0.04	15,15,15,15	0
3	CU	B	602	1/1	0.97	0.04	18,18,18,18	0
3	CU	A	604	1/1	0.98	0.03	14,14,14,14	0
3	CU	B	603	1/1	0.99	0.02	10,10,10,10	0

6.5 Other polymers [i](#)

There are no such residues in this entry.